

wwPDB X-ray Structure Validation Summary Report (i)

Apr 10, 2021 - 08:25 am BST

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
$\operatorname{Resolution}$:	5.74 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

:	4.02b-467
:	1.8.5 (274361), CSD as541be (2020)
:	1.13
:	2.18
:	20191225.v01 (using entries in the PDB archive December 25th 2019)
:	5.8.0158
:	7.0.044 (Gargrove)
:	Engh & Huber (2001)
:	Parkinson et al. (1996)
:	2.18
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1 Overall quality at a glance (i)

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	Whole archive	Similar resolution
	(# Entries)	(# Entries, resolution range(A))
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	А	1260	62%	24% · 12%					
1	В	1260	52%	31% 5% 11%					
1	С	1260	58%	26% • 12%					
1	D	1260	58%	28% · 11%					
2	Е	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 (i)

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,UD P-glucose-glycoprotein glucosyltransferase-like protein.

Mol	Chain	Residues		А	toms		ZeroOcc	AltConf	Trace	
1	Δ	1111	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	А		8882	5671	1509	1675	27	0	0	0
1	р	1120	Total	С	Ν	Ο	S	0	0	0
	D	1120	8955	5718	1522	1688	27	0	0	
1	С	1112	Total	С	Ν	Ο	S	0	0	0
	U	1115	8898	5680	1512	1678	28	0	0	
1	п	1192	Total	С	Ν	Ο	S	0	0	0
		1123	8983	5735	1529	1691	28	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	21	GLU	-	expression tag	UNP G0SB58
А	22	THR	-	expression tag	UNP G0SB58
А	23	GLY	-	expression tag	UNP G0SB58
А	1506	GLY	-	expression tag	UNP G0SB58
A	1507	THR	-	expression tag	UNP G0SB58
А	1508	LYS	-	expression tag	UNP G0SB58
A	1509	HIS	-	expression tag	UNP G0SB58
А	1510	HIS	-	expression tag	UNP G0SB58
А	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
В	21	GLU	-	expression tag	UNP G0SB58
В	22	THR	-	expression tag	UNP G0SB58
В	23	GLY	-	expression tag	UNP G0SB58
В	1506	GLY	-	expression tag	UNP G0SB58
В	1507	THR	-	expression tag	UNP G0SB58
В	1508	LYS	-	expression tag	UNP G0SB58
В	1509	HIS	-	expression tag	UNP G0SB58
В	1510	HIS	-	expression tag	UNP G0SB58



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

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• Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyran ose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	Е	5	Total 61	С 34	N 2	O 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	С	Ν	Ο	0	Ο	0
5	T,	5	39	22	2	15	0	0	
2	Ц	2	Total	С	Ν	0	0	0	0
3	11		39	22	2	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-glucopyranose.



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	A	ton	ns		ZeroOcc	AltConf
5	Λ	1	Total	С	Ν	Ο	0	0
5	A	L	14	8	1	5	0	0
5	Λ	1	Total	С	Ν	Ο	0	0
0	Л	I	14	8	1	5	0	0
5	Λ	1	Total	С	Ν	Ο	0	0
0	Л	T	14	8	1	5	0	0
5	В	1	Total	С	Ν	Ο	0	0
0	D	T	14	8	1	5	0	0
5	В	1	Total	С	Ν	Ο	0	0
0	D	T	14	8	1	5	0	0
5	В	1	Total	С	Ν	Ο	0	0
0	D	T	14	8	1	5	0	0
5	С	1	Total	С	Ν	Ο	0	Ο
0	U	I	14	8	1	5	0	0
5	С	1	Total	С	Ν	Ο	0	0
0	U	I	14	8	1	5	0	0
5	С	1	Total	С	Ν	Ο	0	0
0	U	I	14	8	1	5	0	0
5	П	1	Total	С	Ν	Ο	0	0
0	D	T	14	8	1	5	0	0
5		1	Total	С	Ν	Ο	0	0
		1	14	8	1	5		U
5		1	Total	С	Ν	Ο	0	0
		L	14	8	1	5		

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	1	Total Ca 1 1	0	0
6	В	1	Total Ca 1 1	0	0
6	С	1	Total Ca 1 1	0	0
6	D	1	Total Ca 1 1	0	0



3 Residue-property plots (i)

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-glycoprotei n glucosyltransferase-like protein



 \bullet Molecule 1: UDP-glucose-glycoprotein glucosyltransferase-like protein,
UDP-glucose-glycoprotein n glucosyltransferase-like protein



