



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:35 AM UTC

PDB ID : 3WWG / pdb_00003wwg
Title : Crystal structure of the N-glycan-deficient variant N448A of isopullulanase complexed with isopanose
Authors : Miyazaki, T.; Yashiro, H.; Nishikawa, A.; Tonozuka, T.
Deposited on : 2014-06-17
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

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>.

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

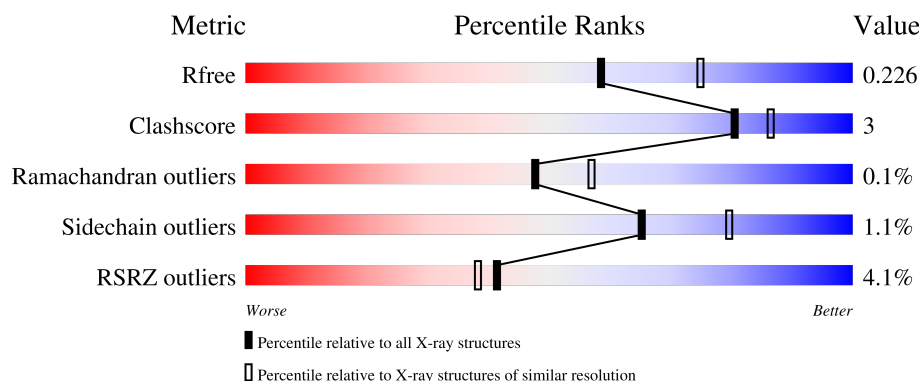
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	549	3% 91% 7%
1	B	549	4% 92% 7%
1	C	549	4% 91% 7%
1	D	549	5% 92% 6%
2	E	2	50% 50%

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Mol	Chain	Length	Quality of chain
3	F	2	50% 50%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17816 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.

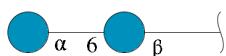
- Molecule 1 is a protein called Isopullulanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	536	Total	C	N	O	S	0	0	0
			4148	2625	692	820	11			
1	B	542	Total	C	N	O	S	0	1	0
			4194	2650	699	834	11			
1	C	541	Total	C	N	O	S	0	0	0
			4186	2647	698	830	11			
1	D	540	Total	C	N	O	S	0	0	0
			4171	2633	697	830	11			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	ARG	-	expression tag	UNP O00105
A	17	GLU	-	expression tag	UNP O00105
A	18	PHE	-	expression tag	UNP O00105
A	19	MET	-	expression tag	UNP O00105
A	448	ALA	ASN	engineered mutation	UNP O00105
B	16	ARG	-	expression tag	UNP O00105
B	17	GLU	-	expression tag	UNP O00105
B	18	PHE	-	expression tag	UNP O00105
B	19	MET	-	expression tag	UNP O00105
B	448	ALA	ASN	engineered mutation	UNP O00105
C	16	ARG	-	expression tag	UNP O00105
C	17	GLU	-	expression tag	UNP O00105
C	18	PHE	-	expression tag	UNP O00105
C	19	MET	-	expression tag	UNP O00105
C	448	ALA	ASN	engineered mutation	UNP O00105
D	16	ARG	-	expression tag	UNP O00105
D	17	GLU	-	expression tag	UNP O00105
D	18	PHE	-	expression tag	UNP O00105
D	19	MET	-	expression tag	UNP O00105
D	448	ALA	ASN	engineered mutation	UNP O00105

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-6)-beta-D-glucopyranose.



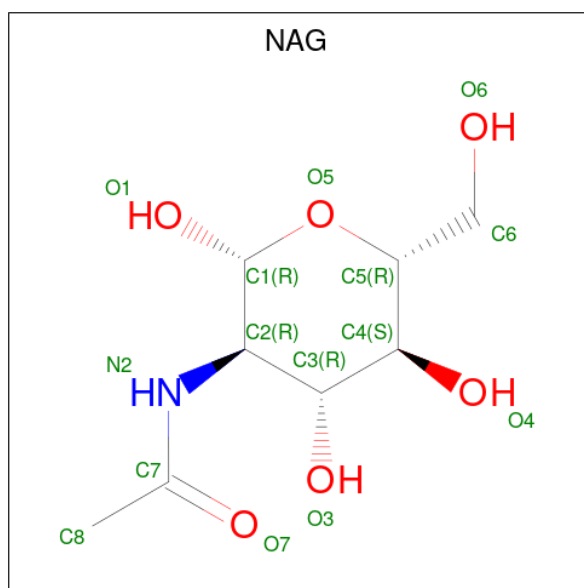
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	F	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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		

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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		
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	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		

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

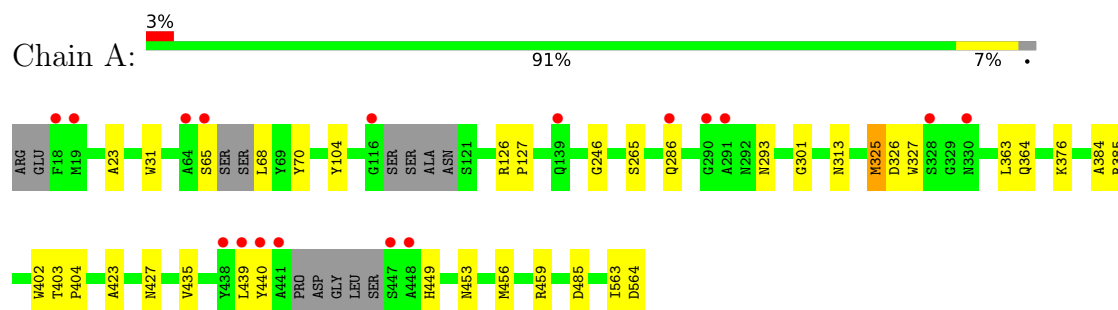
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	182	Total	O	0	0
			182	182		
5	B	175	Total	O	0	0
			175	175		
5	C	137	Total	O	0	0
			137	137		
5	D	129	Total	O	0	0
			129	129		

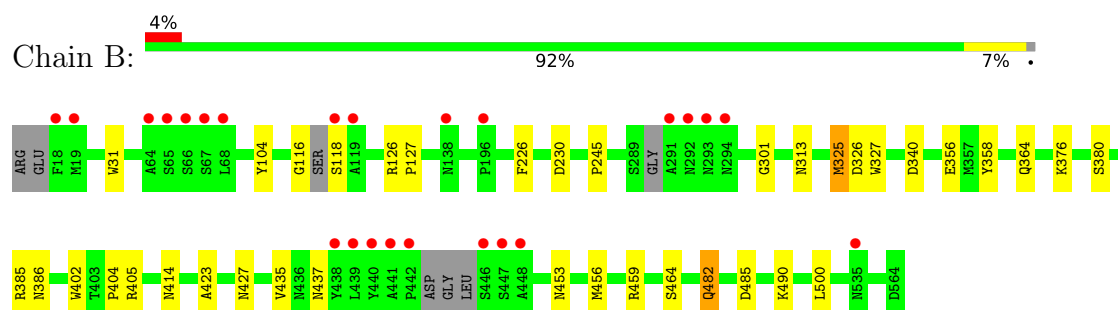
3 Residue-property plots [i](#)

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.

