



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 09:26 PM UTC

PDB ID : 2ADE / pdb\_00002ade  
Title : Crystal structure of fructan 1-exohydrolase IIa from Cichorium intybus in complex with fructose  
Authors : Verhaest, M.; Le Roy, K.; De Ranter, C.J.; Van Laere, A.; Van den Ende, W.; Rabijns, A.  
Deposited on : 2005-07-20  
Resolution : 2.65 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

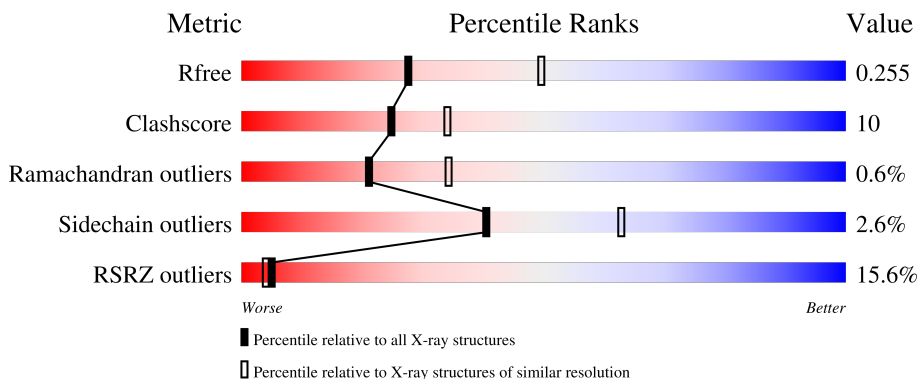
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

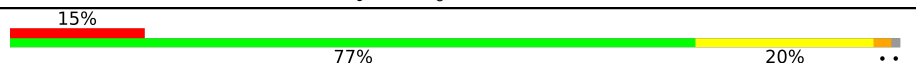


The reported resolution of this entry is 2.65 Å.

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))
$R_{free}$	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	543	
2	B	3	
3	C	2	

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
2	NAG	B	1	X	-	-	-

## 2 Entry composition [i](#)

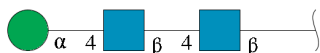
There are 5 unique types of molecules in this entry. The entry contains 4624 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 fructan 1-exohydrolase IIa.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	537	4274	2717	726	816	15	0	0	0

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



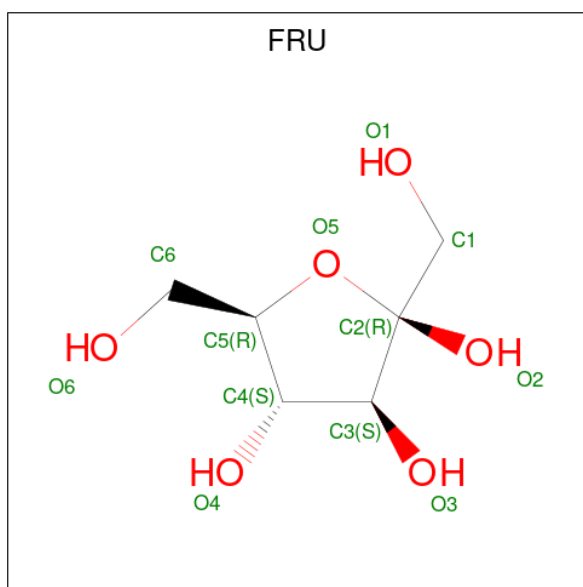
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	3	39	22	2	15	0	0	0

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



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

- Molecule 4 is beta-D-fructofuranose (CCD ID: FRU) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 12 6 6	0	0

