W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Nov 21, 2023 – 03:18 AM JST

PDB ID	:	7EKW
Title	:	Crystal Structure of the Candida Glabrata Glycogen Debranching Enzyme (D535N) in complex with maltotetrose
Authors	:	Shen, M.; Xiang, S.
Deposited on	:	2021-04-07
Resolution	:	3.10 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

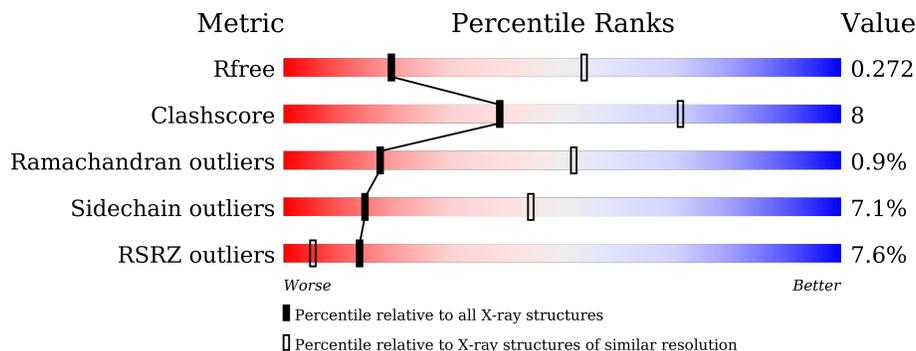|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.10 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	Percentile Ranks	Value
Rfree		0.272
Clashscore		8
Ramachandran outliers		0.9%
Sidechain outliers		7.1%
RSRZ outliers		7.6%

Worse — Better

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 <=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	1536	7% / 77% / 20% / ..
1	B	1536	8% / 76% / 22% / ..
2	C	2	100%

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 24530 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 4-alpha-glucanotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1520	Total	C	N	O	S	0	0	0
			12229	7800	2058	2319	52			
1	B	1526	Total	C	N	O	S	0	0	0
			12278	7830	2066	2330	52			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	535	ASN	ASP	engineered mutation	UNP Q6FSK0
A	1529	LEU	-	expression tag	UNP Q6FSK0
A	1530	GLU	-	expression tag	UNP Q6FSK0
A	1531	HIS	-	expression tag	UNP Q6FSK0
A	1532	HIS	-	expression tag	UNP Q6FSK0
A	1533	HIS	-	expression tag	UNP Q6FSK0
A	1534	HIS	-	expression tag	UNP Q6FSK0
A	1535	HIS	-	expression tag	UNP Q6FSK0
A	1536	HIS	-	expression tag	UNP Q6FSK0
B	535	ASN	ASP	engineered mutation	UNP Q6FSK0
B	1529	LEU	-	expression tag	UNP Q6FSK0
B	1530	GLU	-	expression tag	UNP Q6FSK0
B	1531	HIS	-	expression tag	UNP Q6FSK0
B	1532	HIS	-	expression tag	UNP Q6FSK0
B	1533	HIS	-	expression tag	UNP Q6FSK0
B	1534	HIS	-	expression tag	UNP Q6FSK0
B	1535	HIS	-	expression tag	UNP Q6FSK0
B	1536	HIS	-	expression tag	UNP Q6FSK0

