wwPDB EM Validation Summary Report

May 14, 2024 – 10:16 am BST

PDB ID	:	8R50
EMDB ID	:	EMD-18889
Title	:	Mouse teneurin-3 compact dimer - A1B1 isoform
Authors	:	Gogou, C.; Meijer, D.H.
Deposited on	:	2023-11-15
Resolution	:	3.10 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp
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:

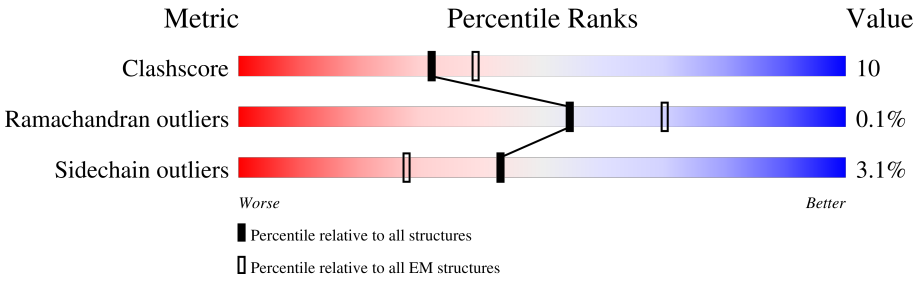
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	2407	59% 19% 22%
1	B	2407	59% 19% 22%
2	C	2	100%
2	D	2	100%
2	E	2	50% 50%
2	F	2	100%
2	G	2	100%
2	H	2	100%
2	I	2	50% 50%

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Mol	Chain	Length	Quality of chain
2	J	2	100%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 29752 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Teneurin-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	1889	Total	C	N	O	S	0	0
			14651	9292	2523	2773	63		
1	A	1889	Total	C	N	O	S	0	0
			14651	9292	2523	2773	63		

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	312	MET	-	initiating methionine	UNP Q9WTS6
B	313	ALA	-	expression tag	UNP Q9WTS6
B	314	ARG	-	expression tag	UNP Q9WTS6
B	315	PRO	-	expression tag	UNP Q9WTS6
B	316	LEU	-	expression tag	UNP Q9WTS6
B	317	CYS	-	expression tag	UNP Q9WTS6
B	318	THR	-	expression tag	UNP Q9WTS6
B	319	LEU	-	expression tag	UNP Q9WTS6
B	320	LEU	-	expression tag	UNP Q9WTS6
B	321	LEU	-	expression tag	UNP Q9WTS6
B	322	LEU	-	expression tag	UNP Q9WTS6
B	323	MET	-	expression tag	UNP Q9WTS6
B	324	ALA	-	expression tag	UNP Q9WTS6
B	325	THR	-	expression tag	UNP Q9WTS6
B	326	LEU	-	expression tag	UNP Q9WTS6
B	327	ALA	-	expression tag	UNP Q9WTS6
B	328	GLY	-	expression tag	UNP Q9WTS6
B	329	ALA	-	expression tag	UNP Q9WTS6
B	330	LEU	-	expression tag	UNP Q9WTS6
B	331	ALA	-	expression tag	UNP Q9WTS6
B	332	GLY	-	expression tag	UNP Q9WTS6
B	333	SER	-	expression tag	UNP Q9WTS6
B	334	HIS	-	expression tag	UNP Q9WTS6
B	335	HIS	-	expression tag	UNP Q9WTS6
B	336	HIS	-	expression tag	UNP Q9WTS6
B	337	HIS	-	expression tag	UNP Q9WTS6

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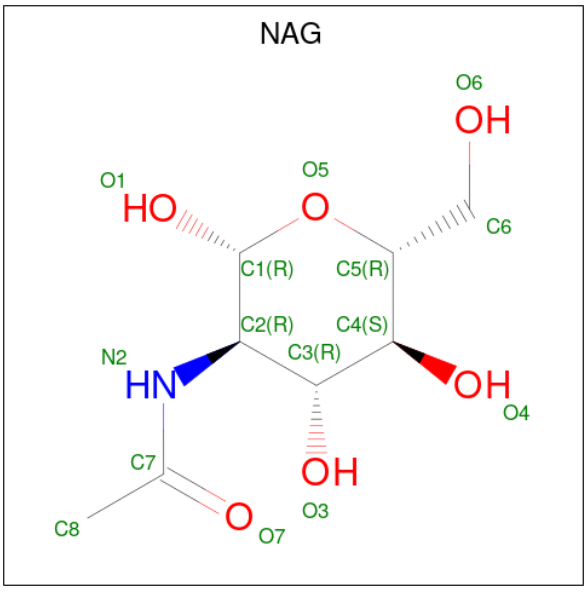
Chain	Residue	Modelled	Actual	Comment	Reference
B	338	HIS	-	expression tag	UNP Q9WTS6
B	339	HIS	-	expression tag	UNP Q9WTS6
B	340	GLY	-	expression tag	UNP Q9WTS6
B	341	SER	-	expression tag	UNP Q9WTS6
B	2332	ILE	THR	conflict	UNP Q9WTS6
B	2716	ALA	-	expression tag	UNP Q9WTS6
B	2717	ALA	-	expression tag	UNP Q9WTS6
B	2718	ALA	-	expression tag	UNP Q9WTS6
A	312	MET	-	initiating methionine	UNP Q9WTS6
A	313	ALA	-	expression tag	UNP Q9WTS6
A	314	ARG	-	expression tag	UNP Q9WTS6
A	315	PRO	-	expression tag	UNP Q9WTS6
A	316	LEU	-	expression tag	UNP Q9WTS6
A	317	CYS	-	expression tag	UNP Q9WTS6
A	318	THR	-	expression tag	UNP Q9WTS6
A	319	LEU	-	expression tag	UNP Q9WTS6
A	320	LEU	-	expression tag	UNP Q9WTS6
A	321	LEU	-	expression tag	UNP Q9WTS6
A	322	LEU	-	expression tag	UNP Q9WTS6
A	323	MET	-	expression tag	UNP Q9WTS6
A	324	ALA	-	expression tag	UNP Q9WTS6
A	325	THR	-	expression tag	UNP Q9WTS6
A	326	LEU	-	expression tag	UNP Q9WTS6
A	327	ALA	-	expression tag	UNP Q9WTS6
A	328	GLY	-	expression tag	UNP Q9WTS6
A	329	ALA	-	expression tag	UNP Q9WTS6
A	330	LEU	-	expression tag	UNP Q9WTS6
A	331	ALA	-	expression tag	UNP Q9WTS6
A	332	GLY	-	expression tag	UNP Q9WTS6
A	333	SER	-	expression tag	UNP Q9WTS6
A	334	HIS	-	expression tag	UNP Q9WTS6
A	335	HIS	-	expression tag	UNP Q9WTS6
A	336	HIS	-	expression tag	UNP Q9WTS6
A	337	HIS	-	expression tag	UNP Q9WTS6
A	338	HIS	-	expression tag	UNP Q9WTS6
A	339	HIS	-	expression tag	UNP Q9WTS6
A	340	GLY	-	expression tag	UNP Q9WTS6
A	341	SER	-	expression tag	UNP Q9WTS6
A	2332	ILE	THR	conflict	UNP Q9WTS6
A	2716	ALA	-	expression tag	UNP Q9WTS6
A	2717	ALA	-	expression tag	UNP Q9WTS6
A	2718	ALA	-	expression tag	UNP Q9WTS6

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

Mol	Chain	Residues	Atoms	AltConf	Trace
2	C	2	Total C N O 28 16 2 10	0	0
2	D	2	Total C N O 28 16 2 10	0	0
2	E	2	Total C N O 28 16 2 10	0	0
2	F	2	Total C N O 28 16 2 10	0	0
2	G	2	Total C N O 28 16 2 10	0	0
2	H	2	Total C N O 28 16 2 10	0	0
2	I	2	Total C N O 28 16 2 10	0	0
2	J	2	Total C N O 28 16 2 10	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