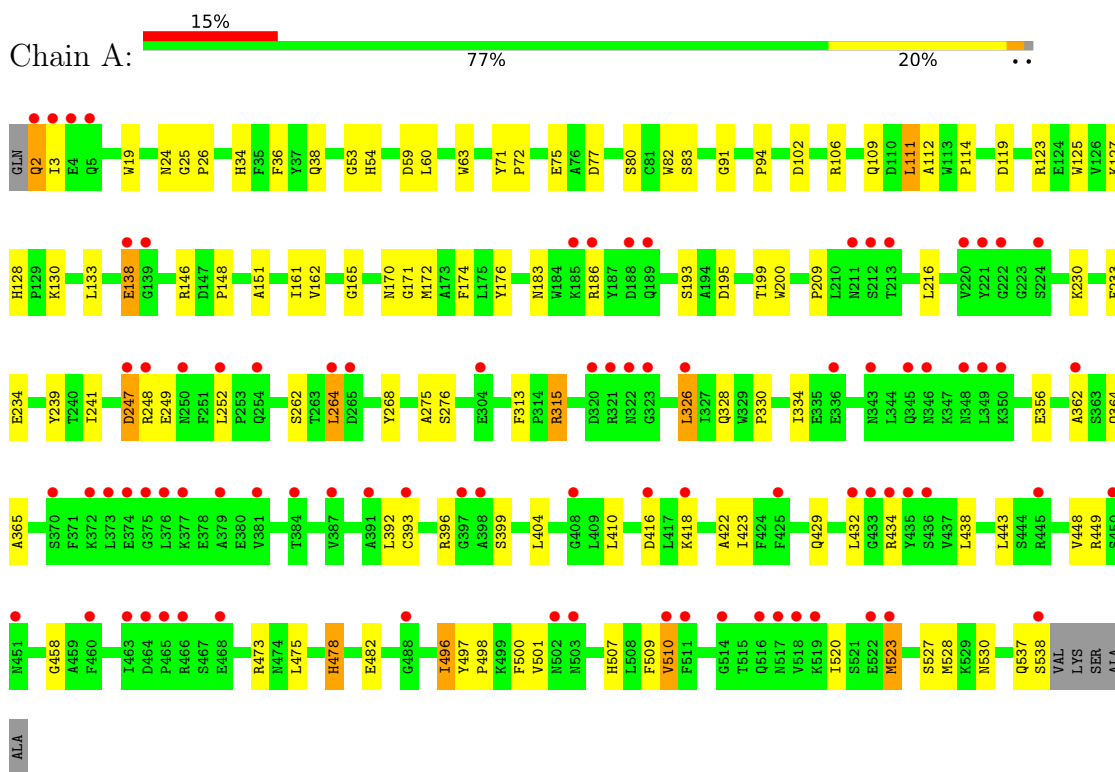
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	271	Total O 271 271	0	0

### 3 Residue-property plots i

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

- Molecule 1: fructan 1-exohydrolase IIa



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



MAG1  
MAG2  
MAG3

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



MAG1  
MAG2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.04Å 139.04Å 182.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.48 – 2.65 29.48 – 2.65	Depositor EDS
% Data completeness (in resolution range)	95.9 (29.48-2.65) 95.8 (29.48-2.65)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.48 (at 2.64Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.239 , 0.251 0.244 , 0.255	Depositor DCC
$R_{free}$ test set	2663 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.8	Xtrriage
Anisotropy	0.459	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 48.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	4624	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, FRU, NAG

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	0.36	0/4397	0.90	10/5988 (0.2%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	83	SER	N-CA-C	7.63	120.16	110.24
1	A	146	ARG	N-CA-C	6.95	117.76	108.38
1	A	53	GLY	N-CA-C	-6.24	104.56	112.54
1	A	268	TYR	N-CA-C	-6.11	104.54	111.14
1	A	91	GLY	N-CA-C	-5.85	107.02	115.27
1	A	510	VAL	N-CA-C	-5.70	100.28	108.48
1	A	527	SER	N-CA-C	-5.69	101.21	110.20
1	A	63	TRP	N-CA-C	5.16	118.00	109.85
1	A	448	VAL	N-CA-C	-5.09	107.79	112.83
1	A	362	ALA	N-CA-C	5.04	118.90	112.34

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4274	0	4062	79	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	39	0	34	4	0
3	C	28	0	25	1	0
4	A	12	0	12	0	0
5	A	271	0	0	7	0
All	All	4624	0	4133	83	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 10.

