



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2020 – 03:58 PM BST

PDB ID : 3PRX  
Title : Structure of Complement C5 in Complex with CVF and SSL7  
Authors : Laursen, N.S.; Andersen, G.R.; Sottrup-Jensen, L.; Andersen, K.R.; Spillner, E.; Braren, I.  
Deposited on : 2010-11-30  
Resolution : 4.30 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.

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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



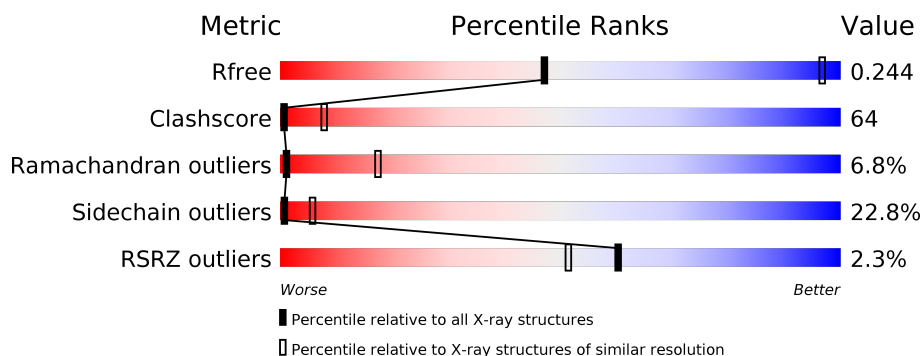
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.30 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	1014 (4.80-3.80)
Clashscore	141614	1077 (4.80-3.80)
Ramachandran outliers	138981	1029 (4.80-3.80)
Sidechain outliers	138945	1012 (4.80-3.80)
RSRZ outliers	127900	1075 (4.90-3.70)





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  $\geq 3$ , 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	<div> <div style="width: 24%; background-color: red;"></div> <div style="width: 50%; background-color: yellow;"></div> <div style="width: 21%; background-color: orange;"></div> <div style="width: 5%; background-color: green;"></div> <div style="width: 0%; background-color: grey;"></div> </div> <p>24% 50% 21% . .</p>
1	C	1676	<div> <div style="width: 3%; background-color: red;"></div> <div style="width: 23%; background-color: green;"></div> <div style="width: 51%; background-color: yellow;"></div> <div style="width: 21%; background-color: orange;"></div> <div style="width: 0%; background-color: grey;"></div> </div> <p>3% 23% 51% 21% . .</p>
2	B	1642	<div> <div style="width: 23%; background-color: green;"></div> <div style="width: 38%; background-color: yellow;"></div> <div style="width: 13%; background-color: orange;"></div> <div style="width: 26%; background-color: grey;"></div> </div> <p>23% 38% 13% 26%</p>
2	D	1642	<div> <div style="width: 22%; background-color: green;"></div> <div style="width: 39%; background-color: yellow;"></div> <div style="width: 12%; background-color: orange;"></div> <div style="width: 26%; background-color: grey;"></div> </div> <p>22% 39% 12% 26%</p>
3	X	231	<div> <div style="width: 11%; background-color: red;"></div> <div style="width: 26%; background-color: green;"></div> <div style="width: 44%; background-color: yellow;"></div> <div style="width: 11%; background-color: orange;"></div> <div style="width: 0%; background-color: grey;"></div> </div> <p>11% 26% 44% 11% . 17%</p>
3	Y	231	<div> <div style="width: 6%; background-color: red;"></div> <div style="width: 24%; background-color: green;"></div> <div style="width: 45%; background-color: yellow;"></div> <div style="width: 13%; background-color: orange;"></div> <div style="width: 0%; background-color: grey;"></div> </div> <p>6% 24% 45% 13% . 17%</p>

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Mol	Chain	Length	Quality of chain
4	E	2	 100%
4	F	2	 50% 50%
4	G	2	 100%
4	H	2	 50% 50%

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
4	NAG	E	1	-	-	-	X
4	NAG	E	2	-	-	-	X
4	NAG	F	1	-	-	-	X
4	NAG	F	2	-	-	-	X
4	NAG	G	2	-	-	-	X
4	NAG	H	1	-	-	-	X
4	NAG	H	2	-	-	-	X



## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 48236 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	1626	Total	C	N	O	S	0	0	0
			12874	8242	2113	2467	52			
1	C	1626	Total	C	N	O	S	0	0	0
			12874	8242	2113	2467	52			

- Molecule 2 is a protein called Cobra venom factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1215	Total	C	N	O	S	0	0	0
			9635	6143	1617	1836	39			
2	D	1215	Total	C	N	O	S	0	0	0
			9635	6143	1617	1836	39			

- Molecule 3 is a protein called Superantigen-like protein 7.

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

- Molecule 4 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
4	E	2	Total	C	N	O		0	0	0
			28	16	2	10				

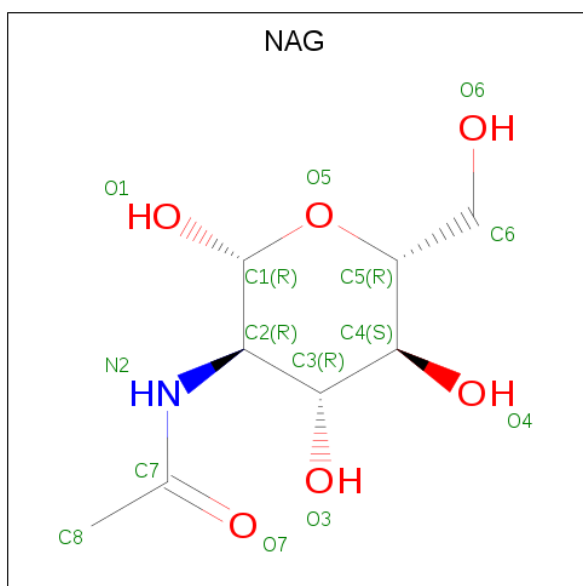
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