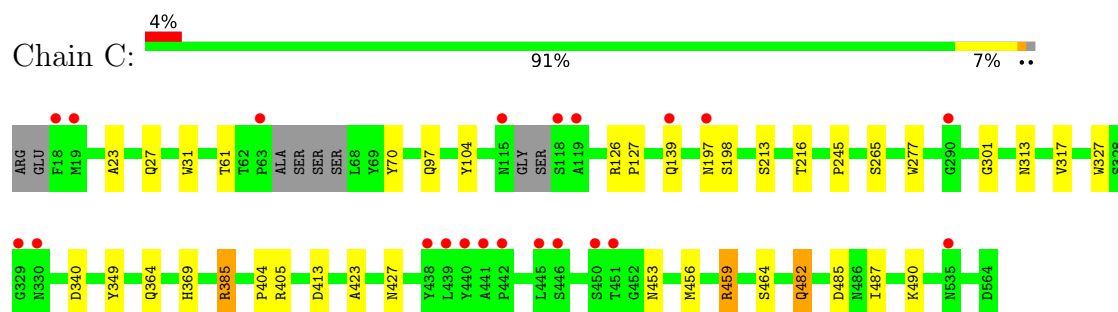
- Molecule 1: Isopullulanase



- Molecule 1: Isopullulanase

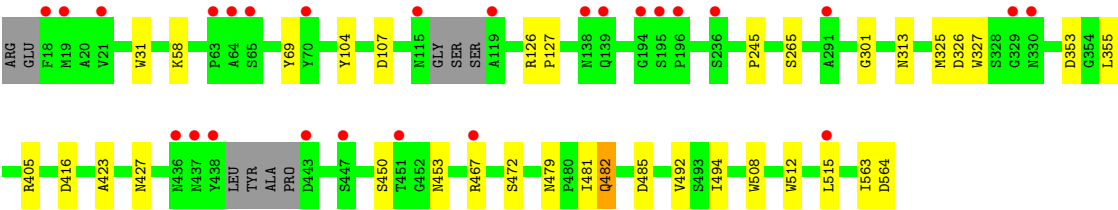


- Molecule 1: Isopullulanase



- Molecule 1: Isopullulanase





● Molecule 2: alpha-D-glucopyranose-(1-6)-beta-D-glucopyranose



● Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.40Å 108.10Å 116.00Å 90.00° 103.90° 90.00°	Depositor
Resolution (Å)	34.04 – 2.20 34.04 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.4 (34.04-2.20) 97.4 (34.04-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.26 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.183 , 0.224 0.191 , 0.226	Depositor DCC
R_{free} test set	5738 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	25.2	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 29.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17816	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: NAG, BGC, GLC

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	0.52	0/4259	0.71	0/5825
1	B	0.52	0/4309	0.72	1/5894 (0.0%)
1	C	0.50	0/4299	0.71	0/5882
1	D	0.48	0/4282	0.70	1/5857 (0.0%)
All	All	0.50	0/17149	0.71	2/23458 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	325	MET	N-CA-C	5.86	118.05	108.55
1	D	508	TRP	N-CA-C	5.40	117.28	109.07

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	4148	0	3895	19	0
1	B	4194	0	3938	24	0
1	C	4186	0	3931	22	0
1	D	4171	0	3915	21	0
2	E	23	0	21	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	23	0	21	0	0
4	A	112	0	104	0	0
4	B	98	0	91	1	0
4	C	126	0	117	0	0
4	D	112	0	104	1	0
5	A	182	0	0	2	0
5	B	175	0	0	0	0
5	C	137	0	0	0	0
5	D	129	0	0	0	0
All	All	17816	0	16137	85	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 3.

