



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:59 AM UTC

PDB ID : 8WG2 / pdb_00008wg2
Title : Crystal structure of GH97 glucodextranase mutant E509Q from *Flavobacterium johnsoniae* in complex with isomaltotriose
Authors : Kurata, R.; Nakamura, S.; Miyazaki, T.
Deposited on : 2023-09-20
Resolution : 2.45 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

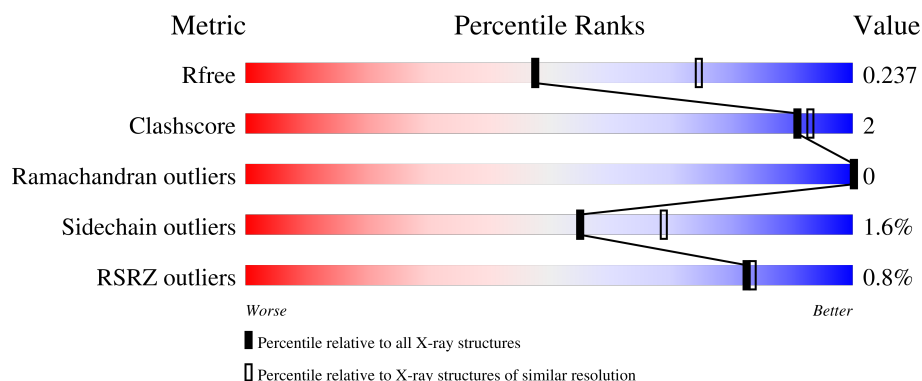
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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.



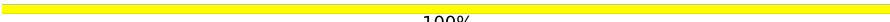
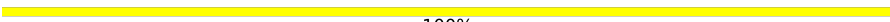
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	685	% 89% 9% ..
1	B	685	% 88% 11% ..
1	C	685	90% 9%
1	D	685	% 88% 11% ..
2	E	3	100%

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Mol	Chain	Length	Quality of chain
2	H	3	 100%
3	F	3	 100%
3	G	3	 67%  33%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 22470 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 Candidate alpha-glucosidase Glycoside hydrolase family 97.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	679	Total	C	N	O	S	0	0	0
			5454	3478	914	1043	19			
1	B	681	Total	C	N	O	S	0	0	0
			5466	3484	917	1046	19			
1	C	684	Total	C	N	O	S	0	0	0
			5484	3494	920	1051	19			
1	D	679	Total	C	N	O	S	0	0	0
			5454	3478	914	1043	19			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	SER	-	expression tag	UNP A5FBI0
A	509	GLN	GLU	engineered mutation	UNP A5FBI0
B	20	SER	-	expression tag	UNP A5FBI0
B	509	GLN	GLU	engineered mutation	UNP A5FBI0
C	20	SER	-	expression tag	UNP A5FBI0
C	509	GLN	GLU	engineered mutation	UNP A5FBI0
D	20	SER	-	expression tag	UNP A5FBI0
D	509	GLN	GLU	engineered mutation	UNP A5FBI0

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



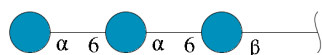
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
2	E	3	Total	C O	0	0	0
			34	18 16			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	H	3	Total	C	O	0	0	0
			34	18	16			

- Molecule 3 is an oligosaccharide called alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	F	3	Total	C	O	0	0	0
			34	18	16			
3	G	3	Total	C	O	0	0	0
			34	18	16			

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

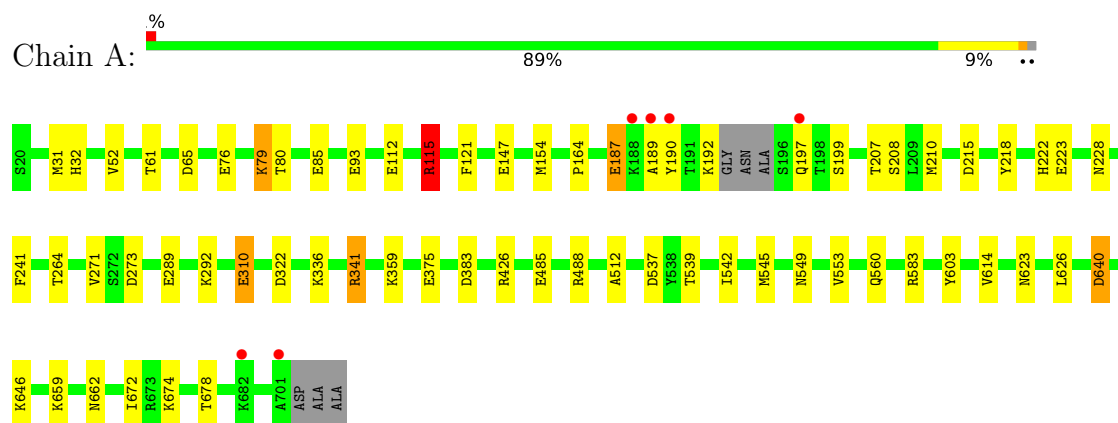
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	144	Total	O	0	0
			144	144		
5	B	88	Total	O	0	0
			88	88		
5	C	108	Total	O	0	0
			108	108		
5	D	132	Total	O	0	0
			132	132		

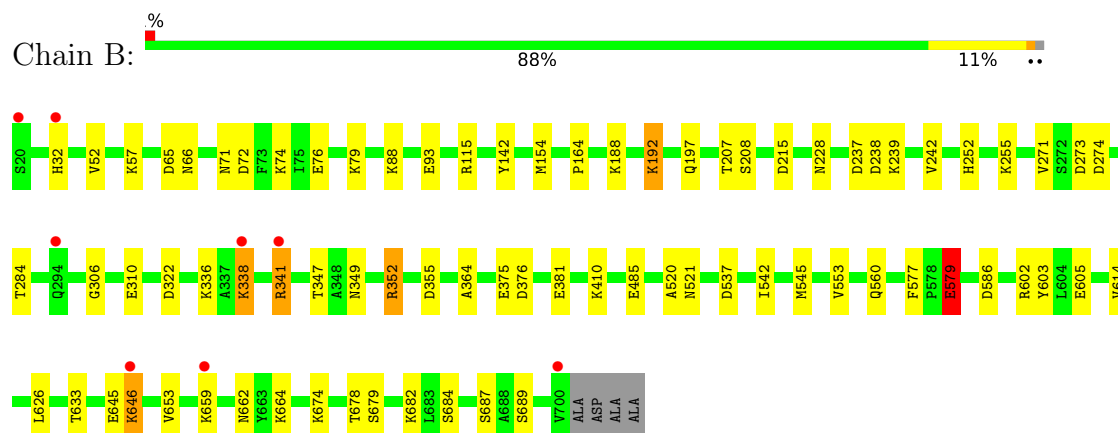
3 Residue-property plots

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.

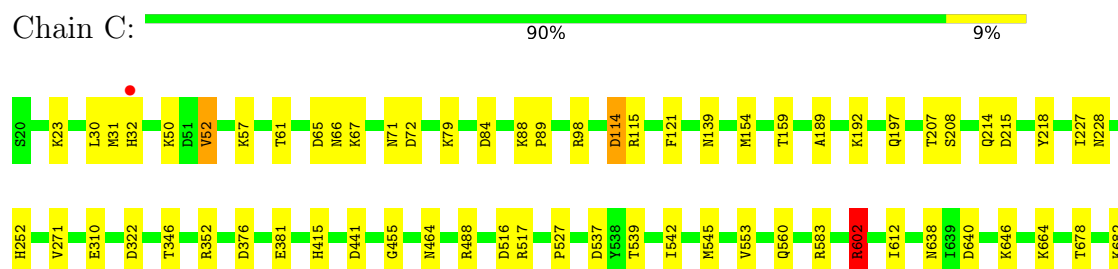
- Molecule 1: Candidate alpha-glucosidase Glycoside hydrolase family 97