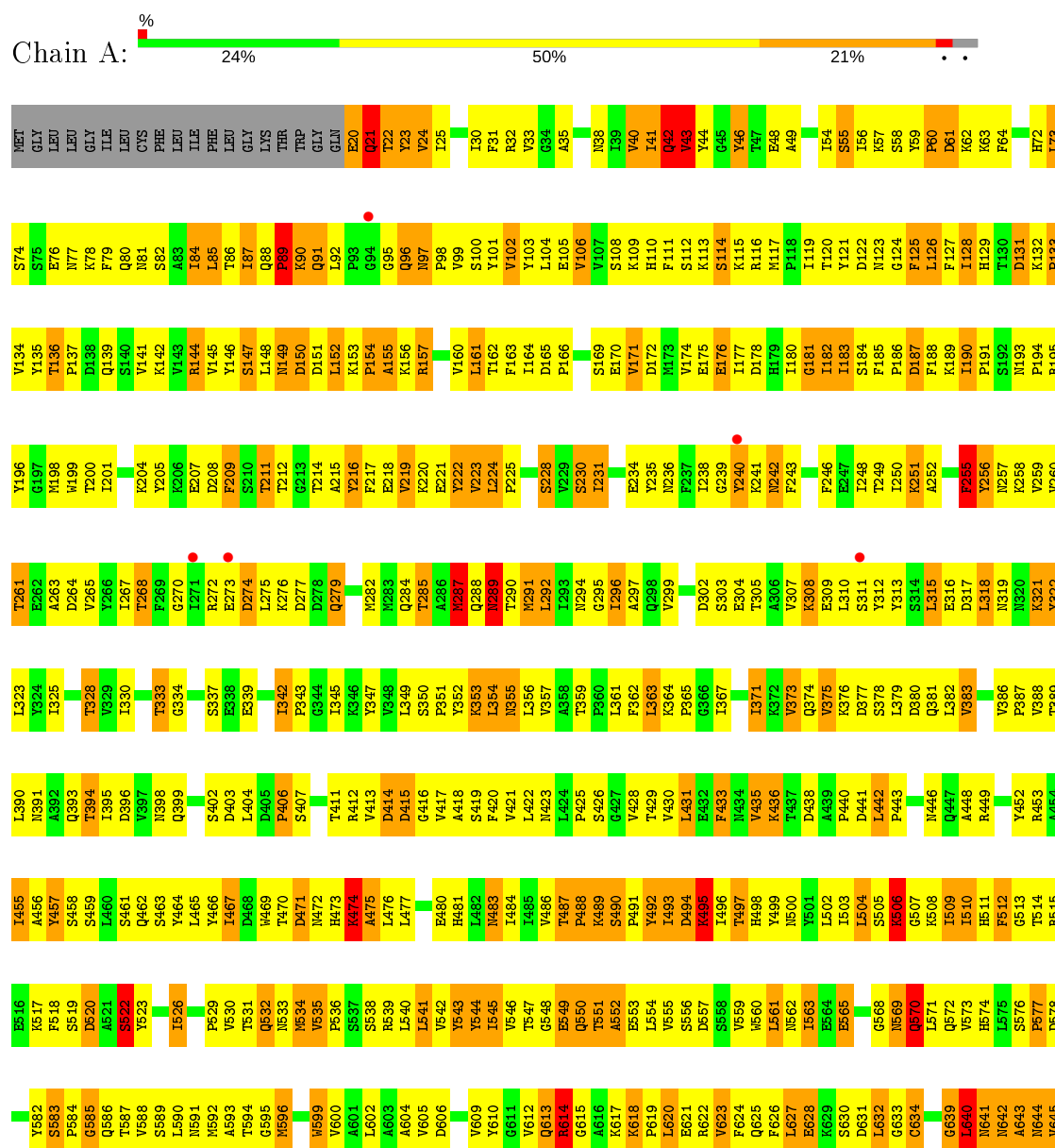
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		



