



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 04:11 AM UTC

PDB ID : 3KM9 / pdb_00003km9
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 types of validation reports are described at

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

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

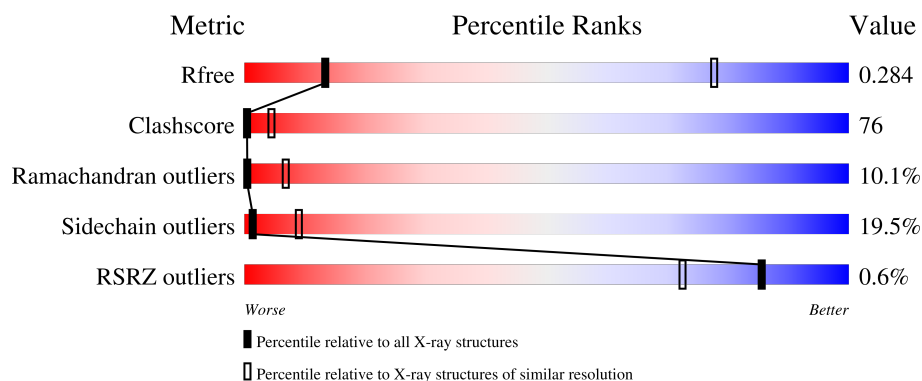
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.20 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}	180053	1004 (4.52-3.88)
Clashscore	190562	1019 (4.50-3.90)
Ramachandran outliers	187476	1020 (4.56-3.84)
Sidechain outliers	187428	1006 (4.56-3.84)
RSRZ outliers	180081	1001 (4.52-3.88)

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

Mol	Chain	Length	Quality of chain
1	A	1676	
1	B	1676	
2	X	103	
2	Y	103	

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Mol	Chain	Length	Quality of chain
3	C	2	 50%50%
3	D	2	 100%

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 (CCD ID: CD) (formula: Cd).

