



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:01 PM UTC

PDB ID : 1V3M / pdb_00001v3m
Title : Crystal structure of F283Y mutant cyclodextrin glycosyltransferase complexed with a pseudo-tetraose derived from acarbose
Authors : Kanai, R.; Haga, K.; Akiba, T.; Yamane, K.; Harata, K.
Deposited on : 2003-11-03
Resolution : 2.00 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

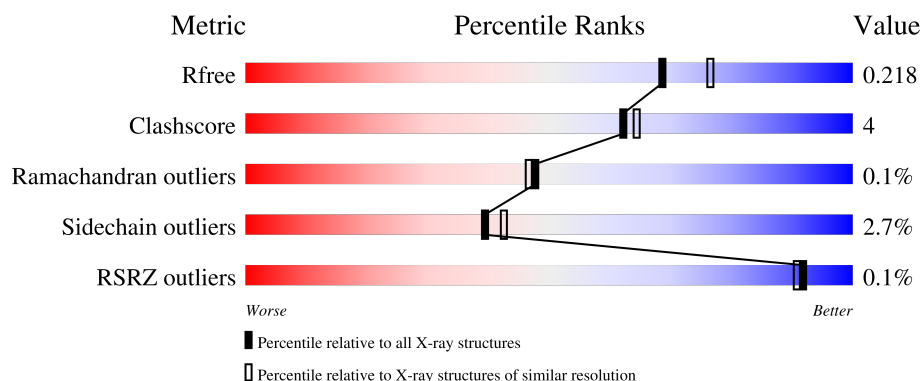
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

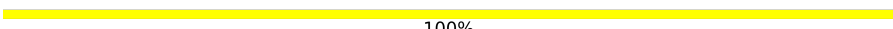
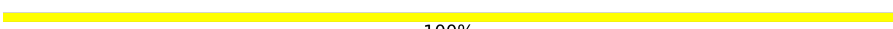
The reported resolution of this entry is 2.00 Å.

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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	686	 83% 15% .
1	B	686	 81% 16% .
2	C	2	 50% 50%
2	D	2	 100%
3	E	2	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GAL	C	1	X	-	-	-
2	GAL	D	1	X	-	-	-
6	GAL	A	731	X	-	-	-
6	GAL	B	811	X	-	-	-
6	GAL	B	831	X	-	-	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 11486 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.

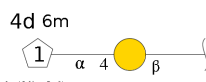
- Molecule 1 is a protein called Cyclomaltodextrin glucanotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	686	Total	C	N	O	S	0	0	0
			5313	3354	906	1037	16			
1	B	686	Total	C	N	O	S	0	0	0
			5313	3354	906	1037	16			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	283	TYR	PHE	engineered mutation	UNP P05618
A	452	PRO	ARG	SEE REMARK 999	UNP P05618
A	454	GLY	ALA	SEE REMARK 999	UNP P05618
B	283	TYR	PHE	engineered mutation	UNP P05618
B	452	PRO	ARG	SEE REMARK 999	UNP P05618
B	454	GLY	ALA	SEE REMARK 999	UNP P05618

- Molecule 2 is an oligosaccharide called 4,6-dideoxy-alpha-D-xylo-hexopyranose-(1-4)-beta-D-galactopyranose.



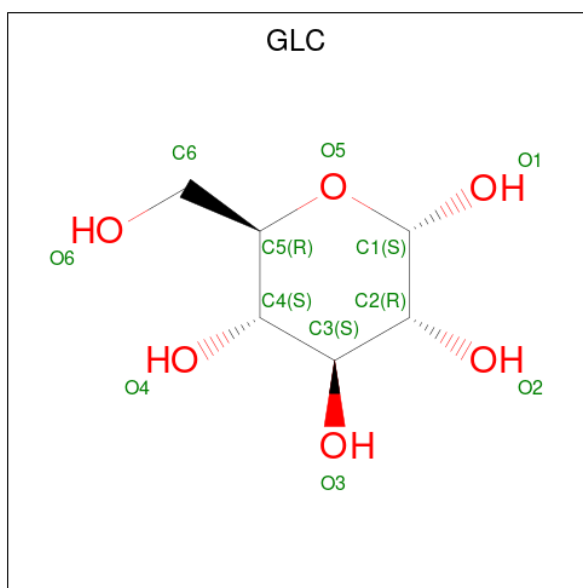
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	2	Total	C	O	0	0	0
			21	12	9			
2	D	2	Total	C	O	0	0	0
			21	12	9			

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



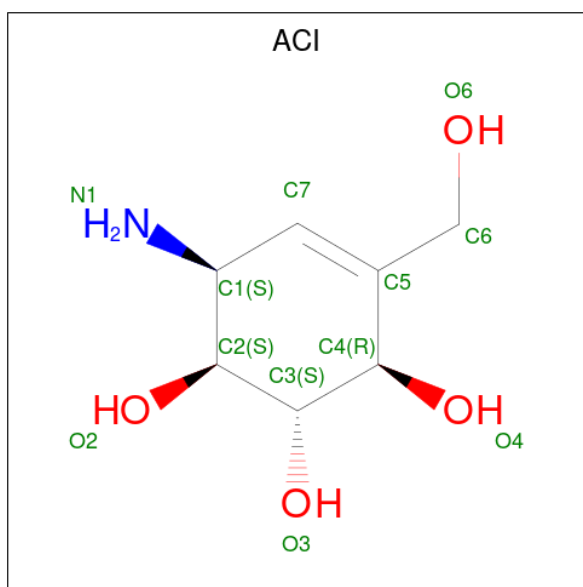
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	E	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 4 is alpha-D-glucopyranose (CCD ID: GLC) (formula: C₆H₁₂O₆).



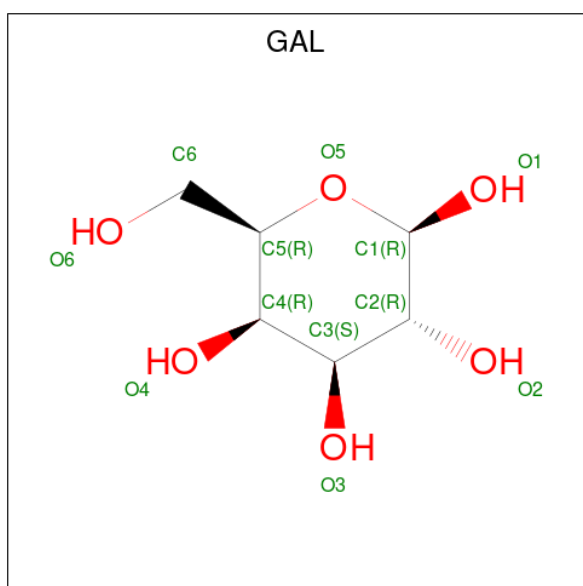
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			12	6	6		
4	A	1	Total	C	O	0	0
			12	6	6		
4	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is 6-AMINO-4-HYDROXYMETHYL-CYCLOHEX-4-ENE-1,2,3-TRIOL (CCD ID: ACI) (formula: C₇H₁₃NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			12	7	1	4		
5	B	1	Total	C	N	O	0	0
			12	7	1	4		

- Molecule 6 is beta-D-galactopyranose (CCD ID: GAL) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			12	6	6		
6	B	1	Total	C	O	0	0
			12	6	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			12	6	6		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Ca	0	0
			2	2		
7	B	2	Total	Ca	0	0
			2	2		

