



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:05 AM UTC

PDB ID : 1UKQ / pdb_00001ukq
Title : Crystal structure of cyclodextrin glucanotransferase complexed with a pseudo-maltotetraose derived from acarbose
Authors : Haga, K.; Kanai, R.; Sakamoto, O.; Harata, K.; Yamane, K.
Deposited on : 2003-09-01
Resolution : 2.00 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

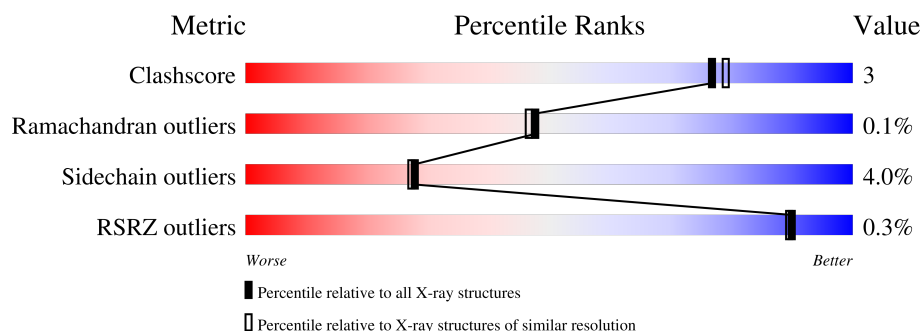
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
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	
1	B	686	
2	C	2	
3	D	2	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 11354 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
			5312	3354	906	1036	16			
1	B	686	Total	C	N	O	S	0	0	0
			5312	3354	906	1036	16			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	452	PRO	ARG	SEE REMARK 999	UNP P05618
A	454	GLY	ALA	SEE REMARK 999	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 alpha-D-quinovopyranose-(1-4)-beta-D-glucopyranose.



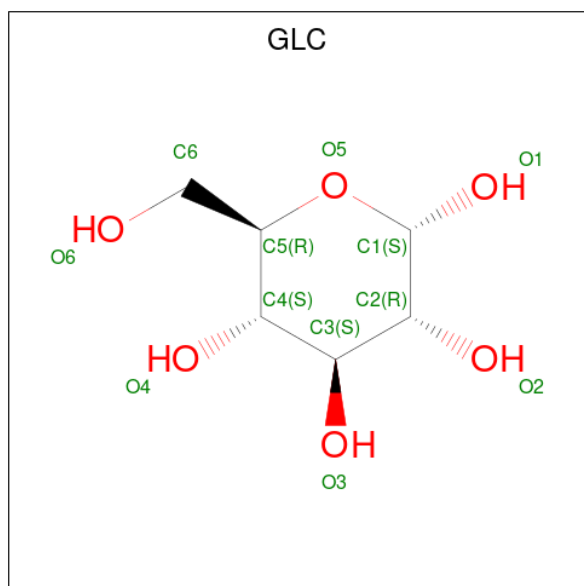
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	2	Total	C	O	0	0	0
			21	12	9			

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



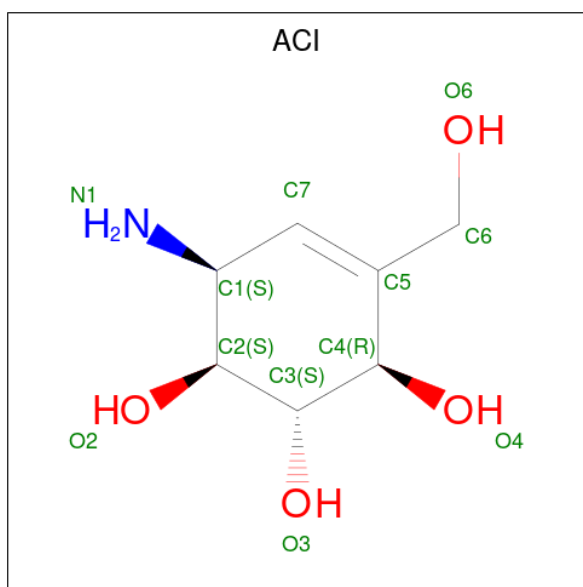
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	D	2	Total	C	O	0	0	0
			21	12	9			

- 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
			12	6	6		
4	B	1	Total	C	O	0	0
			12	6	6		

- 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
			11	7	1	3		
5	B	1	Total	C	N	O	0	0
			11	7	1	3		

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

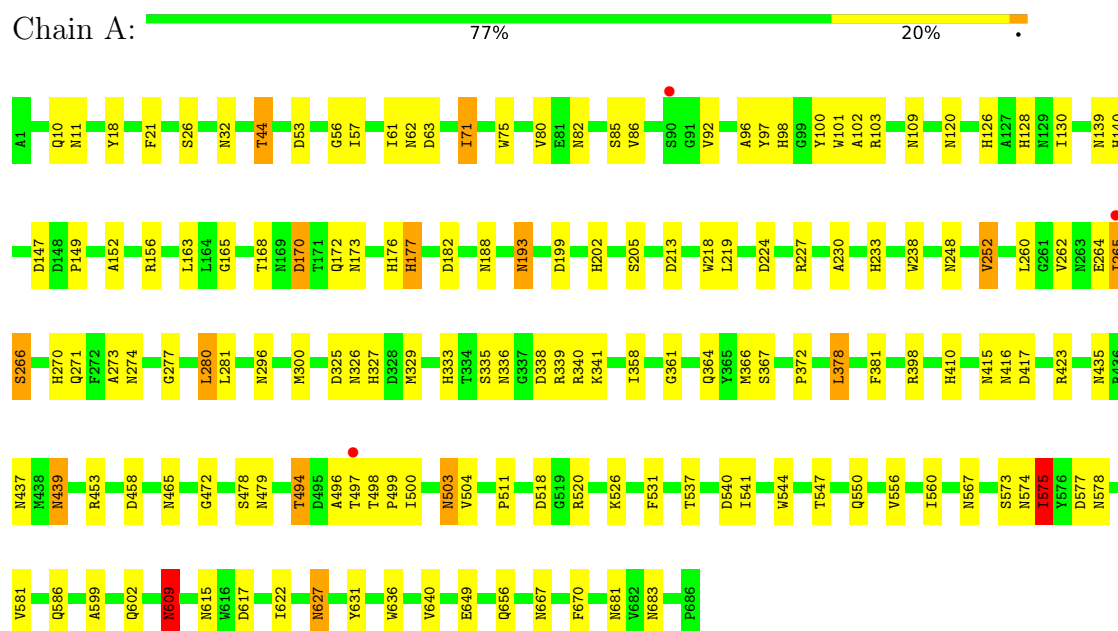
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	339	Total	O	0	0
			339	339		
7	B	299	Total	O	0	0
			299	299		

