



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 9, 2026 – 10:22 PM UTC

PDB ID : 21JI / pdb_000021ji
Title : Crystal structure of isoprimeverose-producing enzyme from *Phaeoacremonium minimum*
Authors : Nakamichi, Y.; Watanabe, M.; Yaoi, K.; Matsuzawa, T.
Deposited on : 2025-12-15
Resolution : 2.80 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:

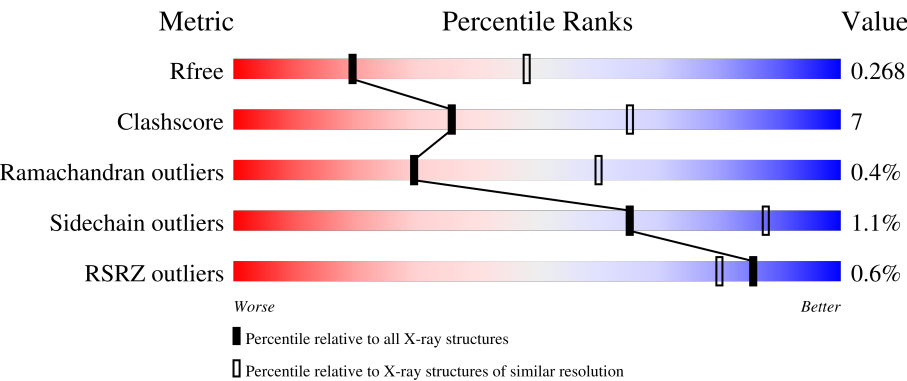
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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.



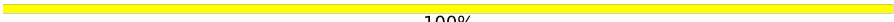



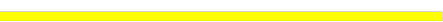
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	871	<div><div></div><div></div><div></div><div></div><div></div></div> <div>72%15%13%</div>
1	B	871	<div><div></div><div></div><div></div><div></div><div></div></div> <div>%73%14%13%</div>
1	C	871	<div><div></div><div></div><div></div><div></div><div></div></div> <div>%65%21%.13%</div>
2	D	3	<div><div></div><div></div><div></div></div> <div>33%33%33%</div>
2	F	3	<div><div></div></div> <div>100%</div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	I	3	 100%
3	E	2	 100%
3	G	2	 100%
3	H	2	 50%  50%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 18089 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 Isoprimeverose-producing oligoxyloglucan hydrolase, beta-glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	757	Total	C	N	O	S	0	1	0
			5809	3692	953	1143	21			
1	B	757	Total	C	N	O	S	0	0	0
			5800	3687	951	1141	21			
1	C	756	Total	C	N	O	S	0	0	0
			5791	3682	950	1138	21			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	PHE	-	linker	UNP A0AA49QB00
A	778	ALA	-	expression tag	UNP R8BKC2
A	779	ALA	-	expression tag	UNP R8BKC2
A	780	ALA	-	expression tag	UNP R8BKC2
A	781	SER	-	expression tag	UNP R8BKC2
A	782	PHE	-	expression tag	UNP R8BKC2
A	783	LEU	-	expression tag	UNP R8BKC2
A	784	GLU	-	expression tag	UNP R8BKC2
A	785	GLN	-	expression tag	UNP R8BKC2
A	786	LYS	-	expression tag	UNP R8BKC2
A	787	LEU	-	expression tag	UNP R8BKC2
A	788	ILE	-	expression tag	UNP R8BKC2
A	789	SER	-	expression tag	UNP R8BKC2
A	790	GLU	-	expression tag	UNP R8BKC2
A	791	GLU	-	expression tag	UNP R8BKC2
A	792	ASP	-	expression tag	UNP R8BKC2
A	793	LEU	-	expression tag	UNP R8BKC2
A	794	ASN	-	expression tag	UNP R8BKC2
A	795	SER	-	expression tag	UNP R8BKC2
A	796	ALA	-	expression tag	UNP R8BKC2
A	797	VAL	-	expression tag	UNP R8BKC2
A	798	ASP	-	expression tag	UNP R8BKC2

Continued on next page...

Continued from previous page...

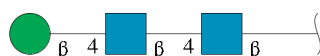
Chain	Residue	Modelled	Actual	Comment	Reference
A	799	HIS	-	expression tag	UNP R8BKC2
A	800	HIS	-	expression tag	UNP R8BKC2
A	801	HIS	-	expression tag	UNP R8BKC2
A	802	HIS	-	expression tag	UNP R8BKC2
A	803	HIS	-	expression tag	UNP R8BKC2
A	804	HIS	-	expression tag	UNP R8BKC2
B	24	PHE	-	linker	UNP A0AA49QB00
B	778	ALA	-	expression tag	UNP R8BKC2
B	779	ALA	-	expression tag	UNP R8BKC2
B	780	ALA	-	expression tag	UNP R8BKC2
B	781	SER	-	expression tag	UNP R8BKC2
B	782	PHE	-	expression tag	UNP R8BKC2
B	783	LEU	-	expression tag	UNP R8BKC2
B	784	GLU	-	expression tag	UNP R8BKC2
B	785	GLN	-	expression tag	UNP R8BKC2
B	786	LYS	-	expression tag	UNP R8BKC2
B	787	LEU	-	expression tag	UNP R8BKC2
B	788	ILE	-	expression tag	UNP R8BKC2
B	789	SER	-	expression tag	UNP R8BKC2
B	790	GLU	-	expression tag	UNP R8BKC2
B	791	GLU	-	expression tag	UNP R8BKC2
B	792	ASP	-	expression tag	UNP R8BKC2
B	793	LEU	-	expression tag	UNP R8BKC2
B	794	ASN	-	expression tag	UNP R8BKC2
B	795	SER	-	expression tag	UNP R8BKC2
B	796	ALA	-	expression tag	UNP R8BKC2
B	797	VAL	-	expression tag	UNP R8BKC2
B	798	ASP	-	expression tag	UNP R8BKC2
B	799	HIS	-	expression tag	UNP R8BKC2
B	800	HIS	-	expression tag	UNP R8BKC2
B	801	HIS	-	expression tag	UNP R8BKC2
B	802	HIS	-	expression tag	UNP R8BKC2
B	803	HIS	-	expression tag	UNP R8BKC2
B	804	HIS	-	expression tag	UNP R8BKC2
C	24	PHE	-	linker	UNP A0AA49QB00
C	778	ALA	-	expression tag	UNP R8BKC2
C	779	ALA	-	expression tag	UNP R8BKC2
C	780	ALA	-	expression tag	UNP R8BKC2
C	781	SER	-	expression tag	UNP R8BKC2
C	782	PHE	-	expression tag	UNP R8BKC2
C	783	LEU	-	expression tag	UNP R8BKC2
C	784	GLU	-	expression tag	UNP R8BKC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	785	GLN	-	expression tag	UNP R8BKC2
C	786	LYS	-	expression tag	UNP R8BKC2
C	787	LEU	-	expression tag	UNP R8BKC2
C	788	ILE	-	expression tag	UNP R8BKC2
C	789	SER	-	expression tag	UNP R8BKC2
C	790	GLU	-	expression tag	UNP R8BKC2
C	791	GLU	-	expression tag	UNP R8BKC2
C	792	ASP	-	expression tag	UNP R8BKC2
C	793	LEU	-	expression tag	UNP R8BKC2
C	794	ASN	-	expression tag	UNP R8BKC2
C	795	SER	-	expression tag	UNP R8BKC2
C	796	ALA	-	expression tag	UNP R8BKC2
C	797	VAL	-	expression tag	UNP R8BKC2
C	798	ASP	-	expression tag	UNP R8BKC2
C	799	HIS	-	expression tag	UNP R8BKC2
C	800	HIS	-	expression tag	UNP R8BKC2
C	801	HIS	-	expression tag	UNP R8BKC2
C	802	HIS	-	expression tag	UNP R8BKC2
C	803	HIS	-	expression tag	UNP R8BKC2
C	804	HIS	-	expression tag	UNP R8BKC2

- Molecule 2 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.



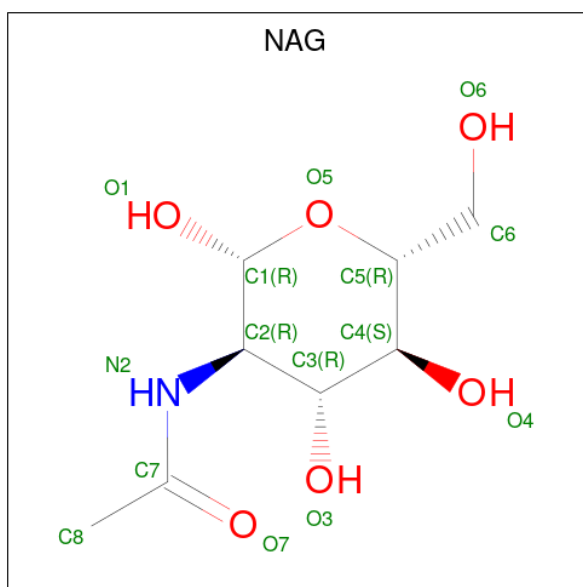
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	F	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	I	3	Total	C	N	O	0	0	0
			39	22	2	15			

- 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
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



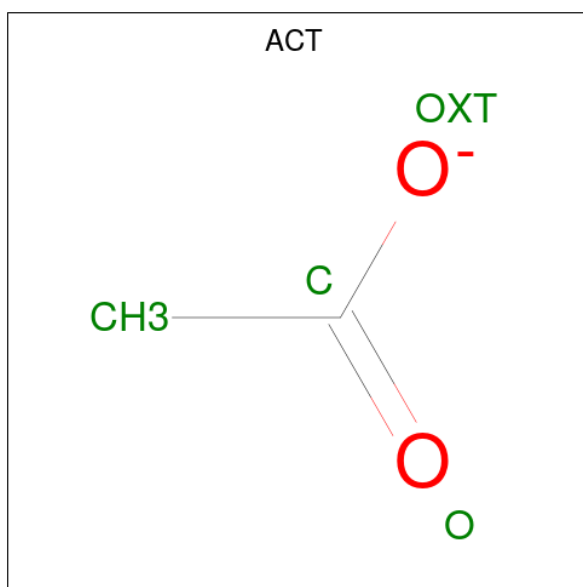
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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	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		

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



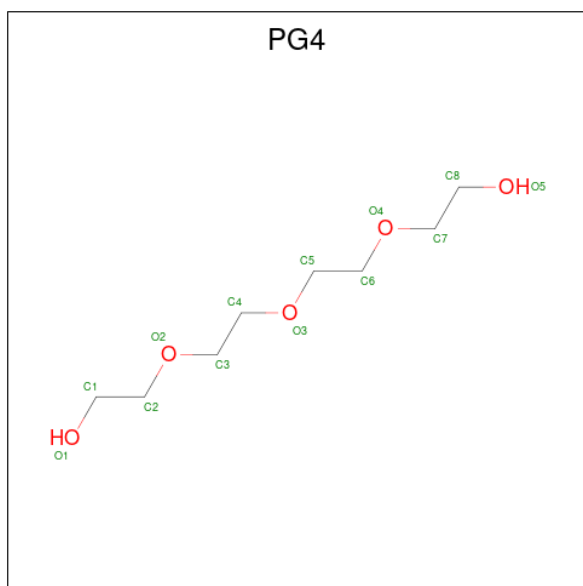
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total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

Continued on next page...

Continued from previous page...

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

- Molecule 6 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).

