



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:33 PM UTC

PDB ID : 6DMF / pdb_00006dmf
Title : Bacteroides ovatus mixed-linkage glucan utilization locus (MLGUL) SGBP-A with cellohexaose
Authors : Koropatkin, N.M.; Bahr, C.M.
Deposited on : 2018-06-05
Resolution : 2.40 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

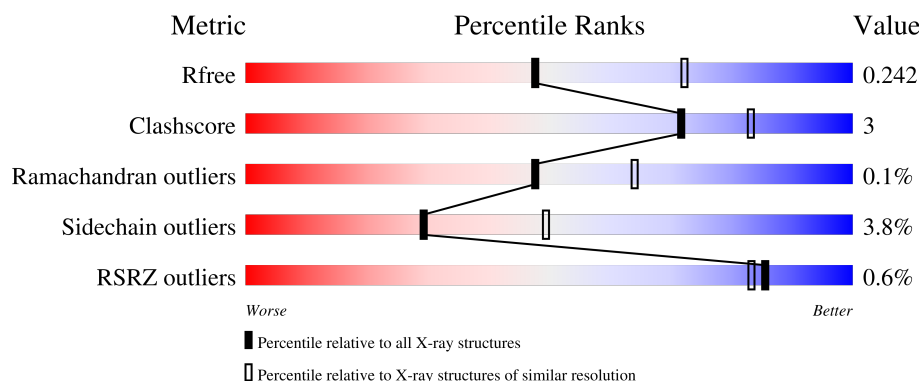
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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.



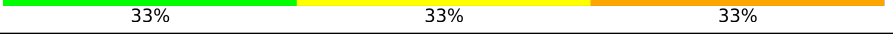
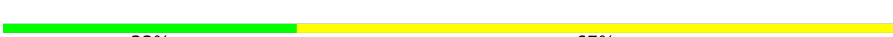
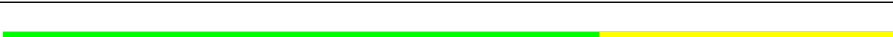
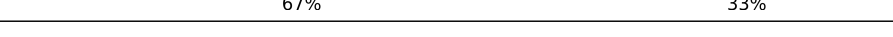
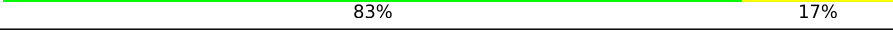
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	520	89% 9% ..
1	B	520	89% 9% ..
1	C	520	90% 8% ..
1	D	520	89% 10% .
1	E	520	90% 9% ..

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Mol	Chain	Length	Quality of chain
1	F	520	 91% 7% ..
1	G	520	 89% 9% .
1	H	520	 88% 10% ..
1	I	520	 89% 8% ..
1	J	520	 89% 9% ..
2	K	5	 60% 40%
3	L	6	 33% 33% 33%
3	M	6	 83% 17%
3	N	6	 67% 33%
3	O	6	 33% 67%
3	P	6	 67% 33%
3	Q	6	 67% 33%
3	R	6	 83% 17%
3	S	6	 67% 33%
3	T	6	 50% 50%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 42441 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 mixed-linkage glucan utilization locus (MLGUL) SGBP-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	513	Total	C	N	O	S	0	0	0
			4072	2572	676	804	20			
1	B	516	Total	C	N	O	S	0	0	0
			4082	2579	680	803	20			
1	C	512	Total	C	N	O	S	0	0	0
			4061	2563	675	803	20			
1	D	519	Total	C	N	O	S	0	0	0
			4103	2592	683	808	20			
1	E	517	Total	C	N	O	S	0	0	0
			4097	2588	681	808	20			
1	F	514	Total	C	N	O	S	0	0	0
			4069	2571	677	801	20			
1	G	512	Total	C	N	O	S	0	0	0
			4041	2552	673	796	20			
1	H	514	Total	C	N	O	S	0	0	0
			4072	2574	677	801	20			
1	I	510	Total	C	N	O	S	0	0	0
			4035	2551	672	792	20			
1	J	512	Total	C	N	O	S	0	0	0
			4053	2561	674	798	20			

There are 10 discrepancies between the modelled and reference sequences:

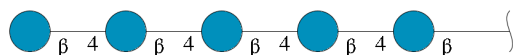
Chain	Residue	Modelled	Actual	Comment	Reference
A	39	ILE	-	expression tag	UNP A7LY27
B	39	ILE	-	expression tag	UNP A7LY27
C	39	ILE	-	expression tag	UNP A7LY27
D	39	ILE	-	expression tag	UNP A7LY27
E	39	ILE	-	expression tag	UNP A7LY27
F	39	ILE	-	expression tag	UNP A7LY27
G	39	ILE	-	expression tag	UNP A7LY27
H	39	ILE	-	expression tag	UNP A7LY27
I	39	ILE	-	expression tag	UNP A7LY27

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Chain	Residue	Modelled	Actual	Comment	Reference
J	39	ILE	-	expression tag	UNP A7LY27

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	K	5	Total	C	O	0	0	0
			56	30	26			

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

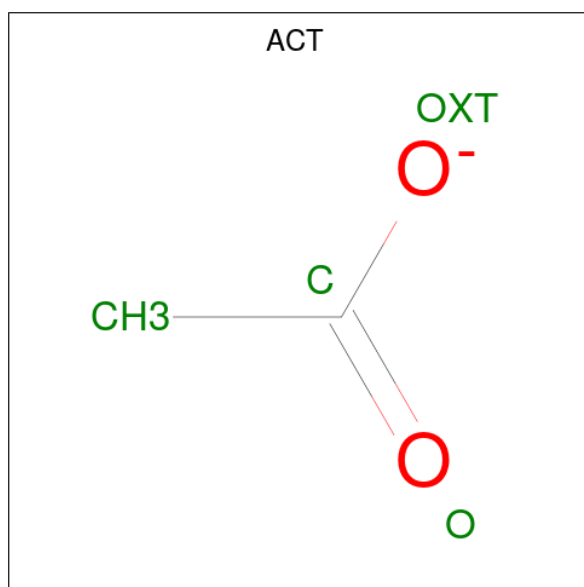


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	L	6	Total	C	O	0	0	0
			67	36	31			
3	M	6	Total	C	O	0	0	0
			67	36	31			
3	N	6	Total	C	O	0	0	0
			67	36	31			
3	O	6	Total	C	O	0	0	0
			67	36	31			
3	P	6	Total	C	O	0	0	0
			67	36	31			
3	Q	6	Total	C	O	0	0	0
			67	36	31			
3	R	6	Total	C	O	0	0	0
			67	36	31			
3	S	6	Total	C	O	0	0	0
			67	36	31			
3	T	6	Total	C	O	0	0	0
			67	36	31			

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0
4	E	1	Total Mg 1 1	0	0
4	F	1	Total Mg 1 1	0	0
4	G	1	Total Mg 1 1	0	0
4	H	1	Total Mg 1 1	0	0
4	I	1	Total Mg 1 1	0	0
4	J	1	Total Mg 1 1	0	0

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	F	1	Total	C	O	0	0
			4	2	2		
5	H	1	Total	C	O	0	0
			4	2	2		
5	I	1	Total	C	O	0	0
			4	2	2		
5	J	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	J	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

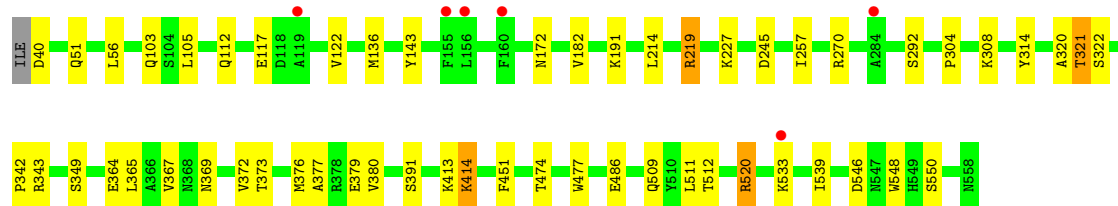
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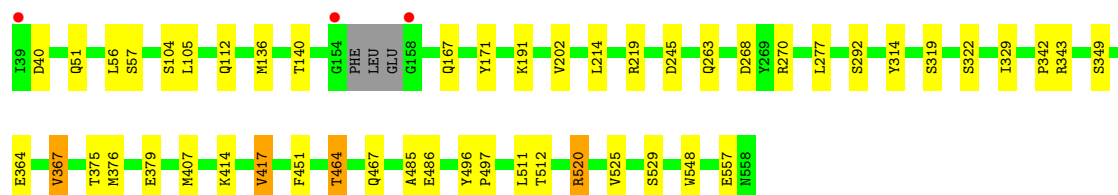
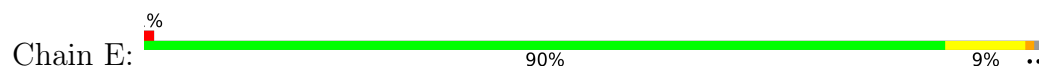
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	E	1	Total C O 4 2 2	0	0
7	G	1	Total C O 4 2 2	0	0
7	G	1	Total C O 4 2 2	0	0
7	G	1	Total C O 4 2 2	0	0
7	G	1	Total C O 4 2 2	0	0
7	G	1	Total C O 4 2 2	0	0
7	H	1	Total C O 4 2 2	0	0
7	I	1	Total C O 4 2 2	0	0

- Molecule 8 is water.

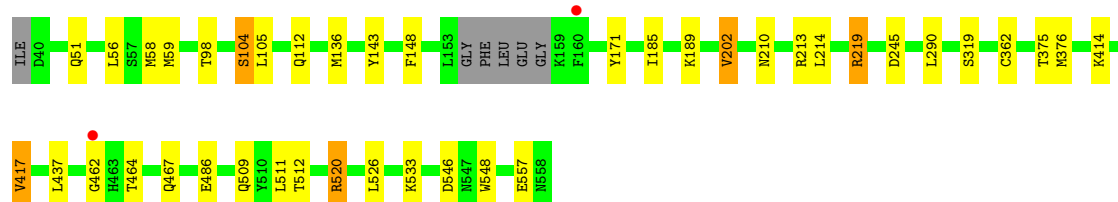
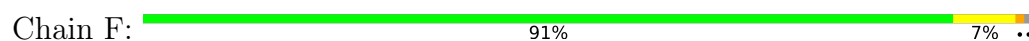
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	110	Total O 110 110	0	0
8	B	129	Total O 129 129	0	0
8	C	98	Total O 98 98	0	0
8	D	88	Total O 88 88	0	0
8	E	115	Total O 115 115	0	0
8	F	59	Total O 59 59	0	0
8	G	90	Total O 90 90	0	0
8	H	87	Total O 87 87	0	0
8	I	64	Total O 64 64	0	0
8	J	104	Total O 104 104	0	0



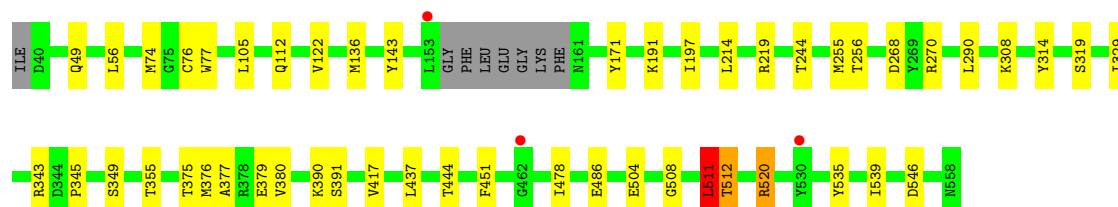
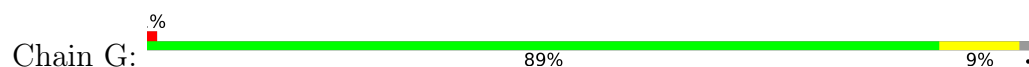
• Molecule 1: mixed-linkage glucan utilization locus (MLGUL) SGBP-B



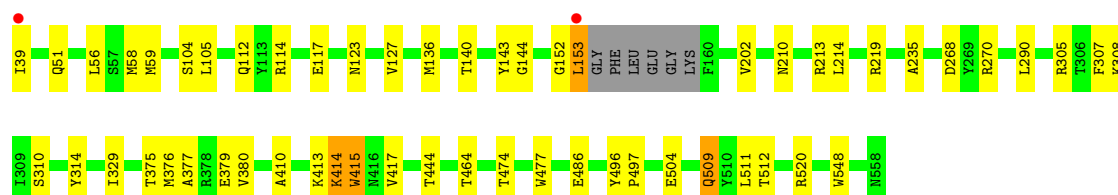
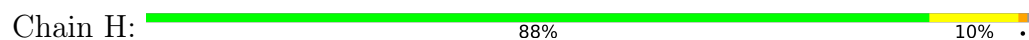
• Molecule 1: mixed-linkage glucan utilization locus (MLGUL) SGBP-B



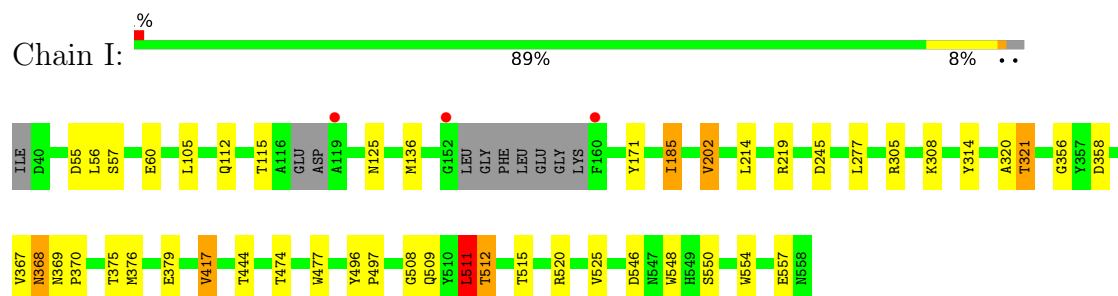
• Molecule 1: mixed-linkage glucan utilization locus (MLGUL) SGBP-B



