Full wwPDB EM Validation Report (i)

Dec 19, 2022 – 12:18 am GMT

PDB ID	:	7BAN
EMDB ID	:	EMD-12125
Title	:	human Teneurin4 Mut C2
Authors	:	Meijer, D.H.; Janssen, B.J.C.
Deposited on	:	2020-12-16
Resolution	:	2.70 Å(reported)

This is a Full wwPDB EM Validation 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 (i) 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 (1)) were used in the production of this report:

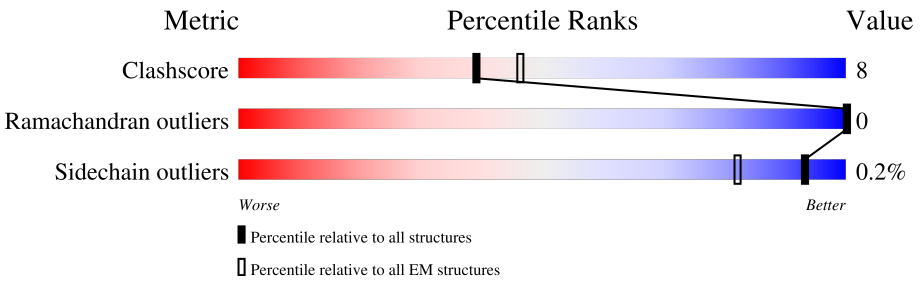
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 2.70 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1932	21% 79% 19% •
1	B	1932	21% 79% 19% •
2	C	2	100%
2	D	2	100%
2	E	2	100%
2	F	2	100% 100%
2	G	2	100%
2	H	2	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	I	2	100%
2	J	2	100% 100%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 30612 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-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1904	15093	9515	2625	2879	74	0	0
1	B	1904	15093	9515	2625	2879	74	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2585	CYS	SER	engineered mutation	UNP Q6N022
B	2585	CYS	SER	engineered mutation	UNP Q6N022

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

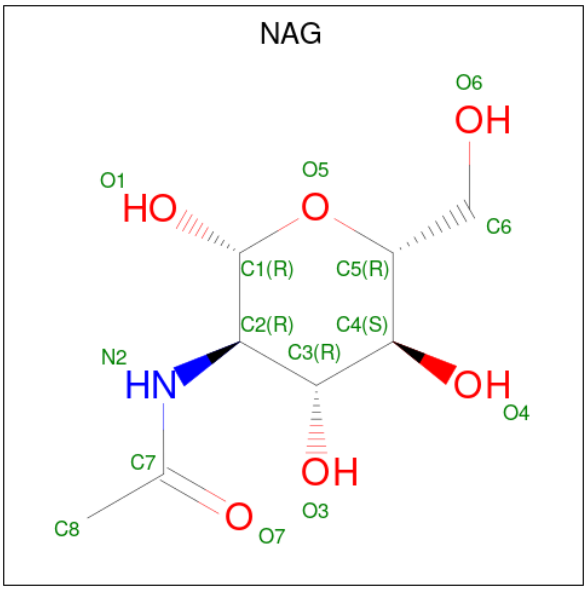
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	C	2	28	16	2	10	0	0
2	D	2	28	16	2	10	0	0
2	E	2	28	16	2	10	0	0
2	F	2	28	16	2	10	0	0
2	G	2	28	16	2	10	0	0
2	H	2	28	16	2	10	0	0
2	I	2	28	16	2	10	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	J	2	28	16	2	10	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	A	1	98	56	7	35	0
3	A	1	98	56	7	35	0
3	A	1	98	56	7	35	0
3	A	1	98	56	7	35	0
3	A	1	98	56	7	35	0
3	A	1	98	56	7	35	0
3	A	1	98	56	7	35	0
3	B	1	98	56	7	35	0
3	B	1	98	56	7	35	0
3	B	1	98	56	7	35	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	B	1	98	56	7	35	0
			Total	C	N	O	
3	B	1	98	56	7	35	0
			Total	C	N	O	
3	B	1	98	56	7	35	0
			Total	C	N	O	
3	B	1	98	56	7	35	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

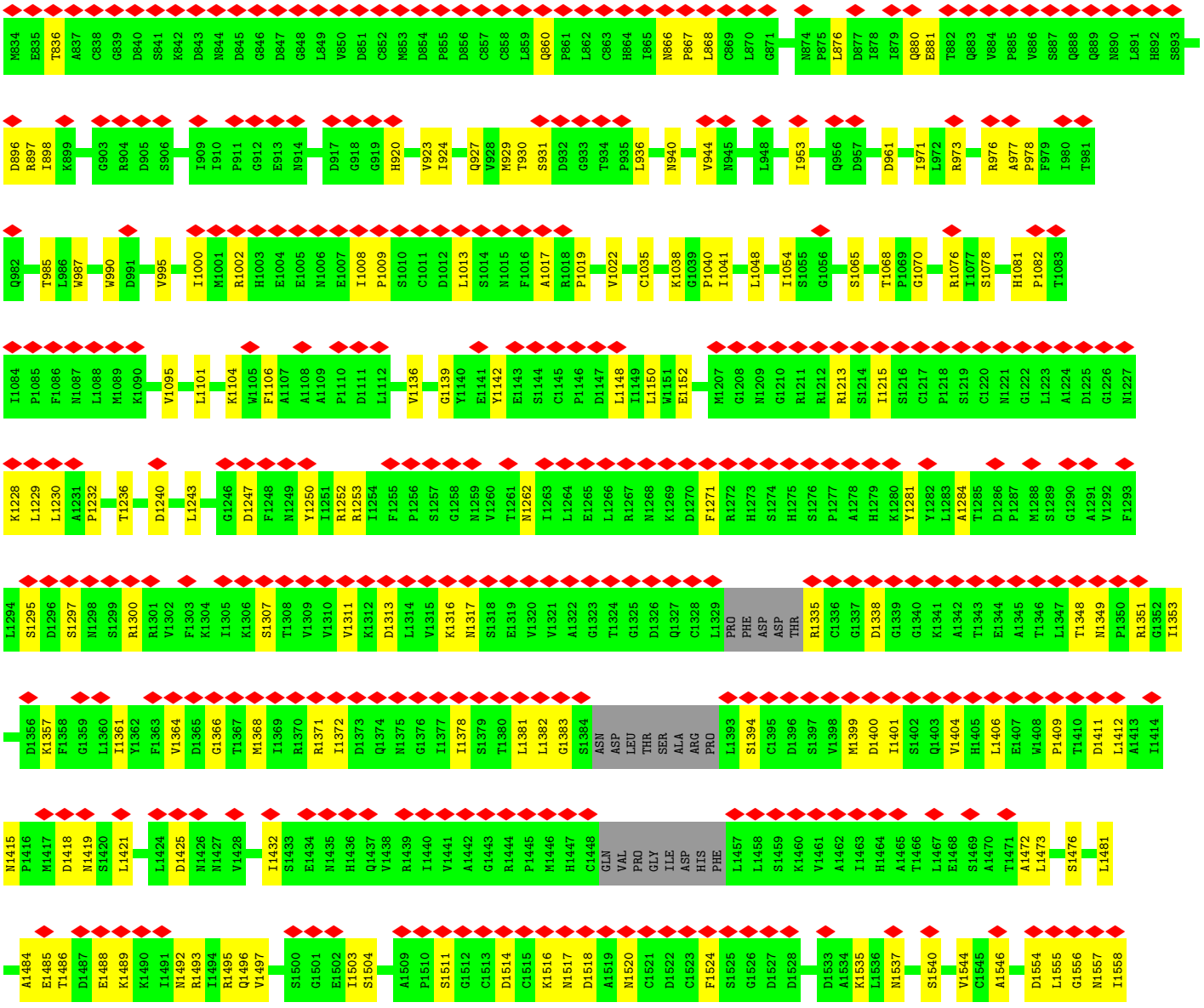
Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
4	A	3	3	3	0
			Total	Ca	
4	B	3	3	3	0

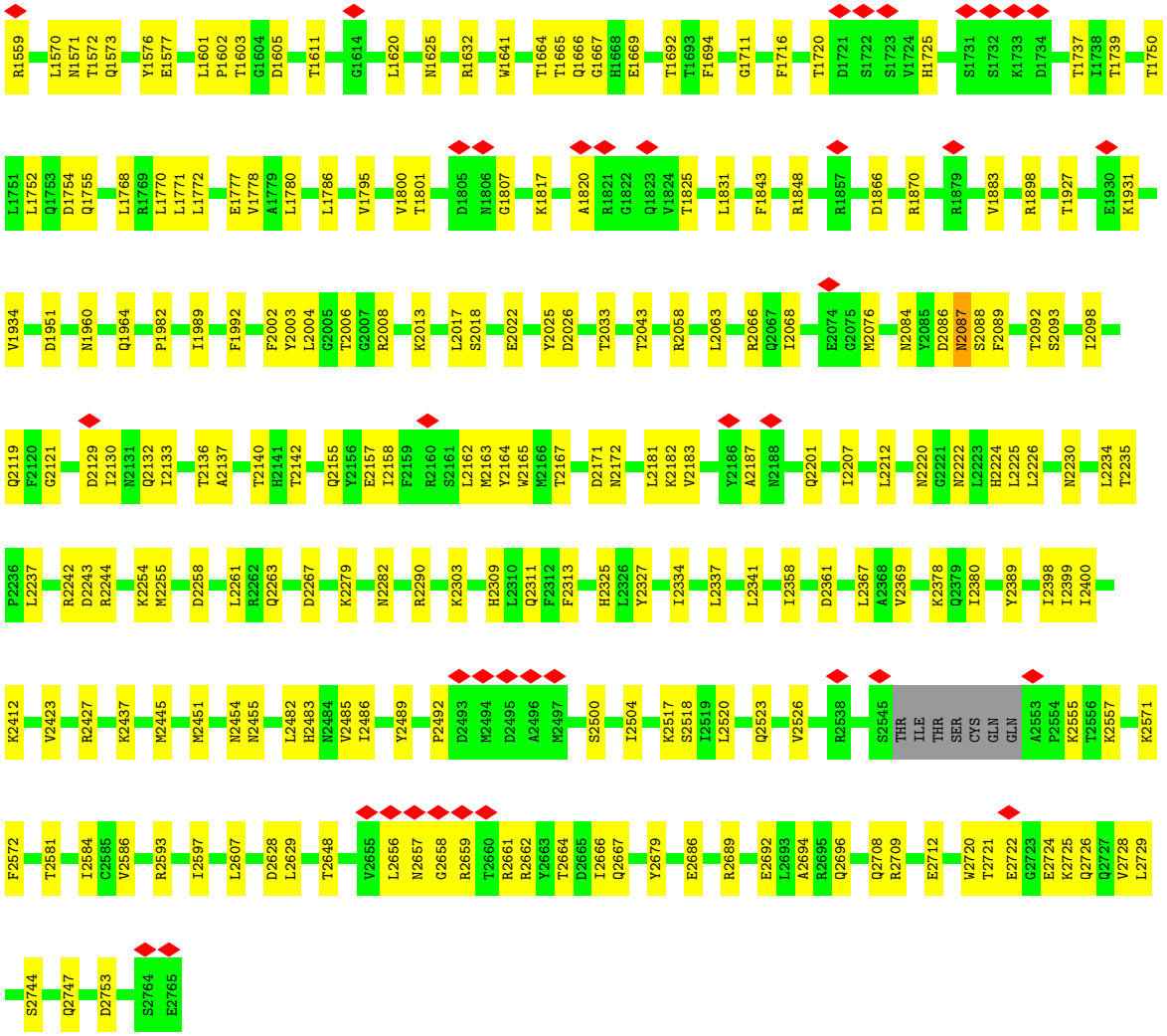
3 Residue-property plots (i)

