



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 07:43 AM UTC

PDB ID : 7P43 / pdb_00007p43
Title : Structure of CgGBE in complex with maltotriose
Authors : Ballut, L.; Conchou, L.; Violot, S.; Galisson, F.; Aghajari, N.
Deposited on : 2021-07-09
Resolution : 1.93 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

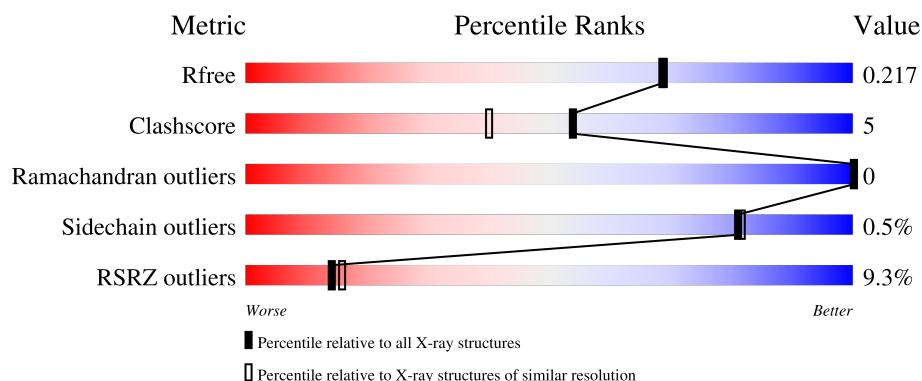
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 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	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	706	2% 91% 7% .
1	B	706	17% 82% 15% .
2	C	3	100%
2	D	3	100%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11641 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 1,4-alpha-glucan-branching enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	687	Total	C	N	O	S	0	0	0
			5551	3552	954	1025	20			
1	B	690	Total	C	N	O	S	0	0	0
			5330	3376	940	996	18			

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



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

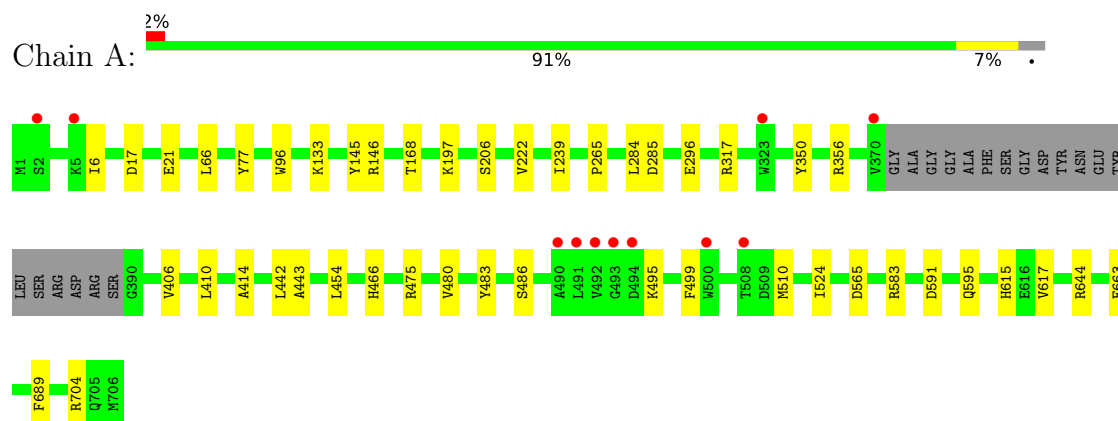
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	552	Total	O	0	0
			552	552		
3	B	140	Total	O	0	0
			140	140		