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Cd	0	0
			2	2		

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

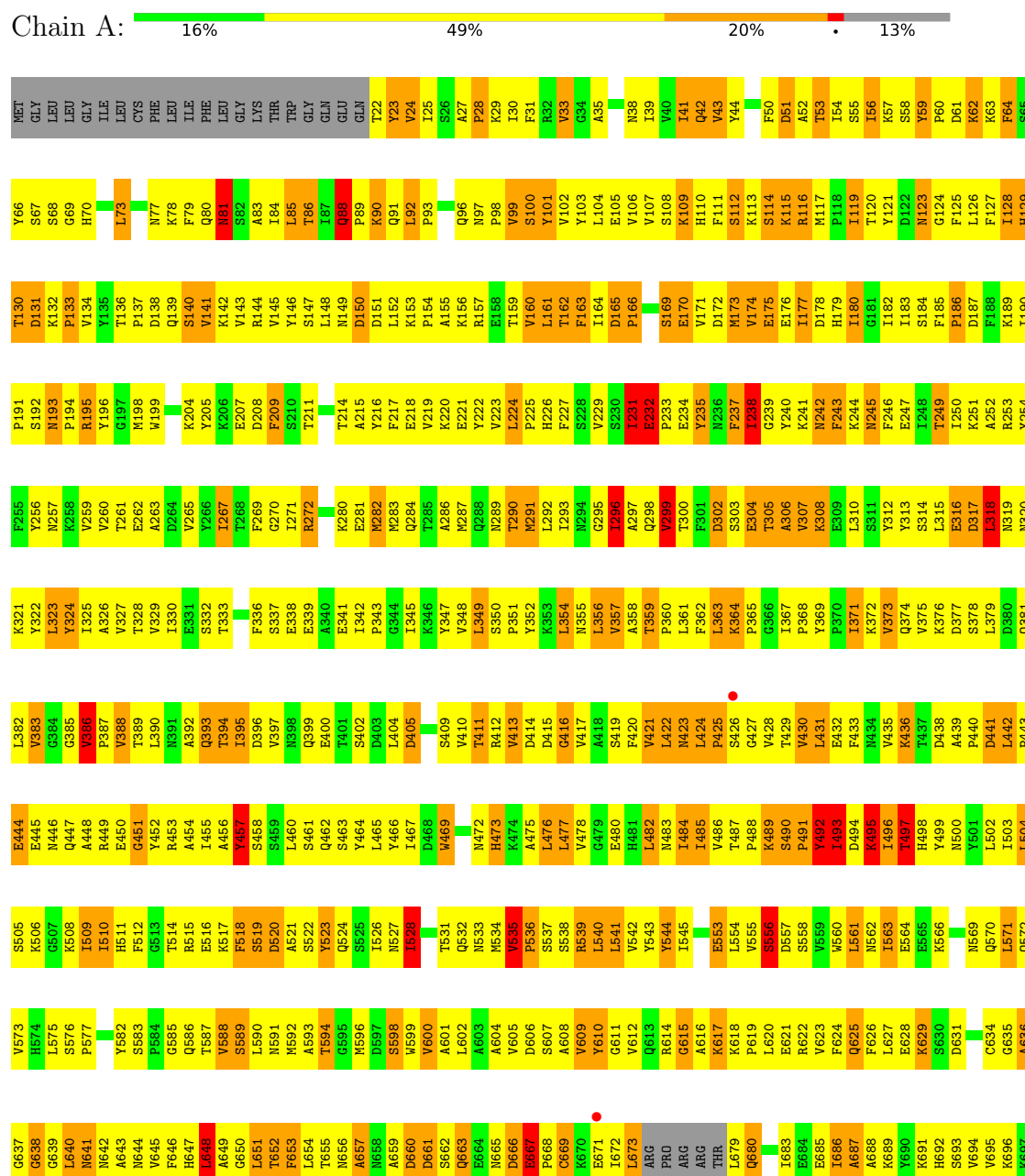


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

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



VAL	Y1509	D1447	G1386	H1324	I1264	P1203	Y1143	A1080	V1015	T952	S891	B822	V760	C698
GLU	S1510	Q1448	GLU	M1325	M1265	Q1204	L1144	F1081	V1016	T953	S892	V823	S761	C699
ASN	T1511	L1449	ALA	Y1326	Y1267	P1205	A1146	A1082	P1017		S893	F824	K762	T700
VAL		F1450	SER	K1327	Y1267	R1206	A1146	L1083	V1018	R956	H894	L825	P763	D701
PHE	I1514	T1451	HIS	M1328	P1269	S1207	R1084	R1084	F1019	K957	L896	E826	E764	G702
VAL	LYS	D1452	TYR	M1329	P1270	I1208	T1148	V1085	Y1020	E958	V896	M827	I765	A703
LYS	ILE	Y1453	ARG		V1270	V1209	V1149	L1086	V1021	F959	T897	B828	B766	C704
TYR	GLN	Q1454	GLY	M1332	I1271	S1210	I1150	G1087	F1022	P960	F898	L829	S767	C705
LYS	LYS	I1455	TYR	F1333	K1272	A1211	Q1088	Q1088	H1023	Y961	T899	P830	B706	V705
ALA	VAL	L1456	GLY	L1334	L1273	L1212	T1152	V1089	Y1024	R962	T899	P830	B706	N707
THR	CYS	D1457	ASN	G1335	L1274	K1213	T1153	N1090	L1025	I963	V900	S832	F769	D708
LEU	GLU	G1458	SER	R1336	S1275	R1214	K1091	K1091	E1026	P964	P902	B833	E771	E709
LEU	GLY	H1459	ASP	P1337	E1276	A1215	A1155	Y1092	T1027	L965	L903	B834	S772	T710
ASP	ALA	V1460	Y1389	V1338	E1277	A1216	F1156	V1093	G1028	D966	E984	R835	C711	C711
ILE	ALA	I1461	R1400	I1339	Q1278	L1217	D1157	E1094	N1029	L967	L905	B836	E712	E712
TYR	CYS	L1462	K1401	V1340	Y1279	L1218	I1158	Q1095	H1030	V968	G906	B837	L774	E713
LYS	LYS	Q1463	I1402	L1341	Y1280	K1219	T1158	Q1096	W1031	P969	L907	B838	E776	R714
THR	CYS	L1464	V1403	L1342	Y1281	G1220	C1166	Q1097	N1032	K970	H908	B839	E777	A715
GLY	VAL	M1465	A1404	M1343	G1282	N1221	L1161	N1098	I1033	T971	N909	B840	H778	A716
GLU	GLU	S1466	C1405	D1344	F1284	P1222	V1162	S1099		E972	I910	L841	L779	R717
ALA	ALA	I1467	A1406	D1345	G1285	F1223	K1163	I1100	S1036	I973	N911		L780	R718
VAL	ASP	Y1468	S1407	L1346	Y1285	I1224	C1101	D1037	D1037	K974	F912	V845	P781	S719
ALA	CYS	L1477	Y1408	I1347	S1286	Y1225	D1165	P1038	P1038	R975	S913	Y846	R782	L720
GLU	GLY	K1409	P1409	V1348	T1287	R1226	S1103	L1039	L1039	I976	L914	N847	R783	G721
LYS	GLN	P1410	K1410	S1349	Q1288	F1227	A1167	L1104	L1040	L977	E915	Y848	K784	P722
ASP	MET	S1411	S1411	T1350	D1289	W1228	L1168	L1105	E1041	S978	T916	R849	Q785	R723
SER	GLN	R1475	R1412	G1351	T1290	K1229	I1169	W1106	K1042	V979			L786	C724
GLU	GLU	Y1476	E1413	F1352	I1291	D1230	K1170	Q1043	Q1043	K980	K920	M853	Q787	T725