All (85) 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:B:453:ASN:HD22	1:B:456:MET:HE2	1.33	0.94
1:D:325:MET:HE3	1:D:355:LEU:HD22	1.58	0.85
1:B:405:ARG:H	1:B:482:GLN:HE21	1.38	0.72
1:B:453:ASN:ND2	1:B:456:MET:HE2	2.05	0.71
1:B:386:ASN:HD22	1:B:414:ASN:HD22	1.37	0.69
1:B:386:ASN:ND2	1:B:414:ASN:HD22	1.94	0.66
1:D:127:PRO:HB3	1:D:416:ASP:OD2	2.00	0.61
1:C:197:ASN:ND2	1:C:213:SER:O	2.29	0.60
1:C:404:PRO:HB2	1:C:456:MET:HE3	1.84	0.59
1:A:286:GLN:HG3	5:A:1134:HOH:O	2.04	0.57
1:C:301:GLY:HA3	1:C:327:TRP:CE2	2.39	0.56
1:B:404:PRO:HB2	1:B:456:MET:HE3	1.87	0.56
1:B:325:MET:O	1:B:326[B]:ASP:CG	2.49	0.56
1:D:450:SER:O	1:D:515:LEU:HA	2.06	0.55
1:D:479:ASN:HD22	1:D:512:TRP:HE1	1.56	0.54
1:D:405:ARG:H	1:D:482:GLN:HE21	1.56	0.53
1:A:404:PRO:HB2	1:A:456:MET:HE3	1.90	0.52
1:B:126:ARG:HA	1:B:127:PRO:C	2.33	0.52
1:D:416:ASP:HB2	1:D:467:ARG:NH2	2.24	0.52
1:D:325:MET:HG2	1:D:326:ASP:N	2.25	0.52
1:C:459:ARG:HA	1:C:485:ASP:O	2.10	0.51
1:C:405:ARG:H	1:C:482:GLN:HE21	1.57	0.51
1:B:301:GLY:HA3	1:B:327:TRP:CE2	2.46	0.50
1:A:453:ASN:ND2	1:A:456:MET:HE2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:325:MET:CE	1:D:355:LEU:HD22	2.36	0.50
1:D:563:ILE:O	1:D:564:ASP:HB2	2.12	0.49
1:C:198:SER:HB3	1:C:216:THR:HB	1.95	0.49
1:D:31:TRP:CZ3	1:D:245:PRO:HB3	2.47	0.49
1:A:126:ARG:HA	1:A:127:PRO:C	2.38	0.48
1:D:325:MET:O	1:D:326:ASP:CG	2.55	0.48
1:B:116:GLY:O	1:B:118:SER:N	2.47	0.48
1:C:404:PRO:HB2	1:C:456:MET:CE	2.43	0.48
1:C:453:ASN:ND2	1:C:456:MET:HE2	2.28	0.48
1:C:126:ARG:HA	1:C:127:PRO:C	2.39	0.47
1:A:325:MET:HG2	1:A:326:ASP:N	2.28	0.47
1:C:464:SER:HA	1:C:490:LYS:O	2.15	0.47
1:A:364:GLN:HA	1:A:385:ARG:O	2.14	0.47
1:C:453:ASN:HD22	1:C:456:MET:HE2	1.78	0.47
1:D:301:GLY:HA3	1:D:327:TRP:CE2	2.50	0.47
1:C:31:TRP:CZ3	1:C:245:PRO:HB3	2.49	0.47
1:A:423:ALA:H	1:A:427:ASN:HD22	1.62	0.46
1:A:31:TRP:CD1	1:A:246:GLY:HA2	2.50	0.46
1:B:402:TRP:CZ2	1:B:435:VAL:HG21	2.51	0.45
1:A:23:ALA:HB2	1:A:70:TYR:CG	2.51	0.45
1:D:126:ARG:HA	1:D:127:PRO:C	2.41	0.45
1:B:404:PRO:HD3	1:B:437:ASN:HD21	1.82	0.45
1:A:23:ALA:HB2	1:A:70:TYR:CD2	2.52	0.45
1:B:459:ARG:HA	1:B:485:ASP:O	2.16	0.45
1:A:402:TRP:CE2	1:A:435:VAL:HG21	2.52	0.45
1:A:449:HIS:HD2	5:A:1138:HOH:O	2.00	0.44
1:D:265:SER:HA	1:D:313:ASN:O	2.17	0.44
1:B:226:PHE:O	1:B:230:ASP:HB3	2.17	0.44
1:B:380:SER:HB2	4:B:1004:NAG:H82	1.97	0.44
1:C:423:ALA:H	1:C:427:ASN:ND2	2.15	0.44
1:D:58:LYS:HB3	1:D:69:TYR:HB3	1.99	0.44
1:C:97:GLN:HE22	1:C:369:HIS:CD2	2.35	0.44
1:D:325:MET:HE3	1:D:355:LEU:CD2	2.37	0.44
1:B:386:ASN:HD22	1:B:414:ASN:ND2	2.09	0.43
1:C:485:ASP:OD2	1:D:485:ASP:OD2	2.36	0.43
1:D:453:ASN:HA	4:D:1005:NAG:H82	1.99	0.43
1:B:325:MET:HE2	1:B:358:TYR:CE2	2.54	0.43
1:A:363:LEU:O	1:A:384:ALA:HA	2.19	0.43
1:D:423:ALA:H	1:D:427:ASN:HD22	1.65	0.43
1:A:301:GLY:HA3	1:A:327:TRP:CE2	2.53	0.42
1:A:439:LEU:HD22	1:A:440:TYR:CZ	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:GLN:OE1	1:C:61:THR:HG21	2.19	0.42
1:C:277:TRP:CD1	1:C:349:TYR:HB3	2.54	0.42
1:B:31:TRP:CZ3	1:B:245:PRO:HB3	2.54	0.42
1:C:385:ARG:HA	1:C:413:ASP:O	2.19	0.42
1:B:356:GLU:OE2	1:B:376:LYS:NZ	2.48	0.42
1:C:23:ALA:HB2	1:C:70:TYR:CG	2.55	0.42
1:A:459:ARG:HA	1:A:485:ASP:O	2.19	0.42
1:A:563:ILE:O	1:A:564:ASP:HB2	2.19	0.42
1:B:464:SER:HA	1:B:490:LYS:O	2.20	0.42
1:D:481:ILE:HG22	1:D:512:TRP:CH2	2.56	0.41
1:B:423:ALA:H	1:B:427:ASN:ND2	2.18	0.41
1:A:423:ALA:H	1:A:427:ASN:ND2	2.17	0.41
1:B:364:GLN:HA	1:B:385:ARG:O	2.21	0.41
1:A:265:SER:HA	1:A:313:ASN:O	2.21	0.41
1:B:405:ARG:N	1:B:482:GLN:HE21	2.13	0.41
1:D:472:SER:HB3	1:D:494:ILE:HG23	2.02	0.41
1:C:423:ALA:H	1:C:427:ASN:HD22	1.68	0.40
1:B:313:ASN:HA	1:B:340:ASP:O	2.20	0.40
1:C:265:SER:HA	1:C:313:ASN:O	2.21	0.40
1:C:313:ASN:HA	1:C:340:ASP:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	528/549 (96%)	501 (95%)	27 (5%)	0	100	100
1	B	535/549 (97%)	507 (95%)	28 (5%)	0	100	100
1	C	535/549 (97%)	504 (94%)	31 (6%)	0	100	100
1	D	534/549 (97%)	497 (93%)	35 (7%)	2 (0%)	30	34
All	All	2132/2196 (97%)	2009 (94%)	121 (6%)	2 (0%)	48	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	107	ASP
1	D	353	ASP

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	453/465 (97%)	446 (98%)	7 (2%)	57	73
1	B	461/465 (99%)	458 (99%)	3 (1%)	76	87
1	C	459/465 (99%)	451 (98%)	8 (2%)	53	69
1	D	458/465 (98%)	455 (99%)	3 (1%)	76	87
All	All	1831/1860 (98%)	1810 (99%)	21 (1%)	65	79

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	SER
1	A	68	LEU
1	A	104	TYR
1	A	293	ASN
1	A	325	MET
1	A	376	LYS
1	A	403	THR
1	B	104	TYR
1	B	482	GLN
1	B	500	LEU
1	C	104	TYR
1	C	139	GLN
1	C	317	VAL
1	C	364	GLN
1	C	385	ARG
1	C	459	ARG
1	C	482	GLN
1	C	487	ILE