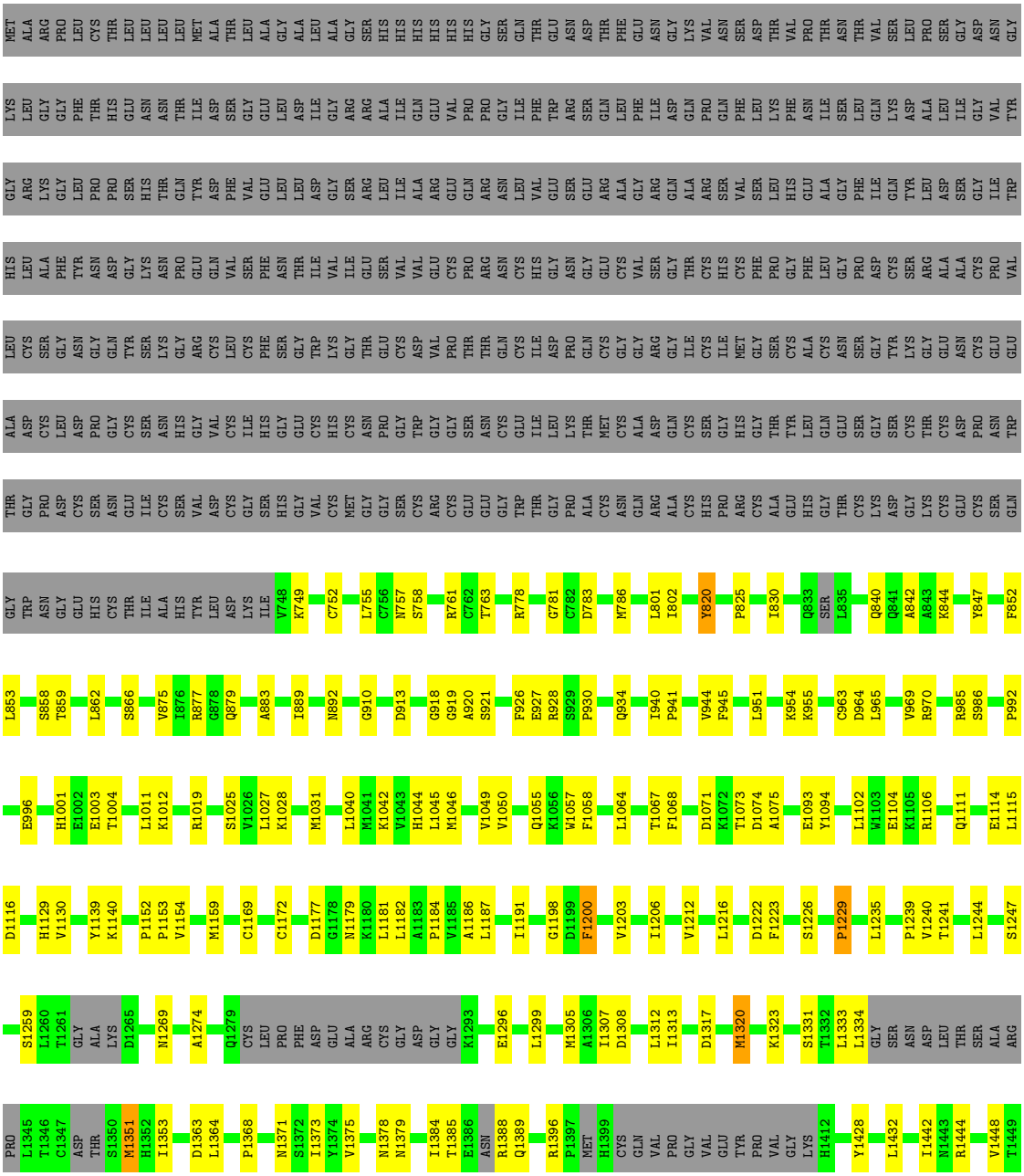
Mol	Chain	Residues	Atoms				AltConf
3	B	1	Total 14	C 8	N 1	O 5	0
3	B	1	Total 14	C 8	N 1	O 5	0
3	B	1	Total 14	C 8	N 1	O 5	0
3	B	1	Total 14	C 8	N 1	O 5	0
3	B	1	Total 14	C 8	N 1	O 5	0
3	B	1	Total 14	C 8	N 1	O 5	0
3	B	1	Total 15	C 8	N 1	O 6	0
3	B	1	Total 14	C 8	N 1	O 5	0
3	A	1	Total 14	C 8	N 1	O 5	0
3	A	1	Total 14	C 8	N 1	O 5	0
3	A	1	Total 14	C 8	N 1	O 5	0
3	A	1	Total 14	C 8	N 1	O 5	0
3	A	1	Total 14	C 8	N 1	O 5	0
3	A	1	Total 14	C 8	N 1	O 5	0
3	A	1	Total 15	C 8	N 1	O 6	0
3	A	1	Total 14	C 8	N 1	O 5	0

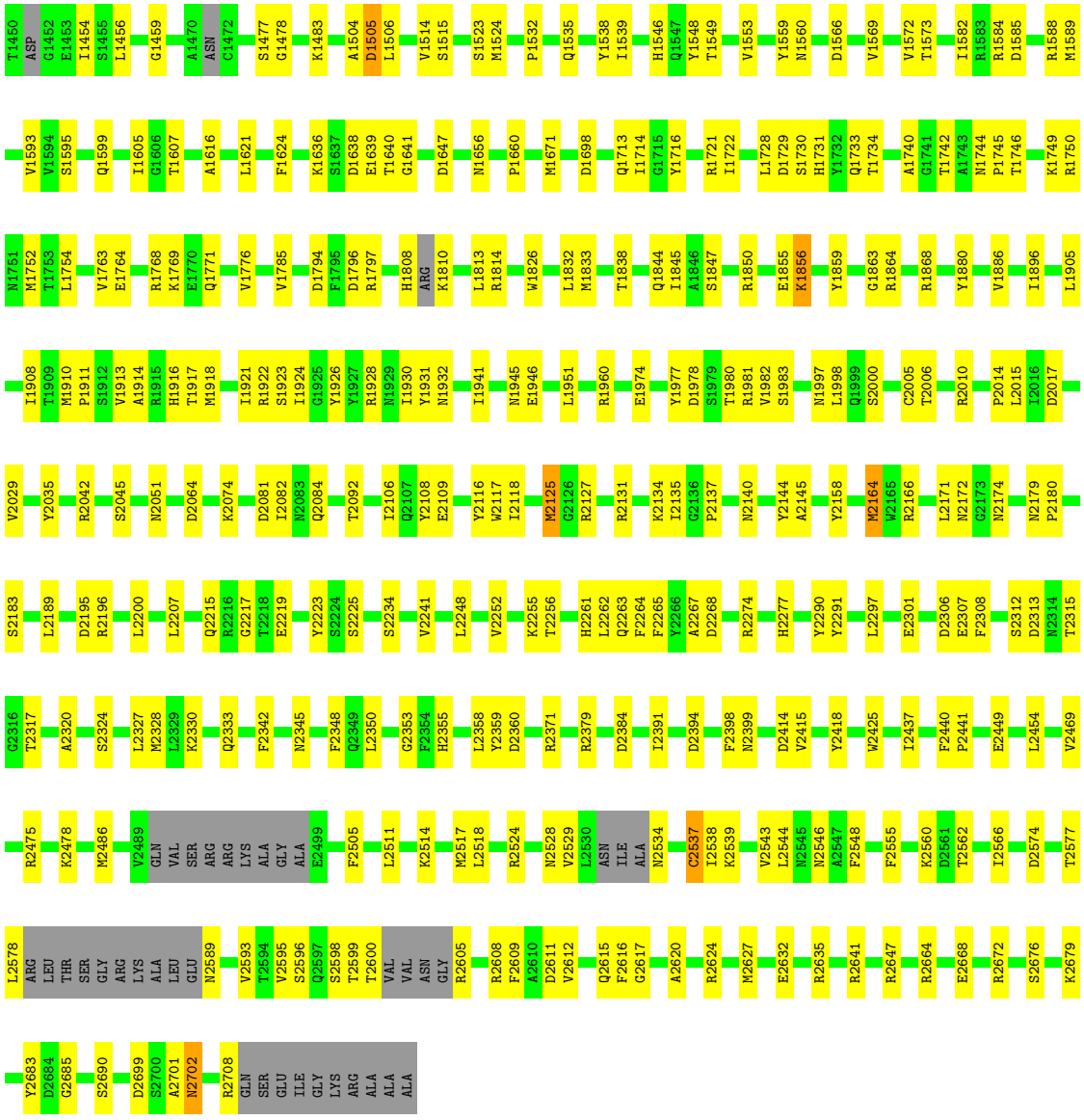
3 Residue-property plots (i)

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. 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. 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: Teneurin-3

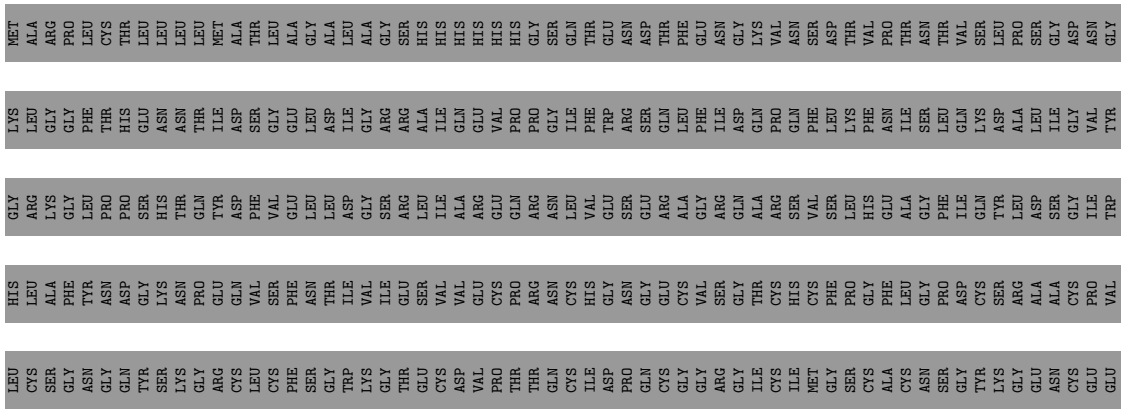
Chain B:

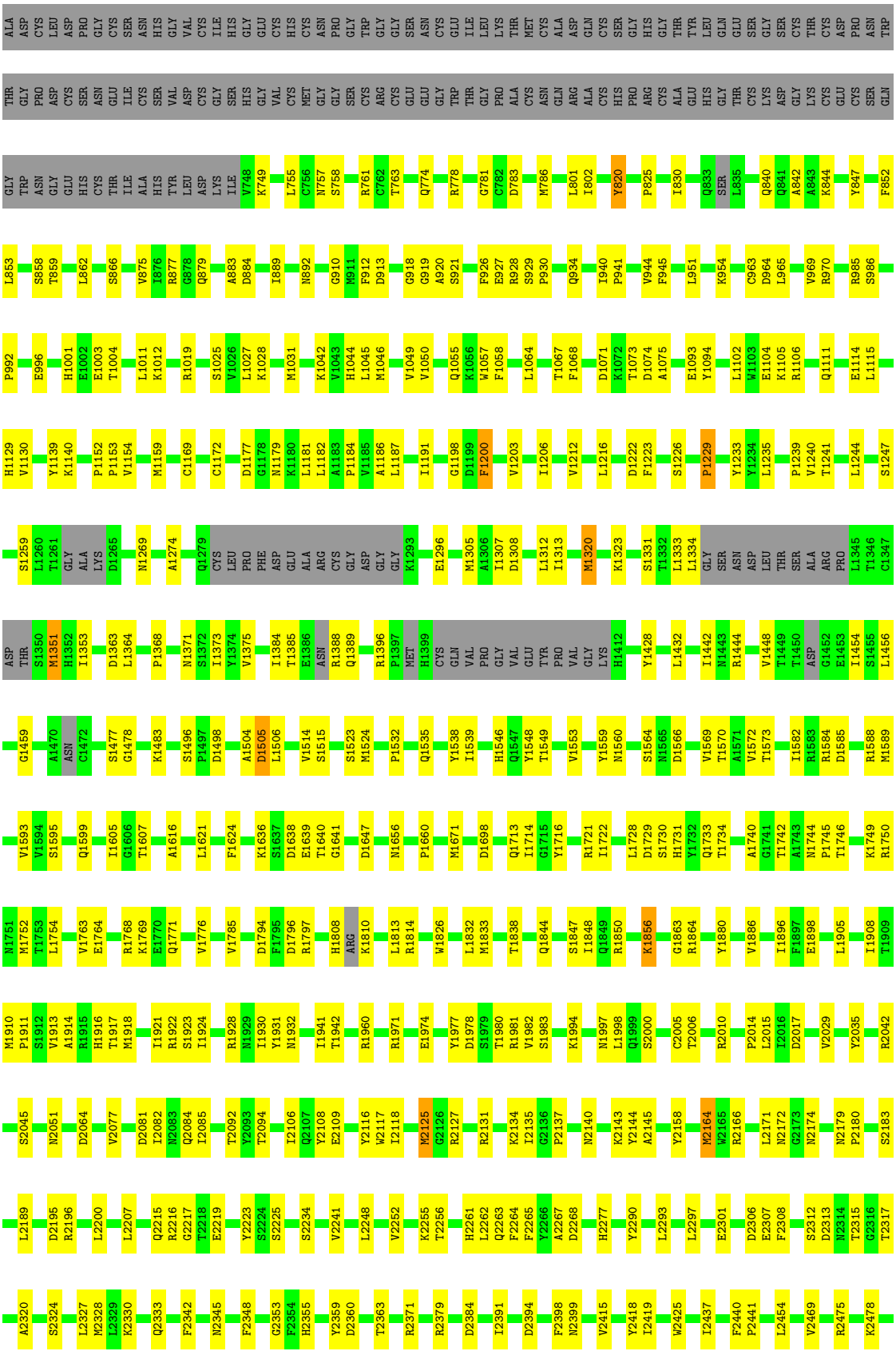


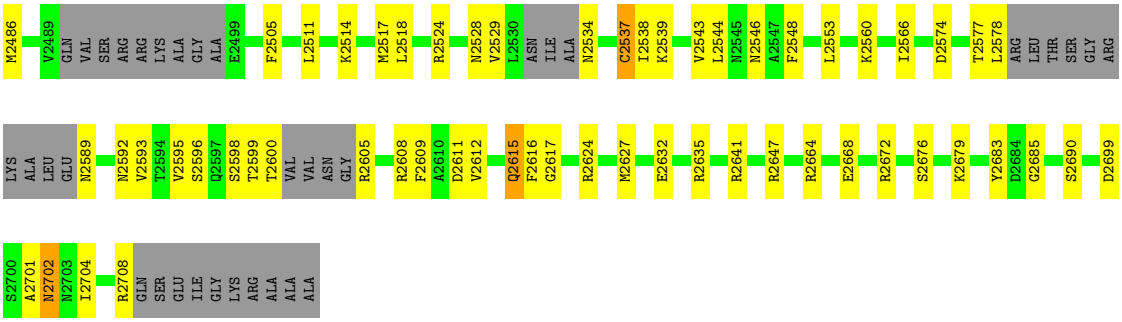


• Molecule 1: Teneurin-3

Chain A:

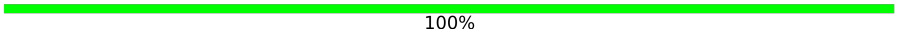



ALA ASP CYS LEU ASP PRO GLY CYS SER ASN HIS GLY VAL CYS ILE HIS GLY GLU CYS HIS CYS ASN PRO GLY CYS TRP GLY GLY SER ASN CYS GLU ILE LEU LYS THR MET CYS ALA ASP GLN CYS SER GLY HIS GLY THR TYR LEU GLN GLU SER GLY SER CYS THR CYS ASP PRO ASN TRP
THR GLY PRO ASP CYS SER ASN GLU ILE CYS SER VAL ASP CYS GLY SER HIS GLY VAL CYS MET GLY GLY SER CYS ARG CYS GLU GLY GLN ARG ALA CYS HIS PRO ARG CYS ALA GLU HIS GLY THR CYS LYS ASP GLY LYS CYS GLU CYS SER GLN
GLY TRP ASN GLY GLU HIS CYS THR ILE ALA HIS TYR LEU ASP LYS ILE V748 K749 L755 C756 N757 S758 R761 C762 T763 Q774 R778 G781 C782 D783 M786 L801 I802 Y820 P825 I830 Q833 SER L835 Q840 Q841 A842 A843 K844 Y847 F852
L853 S858 T859 L862 S866 V875 I876 R877 G878 Q879 A883 D884 I889 N892 G910 M911 F912 D913 G918 G919 A920 S921 F926 E927 R928 S929 P930 Q934 I940 P941 V944 F945 L951 K954 C963 D964 L965 V969 R970 Q984 R985 S986
P992 E996 H1001 E1002 E1003 T1004 L1011 K1012 R1019 S1025 V1026 L1027 K1028 M1031 K1042 V1043 H1044 L1045 M1046 V1049 V1050 Q1055 K1056 W1057 F1058 L1064 T1067 F1068 D1071 K1072 T1073 D1074 A1075 E1093 Y1094 L1102 W1103 E1104 K1105 R1106 Q1111 E1114 L1115
H1129 V1130 Y1139 K1140 P1152 P1153 V1154 M1159 C1169 C1172 D1177 C1178 N1179 K1180 L1181 L1182 A1183 V1184 P1184 V1185 A1186 L1187 I1191 G1198 D1199 F1200 V1203 I1206 V1212 L1216 D1222 F1223 S1226 P1229 Y1233 Y1234 L1235 P1239 V1240 T1241 L1244 S1247
S1259 L1260 T1261 GLY ALA LYS D1265 N1269 A1274 Q1279 CYS LEU PRO PHE ASP GLU ALA ARG CYS GLY ASP GLY GLY K1293 E1296 M1305 A1306 I1307 D1308 L1312 I1313 M1320 K1323 S1331 T1332 L1333 L1334 GLY SER ASN ASP LEU THR SER ALA ARG PRO L1345 T1346 C1347
ASP THR S1350 M1351 H1352 I1353 D1363 L1364 P1368 N1371 S1372 I1373 Y1374 V1375 I1384 T1385 E1386 ASN R1388 Q1389 R1396 P1397 MET H1399 CYS GLN VAL PRO GLY VAL GLU TYR PRO VAL GLY LYS H1412 Y1428 L1432 I1442 M1443 R1444 V1448 T1449 T1450 ASP G1452 E1453 T1454 S1455 L1456
G1459 A1470 ASN C1472 S1477 G1478 K1483 S1496 P1497 D1498 A1504 D1505 L1506 V1514 S1515 S1523 M1524 P1532 Q1535 Y1538 I1539 H1546 Q1547 Y1548 T1549 V1553 Y1559 N1560 S1564 N1565 D1566 V1569 T1570 A1571 V1572 T1573 I1582 R1583 R1584 D1585 R1588 M1589
V1593 Y1594 S1595 Q1599 I1605 G1606 T1607 A1616 L1621 F1624 K1636 S1637 D1638 E1639 T1640 G1641 D1647 N1656 P1660 M1671 D1698 Q1713 I1714 G1715 Y1716 R1721 I1722 L1728 D1729 S1730 H1731 Y1732 Q1733 T1734 A1740 G1741 T1742 A1743 N1744 P1745 T1746 K1749 R1750
N1751 M1752 T1753 L1754 V1763 E1764 R1768 K1769 E1770 Q1771 V1776 V1785 D1794 F1795 D1796 R1797 H1808 ARG K1810 L1813 R1814 W1826 L1832 M1833 T1838 Q1844 S1847 I1848 Q1849 R1850 K1856 G1863 R1864 Y1880 V1886 A1740 I1896 F1897 E1898 L1905 I1908 T1909
M1910 P1911 S1912 V1913 A1914 R1915 H1916 T1917 M1918 I1921 R1922 S1923 I1924 R1928 N1929 I1930 Y1931 N1932 I1941 T1942 R1960 R1971 E1974 Y1977 D1978 S1979 T1980 R1981 V1982 S1983 K1994 N1997 L1998 Q1999 S2000 C2005 T2006 R2010 P2014 L2015 I2016 D2017 V2029 Y2035 R2042
S2045 N2051 D2064 V2077 D2081 I2082 N2083 Q2084 I2085 T2092 Y2093 T2094 I2106 Q2107 Y2108 E2109 Y2116 W2117 I2118 M2125 G2126 R2127 R2131 K2134 I2135 G2136 P2137 N2140 K2143 Y2144 A2145 Y2158 M2164 W2165 R2166 L2171 N2172 G2173 N2174 N2179 P2180 S2183
L2189 D2195 R2196 L2200 L2207 Q2215 R2216 G2217 T2218 E2219 Y2223 S2224 S2225 S2234 V2241 L2248 V2252 K2255 T2256 H2261 L2262 Q2263 F2264 F2265 Y2266 A2267 D2268 H2277 Y2290 L2293 L2297 E2301 D2306 E2307 F2308 S2312 D2313 N2314 T2315 G2316 T2317
A2320 S2324 L2327 M2328 L2329 K2330 Q2333 F2342 N2345 F2348 G2353 F2354 H2355 Y2359 D2360 T2363 R2371 R2379 D2384 I2391 D2394 F2398 N2399 Y2415 Y2418 I2419 W2425 I2437 F2440 P2441 L2454 Y2469 R2475 K2478



