



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2026 – 08:31 AM EDT

PDB ID : 3PRX / pdb\_00003prx  
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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

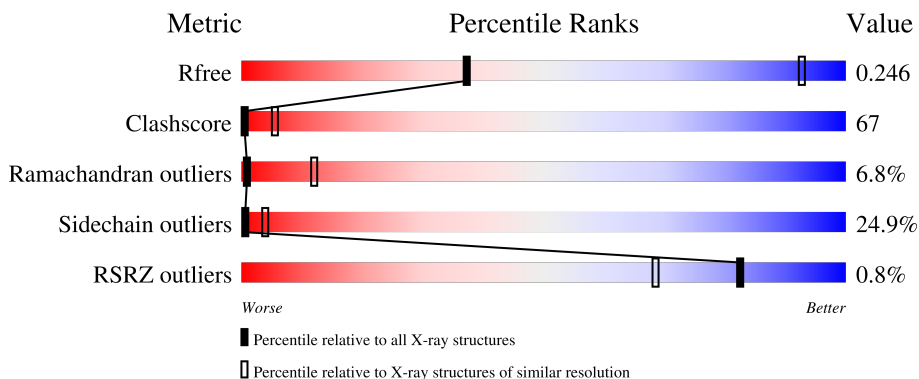
# 1 Overall quality at a glance

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))
$R_{free}$	180053	1052 (4.70-3.90)
Clashscore	190562	1097 (4.70-3.90)
Ramachandran outliers	187476	1001 (4.70-3.90)
Sidechain outliers	187428	1007 (4.72-3.88)
RSRZ outliers	180081	1049 (4.70-3.90)

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	C	1676	
2	B	1642	
2	D	1642	
3	X	231	

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Mol	Chain	Length	Quality of chain
3	Y	231	
4	E	2	
4	F	2	
4	G	2	
4	H	2	

## 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
			Total	C	N	O	S			
1	A	1626	12874	8242	2113	2467	52	0	0	0
1	C	1626	12874	8242	2113	2467	52	0	0	0

- Molecule 2 is a protein called Cobra venom factor.

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

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

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

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



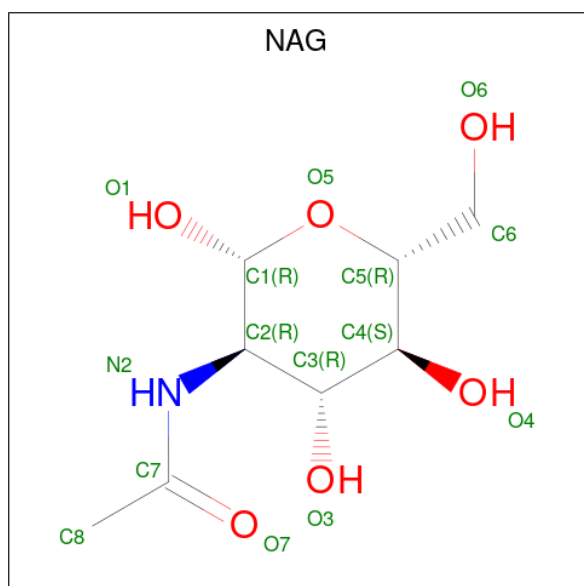
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	E	2	28	16	2	10	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
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 (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

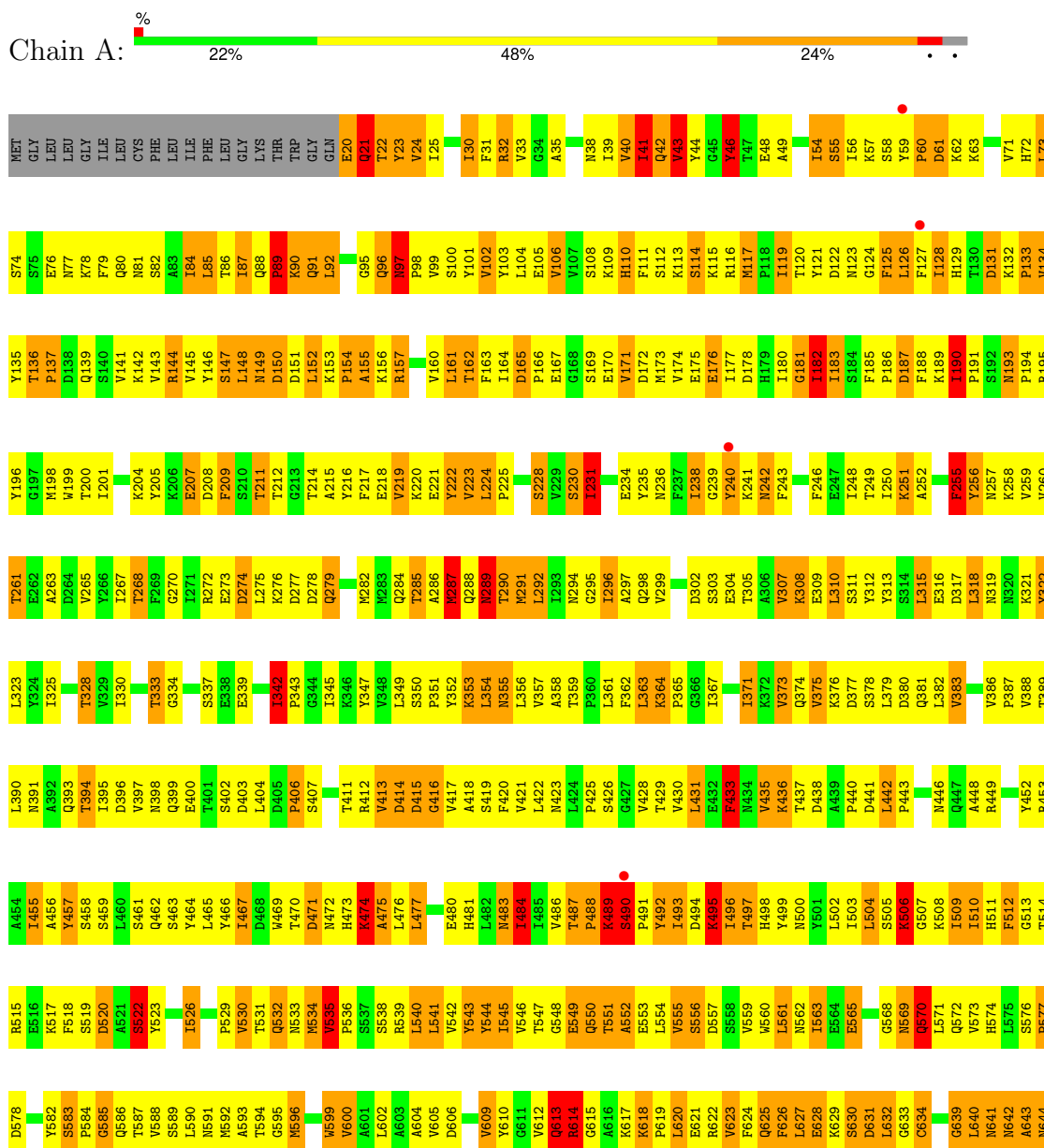


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		

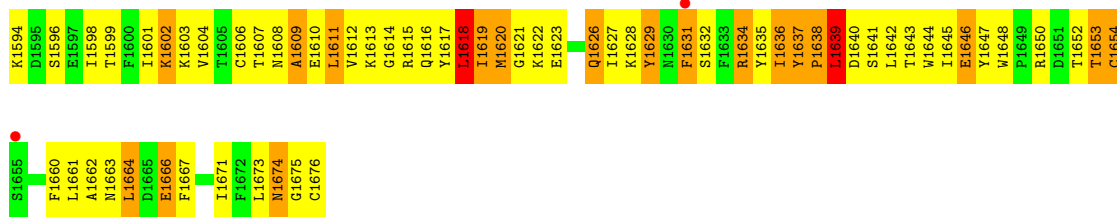
### 3 Residue-property plots

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.