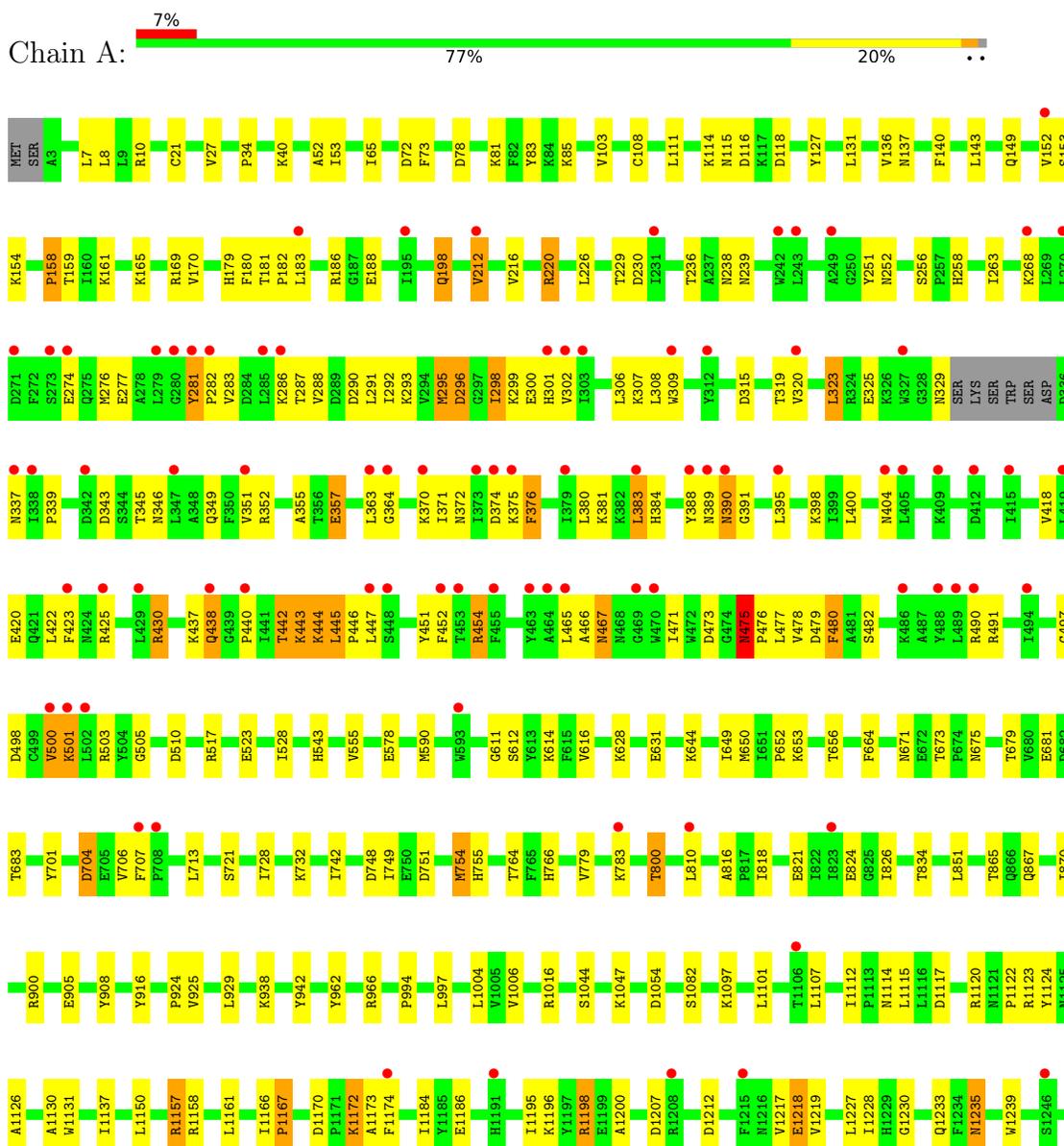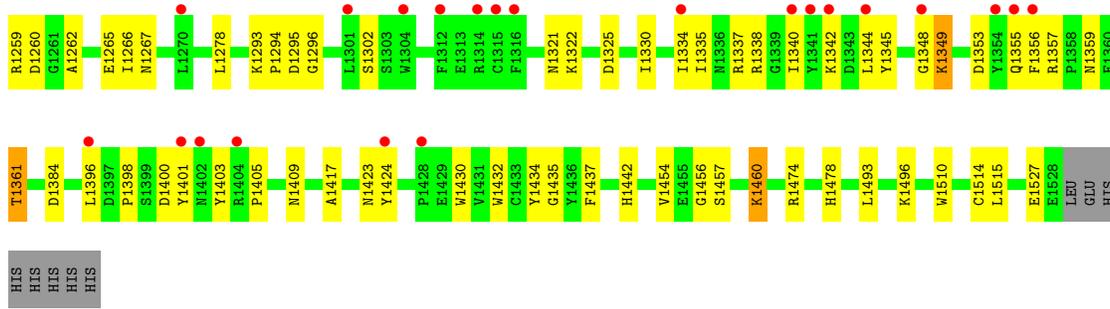- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

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

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: 4-alpha-glucanotransferase

