



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:08 PM UTC

PDB ID : 5CGT / pdb_00005cgt
Title : MALTOTRIOSE COMPLEX OF PRECONDITIONED CYCLODEXTRIN
GLYCOSYLTRANSFERASE MUTANT
Authors : Parsiegla, G.; Schulz, G.E.
Deposited on : 1998-06-06
Resolution : 2.50 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

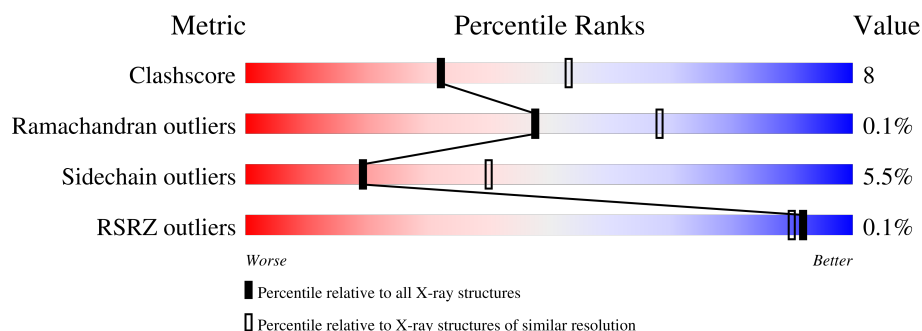
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	684	
2	B	2	
2	C	2	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5516 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 CYCLODEXTRIN GLYCOSYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	684	Total	C	N	O	S	0	0	0
			5264	3322	891	1038	13			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	229	ALA	ASP	engineered mutation	UNP P30920

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



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

- Molecule 3 is alpha-D-glucopyranose (CCD ID: GLC) (formula: C₆H₁₂O₆).



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Ca	0	0
			2	2		

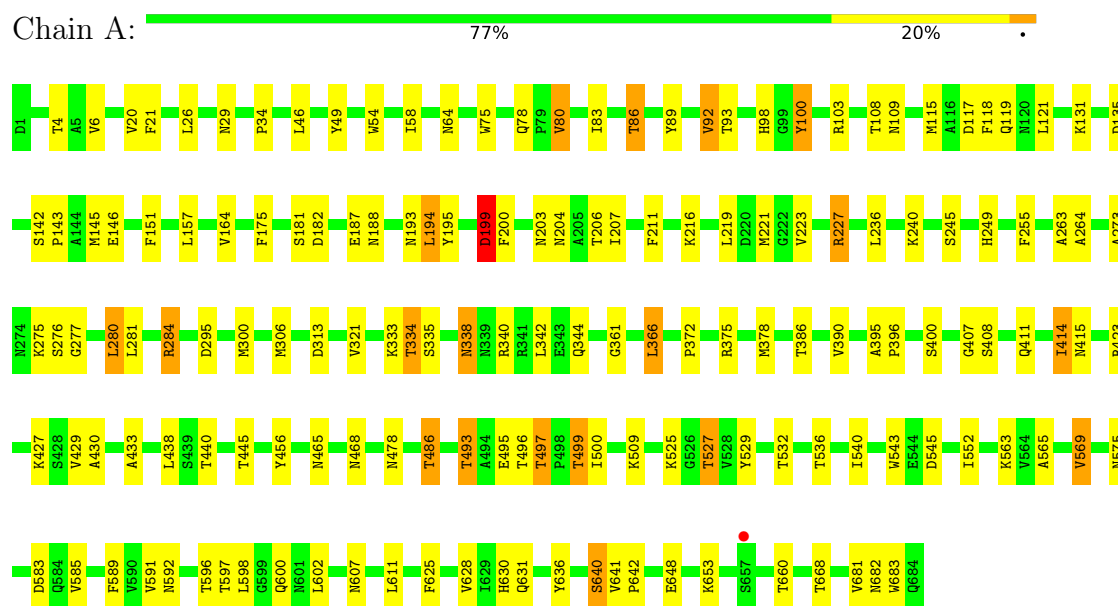
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	192	Total	O	0	0
			192	192		

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: CYCLODEXTRIN GLYCOSYLTRANSFERASE