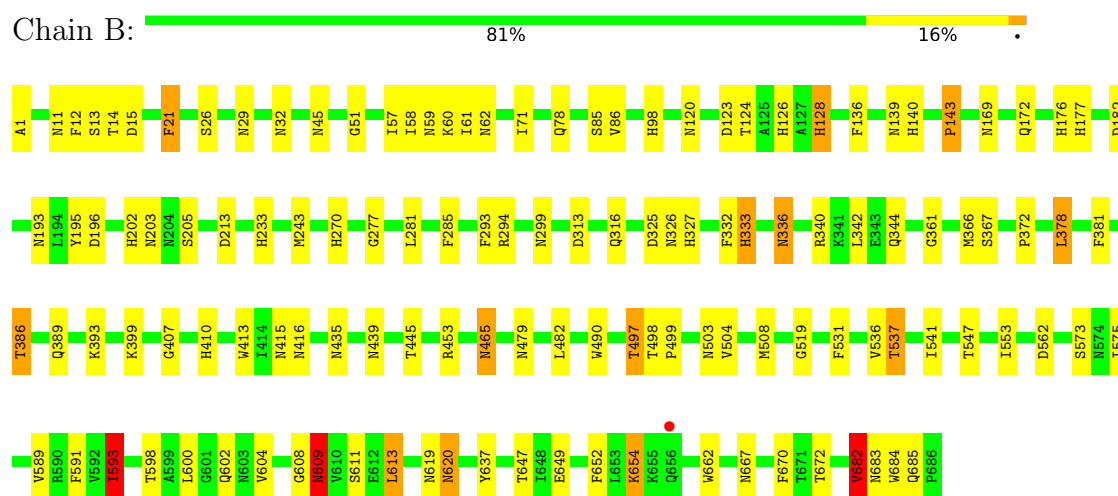
3 Residue-property plots

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: alpha-D-quinovopyranose-(1-4)-beta-D-glucopyranose

Chain C:  100%

EGC1
G6D2

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

Chain D:  50%  50%

GLC1
G6D2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	64.94Å 74.49Å 79.10Å 85.13° 105.02° 101.02°	Depositor
Resolution (Å)	10.00 – 2.00 10.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	87.0 (10.00-2.00) 95.3 (10.00-2.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 2.00Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.184 , 0.246 0.202 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	16.9	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 63.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11354	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% 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, ACI, BGC, G6D, 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	1.01	16/5446 (0.3%)	1.74	115/7429 (1.5%)
1	B	0.98	17/5446 (0.3%)	1.71	85/7429 (1.1%)
All	All	1.00	33/10892 (0.3%)	1.72	200/14858 (1.3%)

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	1
1	B	0	1
All	All	0	2

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	126	HIS	CD2-NE2	-7.71	1.29	1.37
1	A	233	HIS	CD2-NE2	-7.50	1.29	1.37
1	A	126	HIS	CD2-NE2	-7.41	1.29	1.37
1	B	233	HIS	CD2-NE2	-7.30	1.29	1.37
1	B	327	HIS	CD2-NE2	-7.23	1.29	1.37
1	B	140	HIS	CD2-NE2	-7.12	1.30	1.37
1	A	177	HIS	CD2-NE2	-6.89	1.30	1.37
1	A	176	HIS	CD2-NE2	-6.84	1.30	1.37
1	A	202	HIS	CD2-NE2	-6.83	1.30	1.37
1	A	98	HIS	CD2-NE2	-6.79	1.30	1.37
1	A	128	HIS	CD2-NE2	-6.70	1.30	1.37
1	A	333	HIS	CD2-NE2	-6.70	1.30	1.37
1	A	327	HIS	CD2-NE2	-6.69	1.30	1.37
1	A	140	HIS	CD2-NE2	-6.66	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	593	ILE	CA-CB	6.51	1.62	1.54
1	B	333	HIS	CD2-NE2	-6.50	1.30	1.37
1	B	270	HIS	CD2-NE2	-6.36	1.30	1.37
1	B	176	HIS	CD2-NE2	-6.30	1.30	1.37
1	B	98	HIS	CD2-NE2	-6.12	1.31	1.37
1	B	128	HIS	CD2-NE2	-5.94	1.31	1.37
1	B	177	HIS	CD2-NE2	-5.90	1.31	1.37
1	B	126	HIS	CG-ND1	-5.67	1.32	1.38
1	A	270	HIS	CD2-NE2	-5.65	1.31	1.37
1	A	410	HIS	CD2-NE2	-5.61	1.31	1.37
1	B	202	HIS	CD2-NE2	-5.51	1.31	1.37
1	A	176	HIS	CG-ND1	-5.49	1.32	1.38
1	A	80	VAL	CA-CB	5.46	1.61	1.54
1	A	537	THR	CA-CB	5.44	1.63	1.53
1	B	177	HIS	CG-ND1	-5.42	1.32	1.38
1	B	410	HIS	CD2-NE2	-5.29	1.32	1.37
1	A	233	HIS	CG-ND1	-5.07	1.32	1.38
1	B	143	PRO	CA-CB	-5.05	1.47	1.53
1	B	270	HIS	CG-ND1	-5.03	1.32	1.38