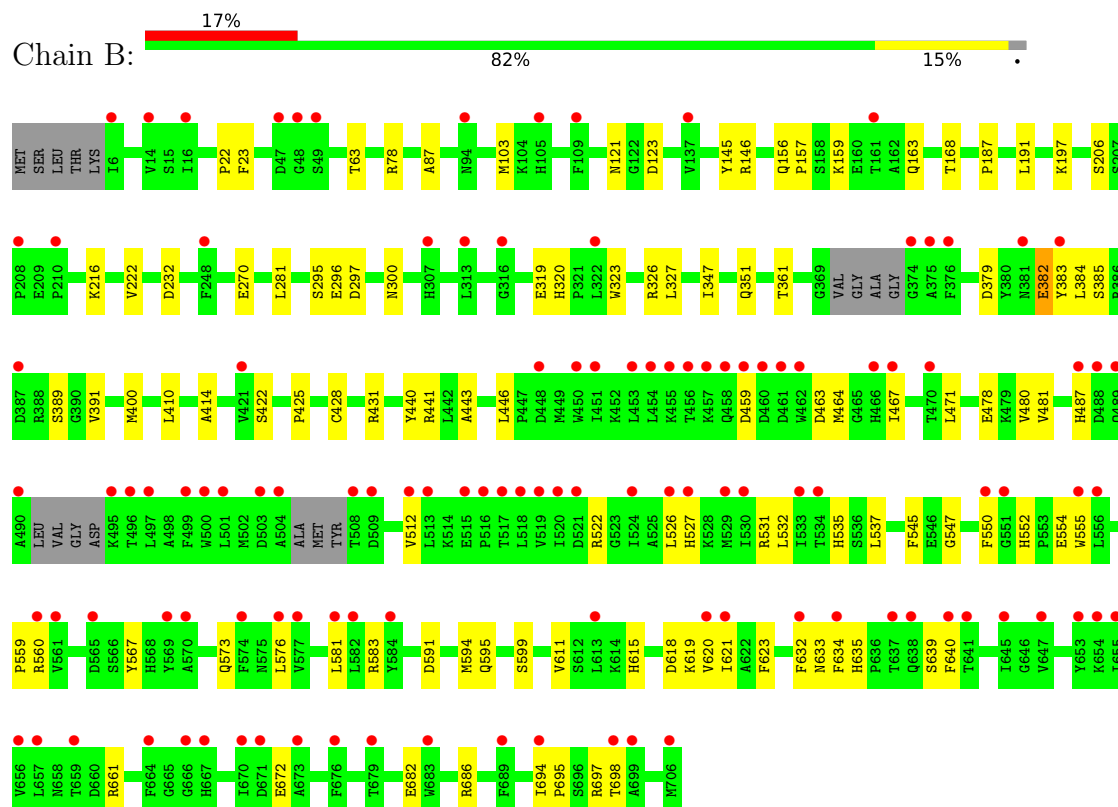
3 Residue-property plots

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: 1,4-alpha-glucan-branching enzyme



- Molecule 1: 1,4-alpha-glucan-branching enzyme



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

Chain C:  100%

GLC1
GLC2
GLC3

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

Chain D:  100%

GLC1
GLC2
GLC3

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	88.72Å 210.70Å 90.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.05 – 1.93 47.05 – 1.93	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.05-1.93) 99.8 (47.05-1.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 1.92Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.192 , 0.217 0.192 , 0.217	Depositor DCC
R_{free} test set	6413 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	31.1	Xtriage
Anisotropy	0.928	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11641	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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: GLC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.52	0/5711	0.65	0/7760
1	B	0.27	0/5476	0.47	0/7453
All	All	0.42	0/11187	0.57	0/15213

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	5551	0	5262	31	0
1	B	5330	0	4809	72	0
2	C	34	0	29	0	0
2	D	34	0	29	0	0
3	A	552	0	0	6	0
3	B	140	0	0	2	0
All	All	11641	0	10129	103	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 5.