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 and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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-4

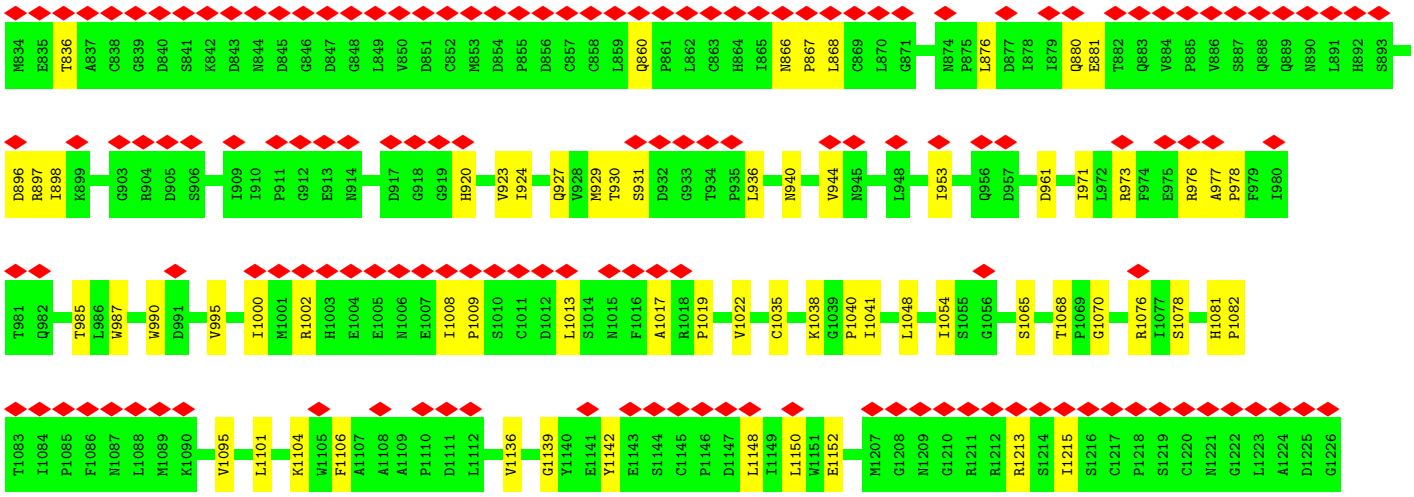
Chain A: 21% 79% 19%

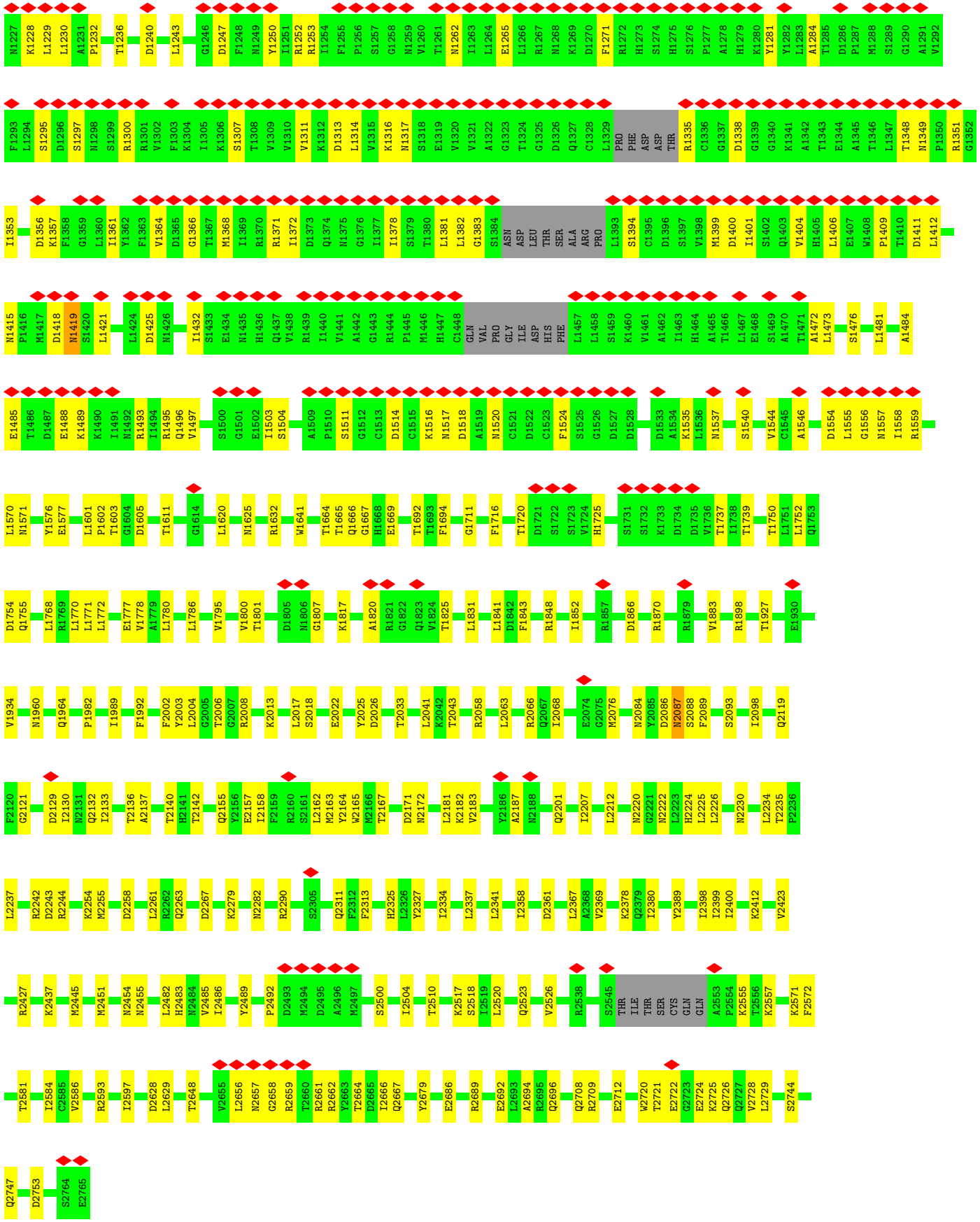




- Molecule 1: Teneurin-4

Chain B:




N1227 K1228 L1229 L1230 A1231 P1232 T1236 D1240 L1243 G1246 D1247 F1248 N1249 Y1250 I1251 R1252 R1253 I1254 F1255 P1256 S1257 G1258 N1259 V1260 T1261 N1262 I1263 L1264 E1265 L1266 R1267 N1268 K1269 D1270 F1271 R1272 H1273 S1274 H1275 S1276 P1277 A1278 H1279 K1280 Y1281 Y1282 L1283 A1284 T1285 D1286 P1287 M1288 S1289 G1290 A1291 V1292
F1293 L1294 S1295 D1296 S1297 N1298 S1299 R1300 R1301 V1302 F1303 K1304 I1305 K1306 S1307 T1308 V1309 V1310 V1311 K1312 D1313 L1314 V1315 K1316 N1317 S1318 E1319 V1320 V1321 A1322 G1323 T1324 G1325 D1326 Q1327 C1328 L1329 PRO PHE ASP ASP THR R1335 G1336 G1337 D1338 G1339 G1340 K1341 A1342 T1343 E1344 A1345 T1346 L1347 T1348 N1349 P1350 R1351 G1352
I1353 D1356 K1357 F1358 G1359 L1360 I1361 Y1362 F1363 V1364 D1365 G1366 T1367 M1368 T1369 R1370 R1371 I1372 D1373 Q1374 N1375 G1376 I1377 I1378 S1379 T1380 L1381 L1382 G1383 S1384 ASN ASP LEU THR SER ALA ARG PRO L1393 S1394 C1395 D1396 S1397 V1398 M1399 D1400 I1401 S1402 Q1403 V1404 H1405 L1406 E1407 W1408 P1409 T1410 D1411 L1412
N1415 P1416 M1417 D1418 N1419 S1420 L1421 L1424 D1425 N1426 I1432 S1433 E1434 N1435 H1436 Q1437 V1438 R1439 I1440 V1441 A1442 G1443 R1444 P1445 M1446 H1447 C1448 GLN VAL PRO GLY ILE ASP HIS PHE L1457 L1458 S1459 K1460 V1461 A1462 I1463 H1464 A1465 T1466 L1467 E1468 S1469 A1470 T1471 A1472 L1473 S1476 L1481 A1484
E1485 T1486 D1487 E1488 K1489 K1490 I1491 N1492 R1493 I1494 R1495 Q1496 V1497 S1500 G1501 E1502 I1503 S1504 A1509 P1510 S1511 G1512 C1513 D1514 C1515 K1516 N1517 D1518 A1519 N1520 C1521 D1522 C1523 F1524 S1525 G1526 D1527 D1528 D1533 A1534 K1535 L1536 N1537 S1540 V1544 C1545 A1546 D1554 L1555 G1556 N1557 I1558 R1559
L1570 N1571 Y1576 E1577 L1601 P1602 T1603 G1604 D1605 T1611 G1614 L1620 N1625 R1632 W1641 T1664 T1665 Q1666 G1667 H1668 E1669 T1692 T1693 F1694 G1711 F1716 T1720 D1721 S1722 S1723 V1724 H1725 S1731 S1732 K1733 D1734 D1735 V1736 T1737 I1738 T1739 T1750 L1751 L1752 Q1753
D1754 Q1755 L1768 R1769 L1770 L1771 L1772 E1777 V1778 A1779 L1780 L1786 V1795 V1800 T1801 D1805 N1806 G1807 K1817 A1820 R1821 G1822 Q1823 V1824 T1825 L1831 L1841 D1842 F1843 R1848 I1852 R1857 D1866 R1870 R1879 V1883 R1898 T1927 E1930
V1934 N1960 Q1964 P1982 I1989 F1992 F2002 Y2003 L2004 G2005 T2006 G2007 R2008 K2013 L2017 S2018 E2022 Y2025 D2026 T2033 L2041 K2042 T2043 R2058 L2063 R2066 Q2067 I2068 E2074 G2075 M2076 N2084 Y2085 D2086 N2087 S2088 F2089 S2093 I2098 Q2119
F2120 G2121 D2129 I2130 N2131 Q2132 I2133 T2136 A2137 T2140 H2141 T2142 Q2155 Y2156 E2157 I2158 F2159 R2160 S2161 L2162 M2163 Y2164 W2165 W2166 T2167 D2171 N2172 L2181 K2182 V2183 Y2186 A2187 N2188 Q2201 I2207 L2212 N2220 G2221 W2222 L2223 H2224 L2225 L2226 N2230 L2234 T2235 P2236
L2237 R2242 D2243 R2244 K2254 M2255 D2258 L2261 R2262 Q2263 D2267 K2279 N2282 R2290 S2305 Q2311 F2312 F2313 H2325 L2326 Y2327 I2334 L2337 L2341 I2358 D2361 L2367 A2368 V2369 K2378 Q2379 I2380 Y2389 I2398 I2399 I2400 K2412 V2423
R2427 K2437 M2445 M2451 N2454 N2455 L2482 H2483 N2484 V2485 I2486 Y2489 P2492 D2493 M2494 D2495 A2496 M2497 S2500 I2504 T2510 K2517 S2518 I2519 L2520 Q2523 V2526 R2538 S2545 THR ILE THR SER CYS GLN GLN A2553 P2554 K2555 T2556 K2557 K2571 F2572
T2581 I2584 C2585 V2586 R2593 I2597 D2628 L2629 T2648 V2655 L2656 N2657 G2658 R2659 T2660 R2661 R2662 Y2663 T2664 D2665 I2666 Q2667 Y2679 E2686 R2689 E2692 L2693 A2694 R2695 Q2696 Q2708 R2709 E2712 W2720 T2721 E2722 G2723 E2724 K2725 Q2726 Q2727 V2728 L2729 S2744
Q2747 D2753 S2764 E2765

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

Chain C: 100%

NAG1 NAG2

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

Chain D: 100%

NAG1 NAG2

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

Chain E: 100%

NAG1 NAG2

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

Chain F: 100% 100%

NAG1 NAG2

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

Chain G: 100%

NAG1 NAG2

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

Chain H: 100%

NAG1 NAG2

• 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, Not provided	
Number of particles used	242300	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.208	Depositor
Minimum map value	-0.131	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.028	Depositor
Map size (Å)	303.12, 303.12, 303.12	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.842, 0.842, 0.842	Depositor

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: CA, 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	0.30	0/15425	0.53	0/20912
1	B	0.30	0/15425	0.53	0/20912
All	All	0.30	0/30850	0.53	0/41824

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	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2025	TYR	Peptide
1	B	2025	TYR	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	15093	0	14709	240	0
1	B	15093	0	14709	238	0
2	C	28	0	25	0	0
2	D	28	0	25	0	0
2	E	28	0	25	0	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	0	0
2	J	28	0	25	0	0
3	A	98	0	91	1	0
3	B	98	0	91	1	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
All	All	30612	0	29800	472	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 8.