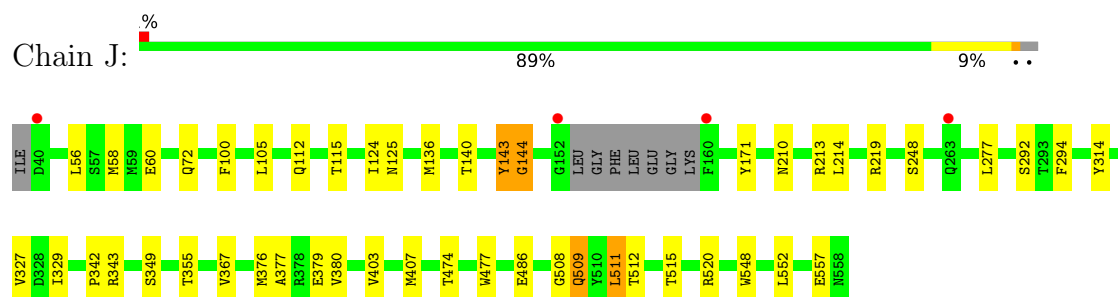
• Molecule 1: mixed-linkage glucan utilization locus (MLGUL) SGBP-B



- Molecule 1: mixed-linkage glucan utilization locus (MLGUL) SGBP-B



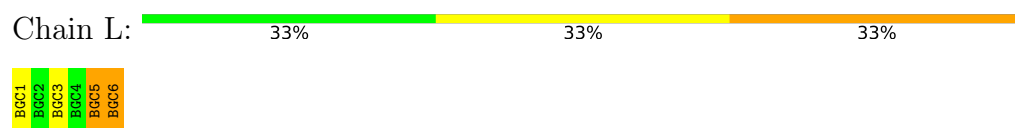
- Molecule 1: mixed-linkage glucan utilization locus (MLGUL) SGBP-B



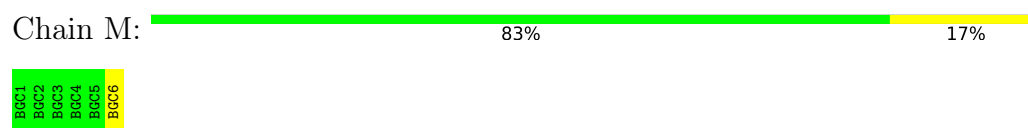
- Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose



- Molecule 3: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose



- Molecule 3: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose



- Molecule 3: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose





- Molecule 3: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose



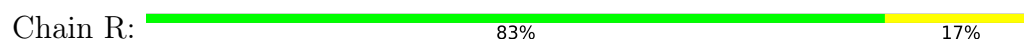
- Molecule 3: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose



- Molecule 3: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose



- Molecule 3: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose



- Molecule 3: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose



- Molecule 3: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	228.84Å 228.84Å 246.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.60 – 2.40 49.60 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.60-2.40) 89.5 (49.60-2.40)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.97 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.190 , 0.242 0.191 , 0.242	Depositor DCC
R_{free} test set	14142 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	28.9	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.023 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	42441	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 57.57 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.3232e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BGC, PEG, EDO, ACT, MG

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	0.62	0/4171	0.97	0/5671
1	B	0.60	0/4181	0.94	3/5684 (0.1%)
1	C	0.60	0/4159	0.95	2/5655 (0.0%)
1	D	0.59	0/4203	0.93	2/5715 (0.0%)
1	E	0.62	0/4196	0.93	0/5703
1	F	0.57	0/4168	0.94	0/5668
1	G	0.58	0/4139	0.95	4/5631 (0.1%)
1	H	0.62	0/4171	0.94	0/5672
1	I	0.59	0/4133	0.96	2/5619 (0.0%)
1	J	0.60	0/4152	0.97	0/5646
All	All	0.60	0/41673	0.95	13/56664 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	2
1	F	0	1
All	All	0	3

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	511	LEU	CA-C-N	6.14	128.84	120.54
1	G	511	LEU	C-N-CA	6.14	128.84	120.54
1	B	511	LEU	CA-C-N	5.92	128.53	120.54
1	B	511	LEU	C-N-CA	5.92	128.53	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	391	SER	CA-C-N	5.81	129.14	120.31
1	G	391	SER	C-N-CA	5.81	129.14	120.31
1	C	511	LEU	CA-C-N	5.55	128.04	120.54
1	C	511	LEU	C-N-CA	5.55	128.04	120.54
1	D	391	SER	CA-C-N	5.46	127.87	120.38
1	D	391	SER	C-N-CA	5.46	127.87	120.38
1	I	511	LEU	CA-C-N	5.42	127.54	120.28
1	I	511	LEU	C-N-CA	5.42	127.54	120.28
1	B	509	GLN	CB-CA-C	-5.01	100.75	110.46