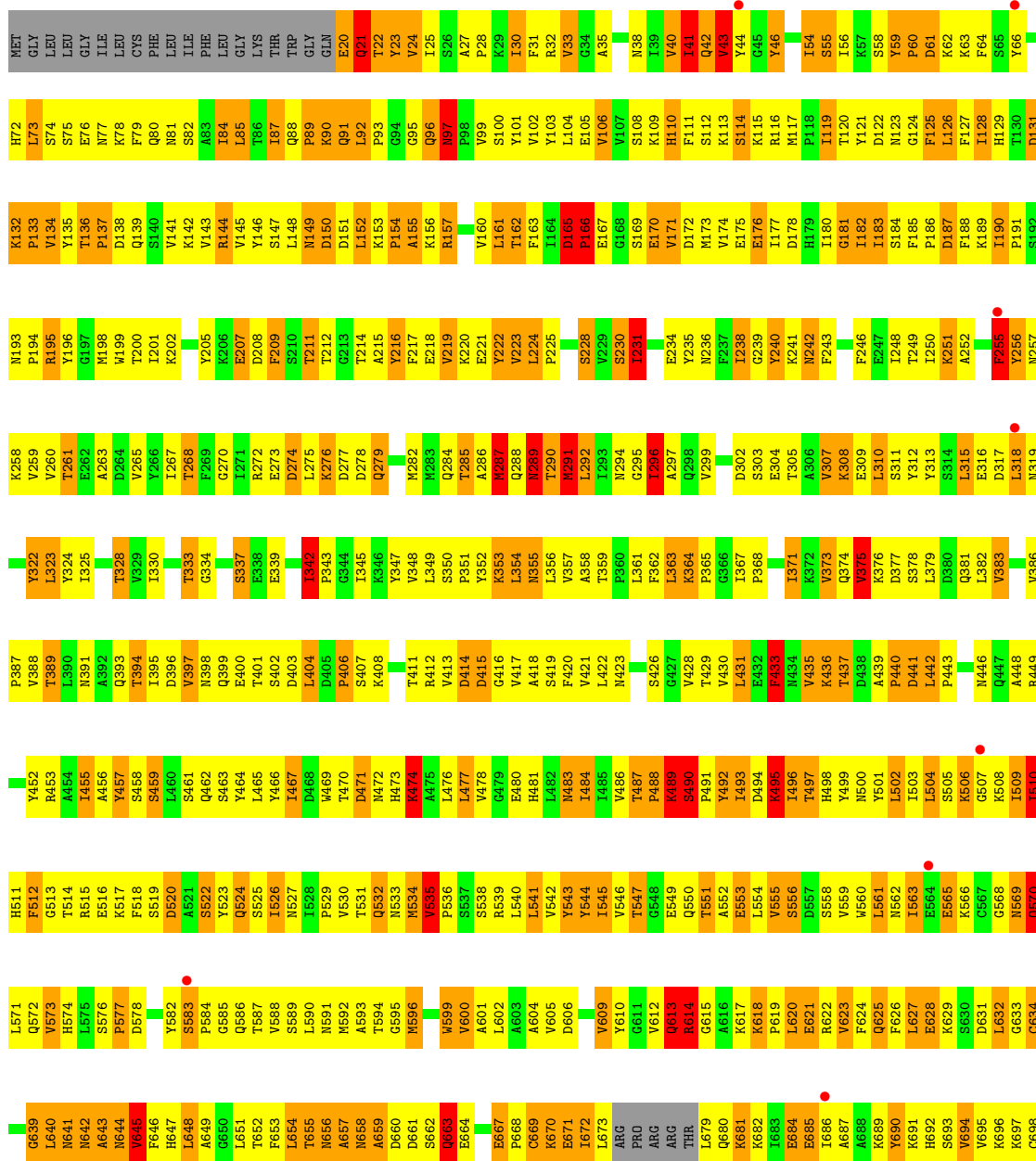
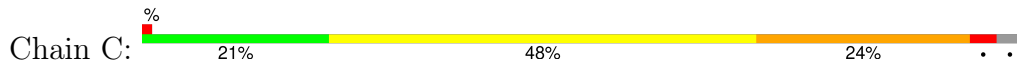
#### ● Molecule 1: Complement C5



Q1534	F1472	S1407	D1345	Y1280	G1220	F1156	V1093	G1028	D966	E904	L839	L774	N706	K645
M1535	L1473	Y1408	L1346	F1283	M1221	D1157	E1094	N1029	L967	L905	Q840	L774	N707	F646
K1409	C1474	K1409	I1347	G1283	P1222	I1158	Q1095	M1029	L968	G906	Q840	L777	D708	H647
E1537	V1475	P1410	V1348	F1284	P1223	C1159	M1096	H1031	P969	L907	C843	H778	E709	L648
E1538	R1476	S1411	S1349	I1285	I1224	P1160	Q1097	W1030	P968	H908	T844	V779	T710	A649
L1539	F1477	L1539	S1350	S1286	I1225	L1161	M1098	I1033	T971	H909	V845	V780	C711	G650
D1540	A1478	E1414	G1351	T1287	R1226	V1162	S1099	F1034	E972	L910	V846	P781	E742	L651
L1541	F1479	S1415	F1352	Q1288	F1227	K1163	L1100	H1035	I973	H911	H847	R782	Q713	T652
T1542	S1416	D1289	D1289	D1289	M1228	I1164	C1101	S1036	K974	F912	H848	R783	Q713	F653
E1481	G1355	S1420	A1293	A1293	D1230	D1165	M1102	P1037	R975	S913	R849	K784	T718	L654
L1482	I1294	H1421	A1357	I1294	D1230	L1166	S1103	P1038	R976	L914	T850	K785	S719	T655
E1483	A1422	A1422	E1295	E1295	M1231	A1167	L1104	P1038	L977	E915	S851	L786	L720	N656
V1485	V1359	V1423	G1296	G1296	Q1233	L1168	L1106	E1041	V979	H911	H853	Q787	G721	A657
R1548	H1360	H1360	H1360	H1297	Q1233	A1171	M1106	K1042	V979	H911	H853	F788	F722	N658
K1549	H1361	D1425	L1361	L1298	K1235	D1172	L1107	Q1043	K980	F918	Q854	A799	R723	A659
Q1550	T1362	I1426	T1362	E1299	K1235	D1172	V1108	Q1044	G981	L919	F855	L790	R723	D660
T1551	T1363	S1427	T1363	E1299	D1236	P1181	E1109	K1044	L982	K920	C856	C724	H725	D661
A1490	V1364	L1428	V1364	S1301	S1237	L1175	M1110	K1048	L983	V928	V857	D792	K726	S662
A1491	V1365	P1429	V1365	L1302	S1238	M1178	Y1111	L1048	V984	V928	K858	S793	K726	O663
K1554	H1366	T1430	H1366	L1303	V1239	M1178	Q1112	L1049	G985	V924	H859	L794	F728	E664
P1555	K1367	G1431	K1367	V1304	P1240	T1179	E1120	M1050	S986	K925	V862	T729	T729	E667
E1556	T1368	I1432	T1368	K1305	M1241	L1180	M1121	M1051	K994	E932	V862	T796	E730	F668
I1557	S1369	S1433	S1369	Q1306	T1242	P1181	Q1122	G1052	E985	E933	E863	C731	C731	P669
A1558	T1370	A1434	T1370	L1307	G1243	A1182	Q1123	M1053	S989	V928	C864	Q800	C732	K670
Y1559	S1371	M1435	S1371	R1308	T1244	Q1183	F1118	L1054	I987	V929	T865	M806	V733	K671
A1560	E1372	E1436	E1372	L1309	A1245	S1184	K1119	S1055	M988	V930	C866	G801	V734	E671
H1498	E1373	E1436	E1373	L1309	R1246	T1185	E1120	M1056	S989	P931	T867	R802	V734	L672
H1499	E1374	E1436	E1374	L1309	M1247	F1186	M1121	M1056	K994	E932	V868	G803	Q737	L673
R1500	C1375	K1440	C1375	I1313	V1248	T1187	Q1123	M1061	E985	E933	E869	R804	L738	ARG
P1501	G1376	K1440	G1376	V1315	T1250	A1189	Y1124	N1061	S989	V934	S870	S805	R739	PRO
D1502	S1376	S1443	S1376	S1316	T1251	I1190	Q1125	Y1064	M988	V936	V872	T807	L742	ARG
K1503	L1379	E1444	L1379	V1317	T1251	S1191	P1126	S1065	S989	E937	V872	G808	S743	THR
Q1504	K1380	E1444	K1380	K1318	V1253	A1192	I1127	Y1066	I989	E937	V872	G808	S743	THR
C1505	I1381	G1445	I1381	H1319	I1253	A1192	K1128	S1067	L1000	S938	D874	L809	L751	L679
L1506	D1382	D1447	D1382	K1320	A1254	Y1193	L1128	S1067	H1001	C810	H875	C810	L752	Q690
M1507	G1321	Q1448	G1321	G1321	L1255	A1194	L1129	V1068	L1002	ASP	M876	V811	H753	K681
S1510	A1322	L1449	A1322	A1322	T1257	L1195	Q1130	V1069	L1003	MET	G877	A812	K755	K682
T1511	D1384	F1450	D1384	H1323	A1257	S1196	Q1131	K1070	P1004	V942	V878	D813	K756	L683
S1512	L1385	F1450	L1385	H1324	S1258	L1197	T1132	G1071	S1007	P943	C883	V814	K756	E684
N1513	H1386	D1451	H1386	H1324	L1259	G1198	L1133	G1072	E685	L944	C883	V815	L751	E685
I1514	E1387	D1452	E1387	M1325	L1259	D1199	P1134	S1073	A1008	D945	V884	L751	L752	L686
L1514	ALA	Y1453	ALA	Y1326	L1261	K1200	V1135	A1074	E1009	P946	V885	K818	H752	A687
LYS	SER	Q1454	SER	K1327	L1262	T1201	E1136	S1075	A1010	R947	Q886	V819	L752	A687
ILE	HIS	I1455	HIS	M1328	D1263	H1202	L1142	T1076	E1011	C948	V887	F820	H753	A688
GLN	TYR	K1456	TYR	T1329	I1264	P1203	M1140	W1077	L1012	L949	V888	K821	K755	K689
LYS	ARG	D1457	ARG	D1330	M1265	Q1204	S1141	W1077	M1013	Y950	E889	D822	K755	V690
VAL	GLY	G1458	GLY	K1331	Y1266	S1210	L1142	L1078	S1014	G951	V891	V823	K756	K691
GLY	TYR	H1459	TYR	N1332	V1267	I1208	Y1143	T1079	S1014	C890	V892	D822	L757	H692
CYS	GLY	W1460	GLY	F1333	M1268	I1208	L1144	F1081	V1015	S891	S892	L825	L758	S693
GLU	ASN	I1461	ASN	L1334	P1269	V1209	T1145	F1082	V1016	S892	S893	E826	P759	V694
ALA	S1397	L1462	S1397	G1335	V1270	S1210	A1146	A1082	P1017	S954	H894	M827	V760	V695
ALA	D1398	Q1463	D1398	L1336	I1271	A1210	F1147	L1083	V1018	H895	V895	M828	V760	K696
C1525	Y1399	L1464	Y1399	K1337	K1272	L1212	T1148	Y1085	Y1020	V896	V896	R829	L765	K697
K1586	L1400	M1465	L1400	F1338	W1273	K1213	V1149	L1086	V1021	T897	V897	P830	L765	C698
T1587	R1401	S1466	R1401	E1339	L1274	I1150	L1150	Q1087	F1022	H898	V898	S767	L765	C699
G1588	I1402	I1467	I1402	I1399	S1275	A1215	Q1087	Q1088	H1023	V961	T899	V768	L765	Y768
E1529	V1403	P1468	V1403	L1341	E1276	A1216	I1152	V1089	Y1024	R862	V900	V834	F770	D701
S1469	A1404	S1469	A1404	L1342	E1277	L1217	M1153	M1090	L1025	I901	V900	H834	F770	G702
A1470	C1405	C1405	C1405	L1343	Q1278	I1218	K1154	K1091	E1026	P902	V900	E837	S771	A703
D1471	A1406	D1471	A1406	D1344	R1279	K1219	A1155	Y1092	T1027	L965	L903	Q838	V773	V705