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	93.50Å 104.90Å 113.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50 10.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	85.0 (10.00-2.50) 79.7 (10.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.57 (at 2.51Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.177 , 0.247 0.184 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	21.4	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 48.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5516	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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: CA, GLC, BGC

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	0.73	0/5395	1.09	34/7362 (0.5%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109	ASN	N-CA-C	-7.69	98.04	109.42
1	A	281	LEU	N-CA-C	-6.84	99.39	110.20
1	A	407	GLY	N-CA-C	6.51	122.47	112.51
1	A	414	ILE	N-CA-C	6.47	115.59	107.70
1	A	275	LYS	N-CA-C	6.37	122.53	114.31
1	A	276	SER	N-CA-C	6.29	118.21	111.36
1	A	648	GLU	N-CA-C	-6.26	99.20	109.40
1	A	575	ASN	N-CA-C	6.20	118.91	110.35
1	A	20	VAL	N-CA-C	6.10	116.65	108.11
1	A	378	MET	CA-C-N	6.02	125.72	119.64
1	A	378	MET	C-N-CA	6.02	125.72	119.64
1	A	100	TYR	N-CA-C	5.99	120.21	113.02
1	A	164	VAL	N-CA-C	-5.93	106.71	111.81
1	A	313	ASP	N-CA-C	5.91	117.80	111.36
1	A	640	SER	N-CA-C	-5.84	100.97	110.20
1	A	400	SER	N-CA-C	5.83	118.86	111.69
1	A	552	ILE	CA-C-N	5.70	125.67	120.03
1	A	552	ILE	C-N-CA	5.70	125.67	120.03
1	A	64	ASN	N-CA-C	5.63	119.46	112.47
1	A	500	ILE	N-CA-C	5.53	116.72	108.54
1	A	80	VAL	N-CA-C	5.47	116.39	110.21
1	A	607	ASN	N-CA-C	5.46	122.43	110.80
1	A	29	ASN	CA-C-N	5.42	125.11	119.64
1	A	29	ASN	C-N-CA	5.42	125.11	119.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	ASN	N-CA-C	-5.33	106.73	113.18
1	A	277	GLY	N-CA-C	-5.27	107.26	114.64
1	A	585	VAL	N-CA-C	-5.22	100.34	108.44
1	A	92	VAL	N-CA-C	5.21	115.60	107.99
1	A	199	ASP	N-CA-C	5.20	117.23	108.96
1	A	211	PHE	N-CA-C	5.18	117.83	111.82
1	A	545	ASP	N-CA-C	5.12	118.31	111.75
1	A	295	ASP	N-CA-C	5.09	119.20	112.89
1	A	135	ASP	N-CA-C	-5.02	102.27	110.20
1	A	117	ASP	N-CA-C	-5.00	105.91	111.36

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	5264	0	5009	83	0
2	B	23	0	21	0	0
2	C	23	0	21	0	0
3	A	12	0	12	0	0
4	A	2	0	0	0	0
5	A	192	0	0	1	0
All	All	5516	0	5063	83	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 8.