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	219	ARG	Sidechain
1	D	270	ARG	Sidechain
1	F	219	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4072	0	3860	23	0
1	B	4082	0	3870	32	0
1	C	4061	0	3851	33	0
1	D	4103	0	3890	26	0
1	E	4097	0	3890	26	0
1	F	4069	0	3854	19	0
1	G	4041	0	3822	26	0
1	H	4072	0	3863	34	0
1	I	4035	0	3824	30	0
1	J	4053	0	3837	25	0
2	K	56	0	48	0	0
3	L	67	0	57	1	0
3	M	67	0	57	0	0
3	N	67	0	57	0	0
3	O	67	0	57	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	P	67	0	57	0	0
3	Q	67	0	57	0	0
3	R	67	0	57	0	0
3	S	67	0	57	0	0
3	T	67	0	57	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
5	C	4	0	3	0	0
5	D	4	0	3	0	0
5	E	4	0	3	0	0
5	F	4	0	3	0	0
5	H	4	0	3	0	0
5	I	4	0	3	0	0
5	J	4	0	3	0	0
6	A	14	0	20	0	0
6	B	14	0	20	0	0
6	J	7	0	10	0	0
7	A	4	0	6	0	0
7	B	8	0	12	0	0
7	C	12	0	18	1	0
7	D	4	0	6	0	0
7	E	16	0	24	1	0
7	G	20	0	30	2	0
7	H	4	0	6	0	0
7	I	4	0	6	0	0
8	A	110	0	0	2	0
8	B	129	0	0	2	0
8	C	98	0	0	4	0
8	D	88	0	0	0	0
8	E	115	0	0	0	0
8	F	59	0	0	0	0
8	G	90	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	87	0	0	0	0
8	I	64	0	0	3	0
8	J	104	0	0	0	0
All	All	42441	0	39307	264	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 (264) 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:D:143:TYR:O	1:D:520:ARG:NH1	1.60	1.31
1:H:51:GLN:NE2	1:H:104:SER:OG	1.87	1.07
1:G:314:TYR:HB2	1:G:376:MET:HE1	1.47	0.97
1:G:143:TYR:O	1:G:520:ARG:NH1	2.05	0.89
1:B:314:TYR:HB2	1:B:376:MET:HE1	1.57	0.84
1:J:314:TYR:HB2	1:J:376:MET:HE1	1.59	0.83
1:A:314:TYR:HB2	1:A:376:MET:HE1	1.60	0.83
1:I:314:TYR:HB2	1:I:376:MET:HE1	1.63	0.79
1:G:268:ASP:OD1	1:G:270:ARG:HD3	1.83	0.79
1:I:520:ARG:NH1	8:I:701:HOH:O	2.00	0.78
1:H:314:TYR:HB2	1:H:376:MET:HE1	1.67	0.77
1:D:219:ARG:NH2	1:D:486:GLU:OE2	2.21	0.74
1:A:520:ARG:NH2	1:A:546:ASP:OD1	2.21	0.73
1:E:329:ILE:HD13	1:E:376:MET:HE2	1.70	0.72
1:A:367:VAL:HG21	1:E:464:THR:HG21	1.72	0.71
1:E:314:TYR:HB2	1:E:376:MET:HE1	1.72	0.71
1:F:362:CYS:SG	1:F:376:MET:CE	2.79	0.70
1:H:219:ARG:HH22	1:H:486:GLU:CD	2.01	0.68
1:F:520:ARG:NH2	1:F:546:ASP:OD1	2.27	0.68
1:D:364:GLU:O	1:D:367:VAL:HG12	1.96	0.65
1:I:115:THR:HG22	1:I:125:ASN:HB2	1.78	0.64
1:H:144:GLY:H	1:H:520:ARG:HH12	1.46	0.64
1:C:185:ILE:HG23	1:C:202:VAL:CG1	2.29	0.63
1:H:105:LEU:HD21	1:H:136:MET:CE	2.29	0.63
1:B:51:GLN:HE22	1:B:103:GLN:HB3	1.64	0.62
1:G:219:ARG:HH22	1:G:486:GLU:CD	2.08	0.62
1:C:329:ILE:HD13	1:C:376:MET:HE2	1.82	0.62
1:E:51:GLN:NE2	1:E:104:SER:OG	2.28	0.61
1:G:329:ILE:HD13	1:G:376:MET:HE2	1.81	0.61
1:B:512:THR:HB	8:B:753:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:432:ALA:HB2	8:C:791:HOH:O	2.00	0.61
1:H:329:ILE:HD13	1:H:376:MET:HE2	1.81	0.61
1:E:376:MET:HE3	1:E:379:GLU:CB	2.30	0.61
1:D:105:LEU:HD21	1:D:136:MET:HE1	1.84	0.60
1:F:362:CYS:SG	1:F:376:MET:HE1	2.42	0.60
1:B:376:MET:HE3	1:B:379:GLU:CB	2.30	0.60
1:I:320:ALA:O	1:I:321:THR:OG1	2.11	0.60
1:D:105:LEU:HD21	1:D:136:MET:CE	2.32	0.60
1:A:367:VAL:HG21	1:E:464:THR:CG2	2.31	0.59
1:B:219:ARG:NH2	1:B:486:GLU:OE2	2.36	0.59
1:G:512:THR:HB	8:G:706:HOH:O	2.02	0.58
1:J:219:ARG:NH2	1:J:486:GLU:OE2	2.36	0.58
1:B:268:ASP:OD1	1:B:270:ARG:HD3	2.04	0.58
1:F:143:TYR:O	1:F:520:ARG:NH1	2.37	0.58
1:J:219:ARG:HH22	1:J:486:GLU:CD	2.10	0.58
1:B:329:ILE:HD13	1:B:376:MET:HE2	1.85	0.58
1:I:185:ILE:HG23	1:I:202:VAL:CG1	2.34	0.58
1:D:219:ARG:HH22	1:D:486:GLU:CD	2.12	0.58
1:I:105:LEU:HD21	1:I:136:MET:CE	2.34	0.58
1:J:329:ILE:HD13	1:J:376:MET:HE2	1.86	0.57
1:J:115:THR:HG22	1:J:125:ASN:HB2	1.85	0.57
1:C:219:ARG:HH22	1:C:486:GLU:CD	2.13	0.57
1:H:219:ARG:NH2	1:H:486:GLU:OE2	2.38	0.56
1:C:314:TYR:HB2	1:C:376:MET:HE1	1.87	0.56
1:B:219:ARG:HH22	1:B:486:GLU:CD	2.13	0.56
1:C:376:MET:HE3	1:C:379:GLU:CB	2.37	0.55
1:B:105:LEU:HD21	1:B:136:MET:CE	2.36	0.55
1:J:58:MET:HE1	1:J:100:PHE:CZ	2.41	0.55
1:A:219:ARG:NH2	1:A:486:GLU:OE2	2.39	0.55
1:G:376:MET:HE3	1:G:379:GLU:CB	2.37	0.55
1:D:51:GLN:HE22	1:D:103:GLN:HE21	1.54	0.54
1:E:171:TYR:OH	1:E:219:ARG:HD2	2.08	0.54
1:E:292:SER:HA	1:E:342:PRO:HB2	1.88	0.54
1:J:105:LEU:HD21	1:J:136:MET:CE	2.37	0.54
1:C:51:GLN:HE22	1:C:103:GLN:HB3	1.71	0.54
1:G:520:ARG:NH2	1:G:546:ASP:OD1	2.41	0.54
1:H:51:GLN:NE2	1:H:104:SER:CB	2.71	0.54
1:H:51:GLN:NE2	1:H:104:SER:HG	2.04	0.54
1:B:105:LEU:HD21	1:B:136:MET:HE1	1.90	0.53
1:F:136:MET:HE3	1:F:148:PHE:CD1	2.44	0.53
1:G:219:ARG:NH2	1:G:486:GLU:OE2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:512:THR:HG21	1:D:245:ASP:HB3	1.90	0.53
1:B:356:GLY:HA3	1:B:376:MET:O	2.09	0.53
1:I:512:THR:HB	8:I:710:HOH:O	2.08	0.53
1:J:140:THR:O	1:J:143:TYR:O	2.27	0.53
1:F:362:CYS:SG	1:F:376:MET:HE3	2.48	0.52
1:H:305:ARG:HA	1:H:308:LYS:HD2	1.91	0.52
1:B:112:GLN:NE2	8:B:704:HOH:O	2.43	0.52
1:H:520:ARG:O	1:H:548:TRP:HB2	2.08	0.52
1:J:171:TYR:OH	1:J:219:ARG:HD2	2.09	0.52
1:A:171:TYR:OH	1:A:219:ARG:HD2	2.10	0.52
1:A:140:THR:O	1:A:143:TYR:O	2.28	0.52
1:B:214:LEU:HG	1:B:232:PHE:CE2	2.45	0.51
1:B:111:ALA:O	1:B:115:THR:HB	2.11	0.51
1:A:314:TYR:HB3	1:A:327:VAL:HB	1.92	0.51
1:C:219:ARG:HA	1:C:493:ARG:HD3	1.92	0.51
1:D:51:GLN:NE2	1:D:103:GLN:NE2	2.58	0.51
1:C:343:ARG:HD2	1:C:349:SER:HA	1.93	0.51
1:F:520:ARG:O	1:F:548:TRP:HB2	2.10	0.51
1:A:115:THR:HG22	1:A:125:ASN:HB2	1.92	0.51
1:A:376:MET:HE3	1:A:379:GLU:CB	2.41	0.50
1:G:377:ALA:O	1:G:380:VAL:HG22	2.11	0.50
1:I:474:THR:O	1:I:477:TRP:HB3	2.11	0.50
1:A:225:PRO:O	8:A:701:HOH:O	2.19	0.50
1:I:305:ARG:HA	1:I:308:LYS:HD2	1.92	0.50
1:E:364:GLU:O	1:E:367:VAL:HG13	2.12	0.50
1:H:123:ASN:O	1:H:127:VAL:HG23	2.11	0.50
1:D:320:ALA:O	1:D:321:THR:CB	2.60	0.50
1:I:60:GLU:OE2	1:I:277:LEU:HD11	2.11	0.50
1:C:376:MET:HE3	1:C:379:GLU:HB2	1.94	0.50
1:G:255:MET:HE3	1:G:270:ARG:HB3	1.94	0.50
1:C:51:GLN:HE22	1:C:103:GLN:CB	2.25	0.49
1:J:210:ASN:HA	1:J:213:ARG:HD3	1.93	0.49
1:D:343:ARG:HD2	1:D:349:SER:HA	1.93	0.49
1:D:520:ARG:NH2	1:D:546:ASP:OD1	2.44	0.49
1:F:245:ASP:HB3	1:I:512:THR:HG21	1.93	0.49
1:C:417:VAL:O	1:C:417:VAL:CG1	2.60	0.49
1:B:60:GLU:HA	1:B:277:LEU:HD21	1.95	0.49
1:E:105:LEU:HD21	1:E:136:MET:CE	2.42	0.49
1:C:219:ARG:NH2	1:C:486:GLU:OE2	2.45	0.49
1:A:329:ILE:HD13	1:A:376:MET:HE2	1.95	0.49
1:B:115:THR:HG22	1:B:125:ASN:OD1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:LEU:HD21	1:C:136:MET:CE	2.42	0.49
1:I:417:VAL:CG1	1:I:417:VAL:O	2.60	0.49
1:H:39:ILE:HG23	1:H:114:ARG:HH12	1.77	0.49
1:J:115:THR:HG21	1:J:124:ILE:HG23	1.95	0.49
1:H:140:THR:O	1:H:143:TYR:O	2.30	0.49
1:H:268:ASP:CG	1:H:270:ARG:HH11	2.19	0.48
1:C:144:GLY:HA3	8:C:780:HOH:O	2.12	0.48
1:B:58:MET:HE3	1:B:96:ILE:HG12	1.95	0.48
1:G:244:THR:O	1:J:512:THR:HB	2.12	0.48
1:J:60:GLU:HA	1:J:277:LEU:HD21	1.94	0.48
1:B:171:TYR:OH	1:B:219:ARG:HD2	2.14	0.48
1:G:105:LEU:HD21	1:G:136:MET:CE	2.43	0.48
1:I:171:TYR:OH	1:I:219:ARG:HD2	2.14	0.48
1:H:144:GLY:N	1:H:520:ARG:HH12	2.11	0.48
1:C:211:SER:O	1:C:214:LEU:HB2	2.14	0.48
1:G:343:ARG:HD2	1:G:349:SER:HA	1.95	0.48
1:H:51:GLN:HE22	1:H:104:SER:CB	2.27	0.48
1:I:508:GLY:HA2	1:I:511:LEU:HD22	1.96	0.48
1:J:474:THR:O	1:J:477:TRP:HB3	2.14	0.48
1:C:512:THR:HG21	1:E:245:ASP:HB3	1.96	0.48
1:D:314:TYR:CE2	1:D:372:VAL:HG13	2.49	0.48
1:H:105:LEU:HD21	1:H:136:MET:HE1	1.96	0.48
1:C:493:ARG:HD3	8:C:775:HOH:O	2.14	0.47
1:F:105:LEU:HD21	1:F:136:MET:CE	2.45	0.47
1:I:520:ARG:O	1:I:548:TRP:HB2	2.13	0.47
1:J:403:VAL:O	1:J:407:MET:HG2	2.13	0.47
1:G:329:ILE:HD13	1:G:376:MET:CE	2.44	0.47
1:E:268:ASP:OD2	1:E:270:ARG:NH1	2.47	0.47
1:A:219:ARG:HH22	1:A:486:GLU:CD	2.21	0.47
1:D:172:ASN:OD1	1:D:227:LYS:HE3	2.15	0.47
1:E:343:ARG:HD2	1:E:349:SER:HA	1.96	0.47
1:E:376:MET:HE3	1:E:379:GLU:HB2	1.96	0.47
1:F:185:ILE:HG23	1:F:202:VAL:HG13	1.96	0.47
1:F:464:THR:HG23	1:G:504:GLU:OE1	2.14	0.47
1:J:508:GLY:HA2	1:J:511:LEU:HD22	1.96	0.47
1:J:376:MET:HE3	1:J:379:GLU:CB	2.45	0.46
1:B:58:MET:HE1	1:B:100:PHE:CZ	2.49	0.46
1:J:377:ALA:O	1:J:380:VAL:HG22	2.15	0.46
1:H:308:LYS:HE3	1:H:444:THR:O	2.15	0.46
1:I:105:LEU:HD21	1:I:136:MET:HE1	1.97	0.46
1:F:51:GLN:NE2	1:F:104:SER:OG	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:314:TYR:HB3	1:J:327:VAL:HB	1.96	0.46
1:D:474:THR:O	1:D:477:TRP:HB3	2.16	0.46
1:A:369:ASN:HA	1:A:370:PRO:HD3	1.81	0.46
1:H:377:ALA:O	1:H:380:VAL:HG22	2.16	0.46
1:A:320:ALA:O	1:A:321:THR:CB	2.63	0.46
1:D:376:MET:HE3	1:D:379:GLU:HB2	1.98	0.45
1:C:140:THR:O	1:C:143:TYR:O	2.34	0.45
1:E:219:ARG:NH2	1:E:486:GLU:OE2	2.48	0.45
1:H:58:MET:HE2	1:H:59:MET:CE	2.46	0.45
1:G:171:TYR:OH	1:G:219:ARG:HD2	2.16	0.45
1:I:60:GLU:HA	1:I:277:LEU:HD21	1.99	0.45
1:B:508:GLY:HA2	1:B:511:LEU:HD22	1.97	0.45
1:B:512:THR:CG2	1:D:245:ASP:HB3	2.47	0.45
1:C:417:VAL:O	1:C:417:VAL:HG12	2.15	0.45
1:C:509:GLN:CD	1:C:509:GLN:H	2.23	0.45
1:F:219:ARG:NH2	1:F:486:GLU:OE2	2.50	0.45
1:B:72:GLN:HA	1:B:294:PHE:HB2	1.98	0.45
1:B:539:ILE:CD1	1:B:546:ASP:HB2	2.47	0.44
1:C:364:GLU:O	1:C:367:VAL:HG13	2.17	0.44
1:E:464:THR:HG22	1:E:467:GLN:H	1.80	0.44
1:I:219:ARG:HD3	1:I:554:TRP:CE2	2.51	0.44
1:G:49:GLN:HE21	1:G:197:ILE:HD12	1.82	0.44
1:C:58:MET:HE2	1:C:59:MET:CE	2.48	0.44
1:E:105:LEU:HD21	1:E:136:MET:HE1	1.98	0.44
1:D:292:SER:HA	1:D:342:PRO:HB2	1.99	0.44
1:G:74:MET:HE3	1:G:345:PRO:HA	1.98	0.44
1:D:51:GLN:NE2	1:D:103:GLN:HE21	2.16	0.44
1:H:152:GLY:HA2	1:H:153:LEU:HG	1.99	0.44
1:J:343:ARG:HD2	1:J:349:SER:HA	1.99	0.44
1:C:268:ASP:OD1	1:C:270:ARG:HD3	2.17	0.44
1:C:356:GLY:HA3	1:C:376:MET:O	2.18	0.44
1:I:496:TYR:HA	1:I:497:PRO:C	2.42	0.44
1:E:520:ARG:O	1:E:548:TRP:HB2	2.17	0.44
1:G:308:LYS:HE3	1:G:444:THR:O	2.18	0.44
1:A:403:VAL:O	1:A:407:MET:HG2	2.18	0.44
1:H:474:THR:O	1:H:477:TRP:HB3	2.18	0.44
1:I:356:GLY:HA3	1:I:376:MET:O	2.18	0.43
1:A:377:ALA:O	1:A:380:VAL:HG22	2.19	0.43
1:F:171:TYR:OH	1:F:219:ARG:HD2	2.18	0.43
1:H:413:LYS:O	1:H:414:LYS:HB2	2.17	0.43
1:G:508:GLY:HA2	1:G:511:LEU:HD22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:377:ALA:O	1:D:380:VAL:HG22	2.18	0.43
1:H:268:ASP:OD2	1:H:270:ARG:NH1	2.51	0.43
1:F:219:ARG:HH22	1:F:486:GLU:CD	2.25	0.43
1:B:462:GLY:HA3	1:B:467:GLN:HB3	2.00	0.43
1:C:307:PHE:HA	1:C:310:SER:O	2.19	0.43
1:C:481:PHE:HB3	7:C:611:EDO:H21	2.00	0.43
1:I:314:TYR:HB2	1:I:376:MET:CE	2.42	0.43
1:D:413:LYS:O	1:D:414:LYS:HB2	2.18	0.43
1:B:369:ASN:HA	1:B:370:PRO:HD3	1.76	0.43
1:G:535:TYR:O	1:G:539:ILE:HG12	2.19	0.43
1:A:496:TYR:HA	1:A:497:PRO:C	2.44	0.43
1:B:403:VAL:O	1:B:407:MET:HG2	2.19	0.43
1:A:256:THR:HA	1:A:391:SER:OG	2.19	0.42
1:F:210:ASN:HA	1:F:213:ARG:HD3	2.00	0.42
1:A:356:GLY:HA3	1:A:376:MET:O	2.18	0.42
1:I:308:LYS:HE3	1:I:444:THR:O	2.19	0.42
1:A:225:PRO:C	8:A:701:HOH:O	2.63	0.42
1:H:268:ASP:CG	1:H:270:ARG:NH1	2.78	0.42
1:H:496:TYR:HA	1:H:497:PRO:C	2.44	0.42
1:B:51:GLN:HE22	1:B:103:GLN:CB	2.32	0.42
1:F:462:GLY:HA3	1:F:467:GLN:HB3	2.01	0.42
1:G:478:ILE:HG22	7:G:608:EDO:H12	2.01	0.42
1:B:509:GLN:HG2	1:D:451:PHE:CE2	2.54	0.42
1:D:520:ARG:O	1:D:548:TRP:HB2	2.20	0.42
1:D:539:ILE:CD1	1:D:546:ASP:HB2	2.50	0.42
1:E:263:GLN:OE1	3:O:1:BGC:H6C1	2.19	0.42
1:C:474:THR:O	1:C:477:TRP:HB3	2.20	0.42
1:G:437:LEU:HD11	7:G:608:EDO:H21	2.02	0.42
1:H:410:ALA:HB1	1:H:415:TRP:CD1	2.54	0.42
1:I:369:ASN:HA	1:I:370:PRO:HD3	1.79	0.42
1:D:304:PRO:O	1:D:308:LYS:HD2	2.21	0.41
1:E:140:THR:O	1:E:167:GLN:NE2	2.53	0.41
1:E:219:ARG:HH22	1:E:486:GLU:CD	2.27	0.41
1:E:485:ALA:HB2	7:E:610:EDO:H22	2.02	0.41
1:H:376:MET:HE3	1:H:379:GLU:CB	2.50	0.41
1:H:210:ASN:HA	1:H:213:ARG:HD3	2.01	0.41
1:C:477:TRP:HB2	8:C:784:HOH:O	2.20	0.41
1:B:140:THR:O	1:B:167:GLN:NE2	2.53	0.41
1:D:320:ALA:O	1:D:321:THR:HB	2.21	0.41
1:E:417:VAL:O	1:E:417:VAL:CG1	2.69	0.41
1:J:72:GLN:HA	1:J:294:PHE:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:520:ARG:O	1:J:548:TRP:HB2	2.20	0.41
1:B:539:ILE:HD12	1:B:546:ASP:HB2	2.03	0.41
1:E:407:MET:HE1	1:E:417:VAL:HG13	2.03	0.41
1:I:368:ASN:HD22	1:I:368:ASN:HA	1.59	0.41
1:I:509:GLN:H	1:I:509:GLN:CD	2.27	0.41
1:F:58:MET:HE2	1:F:59:MET:HE1	2.02	0.41
1:G:76:CYS:O	1:G:77:TRP:C	2.64	0.41
1:B:376:MET:HE3	1:B:379:GLU:HB2	2.03	0.41
1:C:148:PHE:O	1:C:149:SER:C	2.64	0.41
1:H:509:GLN:HE21	1:H:509:GLN:HB2	1.71	0.41
1:I:376:MET:HE3	1:I:379:GLU:HG2	2.01	0.41
1:C:509:GLN:HG2	1:E:451:PHE:CE2	2.56	0.41
1:I:546:ASP:C	8:I:701:HOH:O	2.63	0.41
1:A:462:GLY:HA3	1:A:467:GLN:HB3	2.03	0.41
1:C:464:THR:HG22	1:C:466:ASN:N	2.36	0.41
1:G:451:PHE:CE2	1:J:509:GLN:HG2	2.56	0.41
1:I:358:ASP:OD1	1:I:375:THR:HG22	2.21	0.41
1:A:105:LEU:HD21	1:A:136:MET:HE1	2.03	0.41
1:C:464:THR:HG22	1:C:466:ASN:H	1.86	0.41
1:I:376:MET:HE3	1:I:379:GLU:CB	2.51	0.41
1:H:307:PHE:HA	1:H:310:SER:O	2.20	0.40
3:L:5:BGC:HC	3:L:6:BGC:C1	2.32	0.40
1:I:55:ASP:OD1	1:I:57:SER:HB3	2.21	0.40
1:J:292:SER:HA	1:J:342:PRO:HB2	2.03	0.40
1:J:144:GLY:HA2	1:J:552:LEU:HD22	2.03	0.40
1:H:144:GLY:N	1:H:520:ARG:NH1	2.69	0.40
1:E:496:TYR:HA	1:E:497:PRO:C	2.46	0.40
1:F:417:VAL:O	1:F:417:VAL:CG1	2.69	0.40
1:H:214:LEU:CD1	1:H:235:ALA:HB3	2.52	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	509/520 (98%)	487 (96%)	21 (4%)	1 (0%)	43	58
1	B	512/520 (98%)	492 (96%)	20 (4%)	0	100	100
1	C	508/520 (98%)	489 (96%)	19 (4%)	0	100	100
1	D	517/520 (99%)	500 (97%)	16 (3%)	1 (0%)	43	58
1	E	513/520 (99%)	493 (96%)	20 (4%)	0	100	100
1	F	510/520 (98%)	489 (96%)	20 (4%)	1 (0%)	43	58
1	G	508/520 (98%)	489 (96%)	19 (4%)	0	100	100
1	H	510/520 (98%)	483 (95%)	27 (5%)	0	100	100
1	I	504/520 (97%)	489 (97%)	14 (3%)	1 (0%)	43	58
1	J	508/520 (98%)	493 (97%)	14 (3%)	1 (0%)	43	58
All	All	5099/5200 (98%)	4904 (96%)	190 (4%)	5 (0%)	48	64