DB

THR VAL ARG GLU GLV GLY HIS HIS HIS HIS HIS HIS

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

Chair	n C	: -							5	58%	þ											26	%				•	1	2%				
GLU THR GLY GLN	VAL ALA	ALA S28	530 530			P42 P43	Y44	L45	L49	A52	A53	D55	N56 T57	T58	159 YGO		L64	I67	A75	T76 T77	D78 K70	A80	L81 Y82	L86			M95	L100	F103 K104	L105	A106 L107	A112	
R115 V116 H119	Y122	0 <mark>135</mark>	F142	1144	0148	V161	K162	R174		6/19	V183	L185	K192	S193	F194	1.204	K209	A210	R213	<mark>V214</mark> R215	Y216	V229	E235	1236 V237	1238 1730	AC 74	D242 Y243	I244 V245	ILE ASP	ASP	AKG	THR GLY ALA	
ALA ALA LYS PRO	ALA GLU	GLU ASN	GLN	PRO	VAL	GLY HTS	GIU	THR VAL	IEU	ASP	GLY	GLU	1279 A280	D281	1282 K283	P284	L285 E286	K287	1293	G294 M295	K296	<mark>\$299</mark>	K306	P307 F308	101		K313 L314	T315 0316	D317 F318	P319	K320 Y321	S322 N323	
6326 S331 A332	E333 F334	E335 A336	E337 H338 P000	6340	N341 R342	E343 V344	F345	L346 P347	E348	6.349	L353	400M	L358 H359		D362 R363	Q 364	1365 0366	P367	L370	E377	R378 K370	L380	1381	V384	L387	L389	0392	L397	H400		K407 S408	GLY ASP ASP	
GLU PRO ARG ARG	PHE	SER	ARG	THR	1LE	PHE	E662	D663 K664	N665	999ga	V669 1670	N671	V672	H680	D681 L682		V686 P687	V688	S692	K693	00 <u>7</u> M	L703	00 <mark>70</mark>	I7 12	0715		V7 18	D729	L733 D734	1735	V/36 H737	1742	
L749 D758 K759	L760 L761	D762 F763	F766	D768	L/69 E770	1 788	A789	067N	K798	N802	F803	L806	R809	V810	L811	181 <mark>4</mark>	D818	D819	r 820 K821	R833	836	1837	V840	A843	L844	L847	D851	K852 V853	P856	L857	5858 A859	<mark>A860</mark> K861 L862	
T863 864 V865 T866	A867 L868	5869 1870	I874	6/84	1879 F879	T 884	100 1 V885	R886	F890	K891 Q892	W893	1896	Y897 T898	2899	EC EL	1910	F911	A914	N917	0924	R925	V927	1930	1933	TO26	E937	F944	L945 N946	P947 T948		1955 1955	V956 K957 R958	
F959 Y960 R961 Y962	V963	S966 S967	2968 2969	D971	E9/2 S973	<mark>6974</mark> котб	V976	K977 A978	L979	5980 A981	R982	1900	V986 P987	R988	L.99.1	L992	(995		ABB	W1002 L1003	V1004	K1007	V1010	L1013	D1014	L1016	K1019	D1020 11021	H1029	V1030	L1040	H1044 S1045	
R1046 H1052	<mark>01058</mark> L1059	V1060 L1061	E1062	C00 IN	P1067 H1068	D1071	T1072	01082	F1083	K1084	V1089	1601N	11092 R1093	L1094	K1095 E1096	G1097	R1098	11102	L1105	E1106 S1107	V1108	P1115	D1119	D1120 N1121	T1122 F1102	V1124	V1125 L1126	M1 127	Q1130	L1134	Y1135 P1136	R1137 L1138 R1139	
R1140 K1141 P1142	E1145	V1149 LEU	PRO	THR	LYS SER	GL Y GL Y	GLU	SER GLY	SER	GLY ALA	ARG	LEU	VAL SER	ARG	GLY ILE	LYS	PHE ALA	GLU GLU	GLI	GLY	ARG	ASN	ALA	ALA GLU	ALA THR	TYS	SER VAL	SER LYS	THR GLU	H1197	A1198 E1199	11200 F1203	
A1206 H1209	L1210 Y1211	E1212 R1213		M1217 M1218	M1223	Н1224 Н1225	T1226	N1227 H1228	T1229	V1230 K1231	7 7 1 1 1	r 1204	S1242	11247	E1253	Y1254	M1260	Coot A	1 1702	R1270 01271	01272 11273	E1274	K1275 Q1276	R1277 E1278	11279	F1286	L1290	L1293	S1294 L1295		867L A	A1303	
<mark>V1307</mark> R1308 T1309	L1314	L1319	01329 C1330 P1001	S1332	K1333 V1334	E1335 M1336		W1342 K1343	T1344	61345	L1351	K1354	H1357	I1358	D1365		R1368	A1374	01376 D1376	R1377	A1384	L1395	<mark>01404</mark>	F1405 T1406	11407 D1400	11409	L1412	W1416	L1417 W1418	C1419	E1420 T1421	S1424	