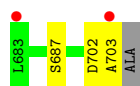


- Molecule 1: Candidate alpha-glucosidase Glycoside hydrolase family 97



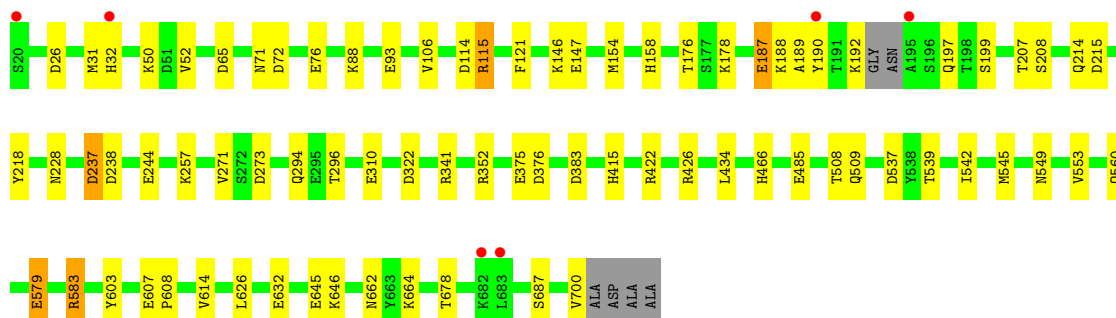
- Molecule 1: Candidate alpha-glucosidase Glycoside hydrolase family 97





- Molecule 1: Candidate alpha-glucosidase Glycoside hydrolase family 97

Chain D: 88% 11% ..



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

Chain E: 100%



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

Chain H: 100%



- Molecule 3: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-beta-D-glucopyranose

Chain F: 100%



- Molecule 3: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-beta-D-glucopyranose

Chain G: 67% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	308.21Å 103.62Å 95.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.16 – 2.45 49.16 – 2.45	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.16-2.45) 100.0 (49.16-2.45)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.85 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.185 , 0.234 0.192 , 0.237	Depositor DCC
R_{free} test set	5817 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	33.6	Xtriage
Anisotropy	0.456	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 31.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	22470	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.81% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BGC, CA, GLC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.04	6/5597 (0.1%)	1.44	41/7589 (0.5%)
1	B	0.94	2/5610 (0.0%)	1.44	50/7608 (0.7%)
1	C	0.96	3/5628 (0.1%)	1.41	40/7633 (0.5%)
1	D	1.00	2/5597 (0.0%)	1.42	49/7589 (0.6%)
All	All	0.99	13/22432 (0.1%)	1.43	180/30419 (0.6%)

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	A	0	2
1	C	0	4
1	D	0	3
All	All	0	9

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	426	ARG	NE-CZ	-6.82	1.25	1.33
1	D	383	ASP	CG-OD1	6.54	1.37	1.25
1	A	512	ALA	CA-CB	-6.17	1.43	1.53
1	C	415	HIS	CG-CD2	-6.06	1.29	1.35
1	D	415	HIS	CG-CD2	-5.78	1.29	1.35
1	A	147	GLU	CD-OE2	5.77	1.36	1.25
1	C	415	HIS	CE1-NE2	-5.66	1.26	1.32
1	A	164	PRO	CA-CB	-5.61	1.46	1.53
1	A	189	ALA	C-N	5.33	1.40	1.33
1	B	164	PRO	CA-CB	-5.22	1.46	1.53
1	B	520	ALA	C-O	-5.22	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	464	ASN	C-O	-5.07	1.17	1.24
1	A	672	ILE	C-O	-5.04	1.18	1.24

