



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 2, 2021 – 12:09 AM EDT

PDB ID : 3KLS  
Title : Structure of complement C5 in complex with SSL7  
Authors : Laursen, N.S.; Gordon, N.; Hermans, S.; Lorenz, N.; Jackson, N.; Wines, B.;  
Spillner, E.; Christensen, J.B.; Jensen, M.; Fredslund, F.; Bjerre, M.; Sottrup-  
Jensen, L.; Fraser, J.D.; Andersen, G.R.  
Deposited on : 2009-11-09  
Resolution : 3.60 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](mailto: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 following versions of software and data (see [references ⓘ](#)) 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 : 2.23.2  
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) : 2.23.2

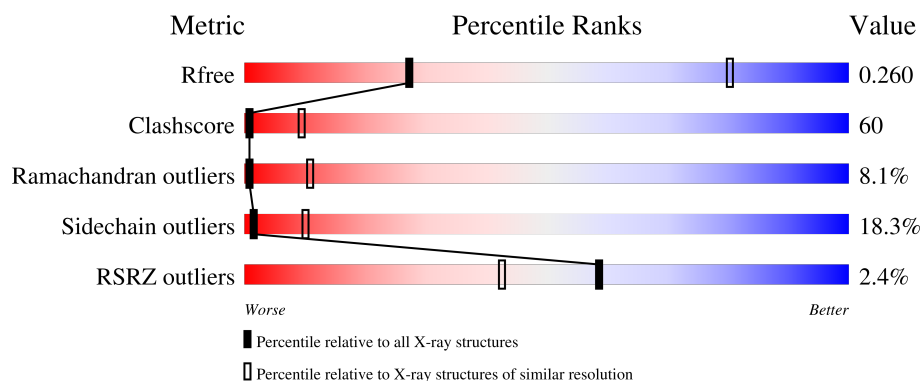
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

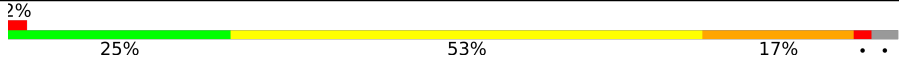
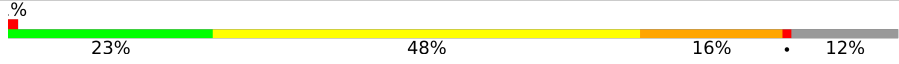
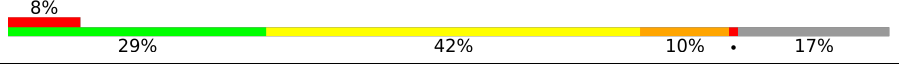
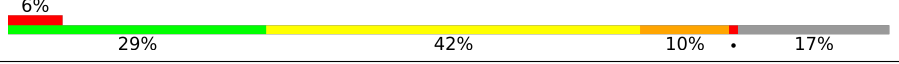

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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  $\geq 3$ , 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	1676	
1	B	1676	
2	X	231	
2	Y	231	
3	C	2	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	D	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	A	1682	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 27683 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 Complement C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1622	Total	C	N	O	S	0	0	0
			12836	8224	2107	2452	53			
1	B	1478	Total	C	N	O	S	0	0	0
			11676	7478	1926	2226	46			

- Molecule 2 is a protein called Exotoxin 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	191	Total	C	N	O	S	0	0	0
			1539	965	267	306	1			
2	Y	191	Total	C	N	O	S	0	0	0
			1539	965	267	306	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	35	GLY	GLU	engineered mutation	UNP Q6GJP2
Y	35	GLY	GLU	engineered mutation	UNP Q6GJP2

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

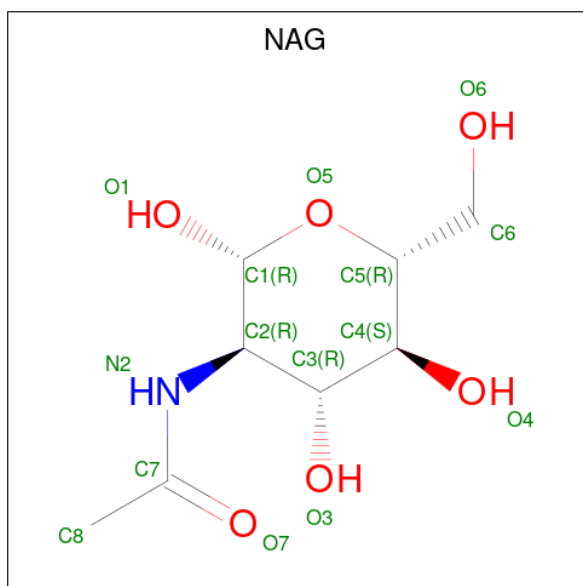


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	Cd	0	0
			5	5		
4	B	4	Total	Cd	0	0
			4	4		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