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Mol	Chain	Res	Type
1	D	104	TYR
1	D	482	GLN
1	D	492	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	88	GLN
1	A	122	ASN
1	A	220	ASN
1	A	386	ASN
1	A	427	ASN
1	A	449	HIS
1	A	516	ASN
1	A	520	GLN
1	B	51	GLN
1	B	88	GLN
1	B	106	HIS
1	B	122	ASN
1	B	220	ASN
1	B	323	ASN
1	B	351	GLN
1	B	386	ASN
1	B	427	ASN
1	B	437	ASN
1	B	482	GLN
1	B	516	ASN
1	C	51	GLN
1	C	97	GLN
1	C	120	ASN
1	C	286	GLN
1	C	323	ASN
1	C	386	ASN
1	C	414	ASN
1	C	427	ASN
1	C	449	HIS
1	C	482	GLN
1	C	516	ASN
1	C	520	GLN
1	C	561	HIS
1	D	51	GLN

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Mol	Chain	Res	Type
1	D	91	GLN
1	D	95	GLN
1	D	192	GLN
1	D	323	ASN
1	D	364	GLN
1	D	386	ASN
1	D	427	ASN
1	D	479	ASN
1	D	482	GLN
1	D	486	ASN

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 ⓘ

4 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	BGC	E	1	2	12,12,12	0.50	0	17,17,17	0.74	0
2	GLC	E	2	2	11,11,12	0.56	0	15,15,17	0.97	1 (6%)
3	GLC	F	1	3	12,12,12	0.58	0	17,17,17	1.36	3 (17%)
3	GLC	F	2	3	11,11,12	0.38	0	15,15,17	0.65	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	BGC	E	1	2	-	2/2/22/22	0/1/1/1
2	GLC	E	2	2	-	0/2/19/22	0/1/1/1
3	GLC	F	1	3	-	2/2/22/22	0/1/1/1
3	GLC	F	2	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1	GLC	O5-C5-C4	2.81	114.75	109.70
3	F	1	GLC	C1-O5-C5	2.63	118.73	113.65
2	E	2	GLC	C1-C2-C3	2.40	113.14	109.64
3	F	1	GLC	C3-C4-C5	2.09	114.02	110.23

There are no chirality outliers.

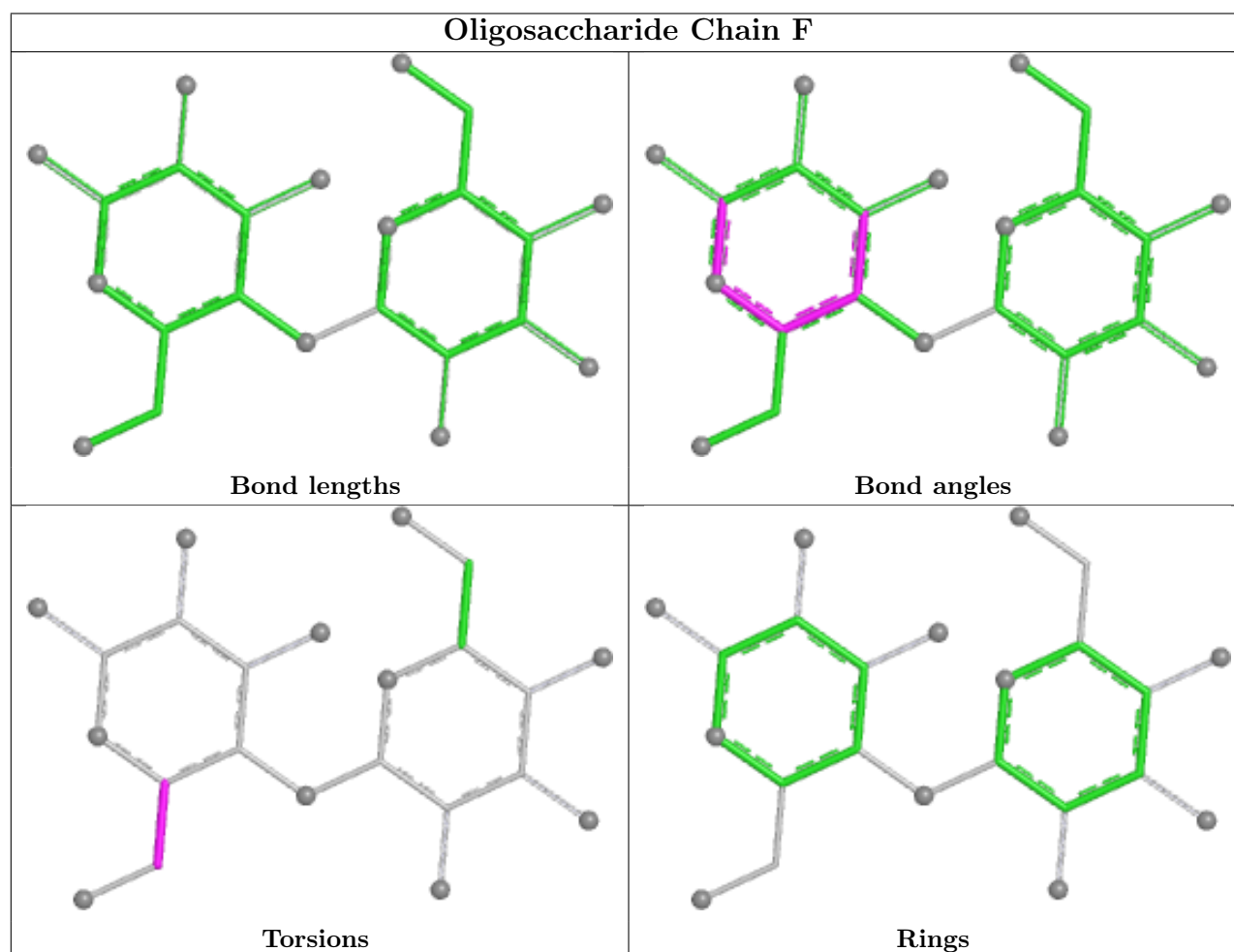
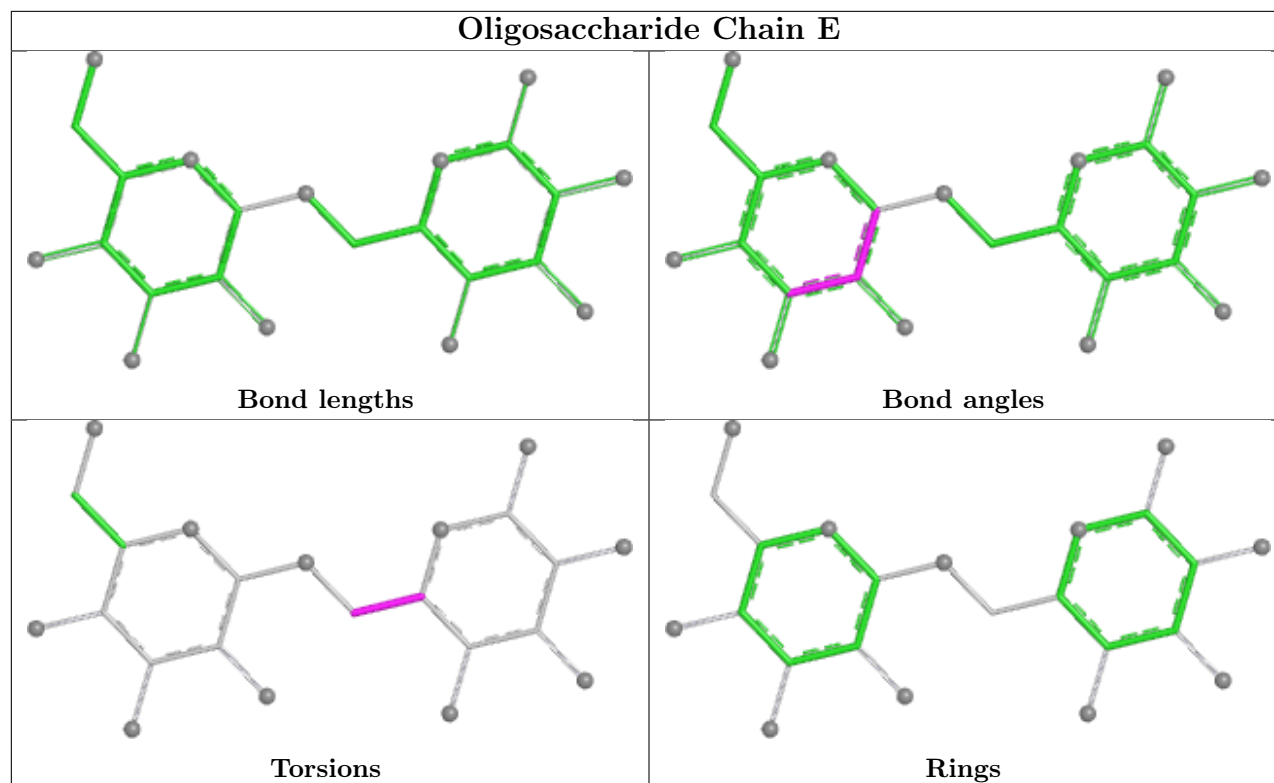
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	1	GLC	C4-C5-C6-O6
3	F	1	GLC	O5-C5-C6-O6
2	E	1	BGC	C4-C5-C6-O6
2	E	1	BGC	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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