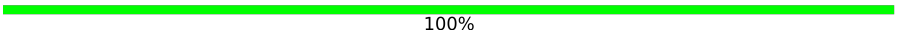
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:



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

Chain D:

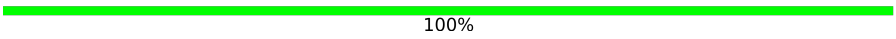


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

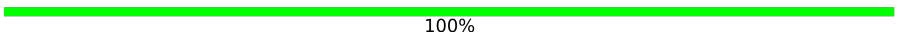
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



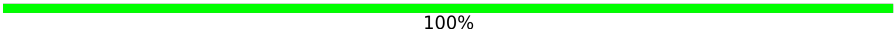
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



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

Chain H:

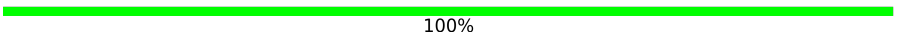


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

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

Chain J:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	57545	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50.0	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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	0.25	0/14968	0.50	0/20337
1	B	0.25	0/14968	0.50	0/20337
All	All	0.25	0/29936	0.50	0/40674

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	14651	0	14020	277	0
1	B	14651	0	14020	273	0
2	C	28	0	25	0	0
2	D	28	0	25	0	0
2	E	28	0	25	4	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	4	0
2	J	28	0	25	0	0
3	A	113	0	106	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	113	0	106	4	0
All	All	29752	0	28452	553	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 10.

The worst 5 of 553 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1913:VAL:HG12	1:B:1913:VAL:O	1.68	0.92
1:A:1913:VAL:HG12	1:A:1913:VAL:O	1.68	0.89
1:A:1312:LEU:HD21	1:A:1323:LYS:HG3	1.66	0.77
1:B:1312:LEU:HD21	1:B:1323:LYS:HG3	1.66	0.77
1:A:1074:ASP:OD1	1:A:1075:ALA:N	2.19	0.76

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 PDB entries followed by that with respect to all EM entries.

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	1858/2407 (77%)	1709 (92%)	148 (8%)	1 (0%)	51 83
1	B	1858/2407 (77%)	1708 (92%)	149 (8%)	1 (0%)	51 83
All	All	3716/4814 (77%)	3417 (92%)	297 (8%)	2 (0%)	54 83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1229	PRO
1	A	1229	PRO

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 PDB entries followed by that with respect to all EM entries.

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	1544/2075 (74%)	1496 (97%)	48 (3%)	40	70
1	B	1544/2075 (74%)	1497 (97%)	47 (3%)	41	71
All	All	3088/4150 (74%)	2993 (97%)	95 (3%)	43	70

5 of 95 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1320	MET
1	A	2042	ARG
1	A	1351	MET
1	A	1671	MET
1	A	2081	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1969	GLN
1	A	2263	GLN
1	A	2534	ASN
1	B	2263	GLN
1	B	1969	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

16 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	$\#\|Z\| > 2$
2	NAG	C	1	2,1	14,14,15	0.19	0	17,19,21	0.41	0
2	NAG	C	2	2	14,14,15	0.20	0	17,19,21	0.42	0
2	NAG	D	1	2,1	14,14,15	0.32	0	17,19,21	0.39	0
2	NAG	D	2	2	14,14,15	0.24	0	17,19,21	0.42	0
2	NAG	E	1	2,1	14,14,15	0.24	0	17,19,21	0.49	0
2	NAG	E	2	2	14,14,15	0.62	1 (7%)	17,19,21	1.27	1 (5%)
2	NAG	F	1	2,1	14,14,15	0.25	0	17,19,21	0.57	0
2	NAG	F	2	2	14,14,15	0.22	0	17,19,21	0.40	0
2	NAG	G	1	2,1	14,14,15	0.20	0	17,19,21	0.40	0
2	NAG	G	2	2	14,14,15	0.21	0	17,19,21	0.42	0
2	NAG	H	1	2,1	14,14,15	0.32	0	17,19,21	0.39	0
2	NAG	H	2	2	14,14,15	0.25	0	17,19,21	0.42	0
2	NAG	I	1	2,1	14,14,15	0.24	0	17,19,21	0.49	0
2	NAG	I	2	2	14,14,15	0.62	0	17,19,21	1.26	1 (5%)
2	NAG	J	1	2,1	14,14,15	0.24	0	17,19,21	0.57	0
2	NAG	J	2	2	14,14,15	0.23	0	17,19,21	0.40	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
2	NAG	C	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	D	2	2	-	1/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	E	2	2	-	5/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	H	2	2	-	1/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	I	2	2	-	5/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2	NAG	C1-C2	2.02	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	2	NAG	C2-N2-C7	4.30	129.03	122.90
2	E	2	NAG	C2-N2-C7	4.30	129.03	122.90

There are no chirality outliers.

5 of 42 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	NAG	O5-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6

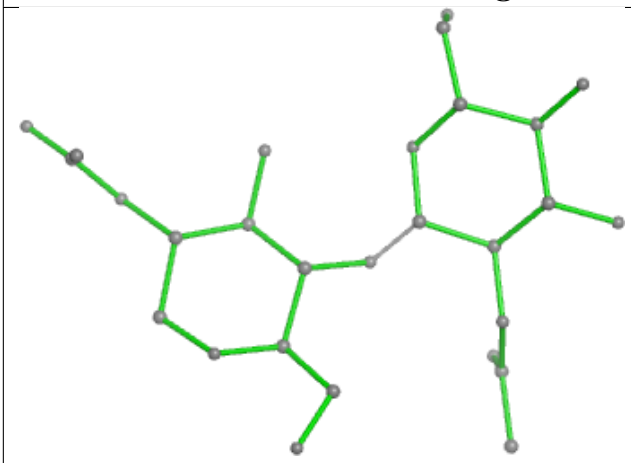
There are no ring outliers.