All (103) 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:464:MET:HE2	1:B:619:LYS:HB3	1.69	0.74
1:A:510:MET:HE3	1:A:583:ARG:HB2	1.73	0.70
1:B:459:ASP:OD2	1:B:697:ARG:NH2	2.27	0.67
1:A:133:LYS:NZ	1:A:296:GLU:OE2	2.29	0.66
1:B:383:TYR:HB2	1:B:384:LEU:HD12	1.77	0.66
1:A:466:HIS:HD2	3:A:1257:HOH:O	1.78	0.65
1:B:428:CYS:HB2	1:B:478:GLU:HB3	1.78	0.64
1:B:361:THR:HG23	1:B:422:SER:HB3	1.80	0.62
1:A:704:ARG:NH1	3:A:806:HOH:O	2.33	0.62
1:B:216:LYS:NZ	1:B:270:GLU:OE1	2.33	0.62
1:A:483:TYR:CE2	1:A:486:SER:HB2	2.36	0.61
1:B:615:HIS:HB3	1:B:618:ASP:O	2.01	0.60
1:B:583:ARG:HG2	1:B:583:ARG:HH11	1.66	0.60
1:B:63:THR:O	1:B:78:ARG:HD3	2.02	0.59
1:B:547:GLY:HA2	1:B:550:PHE:CE1	2.38	0.59
1:B:633:ASN:ND2	1:B:694:ILE:O	2.34	0.59
1:B:639:SER:HB3	1:B:695:PRO:HA	1.83	0.59
1:B:487:HIS:HB3	1:B:545:PHE:CD2	2.38	0.58
1:B:320:HIS:HD2	1:B:323:TRP:H	1.51	0.58
1:A:145:TYR:O	1:A:146:ARG:HD3	2.04	0.57
1:A:410:LEU:HB2	1:A:414:ALA:HB2	1.87	0.57
1:B:471:LEU:HD23	1:B:537:LEU:HD23	1.86	0.57
1:B:121:ASN:ND2	3:B:808:HOH:O	2.39	0.55
1:A:443:ALA:HB2	1:A:480:VAL:CG1	2.36	0.55
1:B:428:CYS:SG	1:B:441:ARG:HB3	2.48	0.54
1:B:464:MET:HB3	1:B:621:ILE:HD11	1.89	0.54
1:B:619:LYS:O	1:B:634:PHE:N	2.37	0.54
1:A:663:GLU:HG2	3:A:883:HOH:O	2.07	0.54
1:A:644:ARG:HG2	1:A:689:PHE:CD2	2.43	0.54
1:B:385:SER:N	1:B:389:SER:OG	2.41	0.54
1:B:661:ARG:NH2	1:B:672:GLU:OE1	2.41	0.53
1:B:463:ASP:O	1:B:467:ILE:HD12	2.09	0.53
1:B:319:GLU:OE1	1:B:320:HIS:N	2.43	0.52
1:B:695:PRO:HD2	1:B:698:THR:HG21	1.92	0.52
1:B:410:LEU:HB2	1:B:414:ALA:HB2	1.92	0.52
1:A:495:LYS:HB3	1:A:499:PHE:HB3	1.92	0.51
1:B:383:TYR:CB	1:B:384:LEU:HD12	2.40	0.51
1:B:535:HIS:CD2	1:B:594:MET:HE3	2.46	0.51
1:B:583:ARG:HG2	1:B:583:ARG:NH1	2.26	0.50
1:B:384:LEU:HD11	1:B:425:PRO:HG2	1.92	0.50
1:B:682:GLU:HA	1:B:686:ARG:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:PRO:HB3	1:A:350:TYR:OH	2.12	0.50
1:B:191:LEU:HD22	3:B:847:HOH:O	2.12	0.50
1:B:512:VAL:HG12	1:B:581:LEU:O	2.11	0.50
1:A:197:LYS:HD2	1:A:595:GLN:OE1	2.12	0.50
1:A:96:TRP:HZ3	1:A:133:LYS:HG3	1.76	0.49
1:A:443:ALA:HB2	1:A:480:VAL:HG13	1.95	0.48
1:B:443:ALA:HB2	1:B:480:VAL:CG1	2.43	0.48
1:B:121:ASN:HB3	1:B:123:ASP:H	1.76	0.48
1:B:87:ALA:HB1	1:B:103:MET:HE3	1.95	0.48
1:B:206:SER:HB3	1:B:222:VAL:HG21	1.96	0.48
1:B:443:ALA:HB1	1:B:446:LEU:HG	1.95	0.47
1:B:320:HIS:CD2	1:B:323:TRP:H	2.30	0.47
1:B:168:THR:HG21	1:B:296:GLU:HG2	1.96	0.47
1:A:66:LEU:HG	1:A:77:TYR:CD1	2.50	0.46