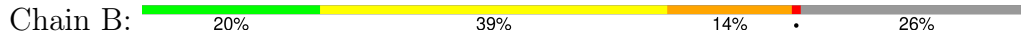
● Molecule 1: Complement C5



Q1534	L1473	S1407	D1345	G1283	M1221	D1157	E1094	M1029	V968	L903	G836	S772	C689
M1555	C1474	Y1408	L1346	G1283	P1222	I1158	Q1095	H1030	P969	E904	E837	W773	Y700
Q1536	R1475	P1409	I1347	F1284	P1223	C1159	M1096	M1031	K970	I905	Q838	L774	D701
E1537	R1476	P1410	V1348	F1284	I1224	P1160	Q1097	N1032	T971	G906	R839	W774	G702
E1538	F1477	S1349	I1349	S1286	R1225	L1161	M1098	I1033	E972	H907	Q840	W777	A703
L1539	R1478	T1350	T1350	S1286	R1226	V1162	S1099	F1034	E973	H908	G843	W778	C704
D1540	I1479	G1351	G1351	Q1288	F1227	K1163	L1100	H1035	K974	N909	G844	W779	V705
L1541	F1480	F1352	D1289	D1289	M1228	I1164	C1101	H1035	R975	I910	T844	W780	N706
T1542	E1481	L1356	T1290	T1290	D1165	D1165	S1037	S1037	R976	N911	W845	W781	V707
L1543	F1482	L1357	A1293	A1293	D1230	T1166	S1103	E1041	L977	F912	W846	W782	E709
L1544	F1483	T1358	L1294	L1294	M1231	A1167	L1104	K1048	S978	S913	W847	W783	T710
E1547	E1484	T1359	E1295	E1295	L1168	L1168	L1105	L1049	K985	L923	W848	W784	T711
R1548	G1486	H1360	G1296	G1296	A1171	Y1106	Q1043	K986	K980	E915	W849	W785	C724
K1549	F1487	V1361	L1297	L1297	H1234	L1107	L1107	E1051	G981	T916	T850	W786	I725
Q1550	F1488	V1362	L1297	L1297	H1234	V1108	V1108	G1052	L982	W917	S951	Q713	I726
T1551	L1488	T1362	L1298	L1298	D1236	L1175	K1047	M1053	L983	F918	S952	Q714	A727
C1552	S1489	T1363	E1299	E1299	S1237	M1110	L1048	L1048	W984	F918	G852	Q715	F728
K1553	P1429	V1364	Y1300	Y1300	S1238	Y1111	L1049	K985	G985	L923	Q854	W791	I729
K1554	T1430	H1366	L1302	L1302	V1239	M1178	K1050	K986	E986	V924	F855	W792	C725
P1555	G1431	H1367	L1303	L1303	P1240	T1179	E1051	K987	L987	K925	C856	W793	I725
F1556	I1432	K1367	L1303	L1303	M1241	L1180	G1052	L988	L988	T926	W857	W794	I726
E1557	T1494	S1369	K1305	K1305	G1243	P1181	M1053	S989	S989	R928	R868	W795	A727
A1558	Y1496	T1370	Q1306	Q1306	T1244	F1118	L1064	A990	A990	R928	L794	W796	F728
Y1559	E1497	S1371	L1307	L1307	A1245	S1184	S1056	V930	S983	V930	W662	W799	I729
A1560	Y1498	E1372	R1308	R1308	R1246	T1185	M1056	V930	S983	V930	W662	W799	E730
Y1561	H1499	E1373	L1309	L1309	M1247	F1186	M1057	P931	G994	P931	E863	W800	V734
K1562	R1500	V1374	I1313	I1313	Y1248	T1187	S1058	V934	E995	V934	G864	Q800	V734
S1563	F1501	C1375	D1314	D1314	E1249	L1188	M1061	K935	G996	K934	R865	Q801	V734
S1564	D1502	S1376	L1315	L1315	E1250	L1189	Y1124	K936	N987	G941	Q802	W802	Q737
K1503	K1503	F1377	V1315	V1315	T1251	I1190	Y1125	E969	N998	S940	C803	W803	Q737
Q1504	E1444	Y1378	S1316	S1316	A1252	S1191	Y1064	S937	W999	F937	S670	L738	L738
C1505	G1445	L1379	Y1317	Y1317	Y1253	S1192	S1065	L1000	L1000	S938	S805	S805	R739
T1506	V1446	K1380	K1318	K1318	A1254	A1193	S1067	T1001	T1001	Y939	W872	S806	R739
S1507	D1447	I1381	H1319	H1319	L1255	Y1194	S1067	H1002	H1002	G941	W808	W808	I742
T1511	F1450	T1383	K1320	K1320	L1256	L1195	M1068	L1003	L1003	S940	D874	W808	S743
Y1512	F1451	Q1384	G1321	G1321	T1257	S1196	W1069	P1004	P1004	V942	H875	W809	HIS
F1513	D1452	I1385	A1322	A1322	S1258	L1197	K1070	K1005	K1005	T943	Q876	C810	LYS
I1514	D1452	I1386	L1323	L1323	L1259	T1198	G1071	G1006	G1006	L944	G877	W811	ASP
I1514	Y1453	I1387	H1324	H1324	M1260	D1199	S1073	S1007	S1007	D945	W878	A812	NET
I1514	Q1454	ALA	N1325	N1325	L1261	K1200	A1074	A1008	A1008	P946	C983	D813	GLN
I1514	Y1455	ALA	K1326	K1326	K1262	T1201	S1075	E1009	E1009	R947	W684	W814	LEU
I1514	I1455	SER	K1327	K1327	I1263	H1202	T1076	A1010	A1010	G948	W685	W814	LEU
I1514	K1456	HIS	M1328	M1328	I1264	H1202	M1077	E1011	E1011	I949	W685	W814	LEU
I1514	D1457	TYR	T1329	T1329	M1265	P1203	L1078	L1012	L1012	Y950	Q886	W815	GLY
I1514	G1458	ARG	D1330	D1330	Y1266	Q1204	L1078	G951	G951	W822	W887	W815	L752
I1514	H1459	GLY	K1331	K1331	V1267	S1207	T1079	S1014	S1014	T952	W888	W819	R753
I1514	L1461	TYR	N1332	N1332	M1268	I1208	F1081	I952	I952	T952	E889	F820	R754
I1514	L1462	ASN	F1333	F1333	P1269	V1209	F1081	V1016	V1016	S954	G890	R821	R755
I1514	L1463	ASN	L1334	L1334	V1270	S1210	A1083	P1017	P1017	R955	W891	W823	L757
I1514	Q1463	S1397	G1335	G1335	I1271	A1211	L1084	W1018	W1018	S892	W892	F824	L758
I1514	M1464	D1398	R1336	R1336	K1272	I1147	V1085	F1019	F1019	E958	S893	L825	P759
I1514	M1465	I1399	F1337	F1337	K1273	T1148	V1086	I1020	I1020	F959	W894	L825	P759
I1514	S1466	K1400	P1338	P1338	V1274	K1213	L1086	F959	F959	W894	W894	E826	P760
I1514	P1467	R1401	E1339	E1339	S1275	R1214	G1087	F1022	F1022	Y961	L895	W827	I765
I1514	L1468	I1402	V1340	V1340	E1276	L1152	Q1088	Y961	Y961	Y961	W896	W827	I765
I1514	S1469	V1403	L1341	L1341	E1277	L1152	Q1088	R962	R962	H023	T897	R829	R766
I1514	D1470	A1404	L1342	L1342	Q1278	L1153	Y1089	Y1024	Y1024	H023	F898	P830	S767
I1514	L1471	C1405	N1343	N1343	I1279	K1154	M1090	P964	P964	L1025	T899	W833	Y768
I1514	F1472	A1406	D1344	D1344	Y1280	A1154	K1091	L965	L965	D966	W900	W834	F769
I1514	F1472	A1406	D1344	D1344	Y1280	F1156	Y1093	L967	L967	L967	P902	W834	F770