### 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.

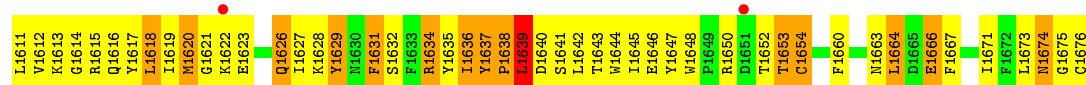
#### • Molecule 1: Complement C5



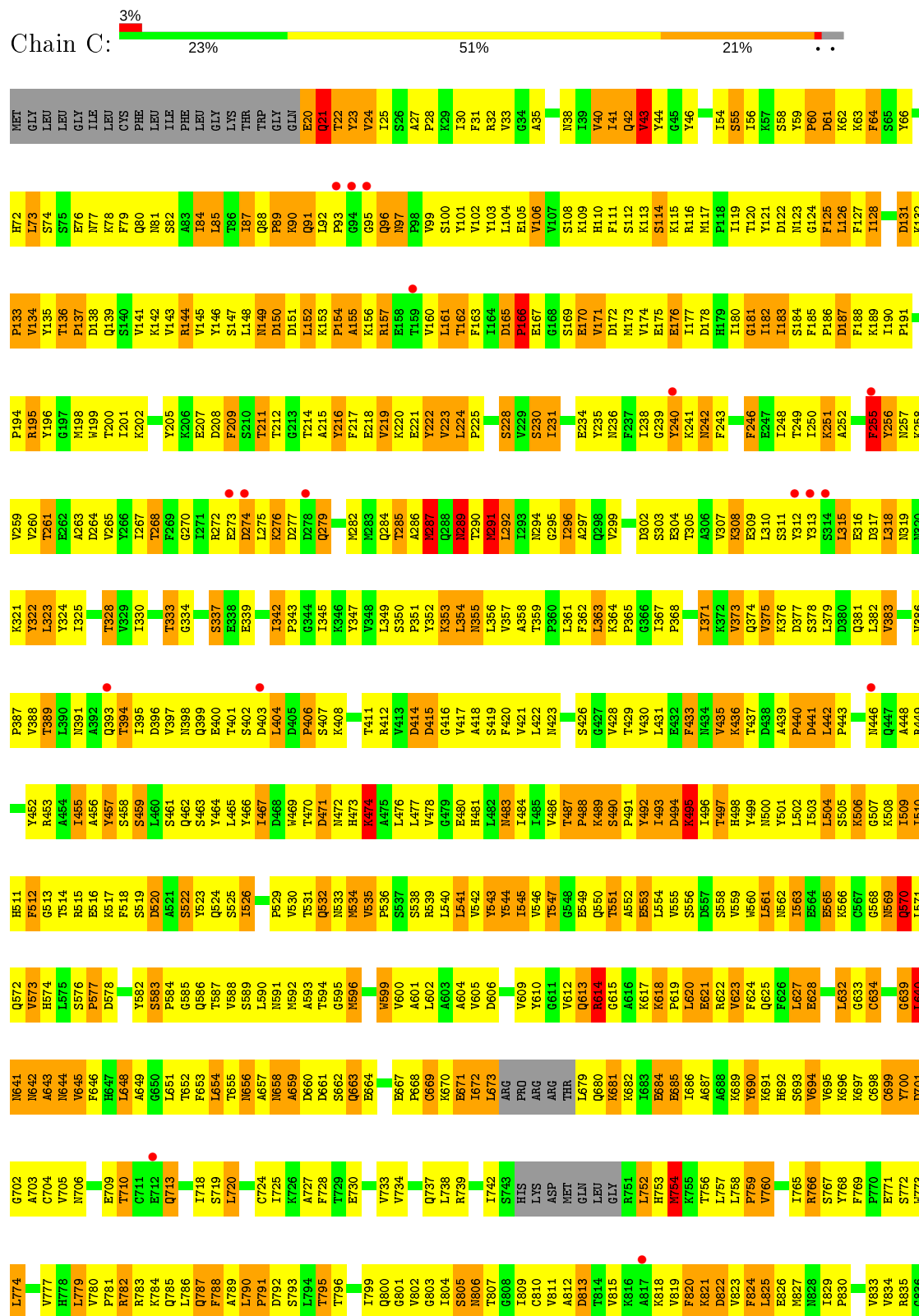


T1551	A1552	C1553	K1554	F1555	E1556	T1557	A1558	Y1559	A1560	A1561	A1562	A1563	A1564	T1565	T1566	S1567	T1568	T1569	E1570	E1571	N1572	V1573	F1574	V1575	K1576	Y1577	I1578	G1579	V1580	V1581	L1582	D1583	Y1584	K1585	T1586	G1587	E1588	A1589	V1590	V1591	A1592	E1593	K1594	D1595	S1596	I1597	T1598	T1599	F1600	I1601	K1602	K1603	V1604	C1605	T1606	N1607	A1608	E1610								
I1426	S1427	L1428	P1429	F1430	E1431	G1432	I1433	E1434	A1435	A1436	L1437	K1438	V1439	K1440	V1441	A1442	G1443	V1444	V1445	V1446	Q1447	Q1448	L1449	F1450	T1451	D1452	I1453	Q1454	L1455	K1456	D1457	G1458	H1459	V1460	L1461	L1462	Q1463	L1464	N1465	P1466	S1467	I1468	A1469	A1470	D1471	F1472	C1473	E1474	V1475	R1476	I1477	F1478	F1479	F1480	E1481	L1482	V1483	C1484	V1485	F1486	A1487	E1488				
S1489	P1490	A1491	K1492	F1493	E1494	V1495	Y1496	E1497	V1498	H1499	R1500	P1501	D1502	L1503	Q1504	C1505	T1506	N1507	S1510	T1511	S1512	N1513	I1514	L1515	L1516	I1517	G1518	G1519	L1520	S1521	V1522	V1523	C1524	C1525	K1526	C1527	V1528	E1529	C1530	C1531	Q1532	Q1533	Q1534	M1535	Q1536	E1537	E1538	L1539	E1540	L1541	L1542	T1543	S1544	C1545	A1546	E1547	T1548	N1549	K1550	E1551						
V1359	H1360	V1361	T1362	F1363	V1364	V1365	H1366	K1367	L1368	A1369	S1370	T1371	E1372	E1373	S1374	L1375	L1376	L1377	K1378	I1379	D1380	D1381	T1382	L1383	Q1384	T1385	I1386	I1387	A1388	L1389	L1390	L1391	L1392	L1393	L1394	L1395	L1396	L1397	L1398	L1399	L1400	L1401	L1402	V1403	A1404	C1405	A1406	S1407	Y1408	K1409	P1410	S1411	L1412	F1413	L1414	M1415	L1416	L1417	L1418	L1419	L1420	L1421	L1422	L1423		
I1294	E1295	G1296	L1297	T1298	E1299	V1300	S1301	L1302	V1303	L1304	K1305	Q1306	L1307	R1308	L1309	I1310	D1311	D1312	D1313	D1314	V1315	S1316	Y1317	K1318	H1319	K1320	G1321	A1322	L1323	H1324	N1325	H1326	L1327	M1328	T1329	D1330	K1331	N1332	F1333	L1334	G1335	R1336	V1337	L1338	L1339	L1340	L1341	L1342	M1343	D1344	D1345	L1346	I1347	V1348	S1349	T1350	G1351	F1352	G1353	L1354	L1355	L1356	A1357	T1358		
V1164	D1165	T1166	A1167	L1168	A1169	D1170	L1171	L1172	L1173	L1174	L1175	T1176	L1177	L1178	L1179	P1180	A1181	Q1182	Q1183	T1184	F1185	F1186	L1187	A1188	I1189	S1190	S1191	A1192	Y1193	A1194	L1195	L1196	L1197	L1198	D1199	K1200	H1201	H1202	P1203	Q1204	S1205	L1206	L1207	L1208	A1209	L1210	L1211	L1212	L1213	L1214	A1215	A1216	L1217	L1218	L1219	G1220	N1221	P1222	P1223	L1224	L1225	L1226	F1227	K1228	D1229	A1230
H1231	L1232	Q1233	H1234	L1235	D1236	S1237	V1238	V1239	N1240	N1241	G1242	T1243	T1244	A1245	R1246	M1247	V1248	E1249	T1250	T1251	A1252	Y1253	A1254	L1255	L1256	L1257	S1258	L1259	N1260	L1261	K1262	L1263	L1264	Y1265	Y1266	V1267	N1268	P1269	V1270	L1271	K1272	L1273	L1274	S1275	E1276	E1277	Q1278	R1279	Y1280	G1281	F1282	Y1283	Y1284	Y1285	L1286	L1287	Q1288	D1289	A1290							
I1294	E1295	G1296	L1297	T1298	E1299	V1300	S1301	L1302	V1303	L1304	K1305	Q1306	L1307	R1308	L1309	I1310	D1311	D1312	D1313	D1314	V1315	S1316	Y1317	K1318	H1319	K1320	G1321	A1322	L1323	H1324	N1325	H1326	L1327	M1328	T1329	D1330	K1331	N1332	F1333	L1334	G1335	R1336	V1337	L1338	L1339	L1340	L1341	L1342	M1343	D1344	D1345	L1346	I1347	V1348	S1349	T1350	G1351	F1352	G1353	L1354	L1355	L1356	A1357	T1358		
V1359	H1360	V1361	T1362	F1363	V1364	V1365	H1366	K1367	L1368	A1369	S1370	T1371	E1372	E1373	S1374	L1375	L1376	L1377	K1378	I1379	D1380	D1381	T1382	L1383	Q1384	T1385	I1386	I1387	A1388	L1389	L1390	L1391	L1392	L1393	L1394	L1395	L1396	L1397	L1398	L1399	L1400	L1401	L1402	V1403	A1404	C1405	A1406	S1407	Y1408	K1409	P1410	S1411	L1412	F1413	L1414	M1415	L1416	L1417	L1418	L1419	L1420	L1421	L1422	L1423		