R1259 D1260 G1261 A1262 E1265 I1266 N1267 L1270 L1278 K1293 P1294 D1295 G1296 L1301 S1302 I1303 W1304 F1312 E1313 R1314 C1315 F1316 N1321 K1322 D1325 I1330 I1334 I1335 N1336 R1337 R1338 G1339 I1340 Y1341 K1342 D1343 L1344 Y1345 G1348 K1349 D1353 Y1354 Q1355 F1356 R1357 P1358 N1359 F1360

T1361 D1384 L1396 D1397 P1398 S1399 D1400 Y1401 N1402 Y1403 R1404 P1405 N1409 A1417 N1423 Y1424 P1428 E1429 W1430 V1431 W1432 C1433 Y1434 G1435 Y1436 F1437 H1442 V1454 E1455 G1456 S1457 K1460 R1474 H1478 L1493 K1496 W1510 C1514 L1515 E1527 E1528 LEU GLU HIS
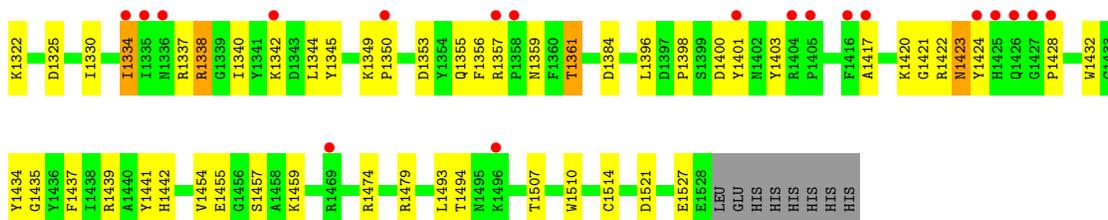
HIS HIS HIS HIS HIS

● **Molecule 1: 4-alpha-glucanotransferase**

8%

Chain B:　　76%　　　　22%

MET SER A3 H4 R5 L8 D13 C21 V27 P31 L35 Y47 I53 I65 D72 F73 D78 K81 V103 Y107 C108 L111 K114 K117 D118 Y127 L131 P142 L143 Q149 S150 K161 E164 R169 V170 A171

S172 H179 P182 L183 Q184 Q198 L199 S208 E209 D230 H235 T236 W242 L243 L244 D245 A249 G250 Y251 N252 H253 S256 P257 H258 L259 I260 S261 A262 I263 D266 K267 K268 L269 L270 D271 F272 S273 E274 Q275 M276 E277 G280 Y281 P282 V283 D284 T287 V288

D289 D290 L291 V294 M295 D296 G297 I298 K299 E300 H301 V302 L306 K307 L308 W309 E310 F311 Y312 V313 V314 Q318 T319 V320 L323 R324 W327 G328 N329 S330 K331 S332 W333 I338 P339 S340 K341 D342 D343 L347 A348 Q349 A355 T356 E357 F360 G361 S362 L363 G364

N369 K370 I371 N372 I373 D374 K375 F376 A377 A378 I379 K382 L383 H384 D387 Y388 N389 N390 I399 L400 N404 L405 P406 F407 Y408 K409 E410 Y411 D412 D413 D414 I415 V418 L419 E420 Q421 L422 F423 N424 R425 I426 K427 I431 D432 D433 H434 G435 K437 Q438 G439 P440 I441 T442

K443 K444 L445 P446 L447 S448 E449 P450 Y451 F452 T453 R454 F455 K456 E462 Y463 A464 L465 A466 N467 M468 W472 L477 F480 A481 Y488 L489 R490 E492 V493 I494 V495 C499 V500 K501 L502 Y513 R517 K520 E523 I528 F529 H543 V555 M572

E578 R587 M590 H605 R608 G611 S612 V616 D630 E631 A635 V643 K644 S647 E648 P652 T656 F664 N671 E672 T673 P674 N675 V680 E681 D682 T683 S695 V700 Y701 D704 E705 V706 Q709 L713 S721 I728

V731 K732 R739 I742 A743 S744 E745 I749 E750 D751 M754 H755 Q761 T764 F765 H766 V779 K783 T800 L810 A816 I822 I823 I826 T834 G835 L851 P852 Q853 T865 Q866 Q867 L868 G869 I870 S893 Y896 R900 A901 E902