All (180) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	579	GLU	CB-CA-C	-14.34	86.94	110.74
1	C	32	HIS	CA-CB-CG	12.60	126.40	113.80
1	A	640	ASP	CB-CA-C	11.53	128.78	109.75
1	A	32	HIS	CA-CB-CG	11.53	125.33	113.80
1	D	32	HIS	CA-CB-CG	11.24	125.04	113.80
1	D	228	ASN	CA-CB-CG	-10.72	101.88	112.60
1	C	228	ASN	CA-CB-CG	-10.38	102.22	112.60
1	B	32	HIS	CA-CB-CG	10.13	123.93	113.80
1	B	322	ASP	CA-CB-CG	9.92	122.52	112.60
1	A	228	ASN	CA-CB-CG	-9.86	102.74	112.60
1	B	228	ASN	CA-CB-CG	-9.21	103.39	112.60
1	B	341	ARG	CB-CG-CD	8.70	131.32	111.30
1	D	187	GLU	CB-CG-CD	8.56	127.15	112.60
1	A	322	ASP	CA-CB-CG	8.53	121.13	112.60
1	A	228	ASN	CB-CA-C	8.39	123.11	111.86
1	D	485	GLU	CG-CD-OE1	-8.35	99.19	118.40
1	A	485	GLU	CG-CD-OE1	-8.30	99.30	118.40
1	D	352	ARG	CD-NE-CZ	8.27	135.97	124.40
1	C	159	THR	CA-CB-OG1	7.88	121.42	109.60
1	C	228	ASN	CB-CA-C	7.81	122.32	111.86
1	D	178	LYS	CG-CD-CE	-7.54	93.97	111.30
1	D	579	GLU	N-CA-CB	7.48	121.74	110.22
1	B	352	ARG	CB-CA-C	-7.39	98.53	110.79
1	B	228	ASN	CB-CA-C	7.36	121.72	111.86
1	B	192	LYS	CB-CA-C	7.29	123.51	114.40
1	B	537	ASP	CA-CB-CG	7.19	119.79	112.60
1	D	50	LYS	CB-CG-CD	7.17	127.79	111.30
1	C	215	ASP	CA-CB-CG	7.10	119.70	112.60
1	A	85	GLU	CB-CG-CD	7.06	124.60	112.60
1	A	189	ALA	CA-C-N	7.03	133.05	122.23
1	A	189	ALA	C-N-CA	7.03	133.05	122.23
1	B	376	ASP	CA-CB-CG	6.94	119.54	112.60
1	B	375	GLU	CB-CG-CD	6.91	124.35	112.60
1	D	322	ASP	CA-CB-CG	6.91	119.51	112.60
1	D	189	ALA	CA-C-N	6.84	132.76	122.23
1	D	189	ALA	C-N-CA	6.84	132.76	122.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	646	LYS	CG-CD-CE	6.75	126.83	111.30
1	A	383	ASP	CA-CB-CG	6.72	119.32	112.60
1	D	646	LYS	CB-CG-CD	6.71	126.73	111.30
1	B	347	THR	CA-CB-OG1	6.70	119.66	109.60
1	D	50	LYS	CG-CD-CE	-6.70	95.88	111.30
1	C	376	ASP	CA-CB-CG	6.69	119.29	112.60
1	D	273	ASP	CA-CB-CG	6.69	119.29	112.60
1	D	310	GLU	CB-CA-C	-6.67	100.13	110.81
1	D	537	ASP	CA-CB-CG	6.55	119.15	112.60
1	A	359	LYS	CB-CG-CD	6.46	126.15	111.30
1	C	516	ASP	CA-CB-CG	6.42	119.02	112.60
1	C	310	GLU	CB-CA-C	-6.39	99.82	110.68
1	D	485	GLU	CG-CD-OE2	6.38	133.06	118.40
1	D	375	GLU	CB-CG-CD	6.37	123.42	112.60
1	D	678	THR	CA-CB-OG1	-6.34	100.09	109.60
1	C	88	LYS	N-CA-CB	6.34	119.39	110.07
1	B	238	ASP	CA-CB-CG	6.33	118.93	112.60
1	C	252	HIS	CA-CB-CG	6.33	120.13	113.80
1	C	352	ARG	NE-CZ-NH1	-6.33	115.17	121.50
1	D	228	ASN	CB-CA-C	6.31	120.32	111.86
1	A	336	LYS	CG-CD-CE	6.30	125.80	111.30
1	A	189	ALA	CA-C-O	-6.30	112.98	120.10
1	B	664	LYS	CB-CA-C	-6.27	99.09	110.56
1	C	678	THR	CA-CB-OG1	-6.24	100.24	109.60
1	B	338	LYS	CG-CD-CE	6.22	125.61	111.30
1	D	215	ASP	CA-CB-CG	6.22	118.82	112.60
1	B	273	ASP	CA-CB-CG	6.19	118.79	112.60
1	B	284	THR	OG1-CB-CG2	-6.18	96.93	109.30
1	D	662	ASN	CA-CB-CG	-6.16	106.44	112.60
1	B	664	LYS	N-CA-CB	6.16	119.73	110.19
1	C	322	ASP	CA-CB-CG	6.13	118.73	112.60
1	A	485	GLU	CG-CD-OE2	6.12	132.47	118.40
1	B	689	SER	CB-CA-C	6.10	118.94	110.16
1	C	664	LYS	N-CA-CB	6.09	119.14	110.13
1	A	375	GLU	CB-CG-CD	6.05	122.88	112.60
1	A	189	ALA	O-C-N	6.05	129.29	122.22
1	A	640	ASP	CA-CB-CG	6.04	118.64	112.60
1	D	352	ARG	CA-CB-CG	6.03	126.16	114.10
1	A	273	ASP	CA-CB-CG	6.02	118.62	112.60
1	B	659	LYS	CB-CA-C	-6.01	99.50	110.63
1	A	215	ASP	CA-CB-CG	5.97	118.57	112.60
1	B	678	THR	CA-CB-OG1	-5.96	100.65	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	664	LYS	N-CA-CB	5.96	118.84	110.07
1	D	646	LYS	CB-CA-C	5.95	119.82	109.65
1	A	79	LYS	CB-CA-C	5.94	120.05	109.65
1	D	583	ARG	CA-CB-CG	5.93	125.96	114.10
1	C	32	HIS	CB-CG-ND1	5.91	131.57	122.70
1	A	537	ASP	CA-CB-CG	5.90	118.50	112.60
1	D	176	THR	CA-CB-OG1	-5.90	100.76	109.60
1	A	310	GLU	N-CA-CB	5.88	118.87	110.06
1	A	289	GLU	CB-CG-CD	5.86	122.56	112.60
1	A	383	ASP	CB-CA-C	5.86	120.03	110.95
1	B	577	PHE	CA-CB-CG	5.86	119.66	113.80
1	B	352	ARG	NE-CZ-NH2	-5.84	113.95	119.20
1	D	76	GLU	N-CA-C	-5.82	105.28	112.90
1	C	537	ASP	CA-CB-CG	5.81	118.41	112.60
1	C	455	GLY	N-CA-C	-5.79	107.59	114.48
1	C	89	PRO	N-CA-CB	5.79	109.46	103.38
1	D	376	ASP	CA-CB-CG	5.78	118.38	112.60
1	C	114	ASP	CA-CB-CG	-5.75	106.85	112.60
1	D	700	VAL	N-CA-CB	-5.72	101.78	111.50
1	B	215	ASP	CA-CB-CG	5.72	118.32	112.60
1	B	274	ASP	CA-CB-CG	5.72	118.32	112.60
1	B	76	GLU	N-CA-C	-5.71	106.44	113.41
1	B	252	HIS	CA-CB-CG	5.69	119.49	113.80
1	B	602	ARG	N-CA-CB	5.69	120.05	110.77
1	C	352	ARG	NE-CZ-NH2	5.68	124.31	119.20
1	C	664	LYS	CB-CA-C	-5.67	101.26	110.79
1	B	255	LYS	N-CA-CB	-5.66	103.06	111.43
1	C	602	ARG	N-CA-CB	5.61	119.58	110.77
1	B	284	THR	CA-CB-OG1	-5.61	101.18	109.60
1	A	115	ARG	CG-CD-NE	5.58	124.27	112.00
1	B	662	ASN	CA-CB-CG	-5.57	107.03	112.60
1	C	346	THR	CA-CB-OG1	-5.57	101.25	109.60
1	B	74	LYS	CB-CG-CD	5.56	124.10	111.30
1	A	61	THR	CA-CB-OG1	-5.56	101.27	109.60
1	B	306	GLY	N-CA-C	5.53	118.81	110.18
1	D	466	HIS	CA-CB-CG	-5.51	108.29	113.80
1	B	586	ASP	CA-CB-CG	5.50	118.10	112.60
1	A	662	ASN	CA-CB-CG	-5.49	107.11	112.60
1	B	381	GLU	CG-CD-OE1	-5.49	105.77	118.40
1	B	633	THR	CA-CB-OG1	-5.47	101.40	109.60
1	C	57	LYS	CG-CD-CE	-5.45	98.77	111.30
1	B	57	LYS	CG-CD-CE	-5.43	98.81	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	189	ALA	CA-C-O	-5.41	113.99	120.10
1	C	352	ARG	N-CA-CB	-5.40	102.18	110.12
1	A	646	LYS	CB-CA-C	5.39	118.86	109.65
1	C	189	ALA	CA-C-O	-5.38	114.02	120.10
1	D	147	GLU	CG-CD-OE1	-5.38	106.04	118.40
1	A	674	LYS	CB-CA-C	-5.37	100.45	109.48
1	A	646	LYS	CB-CG-CD	5.36	123.62	111.30
1	B	352	ARG	N-CA-CB	5.35	117.98	110.12
1	A	310	GLU	CB-CA-C	-5.33	101.61	110.68
1	D	678	THR	OG1-CB-CG2	5.32	119.94	109.30
1	D	539	THR	CA-CB-OG1	5.32	117.57	109.60
1	C	539	THR	CA-CB-OG1	5.30	117.55	109.60
1	D	32	HIS	N-CA-CB	5.29	118.89	110.16
1	A	264	THR	CA-CB-OG1	-5.29	101.67	109.60
1	A	76	GLU	N-CA-C	-5.29	105.97	112.90
1	A	241	PHE	CB-CA-C	5.28	118.94	111.86
1	D	146	LYS	CG-CD-CE	5.28	123.44	111.30
1	B	336	LYS	CB-CG-CD	5.26	123.40	111.30
1	C	61	THR	OG1-CB-CG2	-5.26	98.78	109.30
1	D	158	HIS	CA-CB-CG	5.25	119.05	113.80
1	C	79	LYS	CB-CA-C	5.24	120.01	109.38
1	B	485	GLU	CG-CD-OE2	5.23	130.43	118.40
1	C	640	ASP	CA-CB-CG	5.23	117.83	112.60
1	B	237	ASP	CA-CB-CG	5.23	117.83	112.60
1	D	664	LYS	CB-CA-C	-5.22	102.24	110.86
1	C	682	LYS	CG-CD-CE	5.22	123.31	111.30
1	A	292	LYS	CG-CD-CE	-5.21	99.31	111.30
1	D	296	THR	CA-CB-OG1	-5.20	101.80	109.60
1	C	381	GLU	CG-CD-OE1	-5.20	106.44	118.40
1	C	67	LYS	N-CA-CB	-5.20	103.67	110.59
1	B	352	ARG	CA-CB-CG	5.19	124.48	114.10
1	C	189	ALA	CA-C-N	5.17	130.54	122.26
1	C	189	ALA	C-N-CA	5.17	130.54	122.26
1	A	539	THR	CA-CB-OG1	5.17	117.36	109.60
1	D	237	ASP	CA-CB-CG	5.16	117.76	112.60
1	C	88	LYS	CB-CA-C	-5.15	105.07	110.17
1	C	159	THR	OG1-CB-CG2	-5.15	99.00	109.30
1	A	583	ARG	NE-CZ-NH2	-5.14	114.57	119.20
1	D	106	VAL	N-CA-CB	-5.13	105.21	111.21
1	C	638	ASN	CA-CB-CG	-5.12	107.48	112.60
1	A	678	THR	CA-CB-OG1	-5.12	101.92	109.60
1	C	441	ASP	CB-CA-C	5.12	118.89	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	646	LYS	CB-CG-CD	5.11	123.05	111.30
1	D	26	ASP	CA-CB-CG	5.10	117.70	112.60
1	B	338	LYS	CA-CB-CG	5.10	124.31	114.10
1	A	341	ARG	CG-CD-NE	-5.10	100.78	112.00
1	D	189	ALA	O-C-N	5.10	128.18	122.22
1	C	52	VAL	O-C-N	5.09	126.51	121.98
1	D	88	LYS	N-CA-CB	5.09	117.55	110.07
1	D	238	ASP	CA-CB-CG	5.08	117.67	112.60
1	B	88	LYS	CB-CA-C	-5.06	105.17	110.17
1	D	257	LYS	CG-CD-CE	5.05	122.92	111.30
1	B	310	GLU	N-CA-CB	5.05	117.64	110.06
1	D	244	GLU	CG-CD-OE1	5.04	130.00	118.40
1	B	355	ASP	CA-CB-CG	5.04	117.64	112.60
1	B	242	VAL	N-CA-CB	-5.03	105.10	111.64
1	B	142	TYR	N-CA-CB	5.01	118.60	110.43
1	A	426	ARG	NE-CZ-NH1	-5.01	116.49	121.50
1	D	294	GLN	N-CA-CB	5.00	117.33	110.07
1	A	623	ASN	CB-CA-C	-5.00	101.05	109.50

