



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2020 – 10:42 PM BST

PDB ID : 3KM9
Title : Structure of complement C5 in complex with the C-terminal beta-grasp domain of 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 : 2009-11-10
Resolution : 4.20 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 ⓘ 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 : 2.13.1
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) : 2.13.1

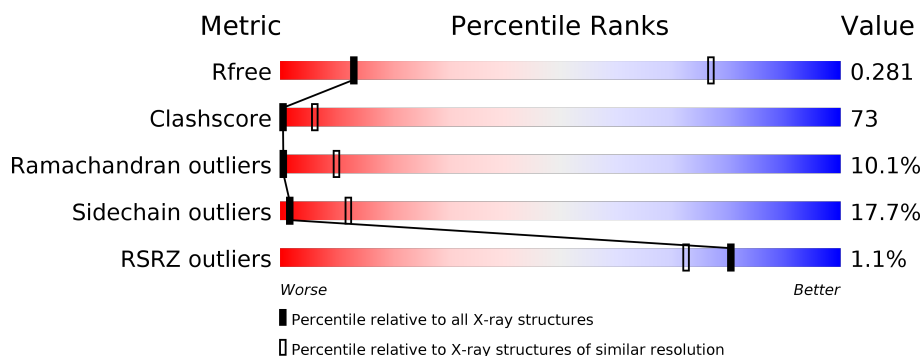
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.20 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	1005 (4.62-3.78)
Clashscore	141614	1044 (4.60-3.80)
Ramachandran outliers	138981	1000 (4.60-3.80)
Sidechain outliers	138945	1007 (4.62-3.78)
RSRZ outliers	127900	1063 (4.70-3.70)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1676	<div> <div>18%</div> <div>50%</div> <div>18%</div> <div>13%</div> </div>
1	B	1676	<div> <div>18%</div> <div>49%</div> <div>18%</div> <div>13%</div> </div>
2	X	103	<div> <div>9%</div> <div>37%</div> <div>52%</div> <div>10%</div> </div>
2	Y	103	<div> <div>5%</div> <div>38%</div> <div>52%</div> <div>9%</div> </div>
3	C	2	<div> <div>50%</div> <div>50%</div> </div>
3	D	2	<div> <div>50%</div> <div>50%</div> </div>

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
3	NAG	C	2	-	-	-	X
3	NAG	D	2	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 24809 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	1459	Total	C	N	O	S	0	0	0
			11541	7396	1903	2200	42			
1	B	1459	Total	C	N	O	S	0	0	0
			11541	7396	1903	2200	42			

- Molecule 2 is a protein called Staphylococcal enterotoxin-like toxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	102	Total	C	N	O	S	0	0	0
			819	517	138	163	1			
2	Y	102	Total	C	N	O	S	0	0	0
			819	517	138	163	1			

- 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	B	2	Total	Cd	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Cd	0	0
			3	3		