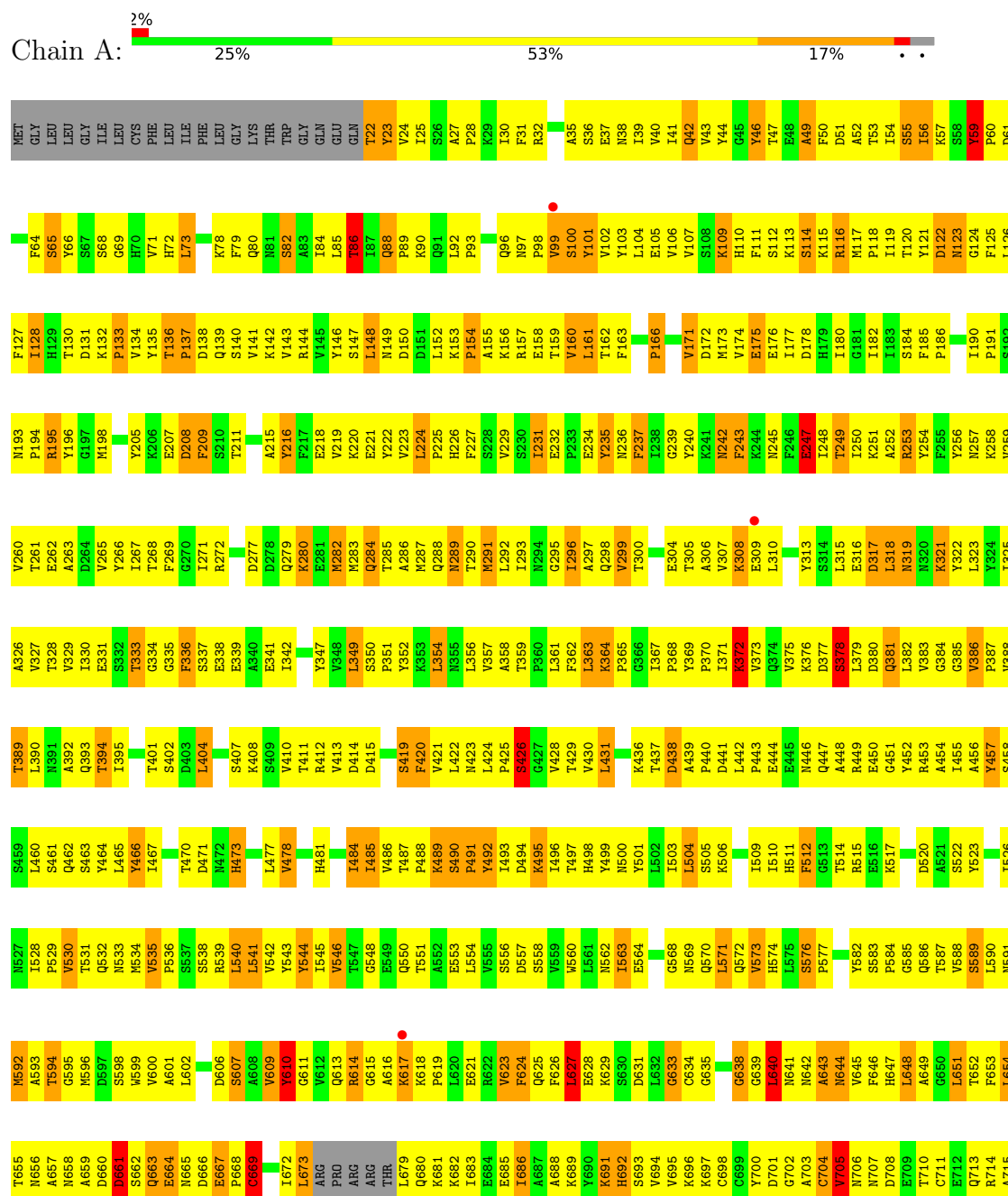


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

### 3 Residue-property plots

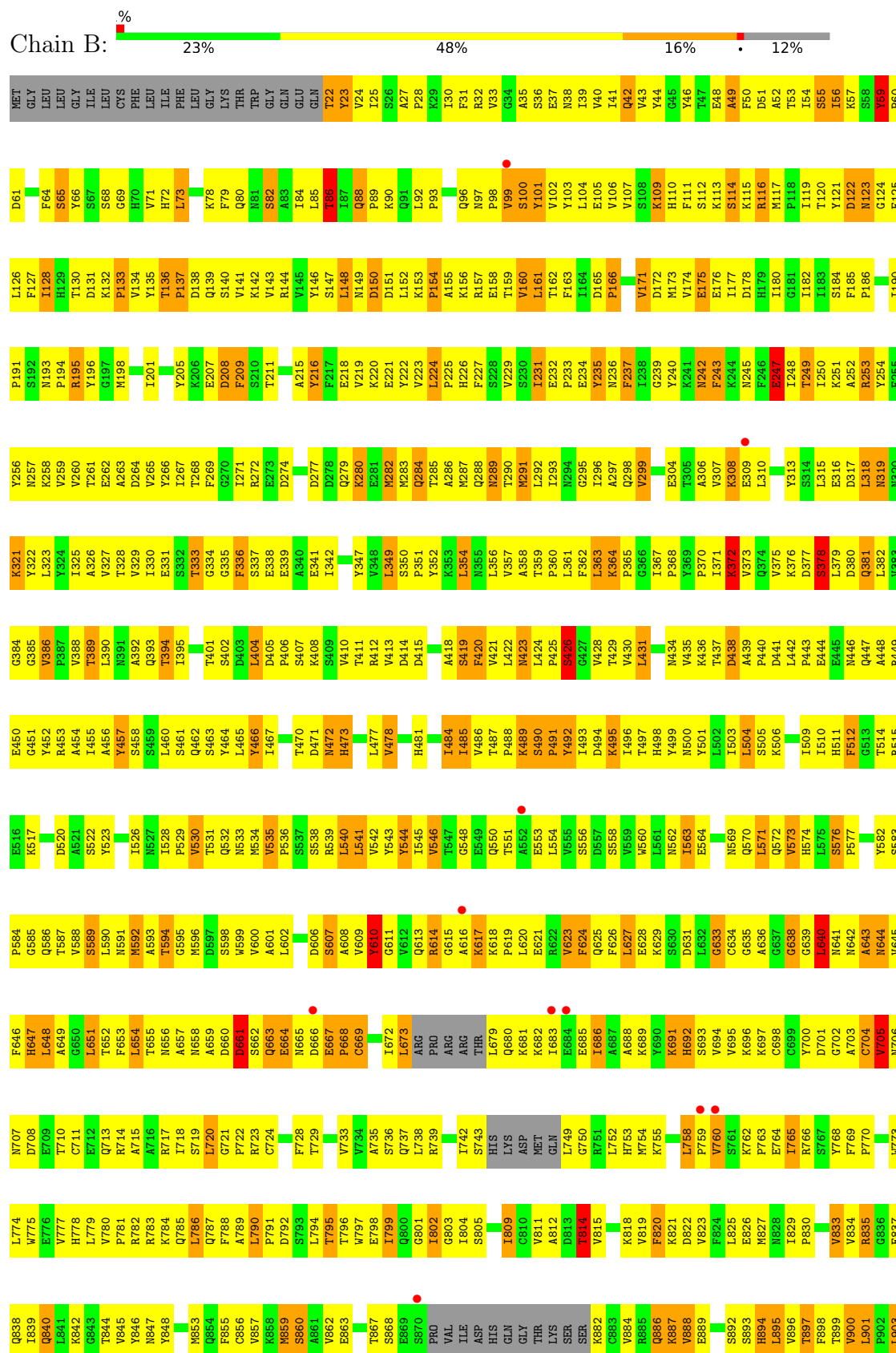
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Complement C5

