WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Jun 26, 2024 – 04:15 AM EDT

PDB ID	:	6TS2
Title	:	Truncated version of Chaetomium thermophilum UDP-Glucose Glucosyl Transferase (UGGT) lacking domain TRXL2 (417-650).
Authors	:	Roversi, P.; Zitzmann, N.
Deposited on	:	2019-12-19
Resolution	:	5.74 Å(reported)

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

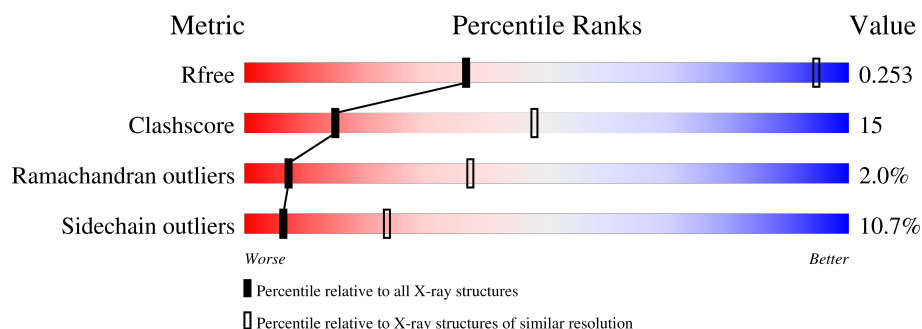|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 5.74 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.
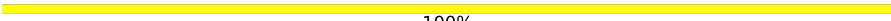
Metric	Percentile Ranks	Value
Rfree		0.253
Clashscore		15
Ramachandran outliers		2.0%
Sidechain outliers		10.7%

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	1006 (7.60-3.86)
Clashscore	141614	1031 (7.58-3.90)
Ramachandran outliers	138981	1002 (7.60-3.86)
Sidechain outliers	138945	1004 (7.60-3.82)

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%

Mol	Chain	Length	Quality of chain
1	A	1260	62% 24% • 12%
1	B	1260	52% 31% 5% 11%
1	C	1260	58% 26% • 12%
1	D	1260	58% 28% • 11%
2	E	5	60% 40%
3	F	3	33% 67%
3	H	3	33% 67%

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Mol	Chain	Length	Quality of chain
4	G	4	100%

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 36079 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 UDP-glucose-glycoprotein glucosyltransferase-like protein,UDP-glucose-glycoprotein glucosyltransferase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1111	Total	C	N	O	S	0	0	0
			8882	5671	1509	1675	27			
1	B	1120	Total	C	N	O	S	0	0	0
			8955	5718	1522	1688	27			
1	C	1113	Total	C	N	O	S	0	0	0
			8898	5680	1512	1678	28			
1	D	1123	Total	C	N	O	S	0	0	0
			8983	5735	1529	1691	28			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	GLU	-	expression tag	UNP G0SB58
A	22	THR	-	expression tag	UNP G0SB58
A	23	GLY	-	expression tag	UNP G0SB58
A	1506	GLY	-	expression tag	UNP G0SB58
A	1507	THR	-	expression tag	UNP G0SB58
A	1508	LYS	-	expression tag	UNP G0SB58
A	1509	HIS	-	expression tag	UNP G0SB58
A	1510	HIS	-	expression tag	UNP G0SB58
A	1511	HIS	-	expression tag	UNP G0SB58
A	1512	HIS	-	expression tag	UNP G0SB58
A	1513	HIS	-	expression tag	UNP G0SB58
A	1514	HIS	-	expression tag	UNP G0SB58
B	21	GLU	-	expression tag	UNP G0SB58
B	22	THR	-	expression tag	UNP G0SB58
B	23	GLY	-	expression tag	UNP G0SB58
B	1506	GLY	-	expression tag	UNP G0SB58
B	1507	THR	-	expression tag	UNP G0SB58
B	1508	LYS	-	expression tag	UNP G0SB58
B	1509	HIS	-	expression tag	UNP G0SB58
B	1510	HIS	-	expression tag	UNP G0SB58

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| Chain	Residue	Modelled	Actual	Comment	Reference
B	1511	HIS	-	expression tag	UNP G0SB58
B	1512	HIS	-	expression tag	UNP G0SB58
B	1513	HIS	-	expression tag	UNP G0SB58
B	1514	HIS	-	expression tag	UNP G0SB58
C	21	GLU	-	expression tag	UNP G0SB58
C	22	THR	-	expression tag	UNP G0SB58
C	23	GLY	-	expression tag	UNP G0SB58
C	1506	GLY	-	expression tag	UNP G0SB58
C	1507	THR	-	expression tag	UNP G0SB58
C	1508	LYS	-	expression tag	UNP G0SB58
C	1509	HIS	-	expression tag	UNP G0SB58
C	1510	HIS	-	expression tag	UNP G0SB58
C	1511	HIS	-	expression tag	UNP G0SB58
C	1512	HIS	-	expression tag	UNP G0SB58
C	1513	HIS	-	expression tag	UNP G0SB58
C	1514	HIS	-	expression tag	UNP G0SB58
D	21	GLU	-	expression tag	UNP G0SB58
D	22	THR	-	expression tag	UNP G0SB58
D	23	GLY	-	expression tag	UNP G0SB58
D	1506	GLY	-	expression tag	UNP G0SB58
D	1507	THR	-	expression tag	UNP G0SB58
D	1508	LYS	-	expression tag	UNP G0SB58
D	1509	HIS	-	expression tag	UNP G0SB58
D	1510	HIS	-	expression tag	UNP G0SB58
D	1511	HIS	-	expression tag	UNP G0SB58
D	1512	HIS	-	expression tag	UNP G0SB58
D	1513	HIS	-	expression tag	UNP G0SB58
D	1514	HIS	-	expression tag	UNP G0SB58

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.
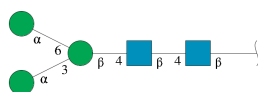
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	E	5	61	34	2	25	0	0	0

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b

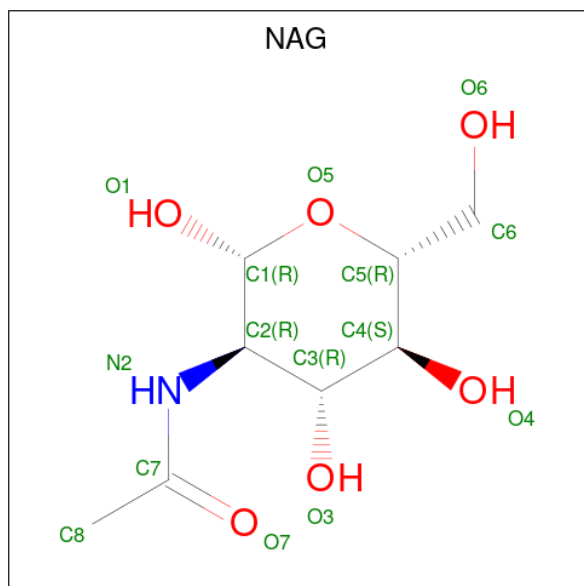eta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.
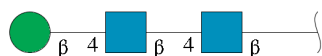
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	3	Total 39	C 22	N 2	O 15	0	0	0
3	H	3	Total 39	C 22	N 2	O 15	0	0	0