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	ARG	Sidechain
1	A	488	ARG	Sidechain
1	C	488	ARG	Sidechain
1	C	517	ARG	Sidechain
1	C	583	ARG	Sidechain
1	C	602	ARG	Sidechain
1	D	115	ARG	Sidechain
1	D	341	ARG	Sidechain
1	D	583	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	5454	0	5238	22	0
1	B	5466	0	5248	17	0
1	C	5484	0	5262	15	0
1	D	5454	0	5238	19	0
2	E	34	0	29	0	0
2	H	34	0	29	0	0
3	F	34	0	28	0	0
3	G	34	0	28	1	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
5	A	144	0	0	1	0
5	B	88	0	0	1	0
5	C	108	0	0	0	0
5	D	132	0	0	1	0
All	All	22470	0	21100	73	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 2.

All (73) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:GLU:HA	1:A:187:GLU:OE1	1.86	0.74
1:A:112:GLU:OE2	1:D:632:GLU:HB3	1.91	0.71
1:A:192:LYS:HA	1:A:197:GLN:HE22	1.58	0.69
1:B:154:MET:HA	1:B:154:MET:HE2	1.74	0.68
1:D:154:MET:HA	1:D:154:MET:HE2	1.77	0.67
1:B:192:LYS:HA	1:B:197:GLN:HE22	1.59	0.67
1:C:192:LYS:HA	1:C:197:GLN:HE22	1.59	0.66
1:D:192:LYS:HA	1:D:197:GLN:HE22	1.59	0.65
1:C:154:MET:HA	1:C:154:MET:HE2	1.82	0.61
1:A:154:MET:HE2	1:A:154:MET:HA	1.82	0.61
1:A:65:ASP:OD2	1:A:115:ARG:NH2	2.36	0.58
1:D:545:MET:HG3	1:D:553:VAL:HB	1.87	0.57
1:C:207:THR:HA	1:C:208:SER:C	2.31	0.55
1:A:310:GLU:HG3	5:A:940:HOH:O	2.05	0.55
1:B:646:LYS:HD2	1:B:679:SER:OG	2.06	0.55
1:D:207:THR:HA	1:D:208:SER:C	2.31	0.55
1:B:207:THR:HA	1:B:208:SER:C	2.32	0.54
1:A:207:THR:HA	1:A:208:SER:C	2.34	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:VAL:HG11	1:B:271:VAL:HG21	1.90	0.53
1:C:65:ASP:OD2	1:C:115:ARG:NH2	2.42	0.53
1:B:605:GLU:HA	5:B:923:HOH:O	2.08	0.53
1:D:65:ASP:OD2	1:D:115:ARG:NH2	2.42	0.52
1:A:190:TYR:CE1	1:A:199:SER:HB3	2.45	0.51
1:A:187:GLU:OE1	1:A:187:GLU:CA	2.59	0.50
1:B:545:MET:HG3	1:B:553:VAL:HB	1.94	0.50
1:A:190:TYR:HD2	1:A:192:LYS:HE3	1.76	0.49
1:B:65:ASP:OD2	1:B:115:ARG:NH2	2.46	0.48
1:B:349:ASN:OD1	1:B:352:ARG:HD3	2.14	0.47
1:C:602:ARG:NH1	1:C:602:ARG:HG2	2.31	0.46
1:A:52:VAL:HG11	1:A:271:VAL:HG21	1.97	0.46
1:A:545:MET:HG3	1:A:553:VAL:HB	1.98	0.45
1:A:549:ASN:OD1	1:A:549:ASN:C	2.59	0.45
1:A:79:LYS:HE3	1:A:80:THR:O	2.16	0.45
1:D:31:MET:HE2	1:D:121:PHE:CG	2.52	0.45
1:B:71:ASN:OD1	1:B:71:ASN:C	2.58	0.45
1:B:653:VAL:HG22	1:B:674:LYS:HG2	1.98	0.45
1:D:52:VAL:HG11	1:D:271:VAL:HG21	1.98	0.45
1:D:93:GLU:OE2	1:D:603:TYR:OH	2.28	0.45
1:B:93:GLU:OE2	1:B:603:TYR:OH	2.28	0.44
1:B:542:ILE:O	1:B:560:GLN:HG3	2.17	0.44
1:A:222:HIS:CG	1:A:223:GLU:H	2.35	0.44
1:A:31:MET:HE2	1:A:121:PHE:CG	2.52	0.44
1:C:31:MET:HE2	1:C:121:PHE:CG	2.53	0.43
1:C:52:VAL:HG11	1:C:271:VAL:HG21	2.00	0.43
1:B:352:ARG:NH2	1:B:579:GLU:OE1	2.50	0.43
1:C:527:PRO:HG2	1:C:612:ILE:HD12	2.00	0.43
1:C:218:TYR:O	1:C:271:VAL:HA	2.18	0.43
1:C:542:ILE:O	1:C:560:GLN:HG3	2.18	0.43
1:A:31:MET:HE2	1:A:121:PHE:CD2	2.53	0.43
1:D:542:ILE:O	1:D:560:GLN:HG3	2.19	0.43
1:C:702:ASP:O	1:C:703:ALA:C	2.62	0.42
1:C:545:MET:HG3	1:C:553:VAL:HB	2.01	0.42
1:A:626:LEU:HD23	1:A:626:LEU:C	2.44	0.42
1:B:521:ASN:OD1	1:B:521:ASN:C	2.61	0.42
1:C:71:ASN:OD1	1:C:71:ASN:C	2.62	0.42
1:C:84:ASP:OD2	1:C:98:ARG:NH2	2.45	0.42
1:C:23:LYS:HE3	1:C:30:LEU:HD13	2.03	0.41
1:D:626:LEU:C	1:D:626:LEU:HD23	2.45	0.41
1:A:210:MET:CE	1:A:218:TYR:HB3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:508:THR:O	1:D:509:GLN:C	2.64	0.41
1:A:542:ILE:O	1:A:560:GLN:HG3	2.21	0.41
1:A:65:ASP:CG	1:A:115:ARG:HH22	2.28	0.41
1:D:190:TYR:CE2	1:D:199:SER:HB3	2.55	0.41
1:B:364:ALA:HA	1:B:410:LYS:O	2.21	0.41
1:D:645:GLU:HG3	5:D:950:HOH:O	2.20	0.41
1:A:93:GLU:OE2	1:A:603:TYR:OH	2.30	0.41
1:D:71:ASN:OD1	1:D:71:ASN:C	2.64	0.41
1:D:549:ASN:OD1	1:D:549:ASN:C	2.64	0.41
1:D:607:GLU:HA	1:D:608:PRO:HD2	1.95	0.41
3:G:1:BGC:O6	3:G:1:BGC:O4	2.33	0.40
1:D:218:TYR:O	1:D:271:VAL:HA	2.21	0.40
1:B:626:LEU:C	1:B:626:LEU:HD23	2.47	0.40
1:D:422:ARG:O	1:D:426:ARG:HG3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	675/685 (98%)	637 (94%)	38 (6%)	0	100	100
1	B	679/685 (99%)	644 (95%)	35 (5%)	0	100	100
1	C	682/685 (100%)	654 (96%)	28 (4%)	0	100	100
1	D	675/685 (98%)	641 (95%)	34 (5%)	0	100	100
All	All	2711/2740 (99%)	2576 (95%)	135 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	580/582 (100%)	575 (99%)	5 (1%)	70	81
1	B	581/582 (100%)	568 (98%)	13 (2%)	45	60
1	C	582/582 (100%)	573 (98%)	9 (2%)	57	70
1	D	580/582 (100%)	570 (98%)	10 (2%)	53	67
All	All	2323/2328 (100%)	2286 (98%)	37 (2%)	55	69

