



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 30, 2024 – 08:13 PM JST

PDB ID : 8WG2
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.

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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

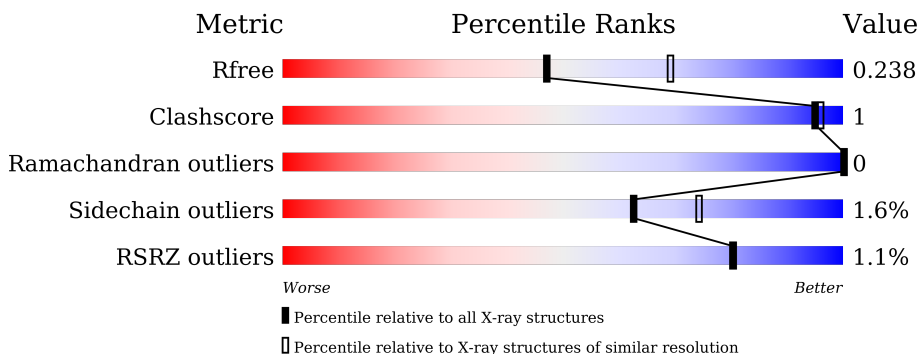
1 Overall quality at a glance

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.



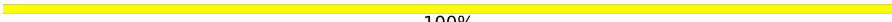
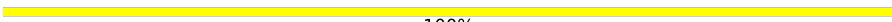
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	 92% 7% ..
1	B	685	 2% 91% 7% ..
1	C	685	 % 93% 7%
1	D	685	 % 91% 7% .
2	E	3	 100%
2	H	3	 100%

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Mol	Chain	Length	Quality of chain
3	F	3	 100%
3	G	3	 100%

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.

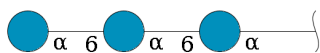
- Molecule 1 is a protein called Candidate alpha-glucosidase Glycoside hydrolase family 97.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
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.



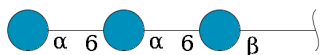
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	E	3	Total	C	O	0	0	0
			34	18	16			

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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 (three-letter code: 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.

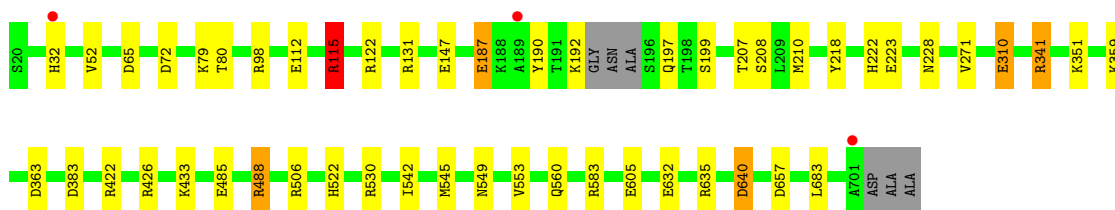
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	144	Total	O	0	0
			144	144		
5	B	88	Total	O	0	0
			88	88		
5	C	108	Total	O	0	0
			108	108		
5	D	132	Total	O	0	0
			132	132		

3 Residue-property plots [i](#)

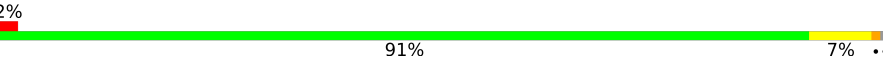
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

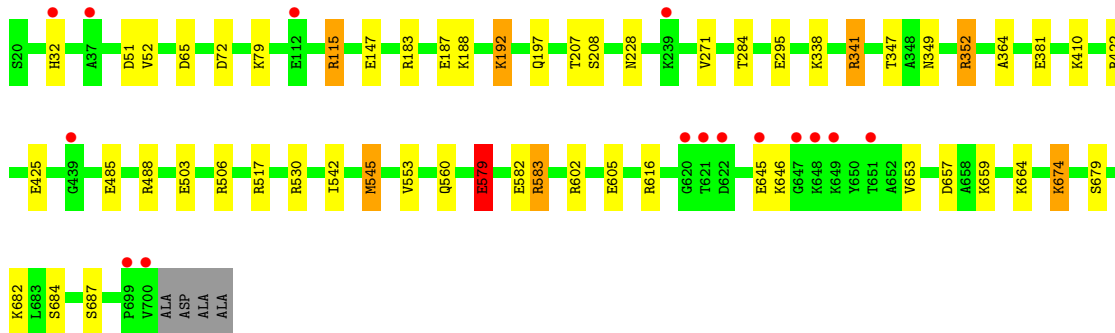
- Molecule 1: Candidate alpha-glucosidase Glycoside hydrolase family 97

Chain A: 

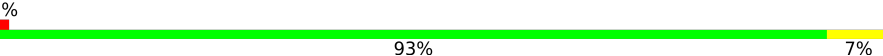


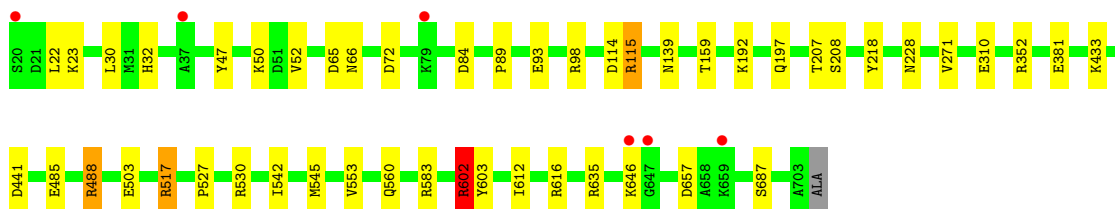
- Molecule 1: Candidate alpha-glucosidase Glycoside hydrolase family 97

Chain B: 