All (472) 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:2242:ARG:HH21	1:B:2244:ARG:HH21	1.25	0.84
1:A:2242:ARG:HH21	1:A:2244:ARG:HH21	1.25	0.83
1:B:1300:ARG:NH1	1:B:1349:ASN:OD1	2.18	0.77
1:B:2119:GLN:NE2	1:B:2121:GLY:O	2.18	0.77
1:B:1300:ARG:NH1	1:B:1348:THR:O	2.19	0.76
1:A:1300:ARG:NH1	1:A:1349:ASN:OD1	2.18	0.76
1:A:2119:GLN:NE2	1:A:2121:GLY:O	2.18	0.76
1:A:1300:ARG:NH1	1:A:1348:THR:O	2.18	0.75
1:A:1213:ARG:HH11	1:A:1229:LEU:HA	1.52	0.74
1:B:1213:ARG:HH11	1:B:1229:LEU:HA	1.52	0.74
1:B:1421:LEU:HB2	1:B:1432:ILE:HB	1.71	0.73
1:A:1421:LEU:HB2	1:A:1432:ILE:HB	1.70	0.72
1:B:2518:SER:HA	1:B:2523:GLN:HE21	1.56	0.71
1:B:2136:THR:HG22	1:B:2137:ALA:H	1.56	0.71
1:A:2136:THR:HG22	1:A:2137:ALA:H	1.56	0.70
1:A:2518:SER:HA	1:A:2523:GLN:HE21	1.56	0.70
1:A:1665:THR:HG22	1:A:1666:GLN:H	1.55	0.70
1:B:1665:THR:HG22	1:B:1666:GLN:H	1.55	0.70
1:B:1848:ARG:NH2	1:B:1866:ASP:O	2.25	0.70
1:A:1848:ARG:NH2	1:A:1866:ASP:O	2.25	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1964:GLN:HG3	1:B:1982:PRO:HD3	1.75	0.69
1:A:1964:GLN:HG3	1:A:1982:PRO:HD3	1.75	0.68
1:B:2279:LYS:HB2	1:B:2290:ARG:HH11	1.58	0.67
1:A:2656:LEU:HB2	1:A:2659:ARG:HB2	1.76	0.67
1:B:2656:LEU:HB2	1:B:2659:ARG:HB2	1.76	0.66
1:B:1473:LEU:HD11	1:B:1481:LEU:HD11	1.78	0.66
1:A:2013:LYS:HB2	1:A:2022:GLU:HB2	1.78	0.66
1:A:2279:LYS:HB2	1:A:2290:ARG:HH11	1.58	0.66
1:A:1473:LEU:HD11	1:A:1481:LEU:HD11	1.77	0.65
1:B:2013:LYS:HB2	1:B:2022:GLU:HB2	1.78	0.65
1:B:2597:ILE:HG22	1:B:2628:ASP:HB3	1.78	0.65
1:A:1311:VAL:HG22	1:A:1313:ASP:H	1.62	0.65
1:B:931:SER:HB3	1:B:1002:ARG:HG2	1.79	0.64
1:B:1311:VAL:HG22	1:B:1313:ASP:H	1.62	0.64
1:A:931:SER:HB3	1:A:1002:ARG:HG2	1.79	0.64
1:A:2597:ILE:HG22	1:A:2628:ASP:HB3	1.79	0.64
1:B:2087:ASN:O	1:B:2087:ASN:ND2	2.27	0.64
1:A:1415:ASN:ND2	1:A:1418:ASP:OD1	2.25	0.63
1:B:1017:ALA:O	1:B:1142:TYR:OH	2.15	0.63
1:B:1725:HIS:CD2	1:B:1739:THR:HG22	2.33	0.63
1:A:1725:HIS:CD2	1:A:1739:THR:HG22	2.33	0.63
1:B:2254:LYS:HB3	1:B:2263:GLN:HB3	1.81	0.63
1:A:1017:ALA:O	1:A:1142:TYR:OH	2.15	0.63
1:A:2254:LYS:HB3	1:A:2263:GLN:HB3	1.81	0.62
1:B:1415:ASN:ND2	1:B:1418:ASP:OD1	2.25	0.62
1:A:2744:SER:OG	1:A:2747:GLN:OE1	2.17	0.61
1:B:2242:ARG:NH2	1:B:2244:ARG:HH21	1.97	0.61
1:B:2267:ASP:OD1	1:B:2282:ASN:ND2	2.33	0.61
3:A:2803:NAG:H3	3:A:2803:NAG:H83	1.83	0.61
1:A:1831:LEU:HD21	1:A:2486:ILE:HD11	1.83	0.61
1:A:1820:ALA:HB2	1:A:1825:THR:HG23	1.83	0.60
1:A:1035:CYS:HB3	1:A:1038:LYS:HG2	1.83	0.60
1:B:1820:ALA:HB2	1:B:1825:THR:HG23	1.83	0.60
3:B:2803:NAG:H3	3:B:2803:NAG:H83	1.83	0.59
1:A:1068:THR:HG22	1:A:1070:GLY:H	1.66	0.59
1:B:1068:THR:HG22	1:B:1070:GLY:H	1.66	0.59
1:B:1035:CYS:HB3	1:B:1038:LYS:HG2	1.83	0.59
1:B:1831:LEU:HD21	1:B:2486:ILE:HD11	1.83	0.59
1:A:2087:ASN:O	1:A:2087:ASN:ND2	2.27	0.59
1:A:2267:ASP:OD1	1:A:2282:ASN:ND2	2.33	0.59
1:A:990:TRP:HE1	1:A:1546:ALA:HB3	1.67	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2686:GLU:OE2	1:A:2689:ARG:NH2	2.29	0.58
1:B:990:TRP:HE1	1:B:1546:ALA:HB3	1.67	0.58
1:B:2158:ILE:HD12	1:B:2163:MET:HG3	1.84	0.58
1:A:2242:ARG:NH2	1:A:2244:ARG:HH21	1.97	0.58
1:B:1778:VAL:HG13	1:B:1800:VAL:HG12	1.85	0.58
1:B:2201:GLN:HG2	1:B:2455:ASN:HB2	1.85	0.58
1:B:2593:ARG:O	1:B:2597:ILE:HG12	2.04	0.57
1:A:2593:ARG:O	1:A:2597:ILE:HG12	2.04	0.57
1:A:1778:VAL:HG13	1:A:1800:VAL:HG12	1.85	0.57
1:B:2744:SER:OG	1:B:2747:GLN:OE1	2.17	0.57
1:A:2158:ILE:HD12	1:A:2163:MET:HG3	1.84	0.57
1:A:2664:THR:HB	1:A:2679:TYR:HB2	1.87	0.57
1:B:2243:ASP:O	1:B:2427:ARG:NH2	2.38	0.57
1:A:2658:GLY:O	1:A:2659:ARG:HD3	2.05	0.56
1:A:2201:GLN:HG2	1:A:2455:ASN:HB2	1.85	0.56
1:A:2230:ASN:HB2	1:A:2389:TYR:HB2	1.87	0.56
1:A:1780:LEU:HD22	1:A:1795:VAL:HG11	1.88	0.56
1:B:2230:ASN:HB2	1:B:2389:TYR:HB2	1.87	0.56
1:A:2063:LEU:HD21	1:A:2089:PHE:HB3	1.88	0.56
1:A:2243:ASP:O	1:A:2427:ARG:NH2	2.38	0.56
1:A:2629:LEU:HD11	1:A:2666:ILE:HD11	1.87	0.56
1:B:2629:LEU:HD11	1:B:2666:ILE:HD11	1.87	0.56
1:B:2664:THR:HB	1:B:2679:TYR:HB2	1.87	0.56
1:B:1081:HIS:HB3	1:B:1082:PRO:HD2	1.88	0.56
1:B:2063:LEU:HD21	1:B:2089:PHE:HB3	1.88	0.56
1:A:1081:HIS:HB3	1:A:1082:PRO:HD2	1.88	0.55
1:B:2658:GLY:O	1:B:2659:ARG:HD3	2.05	0.55
1:B:2628:ASP:OD2	1:B:2679:TYR:OH	2.21	0.55
1:A:1768:LEU:HB2	1:A:1780:LEU:HB2	1.89	0.55
1:A:2722:GLU:O	1:A:2726:GLN:HG2	2.06	0.55
1:B:1768:LEU:HB2	1:B:1780:LEU:HB2	1.88	0.55
1:A:1250:TYR:HB3	1:A:1262:ASN:HD21	1.71	0.55
1:A:2694:ALA:HB1	1:A:2753:ASP:HB3	1.89	0.55
1:B:1780:LEU:HD22	1:B:1795:VAL:HG11	1.88	0.55
1:B:1883:VAL:HG22	1:B:1898:ARG:HD2	1.89	0.55
1:B:2722:GLU:O	1:B:2726:GLN:HG2	2.06	0.55
1:A:1555:LEU:HA	1:A:1558:ILE:HG22	1.89	0.54
1:A:2066:ARG:HH21	1:A:2068:ILE:HD11	1.73	0.54
1:B:1250:TYR:HB3	1:B:1262:ASN:HD21	1.71	0.54
1:A:2026:ASP:OD1	1:A:2026:ASP:N	2.41	0.54
1:B:876:LEU:O	1:B:880:GLN:HG2	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:927:GLN:HG2	1:B:929:MET:HE3	1.89	0.54
1:B:2066:ARG:HH21	1:B:2068:ILE:HD11	1.73	0.54
1:B:2337:LEU:HD11	1:B:2399:ILE:HD11	1.90	0.54
1:B:2518:SER:HA	1:B:2523:GLN:NE2	2.23	0.54
1:B:2694:ALA:HB1	1:B:2753:ASP:HB3	1.89	0.54
1:A:927:GLN:HG2	1:A:929:MET:HE3	1.90	0.53
1:B:1351:ARG:HB2	1:B:1364:VAL:HB	1.90	0.53
1:B:1554:ASP:O	1:B:1558:ILE:HA	2.09	0.53
1:A:876:LEU:O	1:A:880:GLN:HG2	2.08	0.53
1:B:836:THR:O	1:B:860:GLN:NE2	2.33	0.53
1:B:1786:LEU:O	1:B:1817:LYS:NZ	2.38	0.53
1:B:2026:ASP:OD1	1:B:2026:ASP:N	2.41	0.53
1:A:2224:HIS:HA	1:A:2237:LEU:HB2	1.91	0.53
1:A:2628:ASP:OD2	1:A:2679:TYR:OH	2.21	0.53
1:B:1555:LEU:HA	1:B:1558:ILE:HG22	1.89	0.53
1:A:1472:ALA:HB3	1:A:1484:ALA:HB3	1.89	0.53
1:A:1554:ASP:O	1:A:1558:ILE:HA	2.09	0.53
1:A:1228:LYS:O	1:A:1252:ARG:NH2	2.42	0.53
1:A:1883:VAL:HG22	1:A:1898:ARG:HD2	1.89	0.53
1:B:2076:MET:SD	1:B:2311:GLN:NE2	2.81	0.53
1:A:2225:LEU:HG	1:A:2234:LEU:HD12	1.91	0.53
1:A:2518:SER:HA	1:A:2523:GLN:NE2	2.23	0.53
1:B:2224:HIS:HA	1:B:2237:LEU:HB2	1.91	0.53
1:A:1139:GLY:HA2	1:A:1150:LEU:O	2.09	0.53
1:A:2140:THR:HB	1:A:2157:GLU:HB3	1.91	0.53
1:A:2182:LYS:HE3	1:A:2187:ALA:O	2.09	0.53
1:B:2686:GLU:OE2	1:B:2689:ARG:NH2	2.29	0.53
1:A:880:GLN:O	1:B:2662:ARG:NH2	2.39	0.52
1:A:1351:ARG:HB2	1:A:1364:VAL:HB	1.90	0.52
1:A:1665:THR:HG22	1:A:1666:GLN:OE1	2.09	0.52
1:B:1472:ALA:HB3	1:B:1484:ALA:HB3	1.89	0.52
1:B:2006:THR:OG1	1:B:2258:ASP:OD2	2.26	0.52
1:A:2242:ARG:HH21	1:A:2244:ARG:NH2	2.01	0.52
1:B:1665:THR:HG22	1:B:1666:GLN:OE1	2.09	0.52
1:B:2182:LYS:HE3	1:B:2187:ALA:O	2.09	0.52
1:A:1400:ASP:OD1	1:A:1401:ILE:N	2.42	0.52
1:A:1524:PHE:HB3	1:A:1557:ASN:ND2	2.25	0.52
1:A:2129:ASP:OD1	1:A:2130:ILE:N	2.43	0.52
1:A:2337:LEU:HD11	1:A:2399:ILE:HD11	1.90	0.52
1:B:1213:ARG:HD3	1:B:1252:ARG:HH22	1.75	0.52
1:B:2140:THR:HB	1:B:2157:GLU:HB3	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2225:LEU:HG	1:B:2234:LEU:HD12	1.91	0.52
1:B:1228:LYS:O	1:B:1252:ARG:NH2	2.42	0.52
1:B:1524:PHE:HB3	1:B:1557:ASN:ND2	2.25	0.52
1:B:1139:GLY:HA2	1:B:1150:LEU:O	2.09	0.52
1:A:881:GLU:OE1	1:B:2661:ARG:HA	2.10	0.51
1:A:1476:SER:HA	1:A:1544:VAL:HG11	1.92	0.51
1:B:1361:ILE:HB	1:B:1372:ILE:HB	1.92	0.51
1:B:1371:ARG:HH21	1:B:1381:LEU:HD12	1.75	0.51
1:A:1213:ARG:HD3	1:A:1252:ARG:HH22	1.75	0.51
1:A:2076:MET:SD	1:A:2311:GLN:NE2	2.81	0.51
1:B:924:ILE:O	1:B:961:ASP:HA	2.11	0.51
1:A:881:GLU:HG2	1:B:2662:ARG:HB3	1.93	0.51
1:A:898:ILE:HD12	1:A:923:VAL:HG21	1.92	0.51
1:B:1400:ASP:OD1	1:B:1401:ILE:N	2.41	0.51
1:B:1476:SER:HA	1:B:1544:VAL:HG11	1.92	0.51
1:A:1371:ARG:HH21	1:A:1381:LEU:HD12	1.75	0.51
1:A:2006:THR:OG1	1:A:2258:ASP:OD2	2.26	0.51
1:A:924:ILE:O	1:A:961:ASP:HA	2.11	0.51
1:A:836:THR:O	1:A:860:GLN:NE2	2.33	0.51
1:B:1989:ILE:HB	1:B:2002:PHE:HB2	1.93	0.51
1:B:2242:ARG:HH21	1:B:2244:ARG:NH2	2.01	0.51
1:B:898:ILE:HD12	1:B:923:VAL:HG21	1.93	0.51
1:B:1335:ARG:HB3	1:B:1338:ASP:HB3	1.93	0.51
1:A:1000:ILE:O	1:A:1000:ILE:HG13	2.12	0.50
1:A:2482:LEU:HA	1:A:2485:VAL:HG22	1.94	0.50
1:B:2327:TYR:HD1	1:B:2334:ILE:HG13	1.76	0.50
1:A:1368:MET:HG2	1:A:1383:GLY:HA2	1.93	0.50
1:A:1247:ASP:OD2	1:A:1252:ARG:NE	2.44	0.50
1:B:2708:GLN:NE2	1:B:2712:GLU:OE2	2.45	0.50
1:A:2662:ARG:HB3	1:B:881:GLU:HG2	1.92	0.50
1:A:1335:ARG:HB3	1:A:1338:ASP:HB3	1.93	0.50
1:A:1371:ARG:HE	1:A:1381:LEU:HD12	1.76	0.50
1:A:1557:ASN:O	1:A:1559:ARG:HG2	2.12	0.50
1:A:2708:GLN:NE2	1:A:2712:GLU:OE2	2.45	0.50
1:A:1666:GLN:HG2	1:A:1667:GLY:N	2.27	0.50
1:B:1666:GLN:HG2	1:B:1667:GLY:N	2.27	0.50
1:A:1485:GLU:OE2	1:A:1493:ARG:NE	2.44	0.50
1:B:2129:ASP:OD1	1:B:2130:ILE:N	2.43	0.50
1:B:2482:LEU:HA	1:B:2485:VAL:HG22	1.94	0.50
1:A:2648:THR:HG22	1:A:2667:GLN:HB3	1.94	0.50
1:B:1739:THR:OG1	1:B:1750:THR:HB	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1411:ASP:OD1	1:A:1412:LEU:N	2.43	0.50
1:A:1514:ASP:HB2	1:A:1517:ASN:HB2	1.94	0.50
1:A:2327:TYR:HD1	1:A:2334:ILE:HG13	1.76	0.50
1:B:1368:MET:HG2	1:B:1383:GLY:HA2	1.93	0.50
1:B:1557:ASN:O	1:B:1559:ARG:HG2	2.12	0.50
1:A:896:ASP:OD1	1:A:897:ARG:N	2.45	0.49
1:A:1361:ILE:HB	1:A:1372:ILE:HB	1.92	0.49
1:A:1989:ILE:HB	1:A:2002:PHE:HB2	1.93	0.49
1:B:1247:ASP:OD2	1:B:1252:ARG:NE	2.44	0.49
1:B:2648:THR:HG22	1:B:2667:GLN:HB3	1.94	0.49
1:B:896:ASP:OD1	1:B:897:ARG:N	2.45	0.49
1:B:1514:ASP:HB2	1:B:1517:ASN:HB2	1.94	0.49
1:A:1739:THR:OG1	1:A:1750:THR:HB	2.12	0.49
1:A:1313:ASP:HB3	1:A:1316:LYS:HB2	1.94	0.49
1:A:1931:LYS:NZ	1:A:1951:ASP:OD1	2.35	0.49
1:A:1307:SER:O	1:A:1317:ASN:ND2	2.42	0.49
1:A:1632:ARG:HG2	1:A:1641:TRP:CZ2	2.48	0.49
1:A:2661:ARG:HA	1:B:881:GLU:OE1	2.13	0.49
1:A:995:VAL:HG11	1:A:1101:LEU:HB2	1.95	0.49
1:B:944:VAL:HG12	1:B:973:ARG:HB2	1.95	0.49
1:B:1000:ILE:O	1:B:1000:ILE:HG13	2.12	0.49
1:B:1313:ASP:HB3	1:B:1316:LYS:HB2	1.94	0.49
1:B:1371:ARG:HE	1:B:1381:LEU:HD12	1.76	0.49
1:A:1511:SER:HB3	1:A:1535:LYS:NZ	2.28	0.49
1:A:2132:GLN:HG3	1:A:2341:LEU:HD12	1.95	0.49
1:B:1511:SER:HB3	1:B:1535:LYS:NZ	2.28	0.49
1:B:1632:ARG:HG2	1:B:1641:TRP:CZ2	2.48	0.49
1:A:1076:ARG:HG3	1:A:1720:THR:HG21	1.95	0.48
1:B:995:VAL:HG11	1:B:1101:LEU:HB2	1.95	0.48
1:B:1497:VAL:HG22	1:B:1503:ILE:HG12	1.94	0.48
1:B:2207:ILE:HD12	1:B:2212:LEU:HD12	1.95	0.48
1:A:990:TRP:NE1	1:A:1546:ALA:HB3	2.28	0.48
1:A:2207:ILE:HD12	1:A:2212:LEU:HD12	1.95	0.48
1:A:977:ALA:HB3	1:A:978:PRO:HD3	1.95	0.48
1:A:1497:VAL:HG22	1:A:1503:ILE:HG12	1.94	0.48
1:A:2226:LEU:O	1:A:2235:THR:HG22	2.14	0.48
1:A:2662:ARG:HE	1:B:881:GLU:HA	1.79	0.48
1:B:1495:ARG:HH21	1:B:1503:ILE:HG21	1.77	0.48
1:A:1013:LEU:HB2	1:A:1148:LEU:HD11	1.94	0.48
1:B:1013:LEU:HB2	1:B:1148:LEU:HD11	1.94	0.48
1:B:2132:GLN:HG3	1:B:2341:LEU:HD12	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1284:ALA:HB2	1:A:1353:ILE:HG23	1.96	0.48
1:B:1250:TYR:HD2	1:B:1262:ASN:HD21	1.61	0.48
1:B:1364:VAL:HG11	1:B:1409:PRO:HG2	1.96	0.48
1:B:1411:ASP:OD1	1:B:1412:LEU:N	2.43	0.48
1:B:2451:MET:SD	1:B:2454:ASN:HA	2.54	0.48
1:B:1284:ALA:HB2	1:B:1353:ILE:HG23	1.96	0.48
1:B:1076:ARG:NH1	1:B:1078:SER:HB3	2.29	0.48
1:B:2171:ASP:OD1	1:B:2172:ASN:N	2.44	0.48
1:A:2378:LYS:HE3	1:A:2380:ILE:HD11	1.96	0.48
1:A:2451:MET:SD	1:A:2454:ASN:HA	2.54	0.48