All (83) 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:108:THR:HG23	1:A:115:MET:HE2	1.45	0.98
1:A:98:HIS:HD2	1:A:100:TYR:H	1.27	0.82
1:A:653:LYS:HE3	1:A:683:TRP:CZ2	2.31	0.66
1:A:86:THR:HG23	1:A:93:THR:HG23	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:ARG:HH12	1:A:465:ASN:ND2	1.97	0.61
1:A:54:TRP:CZ3	1:A:118:PHE:HB2	2.36	0.60
1:A:75:TRP:CZ2	1:A:227:ARG:HG3	2.38	0.58
1:A:182:ASP:H	1:A:188:ASN:HD21	1.52	0.58
1:A:527:THR:HG23	1:A:565:ALA:HB3	1.87	0.57
1:A:187:GLU:CD	1:A:625:PHE:HB3	2.31	0.56
1:A:641:VAL:HG22	1:A:642:PRO:HD2	1.87	0.55
1:A:386:THR:O	1:A:390:VAL:HG23	2.06	0.55
1:A:445:THR:HG22	1:A:478:ASN:CG	2.31	0.55
1:A:86:THR:CG2	1:A:93:THR:HG23	2.38	0.53
1:A:181:SER:HA	1:A:188:ASN:HD21	1.73	0.53
1:A:219:LEU:HA	1:A:223:VAL:HG22	1.92	0.52
1:A:142:SER:HB2	1:A:143:PRO:CD	2.41	0.51
1:A:264:ALA:O	1:A:284:ARG:HD3	2.09	0.51
1:A:395:ALA:HB3	1:A:396:PRO:HD3	1.93	0.51
1:A:344:GLN:HG2	1:A:486:THR:HG21	1.92	0.51
1:A:204:ASN:ND2	1:A:206:THR:HB	2.25	0.51
1:A:497:THR:O	1:A:499:THR:HG22	2.12	0.50
1:A:361:GLY:HA3	1:A:366:LEU:HD12	1.93	0.50
1:A:495:GLU:HG2	1:A:499:THR:CG2	2.41	0.50
1:A:75:TRP:CE2	1:A:227:ARG:HG3	2.46	0.49
1:A:596:THR:HB	1:A:600:GLN:HB3	1.94	0.49
1:A:427:LYS:HB2	1:A:493:THR:HG22	1.95	0.49
1:A:118:PHE:CD2	1:A:221:MET:HE3	2.47	0.49
1:A:408:SER:O	1:A:423:ARG:HA	2.11	0.49
1:A:338:ASN:HD21	1:A:438:LEU:HD11	1.78	0.49
1:A:597:THR:CG2	1:A:598:LEU:N	2.76	0.49
1:A:273:ALA:HB2	1:A:280:LEU:HD22	1.95	0.48
1:A:263:ALA:O	1:A:284:ARG:HD2	2.13	0.48
1:A:193:ASN:OD1	1:A:199:ASP:HB2	2.14	0.48
1:A:157:LEU:HD22	1:A:200:PHE:CE1	2.49	0.47
1:A:78:GLN:HG2	1:A:80:VAL:HG22	1.96	0.47
1:A:54:TRP:O	1:A:58:ILE:HG13	2.14	0.47
1:A:529:TYR:HB2	1:A:563:LYS:HB3	1.96	0.47
1:A:115:MET:O	1:A:119:GLN:HG3	2.14	0.47
1:A:204:ASN:HD21	1:A:206:THR:HB	1.80	0.46
1:A:240:LYS:HD3	1:A:640:SER:HB3	1.97	0.46
1:A:597:THR:HG22	1:A:598:LEU:N	2.31	0.46
1:A:236:LEU:HD23	1:A:236:LEU:O	2.15	0.46
1:A:300:MET:HB2	1:A:415:ASN:O	2.15	0.45
1:A:592:ASN:HB2	1:A:682:ASN:OD1	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:LYS:NZ	1:A:496:THR:HG22	2.31	0.45
1:A:630:HIS:HB2	1:A:636:TYR:CD1	2.52	0.45
1:A:334:THR:HG23	1:A:335:SER:N	2.32	0.45
1:A:414:ILE:HG12	1:A:415:ASN:N	2.32	0.45
1:A:540:ILE:HG21	1:A:543:TRP:HE3	1.82	0.45
1:A:6:VAL:HG23	1:A:131:LYS:HG2	1.98	0.44
1:A:495:GLU:HG2	1:A:499:THR:HG21	1.99	0.44
1:A:34:PRO:HG2	1:A:49:TYR:CG	2.52	0.44
1:A:255:PHE:CD2	1:A:321:VAL:HG21	2.53	0.44
1:A:219:LEU:HD23	1:A:223:VAL:CG2	2.48	0.44
1:A:236:LEU:HD23	1:A:236:LEU:C	2.42	0.44
1:A:429:VAL:HG12	1:A:430:ALA:N	2.33	0.44
1:A:589:PHE:O	1:A:636:TYR:HA	2.17	0.44
1:A:204:ASN:HD22	1:A:207:ILE:H	1.65	0.43
1:A:427:LYS:HD2	1:A:493:THR:HG21	1.99	0.43
1:A:591:VAL:HA	1:A:681:VAL:O	2.18	0.43
1:A:89:TYR:O	1:A:92:VAL:HG12	2.17	0.43
1:A:227:ARG:HG2	1:A:255:PHE:CE2	2.53	0.43
1:A:142:SER:HB2	1:A:143:PRO:HD2	2.00	0.43
1:A:216:LYS:HD2	1:A:249:HIS:CG	2.54	0.42
1:A:414:ILE:CG1	1:A:415:ASN:N	2.82	0.42
1:A:255:PHE:CD1	1:A:255:PHE:N	2.87	0.42
1:A:456:TYR:O	1:A:468:ASN:HB3	2.20	0.42
1:A:194:LEU:O	1:A:195:TYR:HB2	2.19	0.42
1:A:497:THR:HG22	1:A:569:VAL:HG11	2.00	0.42
1:A:527:THR:HB	1:A:536:THR:HG22	2.02	0.42
1:A:611:LEU:HD23	1:A:611:LEU:HA	1.93	0.42
1:A:306:MET:HE3	1:A:306:MET:HB3	1.92	0.41
1:A:175:PHE:HA	1:A:199:ASP:O	2.21	0.41
1:A:145:MET:HG3	1:A:151:PHE:CD2	2.55	0.41
1:A:83:ILE:HA	1:A:103:ARG:HD3	2.03	0.41
1:A:157:LEU:HD22	1:A:200:PHE:CZ	2.56	0.41
1:A:509:LYS:HE2	1:A:583:ASP:OD1	2.21	0.41
1:A:525:LYS:HD2	1:A:540:ILE:HB	2.02	0.40
1:A:527:THR:HB	1:A:536:THR:CG2	2.50	0.40
1:A:631:GLN:N	1:A:631:GLN:CD	2.79	0.40
1:A:333:LYS:HB3	5:A:741:HOH:O	2.20	0.40
1:A:433:ALA:O	1:A:486:THR:HA	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	682/684 (100%)	649 (95%)	32 (5%)	1 (0%)	48	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	628	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	565/565 (100%)	534 (94%)	31 (6%)	19	40