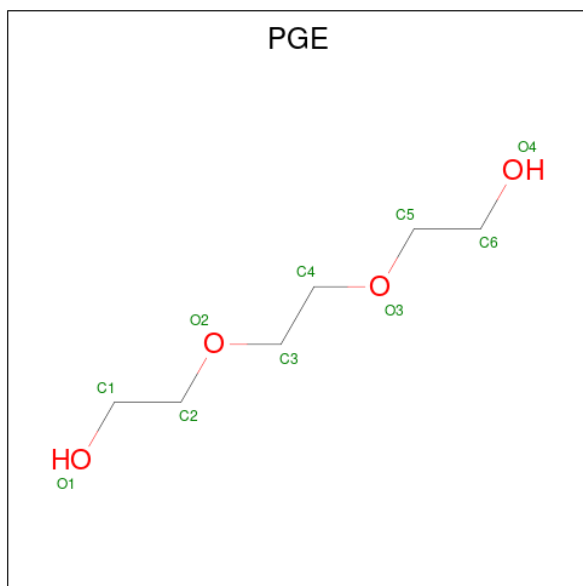


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

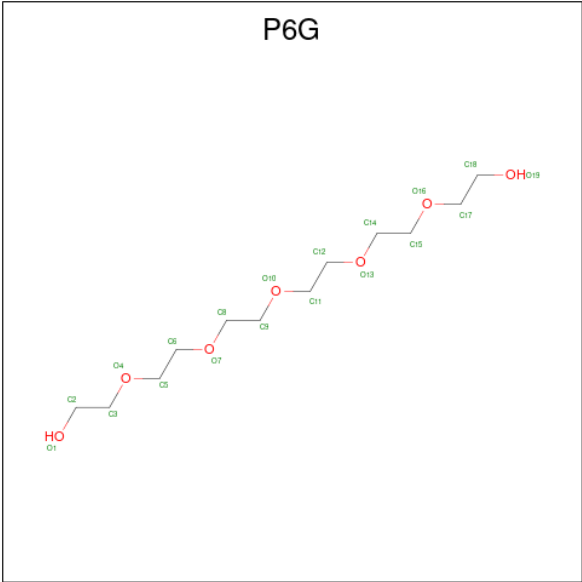
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	B	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 9 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			19	12	7		

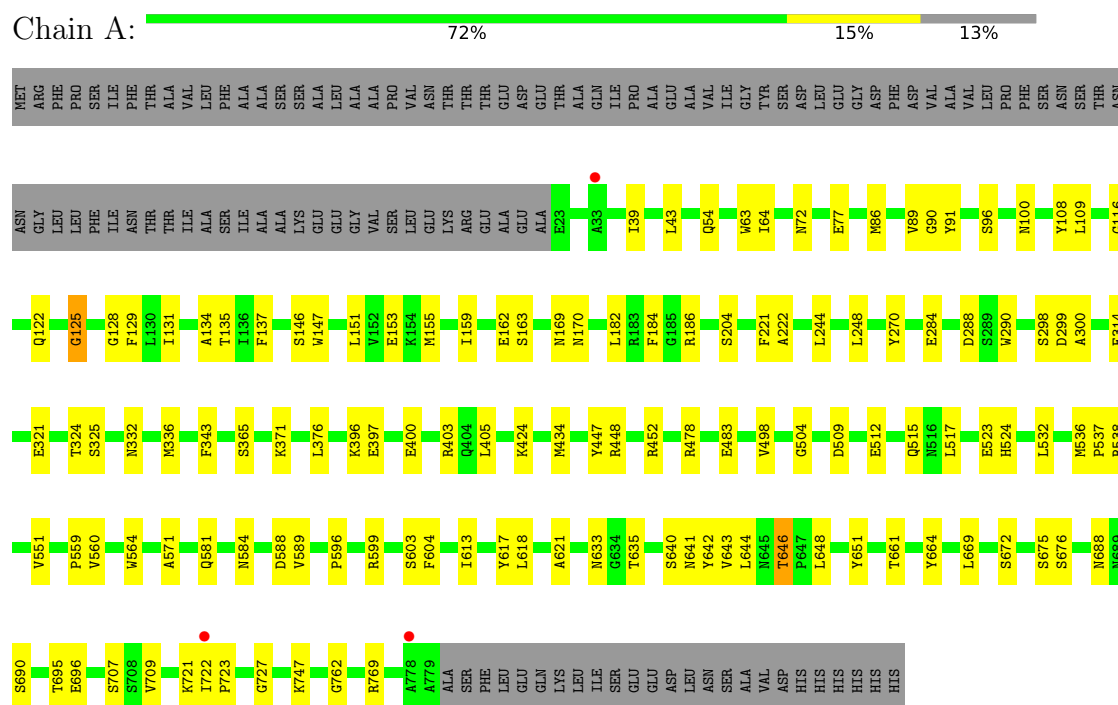
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	17	Total	O	0	0
			17	17		
10	B	15	Total	O	0	0
			15	15		
10	C	15	Total	O	0	0
			15	15		

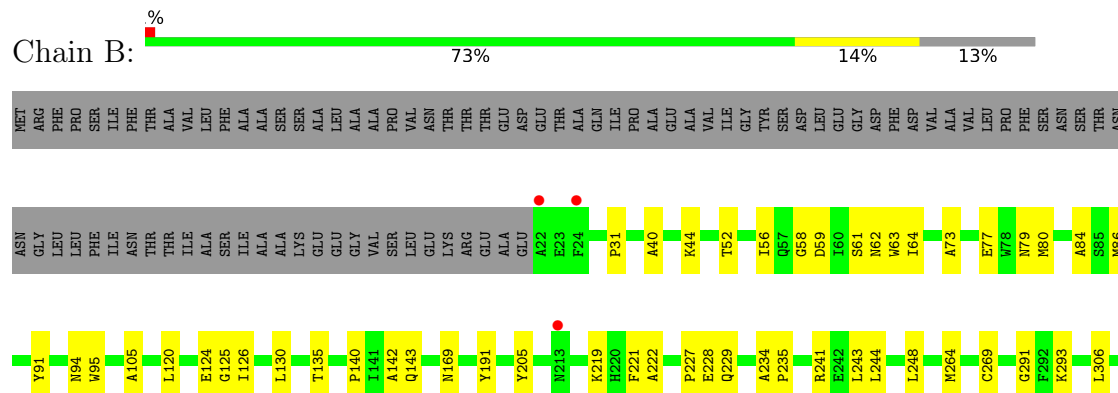
3 Residue-property plots

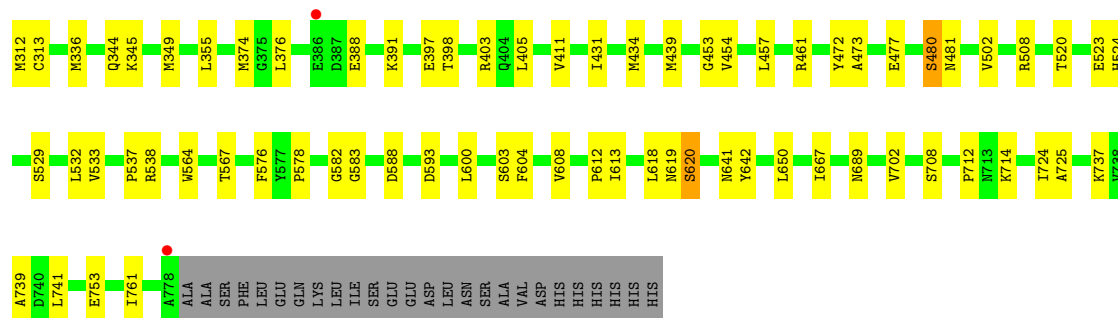
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Isoprimeverose-producing oligoxyloglucan hydrolase,beta-glucosidase

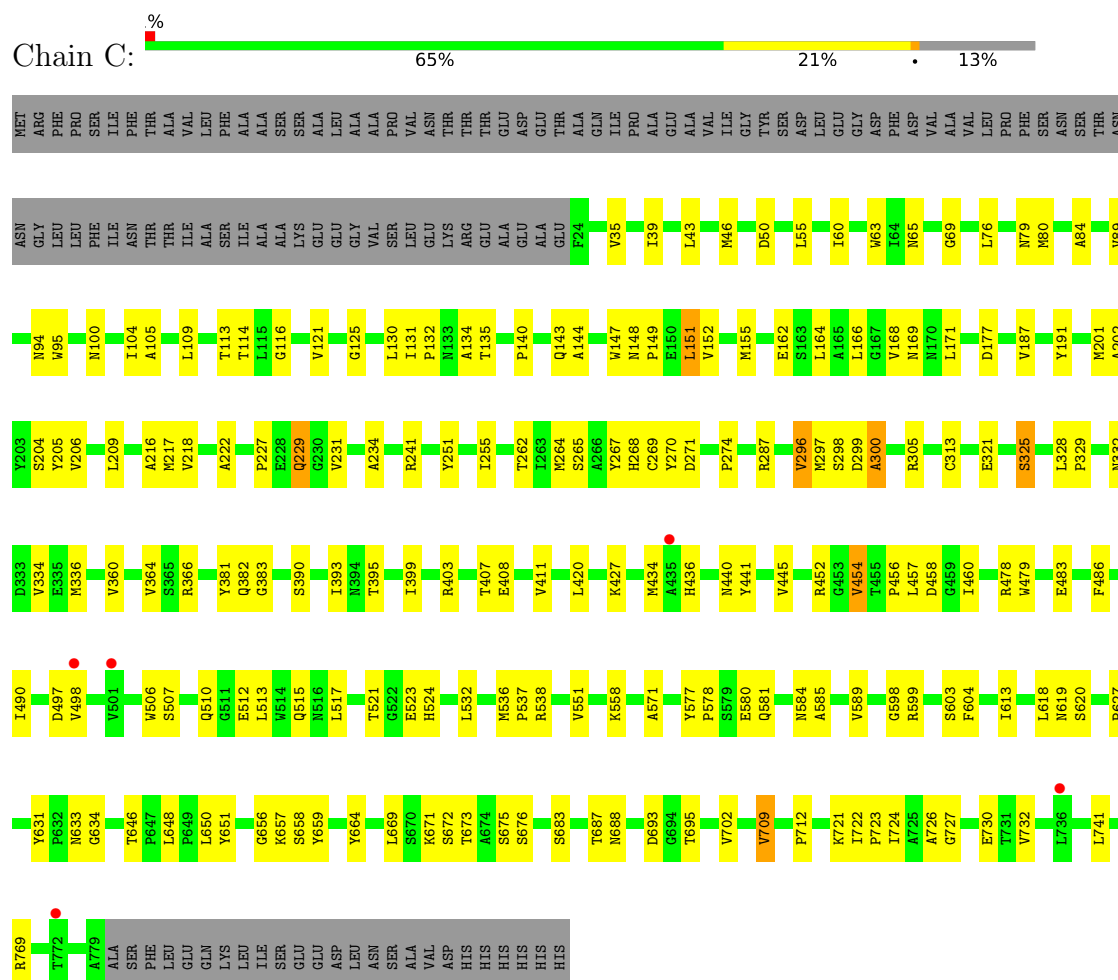


- Molecule 1: Isoprimeverose-producing oligoxyloglucan hydrolase,beta-glucosidase





- Molecule 1: Isoprimeverose-producing oligoxyloglucan hydrolase, beta-glucosidase



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

Chain D: 33% 33% 33%




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

Chain F:  100%

MAG1
MAG2
BMA3

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

Chain I:  100%

MAG1
MAG2
BMA3

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

Chain E:  100%

MAG1
MAG2

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

Chain G:  100%

MAG1
MAG2

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

Chain H:  50% 50%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	186.19Å 74.03Å 184.49Å 90.00° 95.23° 90.00°	Depositor
Resolution (Å)	49.08 – 2.80 49.08 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.08-2.80) 99.1 (49.08-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.216 , 0.268 0.216 , 0.268	Depositor DCC
R_{free} test set	3074 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	64.7	Xtriage
Anisotropy	0.457	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 50.4	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	0.94	EDS
Total number of atoms	18089	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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: BMA, PGE, ACT, CA, NAG, PG4, P6G

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	0.13	0/5944	0.31	0/8105
1	B	0.11	0/5935	0.30	0/8093
1	C	0.12	0/5926	0.30	0/8081
All	All	0.12	0/17805	0.30	0/24279

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 [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	5809	0	5629	71	0
1	B	5800	0	5624	73	0
1	C	5791	0	5619	117	0
2	D	39	0	34	1	0
2	F	39	0	34	1	0
2	I	39	0	34	1	0
3	E	28	0	25	0	0
3	G	28	0	25	0	0
3	H	28	0	25	0	0
4	A	126	0	117	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	98	0	91	3	0
4	C	84	0	78	0	0
5	A	36	0	27	1	0
5	B	40	0	30	1	0
5	C	12	0	9	1	0
6	A	13	0	18	1	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	A	10	0	14	1	0
9	B	19	0	26	0	0
10	A	17	0	0	0	0
10	B	15	0	0	1	0
10	C	15	0	0	1	0
All	All	18089	0	17459	260	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 7.