1:B:379:ASP:O	1:B:382:GLU:HG3	2.15	0.46
1:B:487:HIS:HB3	1:B:545:PHE:HD2	1.80	0.46
1:B:611:VAL:HA	1:B:623:PHE:HB3	1.97	0.45
1:B:320:HIS:HB2	1:B:327:LEU:HD21	1.98	0.45
1:B:522:ARG:HG3	1:B:697:ARG:NH1	2.32	0.45
1:B:573:GLN:HB3	1:B:576:LEU:HG	1.99	0.44
1:B:187:PRO:HG2	1:B:281:LEU:HD23	1.99	0.44
1:A:206:SER:HB3	1:A:222:VAL:HG21	1.99	0.43
1:B:559:PRO:HG2	1:B:567:TYR:CE1	2.52	0.43
1:B:197:LYS:HE3	1:B:232:ASP:OD2	2.18	0.43
1:A:466:HIS:CD2	3:A:1257:HOH:O	2.63	0.43
1:B:347:ILE:O	1:B:351:GLN:HA	2.18	0.43
1:A:406:VAL:HG12	1:A:414:ALA:HB1	2.01	0.43
1:B:560:ARG:HD2	1:B:560:ARG:HA	1.84	0.43
1:B:440:TYR:HB3	1:B:481:VAL:HG23	2.01	0.43
1:A:356:ARG:HD2	1:A:442:LEU:HD11	2.01	0.43
1:B:547:GLY:HA2	1:B:550:PHE:HE1	1.82	0.42
1:B:531:ARG:HH21	1:B:591:ASP:HB2	1.84	0.42
1:B:619:LYS:HB2	1:B:635:HIS:N	2.35	0.42
1:B:545:PHE:CD1	1:B:545:PHE:C	2.97	0.42
1:A:591:ASP:O	1:A:595:GLN:HG2	2.20	0.42
1:B:400:MET:HB3	1:B:431:ARG:CD	2.49	0.42
1:A:475:ARG:HD2	3:A:809:HOH:O	2.20	0.42
1:B:522:ARG:HG2	1:B:526:LEU:HD12	2.01	0.42
1:B:159:LYS:O	1:B:163:GLN:HG2	2.20	0.42
1:A:615:HIS:HE1	1:A:617:VAL:HB	1.85	0.42
1:B:22:PRO:HG2	1:B:23:PHE:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:TRP:CZ3	1:A:133:LYS:HG3	2.54	0.41
1:B:591:ASP:O	1:B:595:GLN:HG2	2.21	0.41
1:A:17:ASP:OD2	1:A:475:ARG:NH2	2.52	0.41
1:A:317:ARG:NH2	3:A:819:HOH:O	2.44	0.41
1:B:527:HIS:O	1:B:531:ARG:HD3	2.19	0.41
1:A:239:ILE:HB	1:A:284:LEU:HD11	2.03	0.41
1:B:156:GLN:HG3	1:B:157:PRO:HD2	2.03	0.41
1:B:197:LYS:NZ	1:B:599:SER:OG	2.45	0.41
1:B:554:GLU:HB3	1:B:555:TRP:H	1.69	0.41
1:B:300:ASN:OD1	1:B:326:ARG:NH1	2.54	0.41
1:B:620:VAL:HA	1:B:632:PHE:O	2.21	0.41
1:A:168:THR:HG21	1:A:296:GLU:HG2	2.03	0.41
1:A:454:LEU:HD23	1:A:454:LEU:HA	1.92	0.41
1:B:487:HIS:H	1:B:487:HIS:CD2	2.38	0.41
1:A:239:ILE:HB	1:A:284:LEU:CD1	2.51	0.41
1:B:618:ASP:HB3	1:B:640:PHE:CZ	2.56	0.41
1:B:163:GLN:HE21	1:B:163:GLN:HA	1.87	0.40
1:B:295:SER:O	1:B:297:ASP:N	2.51	0.40
1:B:550:PHE:CZ	1:B:552:HIS:HD2	2.38	0.40
1:A:6:ILE:HD11	1:A:21:GLU:HG2	2.03	0.40
1:B:145:TYR:C	1:B:146:ARG:HD2	2.47	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	683/706 (97%)	666 (98%)	17 (2%)	0	100	100
1	B	682/706 (97%)	654 (96%)	28 (4%)	0	100	100
All	All	1365/1412 (97%)	1320 (97%)	45 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	582/607 (96%)	579 (100%)	3 (0%)	81	82
1	B	518/607 (85%)	515 (99%)	3 (1%)	78	78
All	All	1100/1214 (91%)	1094 (100%)	6 (0%)	81	82