● Molecule 2: Cobra venom factor

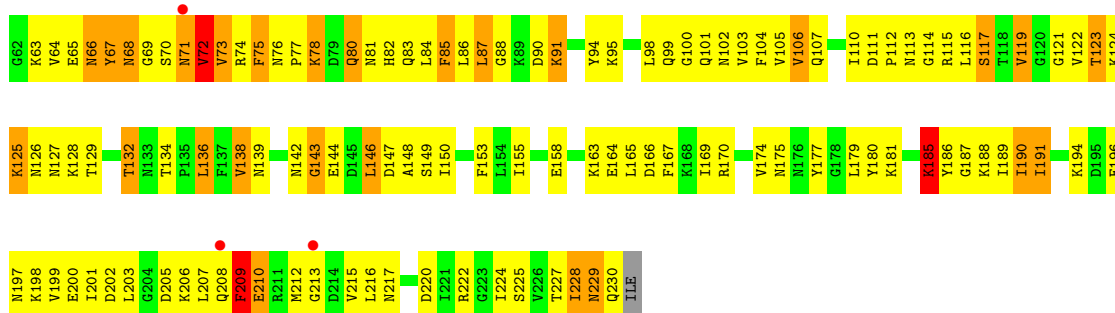


MET	F129	D190	Y253	S326	K397	V462	V526	H599	ASN	ASN	V768
GLU	I130	L191	E256	S327	L398	N463	G527	D600	ALA	GLN	V789
ARG	Q131	V192	E257	D327	L399	F464	N528	T601	SER	GLU	V790
MET	T132	L193	E258	N328	N400	N465	N529	L602	ALA	ARG	V791
ALA	D133	L194	E259	V329	N401	V466	E530	E603	ALA	SER	S793
LEU	K134	G195	G259	V330	N402	K467	I531	K604	ALA	GLU	F794
TYR	F135	T196	V260	Q333	P403	G468	V532	S605	GLU	LEU	T795
LEU	I136	M197	A261	Q334	L404	N469	A533	D606	PHE	LEU	P796
VAL	Y137	R198	F262	I336	P410	N470	D534	F607	GLN	LEU	I800
ALA	R138	I199	V263	I337	P411	N471	S535	G608	ALA	ARG	C801
ALA	P139	V200	L264	V338	T411	S472	S536	G609	GLN	ASP	V802
LEU	G140	A201	F265	I339	T412	I476	V538	A611	ASP	ASP	A803
LEU	S141	K202	G266	V339	T413	K477	K541	G612	LEU	ASP	A804
ILE	P142	Y203	V267	K340	T414	K478	D542	S613	ARG	ARG	B804
GLY	V143	E204	R268	S341	N416	F479	F543	G614	LYS	LYS	P805
PHE	L144	H205	I269	R342	H417	F479	T543	F615	CYS	CYS	R806
PRO	Y145	P206	K270	Q343	C418	Y480	C544	N616	CYS	GLY	E807
GLY	R146	S207	A272	Q344	D419	Y481	N545	N617	GLU	GLU	I808
GLY	G80	E208	K273	I345	L420	L482	G546	L618	ASP	ASP	R809
SER	M81	N209	K274	R346	P421	L483	T547	G619	VAL	VAL	V810
SER	L82	M209	K275	K347	R422	L484	L548	V620	MET	MET	D741
SER	V83	Y210	S275	T348	R423	N485	L555	V621	HIS	HIS	D742
HIS	T84	D151	I276	K349	R424	N486	I556	F622	GLU	GLU	F743
GLY	P85	D151	P277	R424	R424	K486	G487	E622	ASN	ASN	D744
GLY	A23	H152	D278	T350	Q425	K488	I557	L626	PRO	PRO	I745
L24	L88	H152	S279	P351	A426	K488	O557	A627	MET	MET	I746
Y25	I87	ASN	L280	K352	T427	L489	M558	L628	GLY	GLY	S747
T26	E88	THR	L281	I353	K428	F490	P559	L629	GLY	GLY	D748
L27	I89	SER	T281	F354	K429	N491	G560	T629	TYR	TYR	D750
L28	P90	LYS	R282	N430	N430	V492	A561	T630	THR	THR	L818
P90	A91	MET	P284	K355	M430	V492	A562	F631	CYS	CYS	Q819
E1623	P30	P20	P284	G357	T431	C493	M563	S631	THR	THR	P752
A1624	A81	L21	L285	K358	A432	R494	K564	T632	GLU	GLU	K753
L1625	L31	L32	L286	K359	L433	R497	L565	N633	LYS	LYS	M633
Q1626	Q32	Q33	L287	P359	A434	R497	L566	L634	ARG	ARG	L756
L1627	L33	L34	D287	F359	A434	R498	K566	L635	ALA	ALA	W757
K1628	R34	R35	F298	V360	Y435	R498	L567	N636	ALA	ALA	W758
Y1629	Y103	T35	F299	E361	Q436	Q501	L567	T636	LYS	LYS	L759
M1630	M101	D36	F303	L362	T437	Q501	D570	K637	TYR	TYR	R759
F1631	F104	D36	L306	L363	Y444	N502	L503	O638	ILE	ILE	K760
Y1635	Y105	E39	L307	V364	L445	N503	L504	R639	GLN	GLN	D761
I1636	I106	Q40	L309	V365	R446	V504	V504	S640	GLY	GLY	L762
Y1637	Y107	I41	L309	V366	V447	T505	A573	S641	GLY	GLY	L763
P1638	P108	L42	V310	T298	S441	T506	R574	A641	PHE	PHE	T763
L1639	L111	E44	G311	F299	G442	N507	V575	A642	LEU	LEU	E764
D1640	D112	A45	H312	F303	N443	N507	G576	K643	ALA	ALA	E765
S1641	S113	H46	T313	D370	Y444	L445	L577	C644	CYS	CYS	E766
L1642	L114	G47	L314	P378	L445	L445	H508	P645	LYS	LYS	Q769
T1643	T115	D48	L314	P379	V447	S510	H509	Q646	ALA	ALA	S772
W1644	W116	S49	L314	V379	A448	P512	A579	R646	ALA	ALA	S773
I1645	I117	E116	H314	V380	T449	D513	D581	A647	LEU	LEU	T775
E1646	E118	P51	T315	S381	T450	L514	K582	A648	GLU	GLU	M776
Y1647	Y119	K52	L315	E382	S451	L515	L584	A649	ARG	ARG	S777
W1648	W120	Q53	L315	A383	T452	F516	V585	F649	ARG	ARG	F778
P1649	P121	L54	H244	F384	E453	S517	V586	Q649	ARG	ARG	T779
R1650	R122	D55	Y315	H385	K454	R517	L587	A650	TYR	TYR	L780
D1651	D123	I56	I247	H385	K455	F518	N588	A651	SER	SER	R781
T1652	T124	F57	T248	N387	P456	F520	F584	V652	ILE	ILE	I844
T1653	T125	V88	A249	T319	V318	V457	V521	G457	LYS	LYS	V845
C1654	C126	H59	R250	T319	V319	D458	A522	S522	VAL	VAL	R847
F1660	F127	D80	L188	M321	C394	L460	Y523	Q525	ARG	ARG	V848
	F61	D80	L189	T322	P461	Q525	Q525		GLU	GLU	L850










- 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) 96.8 (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)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.208 , 0.261 0.195 , 0.246	Depositor DCC
$R_{free}$ test set	1818 reflections (2.33%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	116.2	Xtrriage
Anisotropy	0.456	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 227.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	48236	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	167.0	wwPDB-VP