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

Mol	Chain	Res	Type
1	A	4	THR
1	A	21	PHE
1	A	26	LEU
1	A	46	LEU
1	A	86	THR
1	A	121	LEU
1	A	146	GLU
1	A	194	LEU
1	A	199	ASP
1	A	227	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	245	SER
1	A	280	LEU
1	A	284	ARG
1	A	334	THR
1	A	338	ASN
1	A	342	LEU
1	A	366	LEU
1	A	372	PRO
1	A	375	ARG
1	A	411	GLN
1	A	440	THR
1	A	486	THR
1	A	493	THR
1	A	497	THR
1	A	499	THR
1	A	527	THR
1	A	532	THR
1	A	569	VAL
1	A	602	LEU
1	A	660	THR
1	A	668	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	A	98	HIS
1	A	120	ASN
1	A	178	ASN
1	A	188	ASN
1	A	204	ASN
1	A	249	HIS
1	A	318	ASN
1	A	338	ASN
1	A	369	ASN
1	A	401	ASN
1	A	465	ASN
1	A	473	ASN
1	A	477	ASN
1	A	547	GLN
1	A	559	ASN
1	A	593	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	600	GLN
1	A	631	GLN
1	A	666	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 ⓘ

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	B	1	2	12,12,12	0.38	0	17,17,17	0.69	0
2	GLC	B	2	2	11,11,12	0.62	0	15,15,17	0.72	1 (6%)
2	BGC	C	1	2	12,12,12	0.27	0	17,17,17	0.96	1 (5%)
2	GLC	C	2	2	11,11,12	0.42	0	15,15,17	0.56	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	BGC	B	1	2	-	0/2/22/22	0/1/1/1
2	GLC	B	2	2	-	1/2/19/22	0/1/1/1
2	BGC	C	1	2	-	0/2/22/22	0/1/1/1
2	GLC	C	2	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	BGC	C4-C3-C2	-3.38	104.89	110.83
2	B	2	GLC	C1-C2-C3	2.34	113.05	109.64

There are no chirality outliers.