ILE	GLU	F1477	L1420	G1353	N1292	M1231	A1171	V1109	K1044	G981	E921	Q854	F788	R726
THR	LEU	R1478	S1415	S1354	A1293	L1232	D1172	E1109	L1045	L982	E921	Q855	A789	A727
PHE	ASP	I1479	E1416	G1355	I1294	Q1233	N1173	N1110	K1046	L983	I922	C856	L790	F728
ILE	LEU	F1480	G1418	L1356	E1295		F1174	Y1111	K1047	V984	L923	B857	B791	T729
LYS	THR	E1481	S1419	A1357	G1296	D1236	L1180	Q1112	K1048	G985	V924	A858	D792	E730
LYS	ILE	L1482	T1358	V1359	T1297	S1237	L1175	D1113	L1049	E986	T926	K859	S793	C731
THR	ALA	E1483	H1422	L1359	T1298	S1238	E1177	N1114	K1050	I987	L926		L794	C732
ALA	GLU	E1484	V1423	H1360	E1299	V1239	N1178	N1115	E1051	L988	L927	V862	T795	V733
CYS	GLU	Y1485	V1423	V1361	Y1300	P1240	T1179	G1116	G1052		E928	V863	T796	V734
THR	THR	G1486	V1424	T1362	S1301	N1241	L1180	S1117	M1053	V991	V929	C864	W797	A735
ASN	ARG	F1487	D1425	T1363	L1302	T1242	F1181	F1118	L1054	L992	V930	L865	E798	
ALA	LYS	L1488	I1426	V1364	L1303	G1243	A1182	K1119	S1055	S993	P931	C866	T799	
GLU	GLN	S1489	S1427	V1365	V1304	T1244	Q1183	E1120	I1056	Q994	E932	T867	Q800	W737
LEU	THR	P1490	H1366	K1366	K1305	A1245	S1184	N1121	M1057	E995	G933	G801	G801	L738
VAL	ALA	A1491	P1429	K1367	Q1306	R1246	F1185	S1122	S1058	G996	V934	S870	I802	R739
LYS	CYS	T1492	L1430	T1368	L1307	M1247	F1186	Q1123	Y1059	I997	K935	PRD	G803	
GLY	LYS	F1493	G1431	S1369	R1308	V1248	T1187		R1060	N998	R936	VAL	I804	I742
ARG	PRO	T1494	I1432	T1370	L1309	E1249	L1188	P1126	M1061	I999	E937	ILE	S805	S743
GLN	GLN	V1495	S1433	S1371	S1310	T1250	A1189	I1127	A1062	L1000	S938	ASP	LYS	
TYR	ILE	Y1496	A1434	E1372	K1311	T1251	I1190	D1063	Y939	T1001	HIS	ASP	LYS	
LEU	ALA	E1497	N1435	E1373	D1312	A1252	S1191	Y1064	H1002	C810	GLN	MET	GLN	
ILE	TYR	Y1498	E1436	V1374	I1313	Y1253	A1192	S1065	G941	L1003	G941	GLY	V811	
MET	ALA	H1499	E1437	G1375	D1314	A1254	Y1193	T1132	V942	P1004	V942	THR	A812	
GLY	TYR	R1500	D1438	S1376	L1255	L1255	A1194	L1133	S1067		T943	LYS	D813	LEU
LYS	LYS	P1501	L1439	F1377	S1316	L1256	P1134	P1134	V1068	S1007	L944	LYS	R751	G750
GLU	VAL	D1502	K1440	Y1378	Y1317	T1257	S1196	V1135	W1069	A1008	D945	SER	R752	
ALA	SER	K1503	A1441	L1379	K1318	L1258	G1197	E1136	K1070	E1009	P946	K882	K816	
LEU	ILE	O1504	L1442	K1380	H1319	S1259	L1498			A1010	R947		H753	
GLN	THR	V1443	V1443	I1381	K1320	N1260	D1199	E1139	T1076	E1011	G948	Q886	K818	
ILE	SER	E1444	E1444	L1382	K1320	L1261	K1200	N1140	Y1077	L1012	L949	R887	B818	
LYS	ILE	M1507	A1322	T1383	A1322	L1262	T1201	S1141	Y950	M1013	F820	V888	L758	
TYR	THR	F1508	V1446		L1323	D1263	H1202	T1079		S1014	G951		K821	P759

Chain B:

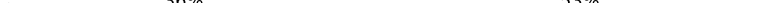


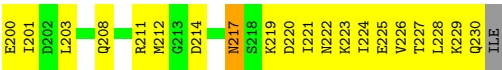
● Molecule 2: Staphylococcal enterotoxin-like toxin

Chain X:

Position	Residue	Probability (%)
S129	Glu	36%
S130	Glu	53%
S131	Glu	53%
S132	Glu	53%
S133	Glu	53%
S134	Glu	53%
S135	Glu	53%
S136	Glu	53%
S137	Glu	53%
S138	Glu	53%
S139	Glu	53%
S140	Glu	53%
S141	Glu	53%
S142	Glu	53%
S143	Glu	53%
S144	Glu	53%
S145	Glu	53%
S146	Glu	53%
S147	Glu	53%
S148	Glu	53%
S149	Glu	53%
S150	Glu	53%
S151	Glu	53%
S152	Glu	53%
S153	Glu	53%
S154	Glu	53%
S155	Glu	53%
S156	Glu	53%
S157	Glu	53%
S158	Glu	53%
S159	Glu	53%
S160	Glu	53%
S161	Glu	53%
S162	Glu	53%
S163	Glu	53%
S164	Glu	53%
S165	Glu	53%
S166	Glu	53%
S167	Glu	53%
S168	Glu	53%
S169	Glu	53%
S170	Glu	53%
S171	Glu	53%
S172	Glu	53%
S173	Glu	53%
S174	Glu	53%
S175	Glu	53%
S176	Glu	53%
S177	Glu	53%
S178	Glu	53%
S179	Glu	53%
S180	Glu	53%
S181	Glu	53%
S182	Glu	53%
S183	Glu	53%
S184	Glu	53%
S185	Glu	53%
S186	Glu	53%
S187	Glu	53%
S188	Glu	53%
S189	Glu	53%
S190	Glu	53%
S191	Glu	53%
S192	Glu	53%
S193	Glu	53%
S194	Glu	53%
S195	Glu	53%
S196	Glu	53%
S197	Glu	53%
S198	Glu	53%
S199	Glu	53%
S200	Glu	53%

- Molecule 2: Staphylococcal enterotoxin-like toxin

Chain X: 



- 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	144.79Å 144.79Å 245.28Å 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 4.14Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.233 , 0.297 0.218 , 0.284	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)	0.30 , 564.4	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	0.84	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.68	3/11793 (0.0%)	1.13	83/16003 (0.5%)
1	B	0.68	1/11793 (0.0%)	1.12	76/16003 (0.5%)
2	X	0.46	0/828	0.83	0/1107
2	Y	0.45	0/828	0.84	0/1107
All	All	0.67	4/25242 (0.0%)	1.11	159/34220 (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	1
1	B	0	2
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1018	VAL	CA-CB	-5.53	1.48	1.54
1	A	430	VAL	CA-CB	-5.28	1.47	1.55
1	A	237	PHE	CA-C	-5.27	1.48	1.53
1	B	1218	VAL	CA-CB	-5.02	1.47	1.54

The worst 5 of 159 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1003	LEU	CA-C-N	13.29	134.15	119.93
1	A	1003	LEU	C-N-CA	13.29	134.15	119.93
1	B	1003	LEU	CA-C-N	10.89	131.58	119.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1003	LEU	C-N-CA	10.89	131.58	119.93
1	B	1278	GLN	OE1-CD-NE2	-10.48	112.12	122.60

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	1801	0
1	B	11541	0	11511	1814	0
2	X	819	0	831	88	0
2	Y	819	0	831	86	0
3	C	28	0	25	2	0
3	D	28	0	25	2	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	3778	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 76.

The worst 5 of 3778 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:698:CYS:SG	1:A:724:CYS:HB2	1.86	1.15
1:B:115:LYS:HG2	1:B:117:MET:HE3	1.21	1.15
1:A:115:LYS:HG2	1:A:117:MET:HE3	1.17	1.13

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	1449/1676 (86%)	1039 (72%)	255 (18%)	155 (11%)	0	6
1	B	1449/1676 (86%)	1026 (71%)	274 (19%)	149 (10%)	0	6
2	X	100/103 (97%)	86 (86%)	9 (9%)	5 (5%)	1	16
2	Y	100/103 (97%)	84 (84%)	11 (11%)	5 (5%)	1	16
All	All	3098/3558 (87%)	2235 (72%)	549 (18%)	314 (10%)	0	7

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 [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	1296/1484 (87%)	1030 (80%)	266 (20%)	1	8
1	B	1296/1484 (87%)	1034 (80%)	262 (20%)	1	9
2	X	93/94 (99%)	87 (94%)	6 (6%)	15	38
2	Y	93/94 (99%)	85 (91%)	8 (9%)	10	30
All	All	2778/3156 (88%)	2236 (80%)	542 (20%)	1	9