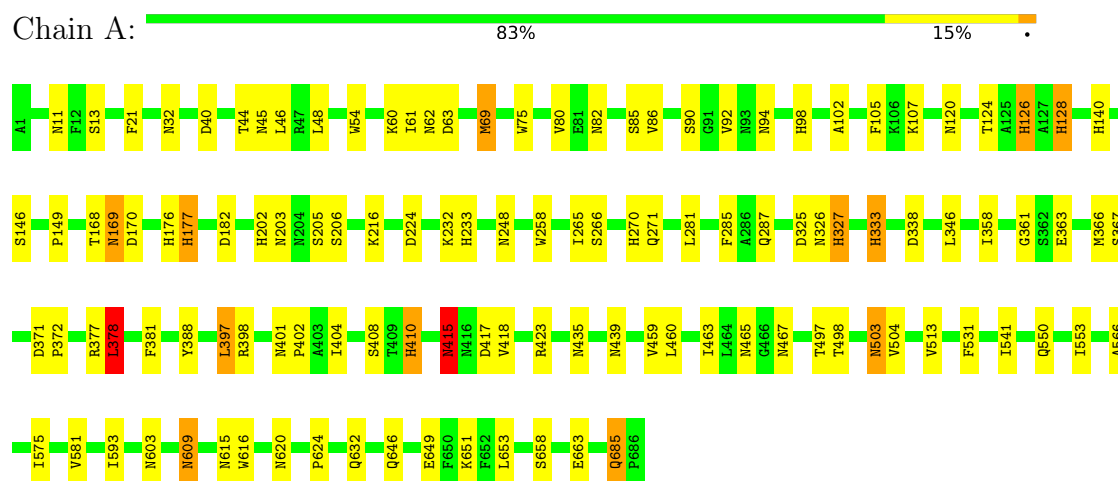
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	342	Total	O	0	0
			342	342		
8	B	343	Total	O	0	0
			343	343		

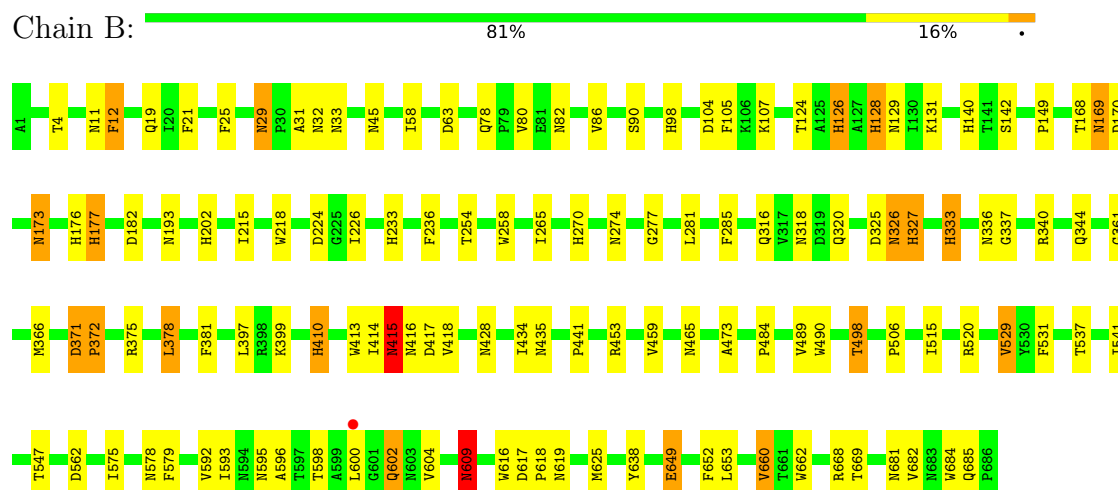
3 Residue-property plots

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: Cyclomaltodextrin glucanotransferase



• Molecule 1: Cyclomaltodextrin glucanotransferase



• Molecule 2: 4,6-dideoxy-alpha-D-xylo-hexopyranose-(1-4)-beta-D-galactopyranose



GAL1
GLD2

- Molecule 2: 4,6-dideoxy-alpha-D-xylo-hexopyranose-(1-4)-beta-D-galactopyranose

Chain D:  100%

GAL1
GLD2

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

Chain E:  100%

GLC1
GLC2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	64.09Å 73.60Å 78.30Å 84.93° 105.12° 101.00°	Depositor
Resolution (Å)	10.00 – 2.00 10.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	92.2 (10.00-2.00) 91.5 (10.00-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.61 (at 2.01Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.163 , 0.218 0.164 , 0.218	Depositor DCC
R_{free} test set	5093 reflections (6.08%)	wwPDB-VP
Wilson B-factor (Å ²)	20.3	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11486	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.75% 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: GLC, GAL, GLD, CA, ACI

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	0.97	14/5447 (0.3%)	1.61	76/7431 (1.0%)
1	B	0.97	17/5447 (0.3%)	1.61	76/7431 (1.0%)
All	All	0.97	31/10894 (0.3%)	1.61	152/14862 (1.0%)

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	140	HIS	CD2-NE2	-7.97	1.29	1.37
1	A	128	HIS	CD2-NE2	-7.45	1.29	1.37
1	A	140	HIS	CD2-NE2	-7.40	1.29	1.37
1	B	126	HIS	CD2-NE2	-7.27	1.29	1.37
1	A	327	HIS	CD2-NE2	-7.21	1.29	1.37
1	A	233	HIS	CD2-NE2	-7.17	1.29	1.37
1	B	128	HIS	CD2-NE2	-7.17	1.29	1.37
1	A	98	HIS	CD2-NE2	-7.07	1.30	1.37
1	A	333	HIS	CD2-NE2	-7.03	1.30	1.37
1	B	98	HIS	CD2-NE2	-6.86	1.30	1.37
1	B	327	HIS	CD2-NE2	-6.83	1.30	1.37
1	A	126	HIS	CD2-NE2	-6.69	1.30	1.37
1	B	176	HIS	CD2-NE2	-6.68	1.30	1.37
1	B	333	HIS	CD2-NE2	-6.67	1.30	1.37
1	A	176	HIS	CD2-NE2	-6.60	1.30	1.37
1	A	177	HIS	CD2-NE2	-6.51	1.30	1.37
1	B	410	HIS	CD2-NE2	-6.46	1.30	1.37
1	B	233	HIS	CD2-NE2	-6.39	1.30	1.37
1	B	270	HIS	CD2-NE2	-6.28	1.30	1.37
1	B	202	HIS	CD2-NE2	-6.20	1.31	1.37
1	A	270	HIS	CD2-NE2	-5.99	1.31	1.37
1	A	202	HIS	CD2-NE2	-5.88	1.31	1.37
1	A	176	HIS	CG-ND1	-5.86	1.31	1.38
1	B	177	HIS	CD2-NE2	-5.55	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	529	VAL	CA-CB	5.50	1.62	1.54
1	A	410	HIS	CD2-NE2	-5.48	1.31	1.37
1	B	270	HIS	CG-ND1	-5.42	1.32	1.38
1	B	140	HIS	CG-ND1	-5.37	1.32	1.38
1	B	128	HIS	CG-ND1	-5.24	1.32	1.38
1	A	177	HIS	CG-ND1	-5.23	1.32	1.38
1	B	414	ILE	CA-CB	5.08	1.60	1.55