All (200) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	325	ASP	CA-CB-CG	9.64	122.24	112.60
1	B	11	ASN	OD1-CG-ND2	-9.06	113.54	122.60
1	A	627	ASN	OD1-CG-ND2	-8.95	113.65	122.60
1	A	398	ARG	NE-CZ-NH2	-8.86	111.23	119.20
1	A	63	ASP	CA-CB-CG	8.66	121.26	112.60
1	B	327	HIS	CB-CG-CD2	-8.24	120.49	131.20
1	B	407	GLY	N-CA-C	8.16	121.30	112.33
1	B	415	ASN	CA-CB-CG	8.14	120.75	112.60
1	A	172	GLN	OE1-CD-NE2	-8.13	114.47	122.60
1	B	541	ILE	N-CA-C	-8.04	93.37	106.32
1	B	453	ARG	CB-CG-CD	-7.94	93.03	111.30
1	B	193	ASN	CA-CB-CG	7.89	120.50	112.60
1	A	126	HIS	CB-CG-CD2	-7.89	120.95	131.20
1	A	627	ASN	CB-CG-ND2	7.83	128.15	116.40
1	A	265	ILE	N-CA-C	-7.82	97.17	108.11
1	A	567	ASN	CA-CB-CG	7.71	120.31	112.60
1	A	62	ASN	N-CA-C	7.70	119.68	111.28
1	A	681	ASN	OD1-CG-ND2	-7.70	114.90	122.60
1	A	277	GLY	N-CA-C	-7.66	104.48	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	537	THR	N-CA-CB	-7.45	99.56	111.62
1	B	45	ASN	OD1-CG-ND2	-7.43	115.17	122.60
1	A	503	ASN	CB-CG-ND2	7.42	127.54	116.40
1	A	32	ASN	CA-CB-CG	7.39	119.99	112.60
1	A	656	GLN	OE1-CD-NE2	-7.29	115.31	122.60
1	A	327	HIS	CB-CG-CD2	-7.23	121.80	131.20
1	A	271	GLN	CA-CB-CG	7.21	128.52	114.10
1	A	156	ARG	N-CA-C	7.08	120.22	110.24
1	A	274	ASN	OD1-CG-ND2	-7.05	115.55	122.60
1	A	61	ILE	N-CA-C	-7.05	103.98	110.82
1	B	12	PHE	CA-CB-CG	7.04	120.84	113.80
1	B	120	ASN	OD1-CG-ND2	-7.03	115.57	122.60
1	A	423	ARG	N-CA-C	-6.86	98.23	109.40
1	A	53	ASP	N-CA-C	6.79	118.11	108.74
1	B	281	LEU	N-CA-C	-6.75	99.67	109.59
1	A	416	ASN	N-CA-C	6.74	119.48	111.33
1	B	435	ASN	OD1-CG-ND2	-6.73	115.87	122.60
1	A	503	ASN	OD1-CG-ND2	-6.73	115.87	122.60
1	A	86	VAL	N-CA-C	-6.73	98.17	107.99
1	A	193	ASN	CA-CB-CG	6.66	119.26	112.60
1	A	575	ILE	N-CA-CB	-6.66	103.46	110.72
1	A	496	ALA	N-CA-C	-6.65	99.75	110.32
1	A	165	GLY	CA-C-N	6.63	127.39	121.82
1	A	165	GLY	C-N-CA	6.63	127.39	121.82
1	B	32	ASN	CA-CB-CG	6.61	119.21	112.60
1	B	182	ASP	CA-CB-CG	6.59	119.19	112.60
1	A	266	SER	CA-C-N	6.58	126.36	119.05
1	A	266	SER	C-N-CA	6.58	126.36	119.05
1	A	437	ASN	OD1-CG-ND2	-6.56	116.04	122.60
1	B	139	ASN	OD1-CG-ND2	-6.56	116.04	122.60
1	A	560	ILE	N-CA-CB	-6.52	103.57	111.00
1	A	518	ASP	CA-CB-CG	6.49	119.09	112.60
1	B	682	VAL	N-CA-CB	-6.47	101.58	112.44
1	B	11	ASN	CB-CG-ND2	6.46	126.09	116.40
1	A	147	ASP	N-CA-C	6.42	119.10	111.71
1	B	293	PHE	CA-CB-CG	-6.42	107.38	113.80
1	A	575	ILE	CA-CB-CG1	-6.40	99.52	110.40
1	A	296	ASN	CB-CG-ND2	6.39	125.98	116.40
1	A	202	HIS	CB-CG-CD2	-6.38	122.90	131.20
1	A	177	HIS	CB-CG-CD2	-6.38	122.91	131.20
1	B	602	GLN	OE1-CD-NE2	-6.38	116.22	122.60
1	A	410	HIS	CA-CB-CG	6.36	120.16	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	416	ASN	N-CA-C	6.36	119.02	111.71
1	B	326	ASN	CA-CB-CG	6.34	118.94	112.60
1	A	100	TYR	N-CA-C	6.31	120.58	113.01
1	A	541	ILE	N-CA-C	-6.28	98.15	107.51
1	A	296	ASN	OD1-CG-ND2	-6.27	116.33	122.60
1	A	120	ASN	OD1-CG-ND2	-6.23	116.37	122.60
1	A	218	TRP	CG-CD2-CE3	6.23	140.13	133.90
1	A	103	ARG	N-CA-C	-6.21	107.54	114.62
1	B	213	ASP	CA-CB-CG	6.20	118.80	112.60
1	B	367	SER	O-C-N	-6.18	116.04	123.03
1	B	128	HIS	CB-CG-CD2	-6.18	123.17	131.20
1	B	609	ASN	OD1-CG-ND2	-6.17	116.43	122.60
1	A	281	LEU	N-CA-C	-6.17	100.71	109.96
1	B	316	GLN	CG-CD-NE2	6.14	125.60	116.40
1	A	213	ASP	CA-CB-CG	6.09	118.69	112.60
1	B	85	SER	N-CA-C	6.09	118.83	110.24
1	B	299	ASN	CA-CB-CG	6.07	118.67	112.60
1	A	683	ASN	OD1-CG-ND2	-6.05	116.55	122.60
1	B	410	HIS	CA-CB-CG	6.03	119.83	113.80
1	B	609	ASN	N-CA-C	6.02	119.68	112.93
1	A	577	ASP	CA-CB-CG	6.02	118.62	112.60
1	A	415	ASN	CA-CB-CG	6.01	118.61	112.60
1	B	553	ILE	CA-C-N	6.01	125.98	120.21
1	B	553	ILE	C-N-CA	6.01	125.98	120.21
1	B	86	VAL	N-CA-C	-6.01	99.04	108.23
1	B	205	SER	N-CA-C	6.00	118.59	111.33
1	B	316	GLN	OE1-CD-NE2	-5.99	116.61	122.60
1	A	670	PHE	CA-CB-CG	-5.94	107.86	113.80
1	A	498	THR	CA-CB-OG1	-5.91	100.74	109.60
1	B	120	ASN	CB-CG-ND2	5.90	125.25	116.40
1	A	44	THR	CA-CB-OG1	-5.88	100.78	109.60
1	A	120	ASN	CA-CB-CG	5.86	118.46	112.60
1	A	333	HIS	CB-CG-CD2	-5.85	123.59	131.20
1	A	152	ALA	CB-CA-C	-5.82	109.85	116.54
1	A	479	ASN	CB-CG-ND2	5.79	125.09	116.40
1	A	139	ASN	OD1-CG-ND2	-5.78	116.82	122.60
1	A	531	PHE	N-CA-C	-5.78	97.90	108.02
1	A	617	ASP	CA-C-N	5.78	125.91	119.32
1	A	617	ASP	C-N-CA	5.78	125.91	119.32
1	B	531	PHE	CA-CB-CG	-5.78	108.03	113.80
1	B	78	GLN	OE1-CD-NE2	-5.77	116.83	122.60
1	A	667	ASN	OD1-CG-ND2	-5.75	116.85	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	416	ASN	OD1-CG-ND2	-5.75	116.86	122.60
1	B	61	ILE	N-CA-C	-5.74	105.25	110.82
1	A	170	ASP	CA-CB-CG	5.73	118.33	112.60
1	A	10	GLN	OE1-CD-NE2	-5.72	116.88	122.60
1	B	327	HIS	CB-CG-ND1	5.72	131.29	122.70
1	A	109	ASN	OD1-CG-ND2	-5.72	116.88	122.60
1	B	313	ASP	N-CA-C	5.70	117.50	111.28
1	B	620	ASN	CB-CG-ND2	5.70	124.96	116.40
1	B	203	ASN	OD1-CG-ND2	-5.69	116.91	122.60
1	B	620	ASN	OD1-CG-ND2	-5.67	116.93	122.60
1	A	540	ASP	CA-CB-CG	5.65	118.25	112.60
1	A	631	TYR	N-CA-C	-5.64	100.73	109.24
1	B	21	PHE	N-CA-C	-5.63	98.07	107.99
1	A	182	ASP	CA-CB-CG	5.60	118.20	112.60
1	B	619	ASN	OD1-CG-ND2	-5.60	117.00	122.60
1	A	339	ARG	CA-CB-CG	-5.58	102.94	114.10
1	B	98	HIS	CB-CG-CD2	-5.58	123.95	131.20
1	A	248	ASN	OD1-CG-ND2	-5.58	117.02	122.60
1	B	685	GLN	OE1-CD-NE2	-5.54	117.06	122.60
1	B	57	ILE	N-CA-C	-5.53	105.13	110.72
1	A	326	ASN	CA-CB-CG	5.52	118.12	112.60
1	B	202	HIS	CB-CG-CD2	-5.51	124.04	131.20
1	B	15	ASP	N-CA-C	5.50	118.95	110.42
1	B	51	GLY	CA-C-N	5.50	125.20	119.92
1	B	51	GLY	C-N-CA	5.50	125.20	119.92
1	A	271	GLN	OE1-CD-NE2	-5.48	117.12	122.60
1	A	458	ASP	CA-CB-CG	5.48	118.08	112.60
1	B	128	HIS	CB-CG-ND1	5.47	130.90	122.70
1	A	102	ALA	N-CA-C	5.46	117.77	110.35
1	A	75	TRP	CG-CD2-CE3	5.45	139.35	133.90
1	B	336	ASN	CA-CB-CG	5.45	118.05	112.60
1	A	479	ASN	OD1-CG-ND2	-5.44	117.16	122.60
1	A	140	HIS	CB-CG-CD2	-5.44	124.13	131.20
1	B	326	ASN	OD1-CG-ND2	-5.43	117.17	122.60
1	B	136	PHE	N-CA-C	-5.41	99.11	108.69
1	A	233	HIS	CB-CG-CD2	-5.40	124.18	131.20
1	B	1	ALA	CA-C-N	5.37	125.35	120.03
1	B	1	ALA	C-N-CA	5.37	125.35	120.03