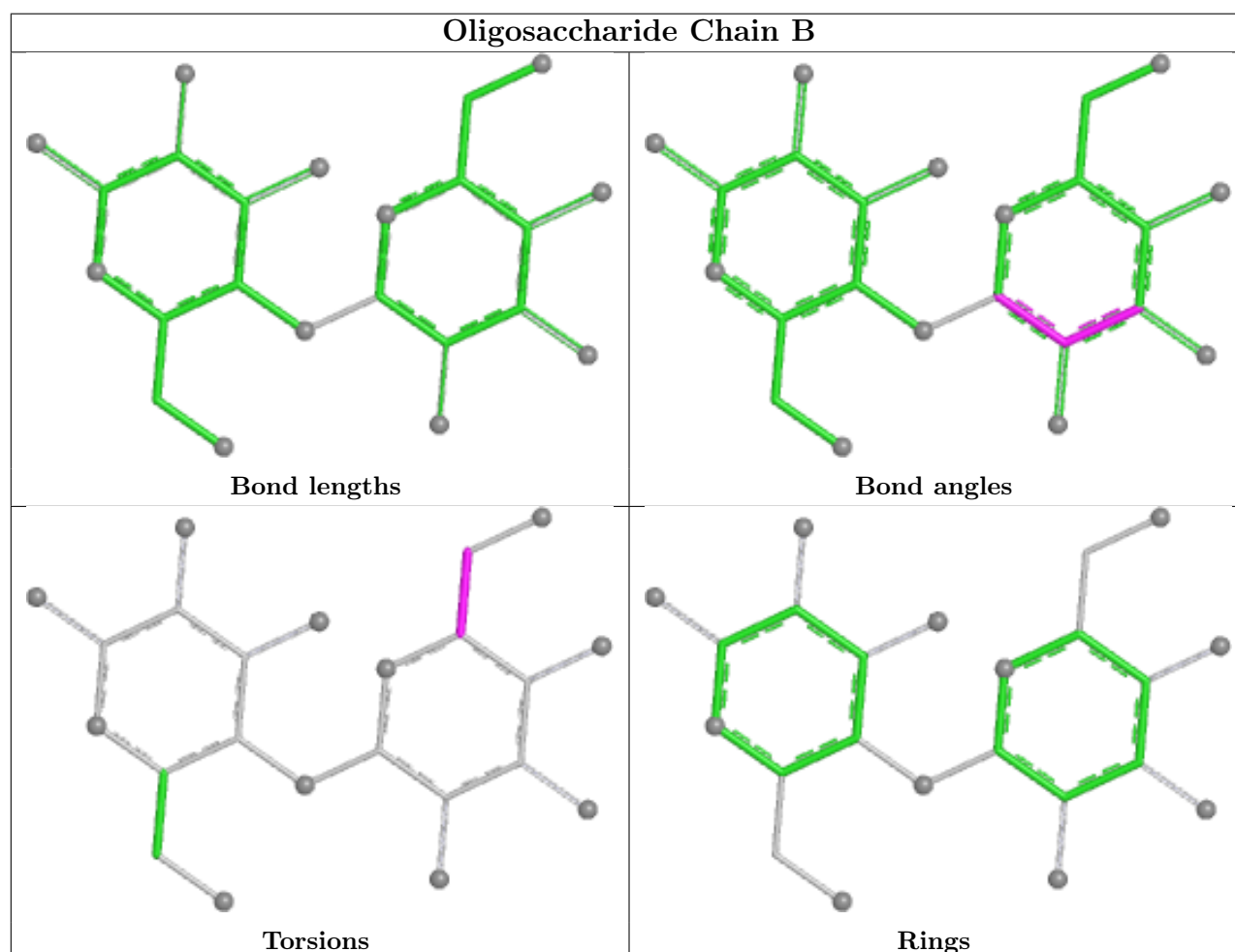
All (1) torsion outliers are listed below:

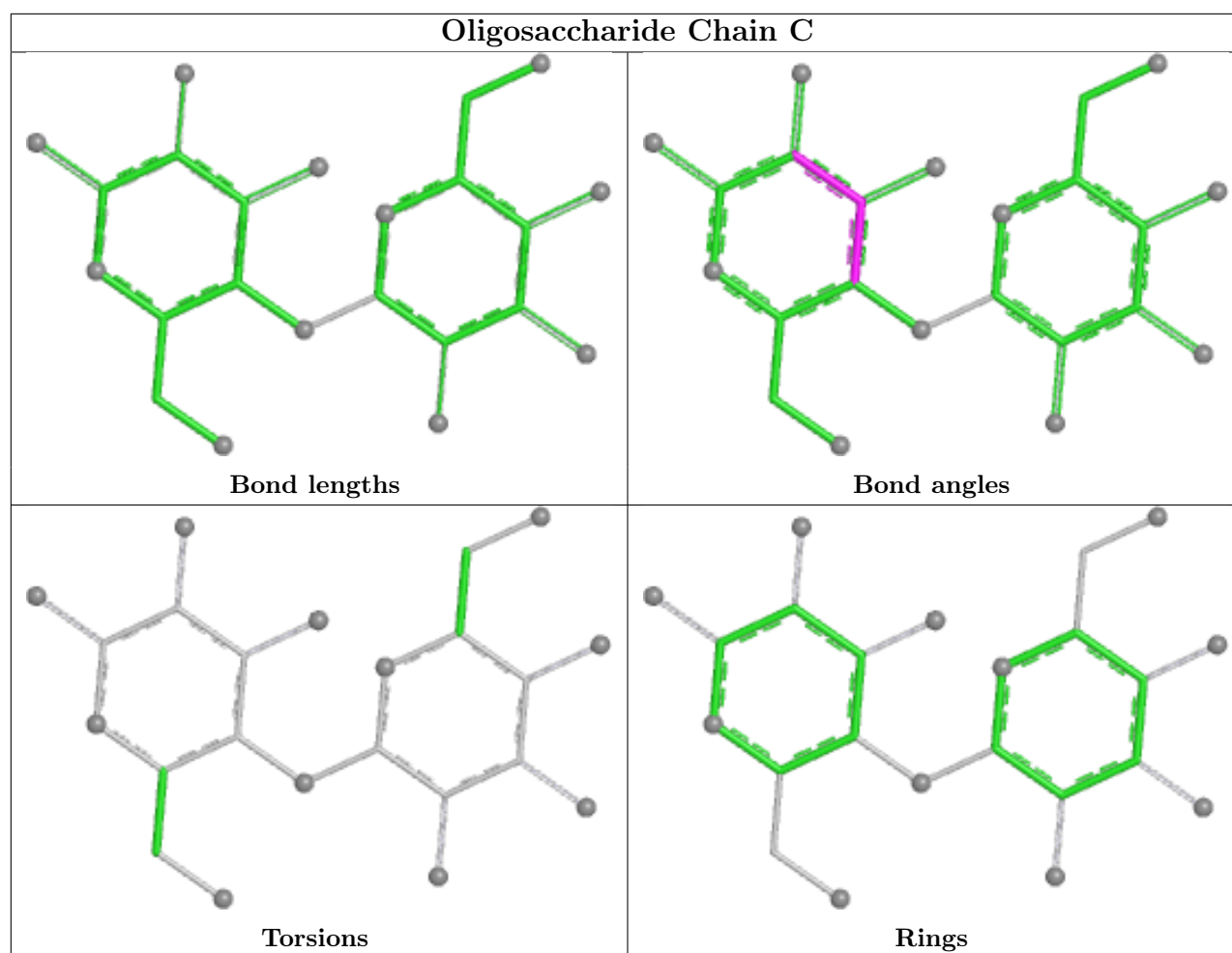
Mol	Chain	Res	Type	Atoms
2	B	2	GLC	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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





5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	$\# Z > 2$
3	GLC	A	711	-	12,12,12	0.59	0	17,17,17	0.80	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
3	GLC	A	711	-	-	2/2/22/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	711	GLC	O5-C5-C6-O6
3	A	711	GLC	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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	684/684 (100%)	-0.91	1 (0%) 92 90	3, 13, 25, 44	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	657	SER	2.4

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](#)