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	285	ASP
1	A	524	ILE
1	A	565	ASP
1	B	382	GLU
1	B	391	VAL
1	B	532	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	220	GLN
1	A	251	GLN
1	A	351	GLN
1	A	458	GLN
1	A	588	ASN
1	A	608	GLN
1	A	628	HIS
1	A	691	GLN
1	B	163	GLN
1	B	184	HIS
1	B	228	HIS
1	B	242	HIS

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Mol	Chain	Res	Type
1	B	320	HIS
1	B	487	HIS
1	B	588	ASN
1	B	596	ASN
1	B	628	HIS

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	GLC	C	1	2	12,12,12	1.42	1 (8%)	17,17,17	0.63	0
2	GLC	C	2	2	11,11,12	1.98	2 (18%)	15,15,17	1.26	2 (13%)
2	GLC	C	3	2	11,11,12	1.75	3 (27%)	15,15,17	1.02	1 (6%)
2	GLC	D	1	2	12,12,12	1.52	1 (8%)	17,17,17	0.73	0
2	GLC	D	2	2	11,11,12	1.88	3 (27%)	15,15,17	1.05	0
2	GLC	D	3	2	11,11,12	1.93	3 (27%)	15,15,17	0.86	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	C	1	2	-	2/2/22/22	0/1/1/1
2	GLC	C	2	2	-	2/2/19/22	0/1/1/1
2	GLC	C	3	2	-	2/2/19/22	0/1/1/1
2	GLC	D	1	2	-	2/2/22/22	0/1/1/1
2	GLC	D	2	2	-	2/2/19/22	0/1/1/1
2	GLC	D	3	2	-	2/2/19/22	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	GLC	O5-C1	5.07	1.52	1.43
2	D	3	GLC	O5-C1	4.76	1.51	1.43
2	D	2	GLC	O5-C1	4.76	1.51	1.43
2	D	1	GLC	O5-C1	4.08	1.52	1.42
2	C	3	GLC	O5-C1	3.88	1.50	1.43
2	C	1	GLC	O5-C1	3.80	1.52	1.42
2	D	3	GLC	O5-C5	2.69	1.48	1.43
2	C	3	GLC	O3-C3	2.67	1.49	1.43
2	C	2	GLC	O5-C5	2.53	1.48	1.43
2	C	3	GLC	O5-C5	2.39	1.48	1.43
2	D	2	GLC	C2-C3	-2.21	1.49	1.52
2	D	2	GLC	O5-C5	2.19	1.47	1.43
2	D	3	GLC	O3-C3	2.09	1.48	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	GLC	C1-C2-C3	2.69	113.57	109.64
2	C	2	GLC	C3-C4-C5	-2.55	105.61	110.23
2	C	2	GLC	O4-C4-C3	2.34	115.89	110.38

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	3	GLC	O5-C5-C6-O6
2	D	2	GLC	O5-C5-C6-O6
2	C	2	GLC	O5-C5-C6-O6
2	D	1	GLC	O5-C5-C6-O6
2	C	1	GLC	O5-C5-C6-O6
2	D	3	GLC	C4-C5-C6-O6