1:B:990:TRP:NE1	1:B:1546:ALA:HB3	2.28	0.48
1:B:2226:LEU:O	1:B:2235:THR:HG22	2.14	0.48
1:A:944:VAL:HG12	1:A:973:ARG:HB2	1.95	0.48
1:B:1537:ASN:ND2	1:B:1556:GLY:HA3	2.29	0.48
1:A:1495:ARG:HH21	1:A:1503:ILE:HG21	1.77	0.47
1:A:1786:LEU:O	1:A:1817:LYS:NZ	2.38	0.47
1:B:868:LEU:HB3	1:B:976:ARG:NH2	2.29	0.47
1:B:1076:ARG:HG3	1:B:1720:THR:HG21	1.95	0.47
1:A:1048:LEU:H	1:A:1065:SER:HB3	1.79	0.47
1:A:1486:THR:OG1	1:A:1492:ASN:OD1	2.31	0.47
1:A:1537:ASN:ND2	1:A:1556:GLY:HA3	2.29	0.47
1:A:868:LEU:HB3	1:A:976:ARG:NH2	2.29	0.47
1:A:2171:ASP:OD1	1:A:2172:ASN:N	2.44	0.47
1:A:2662:ARG:NH2	1:B:880:GLN:O	2.42	0.47
1:B:1518:ASP:OD1	1:B:1520:ASN:N	2.46	0.47
1:B:1605:ASP:OD2	1:B:1848:ARG:NH1	2.43	0.47
1:A:1364:VAL:HG11	1:A:1409:PRO:HG2	1.96	0.47
1:A:1496:GLN:HE21	1:A:1504:SER:HB2	1.80	0.47
1:A:1665:THR:HG22	1:A:1666:GLN:N	2.28	0.47
1:B:1511:SER:HB3	1:B:1535:LYS:HZ2	1.80	0.47
1:A:2133:ILE:HG12	1:A:2142:THR:HG23	1.96	0.47
1:B:2313:PHE:HB2	1:B:2325:HIS:HB2	1.97	0.47
1:A:2279:LYS:HB2	1:A:2290:ARG:NH1	2.29	0.47
1:B:2378:LYS:HE3	1:B:2380:ILE:HD11	1.96	0.47
1:A:1409:PRO:HB3	1:A:1425:ASP:HB2	1.97	0.46
1:B:1496:GLN:HE21	1:B:1504:SER:HB2	1.80	0.46
1:B:2086:ASP:C	1:B:2088:SER:H	2.19	0.46
1:B:2133:ILE:HG12	1:B:2142:THR:HG23	1.96	0.46
1:B:1048:LEU:H	1:B:1065:SER:HB3	1.79	0.46
1:B:1770:LEU:HD13	1:B:2526:VAL:HG11	1.97	0.46
1:A:1250:TYR:HD2	1:A:1262:ASN:HD21	1.61	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2164:TYR:HA	1:A:2182:LYS:O	2.16	0.46
1:B:1409:PRO:HB3	1:B:1425:ASP:HB2	1.97	0.46
1:B:977:ALA:HB3	1:B:978:PRO:HD3	1.95	0.46
1:A:2584:ILE:HG13	1:A:2586:VAL:HG12	1.97	0.46
1:B:1349:ASN:HB2	1:B:1366:GLY:HA2	1.97	0.46
1:B:2164:TYR:HA	1:B:2182:LYS:O	2.16	0.46
1:A:881:GLU:HA	1:B:2662:ARG:HE	1.80	0.46
1:A:2692:GLU:O	1:A:2696:GLN:HG2	2.16	0.46
1:B:1215:ILE:HD11	1:B:1271:PHE:CD1	2.50	0.46
1:B:1992:PHE:CE1	1:B:2557:LYS:HD2	2.51	0.46
1:B:2584:ILE:HG13	1:B:2586:VAL:HG12	1.97	0.46
1:A:1022:VAL:HB	1:A:1078:SER:OG	2.16	0.46
1:A:1076:ARG:NH1	1:A:1078:SER:HB3	2.29	0.46
1:A:2313:PHE:HB2	1:A:2325:HIS:HB2	1.97	0.46
1:B:2136:THR:HG22	1:B:2137:ALA:N	2.28	0.46
1:A:1349:ASN:HB2	1:A:1366:GLY:HA2	1.97	0.46
1:A:1770:LEU:HD13	1:A:2526:VAL:HG11	1.97	0.46
1:A:920:HIS:HB2	1:A:990:TRP:CZ3	2.51	0.46
1:A:1605:ASP:OD2	1:A:1848:ARG:NH1	2.43	0.46
1:A:1992:PHE:CE1	1:A:2557:LYS:HD2	2.51	0.45
1:B:1601:LEU:HB3	1:B:1602:PRO:HD3	1.98	0.45
1:A:1040:PRO:HG2	1:A:1041:ILE:HD12	1.98	0.45
1:B:1485:GLU:OE2	1:B:1493:ARG:NE	2.44	0.45
1:A:1215:ILE:HD11	1:A:1271:PHE:CD1	2.51	0.45
1:A:1572:THR:OG1	1:A:1573:GLN:OE1	2.31	0.45
1:B:920:HIS:HB2	1:B:990:TRP:CZ3	2.51	0.45
1:B:2692:GLU:O	1:B:2696:GLN:HG2	2.16	0.45
1:A:2136:THR:HG22	1:A:2137:ALA:N	2.28	0.45
1:A:1213:ARG:NH1	1:A:1252:ARG:HH21	2.14	0.45
1:B:1989:ILE:HD13	1:B:2004:LEU:HD13	1.97	0.45
1:B:1022:VAL:HB	1:B:1078:SER:OG	2.16	0.45
1:B:1725:HIS:HD2	1:B:1739:THR:HG22	1.80	0.45
1:B:2017:LEU:O	1:B:2018:SER:OG	2.31	0.45
1:A:1297:SER:HA	1:A:1300:ARG:HH21	1.82	0.45
1:A:2607:LEU:HD23	1:A:2607:LEU:HA	1.84	0.45
1:A:1394:SER:HB3	1:A:1399:MET:SD	2.57	0.45
1:A:1770:LEU:CD2	1:A:1778:VAL:HB	2.47	0.45
1:B:1250:TYR:HD2	1:B:1262:ASN:ND2	2.15	0.45
1:B:2720:TRP:HB3	1:B:2724:GLU:HG3	1.99	0.45
1:A:1601:LEU:HB3	1:A:1602:PRO:HD3	1.98	0.45
1:B:1040:PRO:HG2	1:B:1041:ILE:HD12	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1232:PRO:O	1:B:1555:LEU:HD11	2.17	0.45
1:A:2361:ASP:HB3	1:A:2367:LEU:HD11	1.99	0.44
1:B:1666:GLN:HG2	1:B:1667:GLY:H	1.82	0.44
1:A:1095:VAL:HG22	1:A:1136:VAL:HG22	2.00	0.44
1:A:1989:ILE:HD13	1:A:2004:LEU:HD13	1.98	0.44
1:B:1213:ARG:NH1	1:B:1252:ARG:HH21	2.14	0.44
1:B:1495:ARG:NH2	1:B:1503:ILE:HG21	2.32	0.44
1:B:1770:LEU:CD2	1:B:1778:VAL:HB	2.47	0.44
1:A:1725:HIS:HD2	1:A:1739:THR:HG22	1.80	0.44
1:B:1297:SER:HA	1:B:1300:ARG:HH21	1.81	0.44
1:A:1495:ARG:NH2	1:A:1503:ILE:HG21	2.32	0.44
1:A:1771:LEU:HD22	1:A:1777:GLU:OE2	2.18	0.44
1:A:1625:ASN:OD1	1:A:1870:ARG:NH1	2.46	0.44
1:A:1770:LEU:HD12	1:A:1772:LEU:HD21	1.99	0.44
1:B:1095:VAL:HG22	1:B:1136:VAL:HG22	2.00	0.44
1:B:2361:ASP:HB3	1:B:2367:LEU:HD11	1.99	0.44
1:A:1603:THR:HG23	1:A:1843:PHE:CZ	2.53	0.44
1:A:2720:TRP:HB3	1:A:2724:GLU:HG3	1.99	0.44
1:A:2726:GLN:HA	1:A:2729:LEU:HG	1.99	0.44
1:B:987:TRP:HB2	1:B:1357:LYS:HG3	2.00	0.44
1:A:1571:ASN:HD21	1:A:1577:GLU:CD	2.21	0.44
1:A:1692:THR:HG23	1:A:1694:PHE:CE1	2.53	0.44
1:B:1394:SER:HB3	1:B:1399:MET:SD	2.57	0.44
1:B:1488:GLU:HB3	1:B:1516:LYS:HD2	1.99	0.44
1:A:1232:PRO:O	1:A:1555:LEU:HD11	2.17	0.44
1:A:2003:TYR:HB2	1:A:2008:ARG:HB2	2.00	0.44
1:A:2358:ILE:HD12	1:A:2369:VAL:HG22	1.99	0.44
1:B:1236:THR:O	1:B:1243:LEU:HD12	2.17	0.44
1:B:2358:ILE:HD12	1:B:2369:VAL:HG22	1.99	0.44
1:B:940:ASN:HA	1:B:953:ILE:HD13	2.00	0.44
1:A:940:ASN:HA	1:A:953:ILE:HD13	2.00	0.43
1:A:2086:ASP:C	1:A:2088:SER:H	2.19	0.43
1:B:1665:THR:HG22	1:B:1666:GLN:N	2.28	0.43
1:B:2726:GLN:HA	1:B:2729:LEU:HG	1.99	0.43
1:A:1250:TYR:HD2	1:A:1262:ASN:ND2	2.15	0.43
1:A:1927:THR:HB	1:A:1934:VAL:CG1	2.49	0.43
1:A:2398:ILE:HG22	1:A:2400:ILE:H	1.83	0.43
1:B:1603:THR:HG23	1:B:1843:PHE:CZ	2.53	0.43
1:A:2721:THR:O	1:A:2725:LYS:HG3	2.18	0.43
1:B:2003:TYR:HB2	1:B:2008:ARG:HB2	2.00	0.43
1:B:2708:GLN:OE1	1:B:2709:ARG:NH1	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:866:ASN:OD1	1:A:867:PRO:HD2	2.18	0.43
1:A:1236:THR:O	1:A:1243:LEU:HD12	2.17	0.43
1:A:2708:GLN:OE1	1:A:2709:ARG:NH1	2.51	0.43
1:B:1041:ILE:HG21	1:B:1716:PHE:CZ	2.54	0.43
1:B:1960:ASN:OD1	1:B:2220:ASN:ND2	2.51	0.43
1:A:1488:GLU:HB3	1:A:1516:LYS:HD2	1.99	0.43
1:B:1692:THR:HG23	1:B:1694:PHE:HE1	1.84	0.43
1:B:1754:ASP:O	1:B:1755:GLN:HG3	2.18	0.43
1:B:2058:ARG:CZ	1:B:2066:ARG:HD3	2.49	0.43
1:B:2721:THR:O	1:B:2725:LYS:HG3	2.18	0.43
1:A:2058:ARG:CZ	1:A:2066:ARG:HD3	2.49	0.43
1:B:1472:ALA:HB2	1:B:1540:SER:O	2.19	0.43
1:B:1770:LEU:HD12	1:B:1772:LEU:HD21	1.99	0.43
1:A:1692:THR:HG23	1:A:1694:PHE:HE1	1.84	0.43
1:A:2500:SER:O	1:A:2504:ILE:HG12	2.19	0.43
1:B:971:ILE:HD12	1:B:985:THR:HG22	2.01	0.43
1:B:1927:THR:HB	1:B:1934:VAL:CG1	2.49	0.43
1:B:2398:ILE:HG22	1:B:2400:ILE:H	1.83	0.43
1:A:987:TRP:HB2	1:A:1357:LYS:HG3	2.00	0.43
1:A:1754:ASP:O	1:A:1755:GLN:HG3	2.18	0.43
1:B:1692:THR:HG23	1:B:1694:PHE:CE1	2.53	0.43
1:B:1771:LEU:HD22	1:B:1777:GLU:OE2	2.17	0.43
1:B:2255:MET:SD	1:B:2261:LEU:HA	2.59	0.43
1:A:1737:THR:OG1	1:A:1752:LEU:HB3	2.19	0.43
1:A:2483:HIS:HA	1:A:2489:TYR:HB3	2.01	0.43
1:B:1571:ASN:HD21	1:B:1577:GLU:CD	2.22	0.43
1:B:2483:HIS:CD2	1:B:2492:PRO:HD3	2.54	0.43
1:B:2571:LYS:O	1:B:2581:THR:HA	2.19	0.43
1:A:1666:GLN:HG2	1:A:1667:GLY:H	1.82	0.42
1:B:866:ASN:OD1	1:B:867:PRO:HD2	2.18	0.42
1:B:1382:LEU:HD21	1:B:1406:LEU:HD23	2.00	0.42
1:B:1737:THR:OG1	1:B:1752:LEU:HB3	2.19	0.42
1:A:2181:LEU:HD13	1:A:2183:VAL:HG23	2.01	0.42
1:A:2255:MET:SD	1:A:2261:LEU:HA	2.59	0.42
1:B:2181:LEU:HD13	1:B:2183:VAL:HG23	2.01	0.42
1:B:2657:ASN:HB2	1:B:2659:ARG:NH1	2.34	0.42
1:B:1625:ASN:OD1	1:B:1870:ARG:NH1	2.46	0.42
1:B:2155:GLN:HG3	1:B:2162:LEU:HD11	2.02	0.42
1:B:2724:GLU:O	1:B:2728:VAL:HG23	2.20	0.42
1:A:1518:ASP:OD1	1:A:1520:ASN:N	2.46	0.42
1:A:2017:LEU:O	1:A:2018:SER:OG	2.31	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2155:GLN:HG3	1:A:2162:LEU:HD11	2.02	0.42
1:B:920:HIS:HB2	1:B:990:TRP:CE3	2.54	0.42
1:B:2279:LYS:HB2	1:B:2290:ARG:NH1	2.29	0.42
1:B:2483:HIS:HA	1:B:2489:TYR:HB3	2.01	0.42
1:A:1041:ILE:HG21	1:A:1716:PHE:CZ	2.54	0.42
1:A:1570:LEU:HD12	1:A:1576:TYR:CZ	2.55	0.42
1:A:2303:LYS:HD2	1:A:2309:HIS:CE1	2.54	0.42
1:A:2571:LYS:O	1:A:2581:THR:HA	2.19	0.42
1:B:1054:ILE:HG13	1:B:1054:ILE:O	2.19	0.42
1:A:1960:ASN:OD1	1:A:2220:ASN:ND2	2.51	0.42
1:B:930:THR:HB	1:B:936:LEU:HD12	2.02	0.42
1:B:1489:LYS:O	1:B:1514:ASP:HA	2.20	0.42
1:B:1711:GLY:HA2	1:B:2572:PHE:O	2.20	0.42
1:A:1054:ILE:HG13	1:A:1054:ILE:O	2.19	0.42
1:A:1372:ILE:HD13	1:A:1378:ILE:HG22	2.02	0.42
1:A:1382:LEU:HD21	1:A:1406:LEU:HD23	2.00	0.42
1:A:2437:LYS:HG3	1:A:2555:LYS:HD2	2.02	0.42
1:A:930:THR:HB	1:A:936:LEU:HD12	2.02	0.42
1:B:1664:THR:HA	1:B:1669:GLU:HA	2.02	0.42
1:A:920:HIS:HB2	1:A:990:TRP:CE3	2.54	0.42
1:A:971:ILE:HD12	1:A:985:THR:HG22	2.01	0.42
1:A:2033:THR:HB	1:A:2043:THR:HB	2.01	0.42
1:B:1008:ILE:HG13	1:B:1009:PRO:HD3	2.02	0.42
1:B:1801:THR:HA	1:B:1807:GLY:O	2.20	0.42
1:B:2084:ASN:HB2	1:B:2093:SER:HB3	2.02	0.42
1:A:1472:ALA:HB2	1:A:1540:SER:O	2.19	0.42
1:A:2657:ASN:HB2	1:A:2659:ARG:NH1	2.35	0.42
1:B:1524:PHE:HB3	1:B:1557:ASN:HD22	1.85	0.42
1:B:1570:LEU:HD12	1:B:1576:TYR:CZ	2.55	0.42
1:A:1281:TYR:HB2	1:A:1295:SER:O	2.20	0.41
1:A:1711:GLY:HA2	1:A:2572:PHE:O	2.20	0.41
1:A:1801:THR:HA	1:A:1807:GLY:O	2.20	0.41
1:A:2084:ASN:HB2	1:A:2093:SER:HB3	2.02	0.41
1:A:2483:HIS:CD2	1:A:2492:PRO:HD3	2.54	0.41
1:A:2720:TRP:O	1:A:2725:LYS:HE2	2.20	0.41
1:B:1019:PRO:O	1:B:1152:GLU:HG3	2.20	0.41
1:B:2500:SER:O	1:B:2504:ILE:HG12	2.19	0.41
1:A:1489:LYS:O	1:A:1514:ASP:HA	2.20	0.41
1:A:1664:THR:HG22	1:A:1665:THR:O	2.20	0.41
1:A:1213:ARG:HB2	1:A:1230:LEU:CD2	2.51	0.41
1:B:1048:LEU:HB3	1:B:1065:SER:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1104:LYS:HE3	1:B:1106:PHE:CE1	2.56	0.41
1:B:2412:LYS:O	1:B:2423:VAL:HG12	2.21	0.41
1:B:2222:ASN:OD1	1:B:2427:ARG:NH1	2.45	0.41
1:A:1008:ILE:HG13	1:A:1009:PRO:HD3	2.02	0.41
1:B:2033:THR:HB	1:B:2043:THR:HB	2.01	0.41
1:A:944:VAL:HG22	1:A:971:ILE:HG23	2.03	0.41
1:A:1240:ASP:OD2	1:A:1253:ARG:NH2	2.53	0.41
1:B:1265:GLU:N	1:B:1314:LEU:O	2.54	0.41
1:B:2437:LYS:HG3	1:B:2555:LYS:HD2	2.02	0.41
1:A:2165:TRP:CZ3	1:A:2167:THR:HG23	2.55	0.41
1:A:2412:LYS:O	1:A:2423:VAL:HG12	2.21	0.41
1:A:2724:GLU:O	1:A:2728:VAL:HG23	2.20	0.41
1:B:1213:ARG:HB2	1:B:1230:LEU:CD2	2.50	0.41
1:B:1307:SER:O	1:B:1317:ASN:ND2	2.42	0.41
1:B:1664:THR:HG22	1:B:1665:THR:O	2.20	0.41
1:B:2720:TRP:O	1:B:2725:LYS:HE2	2.20	0.41
1:B:1401:ILE:HD12	1:B:1404:VAL:HG21	2.03	0.41
1:B:2165:TRP:CZ3	1:B:2167:THR:HG23	2.55	0.41
1:A:1019:PRO:O	1:A:1152:GLU:HG3	2.20	0.41
1:A:1104:LYS:HE3	1:A:1106:PHE:CE1	2.56	0.41
1:A:1401:ILE:HD12	1:A:1404:VAL:HG21	2.03	0.41
1:A:1611:THR:HB	1:A:1620:LEU:HB3	2.03	0.41
1:A:2086:ASP:O	1:A:2088:SER:N	2.50	0.41
1:A:2098:ILE:HD12	1:A:2334:ILE:HG21	2.02	0.41
1:B:1372:ILE:HD13	1:B:1378:ILE:HG22	2.02	0.41
1:B:1611:THR:HB	1:B:1620:LEU:HB3	2.03	0.41
1:B:2571:LYS:HG2	1:B:2572:PHE:N	2.36	0.41
1:A:1524:PHE:HB3	1:A:1557:ASN:HD22	1.85	0.41
1:A:2520:LEU:H	1:A:2520:LEU:HD23	1.86	0.41
1:B:944:VAL:HG22	1:B:971:ILE:HG23	2.03	0.41
1:B:1281:TYR:HB2	1:B:1295:SER:O	2.20	0.41
1:B:1356:ASP:OD1	1:B:1419:ASN:ND2	2.47	0.40
1:B:1240:ASP:OD2	1:B:1253:ARG:NH2	2.53	0.40
1:A:2084:ASN:O	1:A:2092:THR:HG22	2.22	0.40
1:B:2520:LEU:HD23	1:B:2520:LEU:H	1.86	0.40
1:A:1048:LEU:HB3	1:A:1065:SER:HB2	2.02	0.40
1:A:1664:THR:HA	1:A:1669:GLU:HA	2.02	0.40
1:A:2222:ASN:OD1	1:A:2427:ARG:NH1	2.45	0.40
1:A:2058:ARG:HB3	1:A:2066:ARG:HB2	2.03	0.40
1:B:1841:LEU:HD13	1:B:1852:ILE:HG13	2.04	0.40
1:B:2041:LEU:HB2	1:B:2510:THR:HG21	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2098:ILE:HD12	1:B:2334:ILE:HG21	2.02	0.40