5 of 542 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1056	ILE
1	B	1188	LEU
1	B	1053	MET
1	B	1465	ASN
1	A	1084	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 110 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	110	HIS
1	B	570	GLN
2	Y	192	ASN
1	B	1306	GLN
1	B	139	GLN

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	1.08	1 (5%)
3	NAG	C	2	3	14,14,15	0.48	0	17,19,21	1.01	1 (5%)
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	0.47	0	17,19,21	0.94	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1	1,3	-	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 (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	NAG	C1-O5-C5	3.02	116.23	112.19
3	C	1	NAG	C1-O5-C5	3.01	116.23	112.19
3	D	2	NAG	C1-O5-C5	2.66	115.75	112.19

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

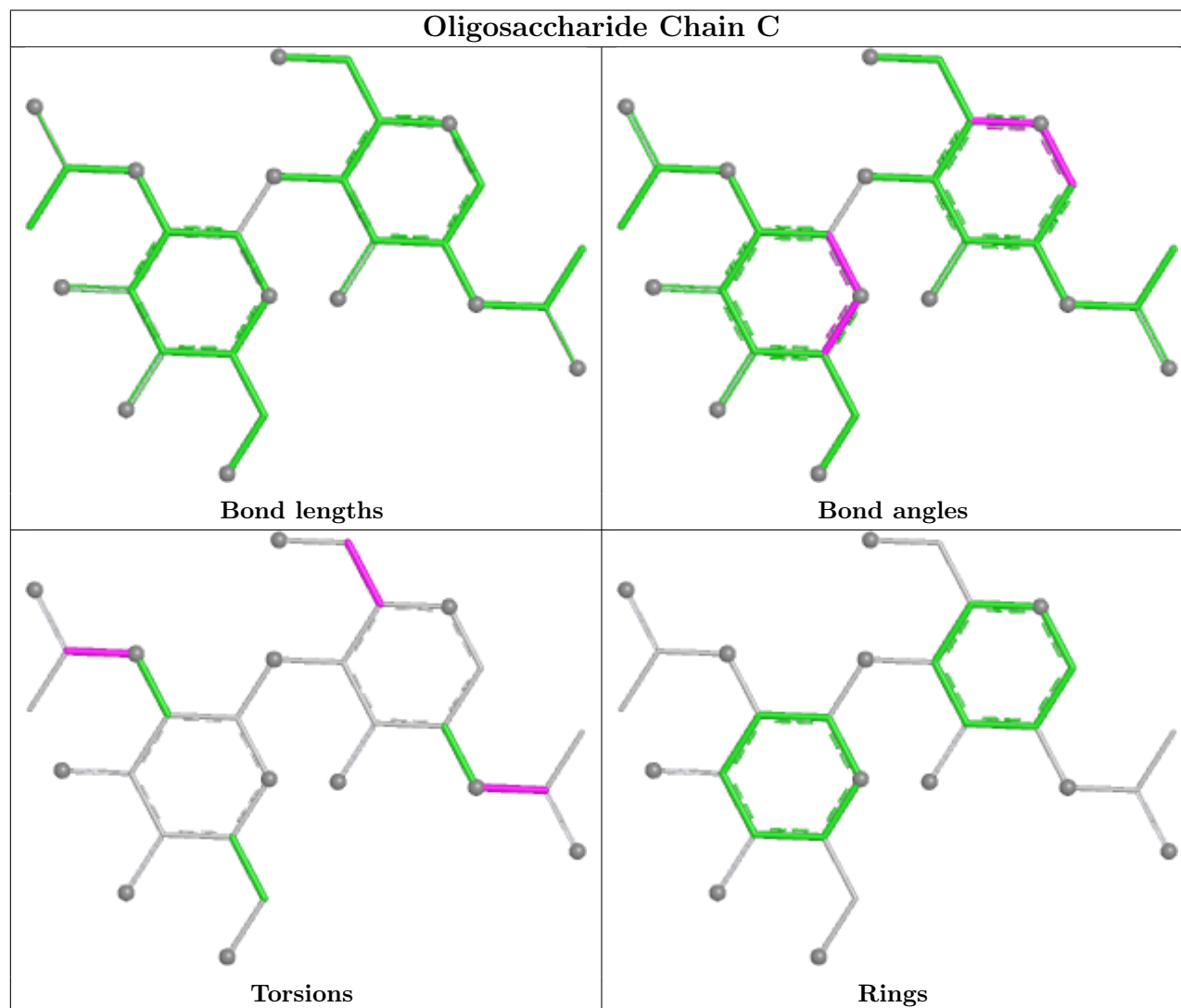
Mol	Chain	Res	Type	Atoms
3	D	2	NAG	C8-C7-N2-C2
3	D	2	NAG	O7-C7-N2-C2
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
3	C	2	NAG	C8-C7-N2-C2