T1427 T1427 T1433 T1433 T1433 T1433 T1433 T1435 M1455 M1455

THR LYS HIS HIS HIS HIS HIS HIS

 \bullet Molecule 1: UDP-glucose-glycoprotein glucosyltransferase-like protein, UDP-glucose-glycoprotein n glucosyltransferase-like protein

Chain	D:						589	%										28	%			•		119	%	I	
GLU THR GLY GLN	VAL ALA ALA	528 P29 S30	135 L35	K36 A37	P42 D43	Y44	V46	L48	T51 AFO	AU2 DEE	N56	T57 T58	I59 Y60	T.64			D78	L81	L86	T 80	M95	L100	C (1 2		L109		T113 P114
R115 V116 E117 A118	H119 Y120 Q121	Q135 F142	1144 1143	01 <u>48</u>	V161 K162	F179	D173		6/T5	1184 1184		K192 S193	F194	1.204	K209		CT 74	R218	<mark>5226</mark> 1227	S228 V229	N230 G231	Y232	1236 1037	1238 1238	R240	D242	1245 1244 V245
ILE ASP ASP ARG	ASP THR GLY	ALA ALA ALA T VS	PRO ALA	GLU GLU	ASP ASP ASP	LYS	LEU	GLY	GLU GLU	VAL	ASP	ASP GLY	GLU GLU	1279 4280	D281	K283	E286	K287	1290	1293 (1294	M295 K296	A297 A298	<mark>\$299</mark>	F308	1312 1919	1314 1314 1515	0316
K320 <mark>Y321</mark> S322	6326 <mark>5327</mark> 0328	S331 A332 F333	F334 E335	A336 E337 U220	R339 1340	N341 R342	E343	F345	1.540 P347 F340	6 349	L353	W354	H359	D362 B363	q 364	1366 0366	F368	T375	R376 E377	R378 K379	L380 1381	V384	L385		1389 L389	<mark>(1392</mark>	L397
H400 A401 E402	K407 S408 GLY	ASP ASP GLU BRD	ARG	PHE ALA TEII	S653 B654	R655 N656	T657	1659 1659		K664	E666	V669	L670 N671	V672 N673		D681	7007	V686 P687	K693		L703	V706		E7 16	Li 11 V7 18	L733	U135 1735 V736
H737 V748 L749	R752	N/58 K759 L760 T761	E101 D762 F763	T764 R765 8766	E / 00 L767 D768		F1774		L/80 A789 N700		F803	L806	R809	TR14		F 820 K 821	E832	R833	R836 1837	VR40	A843	L844	L849	D851	V853	P856	<mark>A859</mark> A860
K861 S864	S872 D873 L874 T874	с/94 1878 1870	D880 D881 N881	A882 P883 Tro 0.1		K891	W893	T896		1909 1910 F011	TTAJ	N917 P918	R925	AQ2A	V929			N946 P947	T948	L954	K957 R958	F959 Y960	R961 V060	1902 V963 1064		E972	6974 6975 K975
V976 A981 R982	F983 V986	r98 / R988	L991 1993 V993	M996 M007	1990 1998 1900	P1000	W1002	V1004	S1006 S1006 V1007			L1013 D1014	N1015 L1016	R1017 T1018		V1030	H1038	11039 L1040	R1046	H1050	01058	L1059 V1060	L1061	M1066	N1066	H1068	F 1009 A1070 D1071
T1072 M1075	Y1080 F1081 Q1082	F1083 K1084 A1085 M1086	P1087 G1088	V1089 Y1090 W1001	11091 11092 11033	L1094	E1096	R1098	I1102	L1105	S1107	V1108	P1115	D1119 D1120	N1121	E1 122 E1 123 	V1125 V1125	L1126 M1127	01130	L1134	Y1135 P1136	R1137 L1138	E4 1.05		GLU BBD	SER	LYS SER
GLY GLU SER	GLY SER GLY	ALA ARG ASN TFU	VAL	ARG GLY TI E	DHF DHF	ALA	ULT 1 PIL	IEU	ARG	ASN	ALA	ALA GLU	ALA THR	LYS SER	VAL	LYS	GLU	H1197 A1198	E1199 I1200	F1203	A1206	<mark>S1207</mark> G1208	H1209	Y1211	R1213 M1213		M1218
M1223 H1224 H1225 T1226	N1227 H1228 T1229	V1230 K1231	r 123 7 11235 E1236	Q1237		R1253	M1760			01271 01271		01276 R1277	E1278 I1279	D1288	V1289		S1294	L1295 D1296	K1297 V1298	A 1303	D1304 D1305	11306 V1307	R1308			C1330 C1330 D1221	L1331 S1332 R1333
V1334 E1335 M1336	W1342 K1343 T1344	61345	K1354	H1357 11358	D1365	01367 01367 81368	F1369		C / CTH	L1378	01380	S1391	L1395	01404	F1405	11406 11407	11409	W1416	L1417 W1418	C1419 F1420	T1421	S1424	T1427	R1432	C1437 M1 430	N1439 D1 440	M1441