All (83) 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:364:GLN:HE22	1:A:530:ASN:HD22	1.14	0.89
1:A:510:VAL:HG11	1:A:520:ILE:HD11	1.54	0.89
3:C:1:NAG:H61	3:C:2:NAG:H82	1.56	0.86
1:A:364:GLN:HE22	1:A:530:ASN:ND2	1.77	0.81
1:A:128:HIS:CD2	1:A:130:LYS:H	1.99	0.81
1:A:128:HIS:HD2	1:A:130:LYS:H	1.30	0.76
1:A:416:ASP:OD1	1:A:418:LYS:HB2	1.92	0.69
1:A:165:GLY:HA2	1:A:199:THR:HG23	1.77	0.66
1:A:410:LEU:HB2	1:A:509:PHE:HB2	1.78	0.65
2:B:2:NAG:HN2	2:B:3:MAN:H2	1.63	0.63
1:A:111:LEU:HB2	1:A:133:LEU:HD22	1.79	0.63
2:B:1:NAG:O4	2:B:2:NAG:H62	1.99	0.63
1:A:72:PRO:HG2	5:A:1169:HOH:O	2.00	0.61
1:A:128:HIS:CD2	1:A:130:LYS:HB2	2.37	0.60
1:A:356:GLU:OE2	1:A:507:HIS:HD2	1.85	0.60
1:A:496:ILE:H	1:A:496:ILE:HD13	1.67	0.59
1:A:434:ARG:HG3	5:A:1243:HOH:O	2.02	0.59
1:A:72:PRO:HB3	1:A:77:ASP:O	2.05	0.56
1:A:330:PRO:HG2	1:A:473:ARG:NH1	2.21	0.56
1:A:230:LYS:HD3	1:A:230:LYS:C	2.31	0.55
1:A:364:GLN:NE2	1:A:530:ASN:HD22	1.94	0.55
1:A:399:SER:O	2:B:1:NAG:H62	2.08	0.54
1:A:233:PHE:HD1	1:A:234:GLU:HG3	1.73	0.53
1:A:313:PHE:CE2	1:A:334:ILE:HB	2.43	0.53
1:A:496:ILE:HD13	1:A:496:ILE:N	2.23	0.53
1:A:54:HIS:HD2	5:A:1003:HOH:O	1.92	0.53
1:A:114:PRO:HD3	1:A:125:TRP:CZ3	2.44	0.52
1:A:393:CYS:SG	1:A:458:GLY:HA3	2.50	0.52
1:A:128:HIS:HD2	1:A:130:LYS:N	2.04	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:MET:HE2	1:A:193:SER:HB2	1.91	0.51
1:A:449:ARG:HD2	5:A:1205:HOH:O	2.10	0.51
1:A:432:LEU:N	1:A:432:LEU:HD22	2.26	0.51
1:A:151:ALA:HB2	1:A:161:ILE:HG22	1.93	0.50
1:A:162:VAL:HA	1:A:174:PHE:O	2.11	0.50
1:A:151:ALA:HB2	1:A:161:ILE:CG2	2.42	0.50
1:A:249:GLU:HA	1:A:249:GLU:OE1	2.12	0.50
1:A:241:ILE:HD11	1:A:326:LEU:HD13	1.94	0.48
1:A:423:ILE:HD12	1:A:423:ILE:N	2.28	0.48
1:A:315:ARG:HE	1:A:328:GLN:NE2	2.11	0.48
1:A:365:ALA:HA	1:A:528:MET:HG2	1.96	0.48
1:A:432:LEU:HD22	1:A:432:LEU:H	1.78	0.48
1:A:510:VAL:HG11	1:A:520:ILE:CD1	2.37	0.48