All (260) 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:C:454:VAL:HG23	1:C:458:ASP:HB2	1.65	0.77
1:C:144:ALA:HA	1:C:201:MET:HE3	1.69	0.74
1:A:314:GLU:N	1:A:314:GLU:OE1	2.25	0.70
1:B:667:ILE:HD12	1:B:761:ILE:HD12	1.75	0.68
1:A:695:THR:HG23	1:A:722:ILE:O	1.94	0.67
1:B:523:GLU:O	1:B:524:HIS:ND1	2.29	0.66
1:C:125:GLY:O	1:C:205:TYR:OH	2.14	0.66
1:A:589:VAL:HG13	1:A:596:PRO:HG3	1.77	0.66
1:B:59:ASP:H	1:B:79:ASN:HD21	1.44	0.66
1:C:523:GLU:O	1:C:524:HIS:ND1	2.29	0.65
1:C:669:LEU:HD23	1:C:672:SER:HA	1.79	0.64
1:A:134:ALA:O	1:A:452:ARG:NH2	2.30	0.64
1:C:657:LYS:NZ	1:C:658:SER:O	2.29	0.64
1:C:604:PHE:HB2	1:C:651:TYR:HB2	1.79	0.63
1:B:529:SER:HA	1:B:608:VAL:HG21	1.80	0.63
1:A:523:GLU:O	1:A:524:HIS:ND1	2.31	0.63
1:C:43:LEU:HA	1:C:46:MET:HE2	1.80	0.63
1:A:696:GLU:HB3	1:A:722:ILE:HD11	1.81	0.62
1:C:35:VAL:O	1:C:39:ILE:HG13	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:403:ARG:HE	1:C:584:ASN:HB3	1.65	0.62
1:A:512:GLU:HA	1:A:515:GLN:HG3	1.81	0.62
1:A:397:GLU:OE1	1:A:397:GLU:N	2.30	0.62
1:B:689:ASN:ND2	4:B:918:NAG:O7	2.33	0.62
1:B:603:SER:HB2	1:B:613:ILE:HG23	1.82	0.61
1:C:521:THR:HG22	1:C:558:LYS:HE2	1.83	0.61
1:B:52:THR:HG22	1:B:56:ILE:HD11	1.82	0.60
1:A:155:MET:HE2	1:A:159:ILE:HD11	1.82	0.60
1:C:113:THR:HG22	1:C:116:GLY:H	1.66	0.60
1:B:306:LEU:HD22	1:B:312:MET:HE2	1.83	0.60
1:A:669:LEU:HD11	1:A:672:SER:HA	1.84	0.59
1:C:513:LEU:HD21	1:C:523:GLU:HB3	1.83	0.58
1:C:532:LEU:HB2	1:C:537:PRO:HG3	1.86	0.58
1:C:515:GLN:HB3	1:C:517:LEU:HD11	1.85	0.57
1:B:714:LYS:NZ	10:B:1001:HOH:O	2.36	0.57
1:B:532:LEU:HB2	1:B:537:PRO:HG3	1.86	0.57
1:B:62:ASN:HD22	1:B:79:ASN:ND2	2.02	0.57
1:B:140:PRO:HA	1:B:143:GLN:HG2	1.87	0.57
1:C:671:LYS:NZ	1:C:673:THR:O	2.28	0.56
1:C:478:ARG:HG2	1:C:479:TRP:CE3	2.40	0.56
1:C:63:TRP:CD2	1:C:76:LEU:HD23	2.41	0.56
1:C:452:ARG:NH1	1:C:580:GLU:OE2	2.39	0.55
1:C:297:MET:HG3	1:C:334:VAL:HG13	1.89	0.55
1:A:54:GLN:OE1	1:A:371:LYS:NZ	2.34	0.55
1:A:581:GLN:OE1	1:A:584:ASN:ND2	2.36	0.55
1:C:130:LEU:HD21	1:C:510:GLN:HG3	1.88	0.55
1:C:94:ASN:ND2	10:C:1003:HOH:O	2.36	0.55
1:B:737:LYS:HE2	1:B:739:ALA:HB3	1.89	0.55
1:B:344:GLN:HG3	1:B:345:LYS:HD2	1.88	0.55
1:B:169:ASN:HD22	1:B:376:LEU:HD21	1.72	0.54
1:A:403:ARG:NH2	1:A:588:ASP:OD2	2.35	0.54
1:B:219:LYS:NZ	5:B:903:ACT:O	2.38	0.54
1:A:270:TYR:HD2	5:A:911:ACT:H1	1.72	0.54
1:B:31:PRO:HD2	4:B:901:NAG:H82	1.90	0.53
1:C:688:ASN:HB3	1:C:727:GLY:H	1.73	0.53
1:C:702:VAL:HG11	1:C:741:LEU:HD22	1.89	0.53
1:B:63:TRP:CD1	1:B:64:ILE:HG12	2.43	0.53
1:B:228:GLU:HG2	1:B:229:GLN:HG3	1.90	0.53
1:C:688:ASN:HB2	1:C:724:ILE:CG2	2.38	0.53
1:C:63:TRP:CZ2	1:C:105:ALA:HB2	2.44	0.53
1:B:143:GLN:HB3	1:B:405:LEU:HD21	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:481:ASN:OD1	1:B:538:ARG:NH1	2.31	0.53
1:C:65:ASN:O	1:C:69:GLY:N	2.42	0.53
1:A:512:GLU:HB3	1:A:517:LEU:HD22	1.91	0.53
1:A:434:MET:HE3	1:A:478:ARG:HD2	1.90	0.53
1:C:551:VAL:HG23	1:C:571:ALA:HB3	1.89	0.53
1:C:633:ASN:HB3	2:I:2:NAG:H82	1.91	0.53
1:B:508:ARG:HH22	4:B:902:NAG:H62	1.74	0.52
1:C:171:LEU:HD12	1:C:209:LEU:HD11	1.91	0.52
1:C:109:LEU:O	1:C:116:GLY:HA2	2.10	0.52
1:B:388:GLU:HG2	1:B:391:LYS:HD2	1.91	0.52
1:C:722:ILE:HD11	1:C:724:ILE:HG12	1.90	0.52
1:C:589:VAL:O	1:C:659:TYR:OH	2.20	0.52
1:C:299:ASP:OD1	1:C:300:ALA:N	2.40	0.52
1:A:244:LEU:HD23	1:A:248:LEU:HD12	1.92	0.51
1:A:688:ASN:HB3	1:A:727:GLY:H	1.75	0.51
1:B:244:LEU:HD23	1:B:248:LEU:HD12	1.92	0.51
1:C:131:ILE:HG13	1:C:132:PRO:HD2	1.93	0.51
1:B:58:GLY:N	1:B:86:MET:O	2.23	0.51
1:C:80:MET:HA	1:C:84:ALA:HB2	1.92	0.51
1:C:147:TRP:CD1	1:C:599:ARG:HB2	2.45	0.51
1:A:72:ASN:ND2	4:A:905:NAG:O7	2.43	0.51
1:C:296:VAL:HG22	1:C:332:ASN:HA	1.92	0.50
1:C:95:TRP:HZ3	1:C:390:SER:HA	1.75	0.50
1:C:202:ALA:O	1:C:206:VAL:HG23	2.12	0.50
1:A:137:PHE:HB2	1:A:155:MET:HE3	1.93	0.50
1:C:131:ILE:HG22	1:C:134:ALA:HB2	1.92	0.50
1:B:235:PRO:HB3	1:B:269:CYS:SG	2.52	0.49
1:C:403:ARG:HB2	1:C:581:GLN:HG3	1.94	0.49
1:A:63:TRP:CD1	1:A:64:ILE:HG12	2.48	0.49
1:B:143:GLN:HG3	1:B:191:TYR:HE1	1.77	0.49
1:C:403:ARG:O	1:C:407:THR:HG23	2.12	0.49
1:A:153:GLU:HB2	1:A:204:SER:HB3	1.94	0.49
1:A:109:LEU:O	1:A:116:GLY:HA2	2.12	0.49
1:A:324:THR:HG22	1:A:343:PHE:CD1	2.48	0.49
1:A:131:ILE:HG22	1:A:134:ALA:HB2	1.95	0.49
1:B:612:PRO:HD2	1:C:229:GLN:HB3	1.94	0.49
1:C:395:THR:O	1:C:399:ILE:HG22	2.13	0.49
1:C:722:ILE:CD1	1:C:724:ILE:HG12	2.43	0.49
1:B:457:LEU:HD21	1:B:461:ARG:HH11	1.77	0.48
1:C:63:TRP:HZ3	1:C:79:ASN:ND2	2.10	0.48
1:C:227:PRO:HB2	1:C:234:ALA:HB3	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:LEU:HD13	1:A:559:PRO:HG2	1.95	0.48
1:B:349:MET:HE2	1:B:355:LEU:HB2	1.95	0.48
1:C:166:LEU:HD11	1:C:393:ILE:HD11	1.95	0.48
1:B:125:GLY:O	1:B:205:TYR:OH	2.29	0.48
1:B:434:MET:HB2	1:B:502:VAL:HG12	1.96	0.48
1:C:408:GLU:HB3	1:C:721:LYS:NZ	2.27	0.48
1:C:599:ARG:HD3	1:C:656:GLY:HA3	1.94	0.48
1:C:603:SER:HB2	1:C:613:ILE:HG23	1.95	0.48
1:B:564:TRP:CD2	2:F:1:NAG:H82	2.48	0.48
1:C:46:MET:HB3	1:C:50:ASP:HB2	1.96	0.48
1:C:633:ASN:OD1	1:C:634:GLY:N	2.47	0.48
1:A:447:TYR:HD2	1:A:448:ARG:N	2.12	0.48
1:C:407:THR:HG22	1:C:585:ALA:HA	1.96	0.48
1:A:532:LEU:HB2	1:A:537:PRO:HG3	1.95	0.47
1:C:121:VAL:HB	1:C:168:VAL:HA	1.96	0.47
1:C:408:GLU:HB3	1:C:721:LYS:HZ3	1.79	0.47
1:C:478:ARG:HE	1:C:506:TRP:CG	2.32	0.47
1:C:478:ARG:HB2	1:C:536:MET:HE2	1.96	0.47
1:B:397:GLU:OE1	1:B:397:GLU:N	2.35	0.47
1:C:420:LEU:HD12	1:C:659:TYR:OH	2.14	0.47
1:B:454:VAL:HG12	1:B:583:GLY:HA3	1.96	0.47
1:B:477:GLU:HB2	1:B:480:SER:HB2	1.97	0.47
1:B:520:THR:HG21	1:B:533:VAL:HG11	1.95	0.47
1:C:100:ASN:O	1:C:104:ILE:HG12	2.14	0.47
1:C:456:PRO:O	1:C:460:ILE:HG13	2.15	0.47
1:C:109:LEU:O	1:C:113:THR:HB	2.14	0.47
1:B:411:VAL:HG11	1:B:600:LEU:HG	1.97	0.47
1:C:618:LEU:HA	1:C:712:PRO:HA	1.96	0.47
1:A:86:MET:SD	1:A:122:GLN:NE2	2.88	0.47
1:C:486:PHE:O	1:C:490:ILE:HG13	2.15	0.46
1:C:140:PRO:HA	1:C:143:GLN:HG2	1.96	0.46
1:C:268:HIS:HE1	1:C:270:TYR:HB2	1.80	0.46
1:A:151:LEU:HB3	1:A:405:LEU:HD13	1.96	0.46
1:C:149:PRO:O	1:C:204:SER:OG	2.22	0.46
1:B:604:PHE:O	1:B:650:LEU:N	2.48	0.46
1:B:293:LYS:HA	1:B:293:LYS:HD3	1.72	0.46
1:C:267:TYR:O	1:C:305:ARG:NH1	2.49	0.46
1:A:664:TYR:CD1	1:A:769:ARG:HG3	2.50	0.46
1:C:675:SER:OG	1:C:676:SER:N	2.49	0.46
1:A:221:PHE:HA	1:A:222:ALA:HA	1.78	0.46
1:C:229:GLN:HG3	1:C:231:VAL:HG23	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:507:SER:HG	1:C:521:THR:HG1	1.64	0.46
1:A:646:THR:HG22	1:A:648:LEU:H	1.81	0.45
1:C:143:GLN:HG3	1:C:191:TYR:HE1	1.81	0.45
1:A:125:GLY:HA2	1:A:128:GLY:O	2.17	0.45
1:A:298:SER:O	1:A:336:MET:HE3	2.16	0.45
1:C:631:TYR:HB2	1:C:633:ASN:OD1	2.15	0.45
1:B:59:ASP:OD2	1:B:91:TYR:OH	2.34	0.45
1:A:603:SER:HB2	1:A:613:ILE:HG23	1.99	0.45
1:A:707:SER:OG	1:A:709:VAL:O	2.31	0.45
1:C:427:LYS:HB2	1:C:497:ASP:H	1.82	0.45
1:A:184:PHE:CE2	1:A:186:ARG:HB2	2.51	0.45
1:B:227:PRO:HB2	1:B:234:ALA:HB3	1.99	0.45
1:B:374:MET:HE2	1:B:374:MET:HB3	1.90	0.45
1:B:403:ARG:HH21	1:B:588:ASP:CG	2.24	0.45
1:C:646:THR:HG22	1:C:648:LEU:H	1.81	0.45
1:A:122:GLN:HA	1:A:170:ASN:O	2.17	0.45
1:A:504:GLY:O	1:A:536:MET:HE1	2.17	0.45
1:B:124:GLU:HB2	1:B:130:LEU:HB2	1.98	0.45
1:C:434:MET:HE3	1:C:478:ARG:HD2	1.99	0.45
1:A:643:VAL:HG12	1:A:644:LEU:HG	1.98	0.44
1:B:40:ALA:O	1:B:44:LYS:HG3	2.17	0.44
1:C:436:HIS:CG	1:C:457:LEU:HD23	2.51	0.44
1:A:129:PHE:CE2	1:A:163:SER:HA	2.51	0.44
1:A:146:SER:O	1:A:721:LYS:NZ	2.43	0.44
1:A:483:GLU:CG	1:A:538:ARG:HH21	2.30	0.44
1:C:512:GLU:HB3	1:C:517:LEU:HD13	1.98	0.44
1:A:299:ASP:OD1	1:A:300:ALA:N	2.41	0.44
1:B:94:ASN:OD1	1:B:95:TRP:N	2.50	0.44
1:B:724:ILE:HG22	1:B:725:ALA:O	2.18	0.44
1:C:264:MET:HE2	1:C:336:MET:HE1	1.99	0.44
1:A:675:SER:OG	1:A:676:SER:N	2.51	0.44
1:C:454:VAL:HG12	1:C:580:GLU:O	2.18	0.44
1:B:142:ALA:HB2	1:B:576:PHE:HB2	1.99	0.44
1:C:55:LEU:C	1:C:334:VAL:HG23	2.42	0.44
1:C:222:ALA:O	1:C:268:HIS:NE2	2.43	0.44
1:A:137:PHE:CB	1:A:155:MET:HE3	2.48	0.44
1:B:61:SER:HA	1:B:64:ILE:O	2.18	0.44
1:B:135:THR:HG21	1:B:398:THR:HG22	1.99	0.44
1:A:396:LYS:NZ	1:A:400:GLU:OE2	2.45	0.43
1:A:604:PHE:HB2	1:A:651:TYR:HB2	2.00	0.43
1:C:328:LEU:HB3	1:C:329:PRO:HD3	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ILE:O	1:A:43:LEU:HB2	2.18	0.43
1:B:63:TRP:CZ2	1:B:105:ALA:HB2	2.54	0.43
1:B:641:ASN:HA	1:B:642:TYR:HA	1.80	0.43
1:C:440:ASN:O	1:C:578:PRO:HD2	2.19	0.43
1:C:693:ASP:OD1	1:C:726:ALA:N	2.34	0.43
1:B:63:TRP:HZ3	1:B:79:ASN:ND2	2.15	0.43
1:B:73:ALA:O	1:B:77:GLU:HG3	2.19	0.43
1:B:221:PHE:HA	1:B:222:ALA:HA	1.74	0.43
1:C:321:GLU:O	1:C:325:SER:OG	2.34	0.43
1:C:619:ASN:O	1:C:620:SER:OG	2.30	0.43
1:A:641:ASN:HA	1:A:642:TYR:HA	1.54	0.43
1:C:187:VAL:HB	1:C:558:LYS:HG2	2.00	0.43
1:C:724:ILE:HD13	1:C:730:GLU:HG3	2.01	0.43
1:A:89:VAL:O	1:A:91:TYR:N	2.51	0.43
1:B:241:ARG:NH1	1:C:271:ASP:O	2.52	0.43
1:B:431:ILE:HA	1:B:473:ALA:O	2.19	0.43
1:B:708:SER:OG	1:B:753:GLU:OE2	2.30	0.43
1:C:155:MET:HB3	1:C:155:MET:HE2	1.80	0.43
1:A:147:TRP:NE1	1:A:599:ARG:HB2	2.34	0.43
1:C:287:ARG:HH21	1:C:366:ARG:HD3	1.84	0.43
1:A:447:TYR:CE2	1:A:448:ARG:HG3	2.53	0.42
1:A:661:THR:H	1:A:690:SER:HB3	1.84	0.42
1:B:702:VAL:HG11	1:B:741:LEU:HD22	1.99	0.42
1:B:588:ASP:HA	1:B:593:ASP:HB2	2.01	0.42
1:A:96:SER:O	1:A:100:ASN:HB2	2.18	0.42
1:C:483:GLU:OE2	1:C:538:ARG:NH1	2.49	0.42
1:C:627:PRO:HG3	1:C:646:THR:HG23	2.02	0.42
1:A:169:ASN:HD22	1:A:376:LEU:HD21	1.84	0.42
1:C:381:TYR:CZ	1:C:383:GLY:HA3	2.55	0.42
1:A:633:ASN:HB3	1:A:635:THR:H	1.84	0.42
1:A:747:LYS:HD2	1:A:747:LYS:HA	1.90	0.42
1:B:80:MET:O	1:B:84:ALA:HB2	2.19	0.42
1:C:144:ALA:HB2	1:C:191:TYR:HD1	1.85	0.42
1:B:619:ASN:O	1:B:620:SER:OG	2.34	0.42
1:C:169:ASN:HD22	1:C:382:GLN:HE22	1.68	0.42
1:A:321:GLU:O	1:A:325:SER:OG	2.27	0.42
1:C:265:SER:OG	1:C:298:SER:HA	2.18	0.42
1:C:441:TYR:HB3	1:C:445:VAL:HG11	2.02	0.42
1:C:664:TYR:CD1	1:C:769:ARG:HD3	2.54	0.42
1:A:290:TRP:HA	8:A:921:PGE:H1	2.01	0.42
1:B:143:GLN:CB	1:B:405:LEU:HD21	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:THR:OG1	1:C:162:GLU:OE2	2.36	0.42
1:C:148:ASN:CG	1:C:151:LEU:HD12	2.45	0.42
1:A:77:GLU:HG2	1:A:108:TYR:OH	2.20	0.42
1:A:551:VAL:HG13	1:A:571:ALA:HB3	2.00	0.41
1:C:152:VAL:HG21	1:C:201:MET:HG3	2.02	0.41
1:C:164:LEU:HD11	1:C:382:GLN:HB2	2.01	0.41
1:C:270:TYR:HD2	5:C:905:ACT:H2	1.85	0.41
1:C:683:SER:HA	1:C:732:VAL:O	2.20	0.41
1:C:269:CYS:HA	1:C:274:PRO:HA	2.01	0.41
1:A:298:SER:HB3	1:A:332:ASN:HD21	1.86	0.41
1:A:613:ILE:HD12	1:A:613:ILE:HA	1.96	0.41
1:B:126:ILE:HD13	1:B:126:ILE:HA	1.87	0.41
1:C:218:VAL:HG21	1:C:255:ILE:HG13	2.02	0.41
1:A:564:TRP:CD2	2:D:1:NAG:H82	2.55	0.41
1:A:135:THR:OG1	1:A:162:GLU:OE2	2.28	0.41
1:A:284:GLU:O	1:A:288:ASP:HB2	2.20	0.41
1:C:177:ASP:OD1	1:C:251:TYR:OH	2.26	0.41
1:C:411:VAL:HG22	1:C:598:GLY:C	2.46	0.41
1:B:120:LEU:HD13	1:B:120:LEU:HA	1.97	0.41
1:C:360:VAL:O	1:C:364:VAL:HG22	2.20	0.41
1:C:695:THR:HA	1:C:723:PRO:HA	2.02	0.41
1:C:241:ARG:HD3	1:C:709:VAL:HG11	2.02	0.41
1:A:762:GLY:HA2	1:A:769:ARG:HG2	2.04	0.41
1:B:376:LEU:HD23	1:B:376:LEU:HA	1.94	0.41
1:B:439:MET:HE2	1:B:453:GLY:HA3	2.02	0.41
6:A:907:PG4:H32	6:A:907:PG4:H12	1.83	0.40
1:B:578:PRO:HB2	1:B:582:GLY:HA3	2.03	0.40
1:C:216:ALA:O	1:C:262:THR:OG1	2.30	0.40
1:C:217:MET:HA	1:C:262:THR:O	2.21	0.40
1:A:617:TYR:CD1	1:A:621:ALA:HB3	2.56	0.40
1:B:618:LEU:HA	1:B:712:PRO:HA	2.02	0.40
1:C:60:ILE:HB	1:C:89:VAL:HG12	2.02	0.40
1:A:424:LYS:HE2	1:A:424:LYS:HB2	1.89	0.40
1:B:291:GLY:O	1:B:293:LYS:HE2	2.21	0.40
1:B:457:LEU:HD11	1:B:472:TYR:HB2	2.03	0.40
1:B:264:MET:HE2	1:B:336:MET:HE1	2.04	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	756/871 (87%)	726 (96%)	26 (3%)	4 (0%)	24	55
1	B	755/871 (87%)	718 (95%)	36 (5%)	1 (0%)	48	77
1	C	754/871 (87%)	709 (94%)	42 (6%)	3 (0%)	30	60
All	All	2265/2613 (87%)	2153 (95%)	104 (5%)	8 (0%)	30	60