 \bullet Molecule 2: 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

Chain E:	60%	40%

NAG1 NAG2 BMA3 MAN4 MAN5

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

Chain F:	33%	67%	
NAG2 BMA3			

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

Chain H: –	33%	67%

NAG1 NAG2 BMA3

 $\bullet \ Molecule \ 4: \ alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose$

Chain G:

100%

NAG 1 NAG 2 BMA 3 MAN 4



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	151.15Å 191.01 Å 158.81 Å	Deperitor
a, b, c, α , β , γ	90.00° 117.70° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	140.60 - 5.74	Depositor
Resolution (A)	140.61 - 5.73	EDS
% Data completeness	74.9 (140.60-5.74)	Depositor
(in resolution range)	63.9(140.61-5.73)	EDS
R _{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.60 (at 5.77 \text{\AA})$	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
D D	0.174 , 0.249	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.187 , 0.253	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.

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.



 $^{^1 {\}rm Intensities}$ estimated from amplitudes.

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: BMA, NAG, MAN, CA

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

Mal	Chain	Bond	lengths	Bond angles					
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5				
1	А	0.45	0/9087	0.66	1/12325~(0.0%)				
1	В	0.46	0/9162	0.68	3/12428~(0.0%)				
1	С	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	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	В	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	В	1274	GLU	C-N-CA	5.23	134.77	121.70
1	А	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 (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	А	8882	0	8770	226	0
1	В	8955	0	8846	326	0



6 TS	2
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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	С	8898	0	8788	270	0
1	D	8983	0	8881	287	0
2	Е	61	0	52	4	0
3	F	39	0	34	0	0
3	Н	39	0	34	0	0
4	G	50	0	43	0	0
5	А	42	0	39	0	0
5	В	42	0	39	0	0
5	С	42	0	39	0	0
5	D	42	0	39	0	0
6	А	1	0	0	0	0
6	В	1	0	0	0	0
6	С	1	0	0	0	0
6	D	1	0	0	0	0
All	All	36079	0	35604	1080	0

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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 (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	А	1101/1260~(87%)	1009 (92%)	78 (7%)	14 (1%)		12	48
1	В	1110/1260~(88%)	947 (85%)	134 (12%)	29 (3%)		5	31
1	С	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	А	332	ALA
1	А	873	ASP
1	А	874	LEU
1	А	876	GLN
1	А	883	PRO

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	Rotameric Outliers		Percentiles		
1	А	965/1088~(89%)	880 (91%)	85~(9%)		10	31	
1	В	974/1088~(90%)	844 (87%)	130~(13%)		4	18	
1	С	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	\mathbf{Res}	Type
1	С	295	MET
1	С	1021	ILE
1	D	1145	GLU
1	С	342	ARG
1	С	820	PHE



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

Mol	Chain	\mathbf{Res}	Type
1	С	230	ASN
1	С	1197	HIS
1	D	1267	HIS
1	С	338	HIS
1	С	738	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

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).