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

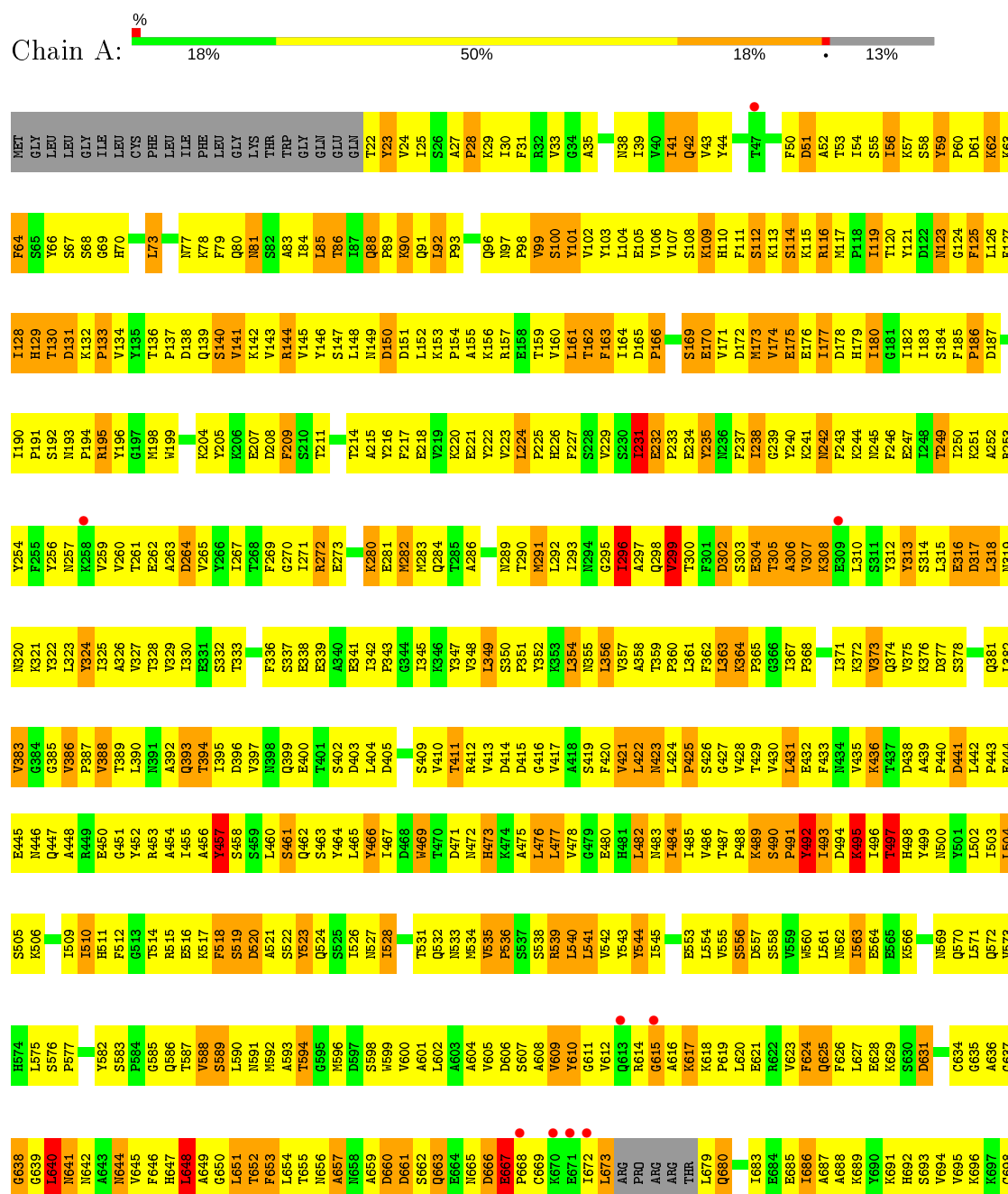


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

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



ASP	THR	CYS	Q1454	ARG	V1270	V1209	V1149	L1086	V1021	K957	L895	F824	C699
SER	LEU	GLU	I1455	GLY	I1271	S1210	I1150	G1087	F1022	E958	V896	F824	C699
THR	LEU	GLY	K1456	THR	K1272	A1211	G1151	Q1088	H1023	E959	V897	L825	Y700
TRP	ASP	ALA	D1457	GLY	W1273	L1212	I1152	V1089	Y1024	F960	F898	E764	D701
ILE	ALA	ASN	G1458	ASN	L1274	K1213	R1153	M1090	L1025	Y961	T899	P830	G702
LYS	LYS	LYS	H1459	SER	S1275	R1214	K1154	K1091	E1026	R962	V900	R765	A703
GLU	LYS	THR	V1460	ASP	E1276	E1215	A1155	V1092	T1027	I963	L901	R766	T704
TRP	GLY	VAL	I1461	ASP	Q1277	A1216	F1156	V1093	G1028	P964	P902	S767	V705
PRO	GLU	VAL	L1462	ASP	Q1278	L1217	D1157	E1094	M1029		I903	V834	V706
ARG	GLU	ALA	Q1463	R1401	R1279	V1218	I1158	Q1095	H1030	V967	E904	R835	D708
ASP	ALA	ALA	L1464	L1341	Y1280	K1219	C1159	M1096	W1031	V968	E905	R836	E709
THR	VAL	CYS	M1465	V1403	G1281	G1230	P1160	Q1097	H1032	K970	G906	E837	C710
ASP	ALA	ASP	M1466	A1404	G1282	M1231	L1161	N1098	I1033	K971	L907	R838	C711
THR	GLU	GLY	I1467	C1405	G1283	P1222	V1162	S1099		T971	H908	R839	E712
CYS	LYS	ASP	P1468	A1406	G1284	P1223	K1163	I1100	S1036	E972	H909	Q840	Q713
SER	ASP	MET		S1407	F1285	I1224	I1164	C1101	D1037	I973	I910	L841	R714
SER	SER	GLN	V1475	K1408	S1286	V1225	D1165	N1102	P1038	K974	H911	V845	A715
CYS	GLU	GLU	R1476	K1409	T1287	R1226	T1166	S1103	L1039	R975	F912	H778	A716