1	B	176	HIS	CB-CG-CD2	-5.36	124.24	131.20
1	B	344	GLN	N-CA-CB	-5.34	102.26	110.01
1	B	465	ASN	CA-CB-CG	-5.34	107.25	112.60
1	B	672	THR	CA-C-N	5.33	125.63	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	672	THR	C-N-CA	5.33	125.63	119.92
1	B	126	HIS	CB-CG-CD2	-5.33	124.27	131.20
1	A	230	ALA	N-CA-C	5.33	118.74	111.39
1	A	609	ASN	N-CA-C	5.31	118.88	112.93
1	A	615	ASN	N-CA-C	5.30	118.51	111.30
1	A	335	SER	CA-C-O	5.29	126.02	120.42
1	B	482	LEU	N-CA-C	-5.29	99.91	108.52
1	A	364	GLN	OE1-CD-NE2	-5.27	117.33	122.60
1	A	586	GLN	OE1-CD-NE2	-5.26	117.34	122.60
1	A	435	ASN	OD1-CG-ND2	-5.26	117.34	122.60
1	A	398	ARG	CG-CD-NE	-5.25	100.44	112.00
1	A	578	ASN	OD1-CG-ND2	-5.25	117.35	122.60
1	B	662	TRP	CE2-CD2-CG	-5.25	100.90	107.20
1	B	667	ASN	OD1-CG-ND2	-5.25	117.35	122.60
1	B	497	THR	N-CA-CB	-5.25	103.38	110.67
1	A	218	TRP	CE2-CD2-CG	-5.24	100.91	107.20
1	B	62	ASN	N-CA-C	5.24	117.90	111.82
1	A	92	VAL	N-CA-C	5.21	116.80	108.87
1	B	589	VAL	O-C-N	-5.20	117.83	123.14
1	B	333	HIS	CB-CG-CD2	-5.20	124.44	131.20
1	A	325	ASP	CA-CB-CG	5.19	117.79	112.60
1	B	285	PHE	CA-CB-CG	5.18	118.98	113.80
1	A	417	ASP	CA-CB-CG	5.18	117.78	112.60
1	B	602	GLN	N-CA-C	-5.18	100.86	109.46
1	A	398	ARG	NE-CZ-NH1	5.17	126.67	121.50
1	A	617	ASP	CA-CB-CG	5.17	117.77	112.60
1	A	636	TRP	CG-CD2-CE3	5.16	139.06	133.90
1	A	188	ASN	OD1-CG-ND2	-5.16	117.44	122.60
1	A	410	HIS	N-CA-CB	-5.15	102.38	110.77
1	A	439	ASN	CA-CB-CG	5.15	117.75	112.60
1	A	494	THR	OG1-CB-CG2	5.15	119.60	109.30
1	B	536	VAL	N-CA-C	-5.12	100.93	108.11
1	A	130	ILE	CA-C-O	5.12	125.91	120.48
1	A	238	TRP	CG-CD2-CE3	5.12	139.02	133.90
1	A	218	TRP	CB-CG-CD1	-5.11	119.23	126.90
1	A	336	ASN	OD1-CG-ND2	-5.10	117.50	122.60
1	A	205	SER	N-CA-C	5.09	118.27	111.75
1	A	98	HIS	CB-CG-CD2	-5.09	124.58	131.20
1	B	327	HIS	N-CA-C	5.08	118.95	112.34
1	A	327	HIS	CB-CG-ND1	5.08	130.32	122.70
1	B	59	ASN	CA-CB-CG	5.08	117.68	112.60
1	A	126	HIS	CB-CG-ND1	5.07	130.31	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	439	ASN	OD1-CG-ND2	-5.07	117.53	122.60
1	A	75	TRP	CG-CD1-NE1	-5.06	103.62	110.20
1	A	252	VAL	N-CA-C	-5.06	100.50	108.90
1	A	92	VAL	CA-CB-CG1	-5.06	101.81	110.40
1	B	29	ASN	CA-C-N	5.05	124.84	119.28
1	B	29	ASN	C-N-CA	5.05	124.84	119.28
1	B	26	SER	CA-C-O	5.03	126.47	120.28
1	B	413	TRP	CE2-CD2-CG	-5.03	101.16	107.20
1	A	300	MET	N-CA-C	5.03	118.52	112.38
1	A	57	ILE	N-CA-C	-5.01	105.66	110.72
1	A	550	GLN	OE1-CD-NE2	-5.01	117.59	122.60
1	B	490	TRP	CE2-CD2-CG	-5.01	101.19	107.20
1	A	270	HIS	CB-CG-CD2	-5.00	124.70	131.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	97	TYR	Sidechain
1	B	195	TYR	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	5312	0	5050	31	0
1	B	5312	0	5050	29	0
2	C	21	0	12	0	0
3	D	21	0	12	1	0
4	A	12	0	11	0	0
4	B	12	0	11	0	0
5	A	11	0	10	0	0
5	B	11	0	10	1	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
7	A	339	0	0	3	0
7	B	299	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	11354	0	10166	60	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (60) 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:18:TYR:HB2	1:A:71:ILE:HG12	1.67	0.76
1:B:340:ARG:HH12	1:B:465:ASN:HD22	1.45	0.64
1:A:149:PRO:HG3	1:A:168:THR:HG21	1.79	0.63
1:A:11:ASN:ND2	7:A:1441:HOH:O	2.31	0.62
1:A:599:ALA:H	1:A:602:GLN:HE21	1.47	0.60
1:B:389:GLN:O	1:B:393:LYS:HG2	2.06	0.55
1:A:170:ASP:OD1	1:A:177:HIS:HE1	1.90	0.54
1:A:273:ALA:HB2	1:A:280:LEU:HD22	1.92	0.52
1:B:593:ILE:HD11	1:B:684:TRP:HA	1.92	0.52
1:A:520:ARG:HH21	1:A:520:ARG:HG2	1.75	0.52
1:A:26:SER:O	1:A:56:GLY:HA3	2.09	0.51
1:A:340:ARG:HH12	1:A:465:ASN:HD22	1.59	0.51
1:A:609:ASN:ND2	1:A:649:GLU:H	2.09	0.51
1:A:82:ASN:ND2	1:A:101:TRP:H	2.09	0.50
1:A:503:ASN:HD22	1:A:504:VAL:H	1.58	0.50
1:B:445:THR:HG22	1:B:479:ASN:ND2	2.26	0.50
1:A:361:GLY:HA3	1:A:366:MET:SD	2.51	0.50
1:A:82:ASN:HD22	1:A:96:ALA:HB1	1.76	0.49
1:A:71:ILE:HD11	1:A:358:ILE:HD12	1.95	0.48
1:A:378:LEU:HD21	1:A:381:PHE:CZ	2.49	0.48
1:B:593:ILE:HG21	1:B:604:VAL:HG11	1.96	0.48
1:A:338:ASP:HB3	1:A:341:LYS:HD3	1.96	0.47
1:B:608:GLY:HA3	1:B:613:LEU:HD23	1.96	0.47
1:A:260:LEU:HD22	1:A:264:GLU:HG2	1.96	0.47
1:B:243:MET:HE2	1:B:277:GLY:O	2.14	0.47
1:B:598:THR:HG22	1:B:654:LYS:HD2	1.95	0.47
1:B:124:THR:O	1:B:128:HIS:HD2	1.98	0.47
1:B:386:THR:HA	1:B:389:GLN:HG3	1.97	0.47
1:B:609:ASN:ND2	1:B:649:GLU:H	2.13	0.46
1:B:499:PRO:HB2	1:B:573:SER:HB3	1.98	0.46
1:B:378:LEU:HD21	1:B:381:PHE:CZ	2.51	0.46
1:A:575:ILE:HD12	1:B:575:ILE:HD11	1.97	0.46
1:A:499:PRO:HB2	1:A:573:SER:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:599:ALA:N	1:A:602:GLN:HE21	2.14	0.46
1:B:378:LEU:HD21	1:B:381:PHE:CE1	2.51	0.45
1:B:58:ILE:HG23	1:B:124:THR:HG21	2.00	0.44
1:B:562:ASP:HB3	1:B:575:ILE:HG23	1.99	0.43
1:A:520:ARG:HD3	1:A:547:THR:HG22	2.00	0.43
1:B:294:ARG:HB2	1:B:332:PHE:CZ	2.52	0.43
1:B:503:ASN:HD22	1:B:504:VAL:H	1.66	0.43
1:B:333:HIS:HB2	1:B:342:LEU:HD22	2.01	0.43
5:B:706:ACI:C7	3:D:2:G6D:C6	2.97	0.43
1:B:361:GLY:HA3	1:B:366:MET:SD	2.59	0.43
1:A:329:MET:HE2	1:A:329:MET:HB3	1.87	0.42
1:B:519:GLY:O	1:B:547:THR:HA	2.19	0.42
1:A:193:ASN:HD22	1:A:199:ASP:HB2	1.84	0.42
1:A:556:VAL:HG23	1:A:581:VAL:HG11	2.01	0.42
1:B:14:THR:HB	1:B:399:LYS:HD3	2.02	0.41
1:A:149:PRO:HD2	7:A:1261:HOH:O	2.21	0.41
1:A:574:ASN:HA	7:A:1378:HOH:O	2.19	0.41
1:A:622:ILE:HG21	1:A:640:VAL:HG22	2.02	0.41
1:B:60:LYS:HD3	1:B:60:LYS:HA	1.85	0.41
1:A:224:ASP:O	1:A:252:VAL:HB	2.21	0.41
1:B:591:PHE:O	1:B:637:TYR:HA	2.21	0.41
1:A:453:ARG:HG2	1:A:472:GLY:C	2.46	0.40
1:B:143:PRO:HB3	1:B:196:ASP:OD1	2.20	0.40
1:B:652:PHE:HE2	1:B:682:VAL:HG11	1.86	0.40
1:A:526:LYS:HA	1:A:544:TRP:CG	2.56	0.40
1:B:508:MET:HE2	1:B:508:MET:HB3	1.97	0.40
1:B:647:THR:HA	1:B:670:PHE:O	2.21	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%)	664 (97%)	20 (3%)	0	100	100
1	B	684/686 (100%)	660 (96%)	23 (3%)	1 (0%)	48	46
All	All	1368/1372 (100%)	1324 (97%)	43 (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%)	540 (96%)	24 (4%)	26	25
1	B	564/564 (100%)	543 (96%)	21 (4%)	30	30
All	All	1128/1128 (100%)	1083 (96%)	45 (4%)	28	27