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranos e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluco pyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	4	Total 50	C 28	N 2	O 20	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

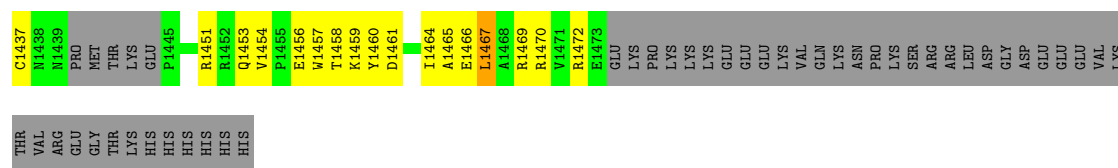| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Ca	0	0
			1	1		
6	B	1	Total	Ca	0	0
			1	1		
6	C	1	Total	Ca	0	0
			1	1		
6	D	1	Total	Ca	0	0
			1	1		

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. 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. 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: UDP-glucose-glycoprotein glucosyltransferase-like protein,UDP-glucose-glycoprotein glucosyltransferase-like protein

• Molecule 1: UDP-glucose-glycoprotein glucosyltransferase-like protein,UDP-glucose-glycoprotein glucosyltransferase-like protein

Chain B:

• Molecule 1: UDP-glucose-glycoprotein glucosyltransferase-like protein,UDP-glucose-glycoprotein glucosyltransferase-like protein

Chain C:

T1427 R1432 T1433 C1437 N1438 N1439 P1440 M1441 A1450 R1451 V1464 W1457 E1463 L1467 A1468 R1469 R1470 V1471 V1472 E1473 GLU LYS PRO LYS LYS LYS GLU GLU GLU LYS VAL GLN LYS ASN PRO LYS SER ARG ARG LEU ASP GLY ASP GLU GLU GLU VAL LYS THR VAL ARG GLU GLY
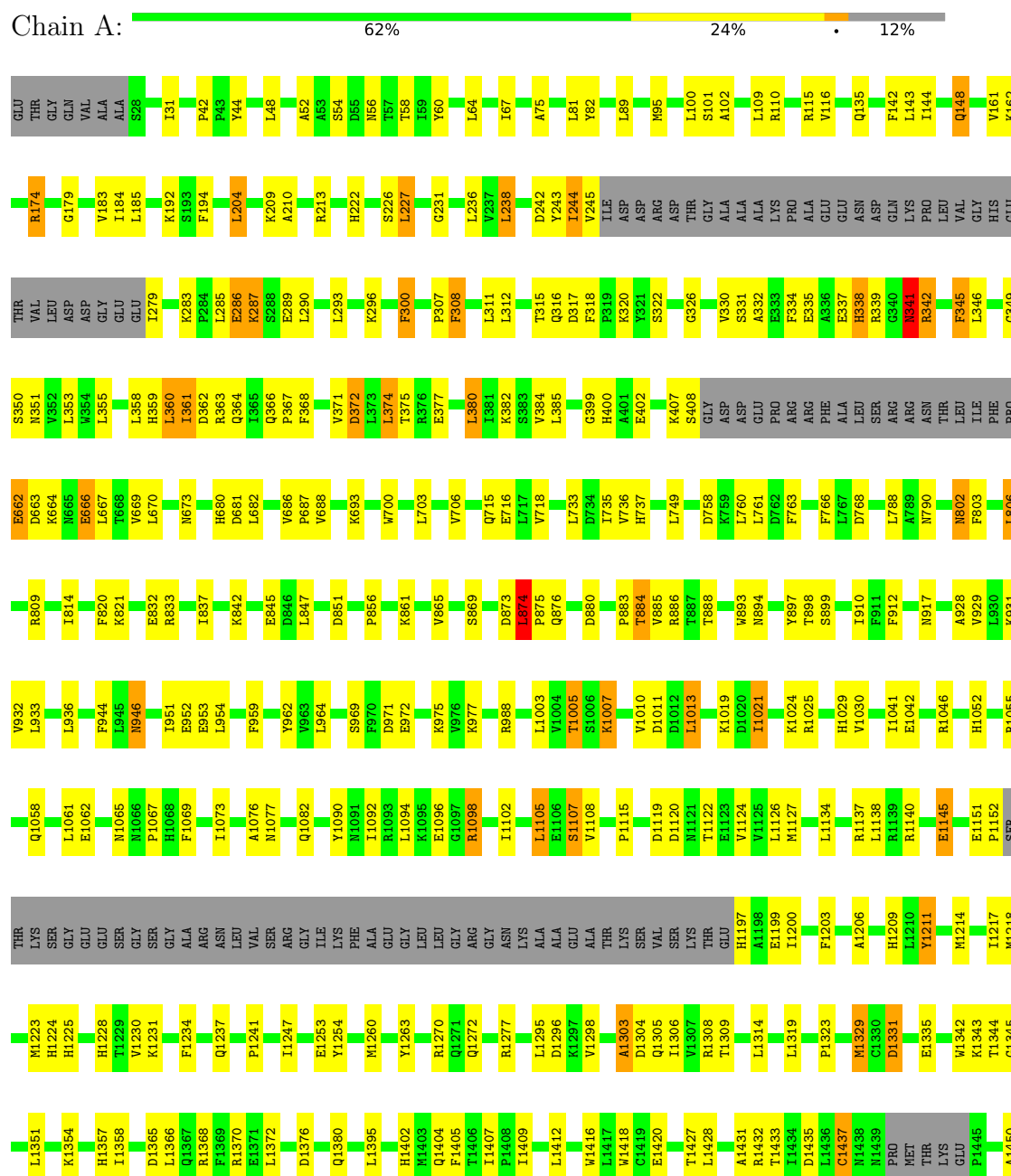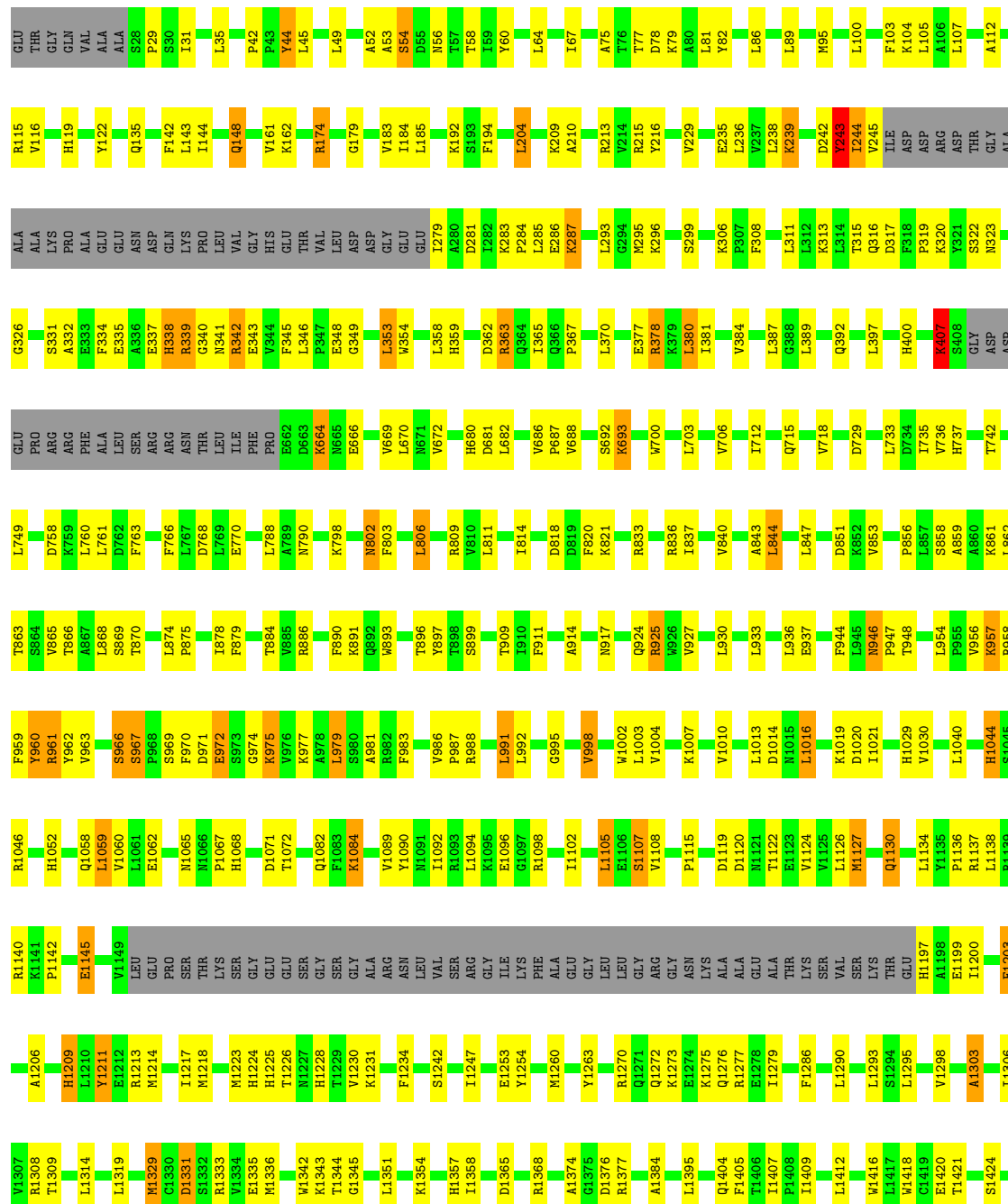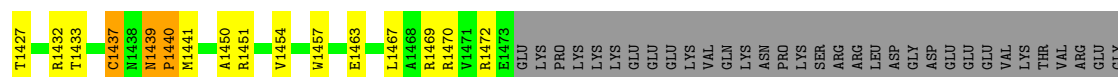
THR LYS HIS HIS HIS HIS HIS HIS