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	187	GLU
1	A	341	ARG
1	A	614	VAL
1	A	640	ASP
1	A	659	LYS
1	B	66	ASN
1	B	72	ASP
1	B	79	LYS
1	B	188	LYS
1	B	239	LYS
1	B	338	LYS
1	B	341	ARG
1	B	579	GLU
1	B	614	VAL
1	B	645	GLU
1	B	682	LYS
1	B	684	SER
1	B	687	SER
1	C	50	LYS
1	C	66	ASN
1	C	72	ASP
1	C	114	ASP
1	C	139	ASN
1	C	214	GLN

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Mol	Chain	Res	Type
1	C	227	ILE
1	C	646	LYS
1	C	687	SER
1	D	72	ASP
1	D	114	ASP
1	D	187	GLU
1	D	188	LYS
1	D	214	GLN
1	D	237	ASP
1	D	434	LEU
1	D	579	GLU
1	D	614	VAL
1	D	687	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	A	100	ASN
1	A	197	GLN
1	A	360	ASN
1	A	423	ASN
1	B	86	ASN
1	B	99	ASN
1	B	100	ASN
1	B	197	GLN
1	B	405	HIS
1	B	509	GLN
1	C	99	ASN
1	C	100	ASN
1	C	197	GLN
1	C	328	GLN
1	C	630	ASN
1	D	99	ASN
1	D	139	ASN
1	D	197	GLN
1	D	380	HIS
1	D	405	HIS
1	D	468	GLN
1	D	630	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 ⓘ

12 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	GLC	E	1	2	12,12,12	1.38	3 (25%)	17,17,17	2.99	9 (52%)
2	GLC	E	2	2,4	11,11,12	0.77	0	15,15,17	1.99	5 (33%)
2	GLC	E	3	2,4	11,11,12	0.87	0	15,15,17	1.79	4 (26%)
3	BGC	F	1	3	12,12,12	1.06	1 (8%)	17,17,17	1.86	4 (23%)
3	GLC	F	2	4,3	11,11,12	0.62	0	15,15,17	2.00	4 (26%)
3	GLC	F	3	4,3	11,11,12	0.63	0	15,15,17	2.12	5 (33%)
3	BGC	G	1	3	12,12,12	1.74	2 (16%)	17,17,17	1.97	7 (41%)
3	GLC	G	2	4,3	11,11,12	0.66	0	15,15,17	1.46	4 (26%)
3	GLC	G	3	4,3	11,11,12	0.54	0	15,15,17	2.44	6 (40%)
2	GLC	H	1	2	12,12,12	1.01	0	17,17,17	1.38	3 (17%)
2	GLC	H	2	2,4	11,11,12	0.46	0	15,15,17	2.32	5 (33%)
2	GLC	H	3	2,4	11,11,12	0.62	0	15,15,17	1.81	5 (33%)

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	GLC	E	1	2	-	2/2/22/22	0/1/1/1
2	GLC	E	2	2,4	-	2/2/19/22	0/1/1/1
2	GLC	E	3	2,4	-	2/2/19/22	0/1/1/1
3	BGC	F	1	3	-	2/2/22/22	0/1/1/1
3	GLC	F	2	4,3	-	1/2/19/22	0/1/1/1
3	GLC	F	3	4,3	-	0/2/19/22	0/1/1/1
3	BGC	G	1	3	-	2/2/22/22	0/1/1/1
3	GLC	G	2	4,3	-	1/2/19/22	0/1/1/1
3	GLC	G	3	4,3	-	0/2/19/22	0/1/1/1
2	GLC	H	1	2	-	1/2/22/22	0/1/1/1
2	GLC	H	2	2,4	-	2/2/19/22	0/1/1/1
2	GLC	H	3	2,4	-	2/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	1	BGC	C1-C2	4.29	1.62	1.52
3	F	1	BGC	C1-C2	2.93	1.59	1.52
2	E	1	GLC	C3-C2	2.47	1.58	1.52
3	G	1	BGC	O5-C1	2.40	1.48	1.42
2	E	1	GLC	C4-C3	2.11	1.57	1.52
2	E	1	GLC	O1-C1	2.08	1.46	1.39

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	2	GLC	C1-O5-C5	6.36	120.70	112.19
2	E	1	GLC	O2-C2-C3	6.03	124.60	110.38
2	E	1	GLC	O2-C2-C1	-5.65	96.20	109.25
3	F	3	GLC	C1-O5-C5	4.81	118.63	112.19
3	G	3	GLC	C1-O5-C5	4.79	118.61	112.19
2	E	2	GLC	O3-C3-C4	4.52	121.04	110.38
3	F	2	GLC	C3-C4-C5	4.48	118.35	110.23
3	F	1	BGC	C3-C4-C5	-4.45	102.16	110.23
3	G	1	BGC	O3-C3-C2	4.30	120.51	110.38
3	F	3	GLC	O2-C2-C3	4.18	118.80	110.15
2	H	3	GLC	O2-C2-C3	4.06	118.56	110.15
3	G	3	GLC	O4-C4-C5	-4.06	99.32	109.32
3	F	1	BGC	O2-C2-C1	4.03	118.55	109.25
2	E	1	GLC	O3-C3-C2	3.89	119.54	110.38
2	E	1	GLC	O4-C4-C5	-3.86	99.81	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	GLC	C1-O5-C5	3.78	120.97	113.65
3	F	2	GLC	O4-C4-C3	-3.77	101.48	110.38
3	G	3	GLC	C2-C3-C4	-3.66	104.43	110.86
3	G	3	GLC	O2-C2-C3	3.38	117.15	110.15
2	H	1	GLC	O3-C3-C2	3.37	118.31	110.38
2	E	1	GLC	O1-C1-C2	3.36	118.72	108.98
3	G	3	GLC	O4-C4-C3	3.30	118.15	110.38
2	E	1	GLC	O5-C5-C4	3.26	115.56	109.70
3	G	1	BGC	O5-C1-C2	3.18	115.89	110.30
2	E	3	GLC	C1-O5-C5	3.17	116.43	112.19
3	F	1	BGC	O4-C4-C5	3.05	116.83	109.32
2	H	2	GLC	O3-C3-C2	-3.00	103.94	110.05
2	H	2	GLC	O4-C4-C5	-2.98	101.99	109.32
2	E	3	GLC	O2-C2-C3	2.96	116.28	110.15
2	H	3	GLC	O4-C4-C3	2.94	117.31	110.38
3	G	2	GLC	O4-C4-C5	2.76	116.12	109.32
3	F	3	GLC	O5-C5-C6	-2.76	102.29	107.66
2	E	2	GLC	C1-O5-C5	2.75	115.88	112.19
3	G	2	GLC	O4-C4-C3	-2.70	104.02	110.38
3	F	2	GLC	C1-O5-C5	2.67	115.77	112.19
2	H	1	GLC	O2-C2-C3	2.66	116.64	110.38
3	F	3	GLC	O3-C3-C2	2.65	115.46	110.05
3	G	1	BGC	O1-C1-C2	2.53	116.34	108.98
2	E	3	GLC	O3-C3-C2	2.51	115.19	110.05
3	F	3	GLC	C2-C3-C4	-2.50	106.46	110.86
2	E	3	GLC	C6-C5-C4	-2.49	106.91	113.02
3	F	1	BGC	C1-O5-C5	-2.43	108.94	113.65
2	H	2	GLC	O3-C3-C4	2.42	116.07	110.38
3	G	3	GLC	O3-C3-C4	2.38	115.98	110.38
2	H	1	GLC	O2-C2-C1	-2.37	103.78	109.25
2	H	3	GLC	C1-O5-C5	2.35	115.33	112.19
3	G	2	GLC	C3-C4-C5	2.33	114.46	110.23
3	G	1	BGC	O3-C3-C4	-2.28	105.00	110.38
3	G	1	BGC	O2-C2-C3	2.27	115.72	110.38
2	H	3	GLC	O4-C4-C5	-2.26	103.75	109.32
2	E	2	GLC	O4-C4-C3	2.26	115.71	110.38
2	H	2	GLC	O4-C4-C3	2.26	115.69	110.38
3	G	1	BGC	O5-C5-C4	2.22	113.69	109.70
2	E	1	GLC	O5-C1-C2	-2.17	106.48	110.30
2	E	2	GLC	O3-C3-C2	-2.12	105.72	110.05
3	F	2	GLC	O3-C3-C2	2.10	114.33	110.05
2	E	2	GLC	O5-C5-C4	-2.09	105.74	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1	BGC	C3-C4-C5	-2.07	106.48	110.23
2	H	3	GLC	C6-C5-C4	-2.06	107.95	113.02
2	E	1	GLC	O4-C4-C3	2.04	115.17	110.38
3	G	2	GLC	C1-O5-C5	2.03	114.91	112.19