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	415	ASN	CA-CB-CG	10.13	122.73	112.60
1	A	398	ARG	NE-CZ-NH2	-8.79	111.29	119.20
1	A	69	MET	CG-SD-CE	-8.78	81.58	100.90
1	A	415	ASN	OD1-CG-ND2	-8.75	113.85	122.60
1	B	98	HIS	CB-CG-CD2	-8.51	120.14	131.20
1	B	327	HIS	CB-CG-CD2	-8.10	120.67	131.20
1	A	415	ASN	CA-CB-CG	8.10	120.70	112.60
1	B	410	HIS	CB-CG-CD2	-8.09	120.68	131.20
1	B	415	ASN	OD1-CG-ND2	-7.85	114.75	122.60
1	B	325	ASP	CA-CB-CG	7.83	120.43	112.60
1	A	327	HIS	CB-CG-CD2	-7.78	121.09	131.20
1	A	216	LYS	CB-CG-CD	-7.62	93.76	111.30
1	B	326	ASN	OD1-CG-ND2	-7.57	115.03	122.60
1	A	98	HIS	CB-CG-CD2	-7.54	121.40	131.20
1	A	550	GLN	OE1-CD-NE2	-7.53	115.07	122.60
1	A	503	ASN	OD1-CG-ND2	-7.51	115.09	122.60
1	A	120	ASN	OD1-CG-ND2	-7.47	115.13	122.60
1	B	169	ASN	CA-CB-CG	-7.44	105.16	112.60
1	A	32	ASN	CA-CB-CG	7.28	119.88	112.60
1	B	29	ASN	OD1-CG-ND2	-7.25	115.35	122.60
1	B	126	HIS	CB-CG-CD2	-7.14	121.92	131.20
1	B	98	HIS	CB-CG-ND1	7.04	133.26	122.70
1	A	398	ARG	CG-CD-NE	-6.83	96.98	112.00
1	B	685	GLN	OE1-CD-NE2	-6.82	115.78	122.60
1	B	609	ASN	N-CA-C	6.82	121.20	113.02
1	B	541	ILE	N-CA-C	-6.73	97.22	107.73
1	A	685	GLN	OE1-CD-NE2	-6.72	115.88	122.60
1	A	531	PHE	N-CA-C	-6.71	96.11	107.99
1	B	609	ASN	OD1-CG-ND2	-6.66	115.94	122.60
1	A	266	SER	CA-C-N	6.62	126.39	119.05
1	A	266	SER	C-N-CA	6.62	126.39	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	415	ASN	CB-CG-ND2	6.59	126.28	116.40
1	B	435	ASN	OD1-CG-ND2	-6.57	116.03	122.60
1	A	333	HIS	CB-CG-CD2	-6.54	122.70	131.20
1	B	63	ASP	CA-CB-CG	6.54	119.14	112.60
1	B	371	ASP	CA-CB-CG	6.50	119.11	112.60
1	A	325	ASP	CA-CB-CG	6.47	119.07	112.60
1	B	327	HIS	CB-CG-ND1	6.46	132.38	122.70
1	A	126	HIS	CB-CG-CD2	-6.44	122.83	131.20
1	A	98	HIS	CB-CG-ND1	6.42	132.33	122.70
1	A	410	HIS	CA-CB-CG	6.36	120.16	113.80
1	B	326	ASN	CA-CB-CG	6.35	118.95	112.60
1	B	595	ASN	OD1-CG-ND2	-6.34	116.26	122.60
1	A	270	HIS	CA-CB-CG	-6.33	107.47	113.80
1	A	435	ASN	OD1-CG-ND2	-6.30	116.30	122.60
1	B	11	ASN	OD1-CG-ND2	-6.26	116.34	122.60
1	A	233	HIS	CA-CB-CG	-6.25	107.56	113.80
1	B	285	PHE	CA-CB-CG	6.23	120.03	113.80
1	A	86	VAL	N-CA-C	-6.21	98.92	107.99
1	A	63	ASP	CA-CB-CG	6.21	118.81	112.60
1	A	182	ASP	CA-CB-CG	6.20	118.80	112.60
1	B	193	ASN	OD1-CG-ND2	-6.18	116.42	122.60
1	A	258	TRP	N-CA-C	-6.10	97.16	108.02
1	A	338	ASP	CA-CB-CG	6.10	118.70	112.60
1	A	467	ASN	OD1-CG-ND2	-6.10	116.50	122.60
1	B	602	GLN	N-CA-C	-6.03	99.88	109.76
1	B	336	ASN	CA-CB-CG	-6.00	106.59	112.60
1	A	541	ILE	N-CA-C	-5.97	98.41	107.73
1	A	233	HIS	CB-CG-CD2	-5.94	123.48	131.20
1	A	327	HIS	CB-CG-ND1	5.93	131.60	122.70
1	B	277	GLY	N-CA-C	-5.91	106.37	114.64
1	B	265	ILE	N-CA-C	-5.89	99.06	107.77
1	B	274	ASN	OD1-CG-ND2	-5.86	116.74	122.60
1	B	416	ASN	N-CA-C	5.84	117.65	111.28
1	A	61	ILE	N-CA-C	-5.84	105.16	110.82
1	A	371	ASP	CA-CB-CG	5.84	118.44	112.60
1	B	78	GLN	OE1-CD-NE2	-5.84	116.76	122.60
1	A	620	ASN	CA-CB-CG	5.83	118.43	112.60
1	A	398	ARG	NE-CZ-NH1	5.83	127.33	121.50
1	B	173	ASN	CA-CB-CG	-5.80	106.80	112.60
1	A	550	GLN	CG-CD-NE2	5.78	125.06	116.40
1	B	142	SER	N-CA-C	5.77	113.20	108.07
1	B	45	ASN	OD1-CG-ND2	-5.74	116.86	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	129	ASN	N-CA-C	5.74	119.34	111.54
1	B	685	GLN	N-CA-C	-5.71	100.36	109.04
1	A	465	ASN	OD1-CG-ND2	-5.70	116.90	122.60
1	A	271	GLN	CB-CA-C	-5.68	101.36	110.79
1	A	498	THR	CA-C-O	-5.67	115.43	120.19
1	A	203	ASN	N-CA-C	-5.67	106.32	113.18
1	A	62	ASN	OD1-CG-ND2	-5.66	116.94	122.60
1	A	415	ASN	CB-CG-ND2	5.63	124.85	116.40
1	B	344	GLN	CB-CA-C	-5.62	101.30	110.85
1	B	32	ASN	CA-CB-CG	5.61	118.21	112.60
1	A	202	HIS	CB-CG-CD2	-5.60	123.92	131.20
1	B	498	THR	CA-CB-OG1	-5.58	101.23	109.60
1	B	258	TRP	N-CA-C	-5.58	98.10	108.02
1	A	140	HIS	CB-CG-CD2	-5.57	123.95	131.20
1	A	270	HIS	CB-CG-CD2	-5.56	123.97	131.20
1	A	377	ARG	CA-C-N	-5.56	112.60	120.49
1	A	377	ARG	C-N-CA	-5.56	112.60	120.49
1	A	281	LEU	N-CA-C	-5.55	101.64	109.96
1	B	182	ASP	CA-CB-CG	5.54	118.14	112.60
1	B	684	TRP	CG-CD2-CE3	5.53	139.43	133.90
1	A	326	ASN	CA-CB-CG	5.52	118.12	112.60
1	B	86	VAL	N-CA-C	-5.51	99.95	107.99
1	A	378	LEU	CA-CB-CG	5.49	135.52	116.30
1	A	128	HIS	CB-CG-CD2	-5.49	124.06	131.20
1	A	616	TRP	CG-CD2-CE3	5.49	139.39	133.90
1	B	333	HIS	CB-CG-CD2	-5.48	124.07	131.20
1	B	11	ASN	CB-CG-ND2	5.47	124.61	116.40
1	B	202	HIS	CB-CG-CD2	-5.46	124.11	131.20
1	A	169	ASN	CA-CB-CG	-5.45	107.15	112.60
1	A	285	PHE	CA-CB-CG	5.45	119.25	113.80
1	A	75	TRP	N-CA-C	-5.42	99.46	108.34
1	B	490	TRP	CE2-CD2-CG	-5.41	100.70	107.20
1	A	205	SER	N-CA-C	5.41	117.93	111.71
1	B	410	HIS	N-CA-CB	-5.41	102.47	110.90
1	B	649	GLU	CA-CB-CG	-5.40	103.30	114.10
1	A	503	ASN	CB-CG-ND2	5.40	124.50	116.40
1	A	287	GLN	OE1-CD-NE2	-5.40	117.20	122.60
1	B	579	PHE	CA-CB-CG	-5.38	108.42	113.80
1	A	439	ASN	CB-CA-C	-5.37	100.63	109.65
1	A	685	GLN	CG-CD-NE2	5.36	124.44	116.40
1	B	531	PHE	N-CA-C	-5.34	97.09	107.62
1	A	632	GLN	OE1-CD-NE2	-5.34	117.26	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	609	ASN	CB-CG-ND2	5.34	124.41	116.40
1	A	102	ALA	N-CA-C	5.33	118.01	110.50
1	A	566	ALA	N-CA-C	-5.33	100.22	108.90
1	B	326	ASN	CB-CG-ND2	5.27	124.31	116.40
1	B	233	HIS	CB-CG-CD2	-5.27	124.35	131.20
1	A	615	ASN	OD1-CG-ND2	-5.27	117.33	122.60
1	B	236	PHE	CA-CB-CG	5.24	119.04	113.80
1	B	104	ASP	CA-CB-CG	5.22	117.82	112.60
1	B	12	PHE	CA-CB-CG	5.21	119.01	113.80
1	A	616	TRP	CE2-CD2-CG	-5.20	100.96	107.20
1	A	265	ILE	N-CA-C	-5.20	100.63	108.12
1	A	45	ASN	OD1-CG-ND2	-5.20	117.40	122.60
1	A	75	TRP	CG-CD2-CE3	5.20	139.10	133.90
1	A	248	ASN	OD1-CG-ND2	-5.20	117.40	122.60
1	B	318	ASN	OD1-CG-ND2	-5.20	117.40	122.60
1	B	281	LEU	N-CA-C	-5.19	102.17	109.96
1	A	581	VAL	N-CA-C	-5.19	100.29	108.23
1	B	685	GLN	CG-CD-NE2	5.19	124.19	116.40
1	B	410	HIS	CB-CG-ND1	5.18	130.48	122.70
1	B	617	ASP	CA-C-N	5.17	124.97	119.28
1	B	617	ASP	C-N-CA	5.17	124.97	119.28
1	B	616	TRP	CE2-CD2-CG	-5.14	101.03	107.20
1	A	54	TRP	CE2-CD2-CG	-5.10	101.08	107.20
1	B	490	TRP	CG-CD2-CE3	5.10	139.00	133.90
1	A	265	ILE	CA-C-O	5.08	125.75	120.36
1	B	218	TRP	CG-CD2-CE3	5.08	138.98	133.90
1	B	660	VAL	N-CA-C	-5.07	101.11	108.36
1	B	19	GLN	OE1-CD-NE2	-5.06	117.54	122.60
1	B	33	ASN	OD1-CG-ND2	-5.06	117.54	122.60
1	B	337	GLY	N-CA-C	-5.04	105.00	113.02
1	A	646	GLN	CA-CB-CG	5.04	124.18	114.10
1	B	320	GLN	OE1-CD-NE2	-5.04	117.56	122.60
1	B	428	ASN	OD1-CG-ND2	-5.04	117.56	122.60
1	B	270	HIS	CA-CB-CG	-5.03	108.77	113.80
1	A	646	GLN	CB-CG-CD	-5.02	104.07	112.60
1	B	684	TRP	CE2-CD2-CG	-5.01	101.19	107.20
1	B	413	TRP	CE2-CD2-CG	-5.00	101.19	107.20