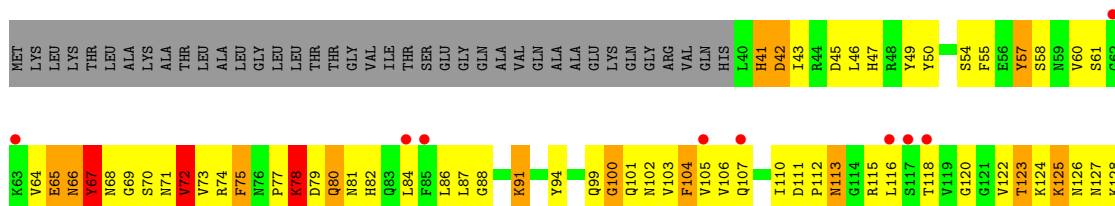


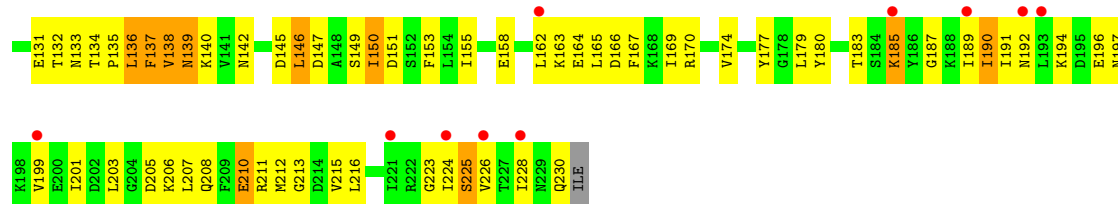
Y1629	S1567	T1506	E1436	E1372	Q1306	P1240	N1178	N1110	K1046	V979	S913	Y846	R783	A716
N1630	I1566	M1507	E1437	E1373	L1307	M1241	T1179	Y1111	K1047	K980	L914	M847	K784	R717
S1632	T1569	F1508	D1438		R1309		L1180	Q1112	K1048	G981	E915	Y848	Q785	T718
R1634	N1573	S1510	A1441	S1376	S1310	T1244	A1245	L1113	L1049	L982			L786	S719
Y1635	F1574	T1511	L1442	Y1377	M1311	A1246	A1182	D1114	K1050	L983			Q787	G721
I1636	F1575	S1512		Y1378	D1312	M1247	Q1183	G1116	G1051	G985			F788	P722
Y1637	V1576	M1513	G1445	K1360	I1313		S1184	S1117	G1052	F855			A789	R723
P1638	K1576	T1514	V1446	I1381	I1314	T1250	T1185	F1118	M1053	E986			L790	C724
L1639	K1515	V1315	D1447	T1382	V1315	T1251	F1186	K1119	S1055	L988			D792	
	L1516		Q1448			A1252	F1187	E1120	I1056				S793	F728
	A1517		L1449	T1383		T1253	L1188	N1121	M1057	S860			L794	T729
	K1518		F1450		K1318	A1254	A1189		S1058	A861			T795	E730
	V1519		K1320	T1386	K1319	L1255	L1190	Y1124	Y1059	V862			T796	
	C1520		G1321	ALA	G1321	L1256	S1191	Q1125	R1060	V863			W797	V733
	E1521		A1453	SER	A1322	T1257	A1192	P1126	G996	E798			V734	A735
	G1522		Q1454	HIS	L1323	S1258	Y1193	I1127	A1062	T799			A736	
	A1523		I1455	TYR	K1324	L1259	A1194	K1128	D1063	G933			S736	
	A1524			ARG	N1326	M1260	L1195		Y1064	Y934			Q800	Q737
	C1525		V1460	GLY	Y1326	L1261	S1196	T1132	S1065	R936			G801	Q737
	K1526		I1461	TYR	I1327	R1262	L1197	L1133	S1066	T1001			I802	L738
	C1527		L1462	GLY	M1328	D1263	F1205	P1134	S1067	I1002			G803	R739
	V1528		Q1463	ASN	T1329	I1264	A1136	V1135	P1068	L1003			I804	
	E1529		L1464	SER	N1332	N1265	H1202	A1137	W1069	Y939			S805	
	A1530		M1465	ASP	F1332	N1266	P1203	R1138	K1070	S940			H806	S743
	D1531		S1466	Y1399	F1333	V1267	P1203	E1139	G1071	A1008			G808	HIS
	C1532		I1467	K1400	L1334	M1268	Q1204	E1139	G1072	Y942			I809	LYS
	G1533		P1468	R1401	G1335	P1269	F1205	N1140	S1073	E1011			ASP	
	M1534			A1402		V1270	R1206	S1141	A1074	L1012			MET	
	Y1535		Y1475	V1403	V1338	I1271	S1207	L1142	S1075	D945			A812	
	Q1536		R1476	A1404	E1339	K1272	I1208	Y1143	T1076	Y1015			D813	L749
	E1537		F1477	C1405	V1340	V1273	V1209	L1144	L1077	P1017			T814	G750
	E1538		R1478	A1406	L1341	T1274	S1210	T1145	W1077	G948			V815	F751
	M1539		L1479	S1407	L1342	L1275	A1211	A1146	T1079	P1018			L752	
	D1540		F1480	Y1408	N1343	E1276	L1212	F1147	A1080	Q886			W818	F753
	L1541		E1481	K1409	D1344	E1278	L1212	T1148	F1081	K887			F820	M754
	T1542		L1482	P1410	V1345	Q1277	V1149	V1149	L1082	K821			K821	K755
	I1543		F1483	S1411	L1346	R1279	A1216	I1150	L1083	F1022			D822	L758