1:A:523:MET:C	1:A:523:MET:HE2	2.39	0.47
1:A:239:TYR:CE1	1:A:326:LEU:HD22	2.50	0.47
1:A:429:GLN:HA	1:A:434:ARG:O	2.15	0.47
1:A:59:ASP:O	1:A:60:LEU:HB2	2.15	0.47
1:A:356:GLU:HB2	1:A:509:PHE:CE1	2.50	0.47
1:A:109:GLN:NE2	1:A:148:PRO:HD3	2.29	0.47
1:A:2:GLN:HE21	1:A:3:ILE:N	2.14	0.46
2:B:2:NAG:HN2	2:B:3:MAN:C2	2.26	0.46
1:A:275:ALA:HA	5:A:1027:HOH:O	2.16	0.46
1:A:171:GLY:HA3	1:A:200:TRP:CD1	2.51	0.45
1:A:71:TYR:O	1:A:127:LYS:NZ	2.48	0.45
1:A:119:ASP:OD2	1:A:123:ARG:HG3	2.17	0.45
1:A:209:PRO:HD3	1:A:216:LEU:HG	1.98	0.45
1:A:38:GLN:OE1	1:A:82:TRP:HA	2.18	0.44
1:A:230:LYS:HE3	1:A:276:SER:OG	2.17	0.44
1:A:111:LEU:CD2	1:A:112:ALA:N	2.80	0.44
1:A:500:PHE:CD1	1:A:500:PHE:C	2.96	0.44
1:A:24:ASN:C	1:A:26:PRO:HD3	2.43	0.43
1:A:19:TRP:CD1	1:A:19:TRP:C	2.96	0.43
1:A:449:ARG:HH21	1:A:497:TYR:HB3	1.83	0.43
1:A:176:TYR:CZ	1:A:186:ARG:HG3	2.54	0.43
1:A:183:ASN:HA	5:A:1141:HOH:O	2.18	0.43
1:A:247:ASP:OD2	1:A:248:ARG:HG2	2.19	0.43
1:A:262:SER:C	1:A:264:LEU:H	2.26	0.43
1:A:24:ASN:O	1:A:36:PHE:HB2	2.19	0.42
1:A:170:ASN:O	1:A:172:MET:HG2	2.19	0.42
1:A:111:LEU:HD23	1:A:112:ALA:H	1.83	0.42
1:A:537:GLN:HB3	1:A:538:SER:H	1.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:PRO:HG2	1:A:114:PRO:HG3	2.00	0.42
1:A:498:PRO:HG2	1:A:501:VAL:HG13	2.02	0.41
1:A:25:GLY:N	1:A:26:PRO:HD3	2.35	0.41
1:A:364:GLN:OE1	1:A:478:HIS:HE1	2.03	0.41
1:A:422:ALA:C	1:A:423:ILE:HD12	2.45	0.41
1:A:396:ARG:HD3	5:A:1076:HOH:O	2.21	0.41
1:A:392:LEU:HD23	1:A:438:LEU:HD22	2.03	0.41
1:A:138:GLU:HA	1:A:138:GLU:OE2	2.20	0.41
1:A:34:HIS:ND1	1:A:54:HIS:HE1	2.20	0.40
1:A:102:ASP:OD2	1:A:106:ARG:HG3	2.21	0.40
1:A:315:ARG:NH1	1:A:482:GLU:OE1	2.54	0.40
1:A:170:ASN:OD1	1:A:195:ASP:HA	2.21	0.40
1:A:75:GLU:OE2	1:A:102:ASP:HB2	2.21	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	535/543 (98%)	503 (94%)	29 (5%)	3 (1%)	21	34