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	723	PRO
1	B	620	SER
1	A	90	GLY
1	C	300	ALA
1	C	577	TYR
1	A	509	ASP
1	C	229	GLN
1	A	125	GLY

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	625/717 (87%)	619 (99%)	6 (1%)	68	88
1	B	624/717 (87%)	620 (99%)	4 (1%)	78	92
1	C	623/717 (87%)	613 (98%)	10 (2%)	55	83

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1872/2151 (87%)	1852 (99%)	20 (1%)	65 87

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	365	SER
1	A	498	VAL
1	A	560	VAL
1	A	618	LEU
1	A	640	SER
1	A	646	THR
1	B	243	LEU
1	B	313	CYS
1	B	480	SER
1	B	567	THR
1	C	114	THR
1	C	151	LEU
1	C	296	VAL
1	C	313	CYS
1	C	325	SER
1	C	454	VAL
1	C	498	VAL
1	C	650	LEU
1	C	687	THR
1	C	709	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	ASN
1	A	531	ASN
1	A	629	HIS
1	B	79	ASN
1	B	332	ASN
1	B	531	ASN
1	B	574	GLN
1	B	619	ASN
1	B	629	HIS
1	C	161	GLN
1	C	232	ASN
1	C	308	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	545	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 ⓘ

15 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	D	1	2,1	14,14,15	0.73	0	17,19,21	1.07	1 (5%)
2	NAG	D	2	2	14,14,15	0.72	0	17,19,21	0.79	0
2	BMA	D	3	2	11,11,12	0.77	0	15,15,17	2.50	6 (40%)
3	NAG	E	1	1,3	14,14,15	0.71	0	17,19,21	0.82	0
3	NAG	E	2	3	14,14,15	0.71	0	17,19,21	0.83	0
2	NAG	F	1	2,1	14,14,15	0.70	0	17,19,21	0.90	0
2	NAG	F	2	2	14,14,15	0.64	0	17,19,21	0.96	2 (11%)
2	BMA	F	3	2	11,11,12	0.77	0	15,15,17	2.76	5 (33%)
3	NAG	G	1	1,3	14,14,15	0.72	0	17,19,21	0.82	0
3	NAG	G	2	3	14,14,15	0.71	0	17,19,21	0.84	0
3	NAG	H	1	1,3	14,14,15	0.67	0	17,19,21	0.91	0
3	NAG	H	2	3	14,14,15	0.73	0	17,19,21	0.96	1 (5%)
2	NAG	I	1	2,1	14,14,15	0.71	0	17,19,21	1.38	2 (11%)
2	NAG	I	2	2	14,14,15	0.74	0	17,19,21	0.98	0
2	BMA	I	3	2	11,11,12	0.84	0	15,15,17	2.66	6 (40%)

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	D	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1
3	NAG	E	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	BMA	F	3	2	-	1/2/19/22	0/1/1/1
3	NAG	G	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	H	2	3	-	1/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	4/6/23/26	0/1/1/1
2	BMA	I	3	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	3	BMA	C1-O5-C5	8.30	123.31	112.19
2	F	3	BMA	C1-O5-C5	8.12	123.06	112.19
2	D	3	BMA	C1-O5-C5	7.62	122.39	112.19
2	F	3	BMA	C1-C2-C3	3.82	115.20	109.64
2	I	1	NAG	C2-N2-C7	3.01	126.94	122.90
2	I	3	BMA	C2-C3-C4	2.70	115.61	110.86
2	F	3	BMA	O4-C4-C3	-2.62	104.21	110.38
2	D	3	BMA	O4-C4-C3	-2.52	104.43	110.38
2	F	3	BMA	O3-C3-C2	-2.52	104.91	110.05
2	F	2	NAG	O4-C4-C3	-2.36	104.81	110.38
2	D	3	BMA	C1-C2-C3	2.35	113.07	109.64
2	D	1	NAG	O5-C1-C2	-2.33	107.69	111.29
2	I	3	BMA	C1-C2-C3	2.31	113.01	109.64
2	F	3	BMA	C2-C3-C4	2.30	114.90	110.86
2	D	3	BMA	C2-C3-C4	2.26	114.83	110.86
2	F	2	NAG	C1-O5-C5	2.23	115.18	112.19
2	I	3	BMA	C3-C4-C5	2.23	114.28	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	3	BMA	O4-C4-C3	-2.22	105.15	110.38
2	I	3	BMA	O3-C3-C2	-2.16	105.64	110.05
2	I	1	NAG	O3-C3-C2	-2.13	104.97	109.40
3	H	2	NAG	C1-O5-C5	2.10	115.00	112.19
2	D	3	BMA	C3-C4-C5	2.10	114.04	110.23
2	D	3	BMA	O3-C3-C2	-2.09	105.78	110.05

There are no chirality outliers.