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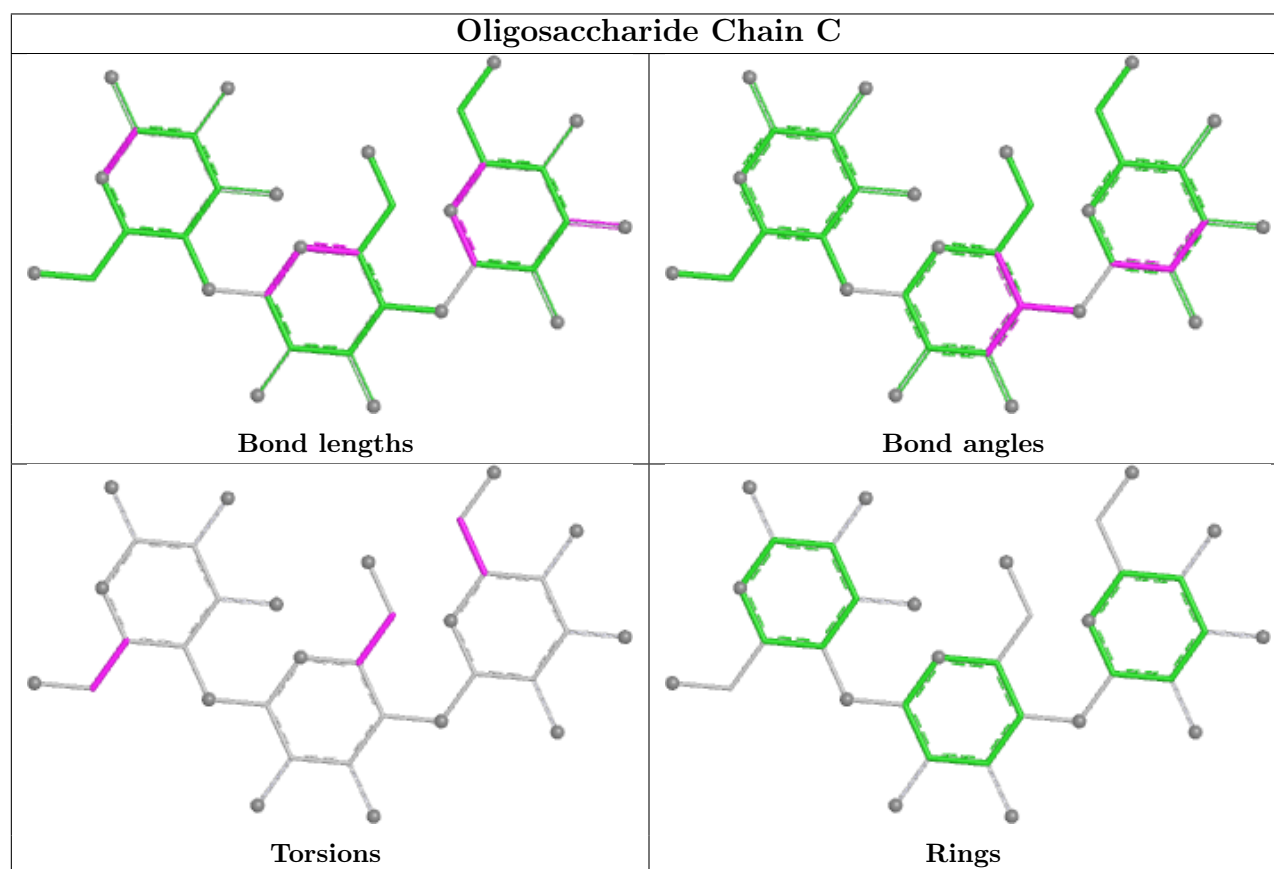
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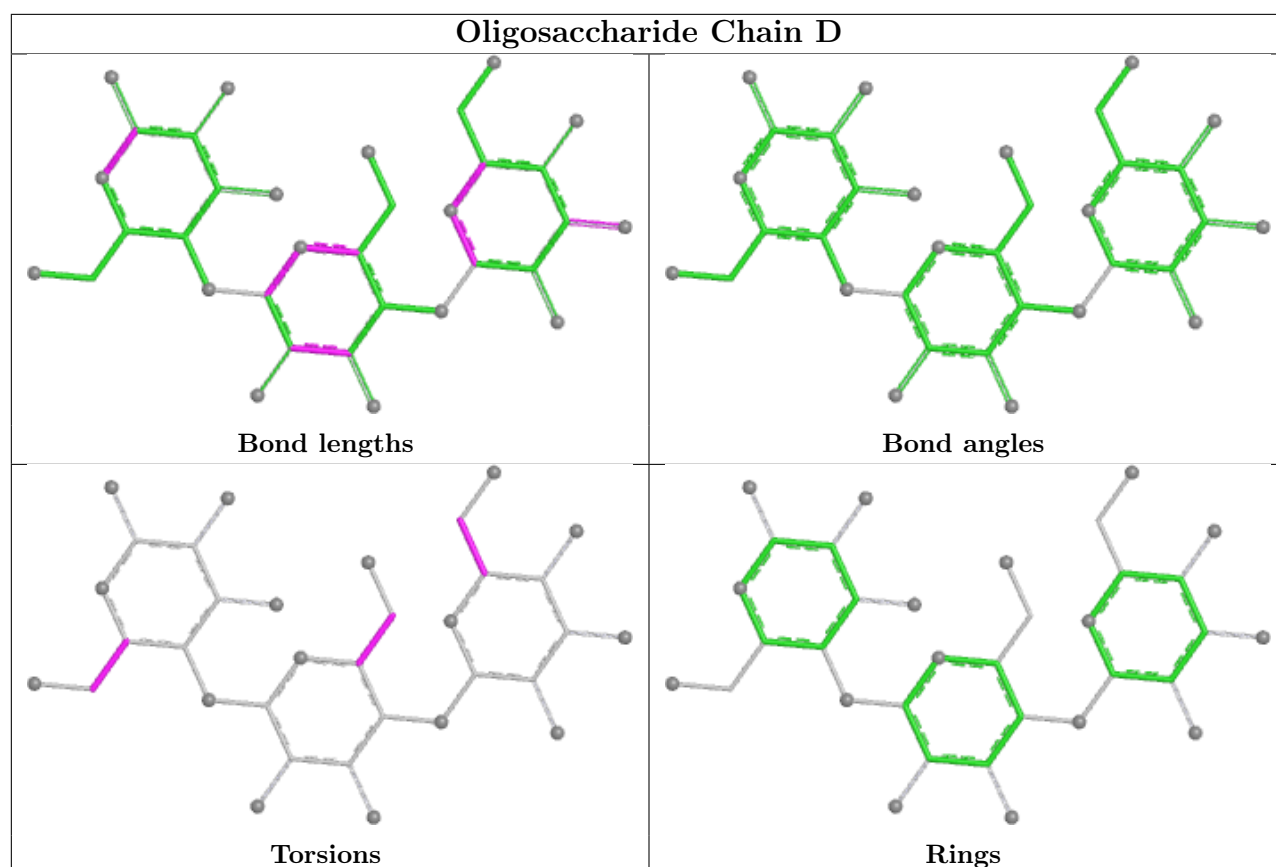
Mol	Chain	Res	Type	Atoms
2	C	1	GLC	C4-C5-C6-O6
2	C	3	GLC	O5-C5-C6-O6
2	D	1	GLC	C4-C5-C6-O6
2	D	2	GLC	C4-C5-C6-O6
2	C	2	GLC	C4-C5-C6-O6
2	C	3	GLC	C4-C5-C6-O6