E905 S909 E910 G911 R912 K923 P924 V925 Y926 K938 Y942 Y962 R966 D972 K973 E974 R989 L997 R1016 T1029 M1042 V1043 S1044 P1053 D1054 A1059 C1074 R1077 S1082 L1083 R1084 L1088 F1103 A1104 K1105 T1106 L1107 K1108 H1109 G1110

L1111 N1114 L1115 L1116 D1117 R1120 R1123 A1126 R1127 D1128 W1131 A1136 I1137 V1155 T1156 R1157 R1158 F1159 P1160 L1161 D1162 D1163 E1164 Y1165 I1166 P1167 Y1168 D1169 D1170 F1174 S1175 Y1176 I1184 R1190 H1191 A1192 A1202 D1207 R1208 V1209 D1212 E1213

N1216 V1217 E1218 V1219 N1220 V1221 D1222 W1223 I1228 H1229 G1230 Q1233 F1234 N1235 C1236 G1237 T1238 W1239 M1240 D1241 K1242 E1245 S1246 E1247 K1248 S1251 V1252 P1255 G1256 T1257 P1258 R1259 D1260 G1261 A1262 I1263 V1264 E1265 I1266 N1267 Q1279 L1280 V1291 T1292 K1293 P1294 D1295 G1296 F1316 N1321

K1322 D1325 I1330 I1334 I1335 N1336 R1337 R1338 G1339 I1340 Y1341 K1342 D1343 L1344 Y1345 K1349 P1350 D1353 Y1354 Q1355 F1356 R1357 P1358 N1359 F1360 T1361 D1384 L1396 D1397 P1398 S1399 D1400 Y1401 N1402 Y1403 R1404 P1405 F1416 A1417 K1420 G1421 R1422 N1423 Y1424 H1425 Q1426 G1427 P1428 W1432 C1433

Y1434 G1435 Y1436 F1437 I1438 R1439 A1440 Y1441 H1442 V1454 E1455 G1456 S1457 A1458 K1459 R1469 R1474 R1479 L1493 T1494 N1495 K1496 T1507 W1510 C1514 D1521 E1527 E1528 LEU GLU HIS HIS HIS HIS HIS HIS

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

Chain C: 100%

GLC1 GLC2

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	160.25Å 198.94Å 134.59Å 90.00° 104.87° 90.00°	Depositor
Resolution (Å)	25.26 – 3.10 99.71 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (25.26-3.10) 99.8 (99.71-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.63 (at 3.13Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.248 , 0.272 0.248 , 0.272	Depositor DCC
R_{free} test set	3769 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	76.4	Xtriage
Anisotropy	0.654	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 49.9	EDS
L-test for twinning [2]	$<|L|> = 0.48, <L^2> = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	24530	wwPDB-VP
Average B, all atoms (Å^2)	101.0	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ 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	0.25	0/12537	0.42	0/16999
1	B	0.24	0/12589	0.41	0/17071
All	All	0.24	0/25126	0.41	0/34070

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	12229	0	11919	173	0
1	B	12278	0	11962	192	0
2	C	23	0	21	0	0
All	All	24530	0	23902	364	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.

The worst 5 of 364 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:1196:LYS:HA	1:A:1218:GLU:HG3	1.47	0.94
1:B:1361:THR:HG21	1:B:1437:PHE:HA	1.61	0.82
1:B:8:LEU:HB2	1:B:652:PRO:HG2	1.64	0.78
1:A:1361:THR:HG21	1:A:1437:PHE:HA	1.65	0.76
1:B:1123:ARG:HH22	1:B:1207:ASP:HB2	1.48	0.76

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	1516/1536 (99%)	1391 (92%)	111 (7%)	14 (1%)	17	52
1	B	1524/1536 (99%)	1408 (92%)	102 (7%)	14 (1%)	17	52
All	All	3040/3072 (99%)	2799 (92%)	213 (7%)	28 (1%)	17	52

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	390	ASN
1	A	440	PRO
1	A	446	PRO
1	A	475	ASN
1	A	476	PRO

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	1338/1354 (99%)	1240 (93%)	98 (7%)	14	43
1	B	1344/1354 (99%)	1251 (93%)	93 (7%)	15	45
All	All	2682/2708 (99%)	2491 (93%)	191 (7%)	14	44

5 of 191 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	349	GLN
1	B	853	GLN
1	B	437	LYS
1	B	543	HIS
1	B	1029	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	349	GLN
1	A	1309	GLN
1	A	1423	ASN
1	B	1229	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 ⓘ