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	PHE
1	A	44	THR
1	A	71	ILE
1	A	85	SER
1	A	163	LEU
1	A	173	ASN
1	A	219	LEU
1	A	227	ARG
1	A	262	VAL
1	A	265	ILE
1	A	266	SER
1	A	280	LEU
1	A	367	SER
1	A	372	PRO
1	A	378	LEU

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Mol	Chain	Res	Type
1	A	439	ASN
1	A	478	SER
1	A	494	THR
1	A	497	THR
1	A	500	ILE
1	A	511	PRO
1	A	575	ILE
1	A	609	ASN
1	A	627	ASN
1	B	13	SER
1	B	21	PHE
1	B	71	ILE
1	B	123	ASP
1	B	169	ASN
1	B	172	GLN
1	B	336	ASN
1	B	372	PRO
1	B	378	LEU
1	B	386	THR
1	B	497	THR
1	B	498	THR
1	B	537	THR
1	B	593	ILE
1	B	609	ASN
1	B	611	SER
1	B	613	LEU
1	B	620	ASN
1	B	654	LYS
1	B	682	VAL
1	B	683	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	10	GLN
1	A	19	GLN
1	A	82	ASN
1	A	94	ASN
1	A	126	HIS
1	A	160	ASN
1	A	177	HIS

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Mol	Chain	Res	Type
1	A	188	ASN
1	A	193	ASN
1	A	333	HIS
1	A	392	GLN
1	A	439	ASN
1	A	465	ASN
1	A	503	ASN
1	A	548	GLN
1	A	550	GLN
1	A	595	ASN
1	A	602	GLN
1	A	603	ASN
1	A	609	ASN
1	A	615	ASN
1	A	619	ASN
1	A	627	ASN
1	B	19	GLN
1	B	120	ASN
1	B	128	HIS
1	B	173	ASN
1	B	239	GLN
1	B	364	GLN
1	B	370	ASN
1	B	465	ASN
1	B	503	ASN
1	B	548	GLN
1	B	595	ASN
1	B	603	ASN
1	B	609	ASN
1	B	632	GLN
1	B	656	GLN

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 ⓘ

4 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGC	C	1	2	12,12,12	1.50	2 (16%)	17,17,17	1.56	6 (35%)
2	G6D	C	2	2,5	9,9,11	2.36	6 (66%)	11,12,16	2.22	4 (36%)
3	GLC	D	1	3	12,12,12	2.49	6 (50%)	17,17,17	1.81	6 (35%)
3	G6D	D	2	5,3	9,9,11	2.12	3 (33%)	11,12,16	2.01	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
2	BGC	C	1	2	-	0/2/22/22	0/1/1/1
2	G6D	C	2	2,5	-	-	0/1/1/1
3	GLC	D	1	3	-	2/2/22/22	0/1/1/1
3	G6D	D	2	5,3	-	-	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2	G6D	C1-C2	4.59	1.63	1.52
3	D	1	GLC	C3-C2	4.31	1.63	1.52
3	D	1	GLC	C1-C2	4.25	1.62	1.52
3	D	1	GLC	C4-C5	4.06	1.61	1.53
2	C	2	G6D	O5-C5	3.71	1.47	1.44
2	C	2	G6D	C3-C2	3.58	1.57	1.52
2	C	1	BGC	C4-C5	3.26	1.60	1.53
3	D	2	G6D	C3-C2	2.85	1.56	1.52
2	C	2	G6D	C4-C5	2.80	1.56	1.52
2	C	1	BGC	C4-C3	2.70	1.59	1.52
3	D	1	GLC	C4-C3	2.43	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	G6D	O5-C1	2.40	1.47	1.43
3	D	1	GLC	O4-C4	2.21	1.48	1.43
2	C	2	G6D	C4-C3	2.17	1.56	1.52
2	C	2	G6D	C1-C2	2.10	1.57	1.52
3	D	2	G6D	O5-C1	2.09	1.47	1.43
3	D	1	GLC	C6-C5	2.00	1.58	1.51