4 monomers are involved in 8 short contacts:

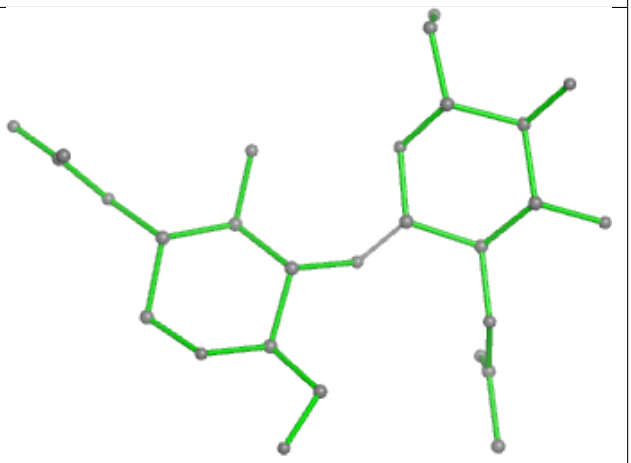
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	2	NAG	4	0
2	I	1	NAG	3	0
2	E	2	NAG	4	0
2	E	1	NAG	3	0

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

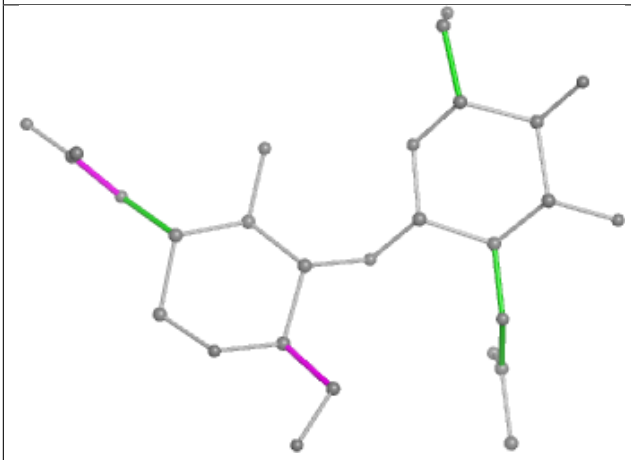
Oligosaccharide Chain C



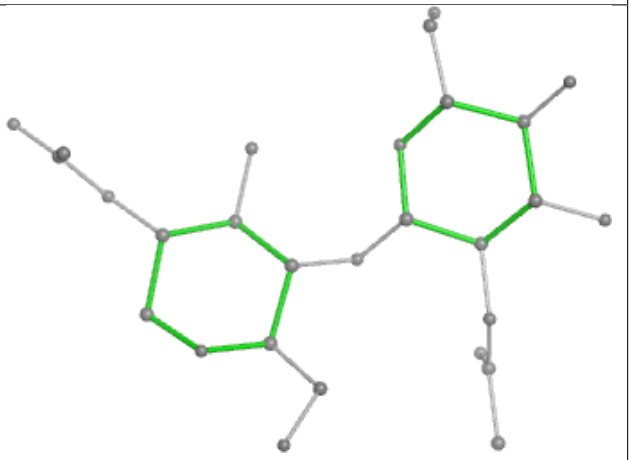
Bond lengths



Bond angles

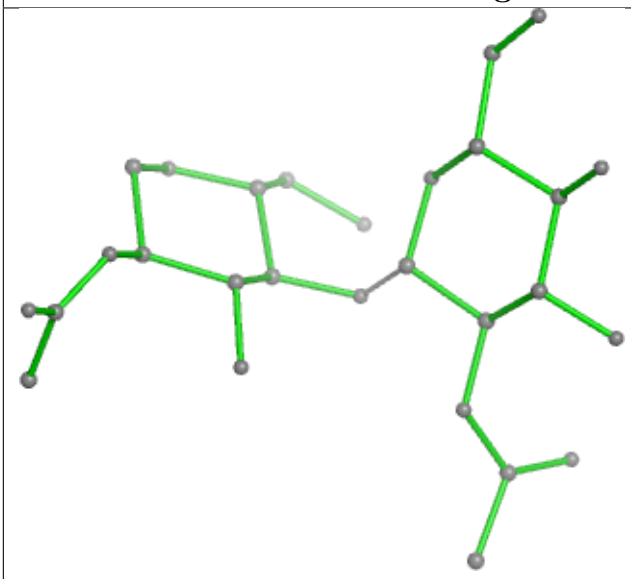


Torsions

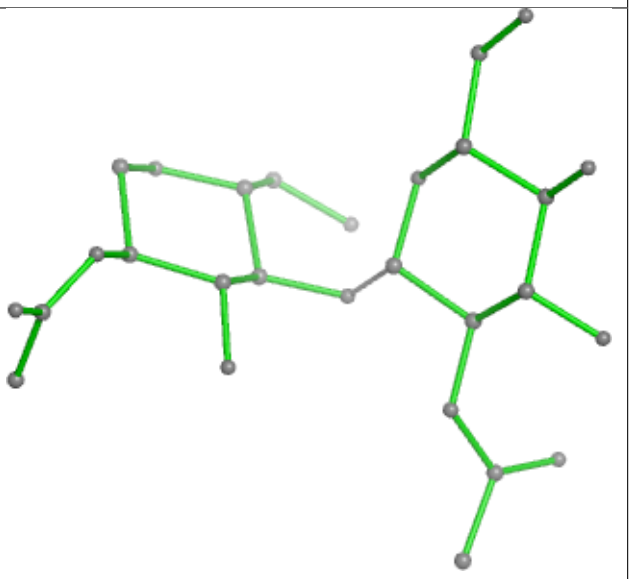


Rings

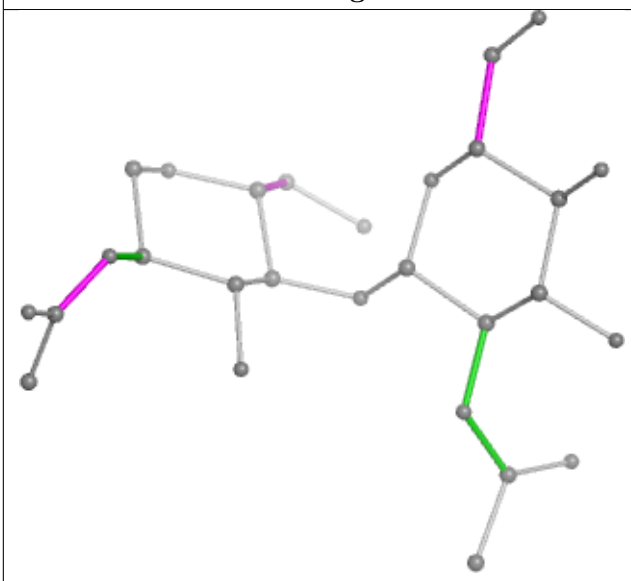
Oligosaccharide Chain D



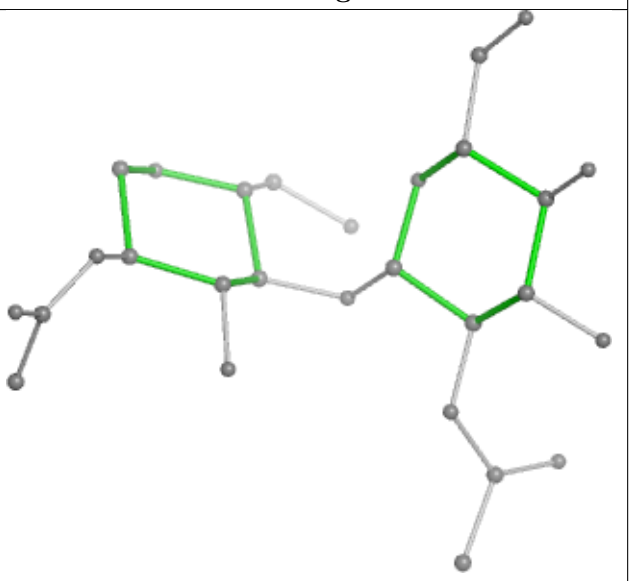
Bond lengths



Bond angles

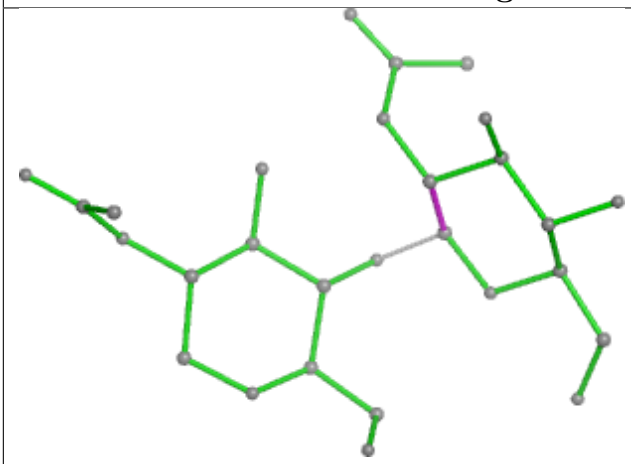


Torsions

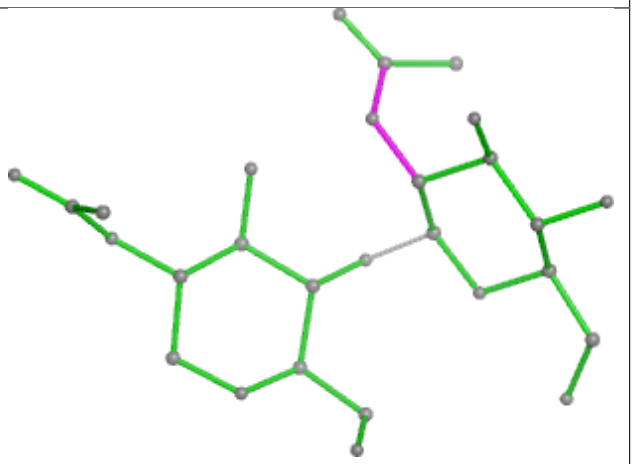


Rings

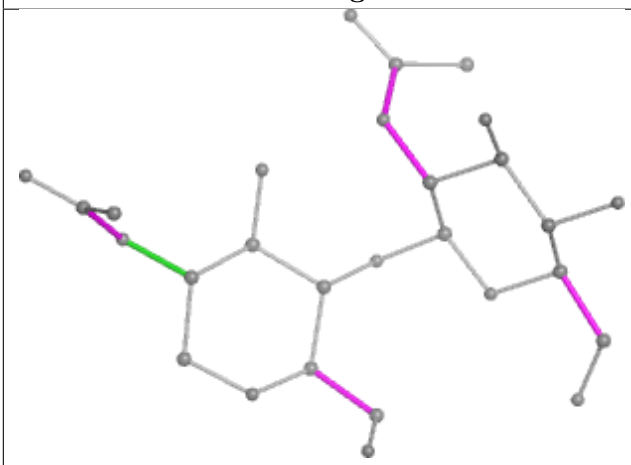
Oligosaccharide Chain E



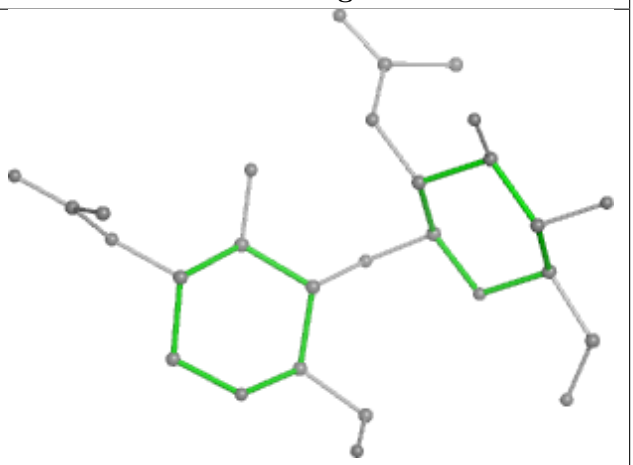
Bond lengths



Bond angles

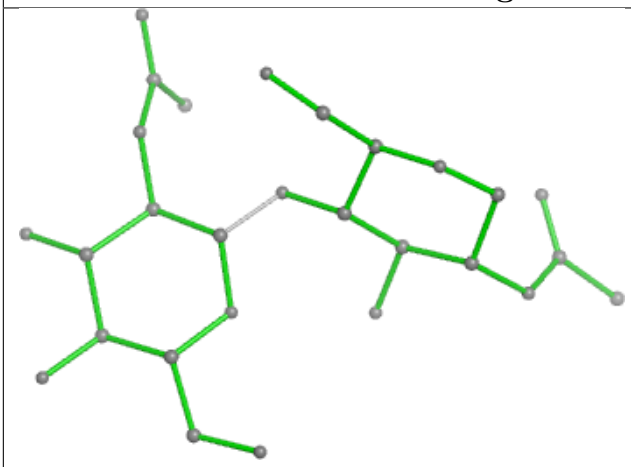


Torsions

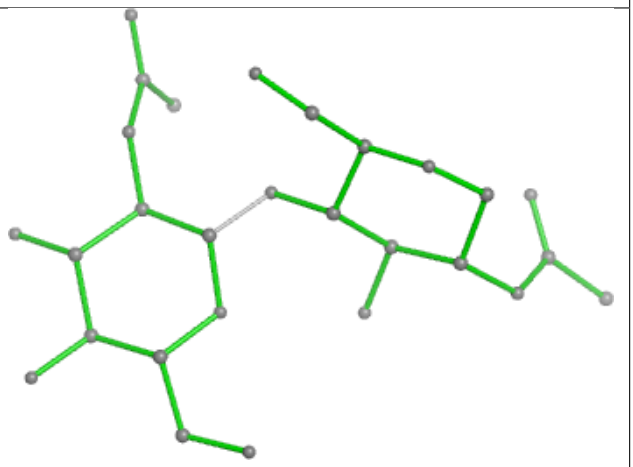


Rings

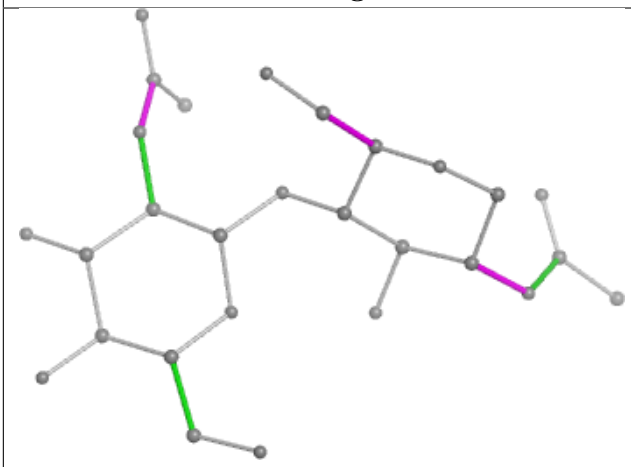