	S1544		E1484	R1412	I1347	Y1280	L1217	G1151	R1084	H1023			W823	P759
	A1545		V1485	E1413	V1348	G1281	V1218	I1152	V1085	Y1024			F824	V760
	E1546		G1486	E1414	S1349	G1282	K1219	R1153	L1086	L1025			L825	
	T1547		F1487	S1415	T1350	G1283	G1220	K1154	G1087	E1026			E958	P763
			L1488		G1351	F1284	N1221	A1155	Q1088	G1028			M827	F764
			S1489		F1352	Y1285	P1222	D1157	V1089	L895			W828	E765
			P1490		L1356	S1286	Y1225	D1157	M1090	P960			I829	I766
			A1491		L1366	T1287	R1226	I1158	K1091	H1030			P830	S767
			T1492		V1359	Q1288	F1227	C1159	Y1092	F898				W768
			F1493		H1360	D1289	Y1227	P1160	N1032	T899				F769
			V1495		V1361	T1290	W1228	L1161	V1093	P964				P770
			Y1496		V1362		K1229	V1162	L965	L901			W834	
			E1497		T1363	I1294	D1230	K1163	D966	P902			R835	
			E1498		V1364	L1297	N1231	I1164	S1036	L903			G836	W773
			Y1498		V1365	T1298	L1232	A1167	S1099	D1037			E837	L774
			H1499		H1366	Q1293	Q1233		I1100	L904			Q838	W775
			R1500		T1367	E1299	H1234	L1168		P969			W776	
			P1501		K1367	Y1300	K1234	I1169	L1104	L1039			R839	E776
			D1502		T1368	S1301	D1236	K1170	E1041	L907			Q840	V777
			K1503		S1369		S1237	W1106	K1042	H908			L841	H778
			Q1504		T1370	L1302	S1238		L1107	N909			K842	L779
			L1505		A1434	L1303	S1238	N1173	Q1043	P910			G843	V780
			C1505		S1371	L1303	V1239	F1174	E1109	L1045			T844	P781
													W845	R782

● Molecule 1: Complement C5

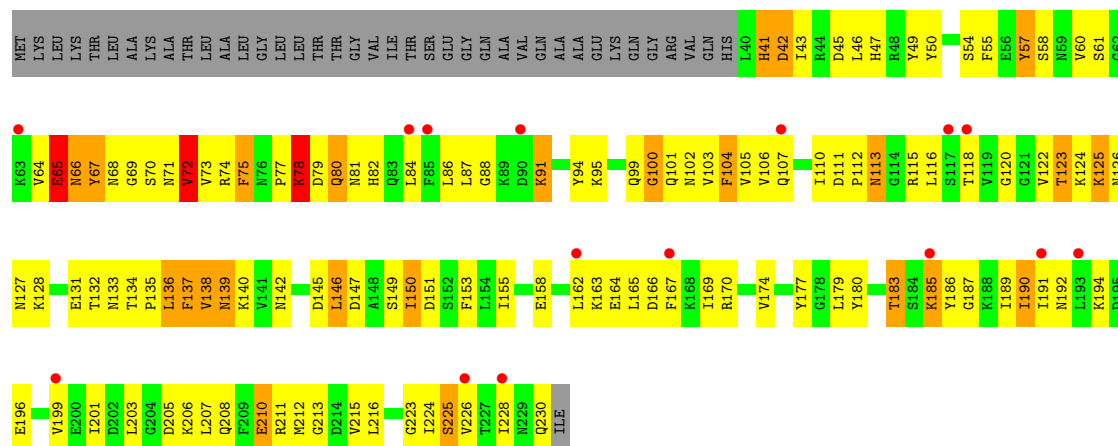








• Molecule 2: Exotoxin 1



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	143.88Å 143.88Å 241.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.05 – 3.60 29.31 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.05-3.60) 99.6 (29.31-3.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.39 (at 3.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.198 , 0.263 0.193 , 0.260	Depositor DCC
$R_{free}$ test set	3224 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	111.0	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 120.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l 0.410 for h,-h-k,-l 0.028 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	27683	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	156.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.59	1/13111 (0.0%)	0.82	7/17784 (0.0%)
1	B	0.60	2/11928 (0.0%)	0.83	6/16183 (0.0%)
2	X	0.33	0/1560	0.56	0/2096
2	Y	0.33	0/1560	0.57	1/2096 (0.0%)
All	All	0.57	3/28159 (0.0%)	0.80	14/38159 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	2
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	247	GLU	CB-CG	5.75	1.63	1.52
1	B	247	GLU	CG-CD	5.70	1.60	1.51
1	A	247	GLU	CB-CG	5.40	1.62	1.52