• Molecule 1: UDP-glucose-glycoprotein glucosyltransferase-like protein,UDP-glucose-glycoprotein glucosyltransferase-like protein
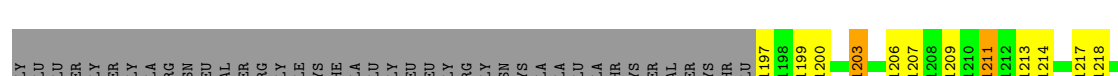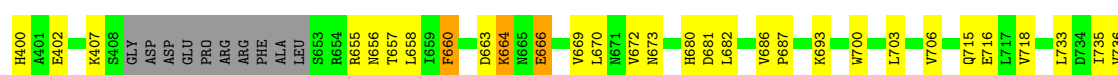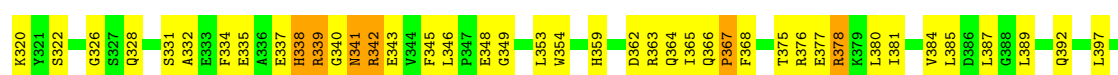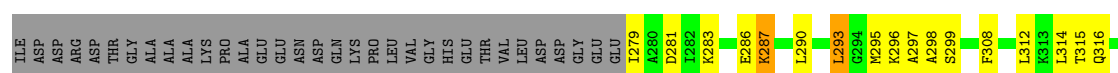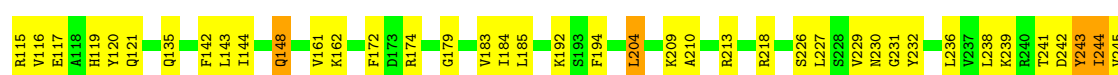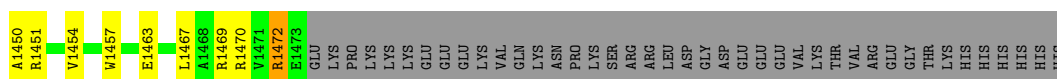
Chain D:

58%　　　　　　28%　　•　　11%

GLU THR GLY VAL ALA ALA S28 P29 S30 I31 L35 K36 A37 P42 P43 Y44 L45 V46 E47 L48 T51 A52 D55 N56 T57 T58 I59 Y60 L64 I67 T77 D78 L81 L86 L89 M95 L100 F103 S108 L109 R110 T111 A112 T113 P114

R115 V116 E117 A118 H119 Y120 Q121 Q135 F142 L143 I144 Q148 V161 K162 F172 D173 R174 G179 V183 I184 L185 K192 S193 F194 L204 K209 A210 R213 R218 S226 L227 S228 V229 N230 G231 Y232 L236 V237 L238 K239 R240 T241 D242 Y243 I244 V245

ILE ASP ASP ARG ASP THR GLY ALA ALA ALA LYS PRO ALA GLU GLU ASN ASP GLN LYS PRO LEU VAL GLY HIS GLU THR VAL LEU ASP ASP GLY GLU I279 A280 D281 I282 K283 E286 K287 L290 L293 G294 M295 K296 A297 A298 S299 F308 L312 K313 L314 T315 Q316

K320 Y321 S322 G326 S327 Q328 S331 A332 E333 F334 E335 A336 E337 H338 R339 G340 N341 R342 E343 V364 F345 L346 P347 E348 G349 L353 W354 H359 D362 R363 Q364 I365 Q366 P367 F368 T375 R376 E377 R378 K379 L380 I381 V384 L385 D386 L387 G388 L389 Q392 L397

H400 A401 E402 K407 S408 GLY ASP ASP GLU PRO ARG ARG PHE ALA LEU S653 R654 R655 N656 T657 L658 I659 F660 D663 K664 N665 E666 V669 L670 N671 V672 N673 H680 D681 L682 V686 P687 K693 W700 L703 V706 Q715 E716 L717 V718 L733 D734 I735 V736

H737 V748 L749 R752 D758 K759 L760 L761 D762 F763 T764 R765 F766 L767 D768 T771 E774 L788 A789 N790 N802 F803 L806 R809 I814 F820 K821 E832 R833 R836 I837 V840 A843 L844 L849 D850 D851 K852 V853 P856 A859 A860

K861 S864 S872 D873 L874 P875 I878 F879 D880 M881 A882 P883 T884 F890 K891 Q892 W893 T896 Y897 T909 I910 F911 N917 P918 R925 A928 V929 L930 L933 N946 P947 T948 L954 K957 R958 F959 Y960 R961 Y962 V963 L964 D971 E972 S973 G974 K975