Xtrriage'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	0.77	5/13151 (0.0%)	1.16	78/17841 (0.4%)
1	C	0.76	4/13151 (0.0%)	1.16	94/17841 (0.5%)
2	B	0.67	0/9833	1.09	58/13345 (0.4%)
2	D	0.69	0/9833	1.11	57/13345 (0.4%)
3	X	0.59	2/1560 (0.1%)	1.02	8/2096 (0.4%)
3	Y	0.61	0/1560	1.04	8/2096 (0.4%)
All	All	0.72	11/49088 (0.0%)	1.13	303/66564 (0.5%)

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

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	210	GLU	C-N	8.37	1.46	1.33
1	A	1002	HIS	ND1-CE1	-6.45	1.26	1.32
1	A	1002	HIS	CG-ND1	6.32	1.45	1.38
1	C	33	VAL	CA-CB	-6.30	1.48	1.54
1	A	1016	VAL	CA-CB	-6.17	1.51	1.54

The worst 5 of 303 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	657	ALA	N-CA-C	-11.21	99.06	111.28
2	B	853	ASN	CA-C-N	11.21	130.99	119.56
2	B	853	ASN	C-N-CA	11.21	130.99	119.56
2	D	853	ASN	CA-C-N	11.10	130.88	119.56
2	D	853	ASN	C-N-CA	11.10	130.88	119.56

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 [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	12874	0	12814	1934	0
1	C	12874	0	12814	1984	0
2	B	9635	0	9630	1143	0
2	D	9635	0	9630	1135	0
3	X	1539	0	1530	175	0
3	Y	1539	0	1530	200	0
4	E	28	0	25	3	0
4	F	28	0	25	4	0
4	G	28	0	25	4	0
4	H	28	0	25	4	0
5	A	14	0	13	1	0
5	C	14	0	13	2	0
All	All	48236	0	48074	6445	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 67.

The worst 5 of 6445 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:HD12	3:X:207:LEU:O	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	8
1	C	1616/1676 (96%)	1179 (73%)	290 (18%)	147 (9%)	0	8
2	B	1203/1642 (73%)	981 (82%)	176 (15%)	46 (4%)	2	19
2	D	1203/1642 (73%)	982 (82%)	177 (15%)	44 (4%)	2	20
3	X	189/231 (82%)	148 (78%)	31 (16%)	10 (5%)	1	15
3	Y	189/231 (82%)	150 (79%)	28 (15%)	11 (6%)	1	14
All	All	6016/7098 (85%)	4605 (76%)	1002 (17%)	409 (7%)	1	12

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%)	1046 (72%)	399 (28%)	0	3
1	C	1445/1484 (97%)	1053 (73%)	392 (27%)	0	3
2	B	1084/1435 (76%)	837 (77%)	247 (23%)	1	6
2	D	1084/1435 (76%)	843 (78%)	241 (22%)	1	6
3	X	175/205 (85%)	141 (81%)	34 (19%)	1	8
3	Y	175/205 (85%)	143 (82%)	32 (18%)	2	10
All	All	5408/6248 (87%)	4063 (75%)	1345 (25%)	0	4

5 of 1345 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1180	LEU
2	D	598	ILE
1	C	1331	LYS
1	C	1179	THR
2	D	54	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 175 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1233	GLN
2	D	528	ASN
1	C	1268	ASN
2	D	152	HIS
2	D	1341	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](#)

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	4,2	14,14,15	1.03	1 (7%)	17,19,21	2.05	5 (29%)
4	NAG	E	2	4	14,14,15	1.04	1 (7%)	17,19,21	2.46	6 (35%)
4	NAG	F	1	4,2	14,14,15	2.08	7 (50%)	17,19,21	3.34	8 (47%)
4	NAG	F	2	4	14,14,15	1.76	2 (14%)	17,19,21	2.30	6 (35%)
4	NAG	G	1	4,2	14,14,15	0.92	1 (7%)	17,19,21	2.00	6 (35%)
4	NAG	G	2	4	14,14,15	1.12	1 (7%)	17,19,21	1.77	4 (23%)
4	NAG	H	1	4,2	14,14,15	2.02	6 (42%)	17,19,21	3.50	8 (47%)
4	NAG	H	2	4	14,14,15	1.64	1 (7%)	17,19,21	2.34	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	4,2	-	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	4,2	-	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	4,2	-	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	4,2	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	5/6/23/26	0/1/1/1

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	2	NAG	C1-C2	5.62	1.60	1.52
4	H	2	NAG	C1-C2	5.45	1.59	1.52
4	F	1	NAG	C1-C2	4.22	1.58	1.52
4	H	1	NAG	C1-C2	3.70	1.57	1.52
4	E	1	NAG	C1-C2	3.11	1.56	1.52

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	NAG	C1-O5-C5	10.20	125.86	112.19
4	F	1	NAG	C1-O5-C5	9.39	124.78	112.19
4	E	2	NAG	C4-C3-C2	6.58	120.66	111.02
4	H	2	NAG	C1-C2-N2	5.97	119.84	110.43
4	F	2	NAG	C1-C2-N2	5.94	119.79	110.43

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

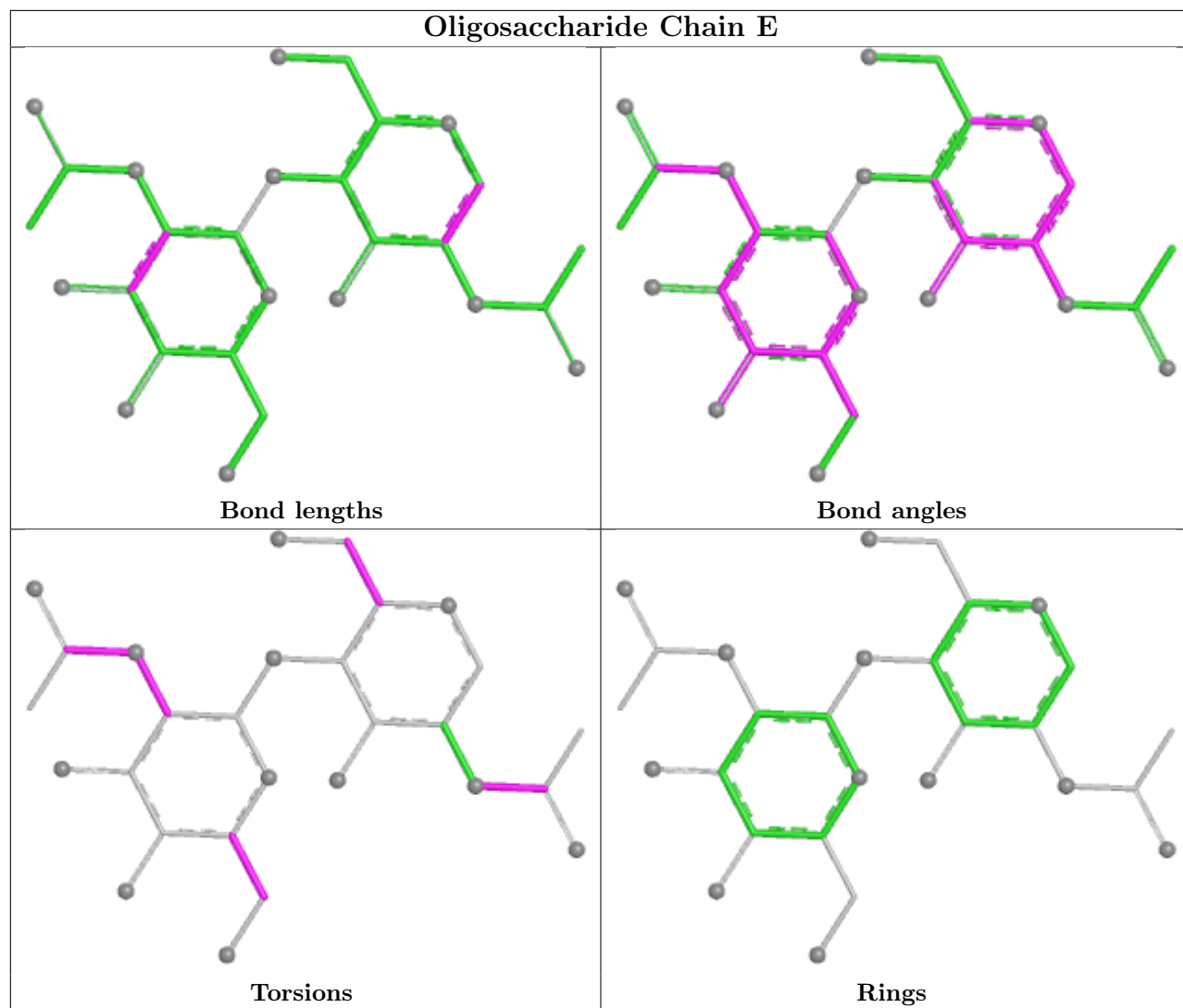
Mol	Chain	Res	Type	Atoms
4	E	1	NAG	C8-C7-N2-C2
4	E	1	NAG	O7-C7-N2-C2
4	E	2	NAG	C1-C2-N2-C7
4	E	2	NAG	O7-C7-N2-C2
4	F	2	NAG	C8-C7-N2-C2