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	GLU
1	A	478	HIS
1	A	80	SER

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	463/467 (99%)	451 (97%)	12 (3%)	40 63

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

Mol	Chain	Res	Type
1	A	2	GLN
1	A	111	LEU
1	A	247	ASP
1	A	252	LEU
1	A	264	LEU
1	A	315	ARG
1	A	326	LEU
1	A	404	LEU
1	A	443	LEU
1	A	475	LEU
1	A	496	ILE
1	A	523	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	54	HIS
1	A	109	GLN
1	A	128	HIS
1	A	177	GLN
1	A	211	ASN
1	A	214	ASN
1	A	227	HIS
1	A	250	ASN
1	A	272	GLN
1	A	325	GLN
1	A	328	GLN
1	A	343	ASN

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Mol	Chain	Res	Type
1	A	345	GLN
1	A	348	ASN
1	A	429	GLN
1	A	431	GLN
1	A	478	HIS
1	A	507	HIS
1	A	517	ASN
1	A	530	ASN
1	A	537	GLN

### 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](#)

5 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	2,1	14,14,15	0.70	0	17,19,21	0.99	1 (5%)
2	NAG	B	2	2	14,14,15	0.80	0	17,19,21	0.86	1 (5%)
2	MAN	B	3	2	11,11,12	0.56	0	15,15,17	0.51	0
3	NAG	C	1	3,1	14,14,15	0.55	0	17,19,21	0.64	0
3	NAG	C	2	3	14,14,15	0.54	0	17,19,21	0.77	1 (5%)

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	2,1	1/1/5/7	1/6/23/26	0/1/1/1
2	NAG	B	2	2	-	5/6/23/26	0/1/1/1
2	MAN	B	3	2	-	1/2/19/22	0/1/1/1
3	NAG	C	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	C2-N2-C7	-2.85	119.08	122.90
3	C	2	NAG	C2-N2-C7	-2.25	119.89	122.90
2	B	2	NAG	C1-O5-C5	2.03	114.90	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1	NAG	C1

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2	NAG	C1-C2-N2-C7
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2
2	B	2	NAG	C4-C5-C6-O6
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
2	B	2	NAG	O5-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
2	B	3	MAN	O5-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 5 short contacts:

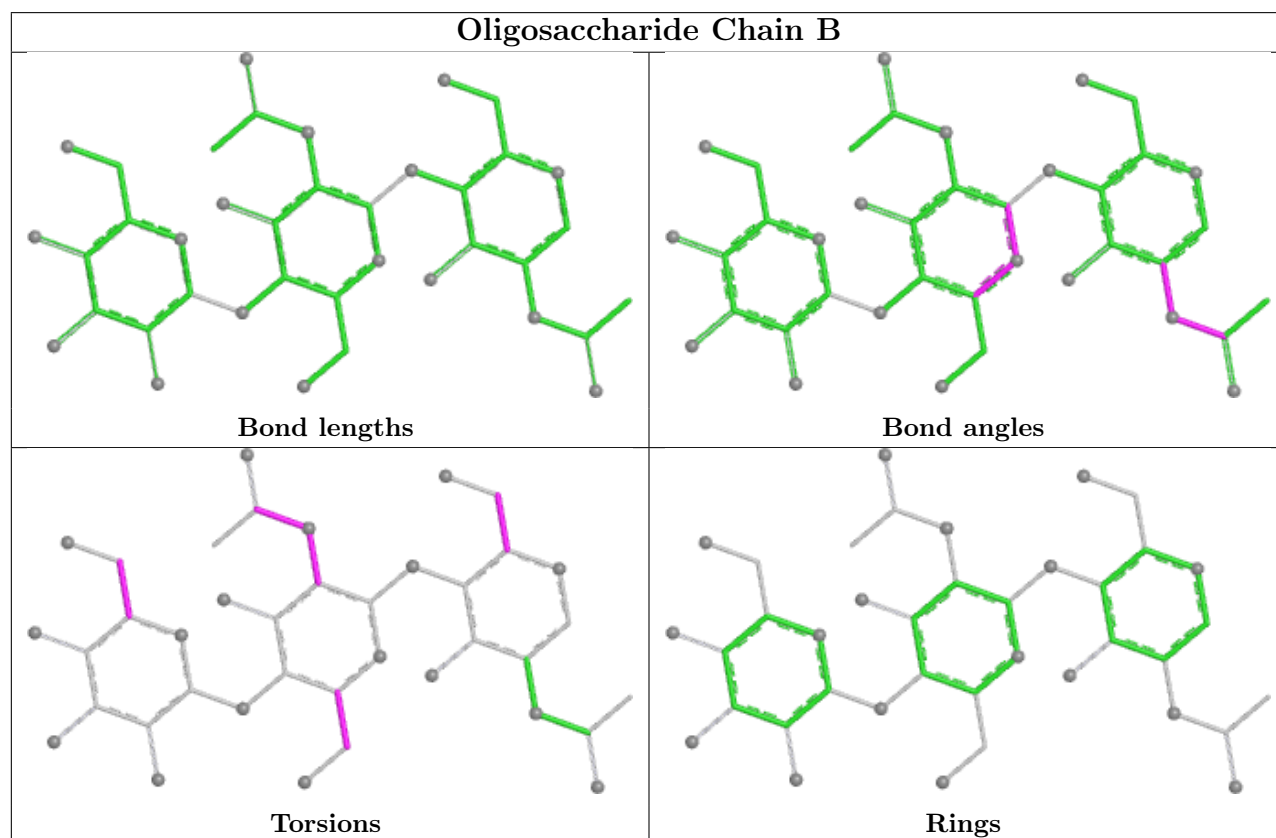
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	3	MAN	2	0
3	C	2	NAG	1	0