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1487	PHE	N-CA-CB	7.79	124.62	110.60
1	A	1303	LEU	CA-CB-CG	6.25	129.68	115.30
1	B	1303	LEU	CA-CB-CG	6.20	129.56	115.30
1	A	1283	GLY	N-CA-C	5.75	127.47	113.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1283	GLY	N-CA-C	5.71	127.37	113.10

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1179	THR	Peptide
1	A	1633	PHE	Peptide
1	A	1635	TYR	Peptide
1	A	651	LEU	Peptide
1	B	651	LEU	Peptide

## 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	12836	0	12796	1596	1
1	B	11676	0	11649	1413	1
2	X	1539	0	1530	162	0
2	Y	1539	0	1530	163	0
3	C	28	0	25	3	0
3	D	28	0	25	2	0
4	A	5	0	0	0	0
4	B	4	0	0	0	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
All	All	27683	0	27581	3288	1

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 60.

The worst 5 of 3288 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1279:ARG:HG3	1:B:1284:PHE:CB	1.60	1.32

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1488:LEU:HD12	1:B:1488:LEU:O	1.31	1.30
1:A:1279:ARG:HG3	1:A:1284:PHE:CB	1.60	1.29
1:A:1486:GLY:O	1:A:1487:PHE:CD2	1.86	1.27
1:B:1323:LEU:HD12	1:B:1324:HIS:H	1.04	1.15

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:955:ARG:NH2	1:B:434:ASN:OD1[3_454]	2.19	0.01

## 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	1612/1676 (96%)	1199 (74%)	273 (17%)	140 (9%)	1	9
1	B	1468/1676 (88%)	1126 (77%)	224 (15%)	118 (8%)	1	11
2	X	189/231 (82%)	150 (79%)	28 (15%)	11 (6%)	1	18
2	Y	189/231 (82%)	150 (79%)	29 (15%)	10 (5%)	2	19
All	All	3458/3814 (91%)	2625 (76%)	554 (16%)	279 (8%)	1	11

5 of 279 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	TYR
1	A	59	TYR
1	A	97	ASN
1	A	209	PHE
1	A	243	PHE

### 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	1438/1484 (97%)	1168 (81%)	270 (19%)	1	9
1	B	1311/1484 (88%)	1055 (80%)	256 (20%)	1	9
2	X	175/205 (85%)	155 (89%)	20 (11%)	5	29
2	Y	175/205 (85%)	154 (88%)	21 (12%)	5	27
All	All	3099/3378 (92%)	2532 (82%)	567 (18%)	1	10

5 of 567 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1069	TRP
1	B	1142	LEU
1	B	1067	SER
1	B	1401	ARG
1	A	1208	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 100 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	288	GLN
1	B	840	GLN
2	Y	176	ASN
1	B	393	GLN
1	B	572	GLN

### 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

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
3	NAG	C	1	1,3	14,14,15	0.58	0	17,19,21	1.41	2 (11%)
3	NAG	C	2	3	14,14,15	0.43	0	17,19,21	1.11	1 (5%)
3	NAG	D	1	1,3	14,14,15	0.57	0	17,19,21	1.13	1 (5%)
3	NAG	D	2	3	14,14,15	0.40	0	17,19,21	1.04	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
3	NAG	C	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	NAG	C1-O5-C5	3.74	117.27	112.19
3	C	2	NAG	C1-O5-C5	3.50	116.93	112.19
3	C	1	NAG	C2-N2-C7	-3.39	118.08	122.90
3	D	2	NAG	C1-O5-C5	3.35	116.73	112.19
3	D	1	NAG	C3-C4-C5	-2.69	105.44	110.24

There are no chirality outliers.

5 of 6 torsion outliers are listed below:



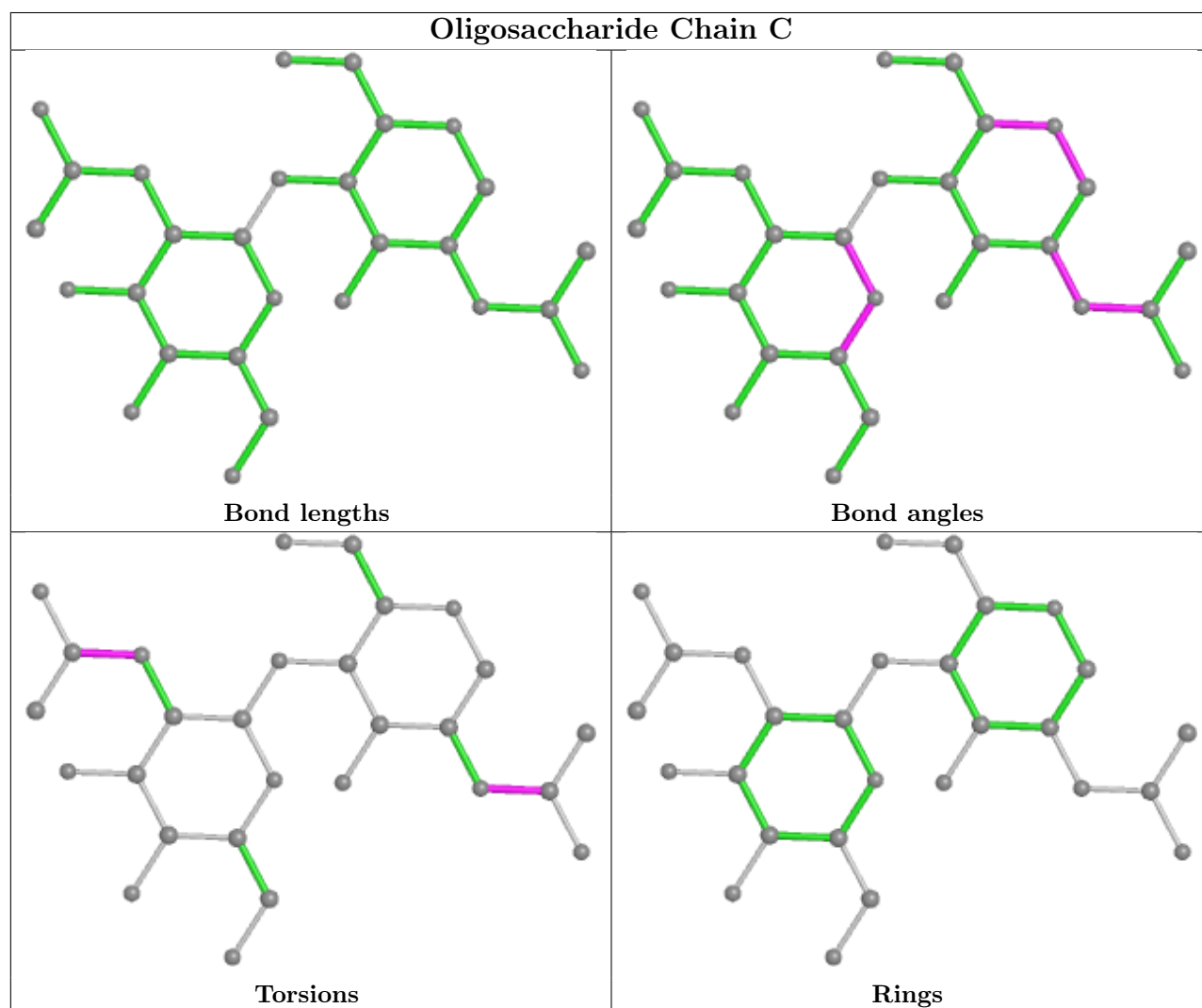
Mol	Chain	Res	Type	Atoms
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
3	D	2	NAG	C8-C7-N2-C2
3	D	2	NAG	O7-C7-N2-C2
3	C	1	NAG	C8-C7-N2-C2

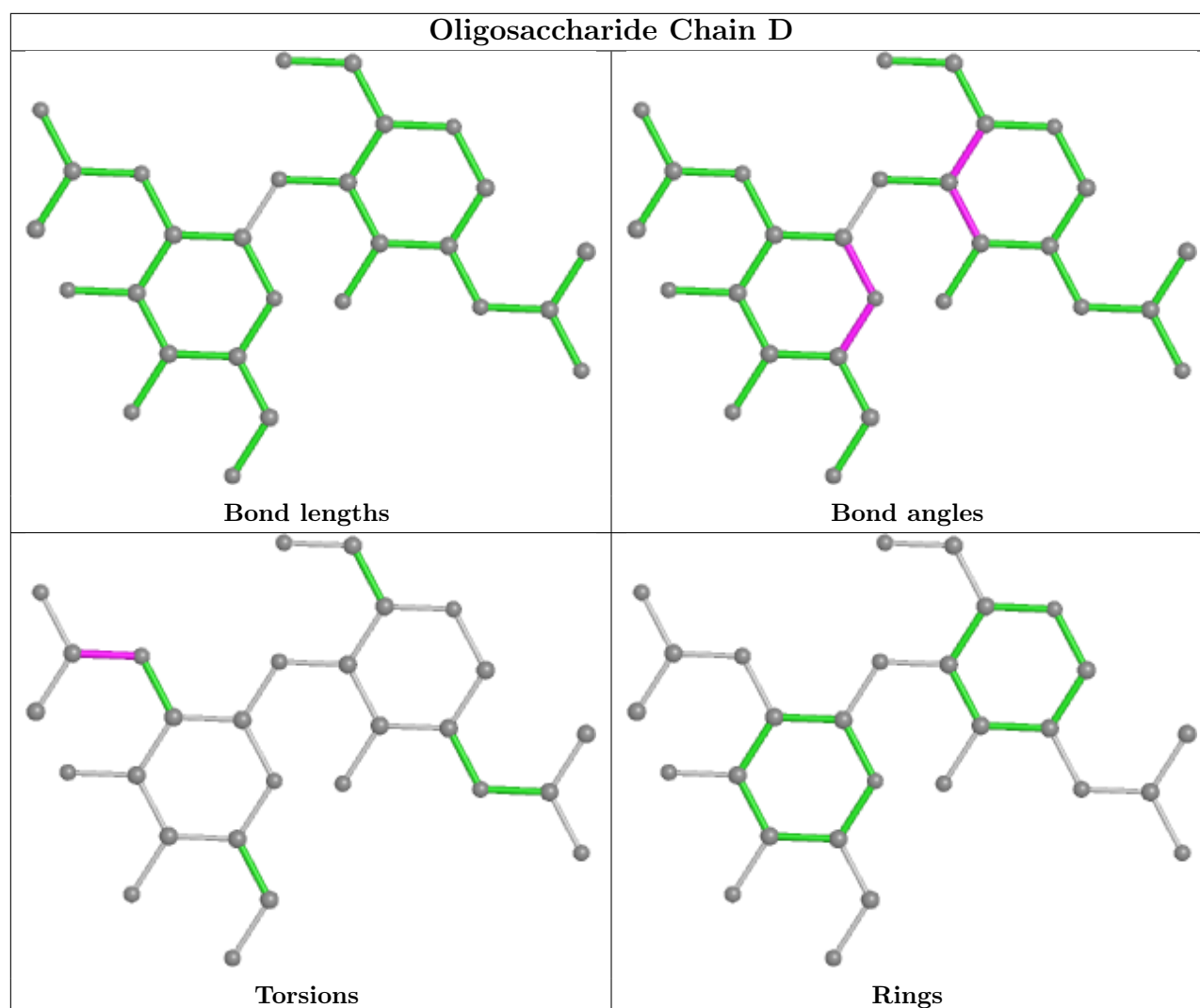
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1	NAG	2	0
3	C	1	NAG	3	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 11 ligands modelled in this entry, 9 are monoatomic - leaving 2 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	1681	1	14,14,15	0.74	0	17,19,21	1.17	1 (5%)
5	NAG	A	1682	1	14,14,15	0.68	0	17,19,21	1.09	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
5	NAG	B	1681	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1682	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1681	NAG	C1-O5-C5	2.21	115.19	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1682	NAG	C8-C7-N2-C2
5	A	1682	NAG	O7-C7-N2-C2
5	B	1681	NAG	C8-C7-N2-C2
5	B	1681	NAG	O7-C7-N2-C2