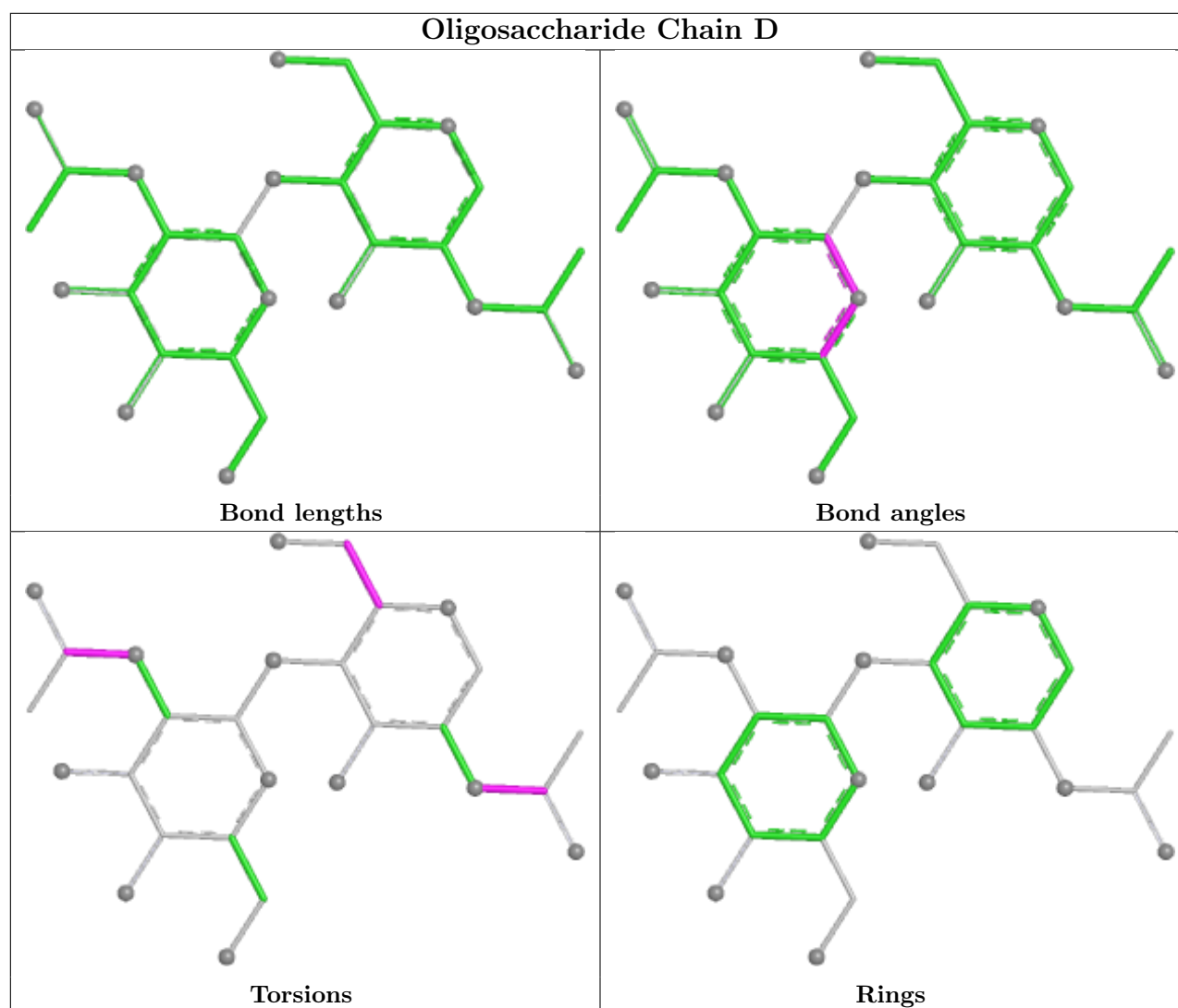
There are no ring outliers.

2 monomers are involved in 4 short contacts:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry [i](#)

Of 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	0.68	0	17,19,21	0.88	1 (5%)
5	NAG	B	1679	1	14,14,15	0.74	1 (7%)	17,19,21	1.01	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1680	1	-	3/6/23/26	0/1/1/1
5	NAG	B	1679	1	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1679	NAG	C1-C2	2.14	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1680	NAG	O5-C5-C6	2.09	111.73	107.66

There are no chirality outliers.