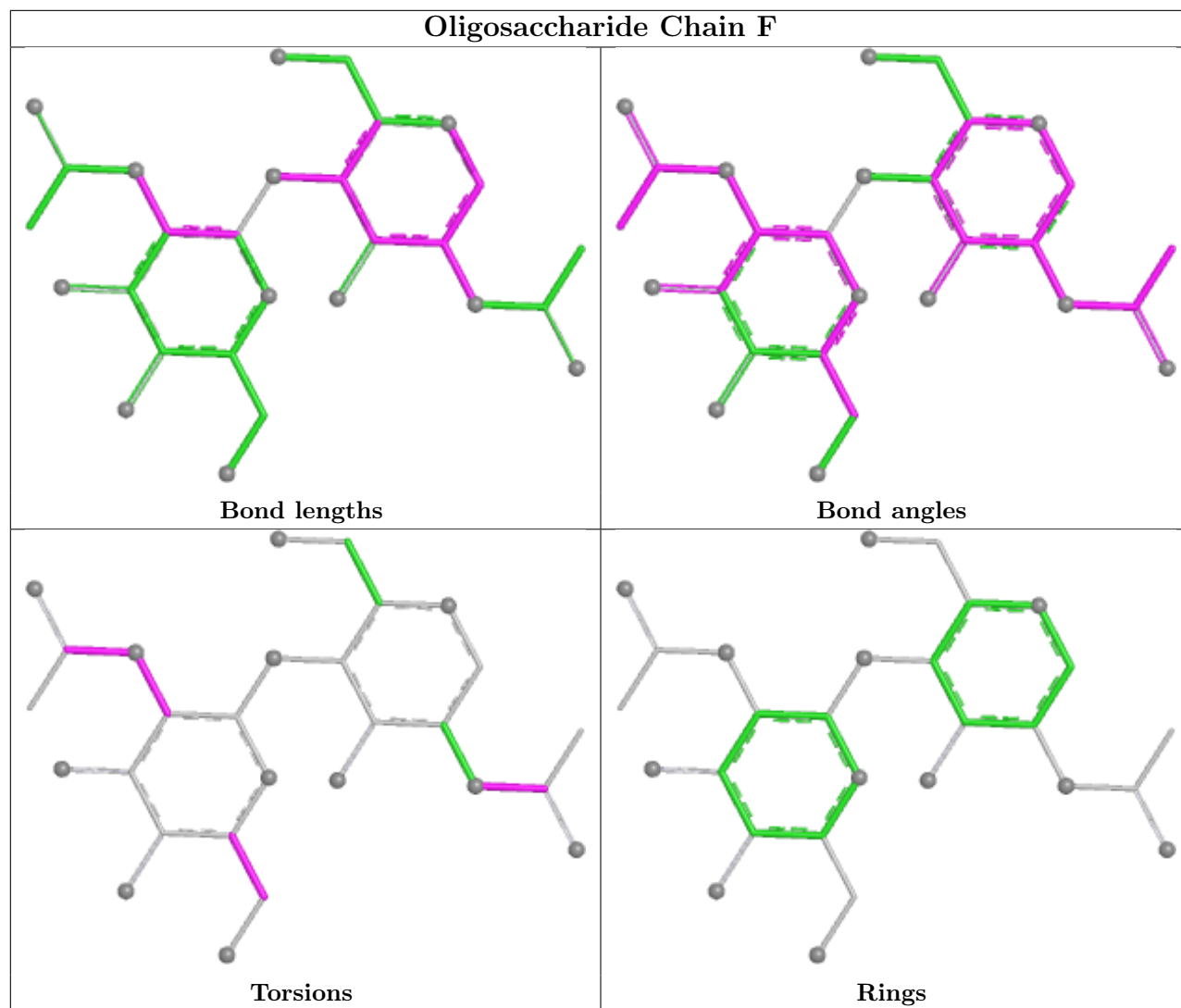
There are no ring outliers.

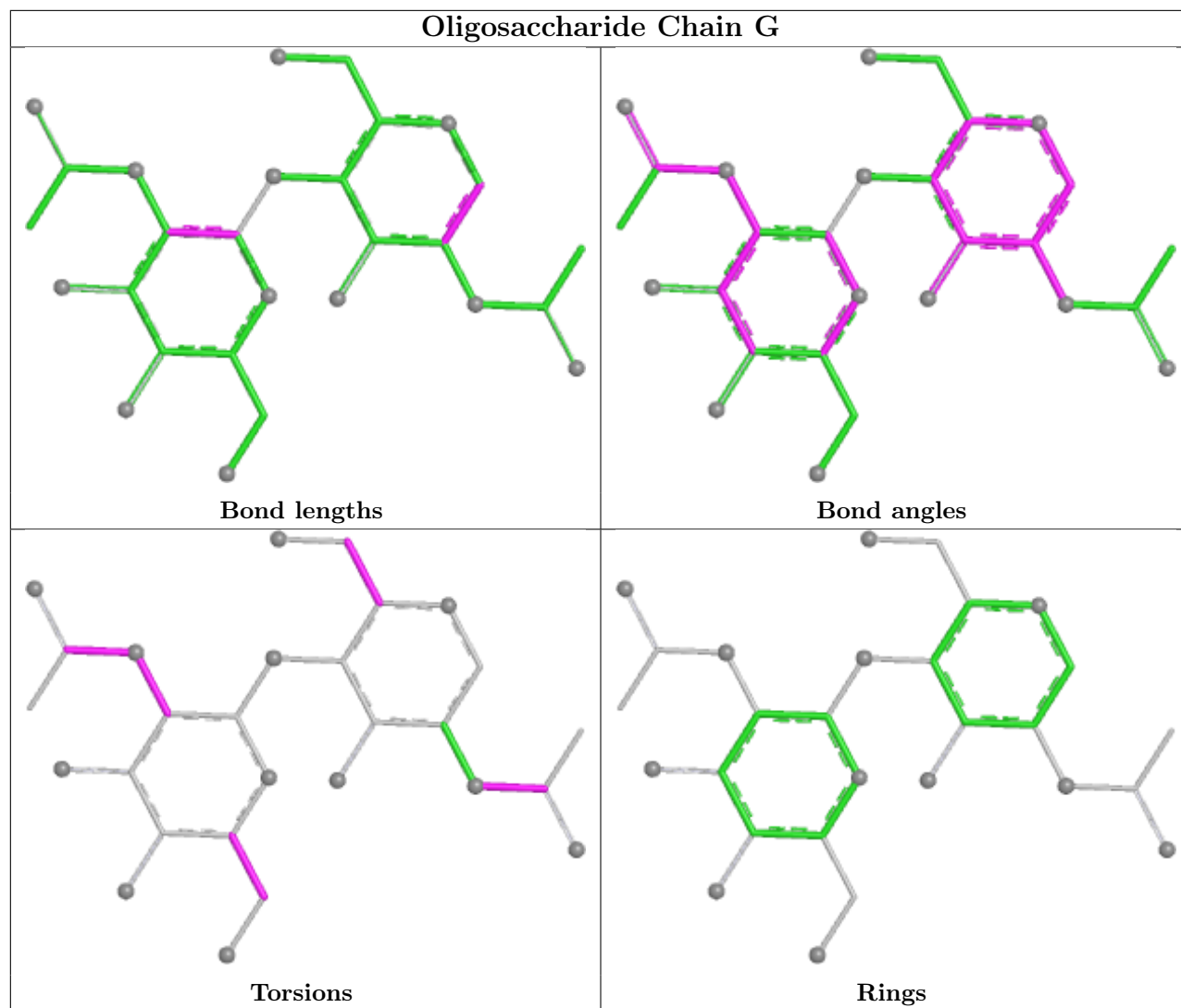
6 monomers are involved in 15 short contacts:

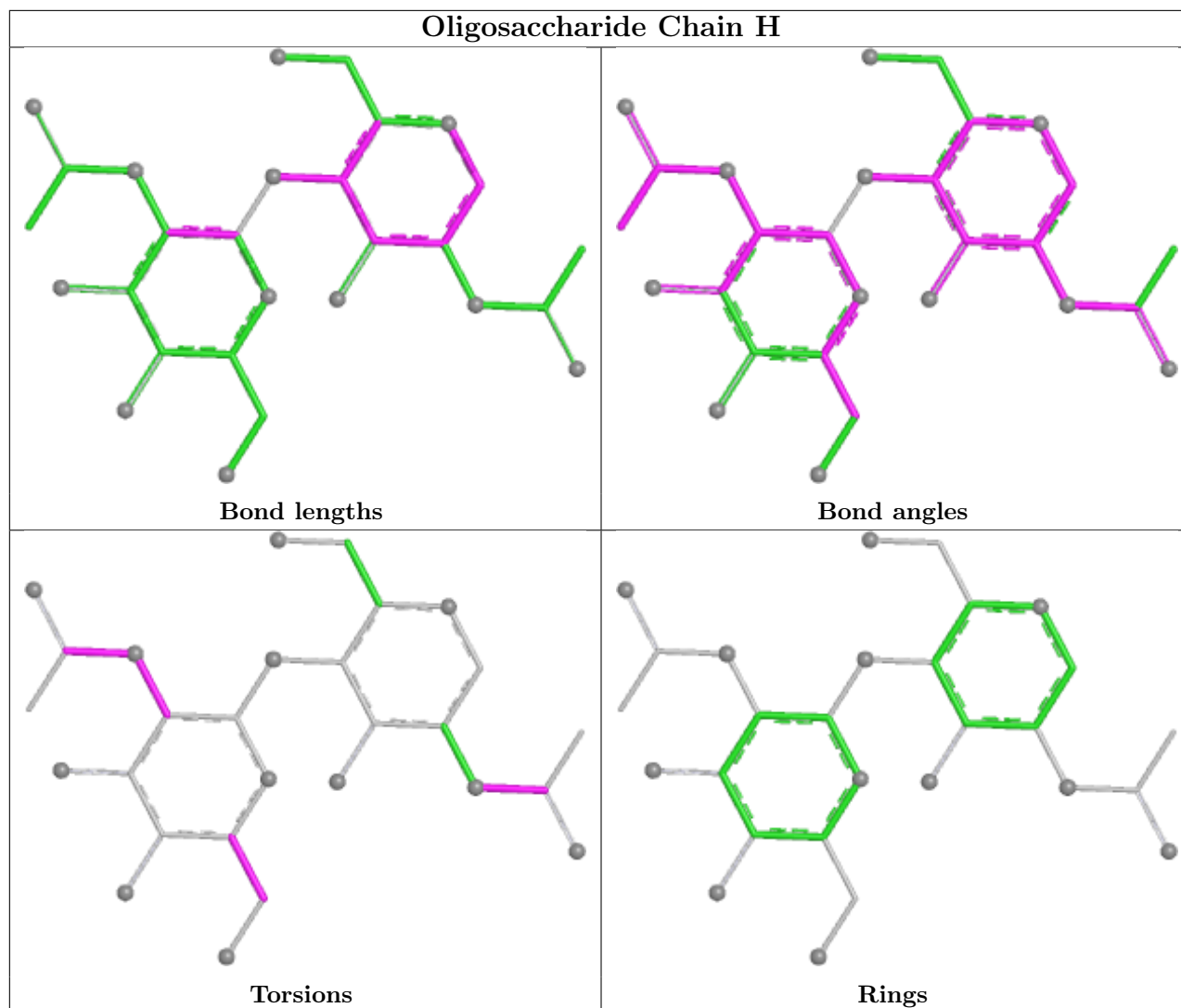
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1	NAG	4	0
4	E	2	NAG	3	0
4	G	1	NAG	4	0
4	E	1	NAG	3	0
4	G	2	NAG	4	0
4	F	1	NAG	4	0

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 [i](#)

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	A	2003	1	14,14,15	1.90	5 (35%)	17,19,21	3.37	12 (70%)
5	NAG	C	2003	1	14,14,15	2.10	4 (28%)	17,19,21	2.63	10 (58%)

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	2003	1	-	2/6/23/26	0/1/1/1
5	NAG	C	2003	1	-	4/6/23/26	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	4.86	1.59	1.52
5	A	2003	NAG	C3-C2	4.43	1.61	1.52
5	C	2003	NAG	C3-C2	4.02	1.60	1.52
5	C	2003	NAG	C4-C5	3.07	1.59	1.53
5	A	2003	NAG	O4-C4	2.32	1.48	1.43

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2003	NAG	C2-N2-C7	5.62	130.43	122.90
5	A	2003	NAG	O7-C7-C8	-5.33	112.57	122.05
5	A	2003	NAG	C4-C3-C2	4.83	118.10	111.02
5	C	2003	NAG	O3-C3-C2	4.39	118.53	109.40
5	A	2003	NAG	O4-C4-C3	4.12	120.10	110.38

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	A	2003	NAG	1	0
5	C	2003	NAG	2	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%)	0.03	15 (0%) 81 66	72, 150, 260, 469	0
1	C	1626/1676 (97%)	0.03	16 (0%) 79 64	60, 153, 277, 515	0
2	B	1215/1642 (73%)	-0.03	5 (0%) 88 77	73, 160, 235, 335	0
2	D	1215/1642 (73%)	-0.01	6 (0%) 87 75	85, 155, 241, 362	0
3	X	191/231 (82%)	0.20	3 (1%) 70 55	99, 230, 333, 437	0
3	Y	191/231 (82%)	0.15	4 (2%) 63 49	95, 195, 300, 385	0
All	All	6064/7098 (85%)	0.02	49 (0%) 82 68	60, 157, 264, 515	0

The worst 5 of 49 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	490	SER	4.0
1	A	1585	TYR	4.0
1	A	874	ASP	3.6
1	C	1585	TYR	3.3
1	A	1279	ARG	3.2

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

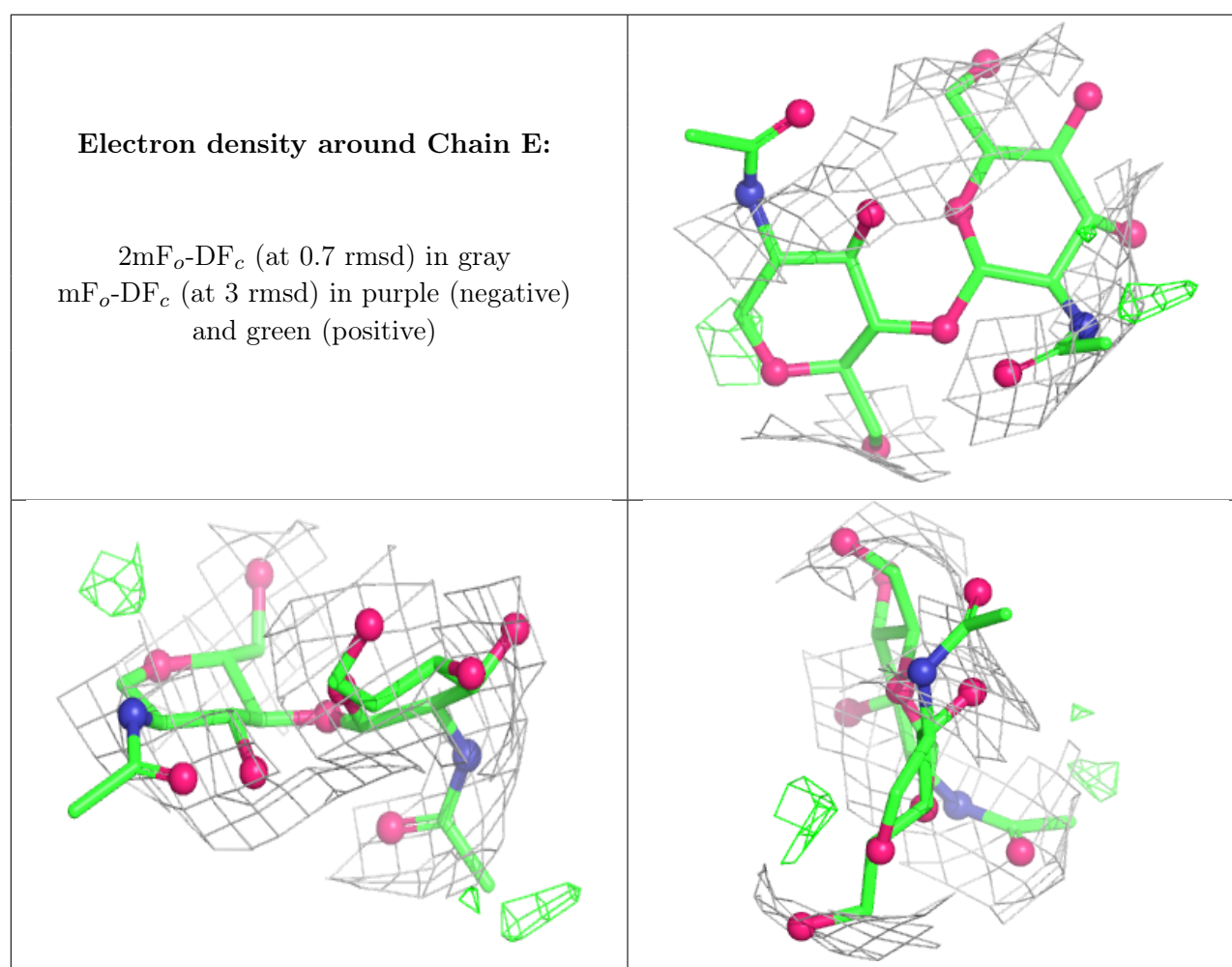
There are no non-standard protein/DNA/RNA residues in this entry.