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	321	THR
1	F	189	LYS
1	A	321	THR
1	I	321	THR
1	J	144	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	436/441 (99%)	418 (96%)	18 (4%)	27	46
1	B	435/441 (99%)	417 (96%)	18 (4%)	27	46
1	C	435/441 (99%)	424 (98%)	11 (2%)	42	64
1	D	437/441 (99%)	417 (95%)	20 (5%)	24	41
1	E	438/441 (99%)	417 (95%)	21 (5%)	23	40
1	F	434/441 (98%)	415 (96%)	19 (4%)	25	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	430/441 (98%)	415 (96%)	15 (4%)	32	53
1	H	435/441 (99%)	420 (97%)	15 (3%)	32	54
1	I	430/441 (98%)	415 (96%)	15 (4%)	32	53
1	J	432/441 (98%)	421 (98%)	11 (2%)	42	64
All	All	4342/4410 (98%)	4179 (96%)	163 (4%)	29	49

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	LEU
1	A	117	GLU
1	A	160	PHE
1	A	214	LEU
1	A	330	THR
1	A	365	LEU
1	A	367	VAL
1	A	369	ASN
1	A	373	THR
1	A	375	THR
1	A	390	LYS
1	A	392	ASP
1	A	417	VAL
1	A	509	GLN
1	A	511	LEU
1	A	512	THR
1	A	515	THR
1	A	529	SER
1	B	108	ILE
1	B	112	GLN
1	B	115	THR
1	B	182	VAL
1	B	202	VAL
1	B	214	LEU
1	B	257	ILE
1	B	319	SER
1	B	365	LEU
1	B	367	VAL
1	B	375	THR
1	B	417	VAL
1	B	464	THR
1	B	504	GLU

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Mol	Chain	Res	Type
1	B	509	GLN
1	B	511	LEU
1	B	512	THR
1	B	515	THR
1	C	40	ASP
1	C	56	LEU
1	C	117	GLU
1	C	185	ILE
1	C	214	LEU
1	C	367	VAL
1	C	509	GLN
1	C	511	LEU
1	C	512	THR
1	C	529	SER
1	C	550	SER
1	D	40	ASP
1	D	56	LEU
1	D	112	GLN
1	D	117	GLU
1	D	122	VAL
1	D	182	VAL
1	D	191	LYS
1	D	214	LEU
1	D	257	ILE
1	D	322	SER
1	D	365	LEU
1	D	369	ASN
1	D	373	THR
1	D	414	LYS
1	D	509	GLN
1	D	511	LEU
1	D	512	THR
1	D	520	ARG
1	D	533	LYS
1	D	550	SER
1	E	40	ASP
1	E	56	LEU
1	E	57	SER
1	E	112	GLN
1	E	191	LYS
1	E	202	VAL
1	E	214	LEU

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Mol	Chain	Res	Type
1	E	277	LEU
1	E	319	SER
1	E	322	SER
1	E	367	VAL
1	E	375	THR
1	E	414	LYS
1	E	417	VAL
1	E	464	THR
1	E	511	LEU
1	E	512	THR
1	E	520	ARG
1	E	525	VAL
1	E	529	SER
1	E	557	GLU
1	F	56	LEU
1	F	98	THR
1	F	104	SER
1	F	112	GLN
1	F	202	VAL
1	F	214	LEU
1	F	290	LEU
1	F	319	SER
1	F	375	THR
1	F	414	LYS
1	F	417	VAL
1	F	437	LEU
1	F	509	GLN
1	F	511	LEU
1	F	512	THR
1	F	520	ARG
1	F	526	LEU
1	F	533	LYS
1	F	557	GLU
1	G	56	LEU
1	G	112	GLN
1	G	122	VAL
1	G	191	LYS
1	G	214	LEU
1	G	256	THR
1	G	290	LEU
1	G	319	SER
1	G	355	THR

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Mol	Chain	Res	Type
1	G	375	THR
1	G	390	LYS
1	G	417	VAL
1	G	511	LEU
1	G	512	THR
1	G	520	ARG
1	H	56	LEU
1	H	112	GLN
1	H	117	GLU
1	H	153	LEU
1	H	202	VAL
1	H	290	LEU
1	H	375	THR
1	H	414	LYS
1	H	415	TRP
1	H	417	VAL
1	H	464	THR
1	H	504	GLU
1	H	509	GLN
1	H	511	LEU
1	H	512	THR
1	I	56	LEU
1	I	112	GLN
1	I	185	ILE
1	I	202	VAL
1	I	214	LEU
1	I	245	ASP
1	I	367	VAL
1	I	368	ASN
1	I	417	VAL
1	I	511	LEU
1	I	512	THR
1	I	515	THR
1	I	525	VAL
1	I	550	SER
1	I	557	GLU
1	J	56	LEU
1	J	112	GLN
1	J	143	TYR
1	J	214	LEU
1	J	248	SER
1	J	355	THR

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Mol	Chain	Res	Type
1	J	367	VAL
1	J	509	GLN
1	J	511	LEU
1	J	515	THR
1	J	557	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	161	ASN
1	A	558	ASN
1	B	51	GLN
1	B	81	ASN
1	B	536	ASN
1	C	51	GLN
1	C	81	ASN
1	C	428	GLN
1	C	490	ASN
1	D	81	ASN
1	D	103	GLN
1	D	125	ASN
1	D	161	ASN
1	D	369	ASN
1	D	480	HIS
1	D	536	ASN
1	E	51	GLN
1	E	66	HIS
1	E	103	GLN
1	E	125	ASN
1	E	206	GLN
1	E	393	ASN
1	E	428	GLN
1	E	509	GLN
1	E	536	ASN
1	F	51	GLN
1	F	66	HIS
1	F	81	ASN
1	F	112	GLN
1	F	161	ASN
1	F	331	GLN
1	F	440	ASN

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Mol	Chain	Res	Type
1	F	558	ASN
1	G	44	GLN
1	G	112	GLN
1	G	125	ASN
1	G	161	ASN
1	G	428	GLN
1	G	536	ASN
1	H	51	GLN
1	H	66	HIS
1	H	81	ASN
1	H	103	GLN
1	H	509	GLN
1	H	531	ASN
1	I	66	HIS
1	I	81	ASN
1	I	112	GLN
1	I	125	ASN
1	I	368	ASN
1	J	81	ASN
1	J	112	GLN
1	J	125	ASN
1	J	536	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 ⓘ