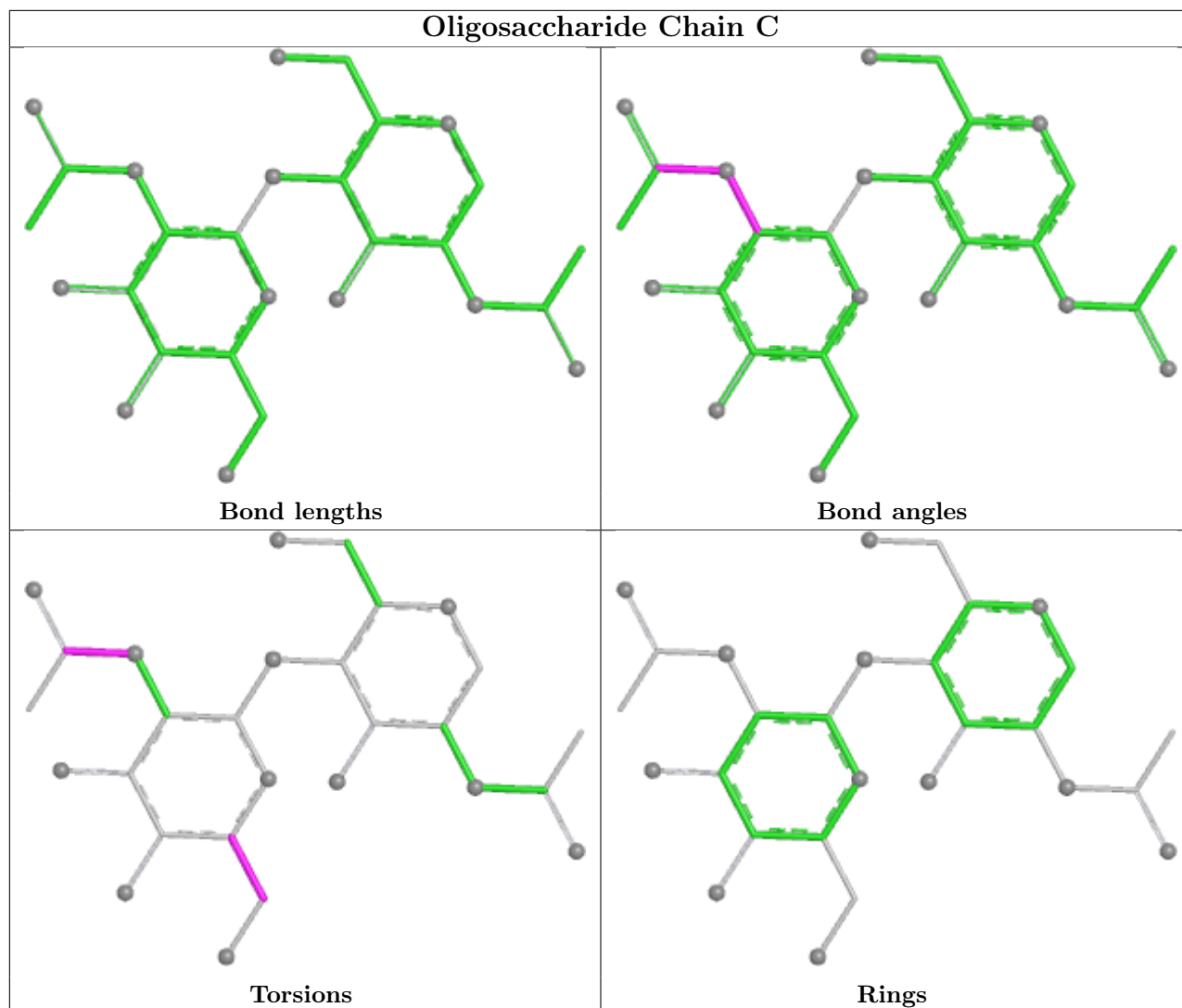
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	NAG	3	0
2	B	1	NAG	2	0
3	C	1	NAG	1	0