Oligosaccharide Chain F



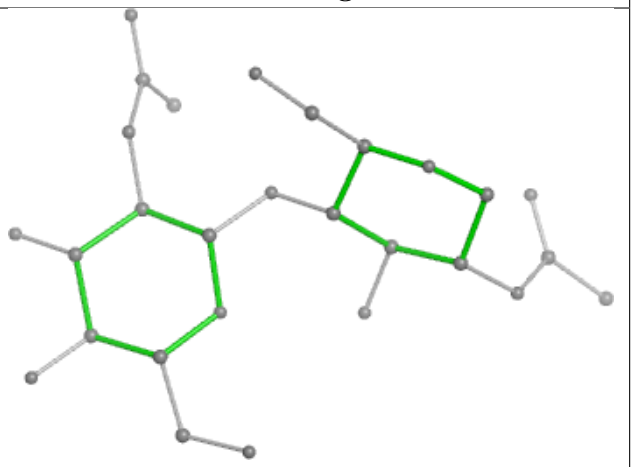
Bond lengths



Bond angles

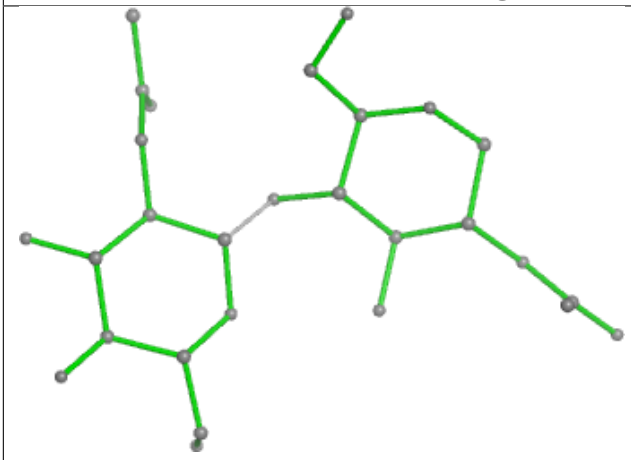


Torsions

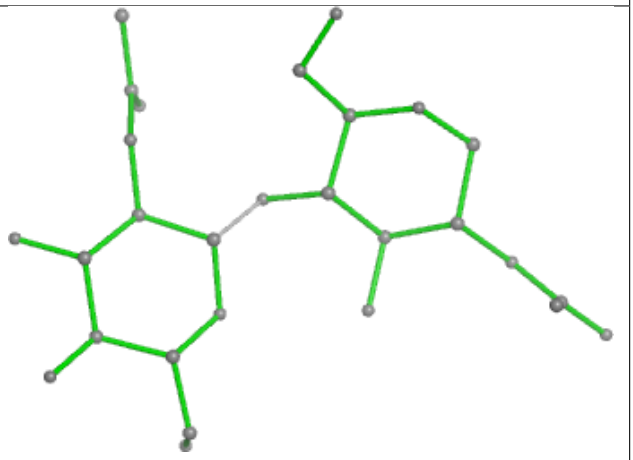


Rings

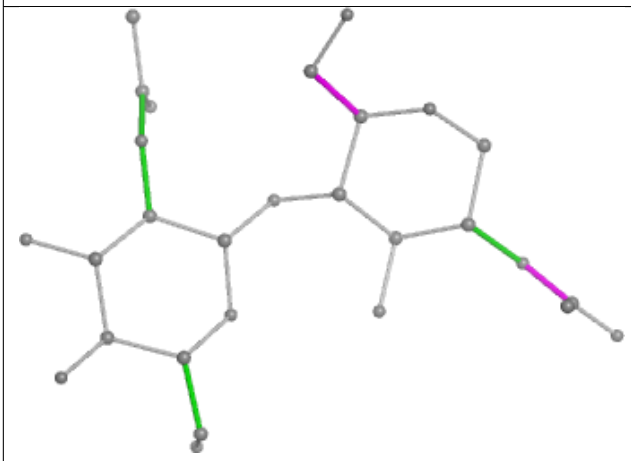
Oligosaccharide Chain G



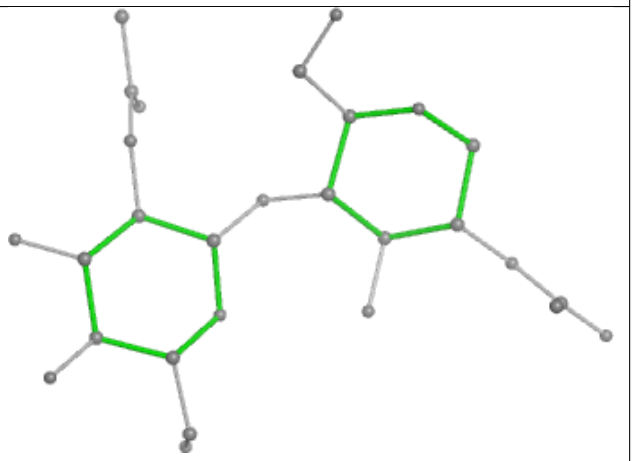
Bond lengths



Bond angles

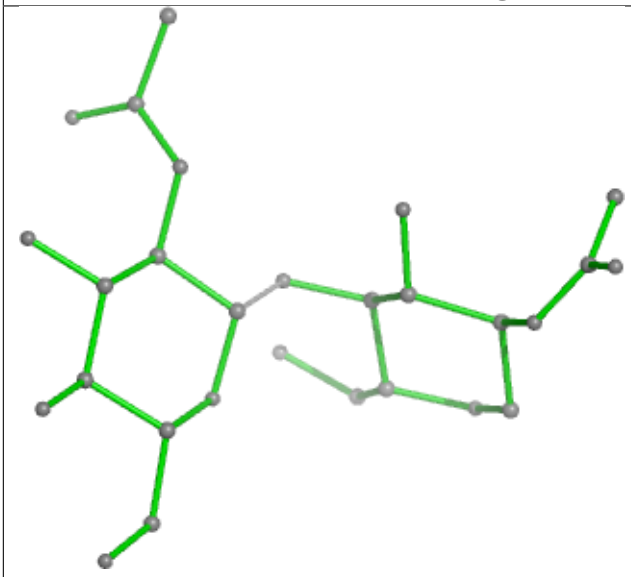


Torsions

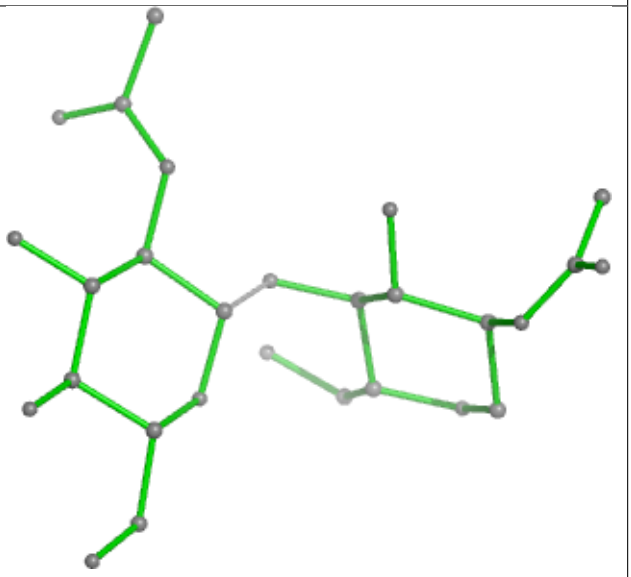


Rings

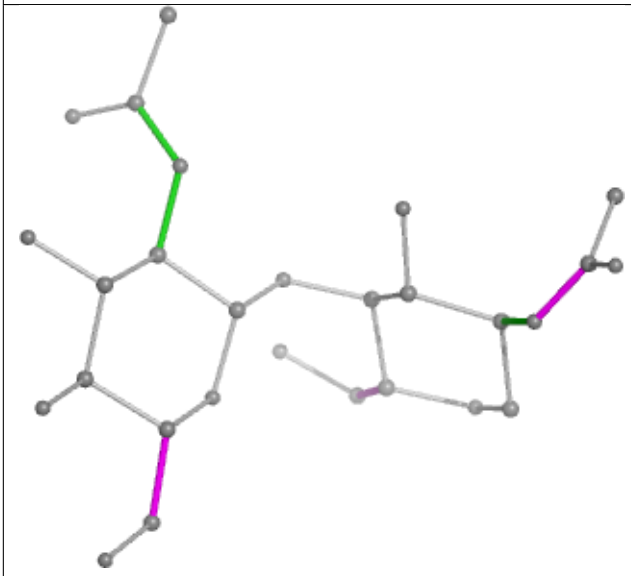
Oligosaccharide Chain H



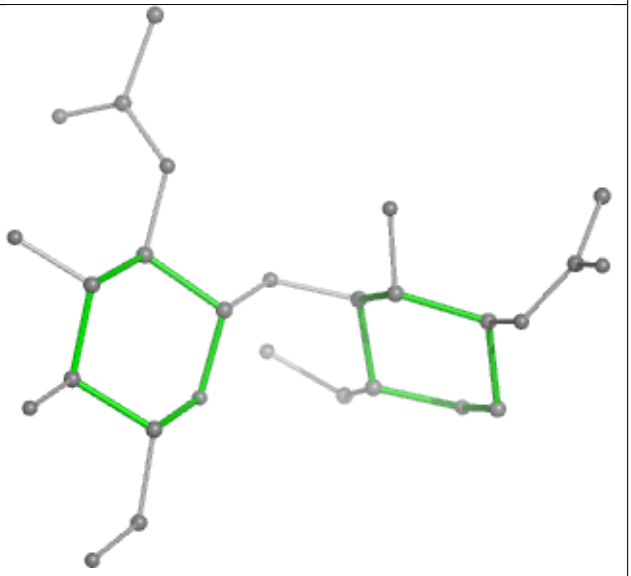
Bond lengths



Bond angles

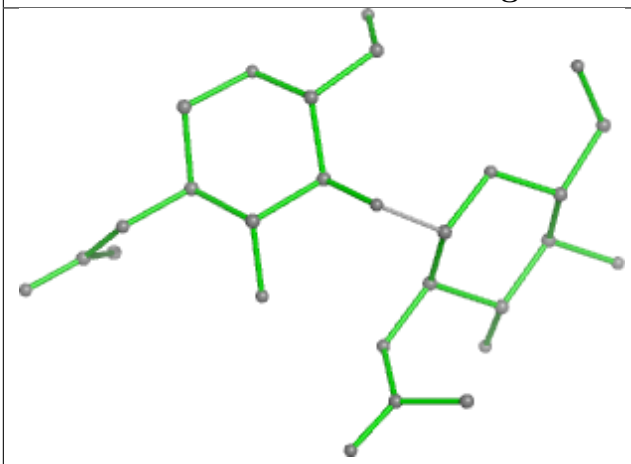


Torsions

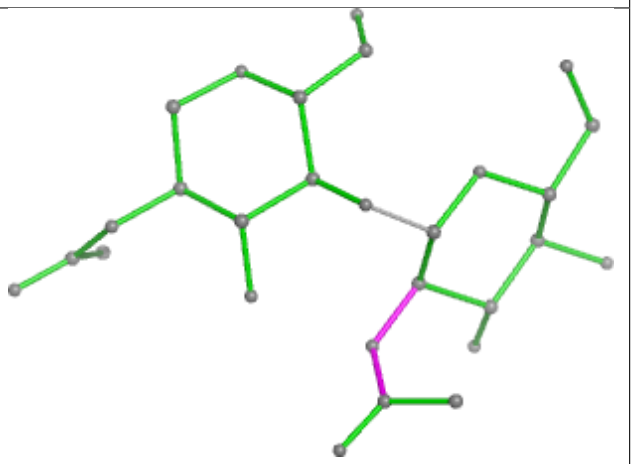


Rings

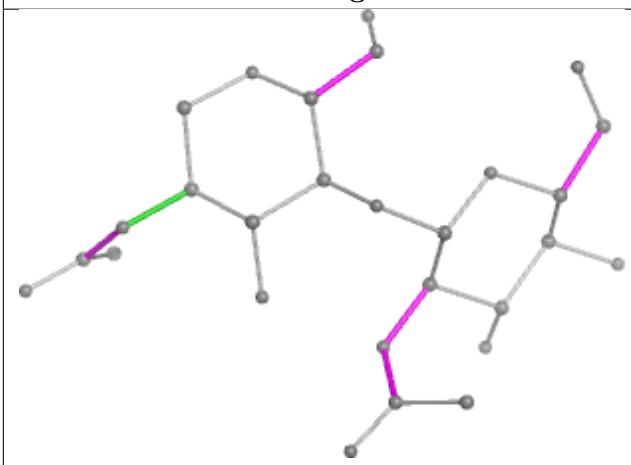
Oligosaccharide Chain I



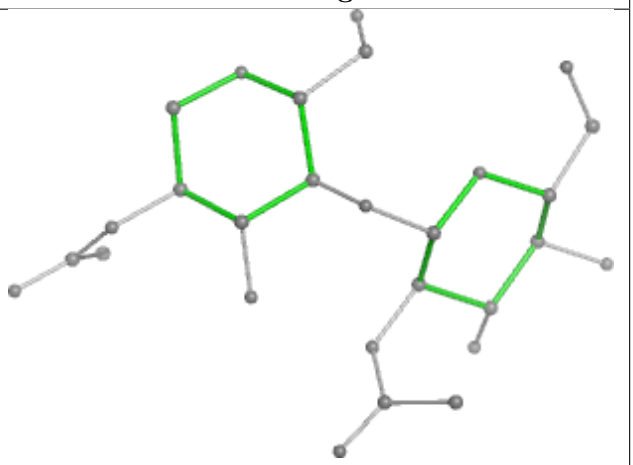
Bond lengths



Bond angles

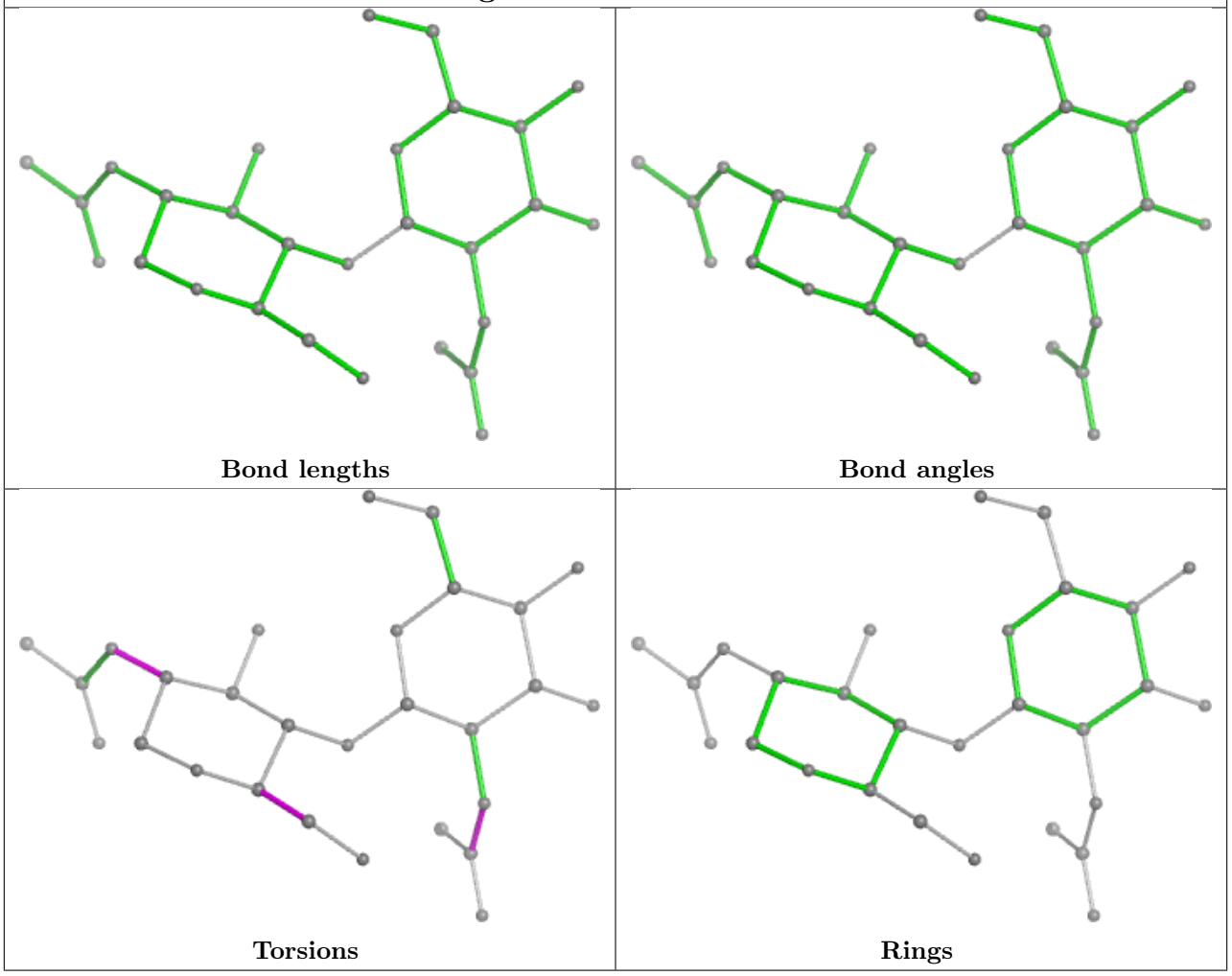


Torsions



Rings

Oligosaccharide Chain J



5.6 Ligand geometry (i)

16 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	$\#\|Z\| > 2$