5 of 6 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	O7-C7-N2-C2
5	B	1679	NAG	C8-C7-N2-C2
5	B	1679	NAG	C3-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%)	-0.22	5 (0%) 90 80	81, 190, 311, 455	0
1	B	1459/1676 (87%)	-0.22	11 (0%) 82 68	85, 190, 308, 475	0
2	X	102/103 (99%)	-0.14	0 100 100	157, 292, 386, 530	0
2	Y	102/103 (99%)	-0.13	2 (1%) 65 50	156, 292, 377, 494	0
All	All	3122/3558 (87%)	-0.22	18 (0%) 85 72	81, 194, 328, 530	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	668	PRO	3.7
1	B	334	GLY	3.3
1	B	666	ASP	2.9
1	A	711	CYS	2.7
1	A	1458	GLY	2.6

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.

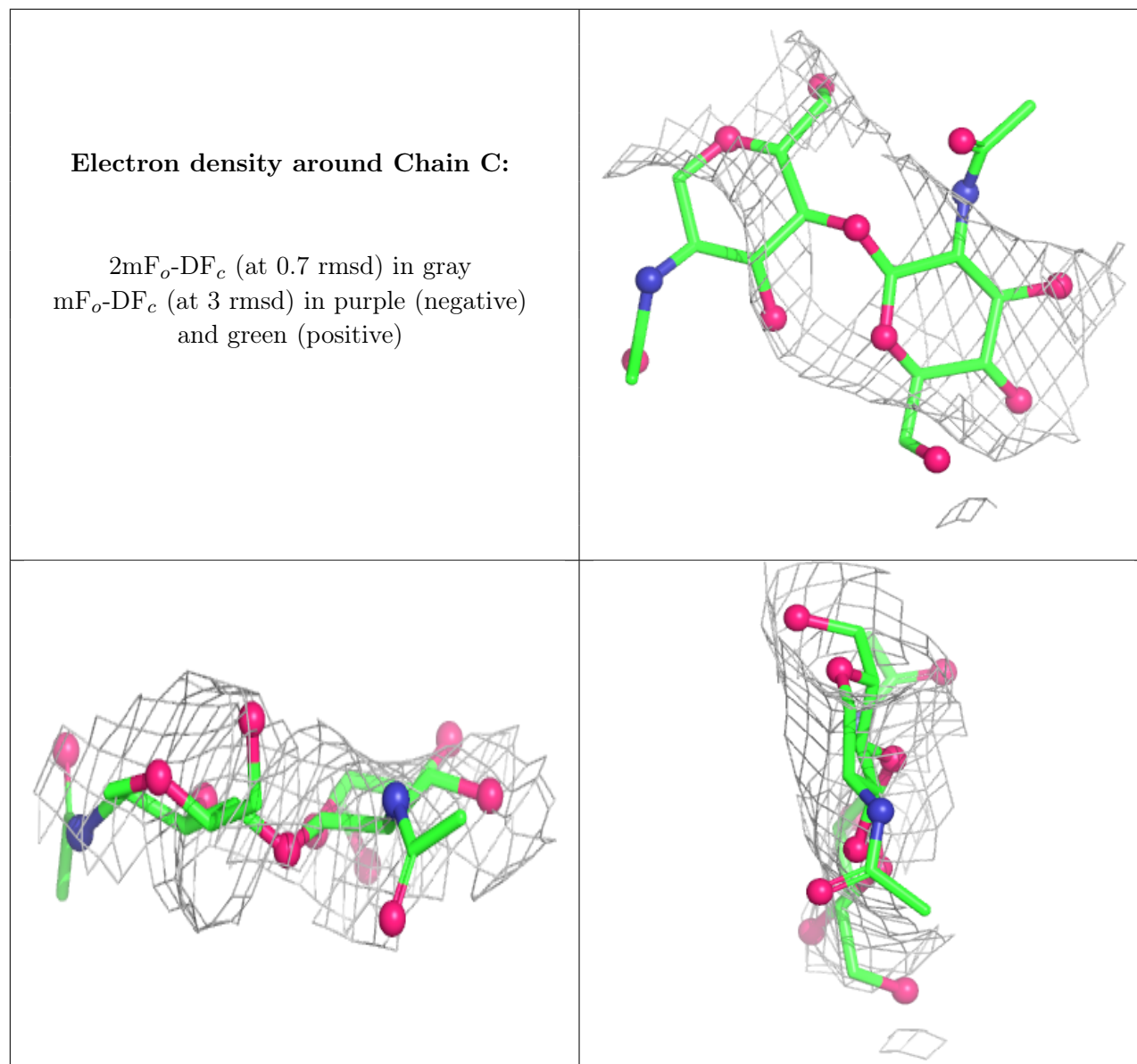
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	C	1	14/15	-	-	293,293,293,293	0
3	NAG	C	2	14/15	-	-	343,343,343,343	0