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1622/1676 (96%)	-0.10	36 (2%) 62 45	60, 136, 275, 372	0
1	B	1478/1676 (88%)	-0.19	13 (0%) 84 73	61, 129, 232, 340	0
2	X	191/231 (82%)	0.28	19 (9%) 7 4	150, 242, 308, 342	0
2	Y	191/231 (82%)	0.29	15 (7%) 12 7	149, 242, 308, 342	0
All	All	3482/3814 (91%)	-0.10	83 (2%) 59 42	60, 140, 279, 372	0

The worst 5 of 83 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1594	LYS	9.7
1	A	1593	GLU	8.6
1	A	1542	THR	6.8
1	A	1630	ASN	5.4
1	A	1522	GLY	5.4

### 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, 95<sup>th</sup> 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.

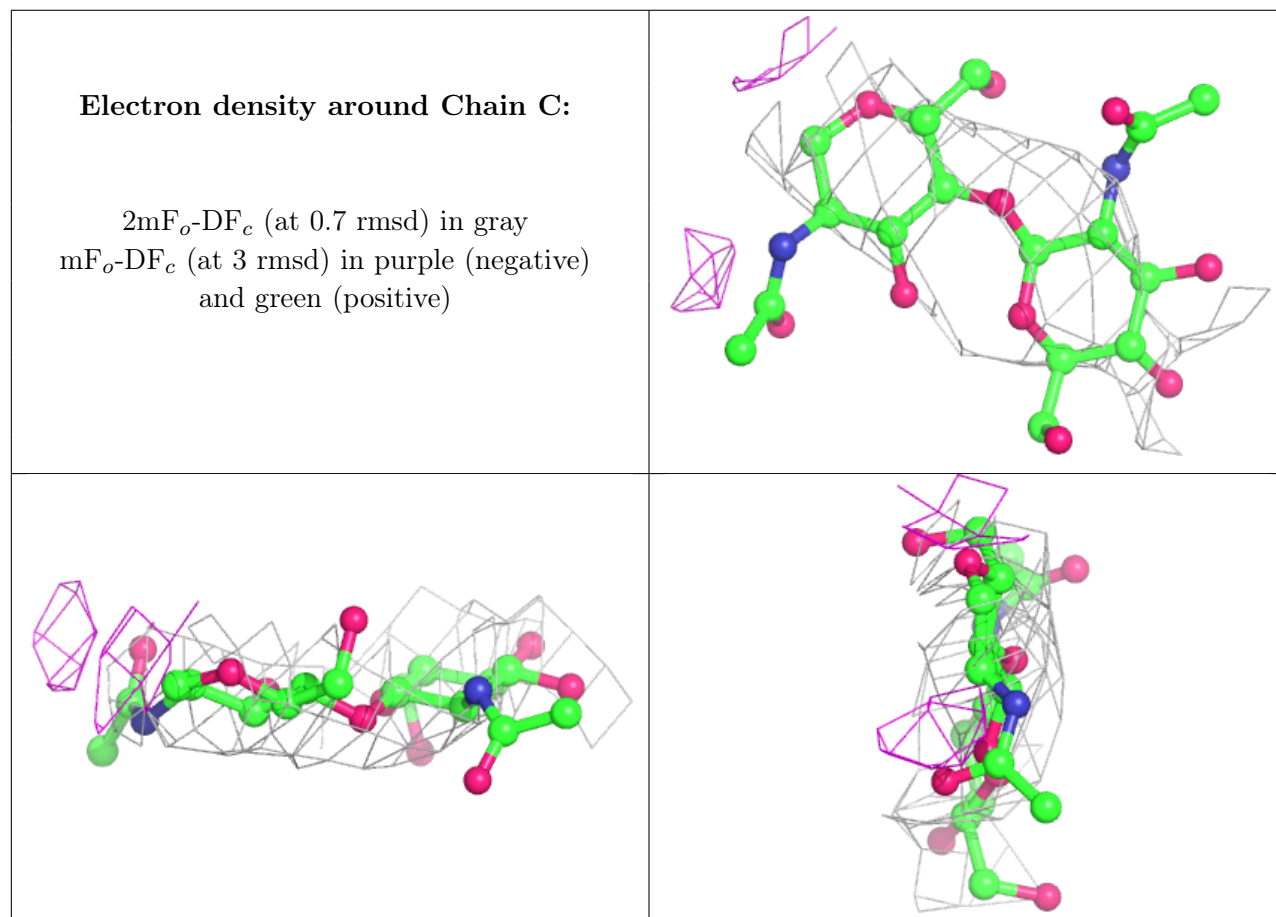
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	C	2	14/15	0.81	0.35	302,303,305,305	0
3	NAG	C	1	14/15	0.82	0.47	304,306,310,312	0