There are no chirality outliers.

All (17) torsion outliers are listed below:

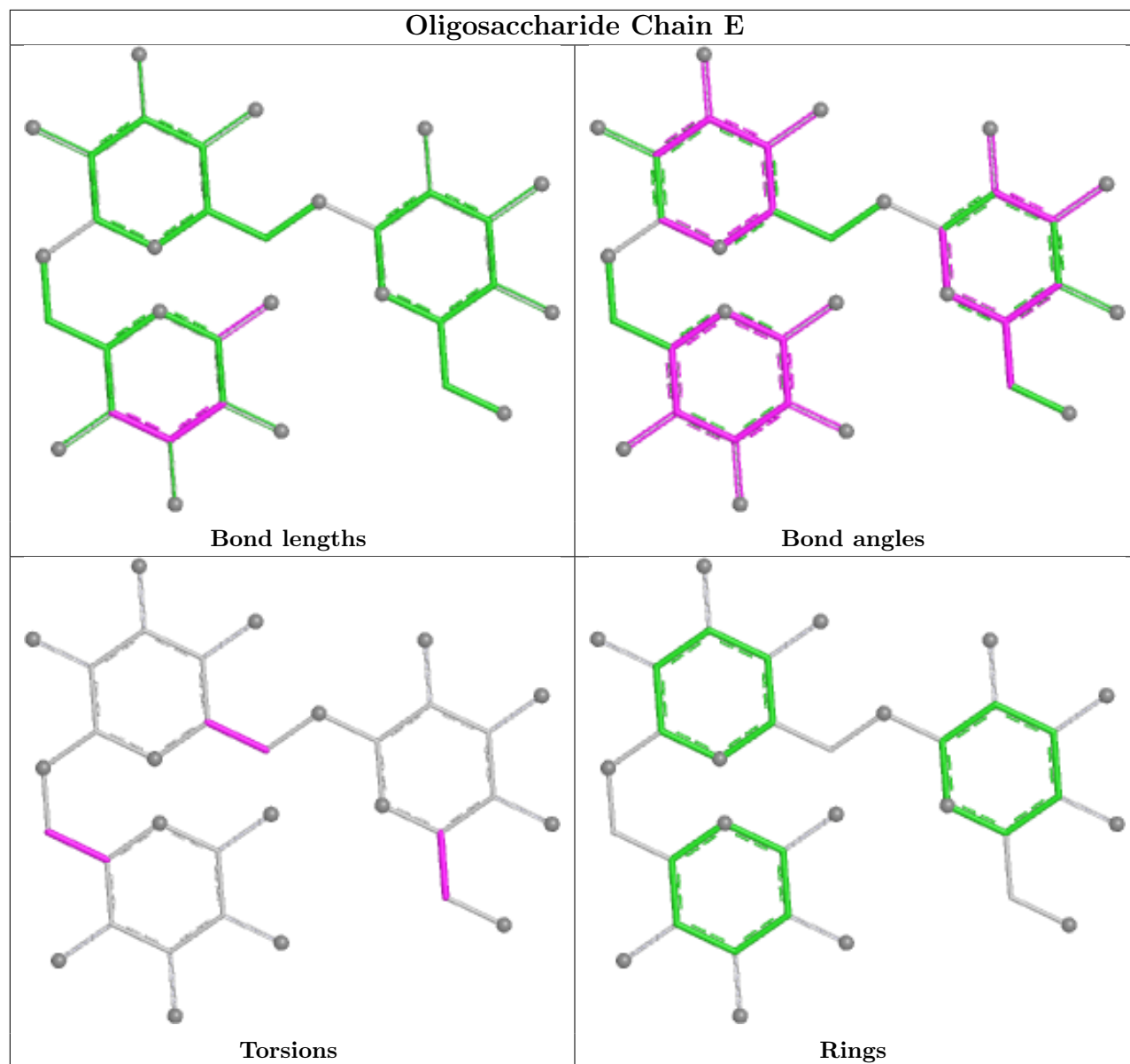
Mol	Chain	Res	Type	Atoms
2	H	2	GLC	O5-C5-C6-O6
3	G	1	BGC	O5-C5-C6-O6
2	H	2	GLC	C4-C5-C6-O6
3	G	1	BGC	C4-C5-C6-O6
3	F	1	BGC	O5-C5-C6-O6
3	F	1	BGC	C4-C5-C6-O6
2	E	1	GLC	O5-C5-C6-O6
2	E	3	GLC	O5-C5-C6-O6
2	H	1	GLC	O5-C5-C6-O6
3	G	2	GLC	O5-C5-C6-O6
3	F	2	GLC	O5-C5-C6-O6
2	H	3	GLC	O5-C5-C6-O6
2	E	3	GLC	C4-C5-C6-O6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