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	687/706 (97%)	-0.04	11 (1%) 70 77	27, 38, 64, 153	0
1	B	690/706 (97%)	1.03	117 (16%) 4 4	39, 70, 118, 184	0
All	All	1377/1412 (97%)	0.50	128 (9%) 14 16	27, 50, 109, 184	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	504	ALA	6.5
1	B	490	ALA	5.8
1	A	493	GLY	4.8
1	B	634	PHE	4.8
1	B	451	ILE	4.8
1	B	453	LEU	4.8
1	B	375	ALA	4.7
1	B	462	TRP	4.6
1	A	490	ALA	4.6
1	B	500	TRP	4.6
1	B	47	ASP	4.5
1	A	370	VAL	4.4
1	B	533	ILE	4.3
1	B	632	PHE	4.3
1	B	561	VAL	4.3
1	B	374	GLY	4.3
1	B	613	LEU	4.2
1	B	495	LYS	4.1
1	B	657	LEU	4.1
1	B	655	ILE	4.0
1	A	492	VAL	4.0
1	B	456	THR	4.0
1	B	520	ILE	4.0
1	B	48	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	653	TYR	3.9
1	B	555	TRP	3.9
1	B	513	LEU	3.9
1	B	458	GLN	3.8
1	B	454	LEU	3.8
1	B	517	THR	3.7
1	A	2	SER	3.7
1	B	664	PHE	3.7
1	B	581	LEU	3.6
1	B	509	ASP	3.6
1	B	556	LEU	3.6
1	B	508	THR	3.6
1	B	518	LEU	3.5
1	B	248	PHE	3.5
1	B	530	ILE	3.4
1	B	16	ILE	3.3
1	B	381	ASN	3.3
1	B	683	TRP	3.3
1	A	5	LYS	3.3
1	B	501	LEU	3.3
1	B	460	ASP	3.3
1	B	105	HIS	3.2
1	B	497	LEU	3.2
1	B	524	ILE	3.2
1	B	515	GLU	3.2
1	B	526	LEU	3.1
1	B	313	LEU	3.1
1	B	450	TRP	3.1
1	B	503	ASP	3.1
1	B	620	VAL	3.1
1	B	455	LYS	3.1
1	B	654	LYS	3.1
1	B	694	ILE	3.0
1	B	14	VAL	3.0
1	B	499	PHE	2.9
1	B	488	ASP	2.9
1	B	670	ILE	2.9
1	B	706	MET	2.9
1	B	519	VAL	2.8
1	B	574	PHE	2.8
1	A	491	LEU	2.8
1	B	679	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	6	ILE	2.8
1	B	576	LEU	2.8
1	B	671	ASP	2.8
1	B	376	PHE	2.8
1	B	521	ASP	2.8
1	B	550	PHE	2.7
1	B	570	ALA	2.7
1	B	689	PHE	2.7
1	B	316	GLY	2.6
1	A	494	ASP	2.6
1	B	569	TYR	2.6
1	B	489	GLN	2.6
1	B	467	ILE	2.6
1	B	109	PHE	2.5
1	B	387	ASP	2.5
1	B	565	ASP	2.5
1	B	551	GLY	2.5
1	B	645	ILE	2.5
1	B	94	ASN	2.5
1	B	466	HIS	2.5
1	B	666	GLY	2.5
1	B	496	THR	2.5
1	B	457	LYS	2.4
1	B	516	PRO	2.4
1	B	322	LEU	2.4
1	B	637	THR	2.4
1	B	699	ALA	2.4
1	B	512	VAL	2.4
1	B	582	LEU	2.4
1	B	461	ASP	2.3
1	B	640	PHE	2.3
1	B	421	VAL	2.3
1	A	323	TRP	2.3
1	B	529	MET	2.3
1	B	621	ILE	2.3
1	B	577	VAL	2.3
1	B	487	HIS	2.3
1	B	527	HIS	2.3
1	B	667	HIS	2.2
1	B	534	THR	2.2
1	B	641	THR	2.2
1	B	698	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	673	ALA	2.2
1	A	500	TRP	2.2
1	B	560	ARG	2.2
1	B	161	THR	2.2
1	B	638	GLN	2.1
1	B	459	ASP	2.1
1	B	137	VAL	2.1
1	B	470	THR	2.1
1	B	210	PRO	2.1
1	B	676	PHE	2.1
1	B	584	TYR	2.1
1	B	659	THR	2.1
1	B	383	TYR	2.1
1	A	508	THR	2.1
1	B	647	VAL	2.1
1	B	208	PRO	2.0
1	B	656	VAL	2.0
1	B	448	ASP	2.0
1	B	49	SER	2.0
1	B	307	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.