All (14) torsion outliers are listed below:

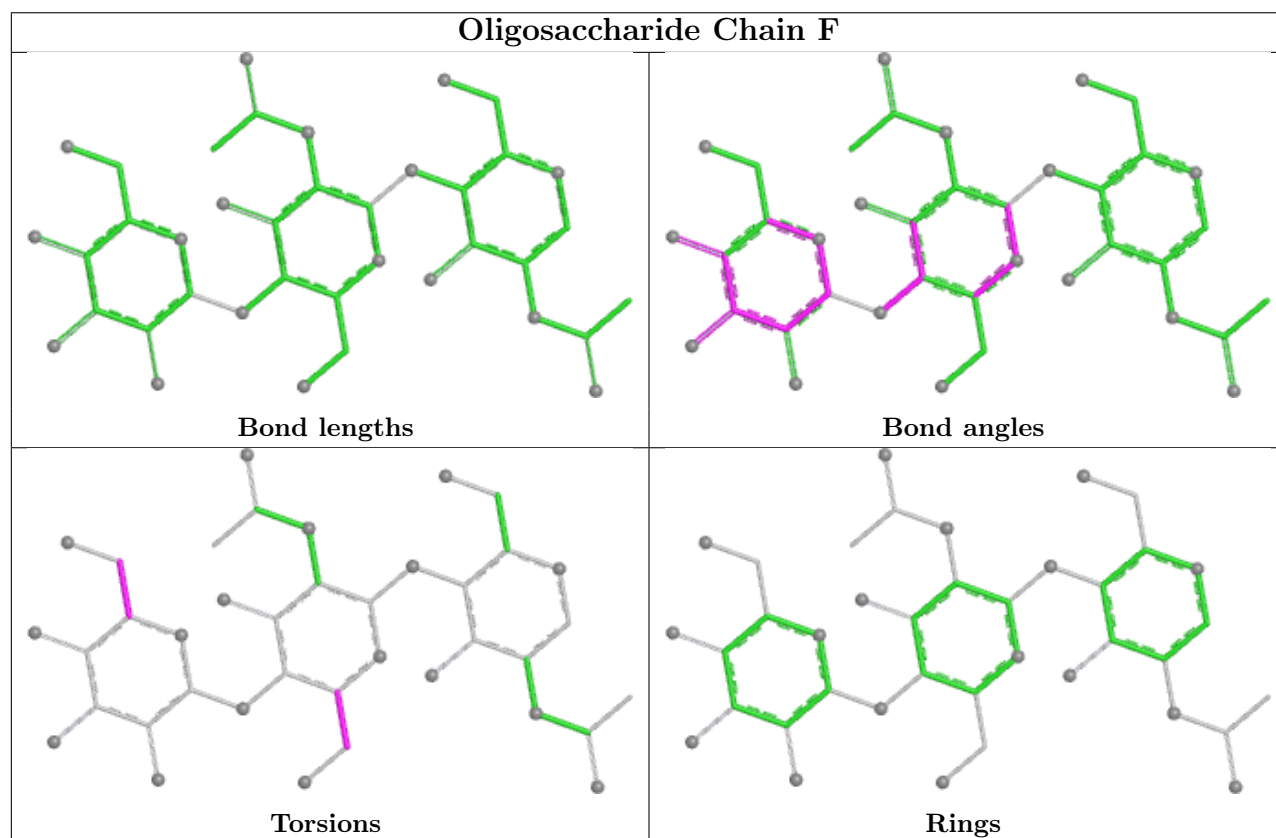
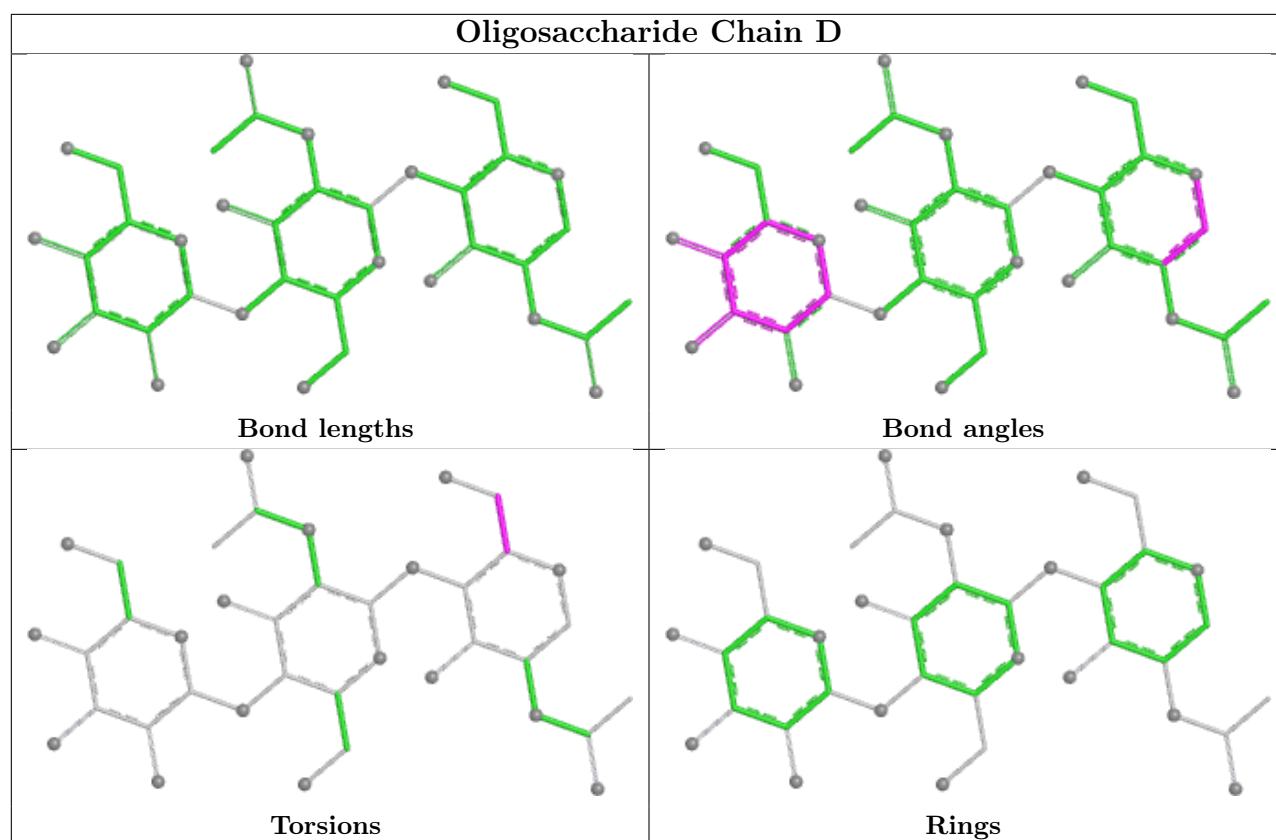
Mol	Chain	Res	Type	Atoms
2	D	1	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	I	2	NAG	C8-C7-N2-C2
2	I	2	NAG	O7-C7-N2-C2
3	G	1	NAG	C8-C7-N2-C2
3	G	1	NAG	O7-C7-N2-C2
2	F	3	BMA	C4-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
3	E	1	NAG	C1-C2-N2-C7
3	H	1	NAG	C1-C2-N2-C7
3	H	2	NAG	C1-C2-N2-C7

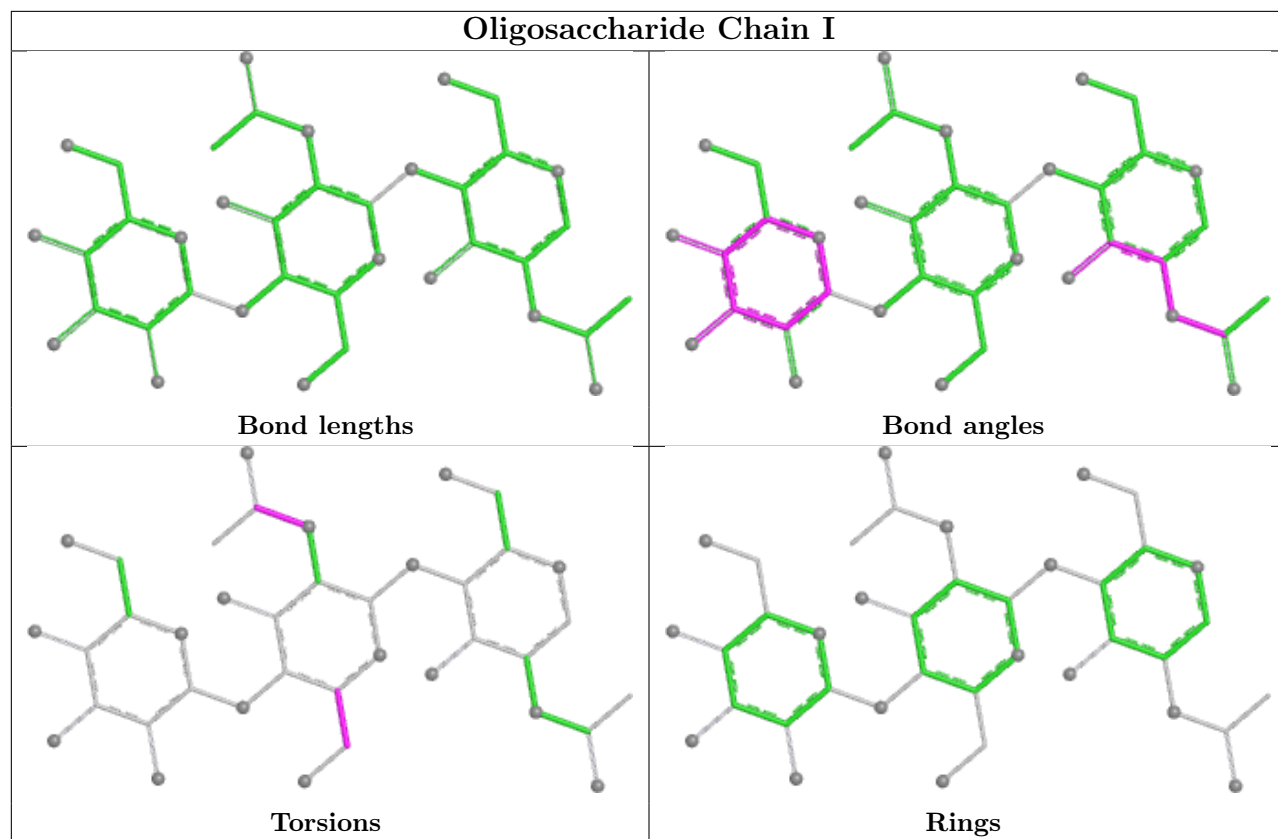
There are no ring outliers.

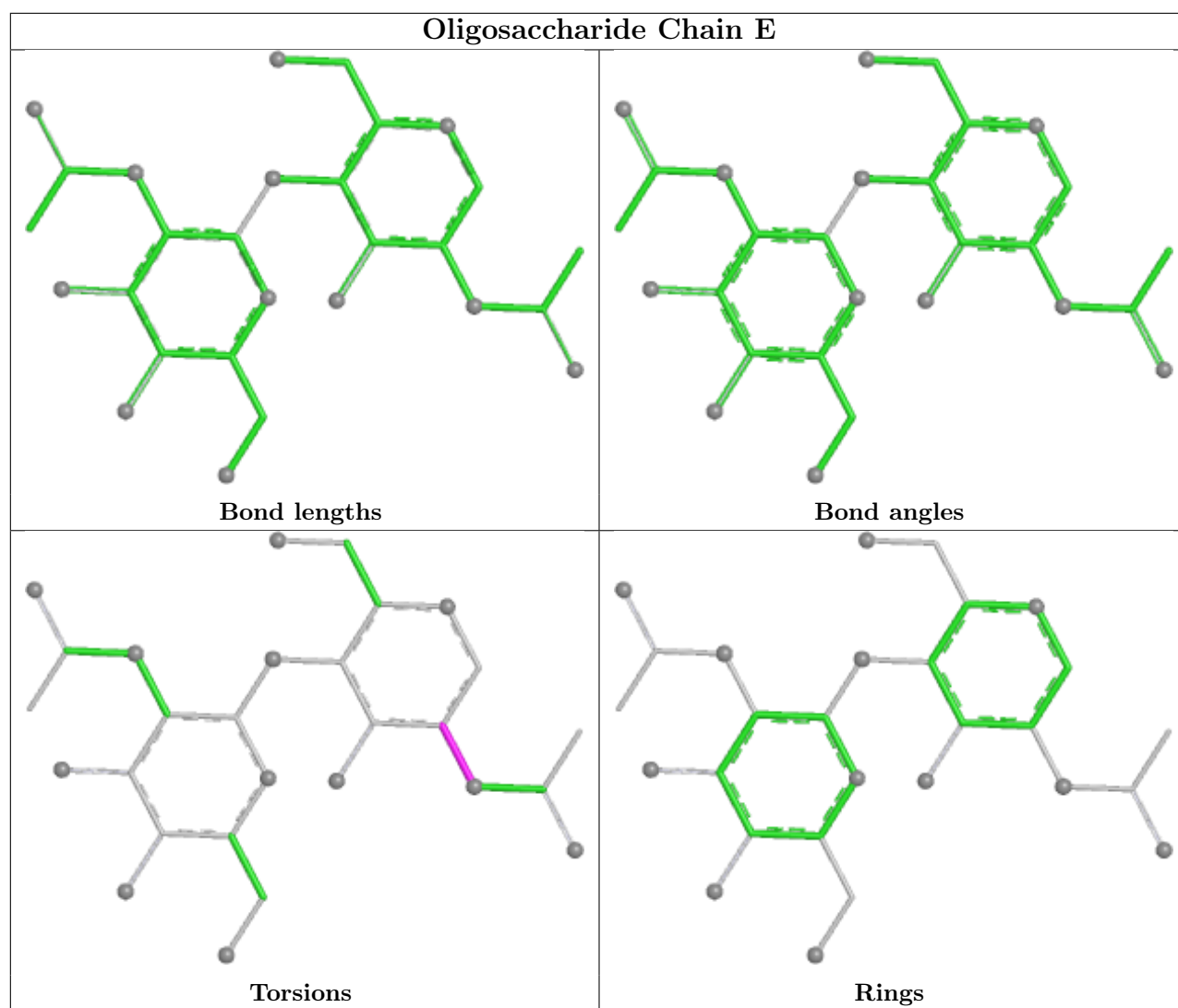
3 monomers are involved in 3 short contacts:

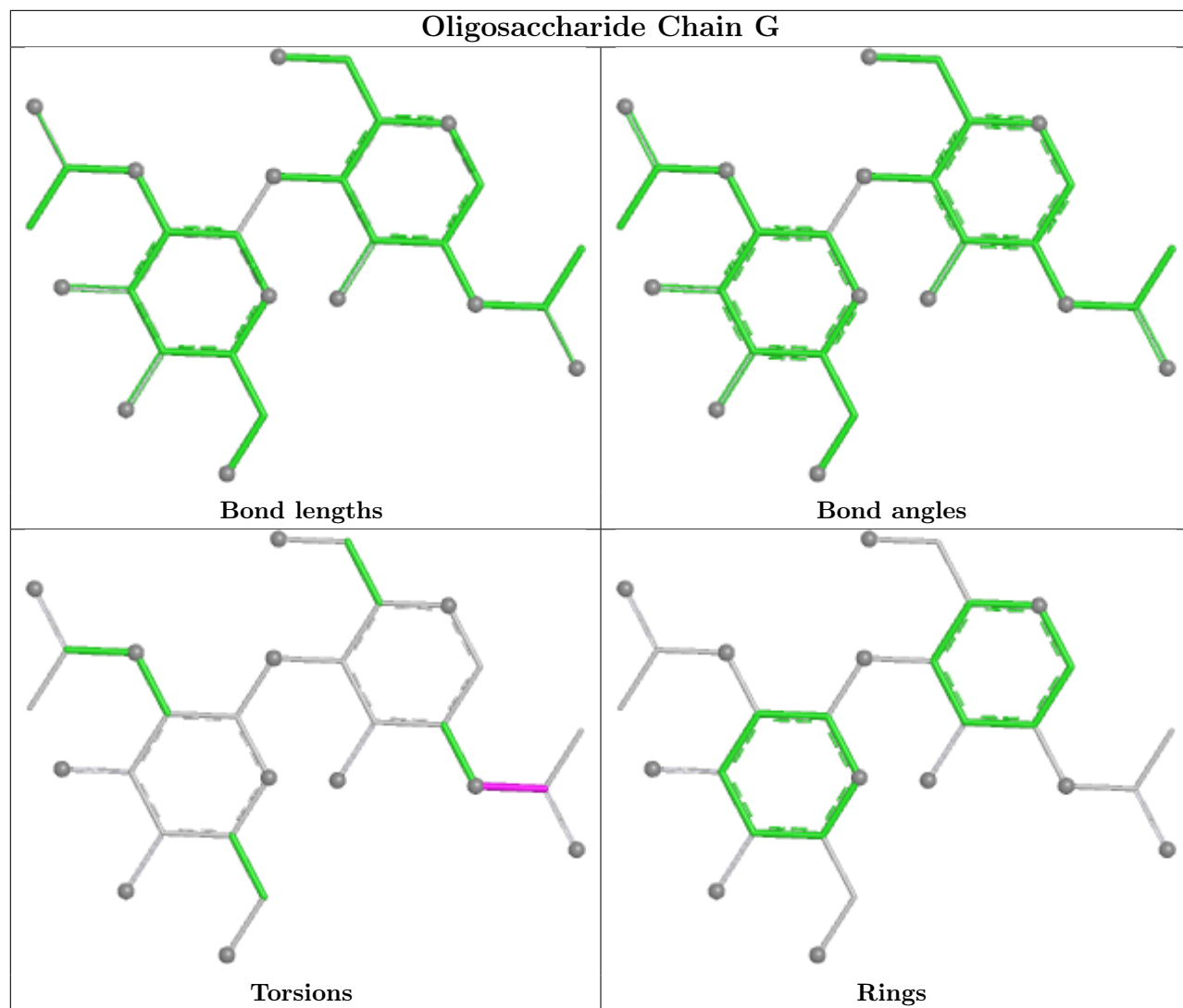
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	1	0
2	I	2	NAG	1	0
2	F	1	NAG	1	0

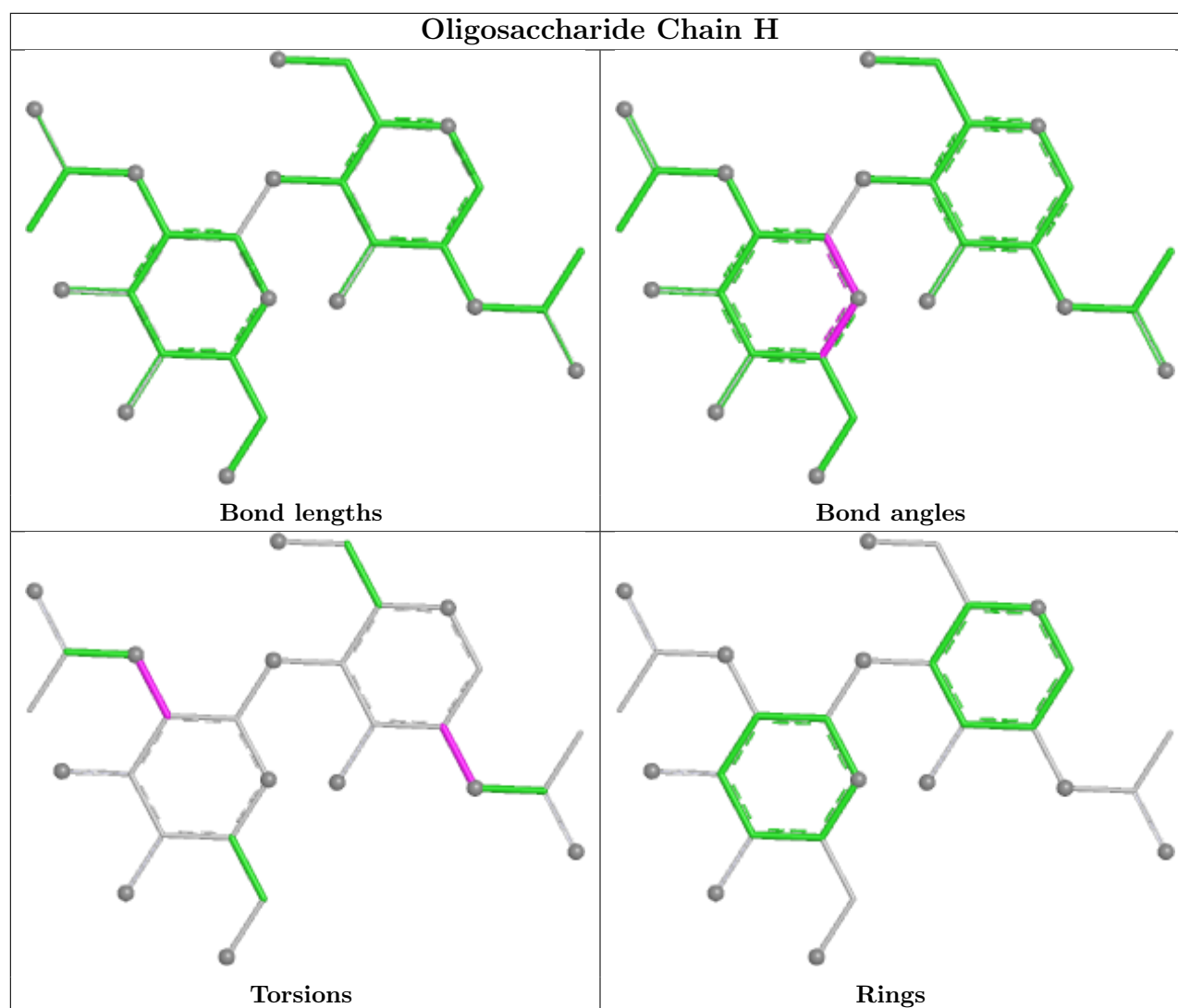
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

Of 50 ligands modelled in this entry, 3 are monoatomic - leaving 47 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	B	917	1	14,14,15	0.69	0	17,19,21	0.80	0
5	ACT	A	910	-	3,3,3	1.15	0	3,3,3	1.19	0
4	NAG	A	918	1	14,14,15	0.68	0	17,19,21	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	906	1	14,14,15	0.75	0	17,19,21	0.99	1 (5%)
5	ACT	B	914	-	3,3,3	1.14	0	3,3,3	1.25	0
4	NAG	A	920	1	14,14,15	0.71	0	17,19,21	0.94	1 (5%)
5	ACT	A	915	-	3,3,3	1.15	0	3,3,3	1.21	0
5	ACT	B	910	-	3,3,3	1.13	0	3,3,3	1.27	0
6	PG4	A	907	-	12,12,12	0.30	0	11,11,11	0.16	0
4	NAG	A	905	1	14,14,15	0.73	0	17,19,21	2.21	3 (17%)
8	PGE	A	921	-	9,9,9	0.33	0	8,8,8	0.50	0
5	ACT	B	915	-	3,3,3	1.14	0	3,3,3	1.22	0
4	NAG	C	903	1	14,14,15	0.73	0	17,19,21	0.81	0
5	ACT	A	913	-	3,3,3	1.14	0	3,3,3	1.20	0
5	ACT	A	917	-	3,3,3	1.15	0	3,3,3	1.19	0
5	ACT	B	909	-	3,3,3	1.14	0	3,3,3	1.21	0
9	P6G	B	907	-	18,18,18	0.31	0	17,17,17	0.16	0
4	NAG	C	908	1	14,14,15	0.70	0	17,19,21	0.80	0
4	NAG	A	903	1	14,14,15	0.73	0	17,19,21	0.96	1 (5%)
5	ACT	B	905	-	3,3,3	1.14	0	3,3,3	1.21	0
4	NAG	A	908	1	14,14,15	0.73	0	17,19,21	0.92	0
4	NAG	B	901	1	14,14,15	0.74	0	17,19,21	0.89	0
5	ACT	B	911	-	3,3,3	1.13	0	3,3,3	1.24	0
5	ACT	B	912	-	3,3,3	1.13	0	3,3,3	1.24	0
5	ACT	B	913	-	3,3,3	1.15	0	3,3,3	1.19	0
4	NAG	B	902	1	14,14,15	0.75	0	17,19,21	0.96	0
4	NAG	C	902	1	14,14,15	0.71	0	17,19,21	0.93	0
4	NAG	B	919	1	14,14,15	0.68	0	17,19,21	1.22	1 (5%)
5	ACT	C	905	-	3,3,3	1.13	0	3,3,3	1.20	0
4	NAG	C	910	1	14,14,15	0.74	0	17,19,21	0.77	0
4	NAG	C	901	1	14,14,15	0.76	0	17,19,21	1.17	1 (5%)
4	NAG	A	919	1	14,14,15	0.69	0	17,19,21	0.78	0
5	ACT	A	904	-	3,3,3	1.12	0	3,3,3	1.30	0
4	NAG	B	918	1	14,14,15	0.67	0	17,19,21	2.13	3 (17%)
4	NAG	A	906	1	14,14,15	0.75	0	17,19,21	0.86	0
4	NAG	A	902	1	14,14,15	0.70	0	17,19,21	0.90	0
5	ACT	A	914	-	3,3,3	1.13	0	3,3,3	1.26	0
4	NAG	C	909	1	14,14,15	0.73	0	17,19,21	1.73	3 (17%)
5	ACT	A	911	-	3,3,3	1.11	0	3,3,3	1.32	0
4	NAG	A	901	1	14,14,15	0.72	0	17,19,21	0.90	0
5	ACT	B	903	-	3,3,3	1.12	0	3,3,3	1.28	0
5	ACT	B	916	-	3,3,3	1.14	0	3,3,3	1.22	0
5	ACT	C	906	-	3,3,3	1.15	0	3,3,3	1.17	0
5	ACT	C	907	-	3,3,3	1.12	0	3,3,3	1.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ACT	A	912	-	3,3,3	1.13	0	3,3,3	1.25	0
4	NAG	B	904	1	14,14,15	0.65	0	17,19,21	0.78	0
5	ACT	A	916	-	3,3,3	1.15	0	3,3,3	1.20	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	B	917	1	-	0/6/23/26	0/1/1/1
4	NAG	A	918	1	-	0/6/23/26	0/1/1/1
4	NAG	B	906	1	-	0/6/23/26	0/1/1/1
4	NAG	A	920	1	-	2/6/23/26	0/1/1/1
6	PG4	A	907	-	-	4/10/10/10	-
4	NAG	A	905	1	-	1/6/23/26	0/1/1/1
8	PGE	A	921	-	-	0/7/7/7	-
4	NAG	C	903	1	-	1/6/23/26	0/1/1/1
9	P6G	B	907	-	-	4/16/16/16	-
4	NAG	C	908	1	-	0/6/23/26	0/1/1/1
4	NAG	A	903	1	-	0/6/23/26	0/1/1/1
4	NAG	A	908	1	-	2/6/23/26	0/1/1/1
4	NAG	B	901	1	-	2/6/23/26	0/1/1/1
4	NAG	B	902	1	-	0/6/23/26	0/1/1/1
4	NAG	C	902	1	-	2/6/23/26	0/1/1/1
4	NAG	B	919	1	-	2/6/23/26	0/1/1/1
4	NAG	C	910	1	-	2/6/23/26	0/1/1/1
4	NAG	C	901	1	-	0/6/23/26	0/1/1/1
4	NAG	A	919	1	-	1/6/23/26	0/1/1/1
4	NAG	B	918	1	-	2/6/23/26	0/1/1/1
4	NAG	A	906	1	-	0/6/23/26	0/1/1/1
4	NAG	A	902	1	-	0/6/23/26	0/1/1/1
4	NAG	C	909	1	-	1/6/23/26	0/1/1/1
4	NAG	A	901	1	-	0/6/23/26	0/1/1/1
4	NAG	B	904	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	905	NAG	C2-N2-C7	7.14	132.46	122.90
4	B	918	NAG	C2-N2-C7	6.75	131.94	122.90
4	C	909	NAG	C2-N2-C7	5.34	130.06	122.90
4	B	918	NAG	C1-C2-N2	4.11	116.91	110.43
4	A	905	NAG	C1-C2-N2	3.82	116.45	110.43
4	B	919	NAG	C2-N2-C7	3.52	127.62	122.90
4	C	901	NAG	C1-O5-C5	3.13	116.38	112.19
4	C	909	NAG	C1-O5-C5	2.59	115.65	112.19
4	A	920	NAG	O5-C1-C2	-2.45	107.50	111.29
4	A	905	NAG	O7-C7-N2	2.38	126.19	121.98
4	B	906	NAG	C2-N2-C7	2.33	126.03	122.90
4	C	909	NAG	O7-C7-N2	2.17	125.81	121.98
4	B	918	NAG	O7-C7-N2	2.06	125.62	121.98
4	A	903	NAG	O5-C1-C2	-2.03	108.15	111.29