2 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	$\#\lvert Z \rvert > 2$	Counts	RMSZ	$\#\lvert Z \rvert > 2$
2	GLC	C	1	2	12,12,12	0.54	0	17,17,17	0.73	0
2	GLC	C	2	2	11,11,12	0.40	0	15,15,17	0.83	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	-	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.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

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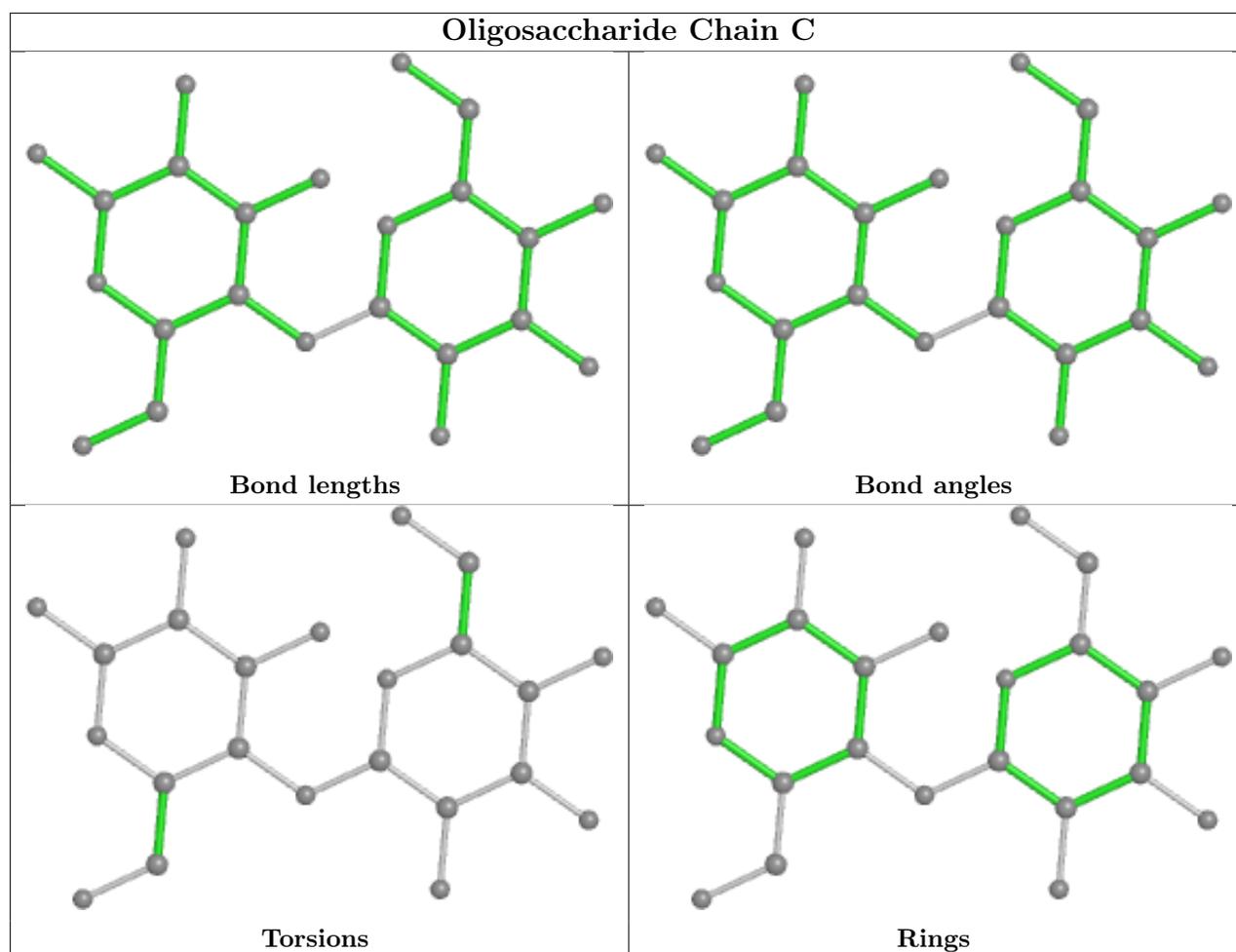
5.6 Ligand geometry (i)