59 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	K	1	2	12,12,12	0.45	0	17,17,17	0.64	0
2	BGC	K	2	2	11,11,12	0.28	0	15,15,17	0.78	0
2	BGC	K	3	2	11,11,12	0.54	0	15,15,17	0.98	1 (6%)
2	BGC	K	4	2	11,11,12	0.55	0	15,15,17	0.73	0
2	BGC	K	5	2	11,11,12	0.57	0	15,15,17	1.21	1 (6%)
3	BGC	L	1	3	12,12,12	0.54	0	17,17,17	1.06	1 (5%)
3	BGC	L	2	3	11,11,12	0.30	0	15,15,17	0.79	0
3	BGC	L	3	3	11,11,12	0.55	0	15,15,17	1.91	2 (13%)
3	BGC	L	4	3	11,11,12	0.44	0	15,15,17	0.79	0
3	BGC	L	5	3	11,11,12	0.36	0	15,15,17	0.98	1 (6%)
3	BGC	L	6	3	11,11,12	0.65	0	15,15,17	1.05	1 (6%)
3	BGC	M	1	3	12,12,12	0.51	0	17,17,17	0.87	0
3	BGC	M	2	3	11,11,12	0.28	0	15,15,17	0.80	0
3	BGC	M	3	3	11,11,12	0.63	0	15,15,17	0.76	0
3	BGC	M	4	3	11,11,12	0.38	0	15,15,17	0.73	0
3	BGC	M	5	3	11,11,12	0.37	0	15,15,17	0.71	0
3	BGC	M	6	3	11,11,12	0.43	0	15,15,17	0.90	1 (6%)
3	BGC	N	1	3	12,12,12	0.48	0	17,17,17	0.90	1 (5%)
3	BGC	N	2	3	11,11,12	0.32	0	15,15,17	1.08	1 (6%)
3	BGC	N	3	3	11,11,12	0.42	0	15,15,17	0.87	0
3	BGC	N	4	3	11,11,12	0.30	0	15,15,17	0.74	0
3	BGC	N	5	3	11,11,12	0.50	0	15,15,17	0.71	0
3	BGC	N	6	3	11,11,12	0.40	0	15,15,17	0.95	0
3	BGC	O	1	3	12,12,12	0.57	0	17,17,17	0.95	0
3	BGC	O	2	3	11,11,12	0.38	0	15,15,17	1.05	2 (13%)
3	BGC	O	3	3	11,11,12	0.35	0	15,15,17	0.74	1 (6%)
3	BGC	O	4	3	11,11,12	0.37	0	15,15,17	0.61	0
3	BGC	O	5	3	11,11,12	0.47	0	15,15,17	1.18	2 (13%)
3	BGC	O	6	3	11,11,12	0.32	0	15,15,17	0.59	0
3	BGC	P	1	3	12,12,12	0.53	0	17,17,17	0.88	0
3	BGC	P	2	3	11,11,12	0.39	0	15,15,17	0.48	0
3	BGC	P	3	3	11,11,12	0.29	0	15,15,17	0.79	0
3	BGC	P	4	3	11,11,12	0.50	0	15,15,17	0.76	1 (6%)
3	BGC	P	5	3	11,11,12	0.39	0	15,15,17	1.12	1 (6%)
3	BGC	P	6	3	11,11,12	0.40	0	15,15,17	0.66	0
3	BGC	Q	1	3	12,12,12	0.48	0	17,17,17	0.58	0
3	BGC	Q	2	3	11,11,12	0.38	0	15,15,17	0.68	0
3	BGC	Q	3	3	11,11,12	0.24	0	15,15,17	0.95	1 (6%)
3	BGC	Q	4	3	11,11,12	0.31	0	15,15,17	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BGC	Q	5	3	11,11,12	0.39	0	15,15,17	1.25	1 (6%)
3	BGC	Q	6	3	11,11,12	0.41	0	15,15,17	0.87	0
3	BGC	R	1	3	12,12,12	0.55	0	17,17,17	1.03	0
3	BGC	R	2	3	11,11,12	0.67	0	15,15,17	0.63	0
3	BGC	R	3	3	11,11,12	0.48	0	15,15,17	0.61	0
3	BGC	R	4	3	11,11,12	0.37	0	15,15,17	0.68	0
3	BGC	R	5	3	11,11,12	0.38	0	15,15,17	1.38	1 (6%)
3	BGC	R	6	3	11,11,12	0.33	0	15,15,17	0.76	0
3	BGC	S	1	3	12,12,12	0.46	0	17,17,17	0.84	1 (5%)
3	BGC	S	2	3	11,11,12	0.36	0	15,15,17	1.70	2 (13%)
3	BGC	S	3	3	11,11,12	0.40	0	15,15,17	0.43	0
3	BGC	S	4	3	11,11,12	0.24	0	15,15,17	0.79	0
3	BGC	S	5	3	11,11,12	0.48	0	15,15,17	0.80	0
3	BGC	S	6	3	11,11,12	0.35	0	15,15,17	0.94	0
3	BGC	T	1	3	12,12,12	0.48	0	17,17,17	0.81	1 (5%)
3	BGC	T	2	3	11,11,12	0.25	0	15,15,17	1.22	2 (13%)
3	BGC	T	3	3	11,11,12	0.60	0	15,15,17	0.60	0
3	BGC	T	4	3	11,11,12	0.35	0	15,15,17	0.74	0
3	BGC	T	5	3	11,11,12	0.28	0	15,15,17	1.16	2 (13%)
3	BGC	T	6	3	11,11,12	0.36	0	15,15,17	0.81	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	K	1	2	-	1/2/22/22	0/1/1/1
2	BGC	K	2	2	-	0/2/19/22	0/1/1/1
2	BGC	K	3	2	-	0/2/19/22	0/1/1/1
2	BGC	K	4	2	-	0/2/19/22	0/1/1/1
2	BGC	K	5	2	-	2/2/19/22	0/1/1/1
3	BGC	L	1	3	-	0/2/22/22	0/1/1/1
3	BGC	L	2	3	-	0/2/19/22	0/1/1/1
3	BGC	L	3	3	-	1/2/19/22	0/1/1/1
3	BGC	L	4	3	-	1/2/19/22	0/1/1/1
3	BGC	L	5	3	-	2/2/19/22	0/1/1/1
3	BGC	L	6	3	-	1/2/19/22	0/1/1/1
3	BGC	M	1	3	-	2/2/22/22	0/1/1/1
3	BGC	M	2	3	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BGC	M	3	3	-	0/2/19/22	0/1/1/1
3	BGC	M	4	3	-	1/2/19/22	0/1/1/1
3	BGC	M	5	3	-	2/2/19/22	0/1/1/1
3	BGC	M	6	3	-	2/2/19/22	0/1/1/1
3	BGC	N	1	3	-	2/2/22/22	0/1/1/1
3	BGC	N	2	3	-	0/2/19/22	0/1/1/1
3	BGC	N	3	3	-	0/2/19/22	0/1/1/1
3	BGC	N	4	3	-	0/2/19/22	0/1/1/1
3	BGC	N	5	3	-	2/2/19/22	0/1/1/1
3	BGC	N	6	3	-	2/2/19/22	0/1/1/1
3	BGC	O	1	3	-	2/2/22/22	0/1/1/1
3	BGC	O	2	3	-	0/2/19/22	0/1/1/1
3	BGC	O	3	3	-	0/2/19/22	0/1/1/1
3	BGC	O	4	3	-	1/2/19/22	0/1/1/1
3	BGC	O	5	3	-	0/2/19/22	0/1/1/1
3	BGC	O	6	3	-	0/2/19/22	0/1/1/1
3	BGC	P	1	3	-	2/2/22/22	0/1/1/1
3	BGC	P	2	3	-	0/2/19/22	0/1/1/1
3	BGC	P	3	3	-	2/2/19/22	0/1/1/1
3	BGC	P	4	3	-	0/2/19/22	0/1/1/1
3	BGC	P	5	3	-	2/2/19/22	0/1/1/1
3	BGC	P	6	3	-	0/2/19/22	0/1/1/1
3	BGC	Q	1	3	-	0/2/22/22	0/1/1/1
3	BGC	Q	2	3	-	0/2/19/22	0/1/1/1
3	BGC	Q	3	3	-	2/2/19/22	0/1/1/1
3	BGC	Q	4	3	-	0/2/19/22	0/1/1/1
3	BGC	Q	5	3	-	1/2/19/22	0/1/1/1
3	BGC	Q	6	3	-	1/2/19/22	0/1/1/1
3	BGC	R	1	3	-	0/2/22/22	0/1/1/1
3	BGC	R	2	3	-	0/2/19/22	0/1/1/1
3	BGC	R	3	3	-	2/2/19/22	0/1/1/1
3	BGC	R	4	3	-	0/2/19/22	0/1/1/1
3	BGC	R	5	3	-	2/2/19/22	0/1/1/1
3	BGC	R	6	3	-	2/2/19/22	0/1/1/1
3	BGC	S	1	3	-	2/2/22/22	0/1/1/1
3	BGC	S	2	3	-	2/2/19/22	0/1/1/1
3	BGC	S	3	3	-	0/2/19/22	0/1/1/1
3	BGC	S	4	3	-	0/2/19/22	0/1/1/1
3	BGC	S	5	3	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BGC	S	6	3	-	2/2/19/22	0/1/1/1
3	BGC	T	1	3	-	1/2/22/22	0/1/1/1
3	BGC	T	2	3	-	0/2/19/22	0/1/1/1
3	BGC	T	3	3	-	0/2/19/22	0/1/1/1
3	BGC	T	4	3	-	0/2/19/22	0/1/1/1
3	BGC	T	5	3	-	2/2/19/22	0/1/1/1
3	BGC	T	6	3	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	3	BGC	C1-O5-C5	5.82	119.98	112.19
3	S	2	BGC	C1-O5-C5	5.35	119.35	112.19
3	R	5	BGC	C1-O5-C5	3.95	117.48	112.19
3	T	2	BGC	C1-O5-C5	3.41	116.75	112.19
3	Q	5	BGC	C1-O5-C5	3.39	116.73	112.19
2	K	5	BGC	C1-O5-C5	3.13	116.39	112.19
3	P	5	BGC	C1-O5-C5	3.06	116.28	112.19
3	O	5	BGC	C1-O5-C5	2.85	116.00	112.19
3	L	3	BGC	O5-C5-C6	-2.82	102.17	107.66
3	O	2	BGC	C1-C2-C3	2.81	113.74	109.64
3	L	1	BGC	O5-C1-C2	-2.81	105.36	110.30
2	K	3	BGC	C1-C2-C3	2.55	113.35	109.64
3	M	6	BGC	O5-C5-C6	2.50	112.53	107.66
3	L	5	BGC	C1-O5-C5	2.41	115.41	112.19
3	L	6	BGC	O5-C5-C6	2.40	112.34	107.66
3	N	2	BGC	C1-O5-C5	2.39	115.39	112.19
3	S	1	BGC	C4-C3-C2	-2.31	106.77	110.83
3	N	1	BGC	O5-C1-C2	-2.29	106.27	110.30
3	T	2	BGC	C6-C5-C4	-2.28	107.41	113.02
3	P	4	BGC	C1-C2-C3	2.27	112.95	109.64
3	O	3	BGC	C1-O5-C5	2.22	115.16	112.19
3	T	5	BGC	C1-O5-C5	2.18	115.11	112.19
3	T	5	BGC	C6-C5-C4	-2.18	107.66	113.02
3	O	5	BGC	C6-C5-C4	-2.13	107.78	113.02
3	T	1	BGC	C4-C3-C2	-2.08	107.17	110.83
3	O	2	BGC	C1-O5-C5	2.08	114.98	112.19
3	S	2	BGC	C6-C5-C4	-2.04	108.01	113.02
3	Q	3	BGC	C6-C5-C4	-2.01	108.09	113.02

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	R	6	BGC	O5-C5-C6-O6
3	M	5	BGC	O5-C5-C6-O6
3	S	6	BGC	O5-C5-C6-O6
2	K	5	BGC	O5-C5-C6-O6
3	P	3	BGC	O5-C5-C6-O6
3	N	1	BGC	C4-C5-C6-O6
3	R	6	BGC	C4-C5-C6-O6
3	M	5	BGC	C4-C5-C6-O6
3	N	1	BGC	O5-C5-C6-O6
3	N	5	BGC	O5-C5-C6-O6
3	O	1	BGC	O5-C5-C6-O6
3	S	1	BGC	O5-C5-C6-O6
3	S	2	BGC	O5-C5-C6-O6
3	O	1	BGC	C4-C5-C6-O6
3	N	5	BGC	C4-C5-C6-O6
3	S	6	BGC	C4-C5-C6-O6
3	M	1	BGC	C4-C5-C6-O6
2	K	5	BGC	C4-C5-C6-O6
3	R	3	BGC	C4-C5-C6-O6
3	S	1	BGC	C4-C5-C6-O6
3	L	5	BGC	O5-C5-C6-O6
3	S	2	BGC	C4-C5-C6-O6
3	M	6	BGC	O5-C5-C6-O6
3	T	5	BGC	O5-C5-C6-O6
3	R	5	BGC	C4-C5-C6-O6
3	M	1	BGC	O5-C5-C6-O6
3	P	3	BGC	C4-C5-C6-O6
3	R	3	BGC	O5-C5-C6-O6
3	M	2	BGC	O5-C5-C6-O6
3	P	5	BGC	C4-C5-C6-O6
3	Q	3	BGC	O5-C5-C6-O6
3	S	5	BGC	O5-C5-C6-O6
3	N	6	BGC	O5-C5-C6-O6
3	N	6	BGC	C4-C5-C6-O6
3	R	5	BGC	O5-C5-C6-O6
3	T	1	BGC	O5-C5-C6-O6
3	Q	6	BGC	O5-C5-C6-O6
3	L	3	BGC	O5-C5-C6-O6
3	P	1	BGC	C4-C5-C6-O6
3	M	4	BGC	O5-C5-C6-O6
3	L	5	BGC	C4-C5-C6-O6
3	M	6	BGC	C4-C5-C6-O6

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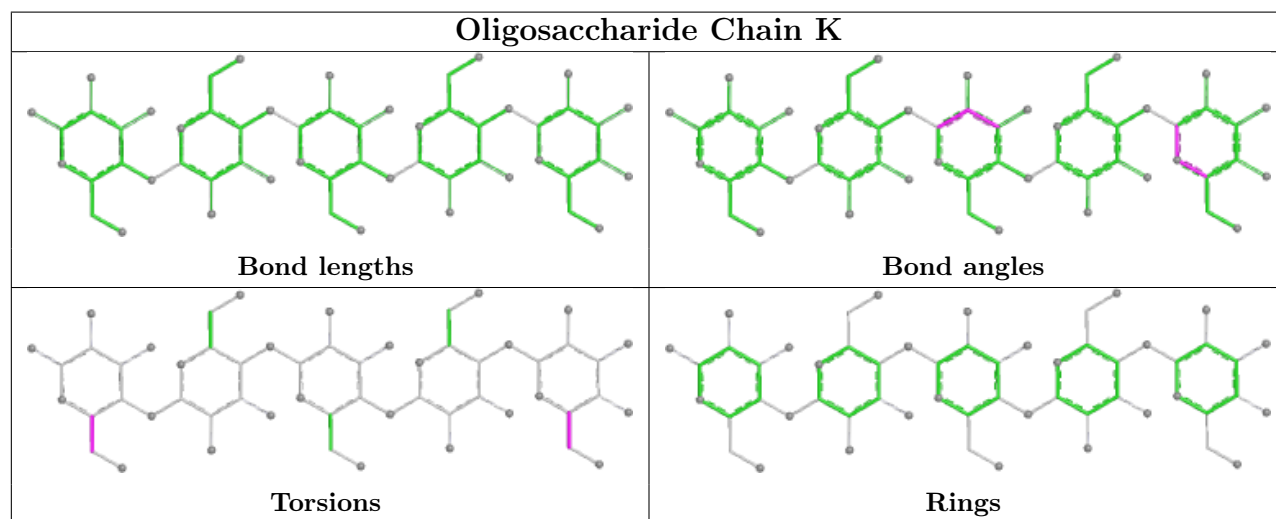
Mol	Chain	Res	Type	Atoms
3	T	5	BGC	C4-C5-C6-O6
3	Q	5	BGC	C4-C5-C6-O6
3	T	6	BGC	O5-C5-C6-O6
3	P	5	BGC	O5-C5-C6-O6
3	L	6	BGC	O5-C5-C6-O6
2	K	1	BGC	C4-C5-C6-O6
3	O	4	BGC	C4-C5-C6-O6
3	P	1	BGC	O5-C5-C6-O6
3	L	4	BGC	O5-C5-C6-O6
3	M	2	BGC	C4-C5-C6-O6
3	Q	3	BGC	C4-C5-C6-O6