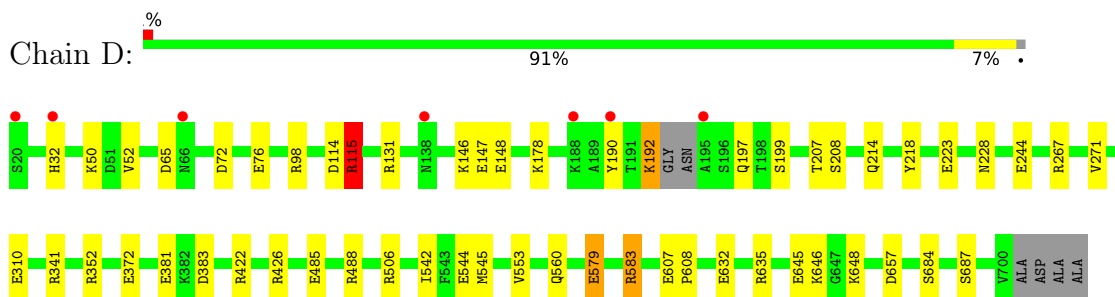


- Molecule 1: Candidate alpha-glucosidase Glycoside hydrolase family 97

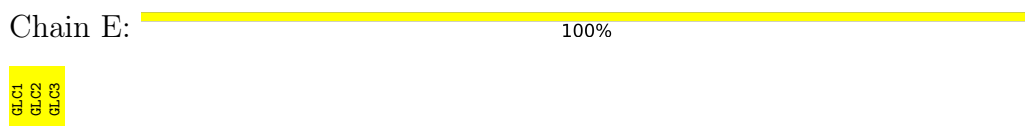
Chain C: 



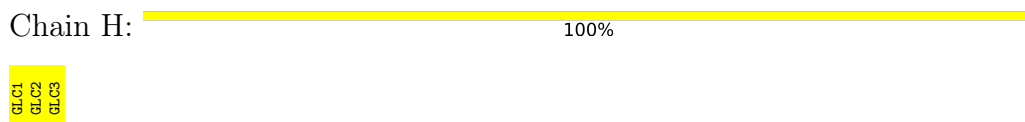
- Molecule 1: Candidate alpha-glucosidase Glycoside hydrolase family 97



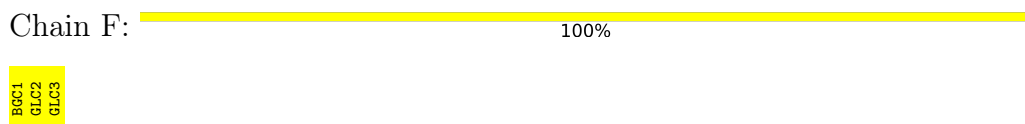
- Molecule 2: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose



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



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



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



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 49.11 – 2.45	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.16-2.45) 100.0 (49.11-2.45)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.85 (at 2.45Å)	Xtrriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.185 , 0.234 0.192 , 0.238	Depositor DCC
R_{free} test set	5817 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	33.6	Xtrriage
Anisotropy	0.456	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 30.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	22470	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.83	5/5597 (0.1%)	1.22	27/7589 (0.4%)
1	B	0.76	5/5610 (0.1%)	1.23	37/7608 (0.5%)
1	C	0.75	0/5628	1.18	23/7633 (0.3%)
1	D	0.82	8/5597 (0.1%)	1.21	32/7589 (0.4%)
All	All	0.79	18/22432 (0.1%)	1.21	119/30419 (0.4%)

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 (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	147	GLU	CD-OE2	9.70	1.36	1.25
1	D	544	GLU	CD-OE2	7.99	1.34	1.25
1	B	582	GLU	CD-OE1	7.62	1.34	1.25
1	D	485	GLU	CD-OE1	-7.22	1.17	1.25
1	B	147	GLU	CD-OE2	6.97	1.33	1.25
1	A	632	GLU	CD-OE1	6.49	1.32	1.25
1	A	426	ARG	NE-CZ	-5.77	1.25	1.33
1	B	582	GLU	CD-OE2	5.71	1.31	1.25
1	A	147	GLU	CD-OE1	5.63	1.31	1.25
1	A	485	GLU	CD-OE2	5.62	1.31	1.25
1	D	148	GLU	CD-OE2	-5.55	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	383	ASP	CG-OD1	5.40	1.37	1.25
1	B	381	GLU	CD-OE1	5.35	1.31	1.25
1	D	485	GLU	CD-OE2	5.35	1.31	1.25
1	D	544	GLU	CD-OE1	5.26	1.31	1.25
1	D	372	GLU	CD-OE2	-5.25	1.19	1.25
1	D	223	GLU	CD-OE2	-5.13	1.20	1.25
1	B	503	GLU	CD-OE1	5.00	1.31	1.25