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](#)

1 ligand is 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	$\# Z  > 2$
4	FRU	A	800	-	11,12,12	1.23	1 (9%)	10,18,18	0.83	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	FRU	A	800	-	-	3/5/24/24	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	800	FRU	O2-C2	3.73	1.47	1.40

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	800	FRU	O1-C1-C2-C3
4	A	800	FRU	O1-C1-C2-O2
4	A	800	FRU	O1-C1-C2-O5

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	537/543 (98%)	1.05	84 (15%) <b>5</b> <b>4</b>	19, 29, 47, 74	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	538	SER	5.3
1	A	321	ARG	5.2
1	A	374	GLU	4.9
1	A	433	GLY	4.8
1	A	350	LYS	4.3
1	A	221	TYR	4.3
1	A	377	LYS	4.3
1	A	211	ASN	4.1
1	A	322	ASN	3.9
1	A	517	ASN	3.9
1	A	188	ASP	3.7
1	A	4	GLU	3.6
1	A	138	GLU	3.6
1	A	372	LYS	3.6
1	A	451	ASN	3.6
1	A	434	ARG	3.5
1	A	189	GLN	3.5
1	A	518	VAL	3.5
1	A	376	LEU	3.5
1	A	450	SER	3.4
1	A	247	ASP	3.4
1	A	3	ILE	3.4
1	A	418	LYS	3.3
1	A	2	GLN	3.3
1	A	345	GLN	3.3
1	A	362	ALA	3.3
1	A	373	LEU	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	250	ASN	3.2
1	A	224	SER	3.1
1	A	468	GLU	3.0
1	A	343	ASN	3.0
1	A	248	ARG	3.0
1	A	436	SER	2.9
1	A	463	ILE	2.9
1	A	391	ALA	2.8
1	A	408	GLY	2.8
1	A	516	GLN	2.8
1	A	222	GLY	2.8
1	A	375	GLY	2.8
1	A	348	ASN	2.7
1	A	346	ASN	2.7
1	A	252	LEU	2.7
1	A	466	ARG	2.7
1	A	370	SER	2.7
1	A	435	TYR	2.6
1	A	519	LYS	2.6
1	A	381	VAL	2.6
1	A	254	GLN	2.6
1	A	265	ASP	2.6
1	A	398	ALA	2.6
1	A	185	LYS	2.5
1	A	379	ALA	2.5
1	A	460	PHE	2.5
1	A	264	LEU	2.4
1	A	212	SER	2.4
1	A	320	ASP	2.4
1	A	139	GLY	2.4
1	A	488	GLY	2.4
1	A	213	THR	2.3
1	A	514	GLY	2.3
1	A	432	LEU	2.3
1	A	503	ASN	2.3
1	A	416	ASP	2.3
1	A	511	PHE	2.3
1	A	522	GLU	2.3
1	A	5	GLN	2.3
1	A	523	MET	2.2
1	A	304	GLU	2.2
1	A	186	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	384	THR	2.1
1	A	445	ARG	2.1
1	A	393	CYS	2.1
1	A	464	ASP	2.1
1	A	323	GLY	2.1
1	A	349	LEU	2.1
1	A	397	GLY	2.1
1	A	387	VAL	2.1
1	A	425	PHE	2.1
1	A	336	GLU	2.1
1	A	465	PRO	2.0
1	A	502	ASN	2.0
1	A	326	LEU	2.0
1	A	220	VAL	2.0
1	A	510	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