There are no chirality outliers.

There are no planarity outliers.

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	5313	0	5050	40	0
1	B	5313	0	5050	46	0
2	C	21	0	20	1	0
2	D	21	0	20	0	0
3	E	23	0	21	0	0
4	A	35	0	34	2	0
4	B	11	0	10	0	0
5	A	12	0	11	1	0
5	B	12	0	11	0	0
6	A	12	0	12	0	0
6	B	24	0	24	0	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
8	A	342	0	0	6	0
8	B	343	0	0	4	0
All	All	11486	0	10263	87	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 4.

All (87) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:GLN:HE22	1:B:578:ASN:HD22	1.33	0.75
1:B:149:PRO:HG3	1:B:168:THR:HG21	1.73	0.71
1:B:340:ARG:HH12	1:B:465:ASN:HD22	1.37	0.71
1:A:90:SER:HB2	4:A:711:GLC:O3	1.96	0.66
1:A:177:HIS:HD2	8:A:1327:HOH:O	1.84	0.59
1:A:333:HIS:HD2	8:A:1528:HOH:O	1.86	0.59
1:A:503:ASN:HD22	1:A:504:VAL:H	1.53	0.57
1:B:333:HIS:HD2	8:B:1591:HOH:O	1.88	0.57
1:A:11:ASN:ND2	8:A:1522:HOH:O	2.37	0.57
1:B:124:THR:O	1:B:128:HIS:HD2	1.88	0.56
1:B:397:LEU:HD21	1:B:459:VAL:HG21	1.88	0.55
1:B:126:HIS:HE1	1:B:224:ASP:OD1	1.90	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:MET:HE1	1:A:363:GLU:HG3	1.88	0.55
1:A:170:ASP:OD1	1:A:177:HIS:HE1	1.90	0.54
1:A:69:MET:HE3	1:A:388:TYR:CD1	2.43	0.53
1:B:609:ASN:ND2	1:B:649:GLU:H	2.07	0.53
1:A:609:ASN:ND2	1:A:649:GLU:H	2.06	0.53
1:B:593:ILE:HG21	1:B:604:VAL:HG11	1.90	0.53
1:A:126:HIS:HE1	1:A:224:ASP:OD2	1.92	0.52
1:B:170:ASP:OD1	1:B:177:HIS:HE1	1.92	0.52
1:B:340:ARG:HH12	1:B:465:ASN:ND2	2.06	0.52
1:A:603:ASN:HB3	1:A:624:PRO:HB3	1.92	0.52
1:A:361:GLY:HA3	1:A:366:MET:SD	2.50	0.51
1:A:415:ASN:HD22	1:A:418:VAL:H	1.58	0.51
1:B:625:MET:HG2	1:B:638:TYR:HB2	1.91	0.51
1:B:80:VAL:HB	1:B:105:PHE:HA	1.92	0.51
1:A:415:ASN:ND2	1:A:417:ASP:H	2.09	0.50
1:B:361:GLY:HA3	1:B:366:MET:SD	2.52	0.50
1:B:649:GLU:HG2	1:B:669:THR:HG22	1.94	0.50
5:A:702:ACI:HN11	2:C:1:GAL:H61	1.77	0.49
1:B:4:THR:HB	1:B:399:LYS:HD2	1.95	0.48
1:A:124:THR:O	1:A:128:HIS:HD2	1.96	0.48
1:A:60:LYS:HA	1:A:60:LYS:HD3	1.75	0.48
1:A:92:VAL:HG13	1:A:94:ASN:HD21	1.79	0.47
1:B:378:LEU:HD21	1:B:381:PHE:CZ	2.49	0.47
1:B:596:ALA:HB1	1:B:604:VAL:HG21	1.95	0.47
1:A:378:LEU:HD11	1:A:381:PHE:CZ	2.49	0.47
1:A:69:MET:HE1	1:A:363:GLU:CG	2.45	0.47
1:B:80:VAL:HA	1:B:107:LYS:O	2.15	0.47
1:B:593:ILE:HD13	1:B:652:PHE:CD2	2.50	0.46
1:A:149:PRO:HG3	1:A:168:THR:HG21	1.97	0.46
1:B:58:ILE:HG23	1:B:124:THR:HG21	1.98	0.45
1:A:92:VAL:HG13	1:A:94:ASN:ND2	2.31	0.45
1:A:397:LEU:HB3	1:A:404:ILE:HD12	1.99	0.45
1:B:441:PRO:HD3	1:B:484:PRO:HG3	1.98	0.45
1:A:346:LEU:HD22	1:A:358:ILE:HD12	1.99	0.45
1:B:506:PRO:HD2	1:B:515:ILE:HG22	1.98	0.45
1:B:29:ASN:HD21	1:B:31:ALA:HB3	1.82	0.45
1:A:408:SER:O	1:A:423:ARG:HA	2.17	0.45
1:B:453:ARG:HH12	1:B:473:ALA:HB2	1.80	0.45
1:B:649:GLU:HA	1:B:668:ARG:O	2.17	0.45
1:A:397:LEU:HD21	1:A:459:VAL:HG11	1.99	0.45
1:A:663:GLU:HB2	1:A:685:GLN:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:651:LYS:HZ1	4:A:721:GLC:H61	1.81	0.44
1:B:592:VAL:HB	1:B:681:ASN:HA	2.00	0.44
1:B:25:PHE:HB3	8:B:1563:HOH:O	2.17	0.44
1:B:418:VAL:HA	1:B:434:ILE:O	2.18	0.44
1:A:40:ASP:HB2	1:A:48:LEU:HD12	1.99	0.43
1:A:232:LYS:HD3	8:A:1623:HOH:O	2.18	0.43
1:A:415:ASN:ND2	1:A:418:VAL:H	2.16	0.43
1:B:410:HIS:HB2	8:B:1139:HOH:O	2.18	0.43
1:A:80:VAL:HB	1:A:105:PHE:HA	2.00	0.43
1:A:410:HIS:HB2	8:A:1367:HOH:O	2.19	0.43
1:B:226:ILE:HB	1:B:254:THR:HG23	2.00	0.43
1:B:21:PHE:HE1	1:B:327:HIS:HB3	1.84	0.42
1:B:598:THR:HB	1:B:602:GLN:HB3	1.99	0.42
1:B:653:LEU:HD12	1:B:660:VAL:HG13	2.02	0.42
1:A:69:MET:HE1	1:A:363:GLU:CB	2.49	0.42
1:B:215:ILE:HD12	1:B:215:ILE:HA	1.88	0.42
1:A:21:PHE:HE2	1:A:327:HIS:HB3	1.84	0.42
1:B:459:VAL:HG22	1:B:489:VAL:HB	2.02	0.42
1:B:415:ASN:ND2	1:B:417:ASP:H	2.19	0.41
1:A:126:HIS:HD2	8:A:1143:HOH:O	2.01	0.41
1:B:371:ASP:HA	1:B:372:PRO:HA	1.93	0.41
1:A:401:ASN:HA	1:A:402:PRO:HD2	1.94	0.41
1:B:177:HIS:HD2	8:B:1579:HOH:O	2.04	0.41
1:B:618:PRO:HG3	1:B:662:TRP:CZ2	2.56	0.41
1:A:80:VAL:HA	1:A:107:LYS:O	2.21	0.41
1:A:146:SER:HA	1:A:168:THR:OG1	2.20	0.41
1:A:513:VAL:HB	1:A:553:ILE:HD12	2.03	0.41
1:A:460:LEU:O	1:A:463:ILE:HG12	2.20	0.40
1:B:12:PHE:CZ	1:B:131:LYS:HD3	2.56	0.40
1:B:593:ILE:HD12	1:B:682:VAL:HG23	2.02	0.40
1:B:372:PRO:HA	1:B:375:ARG:HD2	2.04	0.40
1:B:520:ARG:HD3	1:B:547:THR:HG22	2.02	0.40
1:B:562:ASP:HB3	1:B:575:ILE:HG23	2.03	0.40
1:B:21:PHE:CE1	1:B:327:HIS:HB3	2.57	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	684/686 (100%)	665 (97%)	19 (3%)	0	100	100
1	B	684/686 (100%)	665 (97%)	18 (3%)	1 (0%)	48	46
All	All	1368/1372 (100%)	1330 (97%)	37 (3%)	1 (0%)	48	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	600	LEU