V976 A981 R982 F983 V986 P987 R988 L991 L992 V993 M996 D997 V998 P999 P1000 A1001 W1002 L1003 V1004 T1005 S1006 K1007 V1010 L1013 D1014 N1015 L1016 R1017 I1018 H1029 V1030 H1038 I1039 L1040 R1046 H1052 Q1058 L1059 V1060 L1061 E1062 N1065 N1066 P1067 H1068 F1069 A1070 D1071

T1072 M1075 Y1080 F1081 Q1082 F1083 K1084 A1085 N1086 P1087 G1088 V1089 Y1090 N1091 I1092 R1093 L1094 K1095 E1096 G1097 R1098 I1102 L1105 E1106 S1107 V1108 P1115 D1119 D1120 M1121 T1122 E1123 V1124 V1125 L1126 M1127 Q1130 L1134 Y1135 P1136 R1137 L1138 E1145 L1150 GLU PRO SER THR LYS SER

GLY GLU GLU SER GLY SER GLY ALA ARG ASN LEU VAL SER ARG GLY ILE LYS PHE ALA GLU GLY LEU LEU LEU GLY ARG GLY ASN LYS ALA ALA GLU ALA THR LYS SER VAL SER LYS THR GLU H1197 A1198 E1199 I1200 F1203 A1206 S1207 G1208 H1209 L1210 Y1211 E1212 R1213 M1214 I1217 M1218

M1223 H1224 H1225 T1226 N1227 H1228 T1229 V1230 K1231 F1234 I1235 E1236 Q1237 P1241 K1244 E1253 M1260 Y1263 R1270 Q1271 Q1272 Q1276 R1277 E1278 I1279 D1288 Y1289 L1290 L1293 S1294 L1295 D1296 K1297 V1298 A1303 D1304 Q1305 I1306 V1307 R1308 T1309 L1314 M1329 C1330 D1331 S1332 R1333

V1334 E1335 M1336 W1342 K1343 T1344 G1345 L1351 K1354 H1357 I1358 D1365 L1366 Q1367 R1368 F1369 R1370 A1373 R1377 L1378 R1379 Q1380 S1391 L1395 Q1404 F1405 T1406 I1407 P1408 I1409 W1416 L1417 W1418 C1419 E1420 T1421 S1424 T1427 R1432 C1437 N1438 N1439 P1440 M1441

• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyrano se-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyra nose

Chain E:

• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-ac etamido-2-deoxy-beta-D-glucopyranose

Chain F:

• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-ac etamido-2-deoxy-beta-D-glucopyranose

Chain H:

• Molecule 4: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b eta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	151.15Å 191.01Å 158.81Å 90.00° 117.70° 90.00°	Depositor
Resolution (Å)	140.60 – 5.74 140.61 – 5.73	Depositor EDS
% Data completeness (in resolution range)	74.9 (140.60-5.74) 63.9 (140.61-5.73)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 5.77Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.174 , 0.249 0.187 , 0.253	Depositor DCC
R_{free} test set	829 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å^2)	290.4	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 185.6	EDS
L-test for twinning[2]	$< |L| > = 0.40, < L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.059 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	36079	wwPDB-VP
Average B, all atoms (Å^2)	133.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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 ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CA, MAN, BMA

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	0.45	0/9087	0.66	1/12325 (0.0%)
1	B	0.46	0/9162	0.68	3/12428 (0.0%)
1	C	0.42	0/9104	0.64	2/12349 (0.0%)
1	D	0.43	0/9191	0.65	2/12467 (0.0%)
All	All	0.44	0/36544	0.66	8/49569 (0.0%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	871	ILE	C-N-CA	5.99	136.68	121.70
1	D	875	PRO	C-N-CA	5.67	135.87	121.70
1	D	243	TYR	C-N-CA	5.33	135.04	121.70
1	B	1274	GLU	C-N-CA	5.23	134.77	121.70
1	A	341	ASN	CA-CB-CG	5.15	124.72	113.40

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	8882	0	8770	226	0
1	B	8955	0	8846	326	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	8898	0	8788	270	0
1	D	8983	0	8881	287	0
2	E	61	0	52	4	0
3	F	39	0	34	0	0
3	H	39	0	34	0	0
4	G	50	0	43	0	0
5	A	42	0	39	0	0
5	B	42	0	39	0	0
5	C	42	0	39	0	0
5	D	42	0	39	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
All	All	36079	0	35604	1080	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 15.

The worst 5 of 1080 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:D:78:ASP:HB2	1:D:975:LYS:HA	1.23	1.16
1:B:1376:ASP:HA	1:B:1379:ARG:HD3	1.26	1.15
1:B:1333:ARG:HG3	1:B:1424:SER:HA	1.17	1.13
1:D:1241:PRO:HA	1:D:1244:LYS:HB2	1.32	1.12
1:B:869:SER:HB2	1:B:886:ARG:HE	1.07	1.10

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	1101/1260 (87%)	1009 (92%)	78 (7%)	14 (1%)	12	48
1	B	1110/1260 (88%)	947 (85%)	134 (12%)	29 (3%)	5	31
1	C	1105/1260 (88%)	991 (90%)	98 (9%)	16 (1%)	11	46
1	D	1115/1260 (88%)	987 (88%)	100 (9%)	28 (2%)	5	32
All	All	4431/5040 (88%)	3934 (89%)	410 (9%)	87 (2%)	7	37

5 of 87 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	332	ALA
1	A	873	ASP
1	A	874	LEU
1	A	876	GLN
1	A	883	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	965/1088 (89%)	880 (91%)	85 (9%)	10	31
1	B	974/1088 (90%)	844 (87%)	130 (13%)	4	18
1	C	967/1088 (89%)	864 (89%)	103 (11%)	6	23
1	D	977/1088 (90%)	881 (90%)	96 (10%)	8	26
All	All	3883/4352 (89%)	3469 (89%)	414 (11%)	6	23

5 of 414 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	295	MET
1	C	1021	ILE
1	D	1145	GLU
1	C	342	ARG
1	C	820	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	230	ASN
1	C	1197	HIS
1	D	1267	HIS
1	C	338	HIS
1	C	738	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 ⓘ

15 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	NAG	E	1	2,1	14,14,15	0.31	0	17,19,21	1.12	2 (11%)
2	NAG	E	2	2	14,14,15	0.46	0	17,19,21	2.46	3 (17%)
2	BMA	E	3	2	11,11,12	0.41	0	15,15,17	1.06	2 (13%)
2	MAN	E	4	2	11,11,12	0.95	1 (9%)	15,15,17	1.95	2 (13%)
2	MAN	E	5	2	11,11,12	0.80	0	15,15,17	1.91	2 (13%)
3	NAG	F	1	3,1	14,14,15	0.30	0	17,19,21	1.19	2 (11%)
3	NAG	F	2	3	14,14,15	0.34	0	17,19,21	1.06	1 (5%)
3	BMA	F	3	3	11,11,12	0.31	0	15,15,17	0.49	0
4	NAG	G	1	4,1	14,14,15	0.29	0	17,19,21	1.06	2 (11%)
4	NAG	G	2	4	14,14,15	0.28	0	17,19,21	1.50	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	BMA	G	3	4	11,11,12	0.36	0	15,15,17	0.91	1 (6%)
4	MAN	G	4	4	11,11,12	0.75	0	15,15,17	1.37	2 (13%)
3	NAG	H	1	3,1	14,14,15	0.29	0	17,19,21	1.04	2 (11%)
3	NAG	H	2	3	14,14,15	0.30	0	17,19,21	1.00	2 (11%)
3	BMA	H	3	3	11,11,12	0.30	0	15,15,17	0.42	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	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	BMA	E	3	2	-	0/2/19/22	0/1/1/1
2	MAN	E	4	2	-	0/2/19/22	1/1/1/1
2	MAN	E	5	2	-	1/2/19/22	0/1/1/1
3	NAG	F	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	4/6/23/26	0/1/1/1
3	BMA	F	3	3	-	1/2/19/22	0/1/1/1
4	NAG	G	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	3/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
4	MAN	G	4	4	-	1/2/19/22	0/1/1/1
3	NAG	H	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	4/6/23/26	0/1/1/1
3	BMA	H	3	3	-	1/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	4	MAN	C1-C2	2.02	1.56	1.52