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	905	NAG	C1-C2-N2-C7
4	B	918	NAG	C1-C2-N2-C7
4	C	909	NAG	C3-C2-N2-C7
4	B	901	NAG	C4-C5-C6-O6
4	B	901	NAG	O5-C5-C6-O6
4	B	904	NAG	C4-C5-C6-O6
6	A	907	PG4	O4-C7-C8-O5
4	A	920	NAG	C8-C7-N2-C2
4	A	920	NAG	O7-C7-N2-C2
4	C	902	NAG	C8-C7-N2-C2
4	C	902	NAG	O7-C7-N2-C2
9	B	907	P6G	O1-C2-C3-O4
4	B	904	NAG	O5-C5-C6-O6
9	B	907	P6G	O4-C5-C6-O7
4	C	903	NAG	O5-C5-C6-O6
4	A	919	NAG	O5-C5-C6-O6
4	B	918	NAG	O5-C5-C6-O6
4	C	910	NAG	C4-C5-C6-O6
4	B	919	NAG	C1-C2-N2-C7
4	A	908	NAG	C4-C5-C6-O6
4	A	908	NAG	O5-C5-C6-O6
4	C	910	NAG	O5-C5-C6-O6
4	B	919	NAG	C3-C2-N2-C7
6	A	907	PG4	C1-C2-O2-C3

Continued on next page...

Continued from previous page...

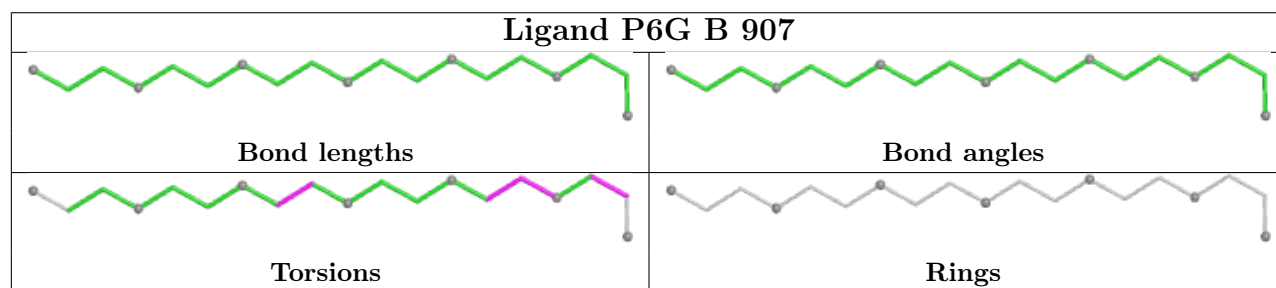
Mol	Chain	Res	Type	Atoms
6	A	907	PG4	C3-C4-O3-C5
6	A	907	PG4	C6-C5-O3-C4
9	B	907	P6G	O10-C11-C12-O13
9	B	907	P6G	C6-C5-O4-C3

There are no ring outliers.

9 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	907	PG4	1	0
4	A	905	NAG	1	0
8	A	921	PGE	1	0
4	B	901	NAG	1	0
4	B	902	NAG	1	0
5	C	905	ACT	1	0
4	B	918	NAG	1	0
5	A	911	ACT	1	0
5	B	903	ACT	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	757/871 (86%)	-0.07	3 (0%) 88 84	24, 58, 79, 95	1 (0%)
1	B	757/871 (86%)	0.04	5 (0%) 84 77	49, 66, 82, 99	0
1	C	756/871 (86%)	0.27	5 (0%) 84 77	51, 77, 98, 111	0
All	All	2270/2613 (86%)	0.08	13 (0%) 85 80	24, 67, 91, 111	1 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	435	ALA	4.1
1	A	722	ILE	2.9
1	B	778	ALA	2.4
1	A	778	ALA	2.3
1	C	736	LEU	2.2
1	C	772	THR	2.2
1	B	22	ALA	2.2
1	B	213	ASN	2.1
1	C	498	VAL	2.1
1	A	33	ALA	2.1
1	B	386	GLU	2.1
1	C	501	VAL	2.0
1	B	24	PHE	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

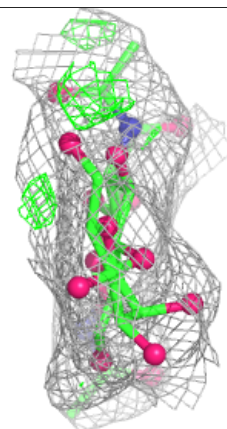
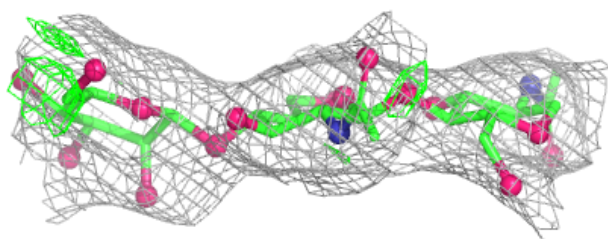
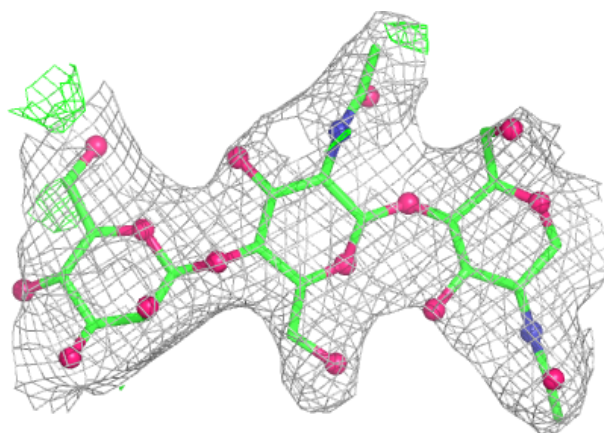
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	BMA	I	3	11/12	0.48	0.12	93,98,100,101	0
3	NAG	G	2	14/15	0.59	0.14	109,117,123,124	0
2	BMA	D	3	11/12	0.63	0.11	89,92,96,105	0
2	BMA	F	3	11/12	0.63	0.12	87,91,97,99	0
2	NAG	I	2	14/15	0.71	0.14	85,89,94,95	0
3	NAG	H	2	14/15	0.73	0.12	92,102,110,112	0
3	NAG	E	2	14/15	0.75	0.10	84,89,97,99	0
3	NAG	G	1	14/15	0.77	0.11	92,96,106,111	0
2	NAG	D	2	14/15	0.81	0.10	71,79,85,89	0
2	NAG	F	2	14/15	0.83	0.11	83,87,91,92	0
3	NAG	H	1	14/15	0.86	0.12	80,88,95,99	0
2	NAG	F	1	14/15	0.86	0.10	72,78,83,90	0
2	NAG	I	1	14/15	0.88	0.10	79,84,87,87	0
2	NAG	D	1	14/15	0.90	0.11	60,71,78,79	0
3	NAG	E	1	14/15	0.92	0.09	69,74,81,84	0

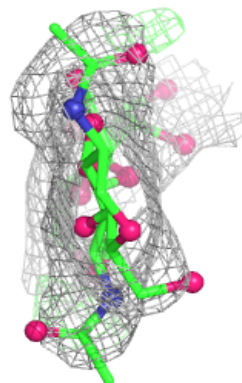
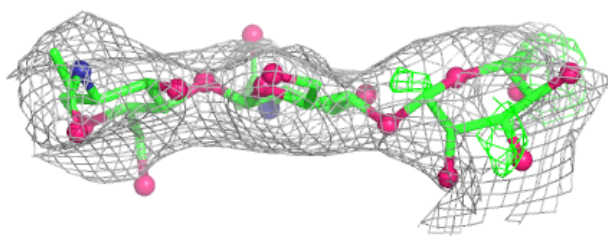
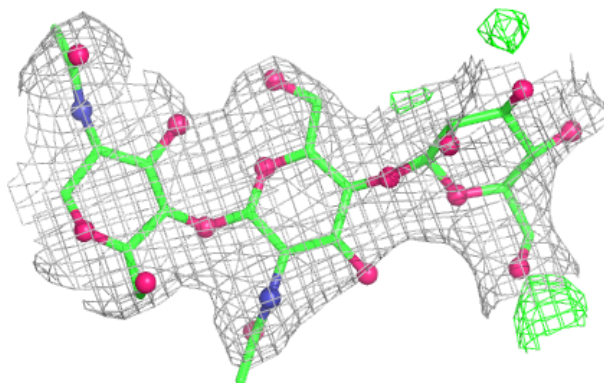
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain D:

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

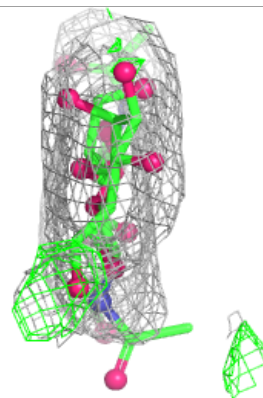
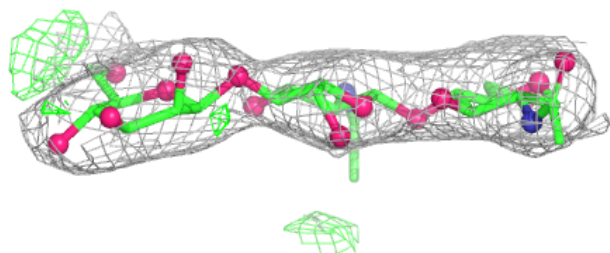
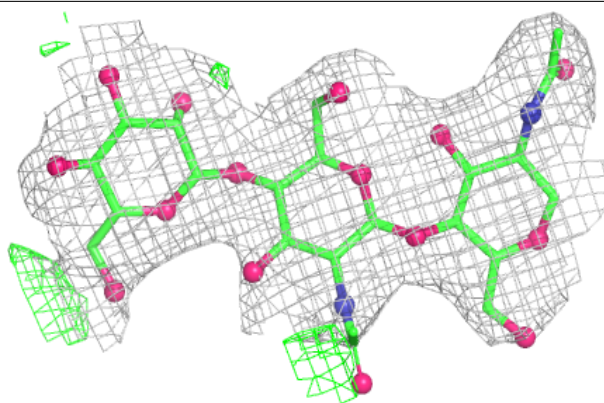
**Electron density around Chain F:**