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	1894/1932 (98%)	1785 (94%)	109 (6%)	0	100	100
1	B	1894/1932 (98%)	1785 (94%)	109 (6%)	0	100	100
All	All	3788/3864 (98%)	3570 (94%)	218 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	1663/1689 (98%)	1659 (100%)	4 (0%)	93	98
1	B	1663/1689 (98%)	1659 (100%)	4 (0%)	93	98
All	All	3326/3378 (98%)	3318 (100%)	8 (0%)	93	98

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1419	ASN
1	A	2087	ASN
1	A	2445	MET
1	A	2517	LYS
1	B	1419	ASN
1	B	2087	ASN
1	B	2445	MET
1	B	2517	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1725	HIS
1	B	1725	HIS
1	B	2155	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	0.28	0	17,19,21	0.50	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	0.35	0	17,19,21	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	D	2	2	14,14,15	0.41	0	17,19,21	0.45	0
2	NAG	E	1	2,1	14,14,15	0.38	0	17,19,21	0.44	0
2	NAG	E	2	2	14,14,15	0.19	0	17,19,21	0.47	0
2	NAG	F	1	2,1	14,14,15	0.28	0	17,19,21	0.38	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	0.28	0	17,19,21	0.50	0
2	NAG	G	2	2	14,14,15	0.20	0	17,19,21	0.42	0
2	NAG	H	1	2,1	14,14,15	0.36	0	17,19,21	0.56	0
2	NAG	H	2	2	14,14,15	0.42	0	17,19,21	0.45	0
2	NAG	I	1	2,1	14,14,15	0.39	0	17,19,21	0.44	0
2	NAG	I	2	2	14,14,15	0.19	0	17,19,21	0.46	0
2	NAG	J	1	2,1	14,14,15	0.29	0	17,19,21	0.38	0
2	NAG	J	2	2	14,14,15	0.23	0	17,19,21	0.41	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	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