32 ligands 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
4	NAG	A	1008	1	14,14,15	0.57	0	17,19,21	2.20	5 (29%)
4	NAG	B	1007	1	14,14,15	0.50	0	17,19,21	1.68	1 (5%)
4	NAG	A	1004	1	14,14,15	0.40	0	17,19,21	1.12	1 (5%)
4	NAG	A	1003	1	14,14,15	0.59	0	17,19,21	0.96	1 (5%)
4	NAG	A	1007	1	14,14,15	0.57	0	17,19,21	0.81	0
4	NAG	B	1002	1	14,14,15	0.60	0	17,19,21	1.52	3 (17%)
4	NAG	D	1004	1	14,14,15	0.49	0	17,19,21	1.21	2 (11%)
4	NAG	C	1001	1	14,14,15	0.65	0	17,19,21	1.11	1 (5%)
4	NAG	B	1006	1	14,14,15	0.57	0	17,19,21	0.78	0
4	NAG	D	1002	1	14,14,15	0.46	0	17,19,21	0.78	0
4	NAG	C	1009	1	14,14,15	0.46	0	17,19,21	1.95	3 (17%)
4	NAG	B	1001	1	14,14,15	0.64	0	17,19,21	1.33	3 (17%)
4	NAG	C	1006	1	14,14,15	0.49	0	17,19,21	1.30	1 (5%)
4	NAG	D	1008	1	14,14,15	0.56	0	17,19,21	1.05	2 (11%)
4	NAG	C	1004	1	14,14,15	0.75	0	17,19,21	1.17	2 (11%)
4	NAG	B	1003	1	14,14,15	0.61	0	17,19,21	1.05	1 (5%)
4	NAG	B	1005	1	14,14,15	0.56	0	17,19,21	1.14	1 (5%)
4	NAG	A	1005	1	14,14,15	0.53	0	17,19,21	0.92	0
4	NAG	C	1003	1	14,14,15	0.58	0	17,19,21	0.87	0
4	NAG	D	1001	1	14,14,15	0.57	0	17,19,21	1.16	2 (11%)
4	NAG	D	1003	1	14,14,15	0.54	0	17,19,21	1.12	1 (5%)
4	NAG	B	1004	1	14,14,15	0.53	0	17,19,21	1.19	1 (5%)
4	NAG	D	1007	1	14,14,15	0.47	0	17,19,21	1.45	2 (11%)
4	NAG	A	1002	1	14,14,15	0.45	0	17,19,21	1.40	3 (17%)
4	NAG	D	1006	1	14,14,15	0.53	0	17,19,21	0.98	0
4	NAG	C	1005	1	14,14,15	0.45	0	17,19,21	0.88	0
4	NAG	C	1007	1	14,14,15	0.56	0	17,19,21	1.02	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	D	1005	1	14,14,15	0.40	0	17,19,21	1.99	6 (35%)
4	NAG	C	1002	1	14,14,15	0.47	0	17,19,21	1.25	1 (5%)
4	NAG	A	1006	1	14,14,15	0.57	0	17,19,21	1.08	1 (5%)
4	NAG	C	1008	1	14,14,15	0.48	0	17,19,21	1.48	3 (17%)
4	NAG	A	1001	1	14,14,15	0.48	0	17,19,21	0.65	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	NAG	A	1008	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1007	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1004	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1003	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1007	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1002	1	-	2/6/23/26	0/1/1/1
4	NAG	D	1004	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1001	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1006	1	-	0/6/23/26	0/1/1/1
4	NAG	D	1002	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1009	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1001	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1006	1	-	0/6/23/26	0/1/1/1
4	NAG	D	1008	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1004	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1003	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1005	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1005	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1003	1	-	2/6/23/26	0/1/1/1
4	NAG	D	1001	1	-	2/6/23/26	0/1/1/1
4	NAG	D	1003	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1004	1	-	0/6/23/26	0/1/1/1
4	NAG	D	1007	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1002	1	-	3/6/23/26	0/1/1/1
4	NAG	D	1006	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1005	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1007	1	-	1/6/23/26	0/1/1/1
4	NAG	D	1005	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1002	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1006	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1008	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1001	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1009	NAG	C1-O5-C5	6.48	120.87	112.19
4	B	1007	NAG	C1-O5-C5	5.73	119.86	112.19
4	A	1008	NAG	C1-O5-C5	5.23	119.19	112.19
4	A	1008	NAG	C2-N2-C7	4.20	128.53	122.90
4	D	1005	NAG	C1-O5-C5	4.06	117.63	112.19
4	D	1005	NAG	C1-C2-N2	4.01	116.76	110.43
4	C	1006	NAG	C1-O5-C5	4.01	117.56	112.19
4	C	1002	NAG	C1-O5-C5	3.96	117.49	112.19
4	B	1002	NAG	C8-C7-N2	3.78	122.39	116.12
4	B	1004	NAG	C1-O5-C5	3.63	117.06	112.19
4	D	1003	NAG	C1-O5-C5	3.63	117.05	112.19
4	D	1005	NAG	O5-C1-C2	-3.61	105.70	111.29
4	C	1008	NAG	C1-O5-C5	3.54	116.93	112.19
4	A	1002	NAG	C1-O5-C5	3.41	116.76	112.19
4	A	1008	NAG	C8-C7-N2	3.26	121.53	116.12
4	C	1004	NAG	C1-O5-C5	3.11	116.36	112.19
4	D	1007	NAG	C1-O5-C5	2.97	116.16	112.19
4	B	1003	NAG	C1-O5-C5	2.89	116.06	112.19
4	A	1002	NAG	O5-C1-C2	-2.84	106.90	111.29
4	C	1001	NAG	C1-C2-N2	-2.76	106.08	110.43
4	D	1007	NAG	O5-C1-C2	-2.73	107.06	111.29
4	B	1001	NAG	C1-O5-C5	2.72	115.83	112.19
4	A	1006	NAG	C1-O5-C5	2.66	115.75	112.19
4	A	1008	NAG	C1-C2-N2	2.63	114.57	110.43
4	A	1008	NAG	C4-C3-C2	-2.62	107.18	111.02
4	C	1009	NAG	C1-C2-N2	2.43	114.26	110.43
4	B	1002	NAG	C2-N2-C7	2.43	126.15	122.90
4	D	1001	NAG	C1-C2-N2	2.42	114.25	110.43
4	C	1009	NAG	C4-C3-C2	-2.36	107.56	111.02
4	A	1004	NAG	O5-C5-C6	2.35	112.24	107.66
4	A	1002	NAG	C8-C7-N2	2.33	119.98	116.12
4	C	1004	NAG	O5-C5-C6	-2.32	103.15	107.66
4	D	1008	NAG	O7-C7-C8	-2.29	117.97	122.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1004	NAG	O5-C1-C2	-2.28	107.76	111.29
4	B	1005	NAG	C4-C3-C2	-2.25	107.72	111.02
4	A	1003	NAG	C1-O5-C5	2.25	115.20	112.19
4	B	1001	NAG	O5-C1-C2	-2.25	107.82	111.29
4	D	1005	NAG	C3-C4-C5	2.23	114.28	110.23
4	D	1004	NAG	C1-O5-C5	2.20	115.14	112.19
4	D	1005	NAG	O5-C5-C4	2.20	116.18	110.83
4	C	1007	NAG	O7-C7-C8	-2.18	118.18	122.05
4	C	1008	NAG	O5-C1-C2	-2.16	107.94	111.29
4	B	1002	NAG	C4-C3-C2	-2.12	107.91	111.02
4	B	1001	NAG	C8-C7-N2	2.11	119.61	116.12
4	C	1007	NAG	O7-C7-N2	2.10	125.69	121.98
4	D	1008	NAG	C1-C2-N2	2.10	113.74	110.43
4	C	1008	NAG	C6-C5-C4	-2.05	107.98	113.02
4	D	1005	NAG	C6-C5-C4	-2.03	108.04	113.02
4	D	1001	NAG	O5-C5-C6	2.00	111.56	107.66