GLN	ILE	GLU	F1477	P1410	F1227	F1227	A1167	L1104	I1040	I976	S913	R779	R717
ALA	THR	LEU	R1478	S1411	M1228	M1228	L1168	L1105	E1041	L977	L914	V780	I718
PHE	PHE	THR	I1479	R1412	R1229	R1229	I1169	W1106	K1042	S978	E915	R847	S719
LEU	LEU	LEU	F1480	E1413	L1291	D1230	K1170	L1107	Q1043	R979	T916	F811	L720
ALA	LYS	THR	E1481	E1414	M1292	M1231	A1171	V1108	K1044	K980	H917	R782	R721
ASN	LYS	ILE	L1482	S1415	A1293	L1232	D1172	E1109	L1045	G981	K920	Q785	P722
LEU	VAL	SER	F1483	K1354	I1294	Q1233	M1173	N1110	K1046	L982	H921	L786	R723
ASP	THR	ALA	E1484	L1356	E1295		F1174	Y1111	K1047	L983	E921	Q787	C724
GLU	CYS	GLU	V1485	A1357	G1296	D1236	L1175	Q1112	L1048	V984	I922	F788	I725
GLY	THR	THR	L1486	T1358	S1297	S1237	L1176	L1113	K1049	G985	L923	R726	K726
PHE	THR	ALA	F1487	V1359	T1298	V1238	E1177	D1114	E1051	R986	V924	L790	A727
GLU	ALA	ARG	L1488	V1423	E1299	E1239	N1178	M1115	K1050	I987	K925	F791	F728
ASP	GLU	GLN	S1489	M1424	P1240	P1240	T1179	G1116	G1052	L988	T926	D792	T729
ILE	LEU	THR	D1425	D1425	M1241	M1241	L1180	S1117	M1053		L927	S793	E730
PHE	VAL	ALA	A1491	L1425	T1242	T1242	P1181	F1118	L1094	V991	R928	C731	C731
ASN	GLY	CYS	T1492	S1427	G1243	G1243	A1182	K1119	S1055	L992	V929	T795	C732
GLY	LYS	LYS	F1493	L1428	V1304	T1244	Q1183	E1120	I1056	S993	V930	T796	V733
ARG	PRO	ARG	P1494	P1429	K1305	A1245	M1121	M1057	Q994	T867	P931	W797	V734
GLN	GLN	GLU	V1495	T1430	R1246	R1246	T1185	S1122	S1058	E995	E932	E798	A735
ILE	THR	ILE	Y1496	G1431	M1247	M1247	F1186	Q1123	Y1059	G996	G933	I799	S736