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	1520/1536 (98%)	0.47	106 (6%)	16	7	46, 97, 175, 203	0
1	B	1526/1536 (99%)	0.49	125 (8%)	11	4	48, 88, 153, 194	0
All	All	3046/3072 (99%)	0.48	231 (7%)	13	5	46, 93, 170, 203	0

The worst 5 of 231 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	313	VAL	6.9
1	B	289	ASP	6.9
1	B	273	SER	6.5
1	B	251	TYR	6.2
1	B	270	LEU	5.8

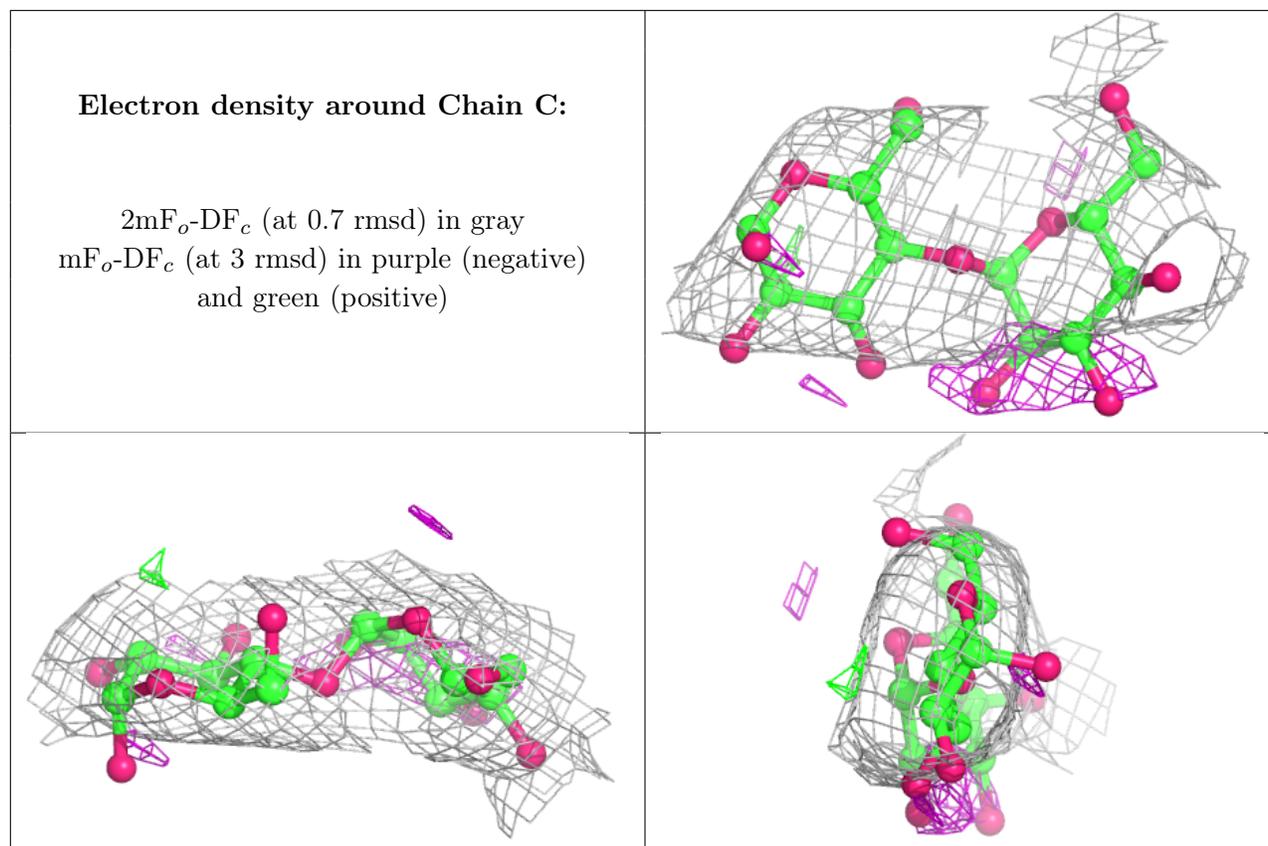## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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	C	2	11/12	0.64	0.36	116,119,128,134	0
2	GLC	C	1	12/12	0.76	0.32	110,110,111,113	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)

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.