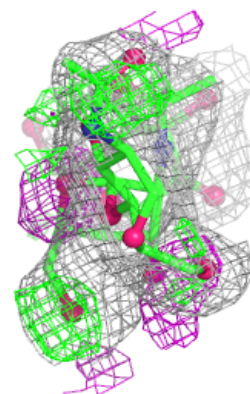
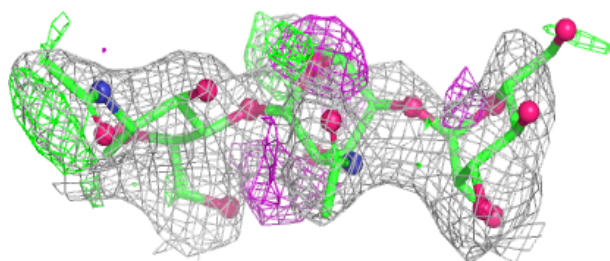
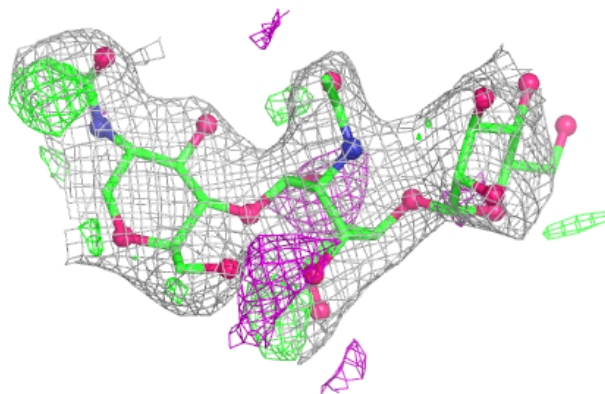
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MAN	B	3	11/12	0.45	0.27	81,83,85,86	0
2	NAG	B	2	14/15	0.67	0.27	53,63,70,74	0
3	NAG	C	2	14/15	0.81	0.16	54,58,63,63	0
2	NAG	B	1	14/15	0.82	0.16	35,38,43,49	0
3	NAG	C	1	14/15	0.91	0.12	39,41,44,49	0

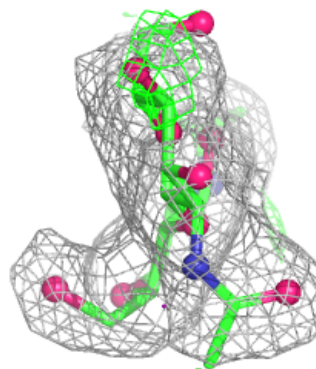
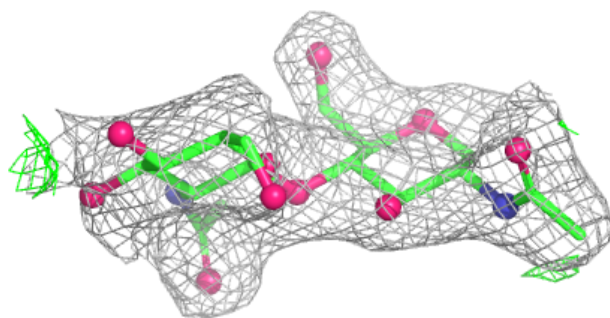
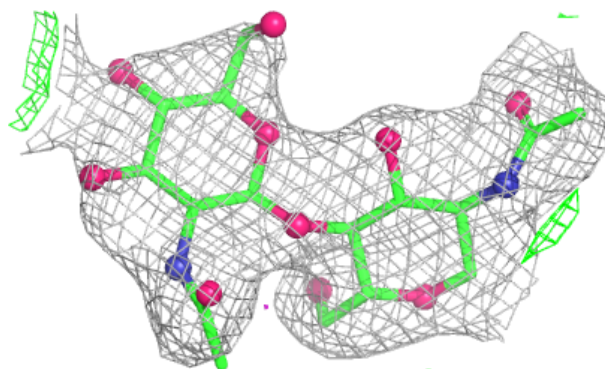
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around Chain B:**

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

**Electron density around Chain C:**

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



## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	FRU	A	800	12/12	0.91	0.14	27,31,35,36	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.