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2	G6D	O2-C2-C1	5.45	121.71	109.22
2	C	2	G6D	O2-C2-C1	4.61	119.77	109.22
3	D	1	GLC	O5-C1-C2	3.50	116.46	110.30
3	D	1	GLC	C1-O5-C5	3.49	120.41	113.65
2	C	2	G6D	C4-C3-C2	-3.10	106.56	110.38
2	C	2	G6D	C1-O5-C5	3.08	116.32	111.80
2	C	2	G6D	O5-C1-C2	-2.87	103.94	110.79
3	D	1	GLC	O4-C4-C5	2.68	115.92	109.32
3	D	1	GLC	C1-C2-C3	2.67	115.79	110.36
2	C	1	BGC	O3-C3-C2	-2.63	104.17	110.38
2	C	1	BGC	C3-C4-C5	2.61	114.97	110.23
3	D	1	GLC	C3-C4-C5	-2.46	105.77	110.23
3	D	2	G6D	O2-C2-C3	-2.43	104.87	110.20
2	C	1	BGC	C6-C5-C4	2.41	118.93	113.02
2	C	1	BGC	O4-C4-C5	-2.37	103.49	109.32
2	C	1	BGC	O5-C1-C2	-2.26	106.32	110.30
3	D	1	GLC	O1-C1-C2	2.04	114.91	108.98
2	C	1	BGC	O3-C3-C4	2.03	115.17	110.38

There are no chirality outliers.

All (2) torsion outliers are listed below:

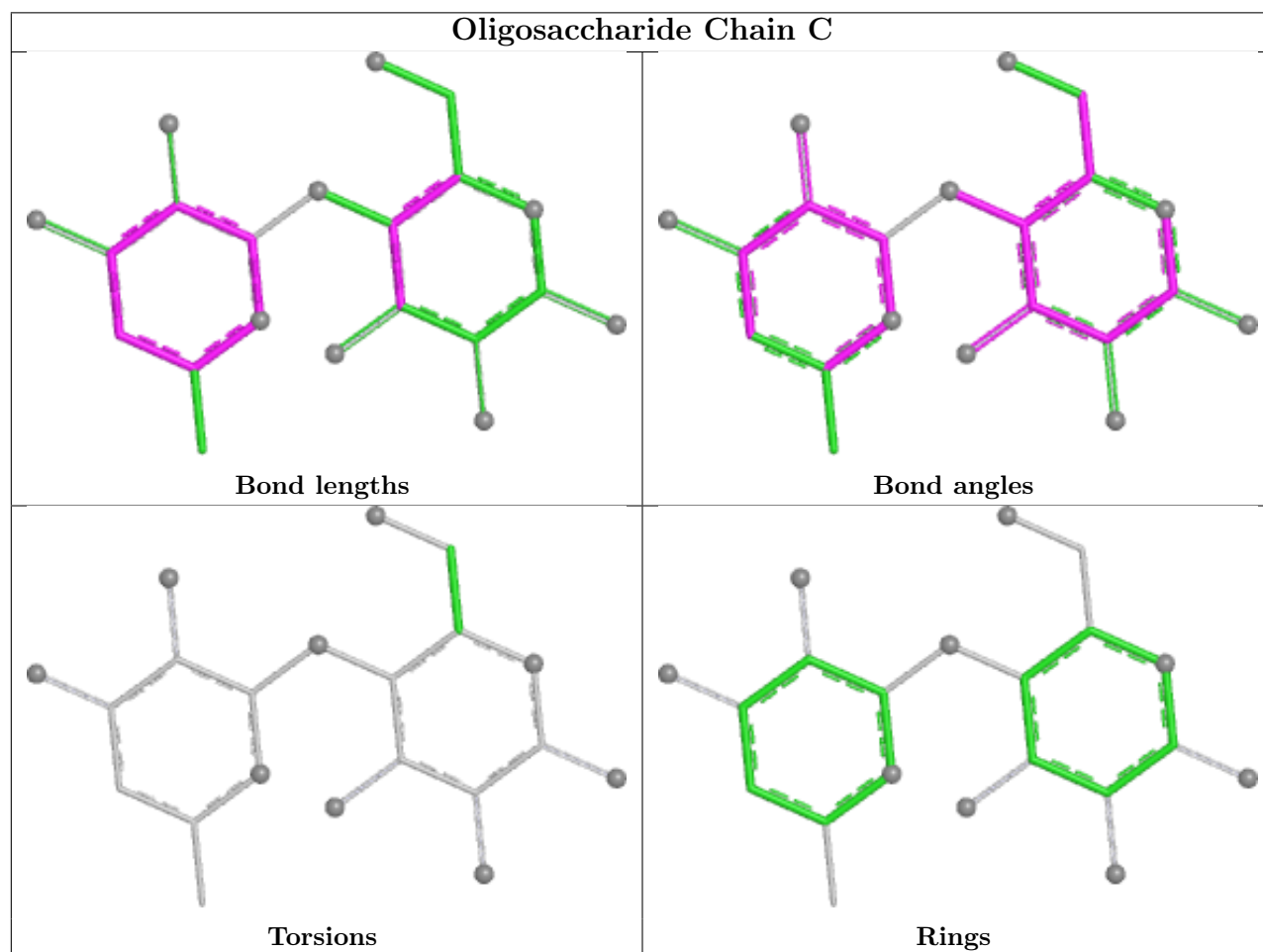
Mol	Chain	Res	Type	Atoms
3	D	1	GLC	O5-C5-C6-O6
3	D	1	GLC	C4-C5-C6-O6