3	NAG	A	2805	1	14,14,15	0.56	0	17,19,21	1.25	1 (5%)
3	NAG	B	2806	1	14,14,15	0.24	0	17,19,21	0.44	0
3	NAG	B	2802	1	14,14,15	0.21	0	17,19,21	0.42	0
3	NAG	B	2804	1	14,14,15	0.23	0	17,19,21	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	A	2808	1	14,14,15	0.22	0	17,19,21	0.41	0
3	NAG	A	2804	1	14,14,15	0.23	0	17,19,21	0.40	0
3	NAG	B	2807	-	15,15,15	0.20	0	21,21,21	0.28	0
3	NAG	A	2806	1	14,14,15	0.22	0	17,19,21	0.43	0
3	NAG	A	2803	1	14,14,15	0.21	0	17,19,21	0.46	0
3	NAG	A	2802	1	14,14,15	0.20	0	17,19,21	0.43	0
3	NAG	B	2801	1	14,14,15	0.19	0	17,19,21	0.42	0
3	NAG	A	2807	-	15,15,15	0.20	0	21,21,21	0.28	0
3	NAG	A	2801	1	14,14,15	0.20	0	17,19,21	0.42	0
3	NAG	B	2805	1	14,14,15	0.56	0	17,19,21	1.26	1 (5%)
3	NAG	B	2803	1	14,14,15	0.21	0	17,19,21	0.46	0
3	NAG	B	2808	1	14,14,15	0.21	0	17,19,21	0.42	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
3	NAG	A	2805	1	-	5/6/23/26	0/1/1/1
3	NAG	B	2806	1	-	2/6/23/26	0/1/1/1
3	NAG	B	2802	1	-	4/6/23/26	0/1/1/1
3	NAG	B	2804	1	-	2/6/23/26	0/1/1/1
3	NAG	A	2808	1	-	2/6/23/26	0/1/1/1