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	352	ARG	NE-CZ-NH2	-12.71	113.95	120.30
1	B	579	GLU	CB-CA-C	-11.73	86.94	110.40
1	A	583	ARG	NE-CZ-NH2	-11.45	114.57	120.30
1	D	383	ASP	CB-CG-OD2	-10.46	108.89	118.30
1	C	352	ARG	NE-CZ-NH1	-10.25	115.17	120.30
1	B	583	ARG	NE-CZ-NH2	-10.18	115.21	120.30
1	D	485	GLU	CG-CD-OE1	-9.55	99.19	118.30
1	A	485	GLU	CG-CD-OE1	-9.50	99.30	118.30
1	A	640	ASP	CB-CA-C	9.19	128.78	110.40
1	A	122	ARG	NE-CZ-NH1	8.92	124.76	120.30
1	D	352	ARG	CD-NE-CZ	8.84	135.97	123.60
1	B	352	ARG	NE-CZ-NH1	8.75	124.67	120.30
1	C	352	ARG	NE-CZ-NH2	8.02	124.31	120.30
1	B	115	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	D	635	ARG	NE-CZ-NH2	-7.81	116.40	120.30
1	B	115	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	A	426	ARG	NE-CZ-NH1	-7.61	116.49	120.30
1	B	341	ARG	CB-CG-CD	7.58	131.32	111.60
1	C	32	HIS	CA-CB-CG	7.53	126.40	113.60
1	D	485	GLU	CG-CD-OE2	7.38	133.06	118.30
1	B	582	GLU	OE1-CD-OE2	7.37	132.14	123.30
1	A	383	ASP	CB-CG-OD2	-7.35	111.69	118.30
1	A	635	ARG	NE-CZ-NH1	7.23	123.92	120.30
1	A	115	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	A	506	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	A	485	GLU	CG-CD-OE2	7.08	132.47	118.30
1	D	115	ARG	NE-CZ-NH2	-7.05	116.77	120.30
1	D	657	ASP	CB-CG-OD2	-6.94	112.05	118.30
1	A	32	HIS	CA-CB-CG	6.90	125.33	113.60
1	A	351	LYS	CD-CE-NZ	6.84	127.44	111.70
1	D	32	HIS	CA-CB-CG	6.73	125.04	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	76	GLU	OE1-CD-OE2	-6.70	115.26	123.30
1	B	192	LYS	CB-CA-C	6.56	123.51	110.40
1	B	341	ARG	NE-CZ-NH2	6.43	123.52	120.30
1	A	228	ASN	CB-CA-C	6.35	123.11	110.40
1	A	310	GLU	OE1-CD-OE2	6.34	130.91	123.30
1	D	115	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	A	98	ARG	NE-CZ-NH1	-6.31	117.14	120.30
1	B	583	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	B	381	GLU	CG-CD-OE1	-6.26	105.77	118.30
1	D	50	LYS	CB-CG-CD	6.23	127.79	111.60
1	D	579	GLU	N-CA-CB	6.19	121.74	110.60
1	C	115	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	C	433	LYS	CD-CE-NZ	-6.18	97.48	111.70
1	C	635	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	D	147	GLU	CG-CD-OE1	-6.13	106.04	118.30
1	D	635	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	D	352	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	B	32	HIS	CA-CB-CG	6.08	123.93	113.60
1	B	485	GLU	CG-CD-OE2	6.07	130.43	118.30
1	D	98	ARG	NE-CZ-NH2	6.07	123.33	120.30
1	A	115	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	D	178	LYS	CG-CD-CE	-5.98	93.97	111.90
1	C	228	ASN	CB-CA-C	5.96	122.32	110.40
1	A	115	ARG	CG-CD-NE	5.94	124.27	111.80
1	B	352	ARG	CB-CA-C	-5.94	98.53	110.40
1	C	381	GLU	CG-CD-OE1	-5.93	106.44	118.30
1	D	131	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	C	159	THR	CA-CB-OG1	5.92	121.42	109.00
1	C	602	ARG	NE-CZ-NH2	5.90	123.25	120.30
1	D	50	LYS	CD-CE-NZ	5.88	125.22	111.70
1	D	352	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	D	244	GLU	CG-CD-OE1	5.85	130.00	118.30
1	D	506	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	D	646	LYS	CB-CG-CD	5.82	126.73	111.60
1	D	352	ARG	CA-CB-CG	5.80	126.16	113.40
1	C	381	GLU	OE1-CD-OE2	5.72	130.16	123.30
1	D	583	ARG	CA-CB-CG	5.71	125.96	113.40
1	B	284	THR	OG1-CB-CG2	-5.68	96.93	110.00
1	D	146	LYS	CD-CE-NZ	-5.68	98.64	111.70
1	A	530	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	C	22	LEU	CB-CG-CD2	-5.67	101.36	111.00
1	B	228	ASN	CB-CA-C	5.66	121.72	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	506	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	B	664	LYS	CB-CA-C	-5.65	99.09	110.40
1	A	131	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	D	544	GLU	OE1-CD-OE2	5.64	130.06	123.30
1	C	485	GLU	CG-CD-OE1	-5.62	107.07	118.30
1	A	359	LYS	CB-CG-CD	5.60	126.15	111.60
1	B	381	GLU	OE1-CD-OE2	5.58	130.00	123.30
1	D	383	ASP	CB-CG-OD1	5.58	123.32	118.30
1	C	530	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	657	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	C	441	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	B	674	LYS	CD-CE-NZ	5.47	124.28	111.70
1	C	616	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	B	545	MET	CG-SD-CE	5.46	108.94	100.20
1	B	659	LYS	CB-CA-C	-5.45	99.50	110.40
1	B	657	ASP	CB-CG-OD2	-5.43	113.41	118.30
1	C	657	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	B	147	GLU	CG-CD-OE1	-5.41	107.48	118.30
1	A	433	LYS	CD-CE-NZ	-5.40	99.28	111.70
1	B	51	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	A	363	ASP	CB-CG-OD1	-5.39	113.45	118.30
1	A	683	LEU	CB-CG-CD1	-5.38	101.85	111.00
1	A	422	ARG	NE-CZ-NH1	-5.35	117.62	120.30
1	C	47	TYR	CB-CG-CD2	5.35	124.21	121.00
1	D	50	LYS	CG-CD-CE	-5.34	95.88	111.90
1	B	530	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	C	485	GLU	CG-CD-OE2	5.33	128.96	118.30
1	B	422	ARG	CD-NE-CZ	5.32	131.04	123.60
1	D	381	GLU	CG-CD-OE1	-5.29	107.71	118.30
1	C	310	GLU	CB-CA-C	-5.29	99.82	110.40
1	B	602	ARG	N-CA-CB	5.25	120.05	110.60
1	A	341	ARG	CG-CD-NE	-5.25	100.78	111.80
1	D	228	ASN	CA-CB-CG	-5.24	101.88	113.40
1	B	187	GLU	OE1-CD-OE2	-5.19	117.07	123.30
1	B	183	ARG	NE-CZ-NH1	-5.15	117.72	120.30
1	C	89	PRO	N-CA-CB	5.13	109.46	103.30
1	D	310	GLU	CB-CA-C	-5.13	100.13	110.40
1	B	485	GLU	CG-CD-OE1	-5.10	108.09	118.30
1	A	605	GLU	CB-CA-C	-5.09	100.22	110.40
1	C	228	ASN	CA-CB-CG	-5.08	102.22	113.40
1	B	347	THR	CA-CB-OG1	5.07	119.66	109.00
1	B	616	ARG	NE-CZ-NH1	5.07	122.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	664	LYS	N-CA-CB	5.07	119.73	110.60
1	C	503	GLU	CG-CD-OE2	5.04	128.38	118.30
1	B	352	ARG	CA-CB-CG	5.04	124.48	113.40
1	B	425	GLU	OE1-CD-OE2	5.00	129.30	123.30

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5454	0	5238	17	0
1	B	5466	0	5248	12	0
1	C	5484	0	5262	12	0
1	D	5454	0	5238	13	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	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
5	A	144	0	0	2	0
5	B	88	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	108	0	0	0	0
5	D	132	0	0	1	0
All	All	22470	0	21100	53	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 1.