### 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.

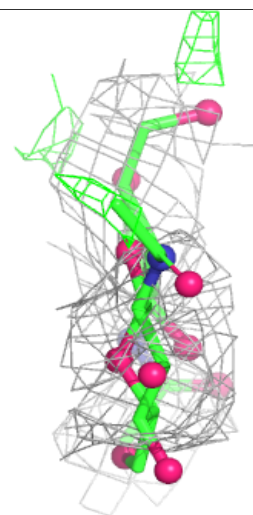
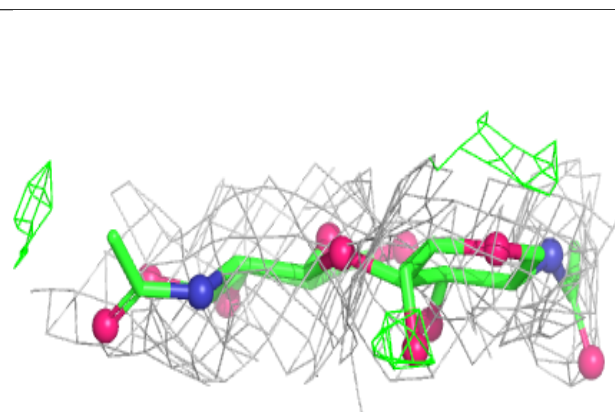
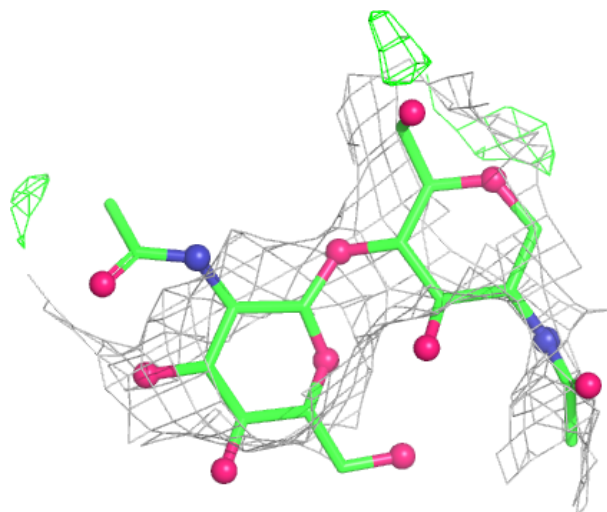
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	E	1	14/15	-	-	278,305,319,322	0
4	NAG	E	2	14/15	-	-	228,239,253,257	0
4	NAG	F	1	14/15	-	-	225,233,240,245	0
4	NAG	F	2	14/15	-	-	297,301,307,310	0
4	NAG	H	1	14/15	0.38	0.15	246,253,258,265	0
4	NAG	H	2	14/15	0.50	0.15	271,274,277,278	0
4	NAG	G	2	14/15	0.63	0.13	228,239,251,252	0
4	NAG	G	1	14/15	0.83	0.13	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.



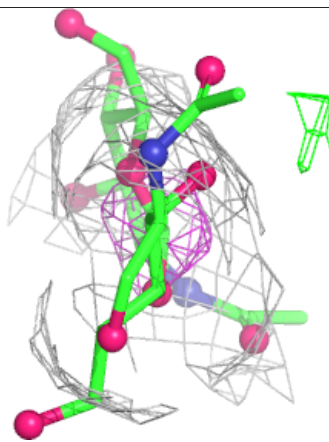
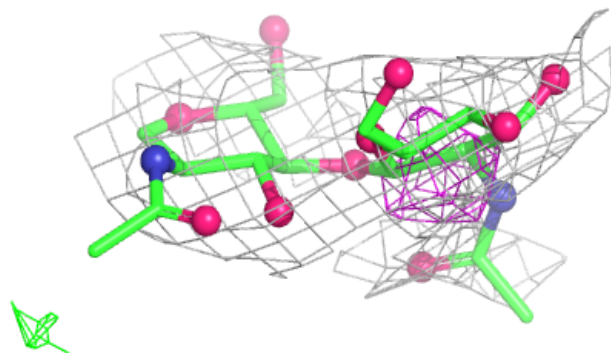
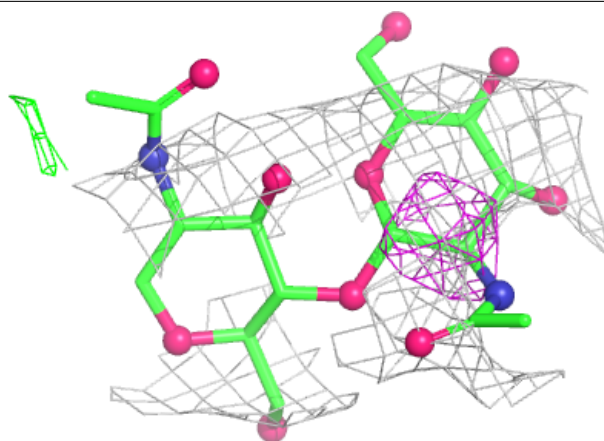
**Electron density around Chain F:**

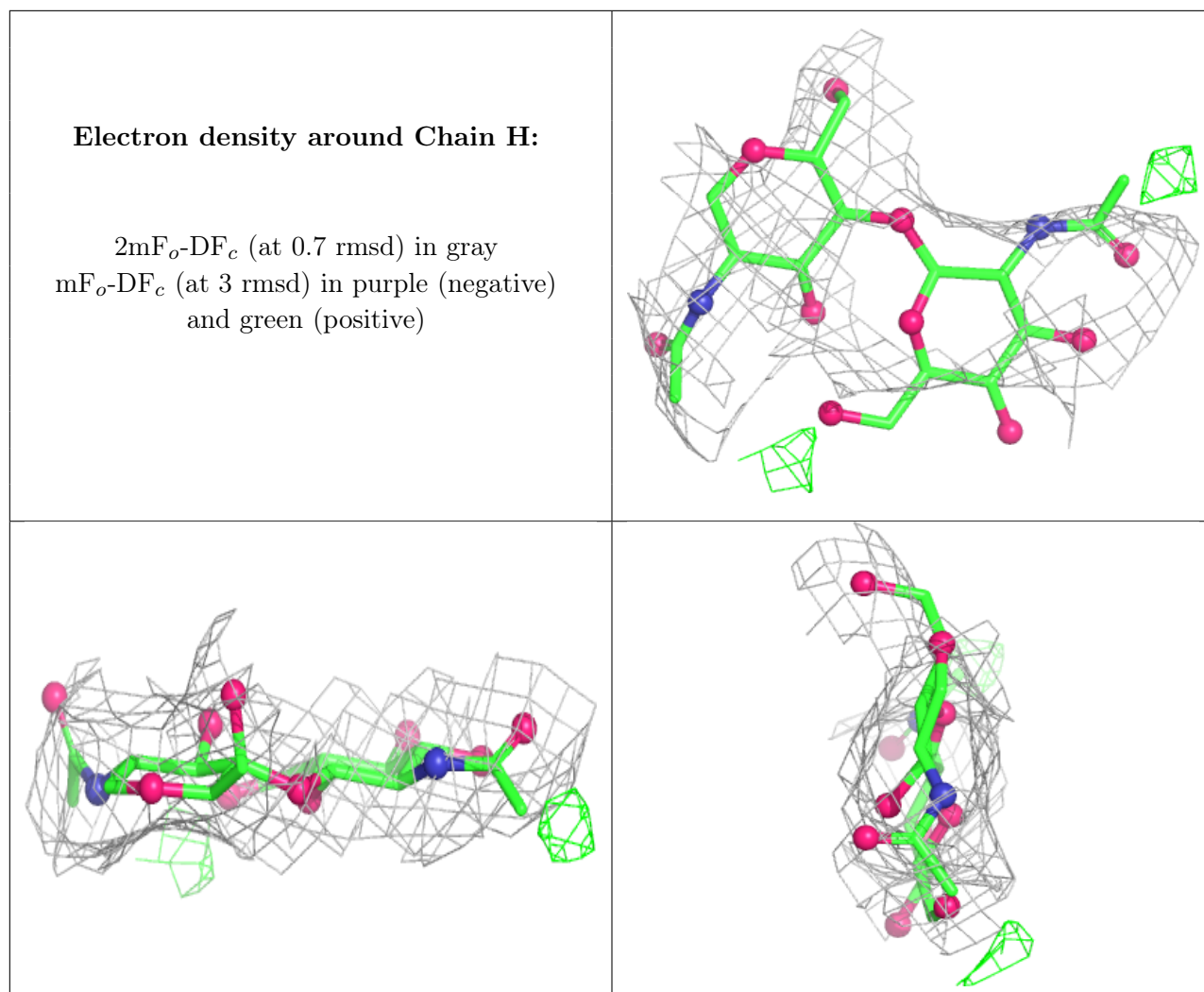
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain G:**

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





## 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	0.77	0.13	177,180,183,183	0
5	NAG	A	2003	14/15	0.82	0.13	166,169,171,172	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.