Mal	True	Chain	Dec	T:nl.	Bo	ond leng	ths	В	ond ang	les
	туре	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
2	NAG	Е	1	2,1	14,14,15	0.31	0	$17,\!19,\!21$	1.12	2 (11%)
2	NAG	Е	2	2	14,14,15	0.46	0	17,19,21	2.46	3 (17%)
2	BMA	Е	3	2	11,11,12	0.41	0	$15,\!15,\!17$	1.06	2 (13%)
2	MAN	Е	4	2	11,11,12	0.95	1 (9%)	$15,\!15,\!17$	1.95	2 (13%)
2	MAN	Е	5	2	11,11,12	0.80	0	$15,\!15,\!17$	1.91	2 (13%)
3	NAG	F	1	1,3	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	1,4	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%)



Mal	Tune	Chain	Chain Res	nain Res		Bo	ond leng	\mathbf{ths}	B	ond ang	les
mor Type C	Ullain	nes		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	Н	1	1,3	14,14,15	0.29	0	17,19,21	1.04	2 (11%)	
3	NAG	Н	2	3	14,14,15	0.30	0	17,19,21	1.00	2 (11%)	
3	BMA	Н	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	Е	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	Е	2	2	-	0/6/23/26	0/1/1/1
2	BMA	Е	3	2	-	0/2/19/22	0/1/1/1
2	MAN	Е	4	2	-	0/2/19/22	1/1/1/1
2	MAN	Е	5	2	-	1/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	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	1,4	-	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	Н	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	Н	2	3	-	4/6/23/26	0/1/1/1
3	BMA	Н	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(A)	$\operatorname{Ideal}(\operatorname{\AA})$
2	Е	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	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	Ε	4	MAN	C1-O5-C5	6.09	120.44	112.19
2	Е	5	MAN	C1-O5-C5	5.86	120.13	112.19
2	Е	2	NAG	O5-C1-C2	-5.82	102.10	111.29
2	Е	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	Ε	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	Н	2	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
2	Е	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	Е	4	MAN	C1-C2-C3-C4-C5-O5

2 monomers are involved in 4 short contacts:

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











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).

Mal	Tuno	Chain	Chain	Pog	Tink	Bo	ond leng	ths	B	ond ang	les
	туре	Unam	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
5	NAG	В	1601	-	14, 14, 15	0.30	0	$17,\!19,\!21$	0.51	0	
5	NAG	D	1605	1	14, 14, 15	0.35	0	$17,\!19,\!21$	0.70	1(5%)	
5	NAG	С	1607	1	14, 14, 15	0.29	0	17, 19, 21	0.56	0	
5	NAG	А	1602	1	14, 14, 15	0.28	0	$17,\!19,\!21$	0.78	1(5%)	
5	NAG	С	1606	1	14,14,15	0.33	0	17,19,21	0.79	1(5%)	
5	NAG	А	1601	-	14,14,15	0.35	0	17,19,21	0.69	0	
5	NAG	С	1601	-	14, 14, 15	0.51	0	$17,\!19,\!21$	0.81	0	
5	NAG	А	1603	1	14, 14, 15	0.34	0	$17,\!19,\!21$	0.78	1(5%)	
5	NAG	В	1602	1	14,14,15	0.36	0	17,19,21	1.17	1 (5%)	
5	NAG	D	1601	-	14,14,15	0.30	0	17,19,21	0.66	0	
5	NAG	D	1606	1	14,14,15	0.30	0	17,19,21	0.75	1(5%)	
5	NAG	В	1603	1	14,14,15	0.37	0	17,19,21	0.98	2 (11%)	

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	В	1601	-	-	0/6/23/26	0/1/1/1
5	NAG	D	1605	1	-	0/6/23/26	0/1/1/1
5	NAG	С	1607	1	-	0/6/23/26	0/1/1/1
5	NAG	А	1602	1	-	0/6/23/26	0/1/1/1
5	NAG	С	1606	1	-	0/6/23/26	0/1/1/1
5	NAG	А	1601	-	-	0/6/23/26	0/1/1/1
5	NAG	С	1601	-	-	0/6/23/26	0/1/1/1
5	NAG	А	1603	1	-	0/6/23/26	0/1/1/1
5	NAG	В	1602	1	-	0/6/23/26	0/1/1/1
5	NAG	D	1601	-	-	0/6/23/26	0/1/1/1
5	NAG	D	1606	1	_	0/6/23/26	0/1/1/1



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Mol	Type	Chain	\mathbf{Res}	Link	Chirals	Torsions	Rings
5	NAG	В	1603	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	В	1602	NAG	C1-O5-C5	4.02	117.64	112.19
5	С	1606	NAG	C1-O5-C5	3.03	116.29	112.19
5	А	1602	NAG	C1-O5-C5	2.94	116.17	112.19
5	В	1603	NAG	C1-O5-C5	2.93	116.17	112.19
5	А	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 (i)

6.1 Protein, DNA and RNA chains (i)

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

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

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

6.3 Carbohydrates (i)

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.











6.4 Ligands (i)

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

6.5 Other polymers (i)

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