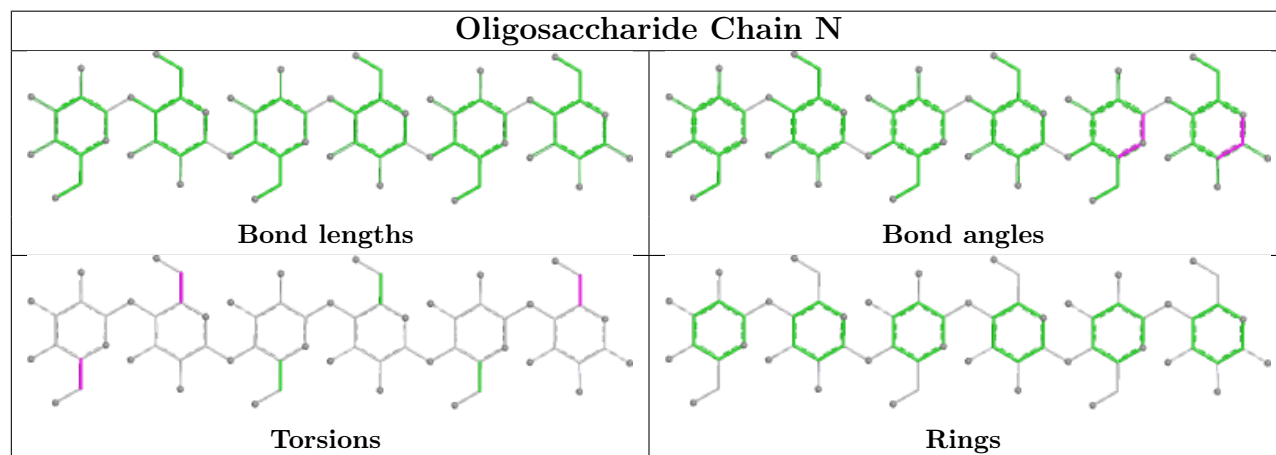
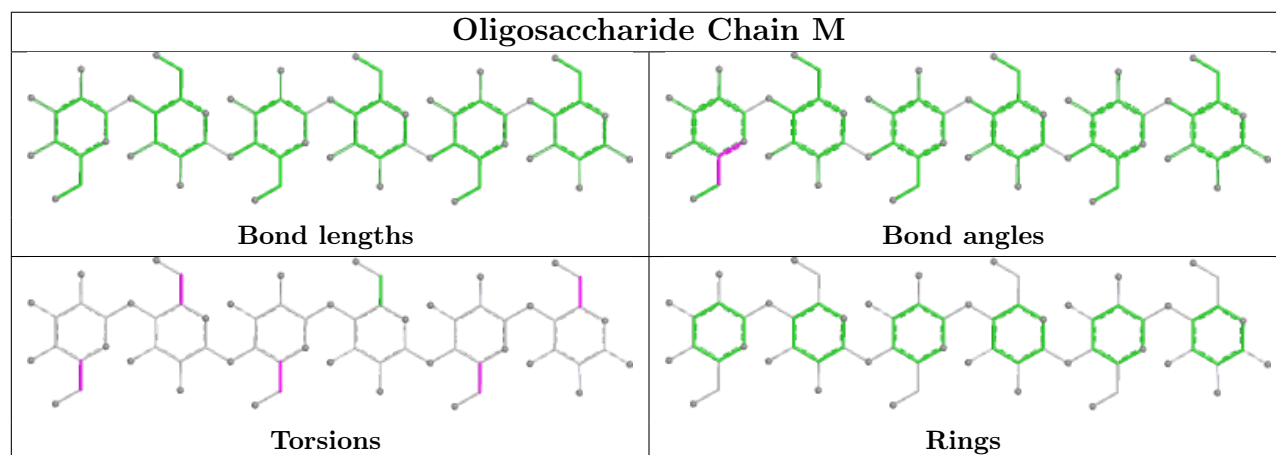
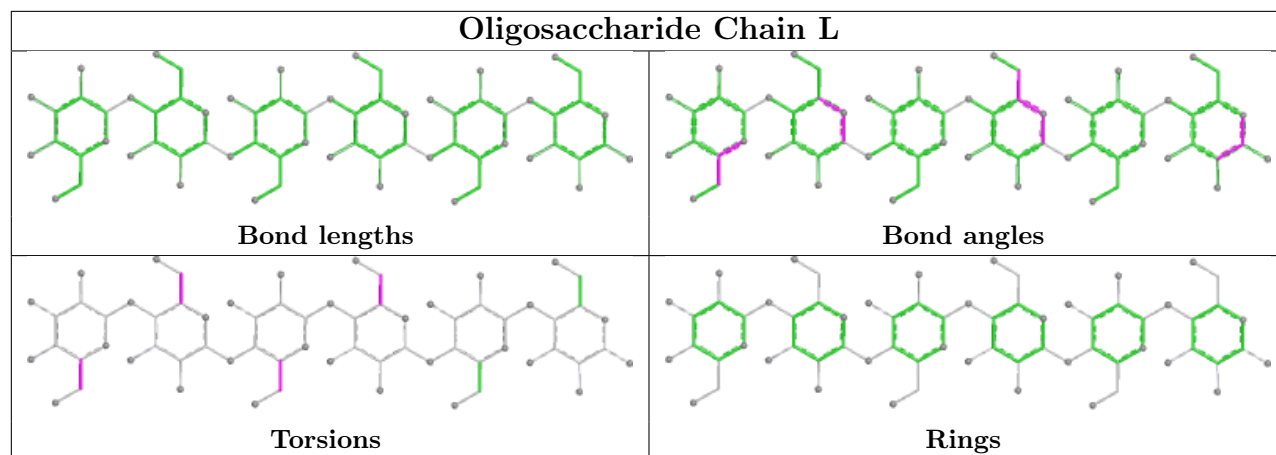
There are no ring outliers.

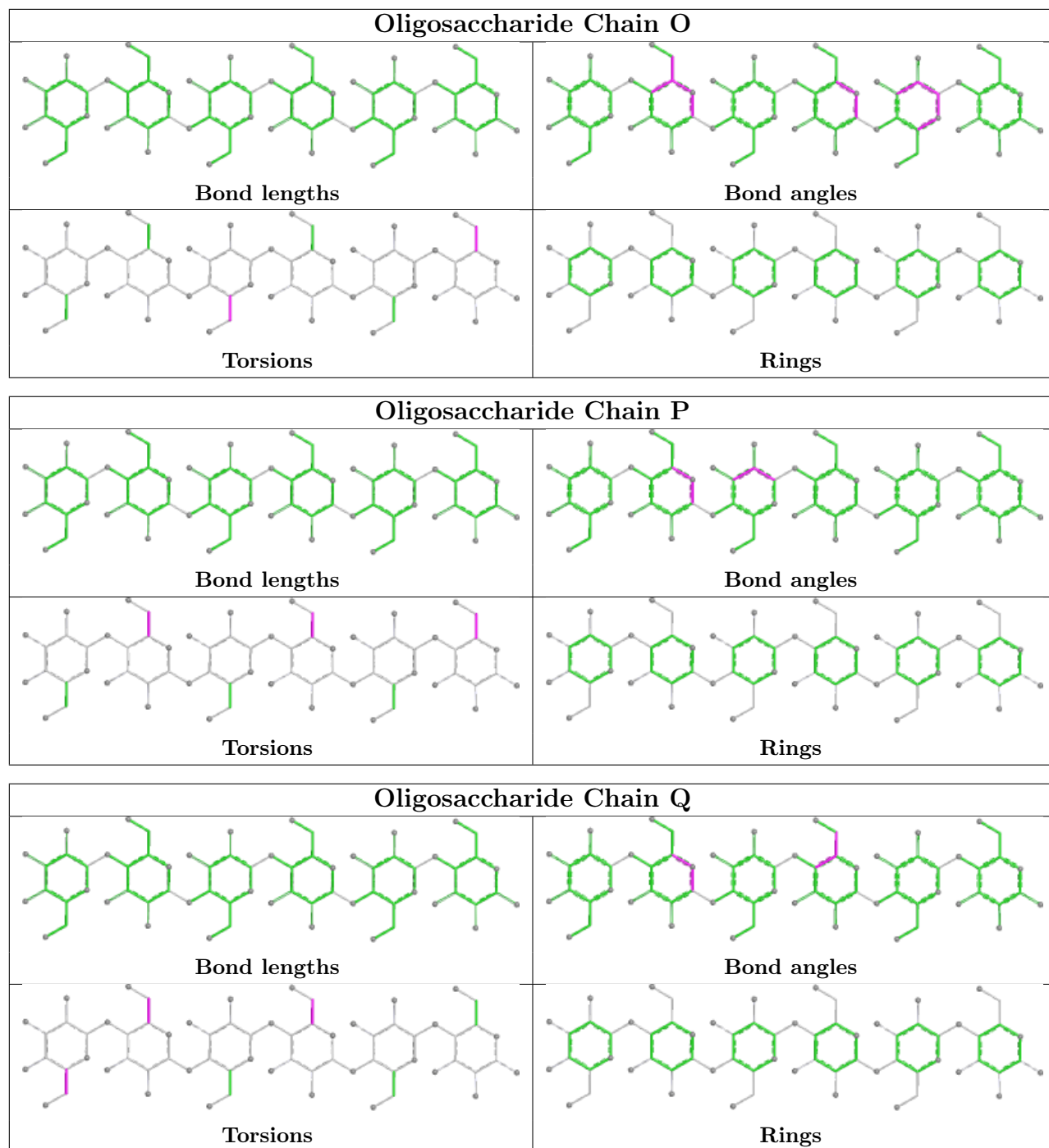
3 monomers are involved in 2 short contacts:

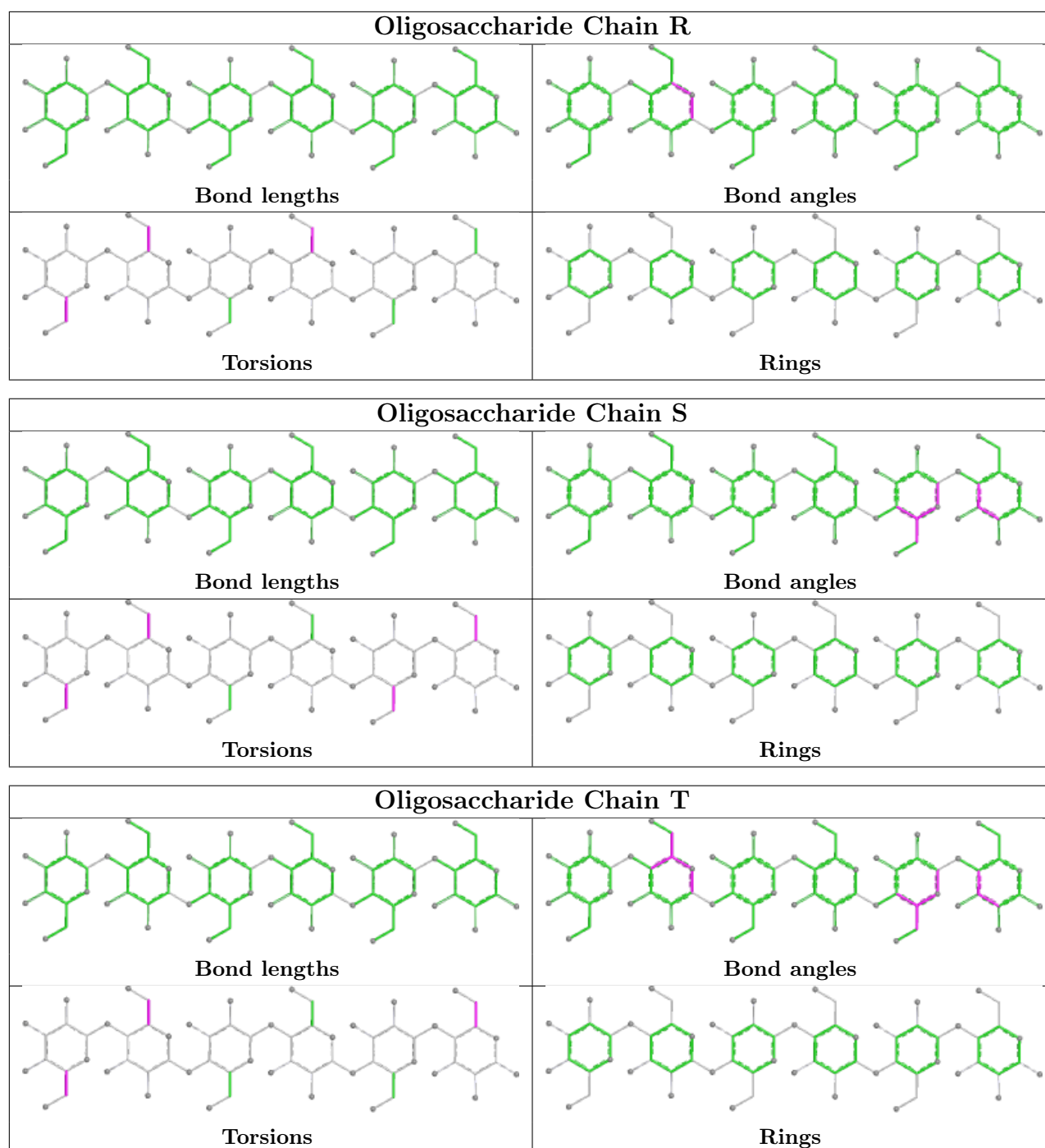
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	O	1	BGC	1	0
3	L	6	BGC	1	0
3	L	5	BGC	1	0