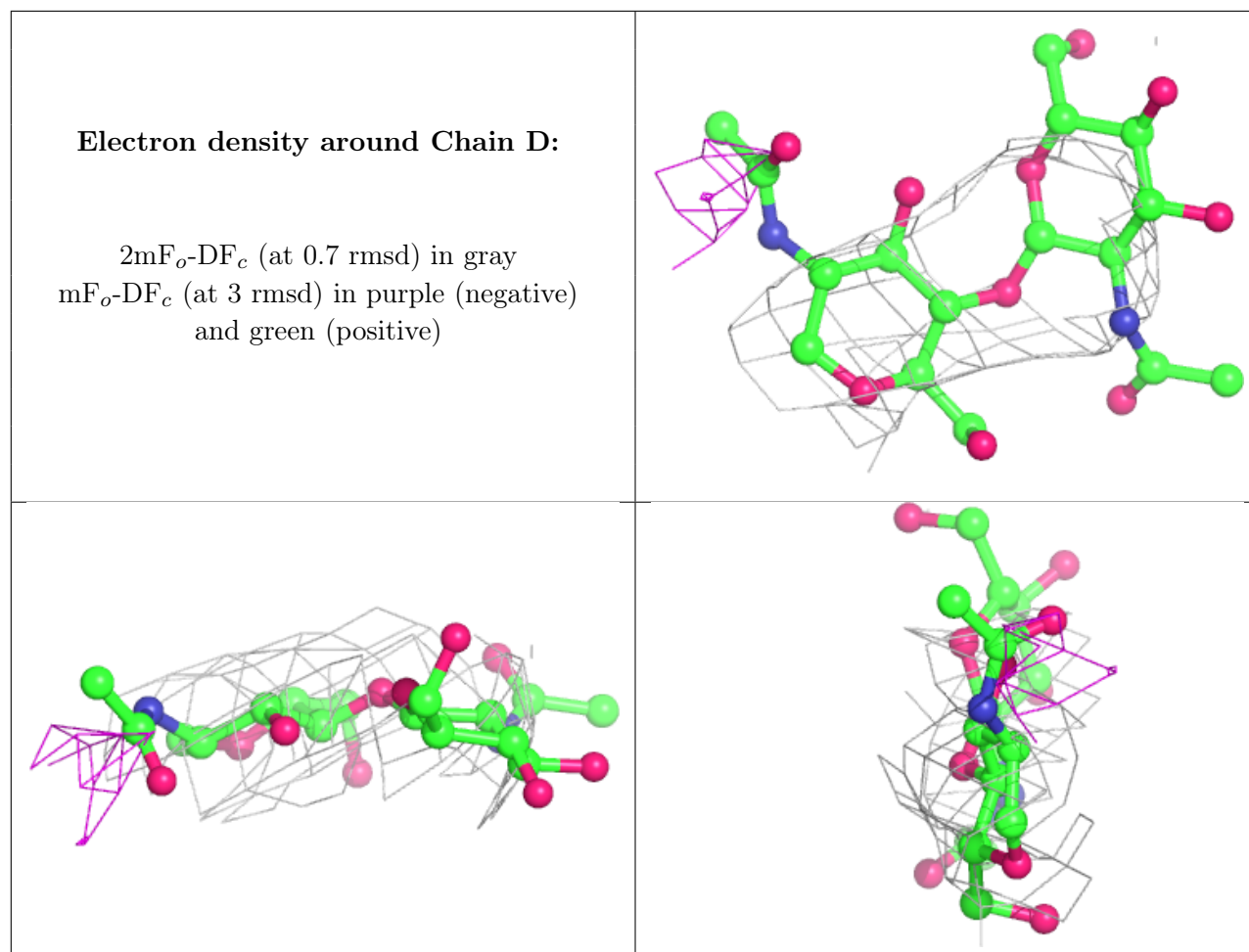
*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	D	1	14/15	0.84	0.49	315,318,321,323	0
3	NAG	D	2	14/15	0.84	0.28	309,312,314,314	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.





## 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	CD	B	1678	1/1	0.39	0.09	271,271,271,271	0
4	CD	A	1681	1/1	0.64	0.15	263,263,263,263	0
5	NAG	A	1682	14/15	0.65	0.58	285,301,311,313	0
4	CD	B	1680	1/1	0.67	0.13	252,252,252,252	0
4	CD	A	1680	1/1	0.81	0.10	241,241,241,241	0
5	NAG	B	1681	14/15	0.81	0.36	268,294,323,333	0
4	CD	A	1679	1/1	0.91	0.08	270,270,270,270	0
4	CD	A	1678	1/1	0.93	0.07	261,261,261,261	0
4	CD	B	1677	1/1	0.93	0.06	255,255,255,255	0
4	CD	B	1679	1/1	0.95	0.12	240,240,240,240	0
4	CD	A	1677	1/1	0.96	0.42	137,137,137,137	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.