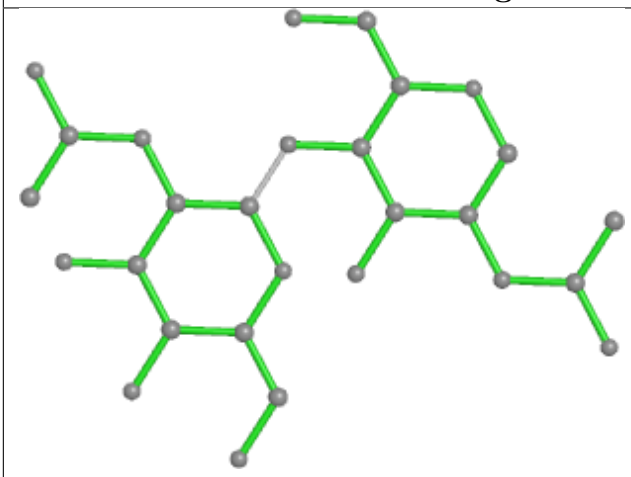
Mol	Chain	Res	Type	Atoms
2	F	2	NAG	C4-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	G	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
2	D	2	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6

There are no ring outliers.

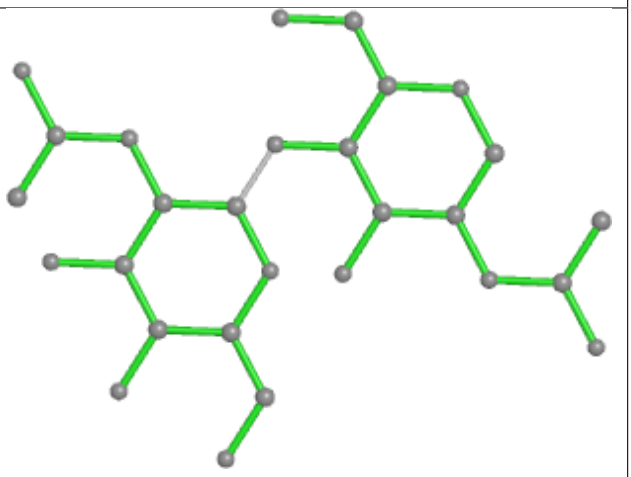
No monomer is involved in short contacts.