LEU	LEU	ALA	E1497	I1432	R1308	V1248	T1157	P1126	R1060	I997	V934	Q800	Q737
ILE	ILE	THR	Y1498	S1433	L1309	E1249	L1188	K1127	M1061	M998	R935	G801	L738
MET	ALA	ALA	H1499	A1434	S1310	T1250	A1189	K1128	A1062	I999	R936	I802	R739
LYS	LYS	LYS	P1501	E1436	D1312	T1251	I1190	L1129	Y1064	L1000	S938	H803	
GLU	VAL	VAL	D1502	E1437	I1313	Y1263	A1192	T1132	S1065	H1002	V939	I804	I742
ALA	ALA	SER	K1503	D1438	L1314	A1294	Y1193	E1136	Y1066	L1003	S940	S805	S743
LEU	LEU	ILE	Q1504	L1439	V1315	L1255	A1194	P1133	S1067		G941	I809	LYS
GLN	GLN	THR	G1505	K1440	S1316	L1256	L1195	P1134	Y1068	S1007	V942	C810	ASP
ILE	ILE	SER	T1506	A1441	Y1317	T1257	S1196	V1135	W1069	E1007	T943	V811	MET
LYS	LYS	ILE	M1507	L1442	K1318	S1258	L1197	E1136	K1070	A1008	L944	A812	GLN
THR	THR	THR	F1508	V1443	H1319	L1259	G1198			E1009	D945	D813	LEU
ASN	ASN	VAL	Y1509	E1444	M1320	M1260	D1199	E1139	T1076	A1010	P946	T814	G750
PHE	PHE	GLU	S1510	G1445	K1321	L1261	K1200	M1140	W1077	E1011	R947	V815	G751
SER	SER	ASN	T1511	V1446	A1322	K1262	T1201	L1012	L1078	L1012	G948	K316	L752
PHE	PHE	VAL		D1447	L1323	D1263	H1202	T1079	T1079		T949	R887	H753
ARG	ARG	PHE	H1514	Q1448	M1324	I1264	Y1143	A1080	V1015	V1015	G951	K318	M754
THR	THR	VAL	LYS	L1449	H1325	M1265	Q1204	F1081	V1016	V1016	T952	V819	K755
ILE	ILE	LYS	ILE	F1450	Y1326	Y1266	F1205	A1082	P1017	P1017	T953	F820	
LYS	LYS	THR	GLN	T1451	K1327	V1267	R1206	L1083	V1018	V1018		S891	L758
PRO	PRO	ASP	LYS	D1452	M1328	M1268	S1207	R1084	F1019	S892		R821	P759
LEU	ALA	ALA	VAL	Y1453	T1329	P1269	I1208	T1148	V1085	Y1020	R956	V823	V760