I1426	S1427	L1428	P1429	F1430	E1431	G1432	I1433	E1434	A1435	A1436	L1437	K1438	V1439	K1440	V1441	A1442	G1443	V1444	V1445	V1446	Q1447	Q1448	L1449	F1450	T1451	D1452	I1453	Q1454	L1455	K1456	D1457	G1458	H1459	V1460	L1461	L1462	Q1463	L1464	N1465	P1466	S1467	I1468	A1469	A1470	D1471	F1472	C1473	E1474	V1475	R1476	I1477	F1478	F1479	F1480	E1481	L1482	V1483	C1484	V1485	F1486	A1487	E1488				
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V1359	H1360	V1361	T1362	F1363	V1364	V1365	H1366	K1367	L1368	A1369	S1370	T1371	E1372	E1373	S1374	L1375	L1376	L1377	K1378	I1379	D1380	D1381	T1382	L1383	Q1384	T1385	I1386	I1387	A1388	L1389	L1390	L1391	L1392	L1393	L1394	L1395	L1396	L1397	L1398	L1399	L1400	L1401	L1402	V1403	A1404	C1405	A1406	S1407	Y1408	K1409	P1410	S1411	L1412	F1413	L1414	M1415	L1416	L1417	L1418	L1419	L1420	L1421	L1422	L1423		
I1294	E1295	G1296	L1297	T1298	E1299	V1300	S1301	L1302	V1303	L1304	K1305	Q1306	L1307	R1308	L1309	I1310	D1311	D1312	D1313	D1314	V1315	S1316	Y1317	K1318	H1319	K1320	G1321	A1322	L1323	H1324	N1325	H1326	L1327	M1328	T1329	D1330	K1331	N1332	F1333	L1334	G1335	R1336	V1337	L1338	L1339	L1340	L1341	L1342	M1343	D1344	D1345	L1346	I1347	V1348	S1349	T1350	G1351	F1352	G1353	L1354	L1355	L1356	A1357	T1358		
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H1231	L1232	Q1233	H1234	L1235	D1236	S1237	V1238	V1239	N1240	N1241	G1242	T1243	T1244	A1245	R1246	M1247	V1248	E1249	T1250	T1251	A1252	Y1253	A1254	L1255	L1256	L1257	S1258	L1259	N1260	L1261	K1262	L1263	L1264	Y1265	Y1266	V1267	N1268	P1269	V1270	L1271	K1272	L1273	L1274	S1275	E1276	E1277	Q1278	R1279	Y1280	G1281	F1282	Y1283	Y1284	Y1285	L1286	L1287	Q1288	D1289	A1290							
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V1359	H1360	V1361	T1362	F1363	V1364	V1365	H1366	K1367	L1368	A1369	S1370	T1371	E1372	E1373	S1374	L1375	L1376	L1377	K1378	I1379	D1380	D1381	T1382	L1383	Q1384	T1385	I1386	I1387	A1388	L1389	L1390	L1391	L1392	L1393	L1394	L1395	L1396	L1397	L1398	L1399	L1400	L1401	L1402	V1403	A1404	C1405	A1406	S1407	Y1408	K1409	P1410	S1411	L1412	F1413	L1414	M1415	L1416	L1417	L1418	L1419	L1420	L1421	L1422	L1423		
I1426	S1427	L1428	P1429	F1430	E1431	G1432	I1433	E1434	A1435	A1436	L1437	K1438	V1439	K1440	V1441	A1442	G1443	V1444	V1445	V1446	Q1447	Q1448	L1449	F1450	T1451	D1452	I1453	Q1454	L1455	K1456	D1457	G1458	H1459	V1460	L1461	L1462	Q1463	L1464	N1465	P1466	S1467	I1468	A1469	A1470	D1471	F1472	C1473	E1474	V1475	R1476	I1477	F1478	F1479	F1480	E1481	L1482	V1483	C1484	V1485	F1486	A1487	E1488				
S1489	P1490	A1491	K1492	F1493	E1494	V1495	Y1496	E1497	V1498	H1499	R1500	P1501	D1502	L1503	Q1504	C1505	T1506	N1507	S1510	T1511	S1512	N1513	I1514	L1515	L1516	I1517	G1518	G1519	L1520	S1521	V1522	V1523	C1524	C1525	K1526	C1527	V1528	E1529	C1530	C1531	Q1532	Q1533	Q1534	M1535	Q1536	E1537	E1538	L1539	E1540	L1541	L1542	T1543	S1544	C1545	A1546	E1547	T1548	N1549	K1550	E1551						
V1359	H1360	V1361	T1362	F1363	V1364	V1365	H1366	K1367	L1368	A1369	S1370	T1371	E1372	E1373	S1374	L1375	L1376	L1377	K1378	I1379	D1380	D1381	T1382	L1383	Q1384	T1385	I1386	I1387	A1388	L1389	L1390	L1391	L1392	L1393	L1394	L1395	L1396	L1397	L1398	L1399	L1400	L1401	L1402	V1403	A1404	C1405	A1406	S1407	Y1408	K1409	P1410	S1411	L1412	F1413	L1414	M1415	L1416	L1417	L1418	L1419	L1420	L1421	L1422	L1423		
I1294	E1295	G1296	L1297	T1298	E1299	V1300	S1301	L1302	V1303	L1304	K1305	Q1306	L1307	R1308	L1309	I1310	D1311	D1312	D1313	D1314	V1315	S1316	Y1317	K1318	H1319	K1320	G1321	A1322	L1323	H1324	N1325	H1326	L1327	M1328	T1329	D1330	K1331	N1332	F1333	L1334	G1335	R1336	V1337	L1338	L1339	L1340	L1341	L1342	M1343	D1344	D1345	L1346	I1347	V1348	S1349	T1350	G1351	F1352	G1353	L1354	L1355	L1356	A1357	T1358		
V1164	D1165	T1166																																																																