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1001	NAG	O5-C5-C6-O6
4	C	1003	NAG	C4-C5-C6-O6
4	D	1001	NAG	C4-C5-C6-O6
4	C	1003	NAG	O5-C5-C6-O6
4	A	1002	NAG	C8-C7-N2-C2
4	A	1002	NAG	O7-C7-N2-C2
4	A	1008	NAG	C8-C7-N2-C2
4	A	1008	NAG	O7-C7-N2-C2
4	B	1001	NAG	C8-C7-N2-C2
4	B	1001	NAG	O7-C7-N2-C2
4	B	1002	NAG	C8-C7-N2-C2
4	B	1002	NAG	O7-C7-N2-C2
4	A	1004	NAG	O5-C5-C6-O6
4	C	1009	NAG	O5-C5-C6-O6
4	A	1002	NAG	C4-C5-C6-O6
4	A	1004	NAG	C4-C5-C6-O6
4	A	1008	NAG	C1-C2-N2-C7
4	C	1007	NAG	C4-C5-C6-O6
4	A	1008	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1004	NAG	1	0
4	D	1005	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q<0.9
1	A	536/549 (97%)	-0.19	17 (3%)	50 47	17, 25, 45, 78	0
1	B	542/549 (98%)	-0.14	24 (4%)	39 36	16, 26, 50, 72	1 (0%)
1	C	541/549 (98%)	0.03	21 (3%)	43 40	18, 29, 53, 79	0
1	D	540/549 (98%)	0.18	26 (4%)	35 32	18, 30, 59, 83	0
All	All	2159/2196 (98%)	-0.03	88 (4%)	41 38	16, 27, 53, 83	1 (0%)