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 42 ligands modelled in this entry, 10 are monoatomic - leaving 32 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	$\# Z > 2$
7	EDO	G	608	-	3,3,3	0.73	0	2,2,2	0.73	0
7	EDO	G	610	-	3,3,3	0.46	0	2,2,2	0.30	0
7	EDO	E	609	-	3,3,3	0.50	0	2,2,2	0.22	0
7	EDO	E	611	-	3,3,3	0.47	0	2,2,2	0.21	0
7	EDO	I	609	-	3,3,3	0.49	0	2,2,2	0.24	0
7	EDO	G	611	-	3,3,3	0.45	0	2,2,2	0.28	0
7	EDO	D	609	-	3,3,3	0.42	0	2,2,2	0.28	0
6	PEG	B	610	-	6,6,6	0.49	0	5,5,5	0.19	0
6	PEG	A	608	-	6,6,6	0.58	0	5,5,5	0.76	0
7	EDO	A	610	-	3,3,3	0.45	0	2,2,2	0.26	0
5	ACT	F	608	-	3,3,3	0.80	0	3,3,3	0.81	0
5	ACT	C	608	-	3,3,3	0.77	0	3,3,3	0.79	0
7	EDO	H	609	-	3,3,3	0.42	0	2,2,2	0.31	0
7	EDO	E	612	-	3,3,3	0.49	0	2,2,2	0.23	0
5	ACT	B	608	-	3,3,3	0.92	0	3,3,3	0.51	0
5	ACT	A	607	-	3,3,3	0.77	0	3,3,3	0.67	0
7	EDO	E	610	-	3,3,3	0.51	0	2,2,2	0.35	0
7	EDO	G	609	-	3,3,3	0.47	0	2,2,2	0.24	0
5	ACT	H	608	-	3,3,3	0.82	0	3,3,3	0.75	0
5	ACT	I	608	-	3,3,3	0.82	0	3,3,3	0.65	0
5	ACT	D	608	-	3,3,3	0.77	0	3,3,3	0.89	0
6	PEG	J	609	-	6,6,6	0.45	0	5,5,5	0.29	0
7	EDO	B	612	-	3,3,3	0.42	0	2,2,2	0.30	0
7	EDO	C	609	-	3,3,3	0.46	0	2,2,2	0.26	0
7	EDO	G	612	-	3,3,3	0.45	0	2,2,2	0.38	0
7	EDO	C	610	-	3,3,3	0.42	0	2,2,2	0.30	0
5	ACT	J	608	-	3,3,3	0.82	0	3,3,3	0.84	0
5	ACT	E	608	-	3,3,3	0.81	0	3,3,3	0.74	0
6	PEG	A	609	-	6,6,6	0.49	0	5,5,5	0.17	0
6	PEG	B	609	-	6,6,6	0.54	0	5,5,5	0.28	0
7	EDO	C	611	-	3,3,3	0.46	0	2,2,2	0.10	0
7	EDO	B	611	-	3,3,3	0.43	0	2,2,2	0.20	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
7	EDO	G	608	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	G	610	-	-	0/1/1/1	-
7	EDO	E	609	-	-	0/1/1/1	-
7	EDO	E	611	-	-	0/1/1/1	-
7	EDO	I	609	-	-	1/1/1/1	-
7	EDO	G	611	-	-	1/1/1/1	-
7	EDO	D	609	-	-	1/1/1/1	-
6	PEG	B	610	-	-	2/4/4/4	-
6	PEG	A	608	-	-	2/4/4/4	-
7	EDO	A	610	-	-	1/1/1/1	-
7	EDO	H	609	-	-	1/1/1/1	-
7	EDO	E	612	-	-	1/1/1/1	-
7	EDO	E	610	-	-	1/1/1/1	-
7	EDO	G	609	-	-	1/1/1/1	-
6	PEG	J	609	-	-	2/4/4/4	-
7	EDO	B	612	-	-	0/1/1/1	-
7	EDO	C	609	-	-	0/1/1/1	-
7	EDO	G	612	-	-	0/1/1/1	-
7	EDO	C	610	-	-	1/1/1/1	-
6	PEG	A	609	-	-	2/4/4/4	-
6	PEG	B	609	-	-	2/4/4/4	-
7	EDO	C	611	-	-	1/1/1/1	-
7	EDO	B	611	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	J	609	PEG	O1-C1-C2-O2
6	A	608	PEG	O2-C3-C4-O4
6	A	609	PEG	O2-C3-C4-O4
7	C	611	EDO	O1-C1-C2-O2
7	E	610	EDO	O1-C1-C2-O2
7	E	612	EDO	O1-C1-C2-O2
7	I	609	EDO	O1-C1-C2-O2
7	A	610	EDO	O1-C1-C2-O2
7	B	611	EDO	O1-C1-C2-O2
7	G	609	EDO	O1-C1-C2-O2
7	G	611	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
6	A	609	PEG	O1-C1-C2-O2
6	B	610	PEG	O1-C1-C2-O2
7	D	609	EDO	O1-C1-C2-O2
7	C	610	EDO	O1-C1-C2-O2
6	B	610	PEG	C4-C3-O2-C2
6	B	609	PEG	O1-C1-C2-O2
7	H	609	EDO	O1-C1-C2-O2
6	A	608	PEG	C1-C2-O2-C3
6	J	609	PEG	C4-C3-O2-C2
6	B	609	PEG	C4-C3-O2-C2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	608	EDO	2	0
7	E	610	EDO	1	0
7	C	611	EDO	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	513/520 (98%)	-0.37	3 (0%) 85 83	19, 30, 53, 79	0
1	B	516/520 (99%)	-0.50	3 (0%) 85 83	16, 27, 46, 78	0
1	C	512/520 (98%)	-0.30	3 (0%) 85 83	19, 32, 58, 87	0
1	D	519/520 (99%)	-0.37	6 (1%) 76 73	18, 34, 55, 79	0
1	E	517/520 (99%)	-0.31	3 (0%) 85 83	19, 31, 52, 75	0
1	F	514/520 (98%)	-0.23	2 (0%) 88 86	20, 39, 63, 81	0
1	G	512/520 (98%)	-0.36	3 (0%) 85 83	21, 32, 56, 72	0
1	H	514/520 (98%)	-0.24	2 (0%) 88 86	20, 35, 56, 76	0
1	I	510/520 (98%)	-0.19	3 (0%) 85 83	24, 39, 59, 70	0
1	J	512/520 (98%)	-0.30	4 (0%) 82 80	19, 34, 58, 85	0
All	All	5139/5200 (98%)	-0.32	32 (0%) 85 83	16, 33, 58, 87	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	39	ILE	6.0
1	E	39	ILE	5.9
1	A	39	ILE	5.2
1	H	39	ILE	4.9
1	H	153	LEU	4.6
1	I	152	GLY	4.2
1	E	154	GLY	3.7
1	J	152	GLY	3.4
1	J	160	PHE	3.3
1	I	119	ALA	3.2
1	I	160	PHE	3.0
1	C	152	GLY	3.0
1	D	533	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	158	GLY	2.7
1	D	156	LEU	2.6
1	F	160	PHE	2.5
1	J	40	ASP	2.5
1	A	530	TYR	2.5
1	C	530	TYR	2.4
1	F	462	GLY	2.4
1	A	160	PHE	2.4
1	D	284	ALA	2.4
1	G	153	LEU	2.3
1	G	530	TYR	2.3
1	B	155	PHE	2.2
1	D	160	PHE	2.2
1	B	160	PHE	2.1
1	D	155	PHE	2.1
1	D	119	ALA	2.1
1	J	263	GLN	2.1
1	B	159	LYS	2.1
1	G	462	GLY	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, 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
3	BGC	O	1	12/12	0.80	0.12	53,63,71,75	0
3	BGC	M	1	12/12	0.83	0.12	54,68,73,74	0
2	BGC	K	1	12/12	0.85	0.11	50,59,66,66	0
3	BGC	P	1	12/12	0.85	0.11	61,67,71,76	0
3	BGC	R	2	11/12	0.85	0.12	49,53,57,57	0
3	BGC	S	1	12/12	0.85	0.11	51,62,72,74	0
3	BGC	T	1	12/12	0.85	0.11	53,57,64,68	0
3	BGC	L	1	12/12	0.86	0.11	53,58,62,65	0
3	BGC	N	1	12/12	0.86	0.11	54,62,64,71	0

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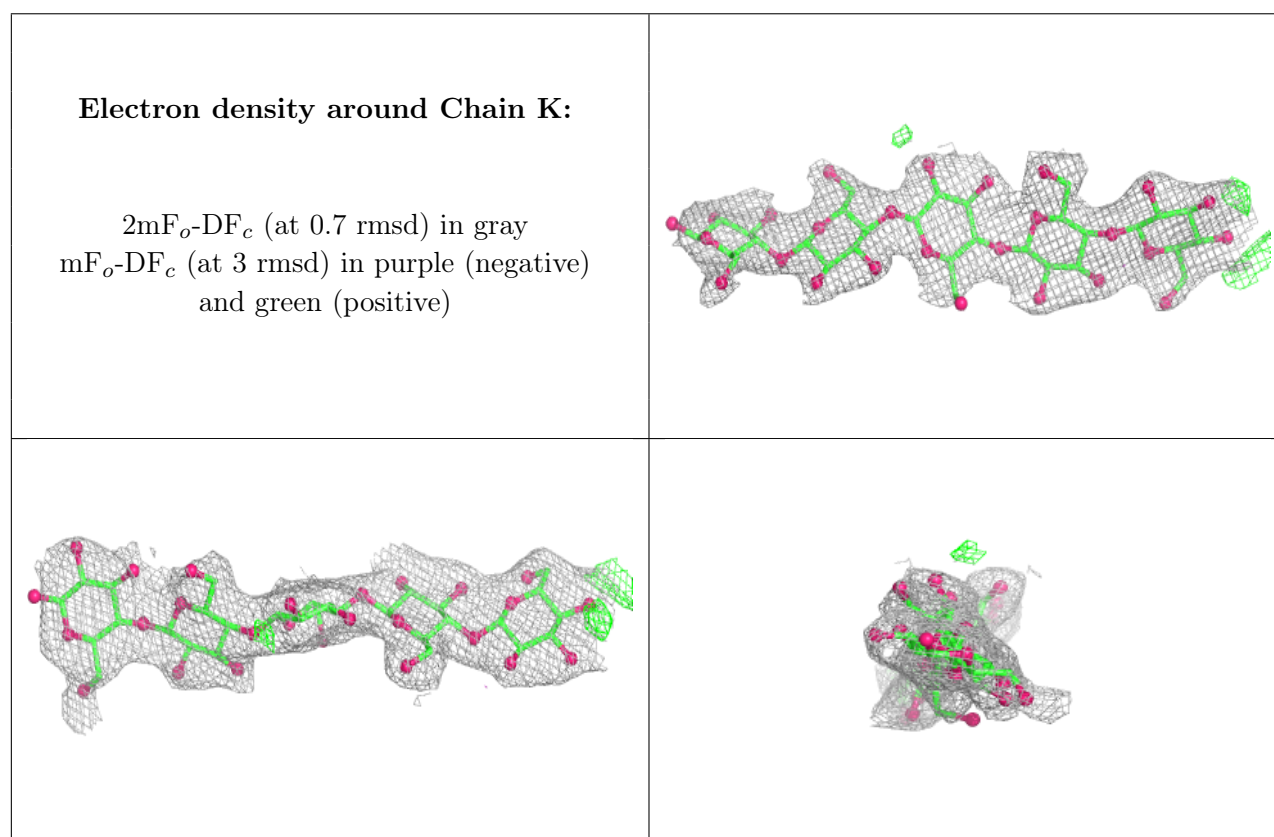
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BGC	R	1	12/12	0.86	0.10	57,63,66,66	0
3	BGC	Q	1	12/12	0.87	0.11	56,59,64,65	0
3	BGC	P	6	11/12	0.88	0.12	63,68,75,76	0
3	BGC	M	2	11/12	0.88	0.11	44,47,58,64	0
3	BGC	N	2	11/12	0.88	0.10	53,55,58,60	0
3	BGC	P	3	11/12	0.89	0.11	60,62,68,74	0
3	BGC	T	2	11/12	0.89	0.11	41,48,52,62	0
3	BGC	L	2	11/12	0.90	0.10	40,43,50,57	0
3	BGC	L	6	11/12	0.91	0.10	42,47,51,53	0
3	BGC	P	4	11/12	0.91	0.09	52,56,59,59	0
3	BGC	N	6	11/12	0.91	0.10	53,58,63,65	0
3	BGC	O	2	11/12	0.92	0.10	43,51,57,58	0
3	BGC	R	6	11/12	0.92	0.09	50,54,60,60	0
2	BGC	K	5	11/12	0.92	0.08	38,42,48,50	0
3	BGC	P	2	11/12	0.92	0.09	49,57,60,61	0
3	BGC	N	4	11/12	0.92	0.08	46,52,57,58	0
3	BGC	T	5	11/12	0.92	0.08	36,39,46,48	0
3	BGC	Q	2	11/12	0.93	0.09	44,46,49,54	0
3	BGC	Q	3	11/12	0.93	0.09	37,41,48,59	0
2	BGC	K	3	11/12	0.93	0.09	37,45,53,58	0
3	BGC	N	3	11/12	0.93	0.07	46,50,52,54	0
3	BGC	R	3	11/12	0.93	0.08	46,47,57,59	0
2	BGC	K	2	11/12	0.93	0.08	47,49,53,55	0
3	BGC	L	3	11/12	0.93	0.07	33,35,42,43	0
3	BGC	S	2	11/12	0.93	0.09	42,45,51,60	0
3	BGC	S	5	11/12	0.93	0.08	39,43,46,49	0
3	BGC	P	5	11/12	0.93	0.09	56,60,66,70	0
3	BGC	M	3	11/12	0.93	0.08	40,43,45,47	0
3	BGC	L	5	11/12	0.93	0.08	34,38,42,46	0
3	BGC	S	4	11/12	0.94	0.07	36,38,42,45	0
3	BGC	O	6	11/12	0.94	0.08	38,40,43,45	0
3	BGC	Q	6	11/12	0.94	0.09	41,44,49,51	0
3	BGC	M	6	11/12	0.94	0.08	44,48,52,62	0
3	BGC	M	4	11/12	0.94	0.07	33,39,41,42	0
3	BGC	O	3	11/12	0.95	0.07	40,41,48,48	0
3	BGC	O	4	11/12	0.95	0.06	33,36,40,42	0
3	BGC	N	5	11/12	0.95	0.08	50,54,63,65	0
3	BGC	M	5	11/12	0.95	0.07	39,42,43,45	0
3	BGC	R	4	11/12	0.95	0.08	45,48,55,62	0
3	BGC	R	5	11/12	0.95	0.08	46,49,52,60	0
3	BGC	T	3	11/12	0.95	0.07	36,39,42,49	0
3	BGC	T	4	11/12	0.95	0.07	32,34,36,36	0

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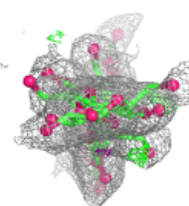
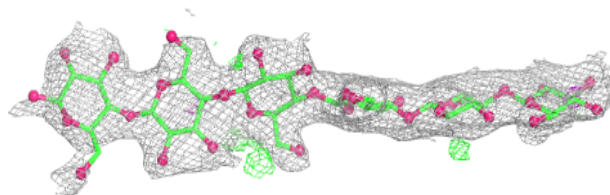
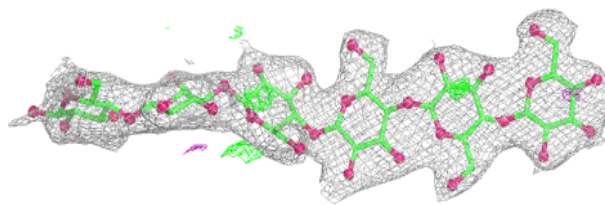
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BGC	Q	5	11/12	0.95	0.07	37,39,44,47	0
3	BGC	S	6	11/12	0.96	0.07	41,44,47,52	0
3	BGC	L	4	11/12	0.96	0.06	32,33,35,35	0
3	BGC	O	5	11/12	0.96	0.07	36,40,47,51	0
3	BGC	S	3	11/12	0.96	0.06	39,42,47,50	0
2	BGC	K	4	11/12	0.96	0.05	35,36,38,40	0
3	BGC	Q	4	11/12	0.96	0.06	32,37,41,42	0
3	BGC	T	6	11/12	0.96	0.09	45,49,57,64	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.