Chain B:



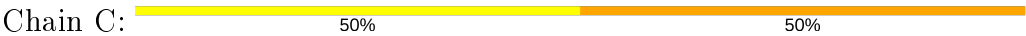
LEU	ASP	LEU	GLY	F1383	V1270	V1209	A1146	A1082	V1015	G951	G880
THR	ASP	THR	ALA	L1394	I1271	S1210	F1147	L1083	V1016	T952	S891
TRP	ILE	TRP	ALA	G1335	K1272	A1211	T1148	R1084	P1017	T953	S892
ILE	TRP	ILE	SER	R1336	M1273	L1212	V1149	L1085	F1018		S893
GLU	LYS	GLU	ASP	V1337	L1274	K1214	G1151	L1086	F1019	R956	H894
LYS	TRP	LYS	ASP	P1338		R1214	G1151	G1087	F1020	K957	L895
VAL	GLY	VAL	ASP	V1339	E1277	E1216	G1152	Q1088	V1021	R958	V896
GLU	GLY	GLU	R1401	V1340	Q1278	A1216	R1153	Q1089	F1022	P959	T897
ALA	ALA	ALA	I1402	L1341	L1279	L1217	K1154	M1090	H1023	F960	F898
ASP	ASP	ASP	V1403	L1342	Y1280	V1218	A1155	K1091	Y1024	Y961	T899
ALA	CYS	ALA	M1343	M1343		K1219	F1156	Y1092	L1025	R962	V900
GLY	GLY	GLY	C1405	D1344	G1283	G1220	D1157	V1093	E1026	P963	L901
GLN	GLN	GLN	F1406	D1345	F1284	M1221	I1158	E1094	T1027	P902	P902
ASP	ASP	ASP	S1407	L1346	Y1285	P1222	C1159	Q1095	G1028	D966	L903
GLN	GLN	GLN	Y1408	T1347	S1286		P1160	M1096	H1029	P967	E904
GLY	GLY	GLY	K1409	V1348	T1287	Y1225	L1161	Q1097	H1030	V968	I905
ILE	GLU	ILE	F1476	S1349	Q1288	R1226	V1162	M1098	W1031	G906	G906
GLU	GLU	GLU	P1410	T1350	D1289	F1227	K1163	S1099	M1032	T971	L907
ALA	THR	ALA	S1411	T1350	R1412	W1228	I1164	I1100	I1033	R972	H908
PRE	ASP	PRE	R1412	G1351	T1290	K1229	D1165		D1037	T973	M909
LEU	LEU	LEU	E1413	F1352	I1291			L1104		R974	I910
ALA	THR	ALA	E1414	G1353	M1292	D1230	L1168		P1038	R975	
THR	THR	THR	S1415	S1354	A1293	M1231	L1105	L1105	L1039	R976	F912
VAL	VAL	VAL		G1355	T1294	L1232	W1106	W1106	S1039	S977	S913
ALA	ALA	ALA	G1418	L1356	E1295	Q1233	D1172	D1172	I1040	S978	S914
CYS	CYS	CYS		A1357	E1296	H1234	M1173	M1173	K1041	S979	E915
THR	THR	THR	H1421	T1358	L1297	K1235	F1174	E1109	K1042	R980	W917
ARG	ARG	ARG	A1422	H1359	T1298	D1236	L1175	M1110	Q1043	G981	
LYS	LYS	LYS	F1423	H1360	E1299	S1237	L1176	Y1111	K1045	L982	K920
GLU	GLN	GLU	M1424	V1361	V1300	S1238	E1177	L1113	K1046	L983	E921
THR	THR	THR	D1425	T1362	S1301	V1239	M1178	L1113	K1047	R984	
ALA	ALA	ALA	T1426	V1363	L1302	P1240	T1179	D1114	K1048	R985	
CYS	CYS	CYS	S1427	V1364	L1303	M1241	L1180	M1115	K1049	R986	L923
LYS	LYS	LYS	L1428	V1365	V1304	T1242	P1181	G1116	K1050	T987	
GLY	GLY	GLY	F1429	H1366	K1305	G1243	Q1182	S1117		R988	K925
PRQ	GLU	PRQ	T1430	K1367	Q1306	T1244	Q1183	F1118			
LEU	ILE	LEU	G1431	T1368	L1307	A1245	S1184	K1119	M1063	T926	
ALA	ALA	ALA	I1432	S1369	R1308	R1246	T1185	E1120	L1054	L927	
TYR	TYR	TYR	S1433	T1370	L1309	M1247	F1186	M121	S1055	R928	
ALA	ALA	ALA	A1434	S1371	S1310	V1248	T1187	Q1122	I1056	S993	
GLY	GLY	GLY	M1435	E1372	M1311	E1249	L1188	Q1123	M1057	V929	
LYS	LYS	LYS	E1436	E1373	D1312	T1250	A1189	S1058	V930	V930	
VAL	VAL	VAL	E1437	V1374	I1313	T1251	I1190	Y1059	E932	P931	
ILE	ILE	ILE	D1438	G1375	D1314	A1252	S1191	Q1125	R1060	G933	
SER	SER	SER	L1439	S1376	V1315	Y1253	A1192	P1126	M1061	V934	
THR	THR	THR	K1440	F1377	S1316	A1294	Y1193	K1128	A1062	K935	
ILE	ILE	ILE	A1441	Y1378	Y1317	L1255	A1194	L1129	D1063	R936	