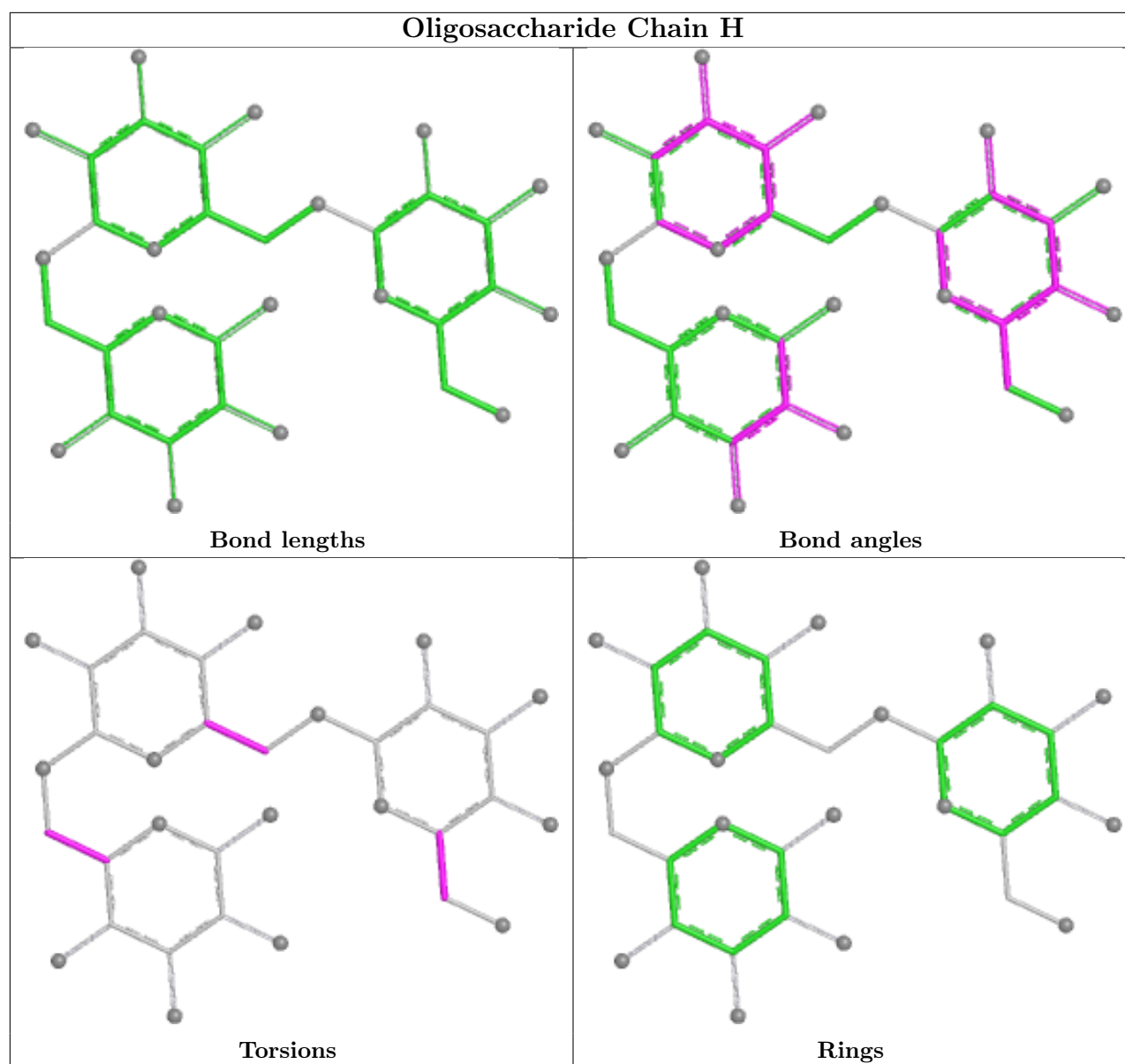
There are no ring outliers.

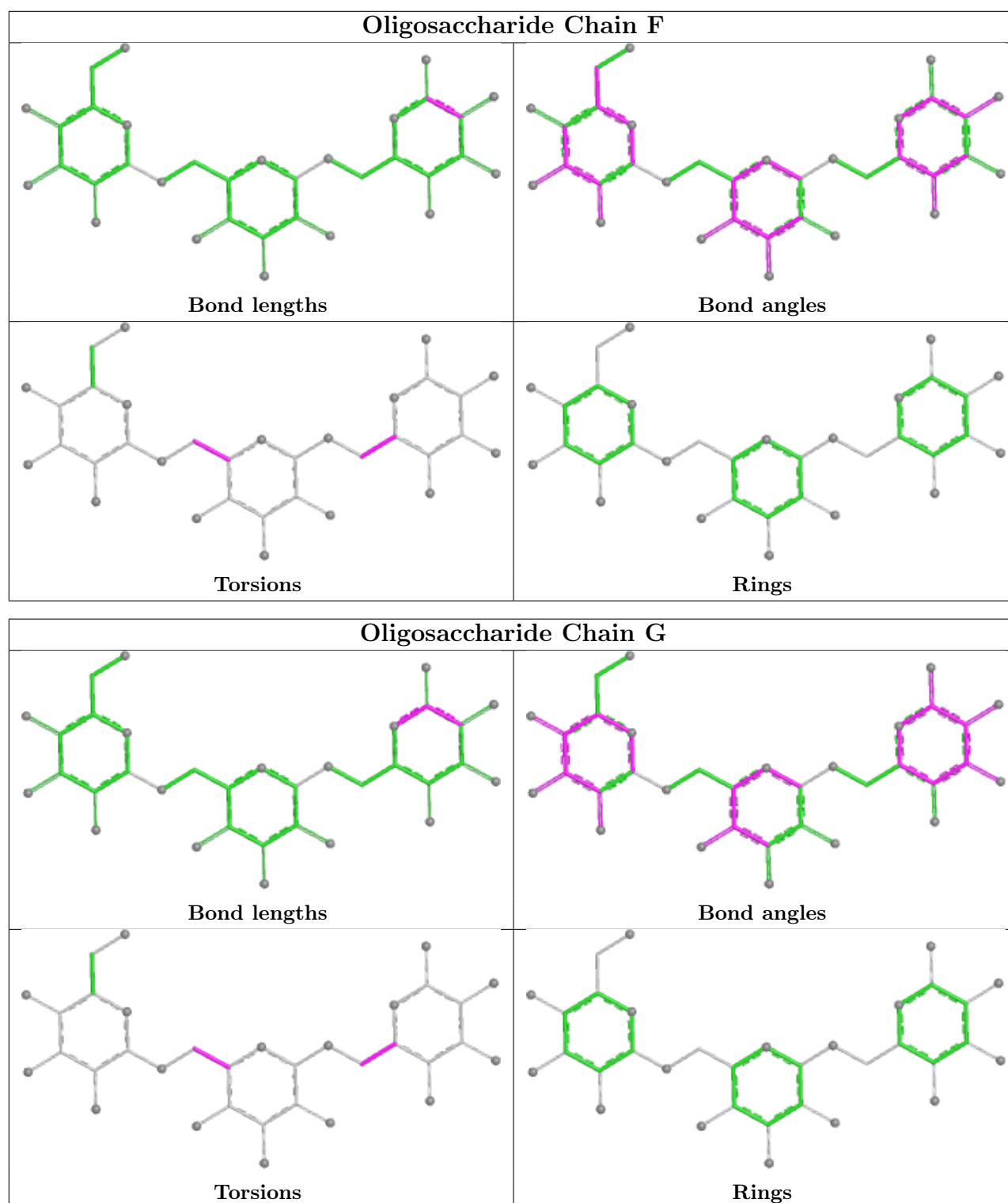
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1	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 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	679/685 (99%)	-0.55	6 (0%) 81 82	18, 31, 57, 89	0
1	B	681/685 (99%)	-0.25	8 (1%) 76 78	22, 42, 71, 97	0
1	C	684/685 (99%)	-0.43	3 (0%) 88 89	17, 38, 64, 88	0
1	D	679/685 (99%)	-0.50	6 (0%) 81 82	18, 35, 59, 91	0
All	All	2723/2740 (99%)	-0.43	23 (0%) 82 83	17, 36, 64, 97	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	195	ALA	3.7
1	C	703	ALA	3.5
1	B	20	SER	3.2
1	A	682	LYS	3.0
1	D	682	LYS	2.9
1	A	189	ALA	2.8
1	B	341	ARG	2.6
1	B	700	VAL	2.6
1	D	32	HIS	2.6
1	B	294	GLN	2.5
1	B	32	HIS	2.5
1	D	190	TYR	2.5
1	B	646	LYS	2.4
1	B	338	LYS	2.3
1	C	32	HIS	2.2
1	A	188	LYS	2.2
1	A	701	ALA	2.2
1	D	20	SER	2.1
1	C	683	LEU	2.1
1	B	659	LYS	2.1
1	A	197	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	683	LEU	2.0
1	A	190	TYR	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](#)