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	564/564 (100%)	546 (97%)	18 (3%)	34	35
1	B	564/564 (100%)	551 (98%)	13 (2%)	44	49
All	All	1128/1128 (100%)	1097 (97%)	31 (3%)	39	42

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	SER
1	A	44	THR
1	A	46	LEU
1	A	82	ASN
1	A	85	SER

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Mol	Chain	Res	Type
1	A	169	ASN
1	A	206	SER
1	A	367	SER
1	A	372	PRO
1	A	378	LEU
1	A	397	LEU
1	A	415	ASN
1	A	497	THR
1	A	575	ILE
1	A	593	ILE
1	A	609	ASN
1	A	653	LEU
1	A	658	SER
1	B	82	ASN
1	B	90	SER
1	B	169	ASN
1	B	173	ASN
1	B	326	ASN
1	B	372	PRO
1	B	378	LEU
1	B	415	ASN
1	B	498	THR
1	B	529	VAL
1	B	537	THR
1	B	609	ASN
1	B	619	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	116	GLN
1	A	126	HIS
1	A	128	HIS
1	A	177	HIS
1	A	316	GLN
1	A	333	HIS
1	A	415	ASN
1	A	479	ASN
1	A	503	ASN
1	A	548	GLN
1	A	578	ASN

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Mol	Chain	Res	Type
1	A	609	ASN
1	B	29	ASN
1	B	55	GLN
1	B	93	ASN
1	B	126	HIS
1	B	128	HIS
1	B	129	ASN
1	B	177	HIS
1	B	270	HIS
1	B	316	GLN
1	B	326	ASN
1	B	333	HIS
1	B	364	GLN
1	B	410	HIS
1	B	415	ASN
1	B	465	ASN
1	B	467	ASN
1	B	479	ASN
1	B	595	ASN
1	B	609	ASN
1	B	620	ASN
1	B	646	GLN
1	B	683	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 ⓘ

6 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	GAL	C	1	2	12,12,12	0.99	1 (8%)	17,17,17	1.42	3 (17%)
2	GLD	C	2	2,5	9,9,10	1.30	1 (11%)	11,12,14	1.95	2 (18%)
2	GAL	D	1	2	12,12,12	1.14	0	17,17,17	1.26	3 (17%)
2	GLD	D	2	2,5	9,9,10	1.09	1 (11%)	11,12,14	1.99	3 (27%)
3	GLC	E	1	3	12,12,12	1.71	3 (25%)	17,17,17	1.13	1 (5%)
3	GLC	E	2	3	11,11,12	0.96	0	15,15,17	1.78	3 (20%)

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	GAL	C	1	2	1/1/5/5	0/2/22/22	0/1/1/1
2	GLD	C	2	2,5	-	-	0/1/1/1
2	GAL	D	1	2	1/1/5/5	1/2/22/22	0/1/1/1
2	GLD	D	2	2,5	-	-	0/1/1/1
3	GLC	E	1	3	-	0/2/22/22	0/1/1/1
3	GLC	E	2	3	-	1/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1	GLC	C4-C5	3.51	1.60	1.53
2	C	2	GLD	C4-C5	2.81	1.56	1.52
3	E	1	GLC	C4-C3	2.72	1.59	1.52
2	D	2	GLD	C4-C5	2.63	1.56	1.52
3	E	1	GLC	C1-C2	2.48	1.58	1.52
2	C	1	GAL	C4-C5	2.25	1.57	1.53

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2	GLC	C1-O5-C5	5.33	119.34	112.19
2	C	2	GLD	C3-C4-C5	5.11	119.31	111.21
2	D	2	GLD	C1-O5-C5	4.35	118.19	111.80
2	C	1	GAL	C3-C4-C5	3.35	116.31	110.23
3	E	1	GLC	C1-O5-C5	3.05	119.55	113.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	GLD	C4-C3-C2	-2.98	106.70	110.38
2	D	1	GAL	C4-C3-C2	-2.82	105.89	110.83
2	C	1	GAL	O2-C2-C1	2.72	115.53	109.25
2	D	2	GLD	C3-C4-C5	-2.31	107.55	111.21
2	C	2	GLD	O2-C2-C1	2.28	114.44	109.22
3	E	2	GLC	O2-C2-C1	2.13	114.10	109.22
2	D	1	GAL	O2-C2-C1	2.11	114.12	109.25
3	E	2	GLC	O2-C2-C3	-2.05	105.91	110.15
2	C	1	GAL	O4-C4-C5	-2.03	104.31	109.32
2	D	1	GAL	O3-C3-C4	2.01	115.11	110.38

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	1	GAL	C4
2	D	1	GAL	C4

All (2) torsion outliers are listed below:

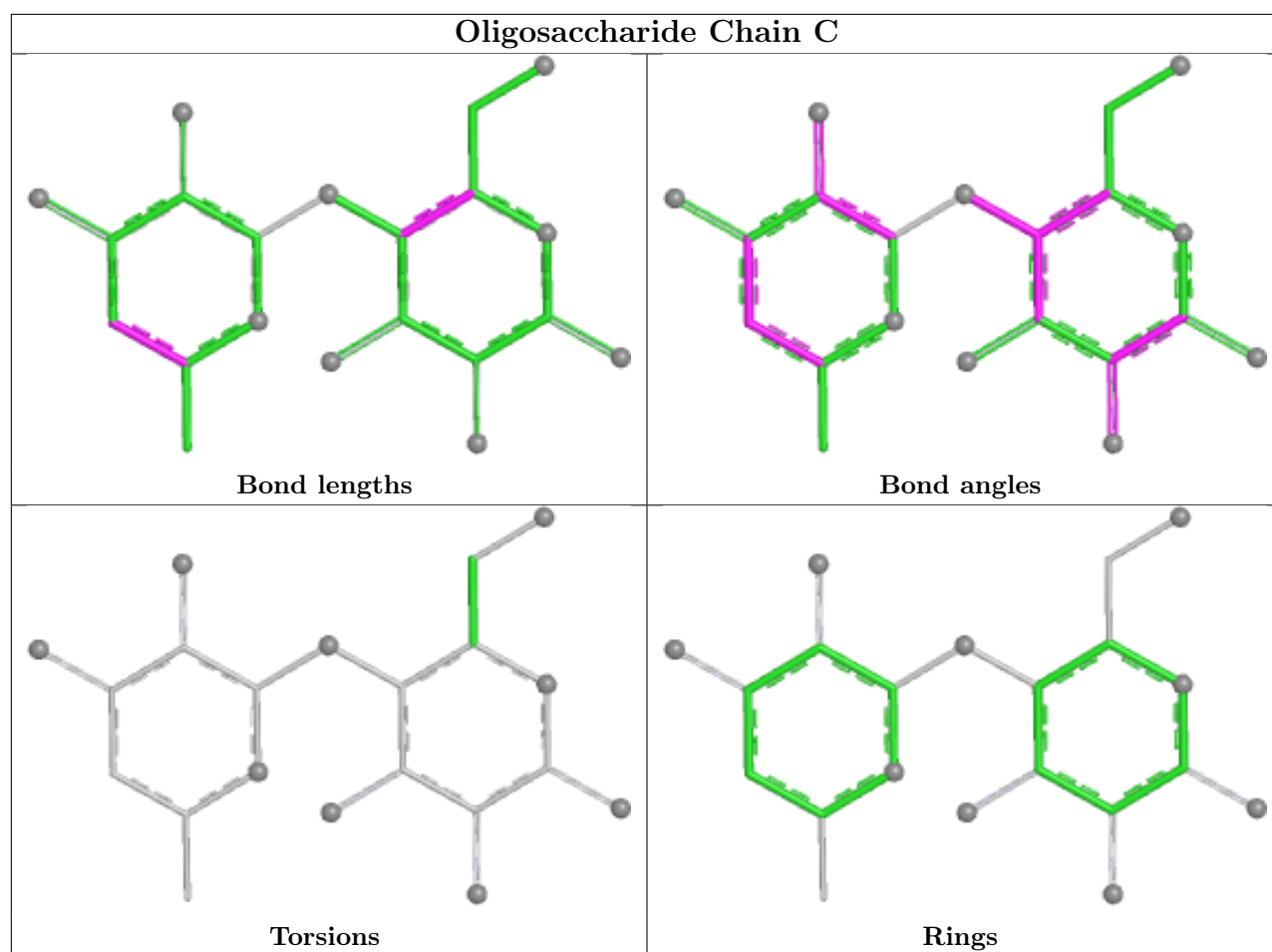
Mol	Chain	Res	Type	Atoms
3	E	2	GLC	O5-C5-C6-O6
2	D	1	GAL	O5-C5-C6-O6

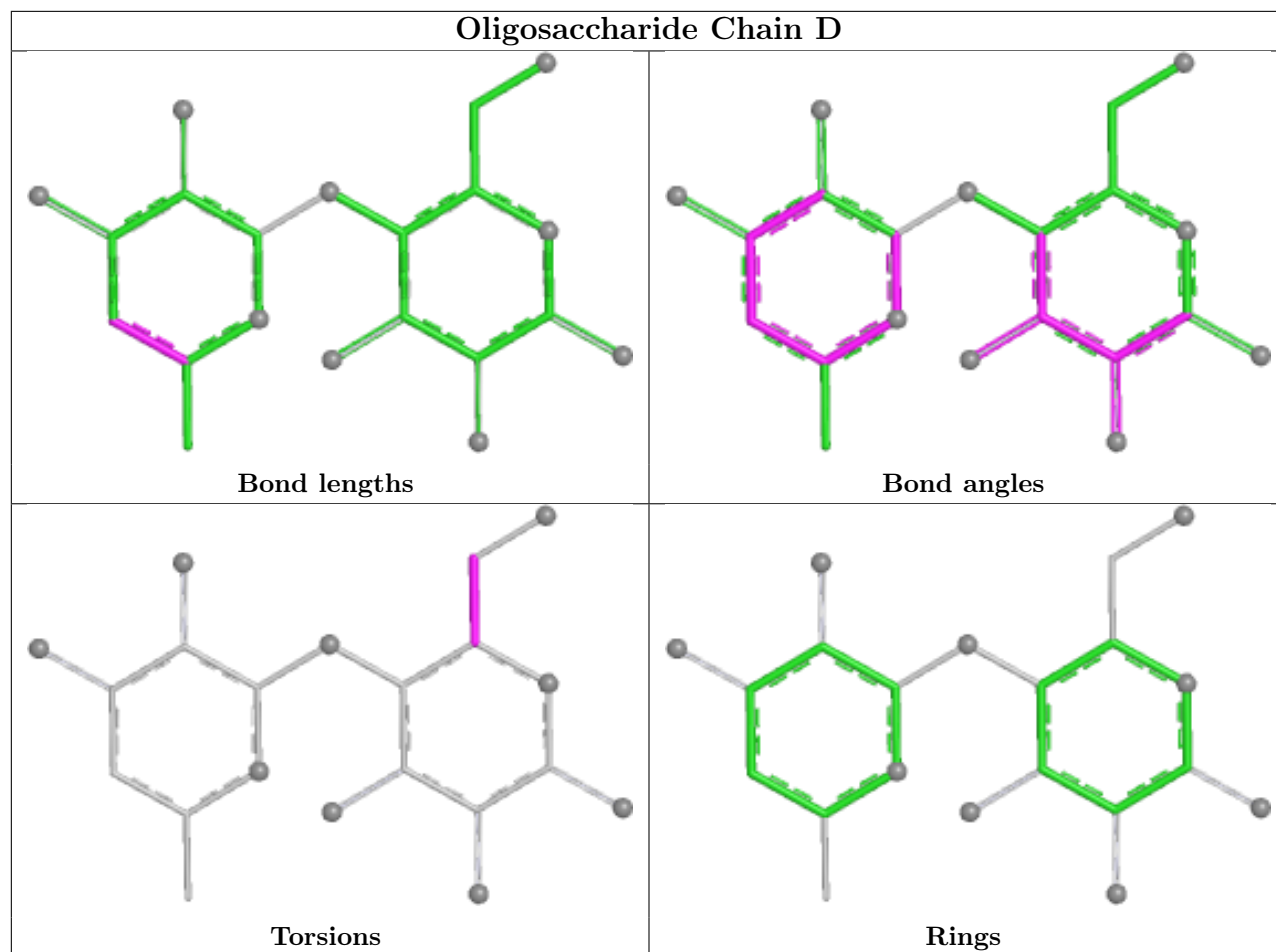
There are no ring outliers.