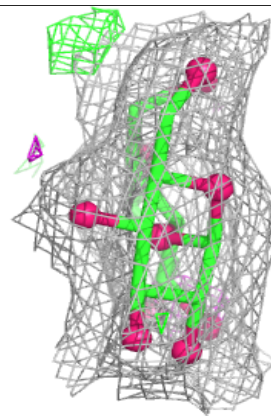
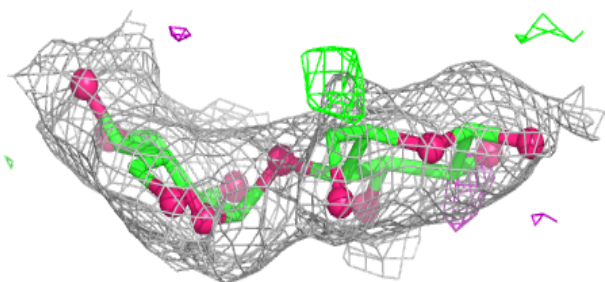
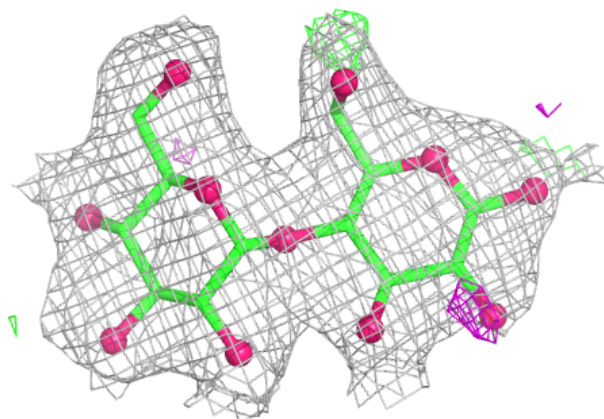
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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	BGC	B	1	12/12	0.90	0.10	26,32,35,37	0
2	GLC	B	2	11/12	0.94	0.06	16,21,22,25	0
2	GLC	C	2	11/12	0.97	0.05	8,10,12,13	0
2	BGC	C	1	12/12	0.98	0.04	5,10,13,14	0

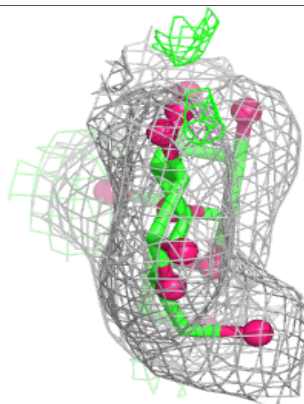
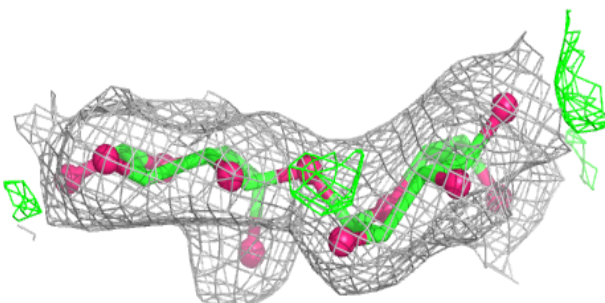
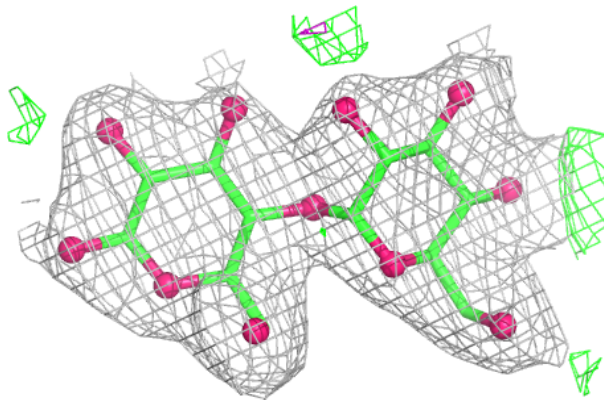
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain B:

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

**Electron density around Chain C:**

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



6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GLC	A	711	12/12	0.82	0.13	28,32,35,36	0
4	CA	A	686	1/1	0.96	0.03	16,16,16,16	0
4	CA	A	685	1/1	0.97	0.02	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.