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

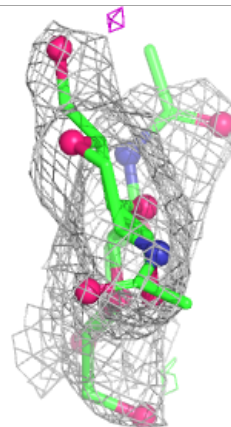
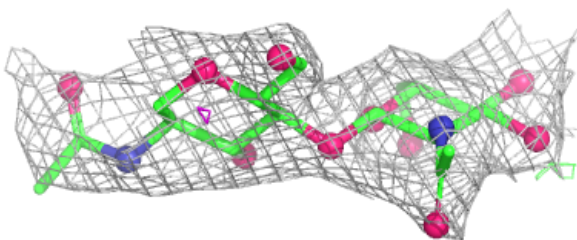
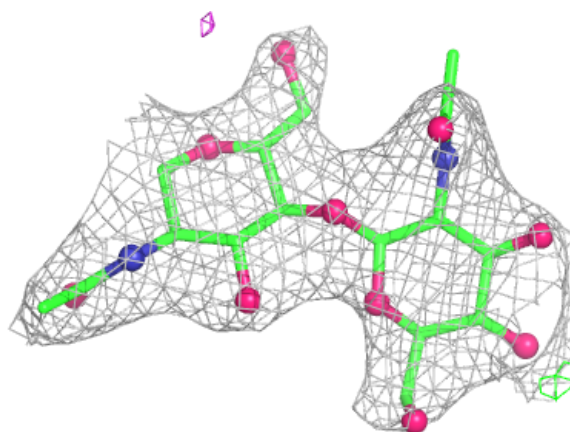


Electron density around Chain I:

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

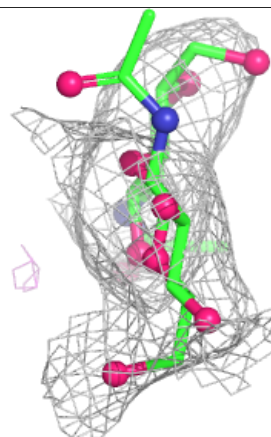
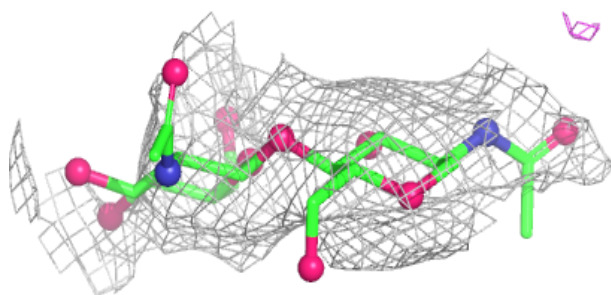
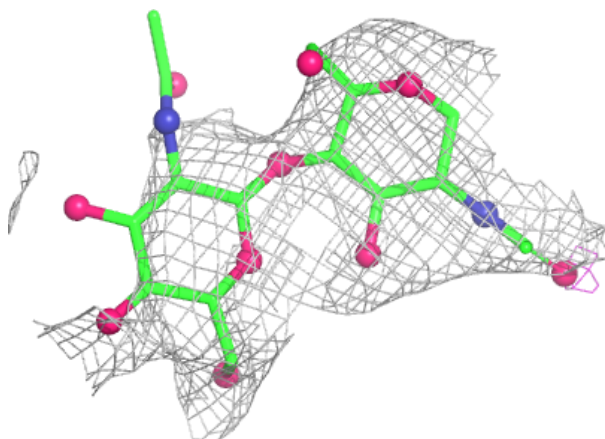
**Electron density around Chain E:**

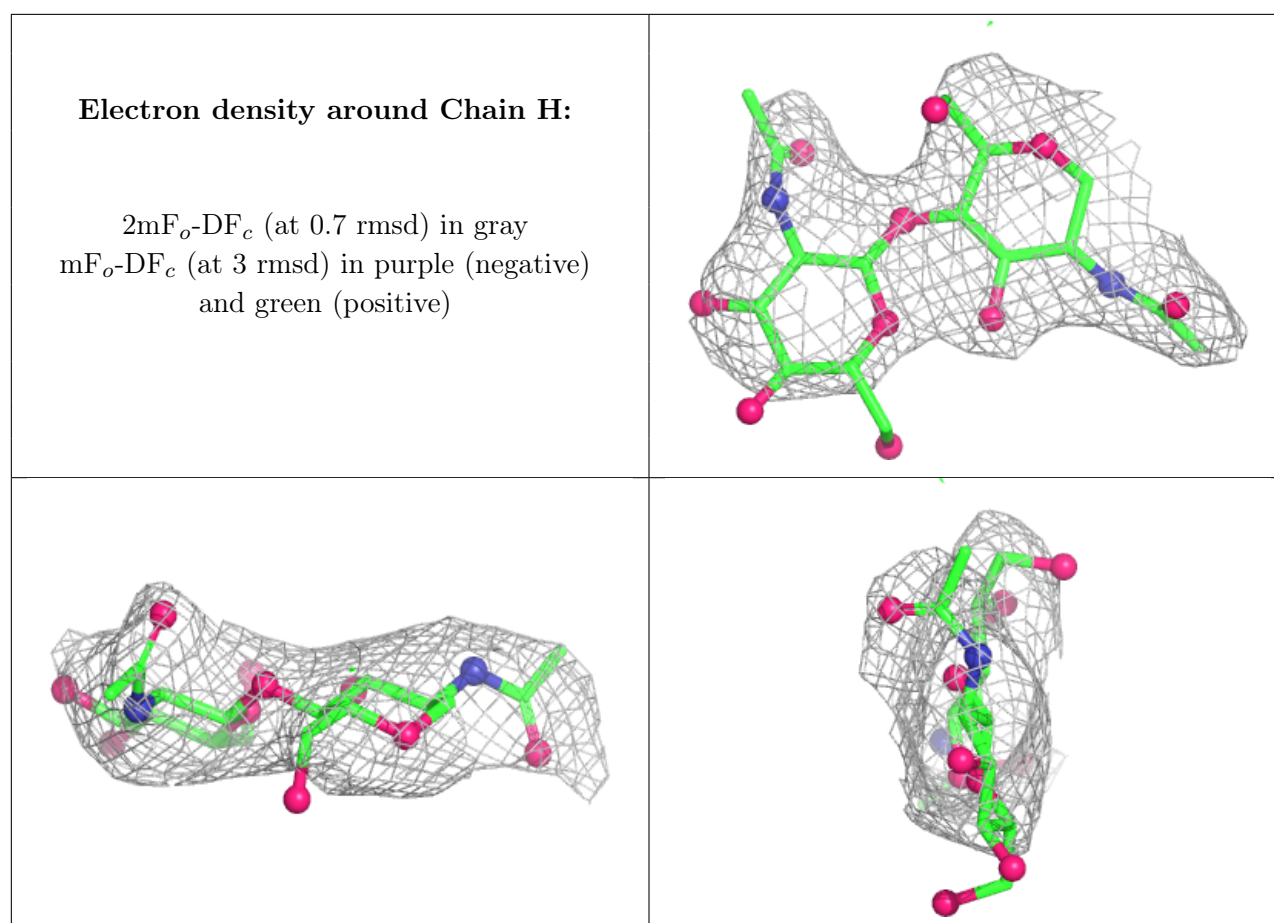
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain G:

$2mF_o-DF_c$ (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, 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
4	NAG	A	920	14/15	0.24	0.14	90,97,112,112	0
4	NAG	C	909	14/15	0.40	0.14	103,109,114,114	0
4	NAG	C	910	14/15	0.41	0.15	90,115,121,124	0
4	NAG	A	918	14/15	0.42	0.16	94,99,106,107	0
4	NAG	C	903	14/15	0.44	0.14	95,106,112,115	0
4	NAG	A	919	14/15	0.46	0.14	88,103,110,114	0
4	NAG	A	905	14/15	0.53	0.16	85,95,99,106	0
4	NAG	C	908	14/15	0.54	0.14	103,111,120,125	0
4	NAG	B	904	14/15	0.56	0.16	81,86,94,96	0
4	NAG	C	902	14/15	0.57	0.13	88,102,105,116	0
4	NAG	C	901	14/15	0.58	0.17	93,99,106,114	0
4	NAG	B	906	14/15	0.60	0.16	85,97,101,106	0

Continued on next page...

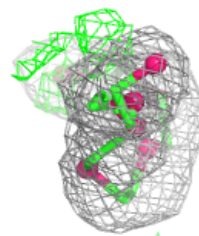
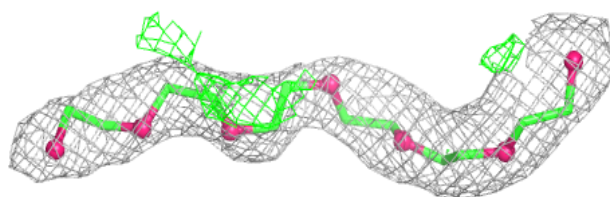
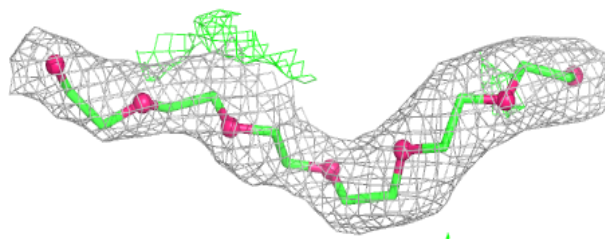
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	A	901	14/15	0.65	0.18	82,96,113,115	0
4	NAG	B	919	14/15	0.65	0.12	97,101,106,106	0
5	ACT	B	916	4/4	0.66	0.14	70,73,78,82	0
4	NAG	B	918	14/15	0.68	0.16	82,88,90,92	0
4	NAG	A	903	14/15	0.69	0.15	87,96,108,109	0
5	ACT	B	914	4/4	0.70	0.18	58,62,72,72	0
5	ACT	B	913	4/4	0.70	0.16	67,68,69,70	0
5	ACT	C	905	4/4	0.71	0.21	63,66,72,75	0
4	NAG	B	917	14/15	0.72	0.12	84,92,97,100	0
4	NAG	A	906	14/15	0.75	0.12	82,89,93,94	0
5	ACT	A	911	4/4	0.76	0.17	51,57,58,62	0
5	ACT	A	914	4/4	0.76	0.16	64,68,69,72	0
5	ACT	B	911	4/4	0.78	0.18	64,65,66,67	0
5	ACT	C	906	4/4	0.78	0.17	72,79,81,86	0
6	PG4	A	907	13/13	0.79	0.16	61,82,86,90	0
5	ACT	A	916	4/4	0.80	0.12	66,70,71,71	0
5	ACT	B	912	4/4	0.80	0.16	69,78,81,86	0
5	ACT	B	903	4/4	0.84	0.14	64,70,71,71	0
5	ACT	B	915	4/4	0.84	0.14	73,75,76,78	0
9	P6G	B	907	19/19	0.84	0.14	65,72,80,84	0
5	ACT	B	909	4/4	0.85	0.21	66,66,66,68	0
5	ACT	A	915	4/4	0.86	0.14	60,63,69,70	0
4	NAG	B	902	14/15	0.86	0.11	76,79,82,83	0
4	NAG	B	901	14/15	0.87	0.12	66,73,78,78	0
5	ACT	B	910	4/4	0.87	0.15	57,59,61,66	0
5	ACT	A	917	4/4	0.87	0.12	55,59,61,65	0
8	PGE	A	921	10/10	0.87	0.10	56,60,65,65	0
5	ACT	A	913	4/4	0.87	0.11	70,70,74,76	0
5	ACT	A	904	4/4	0.88	0.13	40,42,48,50	0
5	ACT	A	910	4/4	0.89	0.13	47,56,59,60	0
5	ACT	A	912	4/4	0.89	0.20	57,60,64,66	0
5	ACT	C	907	4/4	0.89	0.15	58,65,66,71	0
5	ACT	B	905	4/4	0.92	0.10	65,68,68,69	0
4	NAG	A	902	14/15	0.92	0.09	59,63,74,77	0
4	NAG	A	908	14/15	0.92	0.09	67,72,75,78	0
7	CA	B	908	1/1	0.95	0.06	70,70,70,70	0
7	CA	C	904	1/1	0.96	0.06	91,91,91,91	0
7	CA	A	909	1/1	0.99	0.06	65,65,65,65	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around P6G B 907:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.