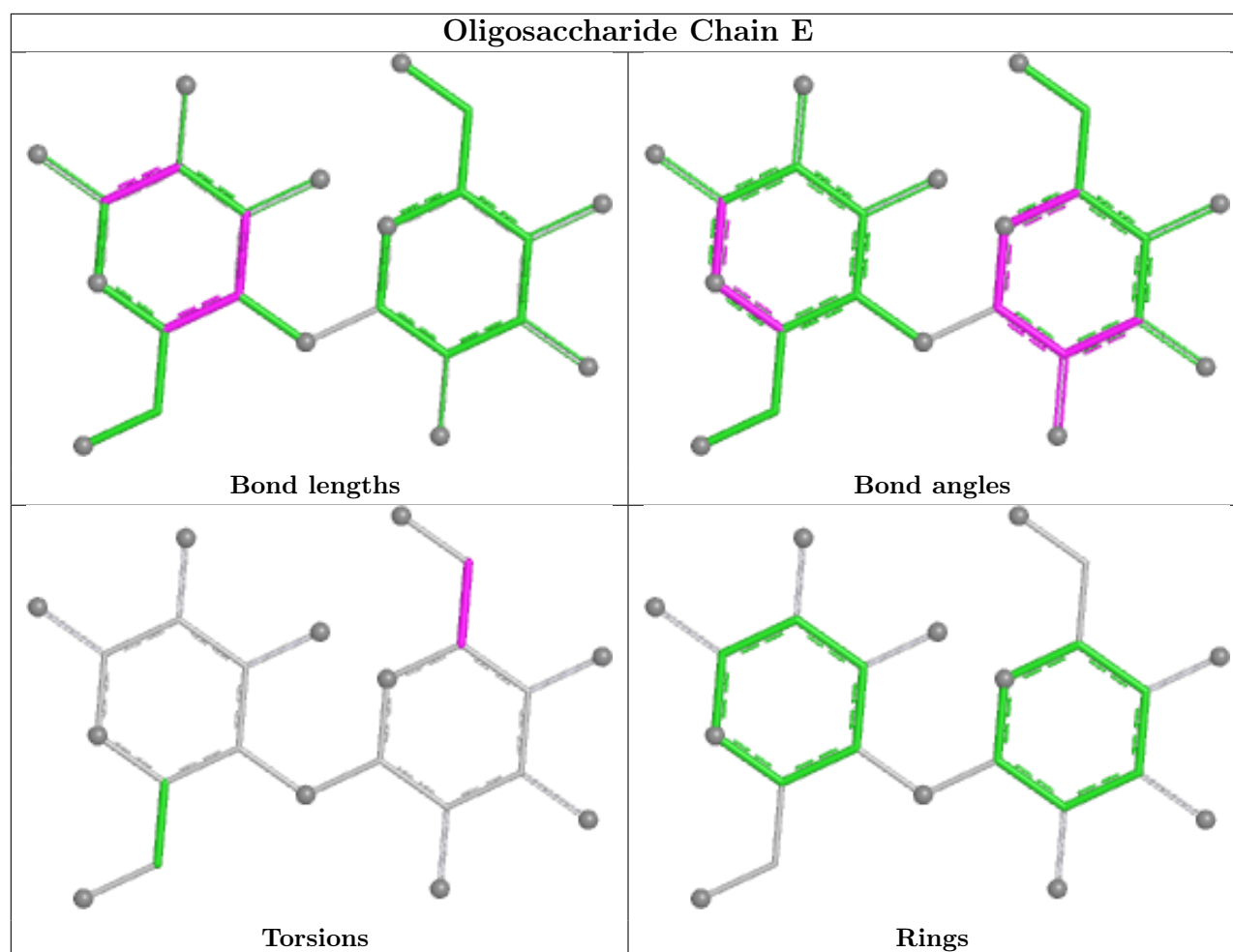
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	GAL	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 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	GLC	B	801	5	11,11,12	1.27	2 (18%)	15,15,17	1.36	2 (13%)
4	GLC	A	711	-	12,12,12	1.06	1 (8%)	17,17,17	1.55	1 (5%)
4	GLC	A	721	-	12,12,12	1.12	1 (8%)	17,17,17	1.55	4 (23%)
6	GAL	A	731	-	12,12,12	1.23	1 (8%)	17,17,17	0.82	1 (5%)
6	GAL	B	811	-	12,12,12	0.97	1 (8%)	17,17,17	1.05	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GAL	B	831	-	12,12,12	0.89	0	17,17,17	0.86	0
4	GLC	A	701	5	11,11,12	0.98	1 (9%)	15,15,17	1.89	6 (40%)
5	ACI	B	802	2,4	12,12,12	2.30	2 (16%)	11,17,17	1.49	2 (18%)
5	ACI	A	702	2,4	12,12,12	2.56	2 (16%)	11,17,17	1.48	2 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GLC	B	801	5	-	2/2/19/22	0/1/1/1
4	GLC	A	711	-	-	1/2/22/22	0/1/1/1
5	ACI	A	702	2,4	-	0/2/22/22	0/1/1/1
4	GLC	A	721	-	-	0/2/22/22	0/1/1/1
6	GAL	B	831	-	1/1/5/5	1/2/22/22	0/1/1/1
6	GAL	B	811	-	1/1/5/5	1/2/22/22	0/1/1/1
6	GAL	A	731	-	1/1/5/5	0/2/22/22	0/1/1/1
5	ACI	B	802	2,4	-	0/2/22/22	0/1/1/1
4	GLC	A	701	5	-	2/2/19/22	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	702	ACI	C4-C5	6.18	1.56	1.51
5	A	702	ACI	C7-C5	5.43	1.40	1.32
5	B	802	ACI	C7-C5	5.40	1.40	1.32
5	B	802	ACI	C4-C5	4.83	1.55	1.51
6	A	731	GAL	C4-C5	3.18	1.59	1.53
4	B	801	GLC	C4-C5	2.74	1.58	1.53
4	A	711	GLC	O5-C1	2.47	1.48	1.42
4	A	721	GLC	C4-C5	2.46	1.58	1.53
6	B	811	GAL	C4-C5	2.42	1.58	1.53
4	A	701	GLC	C4-C5	2.39	1.58	1.53
4	B	801	GLC	C1-C2	2.05	1.57	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	711	GLC	C1-O5-C5	4.67	122.69	113.65
4	A	721	GLC	C1-O5-C5	4.04	121.47	113.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	701	GLC	C1-O5-C5	3.53	116.92	112.19
4	A	701	GLC	C1-C2-C3	3.15	114.23	109.64
5	A	702	ACI	C2-C3-C4	-3.10	105.31	110.22
5	B	802	ACI	C2-C1-N1	-2.81	105.68	111.40
4	B	801	GLC	C1-O5-C5	2.73	115.85	112.19
6	B	811	GAL	O4-C4-C3	-2.65	104.12	110.38
4	A	701	GLC	C3-C4-C5	-2.51	105.67	110.23
4	A	701	GLC	O5-C1-C2	2.49	116.74	110.79
6	A	731	GAL	C1-O5-C5	2.45	118.39	113.65
4	A	721	GLC	O4-C4-C3	-2.42	104.68	110.38
4	A	701	GLC	O4-C4-C5	2.31	115.01	109.32
5	B	802	ACI	C2-C3-C4	-2.28	106.61	110.22
5	A	702	ACI	O2-C2-C1	2.23	113.21	109.04
4	A	721	GLC	O4-C4-C5	2.18	114.70	109.32
4	A	701	GLC	O2-C2-C3	-2.12	105.75	110.15
4	A	721	GLC	O5-C1-C2	2.09	113.97	110.30
4	B	801	GLC	O4-C4-C5	2.01	114.28	109.32

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	731	GAL	C4
6	B	811	GAL	C4
6	B	831	GAL	C4

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	701	GLC	O5-C5-C6-O6
4	A	701	GLC	C4-C5-C6-O6
4	A	711	GLC	O5-C5-C6-O6
6	B	831	GAL	O5-C5-C6-O6
6	B	811	GAL	O5-C5-C6-O6
4	B	801	GLC	C4-C5-C6-O6
4	B	801	GLC	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	711	GLC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	721	GLC	1	0
5	A	702	ACI	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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	686/686 (100%)	-0.97	0 100 100	9, 16, 29, 50	0
1	B	686/686 (100%)	-0.84	1 (0%) 92 91	11, 19, 37, 58	0
All	All	1372/1372 (100%)	-0.91	1 (0%) 92 91	9, 17, 33, 58	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	600	LEU	2.2

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](#)