# • Molecule 1: Complement C5





- Molecule 2: Cobra venom factor









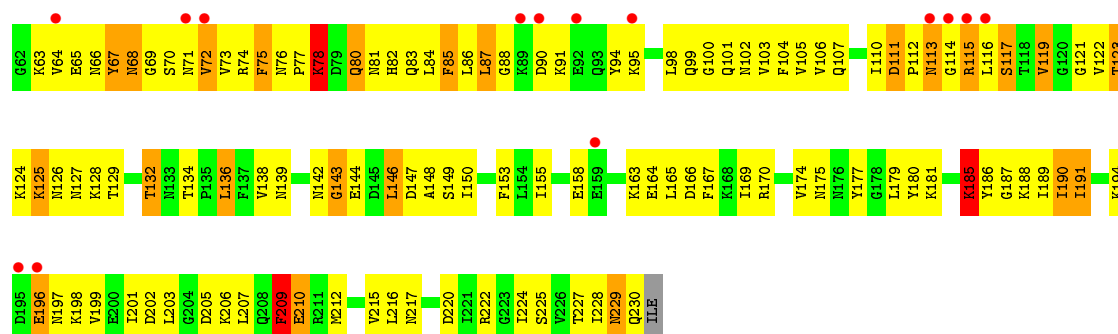












- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 100%

MAG1  
MAG2

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

Chain F: 50% 50%

MAG1  
MAG2

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

Chain G: 100%

MAG1  
MAG2

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

Chain H: 50% 50%

MAG1  
MAG2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	163.65Å 181.96Å 392.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.21 – 4.30 49.21 – 4.30	Depositor EDS
% Data completeness (in resolution range)	96.9 (49.21-4.30) 96.9 (49.21-4.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.83 (at 4.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.208 , 0.261 0.193 , 0.244	Depositor DCC
$R_{free}$ test set	1818 reflections (2.33%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	116.2	Xtriage
Anisotropy	0.456	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 160.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	48236	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	167.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% 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: 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	0.60	1/13151 (0.0%)	0.80	3/17841 (0.0%)
1	C	0.60	0/13151	0.80	5/17841 (0.0%)
2	B	0.53	1/9833 (0.0%)	0.73	2/13345 (0.0%)
2	D	0.54	0/9833	0.74	3/13345 (0.0%)
3	X	0.47	1/1560 (0.1%)	0.67	1/2096 (0.0%)
3	Y	0.49	0/1560	0.69	1/2096 (0.0%)
All	All	0.57	3/49088 (0.0%)	0.77	15/66564 (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	2
1	C	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	210	GLU	C-N	5.35	1.46	1.34
2	B	347	PHE	CB-CG	-5.29	1.42	1.51
1	A	42	GLN	CB-CG	5.16	1.66	1.52

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	347	PHE	CB-CA-C	-7.26	95.88	110.40
2	D	347	PHE	CB-CA-C	-6.90	96.60	110.40

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	640	LEU	CA-CB-CG	6.49	130.23	115.30
1	C	640	LEU	CA-CB-CG	6.30	129.80	115.30
1	A	871	PRO	CA-N-CD	-6.16	102.87	111.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1504	GLN	Peptide
1	A	98	PRO	Peptide
1	C	1504	GLN	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	12874	0	12814	1855	0
1	C	12874	0	12814	1901	0
2	B	9635	0	9630	1082	0
2	D	9635	0	9630	1079	0
3	X	1539	0	1530	166	0
3	Y	1539	0	1530	194	0
4	E	28	0	25	3	0
4	F	28	0	25	3	0
4	G	28	0	25	4	0
4	H	28	0	25	3	0
5	A	14	0	13	1	0
5	C	14	0	13	2	0
All	All	48236	0	48074	6152	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 64.

The worst 5 of 6152 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:1525:CYS:O	1:A:1528:VAL:HG22	1.34	1.25
3:X:207:LEU:O	3:X:207:LEU:HD12	1.32	1.24
3:Y:207:LEU:HD12	3:Y:207:LEU:O	1.32	1.23
1:C:386:VAL:H	1:C:411:THR:HG22	1.03	1.17
1:A:500:ASN:HB2	1:A:543:TYR:CE1	1.79	1.17

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	A	1616/1676 (96%)	1165 (72%)	300 (19%)	151 (9%)	0	12
1	C	1616/1676 (96%)	1179 (73%)	290 (18%)	147 (9%)	1	12
2	B	1203/1642 (73%)	981 (82%)	176 (15%)	46 (4%)	3	27
2	D	1203/1642 (73%)	982 (82%)	177 (15%)	44 (4%)	3	28
3	X	189/231 (82%)	148 (78%)	31 (16%)	10 (5%)	2	22
3	Y	189/231 (82%)	150 (79%)	28 (15%)	11 (6%)	1	20
All	All	6016/7098 (85%)	4605 (76%)	1002 (17%)	409 (7%)	1	17

5 of 409 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	60	PRO
1	A	89	PRO
1	A	96	GLN
1	A	150	ASP



### 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	1445/1484 (97%)	1090 (75%)	355 (25%)	0	4
1	C	1445/1484 (97%)	1098 (76%)	347 (24%)	0	5
2	B	1084/1435 (76%)	849 (78%)	235 (22%)	1	6
2	D	1084/1435 (76%)	855 (79%)	229 (21%)	1	7
3	X	175/205 (85%)	143 (82%)	32 (18%)	1	11
3	Y	175/205 (85%)	142 (81%)	33 (19%)	1	10
All	All	5408/6248 (87%)	4177 (77%)	1231 (23%)	1	6

5 of 1231 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	1480	LEU
1	C	435	VAL
2	D	1480	LEU
2	B	1539	ILE
1	C	161	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 162 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	77	ASN
1	C	658	ASN
3	X	113	ASN
1	C	97	ASN
1	C	294	ASN

### 5.3.3 RNA [i](#)

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 ⓘ

8 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
4	NAG	E	1	2,4	14,14,15	0.96	1 (7%)	17,19,21	2.06	6 (35%)
4	NAG	E	2	4	14,14,15	1.04	1 (7%)	17,19,21	2.50	6 (35%)
4	NAG	F	1	2,4	14,14,15	2.05	7 (50%)	17,19,21	3.28	8 (47%)
4	NAG	F	2	4	14,14,15	1.64	1 (7%)	17,19,21	2.34	6 (35%)
4	NAG	G	1	2,4	14,14,15	0.88	1 (7%)	17,19,21	1.97	6 (35%)
4	NAG	G	2	4	14,14,15	1.07	1 (7%)	17,19,21	1.74	4 (23%)
4	NAG	H	1	2,4	14,14,15	1.99	6 (42%)	17,19,21	3.46	9 (52%)
4	NAG	H	2	4	14,14,15	1.52	1 (7%)	17,19,21	2.32	6 (35%)

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
4	NAG	E	1	2,4	-	4/6/23/26	0/1/1/1
4	NAG	E	2	4	-	5/6/23/26	0/1/1/1
4	NAG	F	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	6/6/23/26	0/1/1/1
4	NAG	G	1	2,4	-	3/6/23/26	0/1/1/1
4	NAG	G	2	4	-	5/6/23/26	0/1/1/1
4	NAG	H	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	6/6/23/26	0/1/1/1