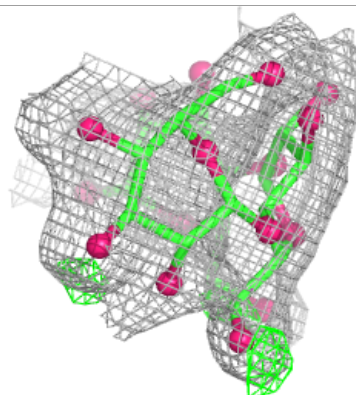
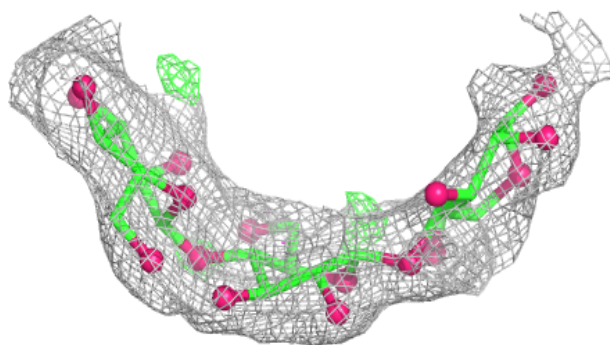
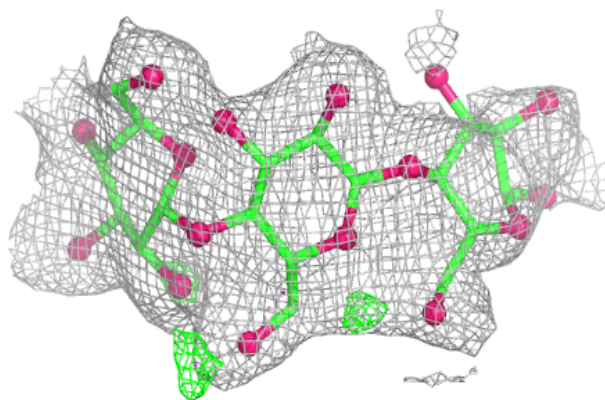
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLC	D	1	12/12	0.57	0.13	100,114,119,119	0
2	GLC	C	1	12/12	0.68	0.13	78,112,121,150	0
2	GLC	D	3	11/12	0.71	0.13	86,93,96,99	0
2	GLC	C	2	11/12	0.79	0.13	65,74,79,84	0
2	GLC	C	3	11/12	0.82	0.10	69,71,76,77	0
2	GLC	D	2	11/12	0.85	0.11	89,94,98,99	0

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.

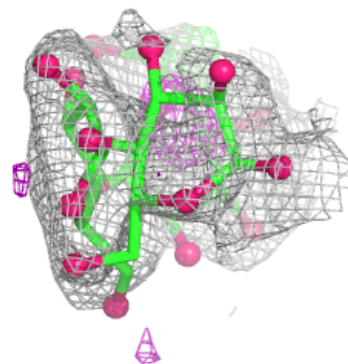
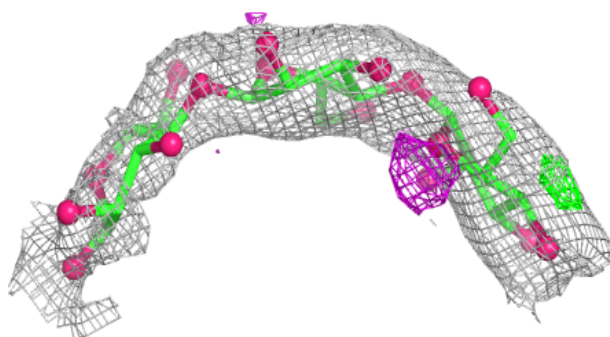
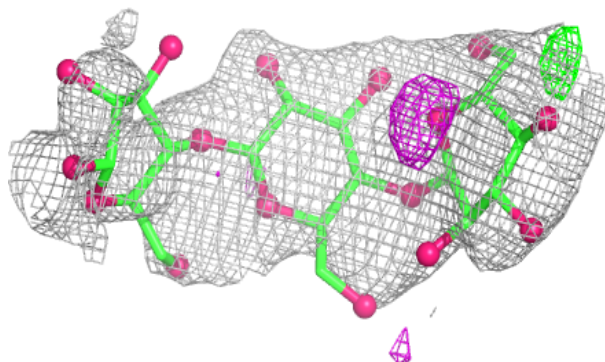
Electron density around Chain C:

$2mF_o-DF_c$ (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 [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.