All (53) 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: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: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:A:522:HIS:ND1	5:A:901:HOH:O	2.32	0.56
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: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:C:207:THR:HA	1:C:208:SER:C	2.31	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:B:207:THR:HA	1:B:208:SER:C	2.32	0.49
1:A:190:TYR:HD2	1:A:192:LYS:HE3	1.76	0.49
1:D:207:THR:HA	1:D:208:SER:C	2.31	0.49
1:B:65:ASP:OD2	1:B:115:ARG:NH2	2.46	0.48
1:A:207:THR:HA	1:A:208:SER:C	2.34	0.47
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:79:LYS:HE3	1:A:80:THR:O	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:645:GLU:OE2	1:D:648:LYS:NZ	2.40	0.44
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:93:GLU:OE2	1:C:603:TYR:OH	2.32	0.43
1:C:542:ILE:O	1:C:560:GLN:HG3	2.18	0.43
1:D:542:ILE:O	1:D:560:GLN:HG3	2.19	0.43
1:C:545:MET:HG3	1:C:553:VAL:HB	2.01	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:A:210:MET:CE	1:A:218:TYR:HB3	2.51	0.41
1:A:542:ILE:O	1:A:560:GLN:HG3	2.21	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:D:607:GLU:HA	1:D:608:PRO:HD2	1.95	0.41
1:A:549:ASN:OD1	1:A:549:ASN:C	2.59	0.40
1:D:218:TYR:O	1:D:271:VAL:HA	2.21	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	580/582 (100%)	575 (99%)	5 (1%)	78	86
1	B	581/582 (100%)	567 (98%)	14 (2%)	49	61
1	C	582/582 (100%)	573 (98%)	9 (2%)	65	76
1	D	580/582 (100%)	571 (98%)	9 (2%)	62	74
All	All	2323/2328 (100%)	2286 (98%)	37 (2%)	62	74

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

Mol	Chain	Res	Type
1	A	72	ASP
1	A	187	GLU
1	A	341	ARG
1	A	488	ARG
1	A	640	ASP
1	B	72	ASP
1	B	79	LYS
1	B	188	LYS
1	B	295	GLU
1	B	338	LYS
1	B	341	ARG
1	B	488	ARG
1	B	517	ARG
1	B	579	GLU
1	B	583	ARG
1	B	645	GLU

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Mol	Chain	Res	Type
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	488	ARG
1	C	517	ARG
1	C	646	LYS
1	C	687	SER
1	D	72	ASP
1	D	114	ASP
1	D	192	LYS
1	D	214	GLN
1	D	267	ARG
1	D	488	ARG
1	D	579	GLU
1	D	684	SER
1	D	687	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	GLN
1	A	405	HIS
1	B	197	GLN
1	B	405	HIS
1	C	197	GLN
1	D	197	GLN
1	D	405	HIS
1	D	468	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

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	1.39	3 (25%)	17,17,17	3.01	9 (52%)
2	GLC	E	2	4,2	11,11,12	0.79	0	15,15,17	2.08	6 (40%)
2	GLC	E	3	4,2	11,11,12	0.86	0	15,15,17	1.84	4 (26%)
3	BGC	F	1	3	12,12,12	1.04	1 (8%)	17,17,17	1.88	4 (23%)
3	GLC	F	2	4,3	11,11,12	0.63	0	15,15,17	2.09	5 (33%)
3	GLC	F	3	4,3	11,11,12	0.65	0	15,15,17	2.20	5 (33%)
3	BGC	G	1	3	12,12,12	1.71	2 (16%)	17,17,17	1.99	7 (41%)
3	GLC	G	2	4,3	11,11,12	0.67	0	15,15,17	1.50	5 (33%)
3	GLC	G	3	4,3	11,11,12	0.55	0	15,15,17	2.48	6 (40%)
2	GLC	H	1	2	12,12,12	1.01	0	17,17,17	1.40	3 (17%)
2	GLC	H	2	4,2	11,11,12	0.48	0	15,15,17	2.34	6 (40%)
2	GLC	H	3	4,2	11,11,12	0.63	0	15,15,17	1.87	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	4,2	-	2/2/19/22	0/1/1/1
2	GLC	E	3	4,2	-	2/2/19/22	0/1/1/1
3	BGC	F	1	3	-	2/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	4,2	-	2/2/19/22	0/1/1/1
2	GLC	H	3	4,2	-	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	4.15	1.62	1.52
3	F	1	BGC	C1-C2	2.84	1.59	1.52
2	E	1	GLC	C3-C2	2.52	1.58	1.52
3	G	1	BGC	O5-C1	2.34	1.48	1.42
2	E	1	GLC	C4-C3	2.15	1.57	1.52
2	E	1	GLC	O1-C1	2.04	1.46	1.39

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	2	GLC	C1-O5-C5	6.28	120.70	112.19
2	E	1	GLC	O2-C2-C3	6.16	124.60	110.35
2	E	1	GLC	O2-C2-C1	-5.59	96.20	109.16
3	F	3	GLC	C1-O5-C5	4.75	118.63	112.19
3	G	3	GLC	C1-O5-C5	4.74	118.61	112.19
2	E	2	GLC	O3-C3-C4	4.62	121.04	110.35
3	F	2	GLC	C3-C4-C5	4.55	118.35	110.24
3	F	1	BGC	C3-C4-C5	-4.53	102.16	110.24
3	G	1	BGC	O3-C3-C2	4.40	120.51	110.35
3	F	3	GLC	O2-C2-C3	4.33	118.80	110.14
2	H	3	GLC	O2-C2-C3	4.21	118.56	110.14
3	F	1	BGC	O2-C2-C1	4.05	118.55	109.16
3	G	3	GLC	O4-C4-C5	-4.02	99.32	109.30
2	E	1	GLC	O3-C3-C2	3.98	119.54	110.35
2	E	1	GLC	C1-O5-C5	3.87	120.97	113.66
3	F	2	GLC	O4-C4-C3	-3.83	101.48	110.35
2	E	1	GLC	O4-C4-C5	-3.82	99.81	109.30
3	G	3	GLC	C2-C3-C4	-3.74	104.43	110.89
3	G	3	GLC	O2-C2-C3	3.50	117.15	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	GLC	O3-C3-C2	3.44	118.31	110.35
2	E	1	GLC	O1-C1-C2	3.44	118.72	109.03
3	G	3	GLC	O4-C4-C3	3.38	118.15	110.35
2	E	1	GLC	O5-C5-C4	3.23	115.56	109.69
2	H	2	GLC	O3-C3-C2	-3.16	103.94	109.99
3	G	1	BGC	O5-C1-C2	3.14	115.89	110.28
3	F	3	GLC	O5-C5-C6	-3.13	102.29	107.20
2	E	3	GLC	C1-O5-C5	3.13	116.43	112.19
2	E	3	GLC	O2-C2-C3	3.06	116.28	110.14
3	F	1	BGC	O4-C4-C5	3.04	116.83	109.30
2	H	3	GLC	O4-C4-C3	3.01	117.31	110.35
2	H	2	GLC	O4-C4-C5	-2.94	101.99	109.30
3	F	3	GLC	O3-C3-C2	2.86	115.46	109.99
3	G	2	GLC	O4-C4-C5	2.75	116.12	109.30
3	G	2	GLC	O4-C4-C3	-2.74	104.02	110.35
2	H	1	GLC	O2-C2-C3	2.72	116.64	110.35
2	E	2	GLC	C1-O5-C5	2.72	115.88	112.19
2	E	3	GLC	O3-C3-C2	2.71	115.19	109.99
3	F	2	GLC	C1-O5-C5	2.64	115.77	112.19
2	E	3	GLC	C6-C5-C4	-2.60	106.91	113.00
3	G	1	BGC	O1-C1-C2	2.59	116.34	109.03
3	F	3	GLC	C2-C3-C4	-2.56	106.46	110.89
3	F	1	BGC	C1-O5-C5	-2.50	108.94	113.66
2	H	2	GLC	O3-C3-C4	2.48	116.07	110.35
3	G	3	GLC	O3-C3-C4	2.43	115.98	110.35
3	G	2	GLC	C3-C4-C5	2.37	114.46	110.24
3	G	1	BGC	O2-C2-C3	2.32	115.72	110.35
2	H	1	GLC	O2-C2-C1	-2.32	103.78	109.16
2	E	2	GLC	O4-C4-C3	2.32	115.71	110.35
2	H	3	GLC	C1-O5-C5	2.32	115.33	112.19
3	G	1	BGC	O3-C3-C4	-2.31	105.00	110.35
2	H	2	GLC	O4-C4-C3	2.31	115.69	110.35
3	F	2	GLC	C1-C2-C3	2.28	112.47	109.67
3	F	2	GLC	O3-C3-C2	2.27	114.33	109.99
2	H	3	GLC	O4-C4-C5	-2.24	103.75	109.30
2	E	2	GLC	O3-C3-C2	-2.23	105.72	109.99
3	G	1	BGC	O5-C5-C4	2.20	113.69	109.69
2	H	3	GLC	C6-C5-C4	-2.16	107.95	113.00
2	E	1	GLC	O5-C1-C2	-2.13	106.48	110.28
3	G	1	BGC	C3-C4-C5	-2.11	106.48	110.24
2	E	2	GLC	O5-C5-C4	-2.09	105.74	110.83
3	G	2	GLC	O5-C5-C6	-2.09	103.93	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	GLC	O4-C4-C3	2.09	115.17	110.35
2	E	2	GLC	O2-C2-C1	-2.04	104.98	109.15
2	H	2	GLC	O2-C2-C1	-2.04	104.98	109.15
3	G	2	GLC	C1-O5-C5	2.01	114.91	112.19