The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	2	NAG	C1-C2	5.13	1.60	1.52
4	H	2	NAG	C1-C2	4.97	1.59	1.52
4	F	1	NAG	C1-C2	3.85	1.58	1.52
4	H	1	NAG	C1-C2	3.38	1.57	1.52
4	F	1	NAG	O5-C1	3.13	1.48	1.43

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	NAG	C1-O5-C5	10.09	125.86	112.19
4	F	1	NAG	C1-O5-C5	9.29	124.78	112.19
4	E	2	NAG	C4-C3-C2	6.58	120.66	111.02
4	H	2	NAG	C1-C2-N2	5.47	119.84	110.49
4	F	2	NAG	C1-C2-N2	5.45	119.79	110.49

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	1	NAG	C8-C7-N2-C2
4	E	1	NAG	O7-C7-N2-C2
4	H	2	NAG	C8-C7-N2-C2
4	H	2	NAG	O7-C7-N2-C2
4	G	2	NAG	C1-C2-N2-C7

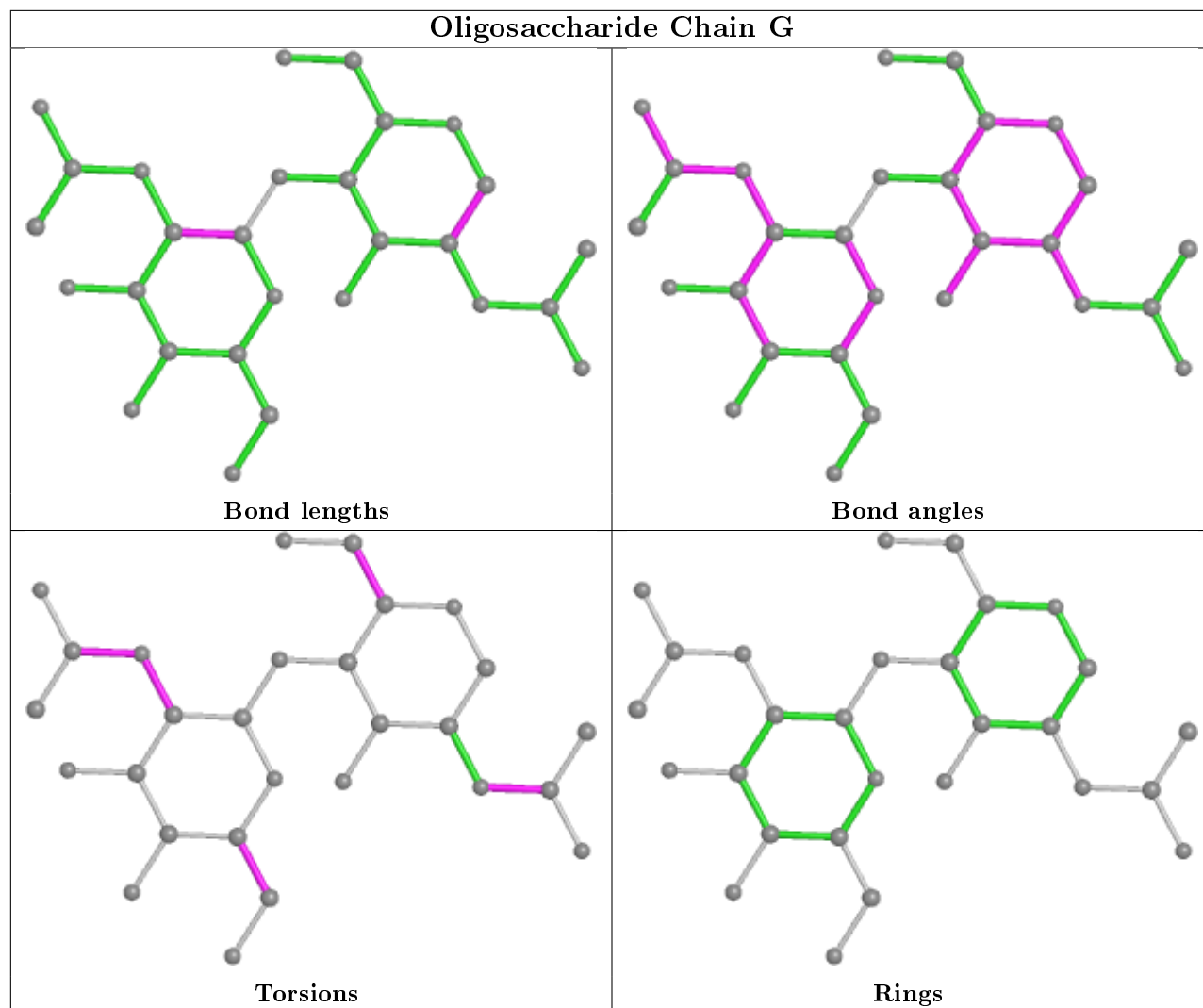
There are no ring outliers.

6 monomers are involved in 13 short contacts:

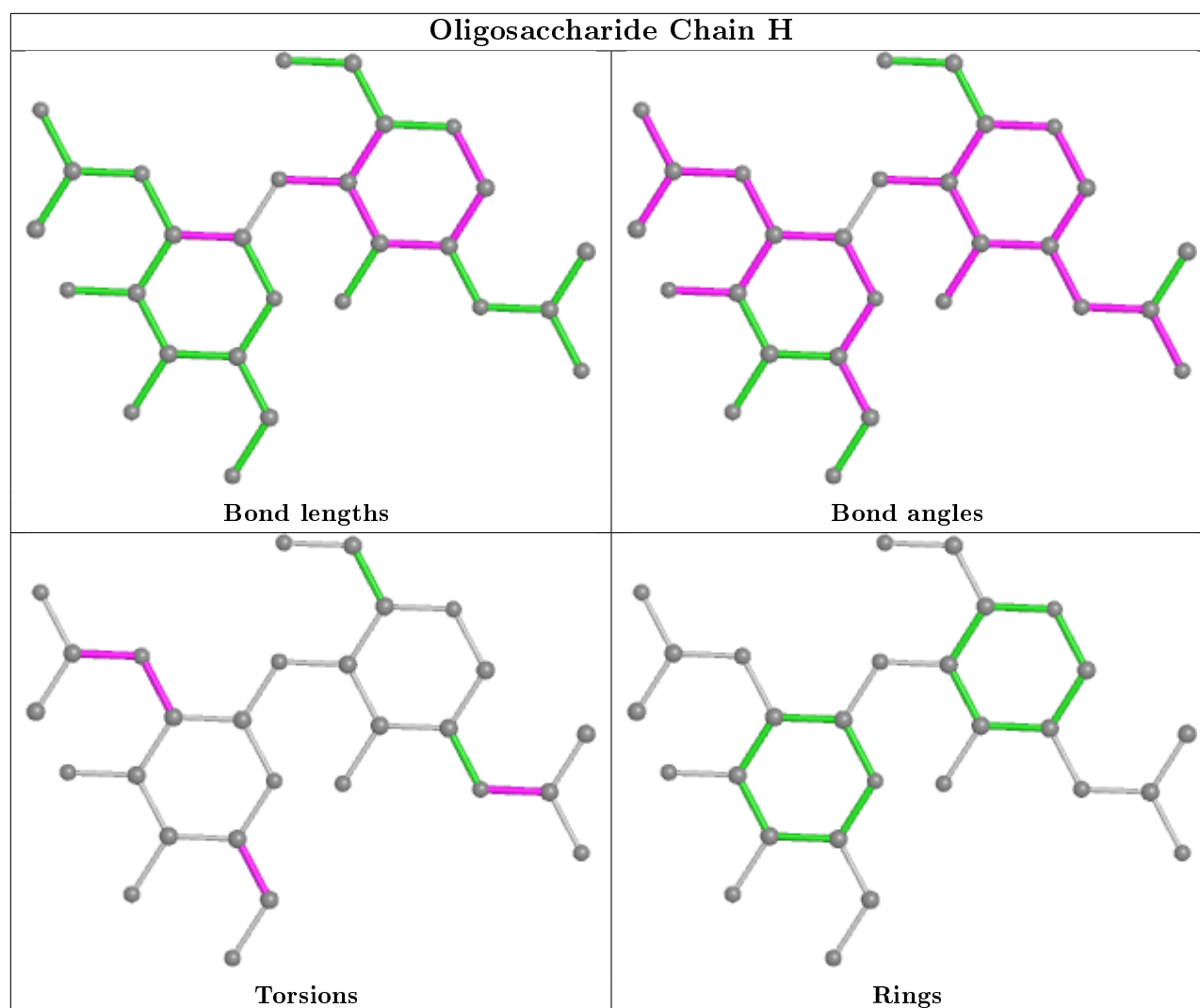
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1	NAG	3	0
4	F	1	NAG	3	0
4	G	2	NAG	4	0
4	H	1	NAG	3	0
4	E	2	NAG	3	0
4	G	1	NAG	4	0

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 ⓘ

2 ligands 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	$\# Z  > 2$
5	NAG	C	2003	1	14,14,15	2.04	4 (28%)	17,19,21	2.60	10 (58%)
5	NAG	A	2003	1	14,14,15	1.89	5 (35%)	17,19,21	3.34	13 (76%)



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	C	2003	1	-	4/6/23/26	0/1/1/1
5	NAG	A	2003	1	-	2/6/23/26	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	2003	NAG	C1-C2	4.43	1.59	1.52
5	A	2003	NAG	C3-C2	4.37	1.61	1.52
5	C	2003	NAG	C3-C2	3.97	1.60	1.52
5	C	2003	NAG	C4-C5	3.10	1.59	1.53
5	A	2003	NAG	O4-C4	2.43	1.48	1.43

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2003	NAG	C2-N2-C7	5.28	130.43	122.90
5	A	2003	NAG	O7-C7-C8	-5.11	112.57	122.06
5	A	2003	NAG	C4-C3-C2	4.83	118.10	111.02
5	C	2003	NAG	O3-C3-C2	4.38	118.53	109.47
5	A	2003	NAG	O4-C4-C3	4.22	120.10	110.35

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	2003	NAG	O5-C5-C6-O6
5	A	2003	NAG	O5-C5-C6-O6
5	C	2003	NAG	C4-C5-C6-O6
5	A	2003	NAG	C4-C5-C6-O6
5	C	2003	NAG	C8-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	2003	NAG	2	0
5	A	2003	NAG	1	0



## 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	1626/1676 (97%)	-0.04	19 (1%) 79 70	72, 150, 260, 469	0
1	C	1626/1676 (97%)	0.03	42 (2%) 56 46	60, 153, 277, 515	0
2	B	1215/1642 (73%)	0.02	21 (1%) 70 61	73, 160, 235, 335	0
2	D	1215/1642 (73%)	-0.03	16 (1%) 77 68	85, 155, 241, 362	0
3	X	191/231 (82%)	0.68	26 (13%) 3 3	99, 230, 333, 437	0
3	Y	191/231 (82%)	0.41	15 (7%) 12 11	95, 195, 300, 385	0
All	All	6064/7098 (85%)	0.03	139 (2%) 60 51	60, 157, 264, 515	0

The worst 5 of 139 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	X	112	PRO	11.8
3	Y	114	GLY	6.8
3	X	113	ASN	5.6
1	C	1651	ASP	5.6
3	X	114	GLY	5.6