SER	SER	SER	L1442	L1379	H1318	L1256	L1195		Y1064	E937	
LYS	LYS	LYS	V1443	K1380	H1319	T1257	S1196	S1065	L1000	T1001	
THR	THR	THR	E1444	I1381	K1320	S1258	L1197	H1002	S938	H002	
ASN	VAL	ASN	G1445	T1382	G1321	L1259	G1193	L1133	Y1066	Y939	
ASN	ASN	ASN	V1446	T1383	A1322	M1260	D1199	P1134	S1067	S940	
VAL	VAL	VAL	D1447		L1323	L1261	K1200	V1135	W1069	G941	
PHE	PHE	PHE	L1448	G1386	L1324	K1262	T1201	E1136	S1007	G1006	
ARG	ARG	ARG	Q1449	GLU	H1324	L1261	H1202	A1008	T943	T943	
LYS	LYS	LYS	F1450	ALA	V1326	D1263	P1203	N1140	D945	D945	
TYR	TYR	TYR	T1451	SER	K1327	N1265	Q1204	S1141	W1077	P946	
LYS	LYS	LYS	D1452	HIS	M1328	Y1266	F1205	L1142	L1078	R947	
LEU	LEU	LEU	Y1453	TYR	T1329	Y1267	R1206	Y1143	T1079	G948	
ASP	ASP	ASP	Q1454	ARG	M1268	N1268	S1207	L1144	A1080	I949	
GLY	GLY	GLY	I1455		P1269		T1208	T1145	F1081	S1014	
LEU	THR	LEU									
THR	THR	THR									
TRP	TRP	TRP									
ILE	ILE	ILE									
GLU	GLU	GLU									
LYS	LYS	LYS									
VAL	VAL	VAL									
GLY	GLY	GLY									
ASP	ASP	ASP									
THR	THR	THR									
ALA	ALA	ALA									
GLY	GLY	GLY									
LEU	LEU	LEU									
ALA	ALA	ALA									
GLY	GLY	GLY									
LEU	LEU	LEU									
ALA	ALA	ALA									
GLY	GLY	GLY									
LEU	LEU	LEU									
ALA	ALA	ALA									
GLY	GLY	GLY									
LEU	LEU	LEU									
ALA	ALA	ALA									
GLY	GLY	GLY									
LEU	LEU	LEU									
ALA	ALA	ALA									
GLY	GLY	GLY									
LEU	LEU	LEU									
ALA	ALA	ALA									
GLY	GLY	GLY									
LEU	LEU	LEU									
ALA	ALA	ALA									
GLY	GLY	GLY									
LEU	LEU	LEU									
ALA	ALA	ALA									
GLY	GLY	GLY									
LEU	LEU	LEU									
ALA	ALA	ALA									
GLY	GLY	GLY									
LEU	LEU	LEU									
ALA	ALA	ALA									
GLY	GLY	GLY									
LEU	LEU	LEU									
ALA	ALA	ALA									
GLY	GLY	GLY									
LEU	LEU	LEU									
ALA	ALA	ALA									
GLY	GLY	GLY									
LEU	LEU	LEU									
ALA	ALA	ALA									
GLY	GLY	GLY									
LEU	LEU	LEU									
ALA	ALA	ALA									
GLY	GLY	GLY									
LEU	LEU	LEU									
ALA	ALA	ALA									
GLY	GLY	GLY									
LEU	LEU	LEU									
ALA	ALA	ALA									
GLY	GLY	GLY									
LEU	LEU	LEU									
ALA	ALA	ALA									
GLY	GLY	GLY									
LEU	LEU	LEU									
ALA	ALA	ALA									
GLY	GLY	GLY									
LEU	LEU	LEU									
ALA	ALA	ALA									
GLY	GLY	GLY									
LEU	LEU	LEU									
ALA	ALA	ALA									
GLY	GLY	GLY									
LEU	LEU	LEU									
ALA	ALA	ALA									
GLY	GLY	GLY									
LEU	LEU	LEU									
ALA	ALA	ALA									
GLY	GLY	GLY									
LEU	LEU	LEU									
ALA	ALA	ALA									
GLY	GLY	GLY									
LEU	LEU	LEU									
ALA	ALA	ALA									
GLY	GLY	GLY									
LEU	LEU	LEU									
ALA	ALA	ALA									
GLY	GLY	GLY									
LEU	LEU	LEU									
ALA	ALA	ALA									
GLY	GLY	GLY									
LEU	LEU	LEU									
ALA	ALA	ALA									
GLY	GLY	GLY									
LEU	LEU	LEU									
ALA	ALA	ALA									
GLY	GLY	GLY									
LEU	LEU	LEU									
ALA	ALA	ALA									
GLY	GLY	GLY									