There are no chirality outliers.

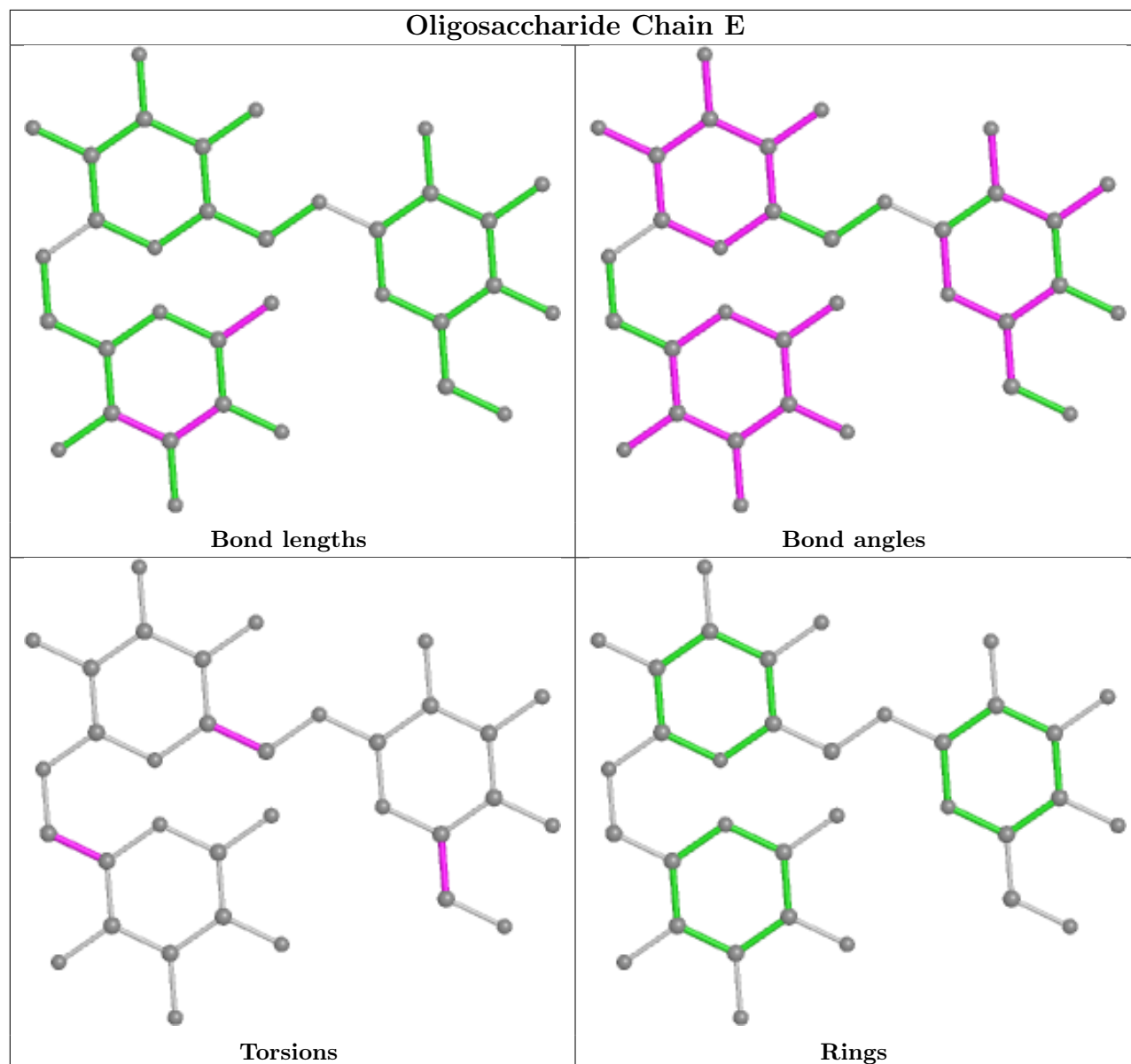
All (17) torsion outliers are listed below:

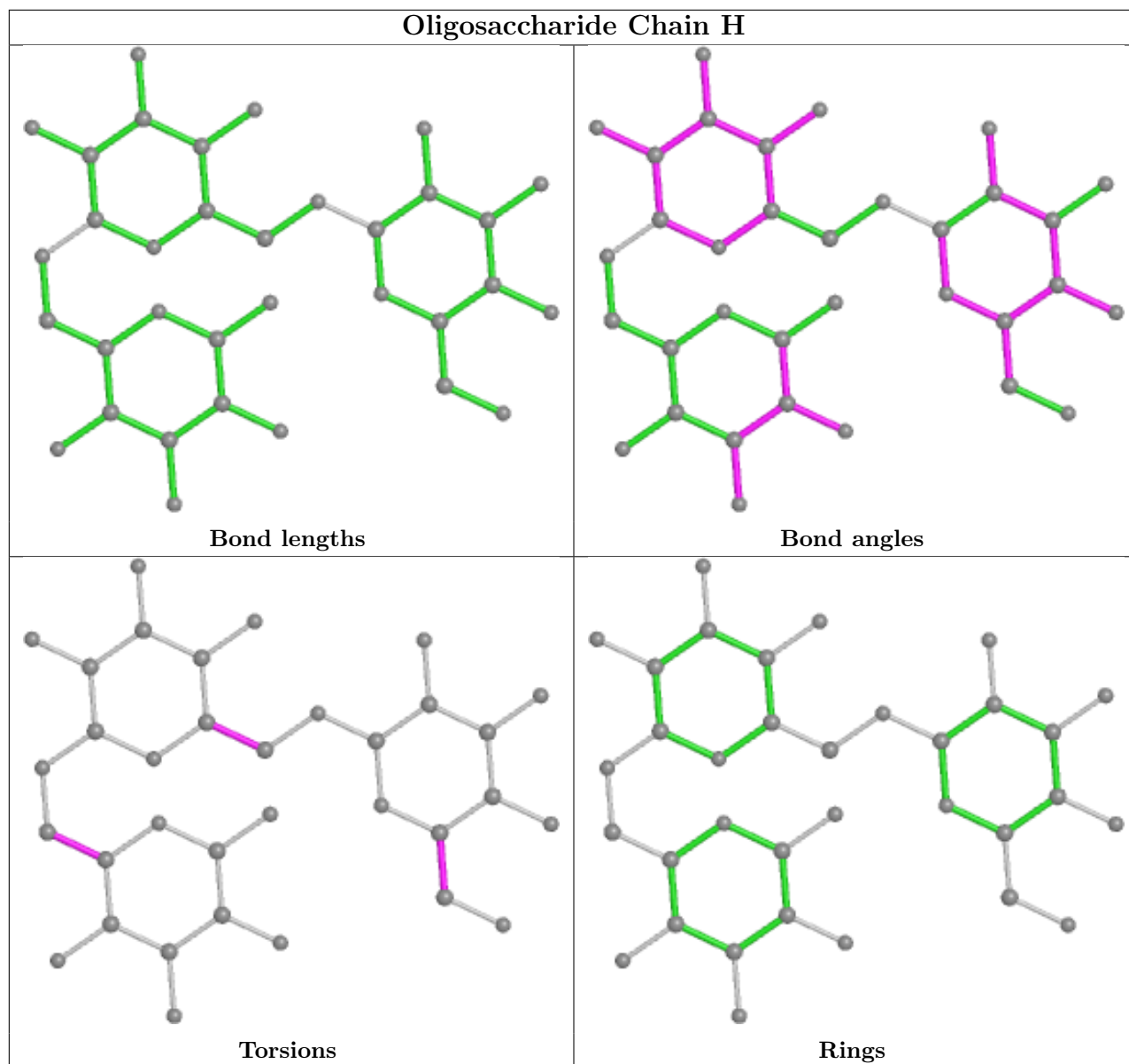
Mol	Chain	Res	Type	Atoms
2	H	2	GLC	O5-C5-C6-O6
3	G	1	BGC	C4-C5-C6-O6
3	G	1	BGC	O5-C5-C6-O6
2	H	2	GLC	C4-C5-C6-O6
3	F	1	BGC	O5-C5-C6-O6
3	F	1	BGC	C4-C5-C6-O6
2	E	1	GLC	O5-C5-C6-O6
2	E	3	GLC	O5-C5-C6-O6
2	H	1	GLC	O5-C5-C6-O6
3	G	2	GLC	O5-C5-C6-O6
3	F	2	GLC	O5-C5-C6-O6
2	H	3	GLC	O5-C5-C6-O6
2	E	3	GLC	C4-C5-C6-O6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

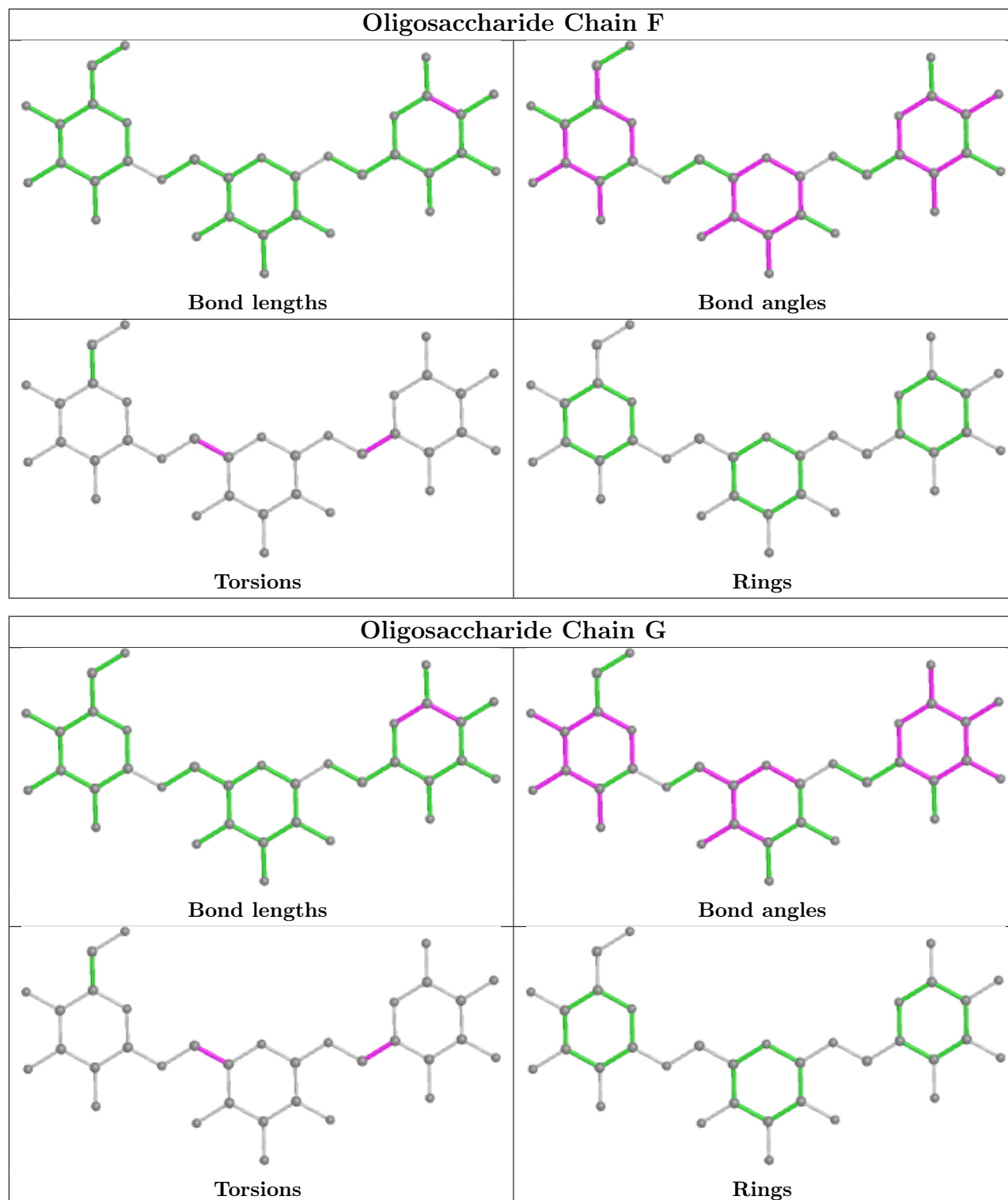
There are no ring outliers.