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	4	MAN	C1-O5-C5	6.09	120.44	112.19
2	E	5	MAN	C1-O5-C5	5.86	120.13	112.19
2	E	2	NAG	O5-C1-C2	-5.82	102.10	111.29
2	E	2	NAG	C1-C2-N2	5.72	120.27	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	2	NAG	C1-O5-C5	4.98	118.93	112.19

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	2	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
2	E	5	MAN	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
4	G	4	MAN	O5-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	4	MAN	C1-C2-C3-C4-C5-O5

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	NAG	4	0
2	E	2	NAG	4	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.

Oligosaccharide Chain E

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain F

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain H

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain G

Bond lengths

Bond angles

Torsions

Rings
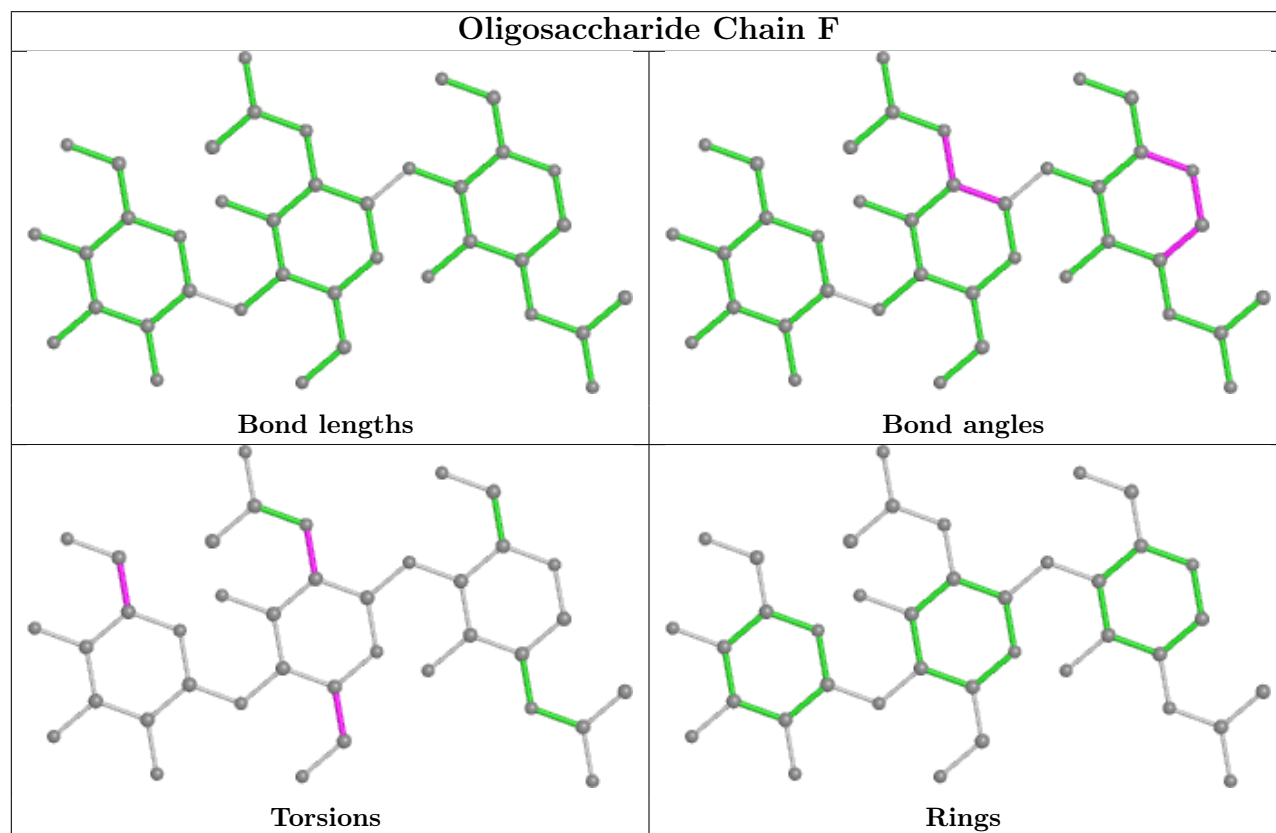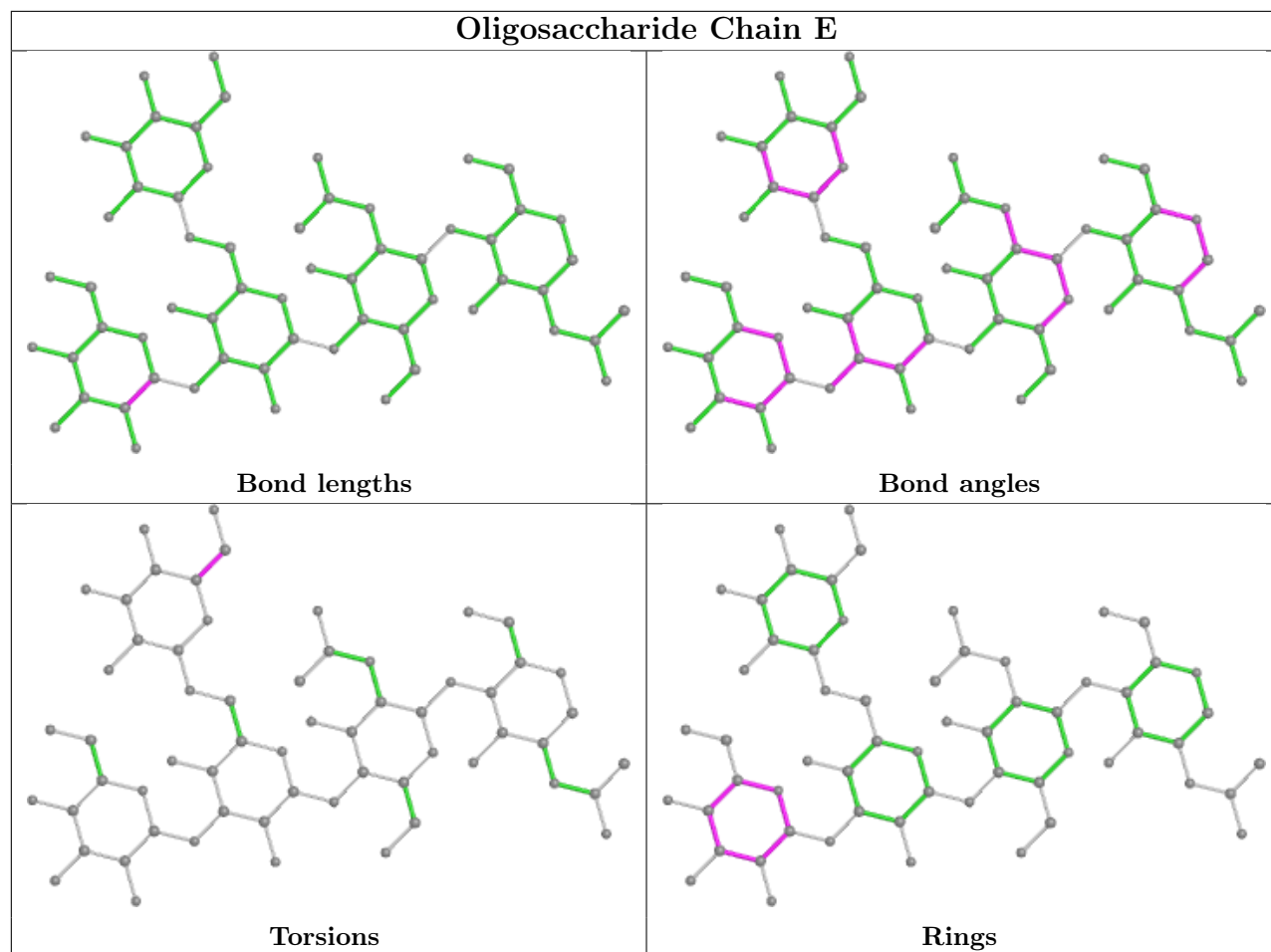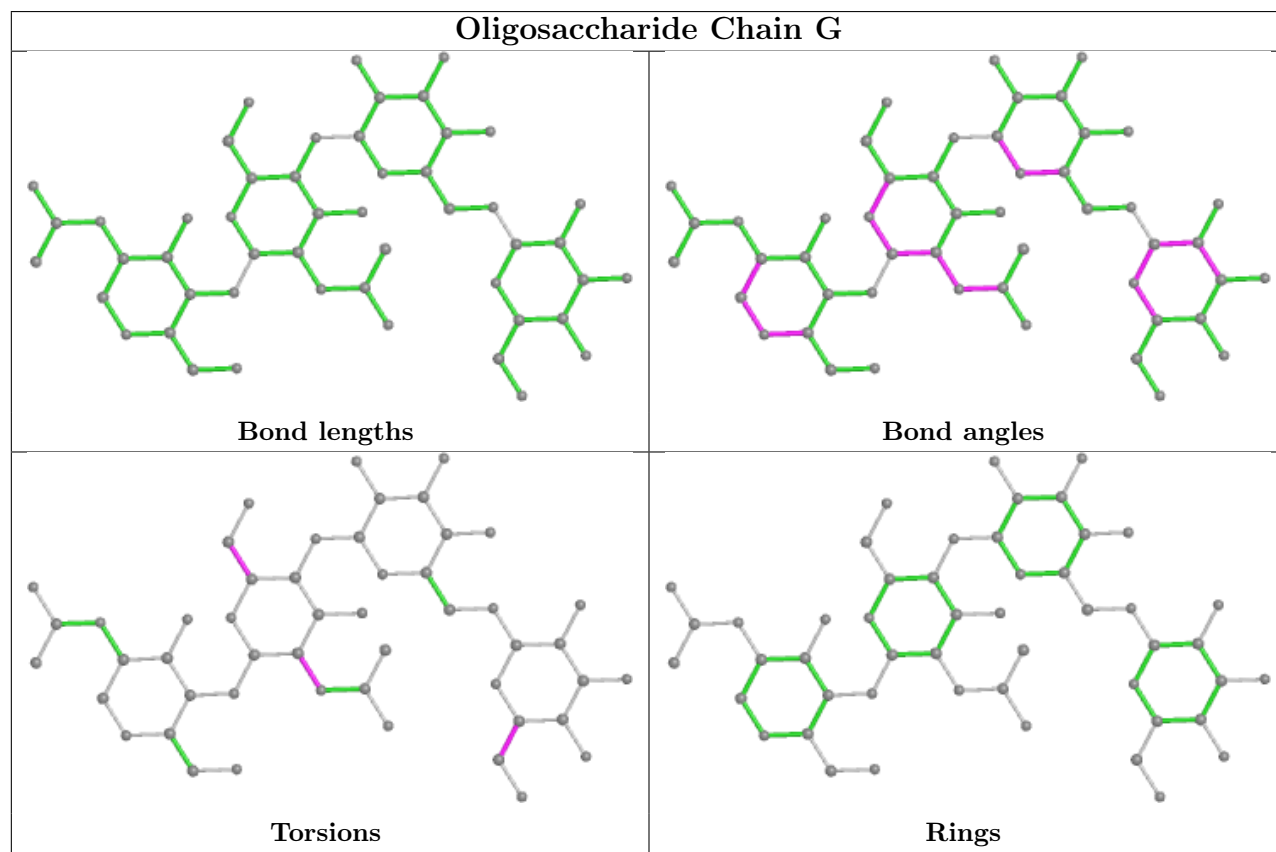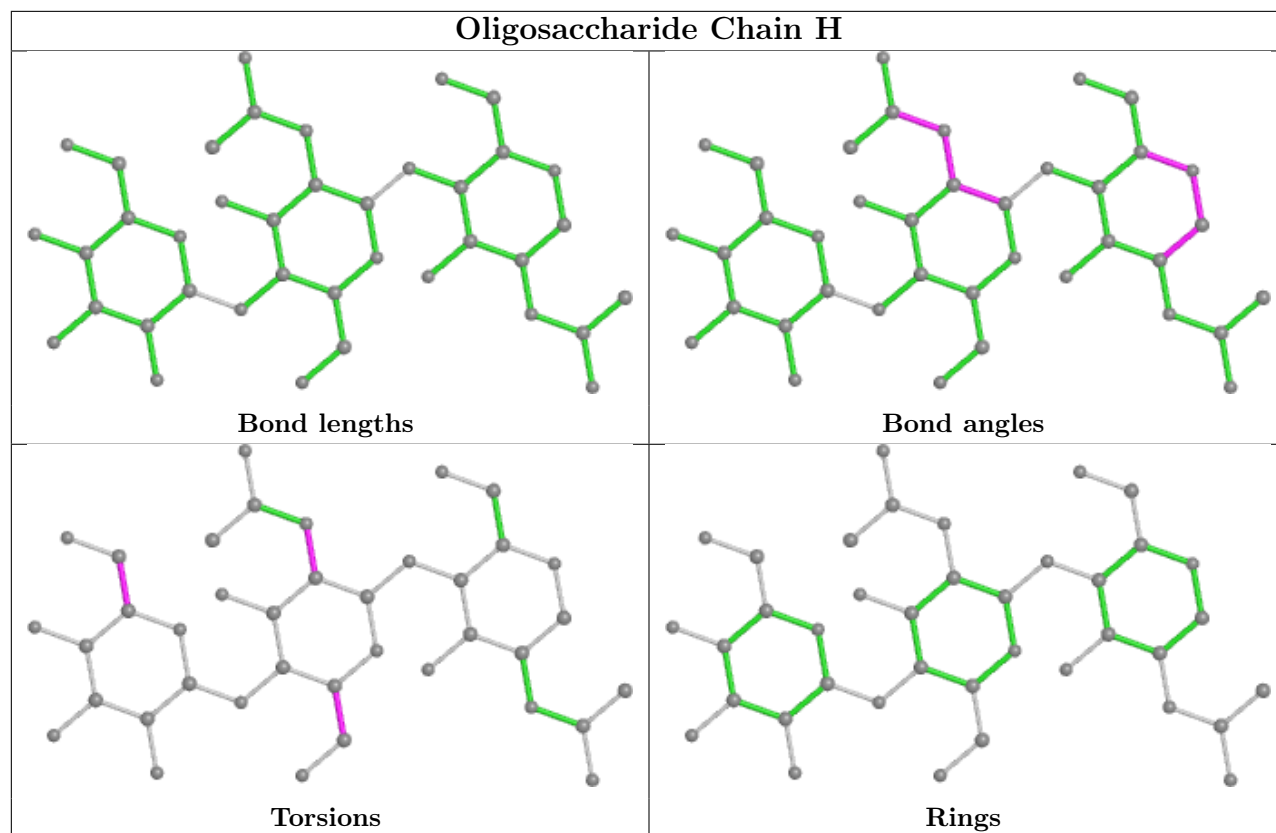
5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	$\#|Z| > 2$
5	NAG	B	1601	-	14,14,15	0.30	0	17,19,21	0.51	0
5	NAG	A	1601	-	14,14,15	0.35	0	17,19,21	0.69	0
5	NAG	A	1602	1	14,14,15	0.28	0	17,19,21	0.78	1 (5%)
5	NAG	B	1603	1	14,14,15	0.37	0	17,19,21	0.98	2 (11%)
5	NAG	C	1601	-	14,14,15	0.51	0	17,19,21	0.81	0
5	NAG	D	1601	-	14,14,15	0.30	0	17,19,21	0.66	0
5	NAG	D	1605	1	14,14,15	0.35	0	17,19,21	0.70	1 (5%)
5	NAG	C	1606	1	14,14,15	0.33	0	17,19,21	0.79	1 (5%)
5	NAG	C	1607	1	14,14,15	0.29	0	17,19,21	0.56	0
5	NAG	D	1606	1	14,14,15	0.30	0	17,19,21	0.75	1 (5%)
5	NAG	A	1603	1	14,14,15	0.34	0	17,19,21	0.78	1 (5%)
5	NAG	B	1602	1	14,14,15	0.36	0	17,19,21	1.17	1 (5%)