● Molecule 2: Staphylococcal enterotoxin-like toxin



● 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, α , β , γ	144.79 Å 144.79 Å 245.28 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.75 – 4.20 49.75 – 4.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.75-4.20) 99.8 (49.75-4.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 4.14 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.233 , 0.297 0.215 , 0.281	Depositor DCC
R_{free} test set	2039 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	115.5	Xtriage
Anisotropy	0.855	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.19 , 90.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.044 for -h,-k,l 0.397 for h,-h-k,-l 0.045 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	24809	wwPDB-VP
Average B, all atoms (Å ²)	205.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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: NAG, CD

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	0.53	0/11793	0.77	6/16003 (0.0%)
1	B	0.53	0/11793	0.77	5/16003 (0.0%)
2	X	0.34	0/828	0.54	0/1107
2	Y	0.34	0/828	0.56	1/1107 (0.1%)
All	All	0.52	0/25242	0.75	12/34220 (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	1
1	B	0	2
All	All	0	3

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	264	ASP	CB-CG-OD1	-8.57	110.58	118.30
1	B	640	LEU	CA-CB-CG	7.23	131.94	115.30
1	B	1374	VAL	CB-CA-C	-6.61	98.85	111.40
1	A	640	LEU	CA-CB-CG	6.51	130.28	115.30
1	A	1195	LEU	CA-CB-CG	-5.71	102.17	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	651	LEU	Peptide
1	B	1179	THR	Peptide
1	B	651	LEU	Peptide

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	11541	0	11511	1721	0
1	B	11541	0	11511	1730	0
2	X	819	0	831	85	0
2	Y	819	0	831	83	0
3	C	28	0	25	2	0
3	D	28	0	25	3	0
4	A	3	0	0	0	0
4	B	2	0	0	0	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
All	All	24809	0	24760	3610	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 73.

The worst 5 of 3610 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:535:VAL:HG23	1:A:536:PRO:HD3	1.21	1.17
1:A:698:CYS:SG	1:A:724:CYS:CB	2.33	1.16
1:A:698:CYS:SG	1:A:724:CYS:HB2	1.86	1.15
1:A:968:VAL:HG12	1:A:1368:THR:HG22	1.19	1.13
1:B:535:VAL:HG23	1:B:536:PRO:HD3	1.29	1.13

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	1449/1676 (86%)	1039 (72%)	255 (18%)	155 (11%)	0	8
1	B	1449/1676 (86%)	1026 (71%)	274 (19%)	149 (10%)	0	9
2	X	100/103 (97%)	86 (86%)	9 (9%)	5 (5%)	2	23
2	Y	100/103 (97%)	84 (84%)	11 (11%)	5 (5%)	2	23
All	All	3098/3558 (87%)	2235 (72%)	549 (18%)	314 (10%)	0	10

5 of 314 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	TYR
1	A	86	THR
1	A	97	ASN
1	A	99	VAL
1	A	170	GLU