No monomer is involved in short contacts.

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







5.6 Ligand geometry [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%)	-0.38	3 (0%) 92 93	18, 31, 57, 89	0
1	B	681/685 (99%)	-0.11	15 (2%) 62 58	22, 42, 71, 97	0
1	C	684/685 (99%)	-0.39	6 (0%) 84 85	17, 38, 64, 88	0
1	D	679/685 (99%)	-0.36	7 (1%) 82 83	18, 35, 59, 91	0
All	All	2723/2740 (99%)	-0.31	31 (1%) 80 80	17, 36, 64, 97	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	700	VAL	4.3
1	D	20	SER	3.6
1	A	701	ALA	3.5
1	B	647	GLY	3.3
1	D	66	ASN	3.2
1	D	188	LYS	3.1
1	C	659	LYS	3.0
1	D	190	TYR	2.8
1	B	620	GLY	2.8
1	C	646	LYS	2.7
1	B	699	PRO	2.5
1	D	32	HIS	2.5
1	B	37	ALA	2.5
1	B	645	GLU	2.4
1	C	647	GLY	2.4
1	C	20	SER	2.3
1	B	651	THR	2.3
1	A	189	ALA	2.3
1	B	239	LYS	2.3
1	B	621	THR	2.3
1	B	622	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	195	ALA	2.2
1	B	439	GLY	2.2
1	B	648	LYS	2.2
1	C	79	LYS	2.1
1	B	649	LYS	2.1
1	C	37	ALA	2.1
1	B	112	GLU	2.1
1	B	32	HIS	2.0
1	D	138	ASN	2.0
1	A	32	HIS	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](#)

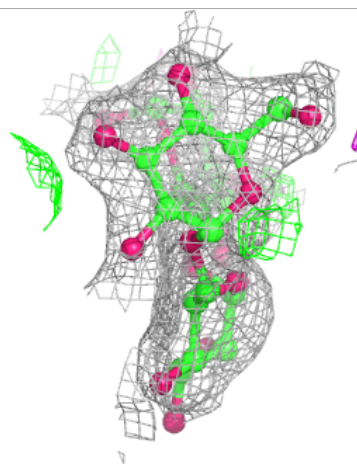
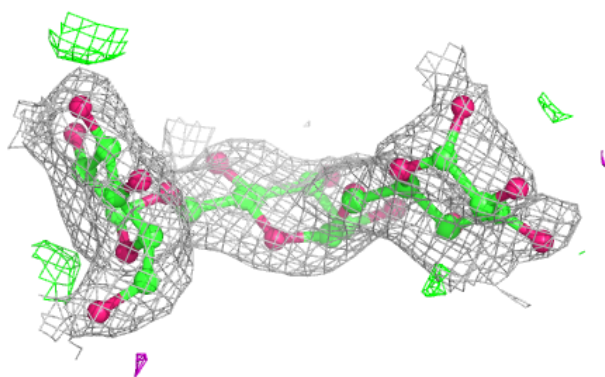
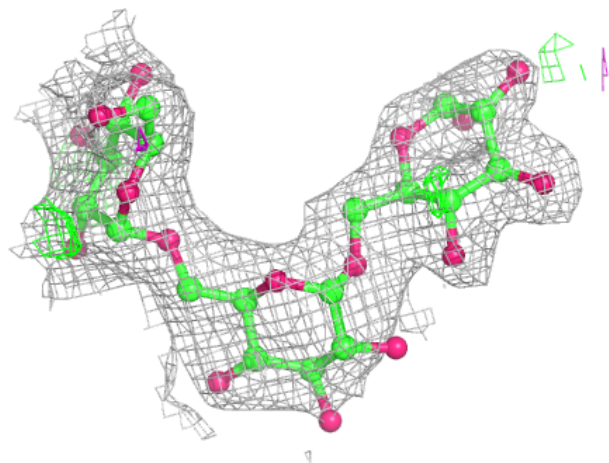
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BGC	F	1	12/12	0.83	0.22	43,61,71,86	0
3	BGC	G	1	12/12	0.84	0.20	47,64,70,76	0
2	GLC	E	1	12/12	0.86	0.14	42,53,60,65	0
2	GLC	H	1	12/12	0.92	0.13	38,48,53,54	0
2	GLC	E	2	11/12	0.93	0.15	40,56,74,77	0
3	GLC	G	2	11/12	0.95	0.14	28,37,46,48	0
2	GLC	H	2	11/12	0.96	0.11	33,42,49,55	0
2	GLC	E	3	11/12	0.97	0.12	23,28,33,35	0
3	GLC	F	2	11/12	0.97	0.14	29,33,39,39	0
2	GLC	H	3	11/12	0.98	0.14	22,27,31,33	0
3	GLC	G	3	11/12	0.98	0.10	26,30,34,34	0
3	GLC	F	3	11/12	0.99	0.13	23,28,30,34	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.