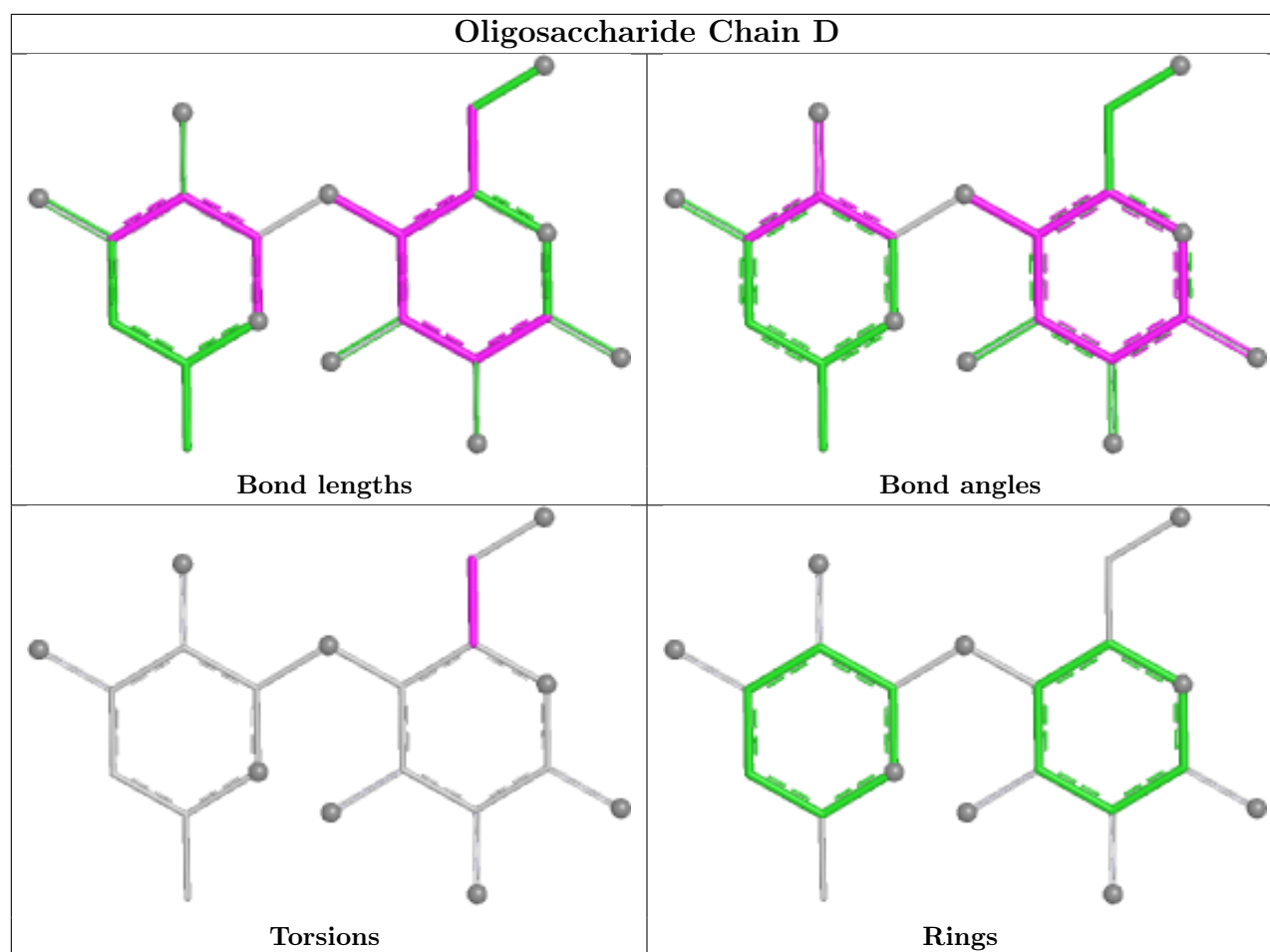
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	2	G6D	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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	A	701	5	12,12,12	1.74	4 (33%)	17,17,17	1.99	5 (29%)
5	ACI	A	702	2,4	11,11,12	2.08	4 (36%)	8,15,17	1.72	3 (37%)
5	ACI	B	706	3,4	11,11,12	1.45	2 (18%)	8,15,17	1.45	2 (25%)
4	GLC	B	705	5	12,12,12	1.76	4 (33%)	17,17,17	1.58	4 (23%)

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	A	701	5	-	0/2/22/22	0/1/1/1
5	ACI	A	702	2,4	-	1/2/18/22	0/1/1/1
5	ACI	B	706	3,4	-	1/2/18/22	0/1/1/1
4	GLC	B	705	5	-	0/2/22/22	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	702	ACI	C4-C5	3.71	1.58	1.50
4	B	705	GLC	C1-C2	3.57	1.60	1.52
5	A	702	ACI	C6-C5	3.47	1.56	1.51
4	A	701	GLC	C1-C2	3.11	1.59	1.52
5	A	702	ACI	C7-C5	3.03	1.42	1.33
4	B	705	GLC	C3-C2	2.89	1.59	1.52
4	B	705	GLC	O1-C1	2.88	1.48	1.39
4	A	701	GLC	C4-C3	2.82	1.59	1.52
5	B	706	ACI	C4-C5	2.67	1.56	1.50
5	B	706	ACI	C7-C5	2.66	1.41	1.33
5	A	702	ACI	C1-C7	2.45	1.55	1.50
4	B	705	GLC	C4-C5	2.09	1.57	1.53
4	A	701	GLC	C4-C5	2.07	1.57	1.53
4	A	701	GLC	C6-C5	2.06	1.58	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	701	GLC	O5-C1-C2	3.88	117.12	110.30
4	A	701	GLC	C1-O5-C5	3.83	121.06	113.65
4	A	701	GLC	C6-C5-C4	3.14	120.73	113.02
5	B	706	ACI	C2-C1-N1	-2.84	105.63	111.40
4	B	705	GLC	O5-C1-C2	2.83	115.28	110.30
4	A	701	GLC	C3-C4-C5	-2.81	105.14	110.23
5	A	702	ACI	C3-C4-C5	2.61	116.21	111.94
5	B	706	ACI	O3-C3-C4	2.40	114.71	109.38
4	A	701	GLC	C1-C2-C3	-2.40	105.47	110.36
5	A	702	ACI	O3-C3-C4	2.24	114.36	109.38
4	B	705	GLC	C1-C2-C3	2.23	114.91	110.36
4	B	705	GLC	O3-C3-C4	-2.23	105.12	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	705	GLC	O6-C6-C5	-2.14	104.04	111.33
5	A	702	ACI	C2-C1-N1	-2.07	107.19	111.40

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	702	ACI	C7-C5-C6-O6
5	B	706	ACI	C7-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	706	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%)	-0.41	3 (0%) 88 88	5, 13, 25, 40	0
1	B	686/686 (100%)	-0.24	1 (0%) 92 91	7, 17, 33, 46	0
All	All	1372/1372 (100%)	-0.32	4 (0%) 90 89	5, 15, 30, 46	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	656	GLN	2.3
1	A	497	THR	2.2
1	A	90	SER	2.1
1	A	265	ILE	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.