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	1296/1484 (87%)	1061 (82%)	235 (18%)	1	11
1	B	1296/1484 (87%)	1051 (81%)	245 (19%)	1	10
2	X	93/94 (99%)	87 (94%)	6 (6%)	17	44
2	Y	93/94 (99%)	86 (92%)	7 (8%)	13	40
All	All	2778/3156 (88%)	2285 (82%)	493 (18%)	2	12

5 of 493 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1465	ASN
1	B	184	SER
1	B	1313	ILE
1	A	1496	TYR
1	B	73	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 98 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1463	GLN
1	B	139	GLN
1	B	1366	HIS
1	A	1465	ASN
1	B	77	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

4 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	C	1	1,3	14,14,15	0.53	0	17,19,21	1.06	1 (5%)
3	NAG	C	2	3	14,14,15	0.48	0	17,19,21	1.07	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	D	1	1,3	14,14,15	0.56	0	17,19,21	0.96	0
3	NAG	D	2	3	14,14,15	0.48	0	17,19,21	1.01	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
3	NAG	C	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	4/6/23/26	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	2	NAG	C1-O5-C5	2.98	116.23	112.19
3	C	1	NAG	C1-O5-C5	2.98	116.23	112.19
3	D	2	NAG	C1-O5-C5	2.63	115.75	112.19
3	D	2	NAG	O5-C5-C6	2.20	110.65	107.20
3	C	2	NAG	O5-C5-C6	2.07	110.45	107.20

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

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

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1	NAG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	NAG	2	0
3	D	2	NAG	1	0

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 5 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	A	1680	1	14,14,15	0.65	0	17,19,21	1.00	1 (5%)
5	NAG	B	1679	1	14,14,15	0.70	0	17,19,21	1.10	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	A	1680	1	-	4/6/23/26	0/1/1/1
5	NAG	B	1679	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1680	NAG	O5-C5-C6	2.89	111.73	107.20
5	B	1679	NAG	O5-C5-C6	2.55	111.21	107.20

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1680	NAG	C8-C7-N2-C2
5	A	1680	NAG	O7-C7-N2-C2
5	B	1679	NAG	C8-C7-N2-C2
5	B	1679	NAG	O7-C7-N2-C2
5	B	1679	NAG	C1-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1459/1676 (87%)	-0.62	11 (0%) 86 79	81, 190, 311, 455	0
1	B	1459/1676 (87%)	-0.63	10 (0%) 87 82	85, 190, 308, 475	0
2	X	102/103 (99%)	0.04	9 (8%) 10 9	157, 292, 386, 530	0
2	Y	102/103 (99%)	0.02	5 (4%) 29 25	156, 292, 377, 494	0
All	All	3122/3558 (87%)	-0.58	35 (1%) 80 72	81, 194, 328, 530	0

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	671	GLU	4.8
2	Y	193	LEU	4.4
2	X	193	LEU	4.4
1	B	671	GLU	4.0
1	A	670	LYS	3.6

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	C	2	14/15	0.66	0.46	343,343,343,343	0
3	NAG	D	2	14/15	0.73	0.50	363,363,363,363	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	D	1	14/15	0.79	0.30	280,280,280,280	0
3	NAG	C	1	14/15	0.85	0.28	293,293,293,293	0

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	CD	A	1679	1/1	0.22	0.12	402,402,402,402	0
4	CD	B	1678	1/1	0.39	0.11	397,397,397,397	0
5	NAG	A	1680	14/15	0.51	0.36	301,301,301,301	0
5	NAG	B	1679	14/15	0.59	0.35	290,290,290,290	0
4	CD	A	1678	1/1	0.87	0.44	481,481,481,481	0
4	CD	A	1677	1/1	0.89	0.09	229,229,229,229	1
4	CD	B	1677	1/1	0.90	0.38	466,466,466,466	0

6.5 Other polymers [i](#)

There are no such residues in this entry.