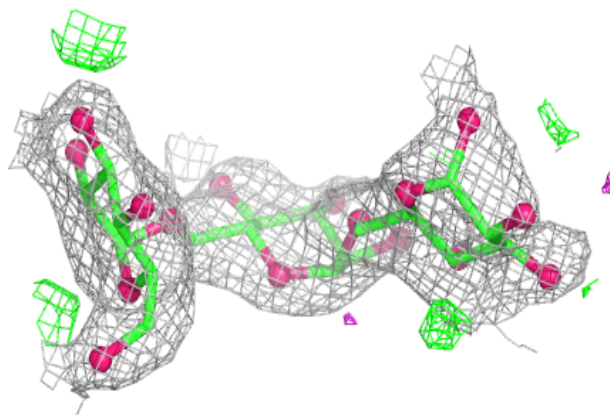
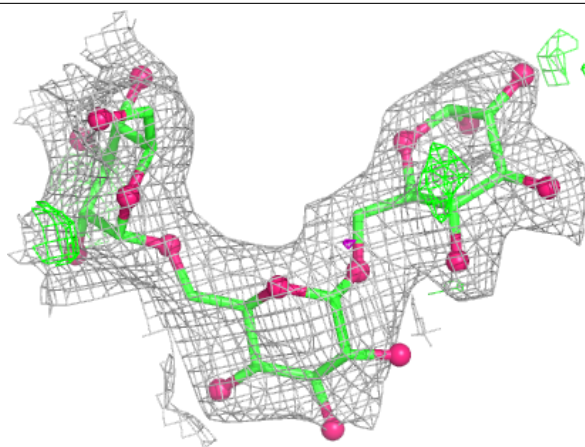
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	F	1	12/12	0.85	0.12	43,61,71,86	0
2	GLC	E	1	12/12	0.86	0.11	42,53,60,65	0
2	GLC	E	2	11/12	0.89	0.11	40,56,74,77	0
3	BGC	G	1	12/12	0.89	0.10	47,64,70,76	0
2	GLC	H	1	12/12	0.92	0.08	38,48,53,54	0
2	GLC	H	2	11/12	0.95	0.07	33,42,49,55	0
3	GLC	G	2	11/12	0.95	0.08	28,37,46,48	0
2	GLC	E	3	11/12	0.96	0.06	23,28,33,35	0
3	GLC	F	2	11/12	0.97	0.05	29,33,39,39	0
3	GLC	G	3	11/12	0.97	0.05	26,30,34,34	0
3	GLC	F	3	11/12	0.98	0.05	23,28,30,34	0
2	GLC	H	3	11/12	0.98	0.05	22,27,31,33	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.

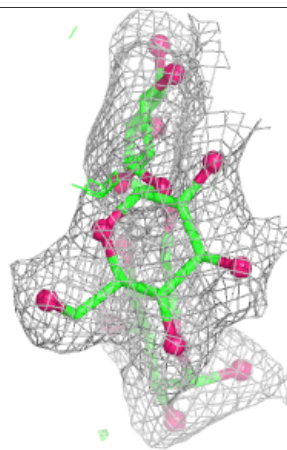
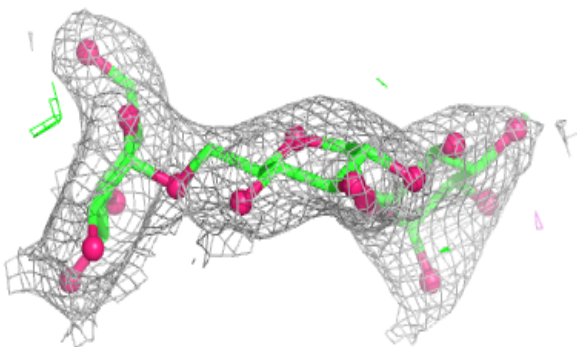
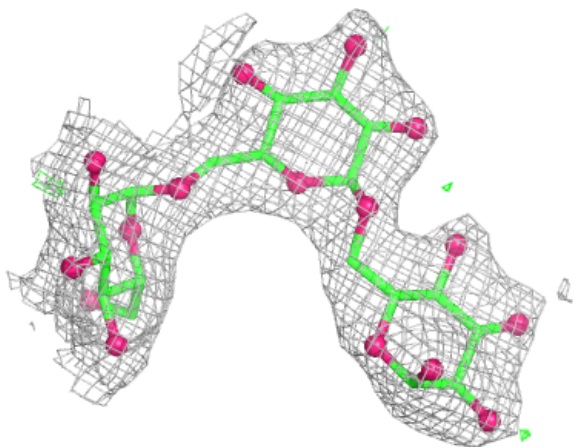
Electron density around Chain E:

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



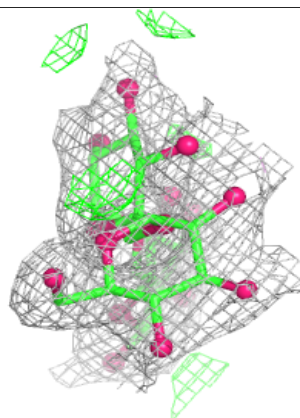
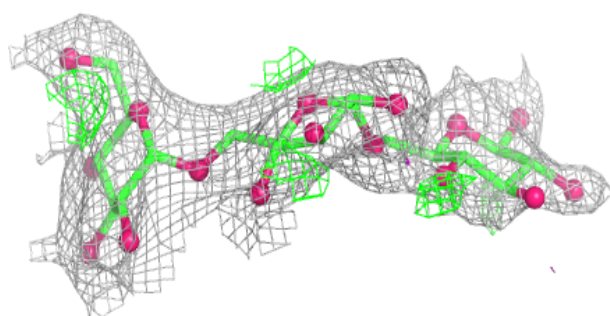
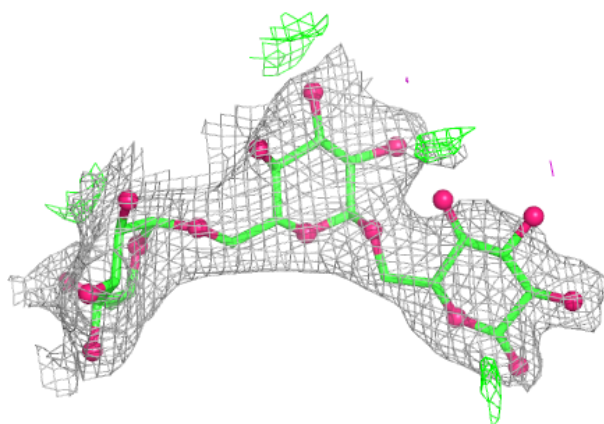
Electron density around Chain H:

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

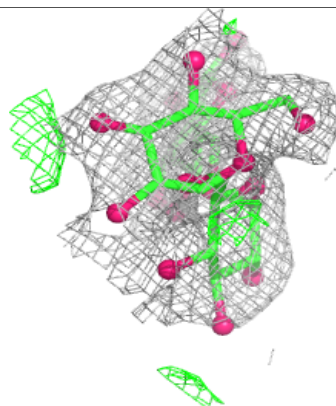
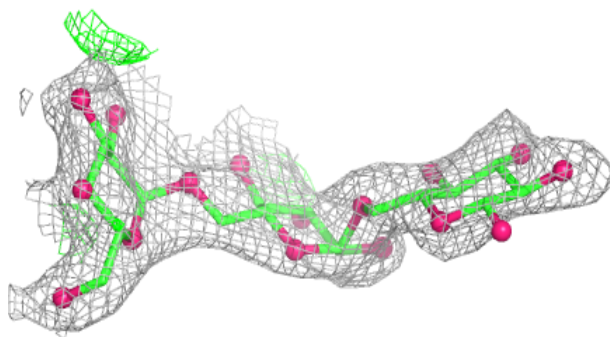
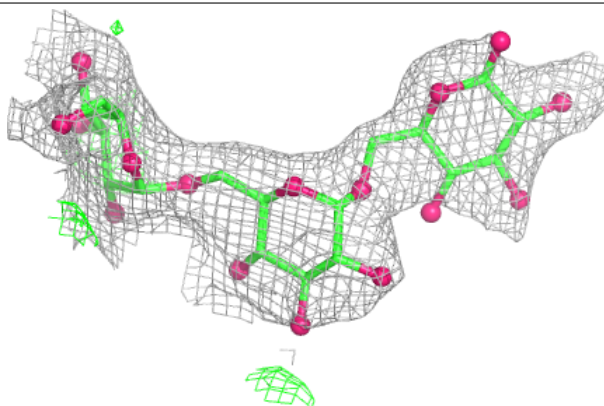


Electron density around Chain F:

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

**Electron density around Chain 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	CA	A	800	1/1	0.98	0.05	34,34,34,34	0
4	CA	B	800	1/1	0.99	0.04	34,34,34,34	0
4	CA	C	800	1/1	0.99	0.02	42,42,42,42	0
4	CA	D	800	1/1	0.99	0.06	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.