3	NAG	A	2804	1	-	2/6/23/26	0/1/1/1
3	NAG	B	2807	-	-	4/6/26/26	0/1/1/1
3	NAG	A	2806	1	-	2/6/23/26	0/1/1/1
3	NAG	A	2803	1	-	4/6/23/26	0/1/1/1
3	NAG	A	2802	1	-	4/6/23/26	0/1/1/1
3	NAG	B	2801	1	-	1/6/23/26	0/1/1/1
3	NAG	A	2807	-	-	4/6/26/26	0/1/1/1
3	NAG	A	2801	1	-	1/6/23/26	0/1/1/1
3	NAG	B	2805	1	-	5/6/23/26	0/1/1/1
3	NAG	B	2803	1	-	4/6/23/26	0/1/1/1
3	NAG	B	2808	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	2805	NAG	C2-N2-C7	4.29	129.01	122.90
3	A	2805	NAG	C2-N2-C7	4.26	128.97	122.90

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2804	NAG	O5-C5-C6-O6
3	B	2805	NAG	O5-C5-C6-O6
3	A	2804	NAG	O5-C5-C6-O6
3	A	2805	NAG	O5-C5-C6-O6
3	B	2804	NAG	C4-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2805	NAG	2	0
3	B	2807	NAG	1	0
3	A	2803	NAG	1	0
3	A	2807	NAG	1	0
3	B	2805	NAG	2	0
3	B	2803	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 Map visualisation

This section contains visualisations of the EMDB entry EMD-18889. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.