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
5	NAG	B	1601	-	-	0/6/23/26	0/1/1/1
5	NAG	A	1601	-	-	0/6/23/26	0/1/1/1
5	NAG	A	1602	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1603	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1601	-	-	0/6/23/26	0/1/1/1
5	NAG	D	1601	-	-	0/6/23/26	0/1/1/1
5	NAG	D	1605	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1606	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1607	1	-	0/6/23/26	0/1/1/1
5	NAG	D	1606	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1603	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	1602	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1602	NAG	C1-O5-C5	4.02	117.64	112.19
5	C	1606	NAG	C1-O5-C5	3.03	116.29	112.19
5	A	1602	NAG	C1-O5-C5	2.94	116.17	112.19
5	B	1603	NAG	C1-O5-C5	2.93	116.17	112.19
5	A	1603	NAG	C1-O5-C5	2.78	115.96	112.19

There are no chirality outliers.

There are no torsion outliers.

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 ⓘ

6.1　Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3　Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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 E:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
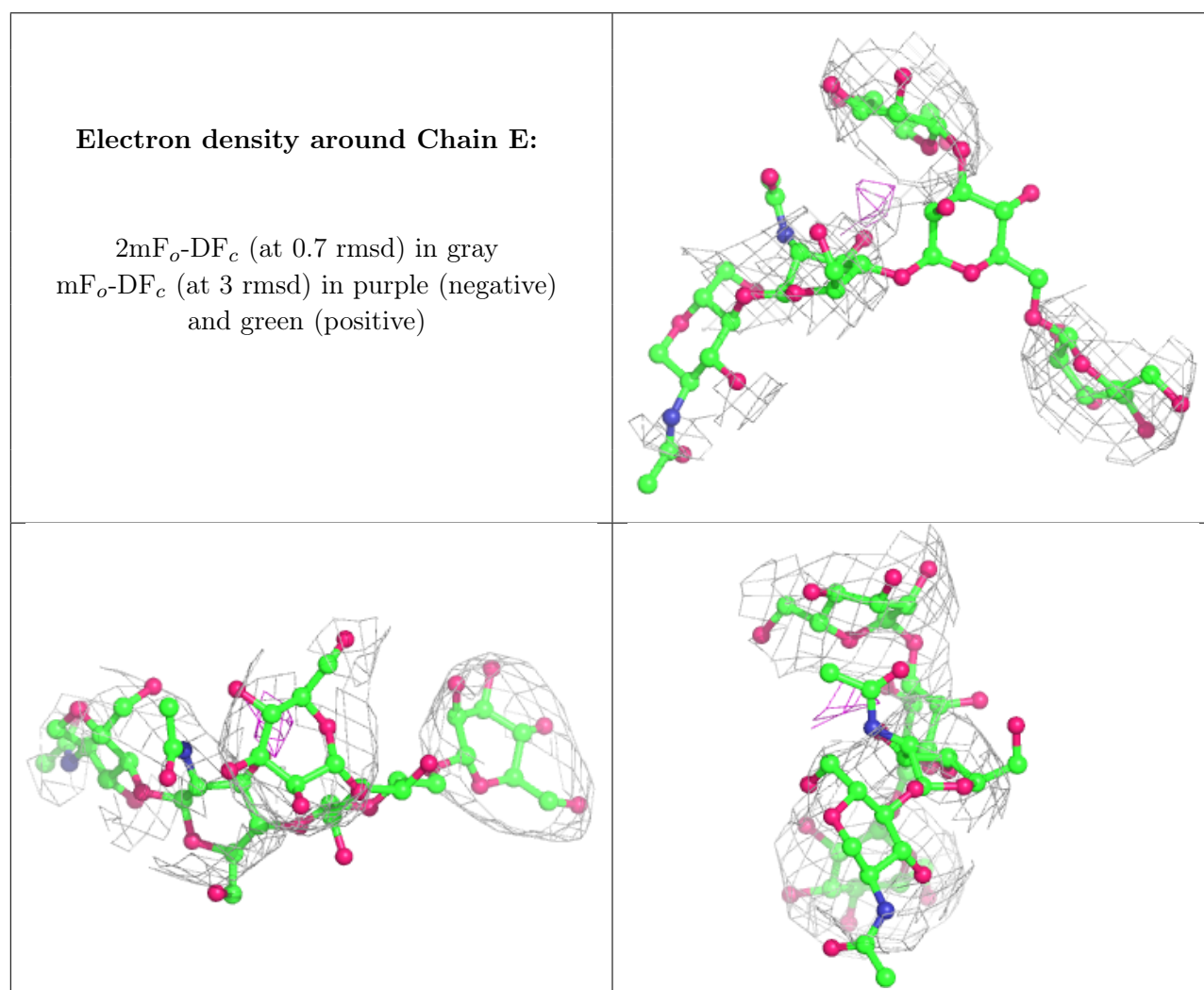
Electron density around Chain F:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
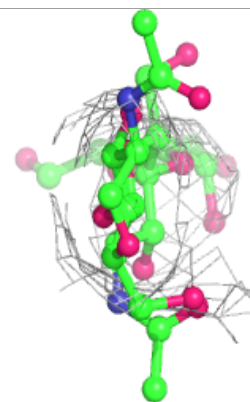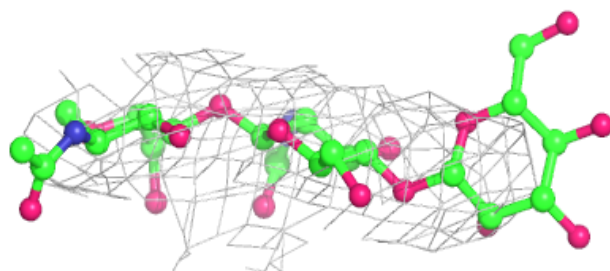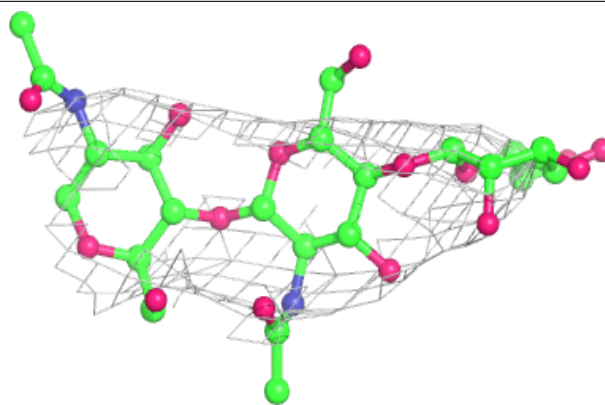
Electron density around Chain H:

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

Electron density around Chain G:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
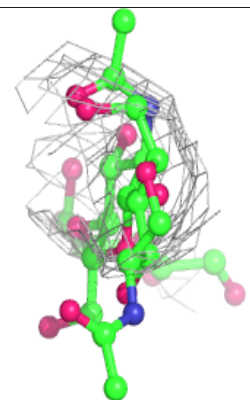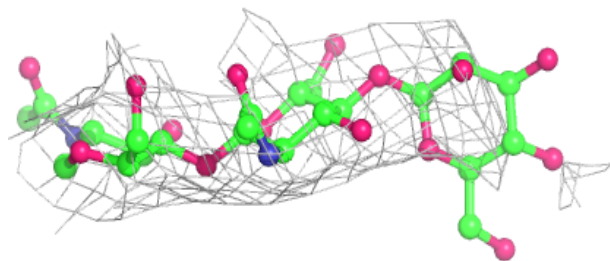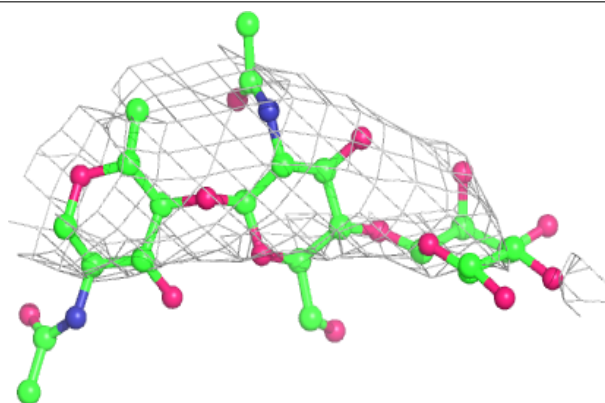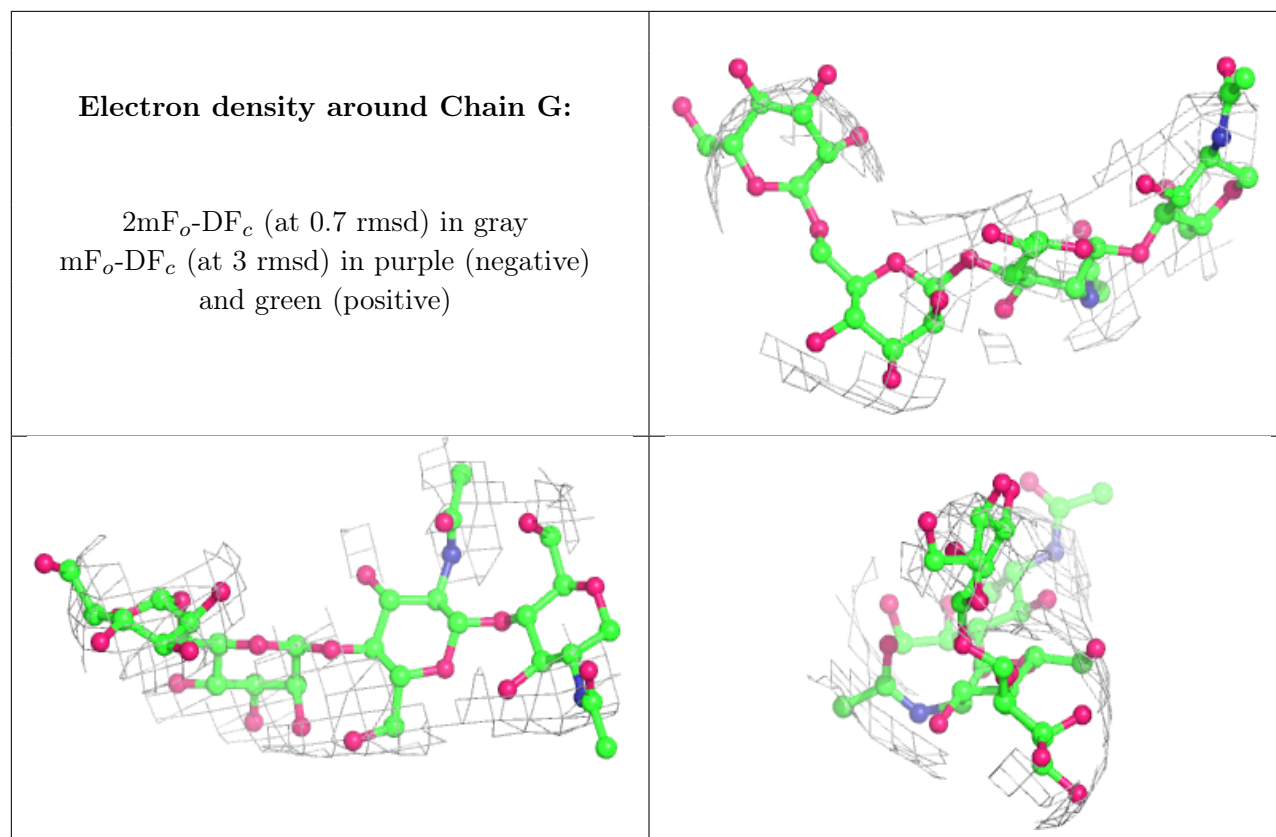
6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.