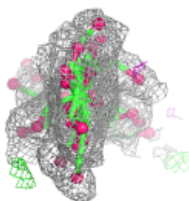
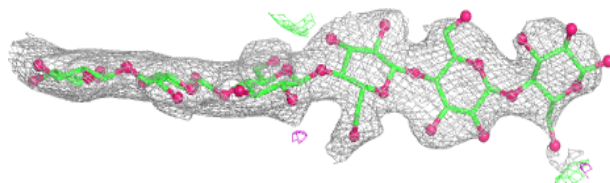
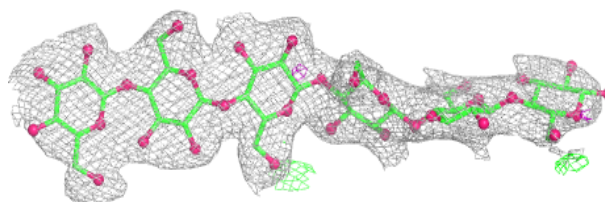


Electron density around Chain L:

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

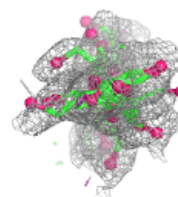
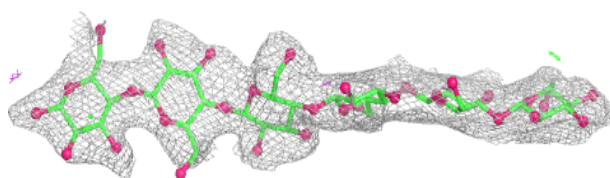
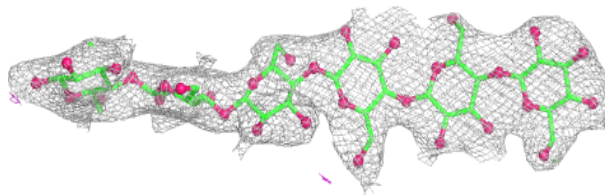
**Electron density around Chain M:**

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

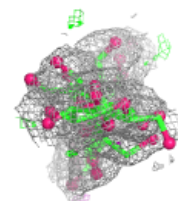
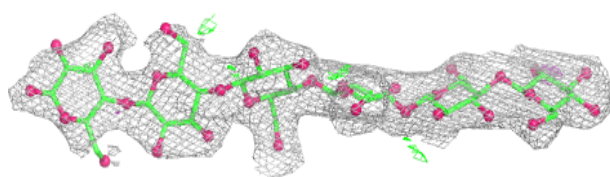
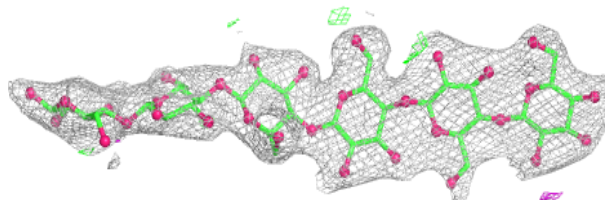


Electron density around Chain N:

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

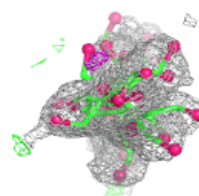
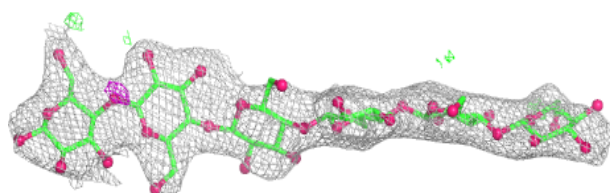
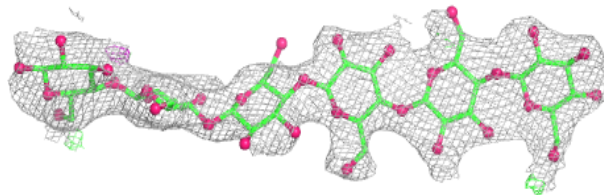
**Electron density around Chain O:**

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

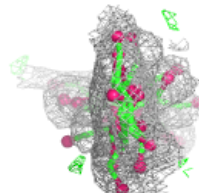
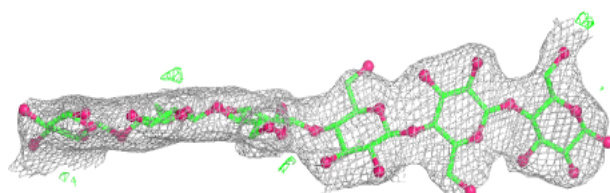
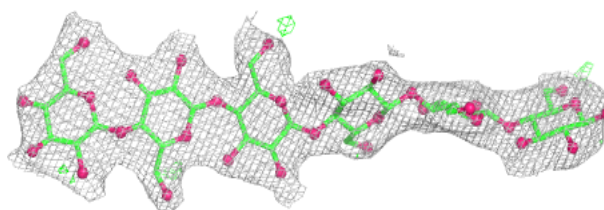


Electron density around Chain P:

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

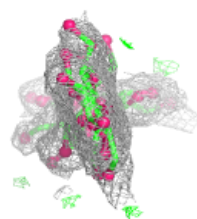
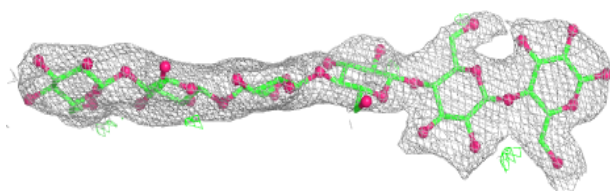
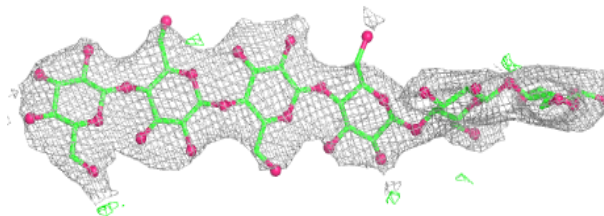
**Electron density around Chain Q:**

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

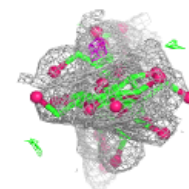
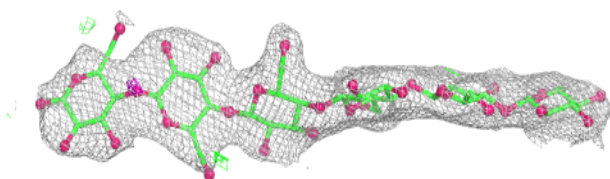
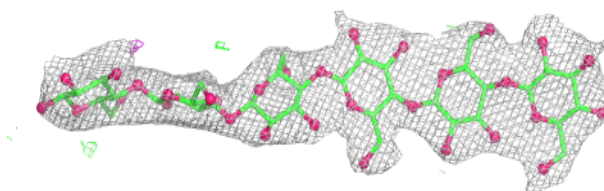


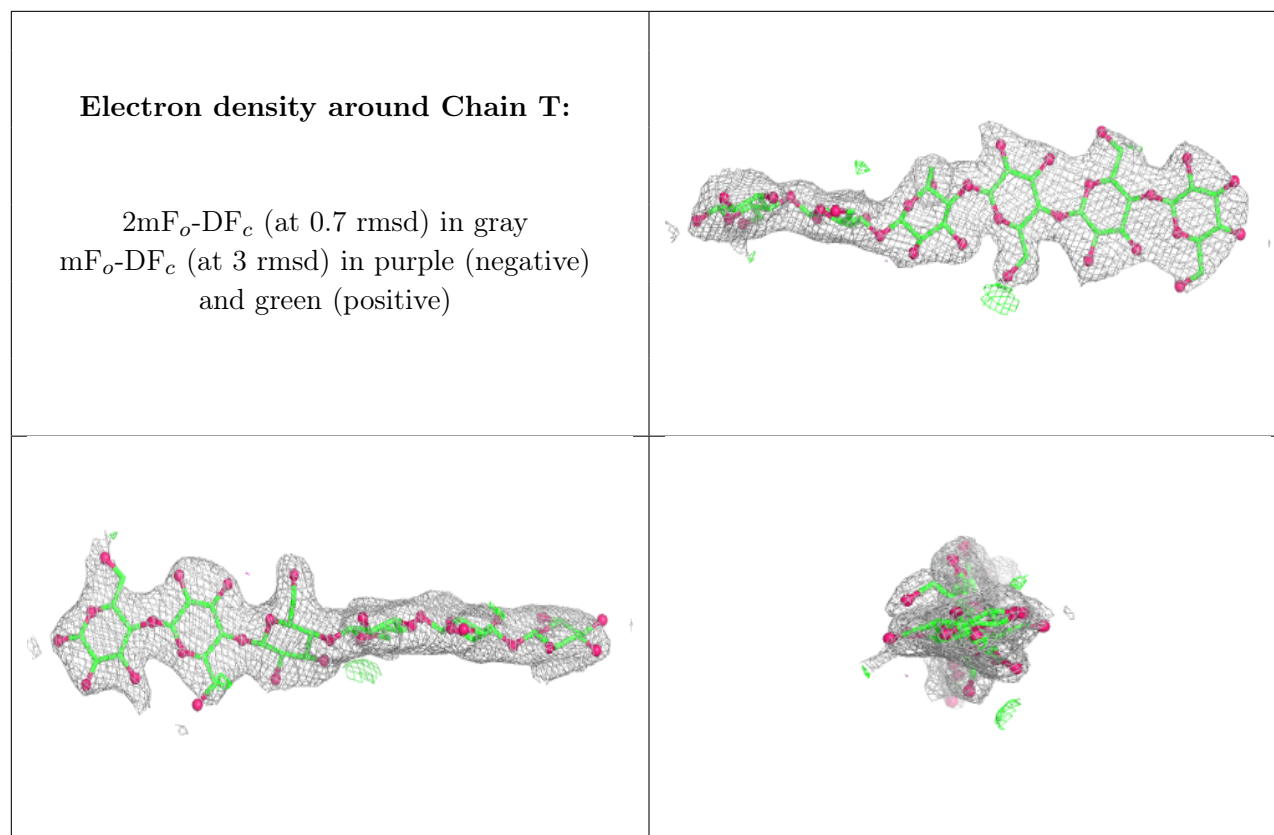
Electron density around Chain R:

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

**Electron density around Chain S:**

$2mF_o-DF_c$ (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
5	ACT	E	608	4/4	0.66	0.26	42,51,53,64	0
5	ACT	I	608	4/4	0.66	0.25	52,53,56,57	0
5	ACT	D	608	4/4	0.68	0.27	53,53,54,57	0
5	ACT	J	608	4/4	0.75	0.19	48,49,54,58	0
5	ACT	H	608	4/4	0.76	0.17	66,69,70,74	0
5	ACT	B	608	4/4	0.77	0.15	38,42,43,50	0
5	ACT	A	607	4/4	0.81	0.20	54,56,58,60	0
7	EDO	G	612	4/4	0.81	0.18	44,46,50,51	0
7	EDO	C	609	4/4	0.84	0.31	51,53,53,53	0
6	PEG	B	610	7/7	0.84	0.23	56,57,60,61	0
5	ACT	F	608	4/4	0.85	0.17	51,55,57,57	0
7	EDO	E	609	4/4	0.86	0.25	52,55,56,56	0
7	EDO	G	610	4/4	0.86	0.17	54,57,57,58	0
5	ACT	C	608	4/4	0.86	0.19	47,51,54,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	EDO	G	608	4/4	0.87	0.22	41,47,50,52	0
7	EDO	G	609	4/4	0.87	0.18	50,57,58,59	0
7	EDO	G	611	4/4	0.88	0.21	54,55,56,57	0
6	PEG	A	609	7/7	0.88	0.19	52,57,64,66	0
7	EDO	H	609	4/4	0.88	0.13	52,54,55,57	0
6	PEG	B	609	7/7	0.90	0.15	49,53,61,62	0
6	PEG	A	608	7/7	0.90	0.17	36,45,58,62	0
7	EDO	E	610	4/4	0.90	0.17	43,47,50,52	0
7	EDO	I	609	4/4	0.91	0.18	54,57,58,59	0
7	EDO	E	612	4/4	0.92	0.13	65,67,68,68	0
7	EDO	D	609	4/4	0.92	0.16	56,63,63,65	0
7	EDO	B	612	4/4	0.92	0.21	54,54,55,55	0
6	PEG	J	609	7/7	0.92	0.14	52,52,56,56	0
7	EDO	A	610	4/4	0.93	0.22	46,47,51,52	0
7	EDO	C	610	4/4	0.94	0.15	47,50,51,51	0
7	EDO	E	611	4/4	0.94	0.12	48,49,52,53	0
7	EDO	C	611	4/4	0.96	0.09	36,37,38,38	0
4	MG	C	607	1/1	0.98	0.06	50,50,50,50	0
7	EDO	B	611	4/4	0.98	0.05	36,37,37,39	0
4	MG	J	607	1/1	0.98	0.03	43,43,43,43	0
4	MG	H	607	1/1	0.99	0.04	51,51,51,51	0
4	MG	I	607	1/1	0.99	0.03	55,55,55,55	0
4	MG	A	606	1/1	0.99	0.08	45,45,45,45	0
4	MG	D	607	1/1	0.99	0.04	44,44,44,44	0
4	MG	E	607	1/1	0.99	0.09	54,54,54,54	0
4	MG	F	607	1/1	0.99	0.04	52,52,52,52	0
4	MG	G	607	1/1	0.99	0.03	53,53,53,53	0
4	MG	B	607	1/1	1.00	0.03	48,48,48,48	0

6.5 Other polymers

There are no such residues in this entry.