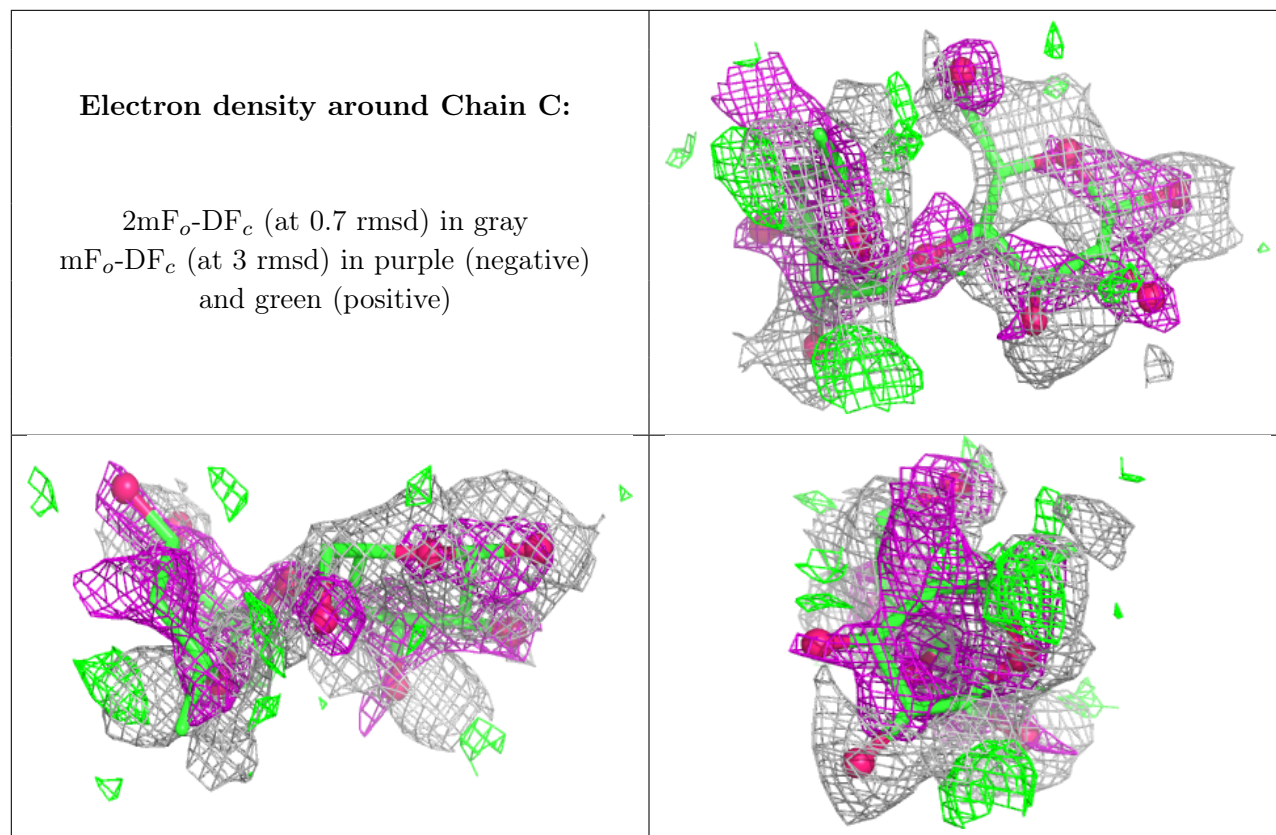
6.3 Carbohydrates [i](#)

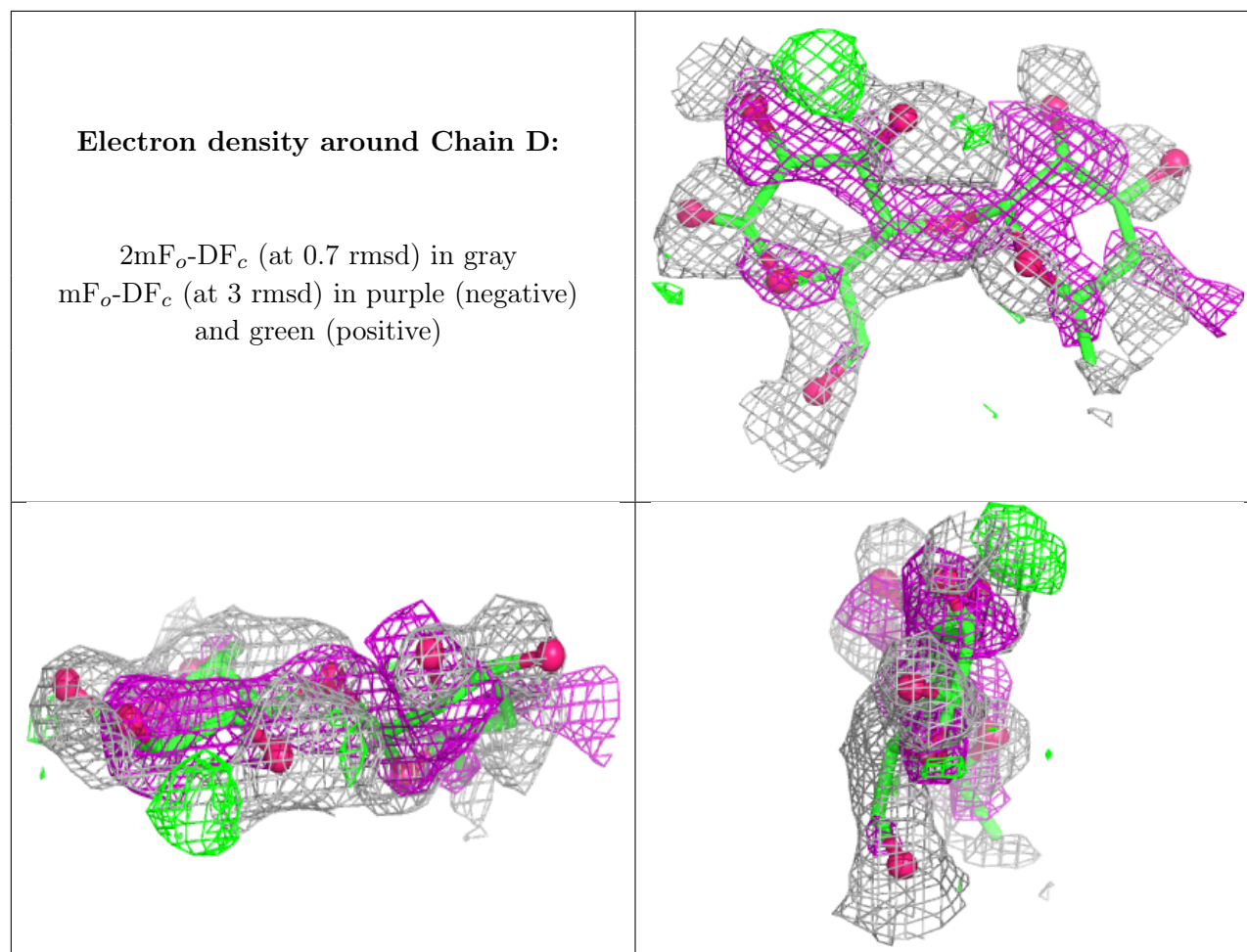
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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	G6D	D	2	9/11	0.44	0.15	20,23,29,32	0
2	G6D	C	2	9/11	0.47	0.17	20,25,31,31	0
3	GLC	D	1	12/12	0.60	0.14	19,26,29,32	0
2	BGC	C	1	12/12	0.64	0.11	17,23,26,28	0

The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.





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	B	705	12/12	0.53	0.32	19,26,30,31	0
5	ACI	B	706	11/12	0.61	0.24	18,23,28,30	0
5	ACI	A	702	11/12	0.63	0.25	20,24,27,27	0
4	GLC	A	701	12/12	0.68	0.27	15,23,27,30	0
6	CA	B	690	1/1	0.87	0.07	18,18,18,18	0
6	CA	B	689	1/1	0.89	0.06	16,16,16,16	0
6	CA	A	688	1/1	0.90	0.07	17,17,17,17	0
6	CA	A	687	1/1	0.93	0.05	9,9,9,9	0

6.5 Other polymers [i](#)

There are no such residues in this entry.