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	438	TYR	5.5
1	B	442	PRO	4.8
1	B	448	ALA	4.7
1	A	441	ALA	4.6
1	A	65	SER	4.2
1	D	437	ASN	4.2
1	A	447	SER	4.1
1	A	448	ALA	4.0
1	C	329	GLY	4.0
1	D	196	PRO	4.0
1	D	194	GLY	3.9
1	D	64	ALA	3.8
1	C	438	TYR	3.7
1	C	330	ASN	3.6
1	D	436	ASN	3.6
1	D	443	ASP	3.6
1	D	119	ALA	3.6
1	C	63	PRO	3.6
1	A	438	TYR	3.4
1	C	451	THR	3.4
1	A	440	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	139	GLN	3.3
1	B	64	ALA	3.3
1	D	18	PHE	3.3
1	A	291	ALA	3.3
1	B	440	TYR	3.3
1	B	291	ALA	3.2
1	D	329	GLY	3.2
1	A	439	LEU	3.2
1	B	447	SER	3.1
1	B	441	ALA	3.1
1	B	67	SER	3.1
1	D	195	SER	2.9
1	C	115	ASN	2.9
1	D	19	MET	2.8
1	C	118	SER	2.8
1	C	440	TYR	2.8
1	B	446	SER	2.8
1	C	290	GLY	2.8
1	B	68	LEU	2.7
1	A	18	PHE	2.7
1	C	535	ASN	2.7
1	A	116	GLY	2.7
1	A	290	GLY	2.7
1	C	119	ALA	2.6
1	B	293	ASN	2.6
1	C	442	PRO	2.5
1	D	63	PRO	2.5
1	C	197	ASN	2.5
1	B	119	ALA	2.5
1	D	515	LEU	2.4
1	A	330	ASN	2.4
1	D	65	SER	2.4
1	C	445	LEU	2.4
1	B	438	TYR	2.4
1	A	64	ALA	2.4
1	C	441	ALA	2.4
1	D	291	ALA	2.4
1	D	447	SER	2.4
1	C	18	PHE	2.4
1	C	19	MET	2.4
1	C	439	LEU	2.4
1	D	467	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	139	GLN	2.4
1	B	294	ASN	2.3
1	D	70	TYR	2.3
1	A	19	MET	2.3
1	C	450	SER	2.3
1	B	19	MET	2.3
1	B	18	PHE	2.2
1	B	138	ASN	2.2
1	B	66	SER	2.2
1	B	439	LEU	2.2
1	D	115	ASN	2.2
1	A	139	GLN	2.2
1	D	451	THR	2.2
1	D	138	ASN	2.2
1	A	328	SER	2.2
1	D	236	SER	2.2
1	B	292	ASN	2.1
1	A	286	GLN	2.1
1	B	196	PRO	2.1
1	B	535	ASN	2.1
1	B	65	SER	2.1
1	B	118	SER	2.1
1	D	330	ASN	2.1
1	C	446	SER	2.0
1	D	21	VAL	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, 95th 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.

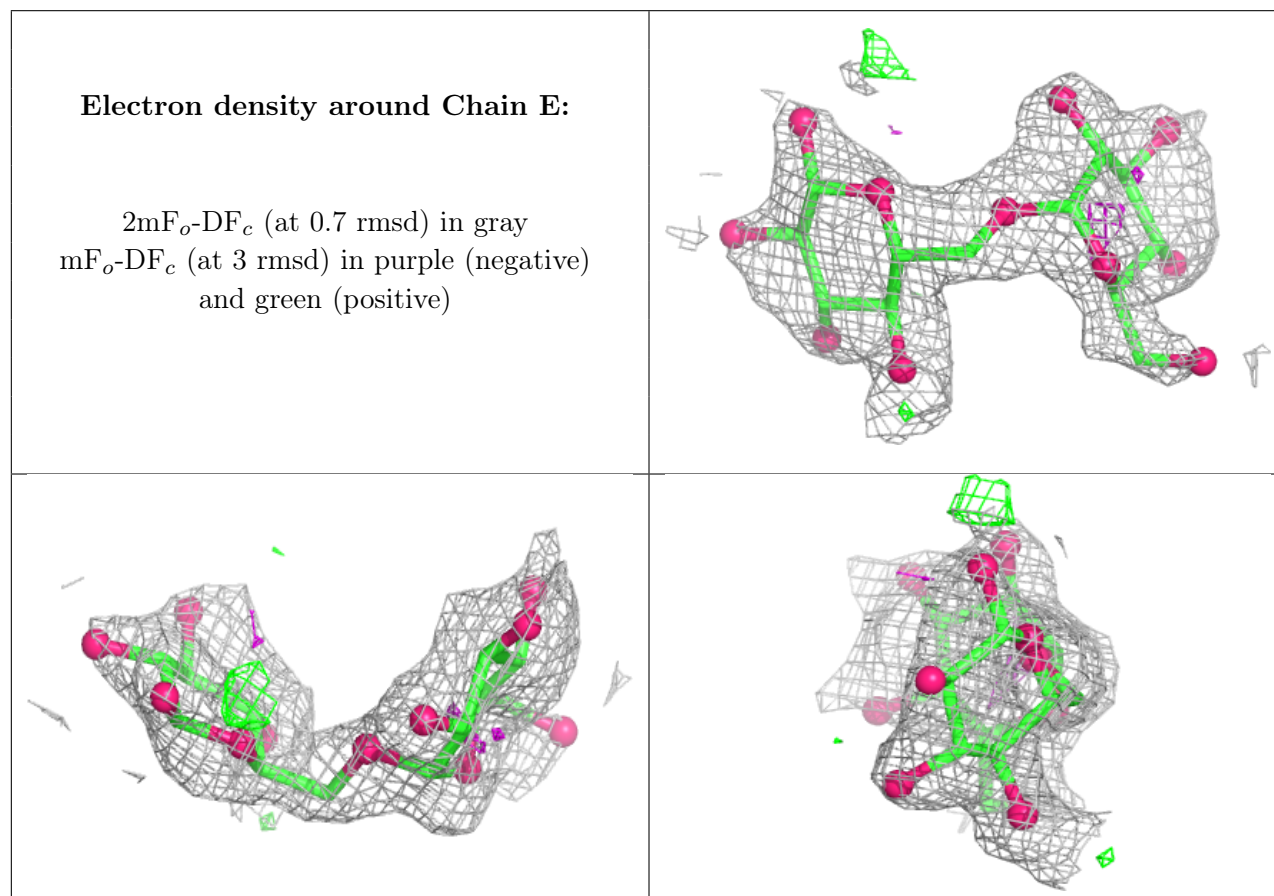
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLC	E	2	11/12	0.63	0.19	66,71,74,75	0
2	BGC	E	1	12/12	0.83	0.14	60,63,65,67	0
3	GLC	F	1	12/12	0.85	0.10	48,51,52,52	0