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

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

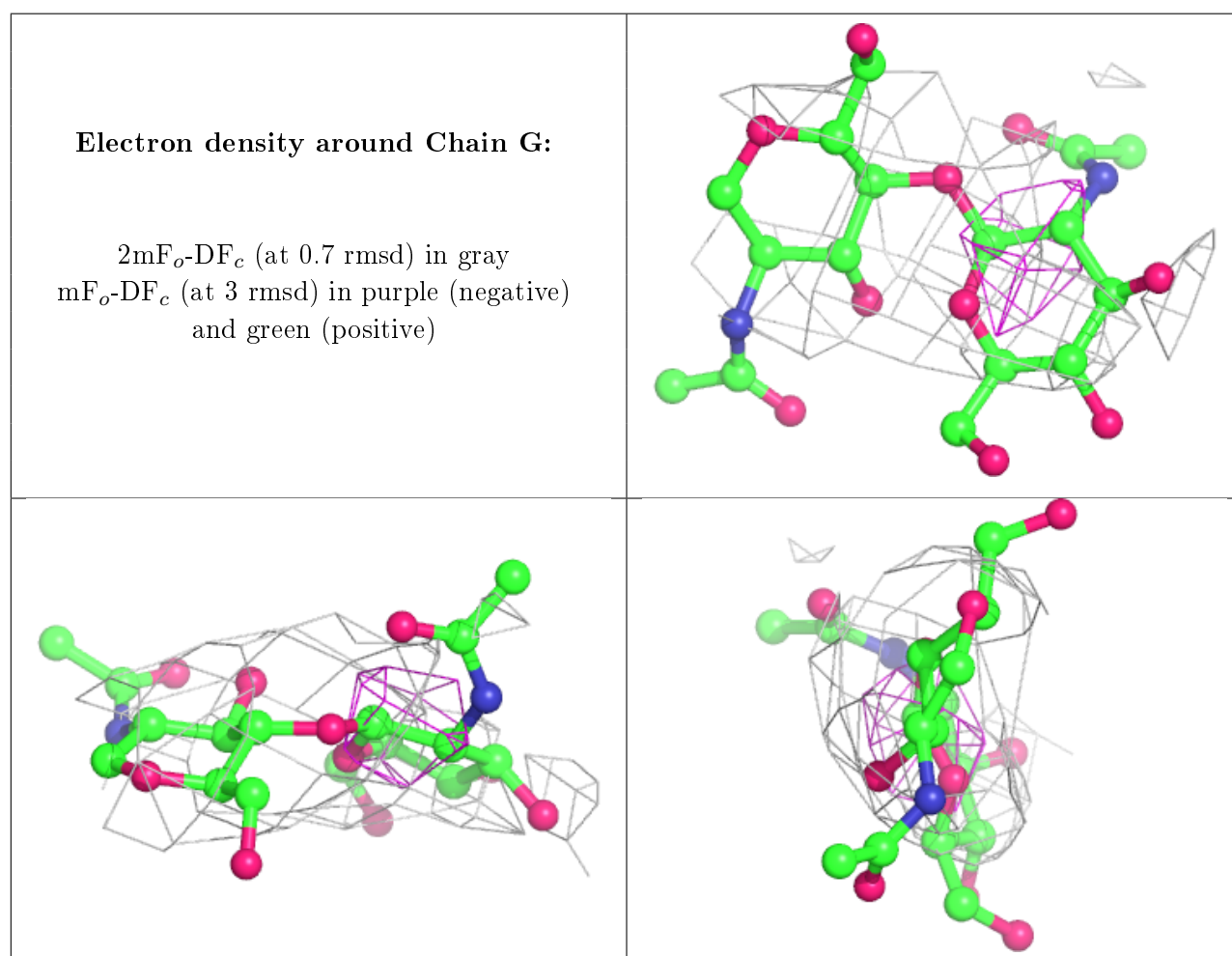
### 6.3 Carbohydrates [i](#)

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, 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.

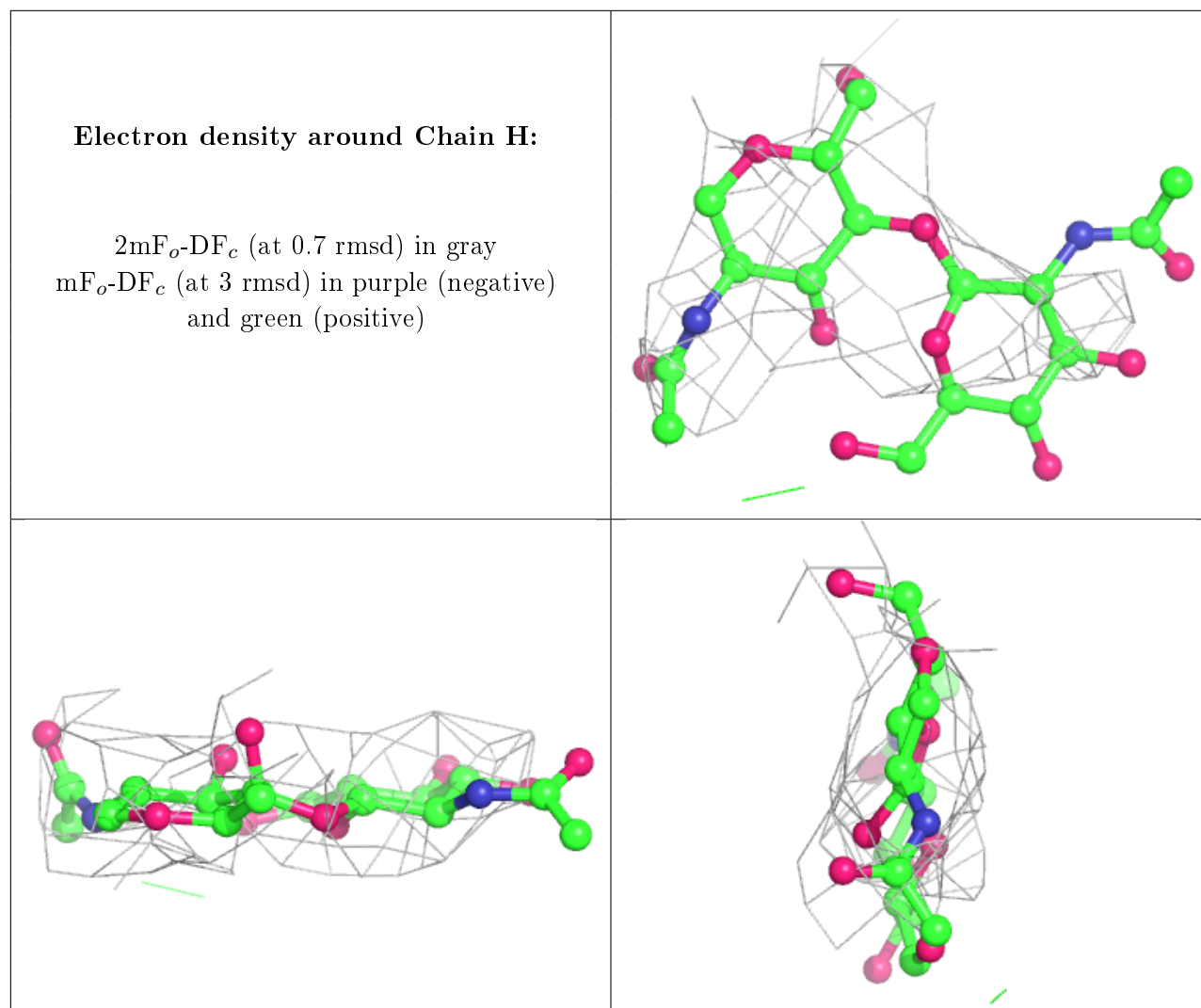


Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	F	1	14/15	0.24	0.78	225,233,240,245	0
4	NAG	H	1	14/15	0.54	0.54	246,253,258,265	0
4	NAG	F	2	14/15	0.55	0.79	297,301,307,310	0
4	NAG	G	2	14/15	0.66	0.60	228,239,251,252	0
4	NAG	H	2	14/15	0.72	0.85	271,274,277,278	0
4	NAG	E	2	14/15	0.72	0.69	228,239,253,257	0
4	NAG	E	1	14/15	0.73	0.55	278,305,319,322	0
4	NAG	G	1	14/15	0.89	0.41	228,253,282,288	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
5	NAG	C	2003	14/15	0.73	0.39	177,180,183,183	0
5	NAG	A	2003	14/15	0.78	0.29	166,169,171,172	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.