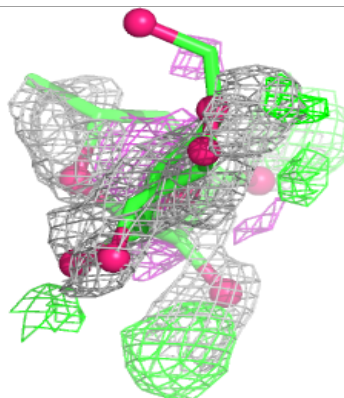
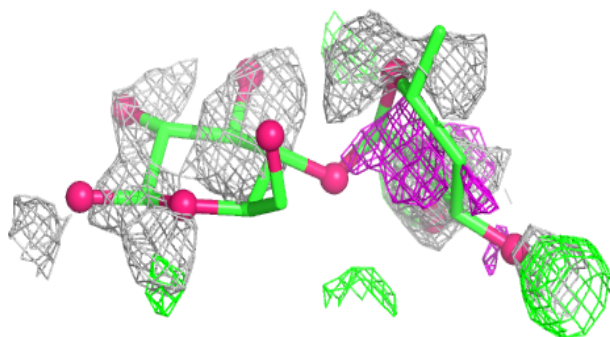
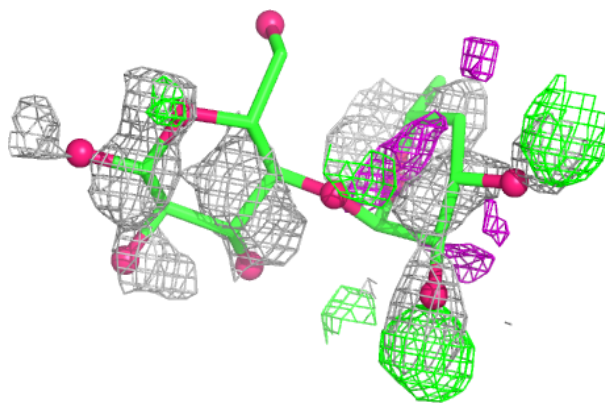
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GAL	D	1	12/12	0.45	0.16	74,78,79,81	0
2	GLD	C	2	9/10	0.46	0.17	60,64,65,66	0
3	GLC	E	1	12/12	0.56	0.12	71,72,73,73	0
2	GAL	C	1	12/12	0.61	0.13	70,73,76,77	0
2	GLD	D	2	9/10	0.72	0.12	72,74,75,75	0
3	GLC	E	2	11/12	0.72	0.12	70,71,72,74	0

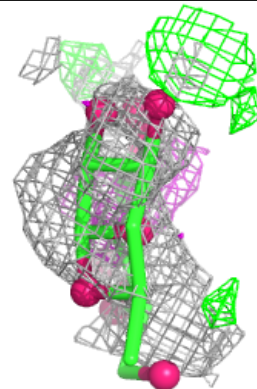
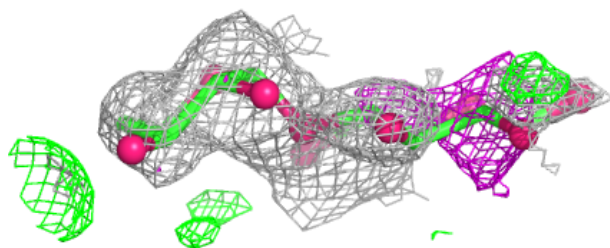
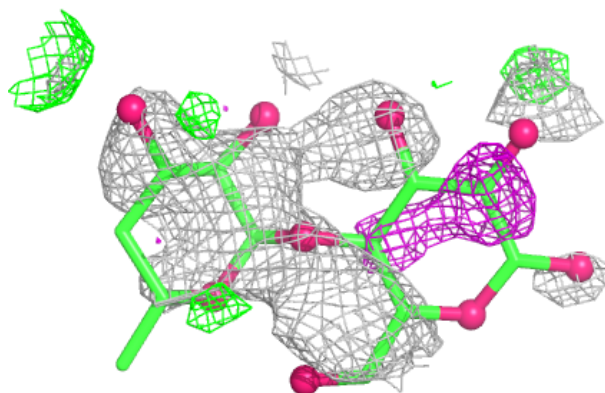
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

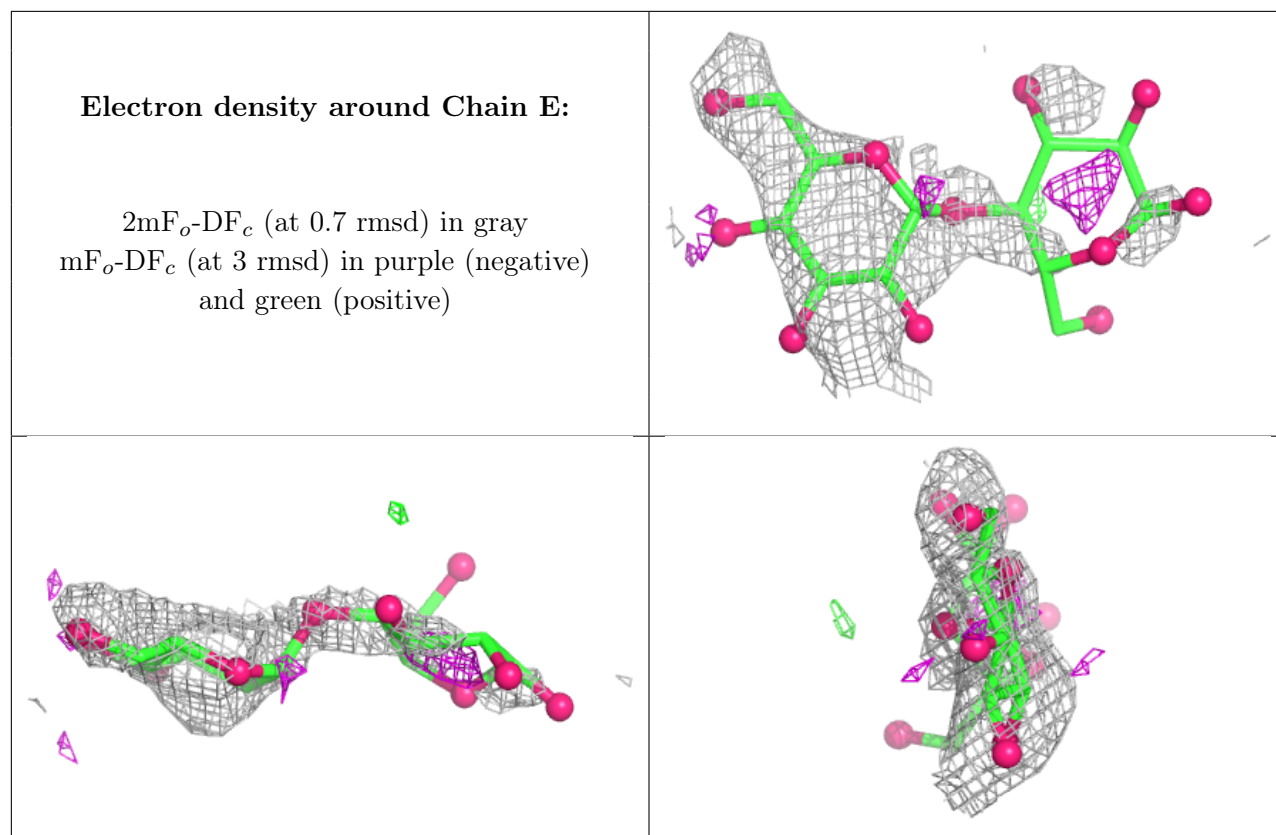
Electron density around Chain C:

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

**Electron density around Chain D:**

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





6.4 Ligands ⓘ

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	GLC	A	711	12/12	0.30	0.18	71,74,75,76	0
6	GAL	B	811	12/12	0.39	0.16	76,79,79,79	0
4	GLC	B	801	11/12	0.44	0.16	70,72,73,74	0
5	ACI	A	702	12/12	0.50	0.16	62,67,70,70	0
4	GLC	A	721	12/12	0.57	0.14	68,70,71,72	0
6	GAL	A	731	12/12	0.62	0.16	59,61,62,63	0
4	GLC	A	701	11/12	0.63	0.15	64,69,70,71	0
6	GAL	B	831	12/12	0.64	0.14	73,76,79,79	0
5	ACI	B	802	12/12	0.65	0.13	64,68,71,71	0
7	CA	A	687	1/1	0.92	0.05	13,13,13,13	0
7	CA	B	690	1/1	0.92	0.05	19,19,19,19	0
7	CA	A	688	1/1	0.95	0.07	18,18,18,18	0
7	CA	B	689	1/1	0.96	0.05	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.