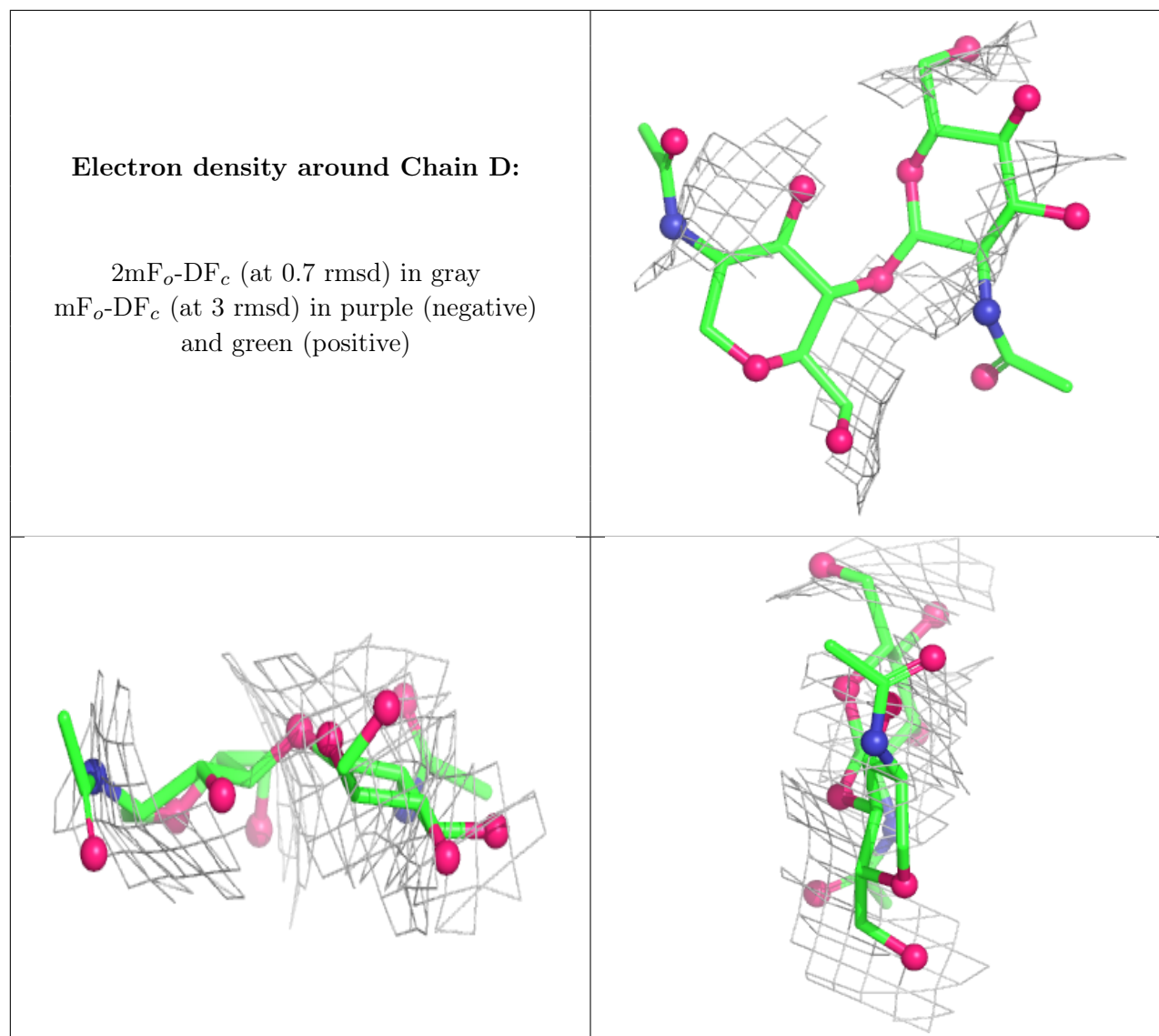
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	D	1	14/15	-	-	280,280,280,280	0
3	NAG	D	2	14/15	-	-	363,363,363,363	0

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, 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
4	CD	A	1677	1/1	0.88	0.15	229,229,229,229	1
5	NAG	B	1679	14/15	0.92	0.08	290,290,290,290	0
5	NAG	A	1680	14/15	0.95	0.07	301,301,301,301	0
4	CD	A	1679	1/1	0.95	0.07	402,402,402,402	0
4	CD	B	1678	1/1	0.96	0.06	397,397,397,397	0
4	CD	B	1677	1/1	0.98	0.07	466,466,466,466	0
4	CD	A	1678	1/1	0.98	0.11	481,481,481,481	0

6.5 Other polymers [i](#)

There are no such residues in this entry.