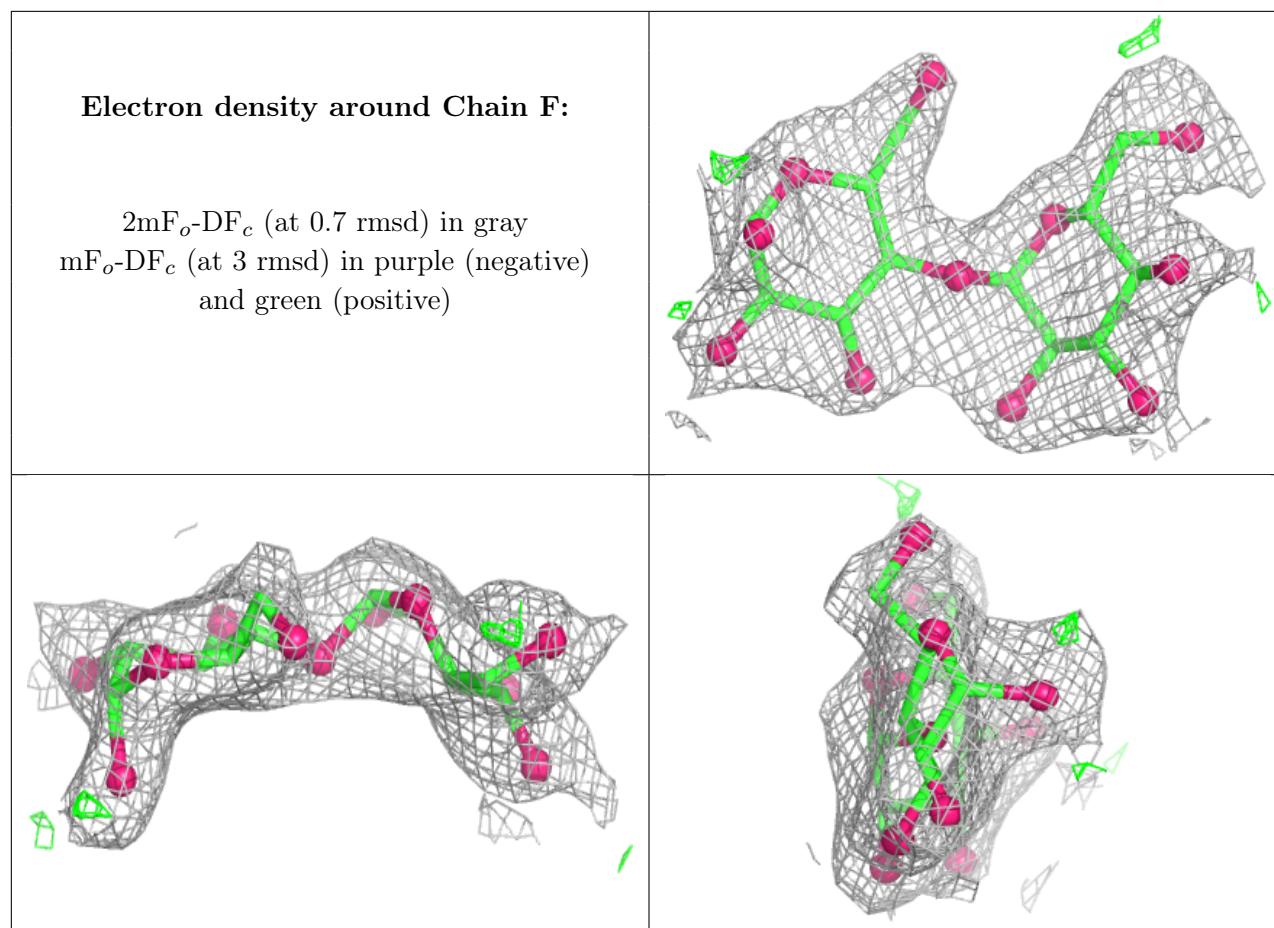
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GLC	F	2	11/12	0.88	0.10	43,46,48,49	0

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.





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, 95th 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	C	1003	14/15	0.65	0.20	76,80,82,82	0
4	NAG	D	1005	14/15	0.66	0.17	47,60,63,64	0
4	NAG	D	1001	14/15	0.67	0.17	61,63,65,66	0
4	NAG	B	1001	14/15	0.68	0.17	48,56,66,67	0
4	NAG	C	1006	14/15	0.74	0.15	47,54,57,57	0
4	NAG	C	1009	14/15	0.74	0.15	59,62,64,64	0
4	NAG	A	1008	14/15	0.77	0.13	46,50,53,54	0
4	NAG	D	1003	14/15	0.78	0.15	52,55,56,56	0
4	NAG	D	1004	14/15	0.79	0.14	44,49,53,55	0
4	NAG	C	1001	14/15	0.81	0.15	45,52,60,60	0
4	NAG	A	1001	14/15	0.81	0.13	43,44,47,48	0
4	NAG	B	1007	14/15	0.82	0.13	51,54,56,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	C	1004	14/15	0.82	0.12	39,44,46,47	0
4	NAG	C	1005	14/15	0.82	0.13	45,51,55,56	0
4	NAG	C	1008	14/15	0.84	0.11	32,39,44,48	0
4	NAG	A	1004	14/15	0.84	0.12	41,46,48,49	0
4	NAG	A	1005	14/15	0.85	0.11	41,44,47,48	0
4	NAG	B	1003	14/15	0.85	0.11	41,44,46,46	0
4	NAG	B	1004	14/15	0.85	0.12	42,45,52,53	0
4	NAG	D	1007	14/15	0.87	0.10	31,38,41,44	0
4	NAG	A	1007	14/15	0.88	0.10	31,33,38,40	0
4	NAG	C	1002	14/15	0.89	0.10	34,37,40,41	0
4	NAG	B	1006	14/15	0.90	0.08	32,36,39,43	0
4	NAG	A	1002	14/15	0.90	0.10	37,40,41,42	0
4	NAG	B	1002	14/15	0.90	0.09	35,37,40,44	0
4	NAG	D	1002	14/15	0.91	0.09	38,42,45,47	0
4	NAG	A	1003	14/15	0.92	0.08	33,34,36,36	0
4	NAG	D	1008	14/15	0.93	0.08	30,31,36,38	0
4	NAG	A	1006	14/15	0.97	0.06	18,19,19,20	0
4	NAG	D	1006	14/15	0.97	0.05	20,21,22,22	0
4	NAG	B	1005	14/15	0.97	0.05	20,20,21,21	0
4	NAG	C	1007	14/15	0.97	0.05	20,21,22,23	0

6.5 Other polymers

There are no such residues in this entry.