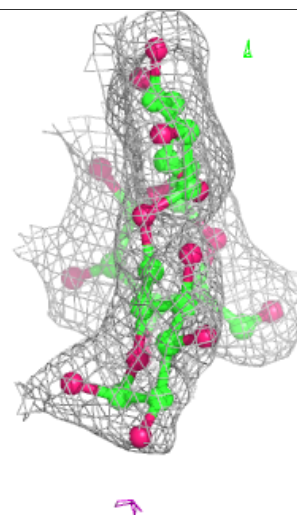
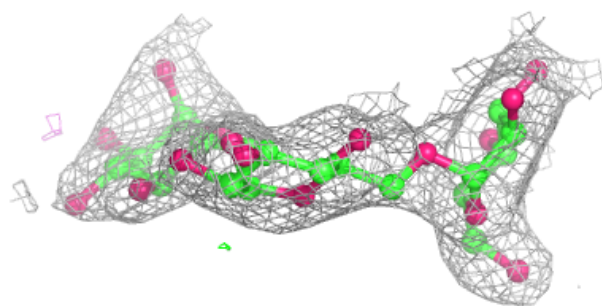
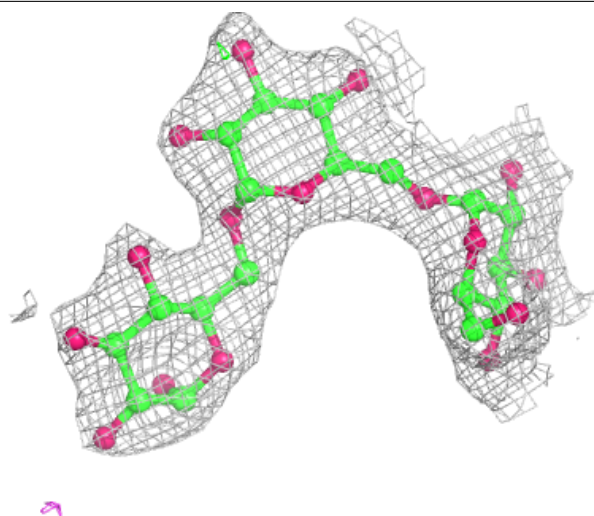
Electron density around Chain E:

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



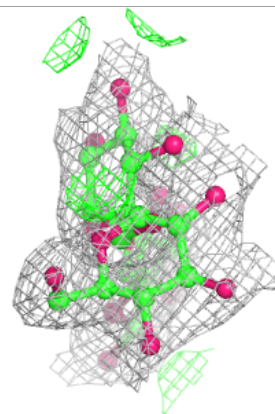
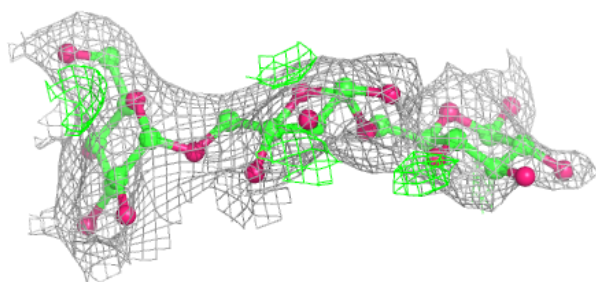
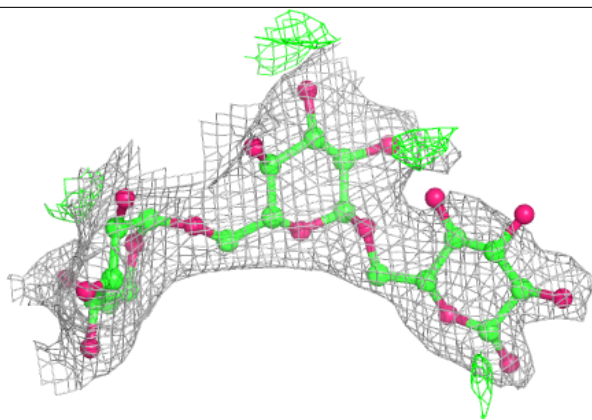
Electron density around Chain H:

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

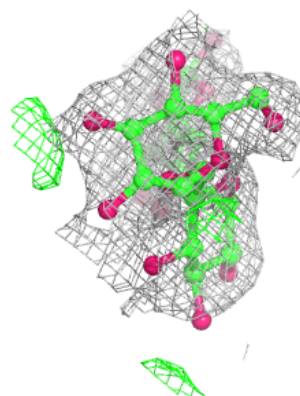
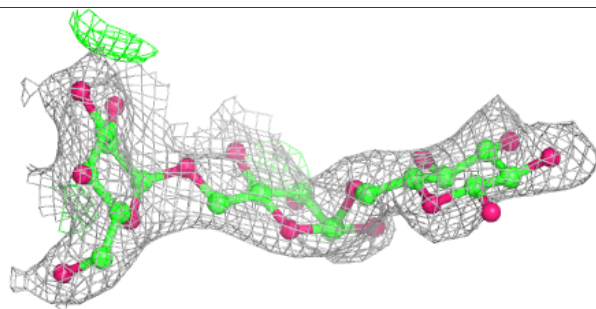
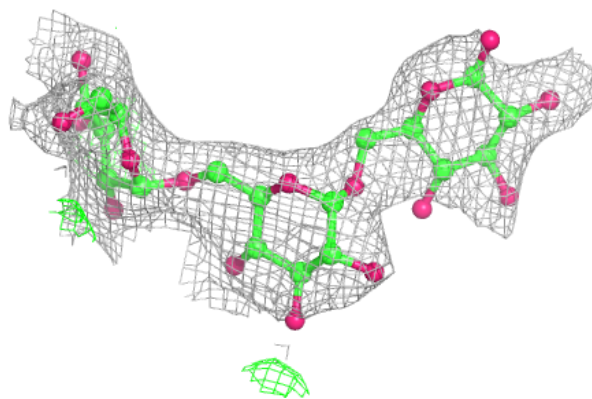


Electron density around Chain F:

$2mF_o-DF_c$ (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	0.97	0.08	34,34,34,34	0
4	CA	C	800	1/1	0.98	0.09	42,42,42,42	0
4	CA	D	800	1/1	0.98	0.04	39,39,39,39	0
4	CA	B	800	1/1	1.00	0.09	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.