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

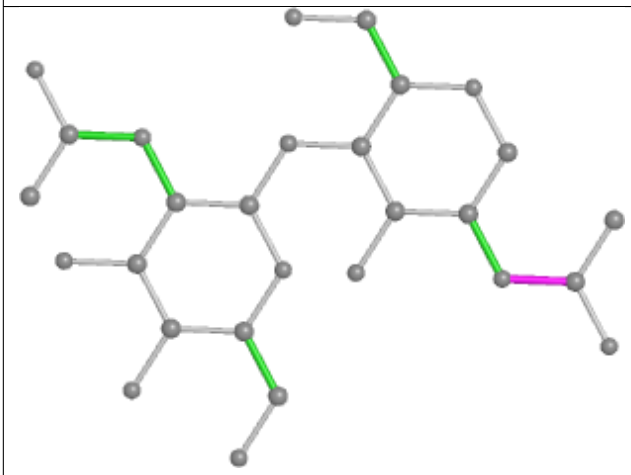
Oligosaccharide Chain C



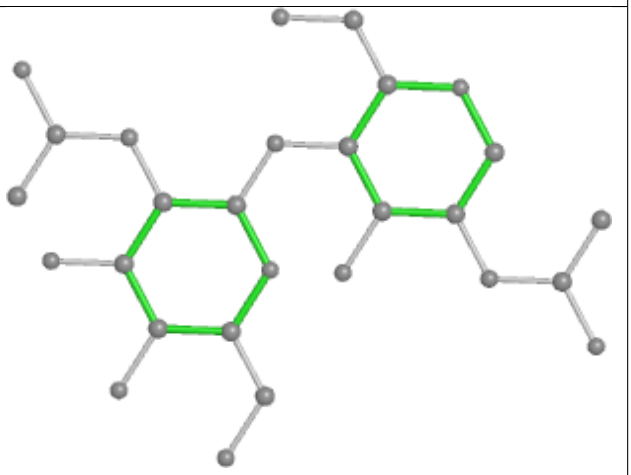
Bond lengths



Bond angles

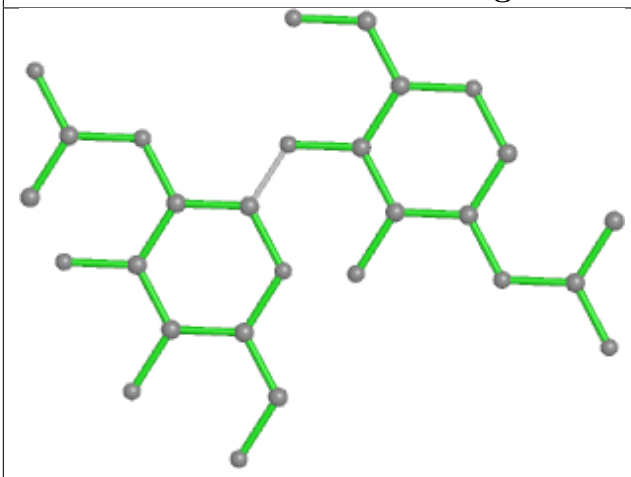


Torsions

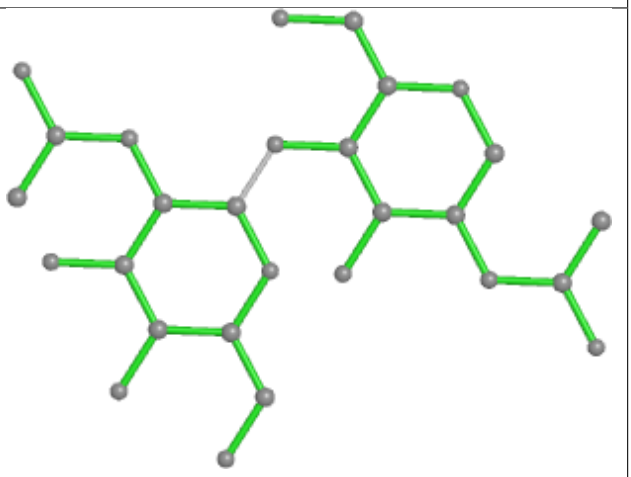


Rings

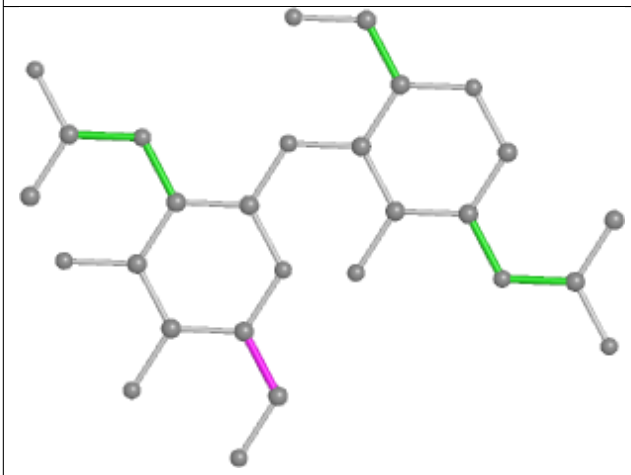
Oligosaccharide Chain D



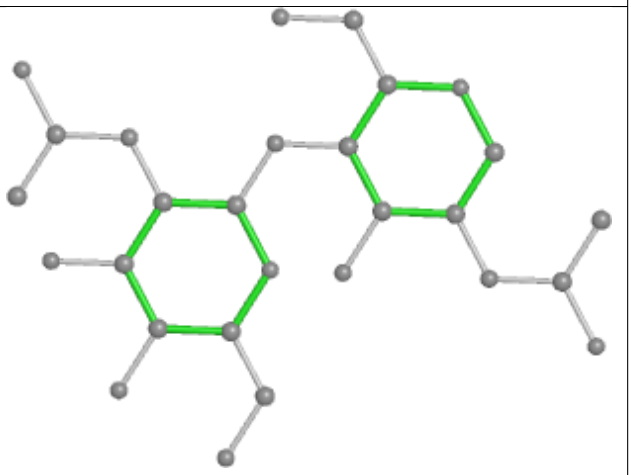
Bond lengths



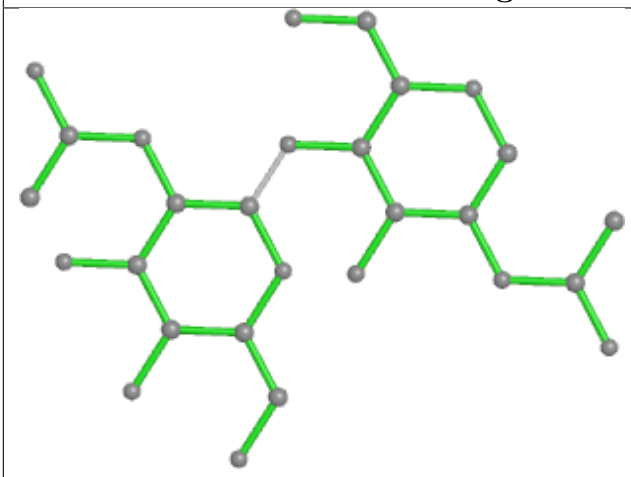
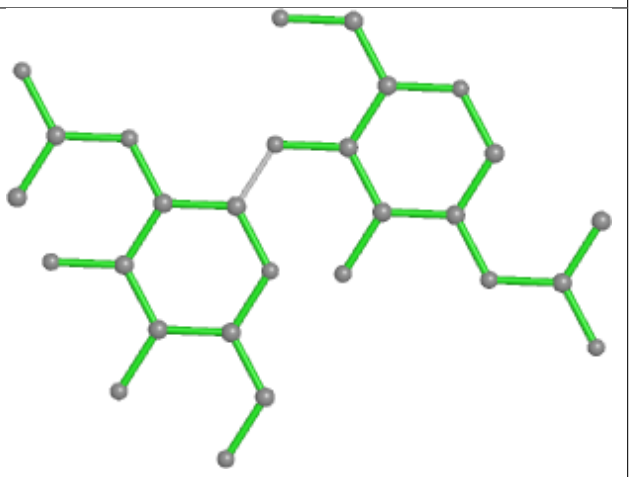
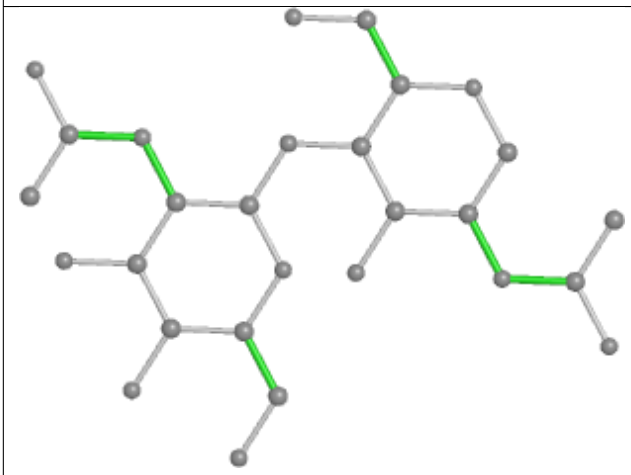
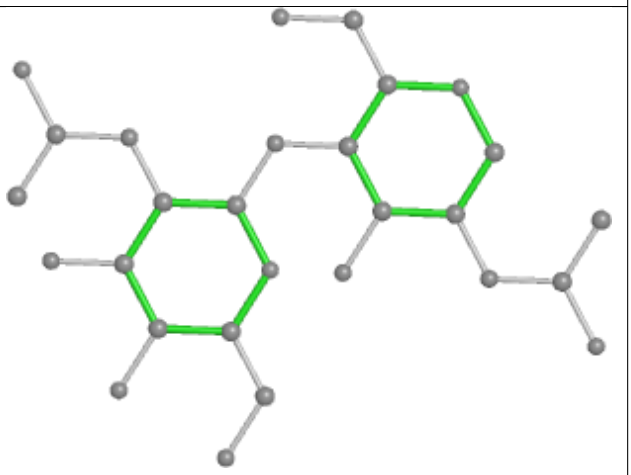
Bond angles



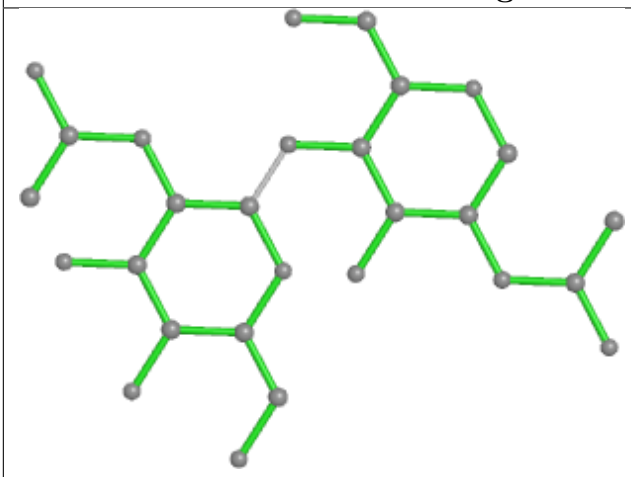
Torsions



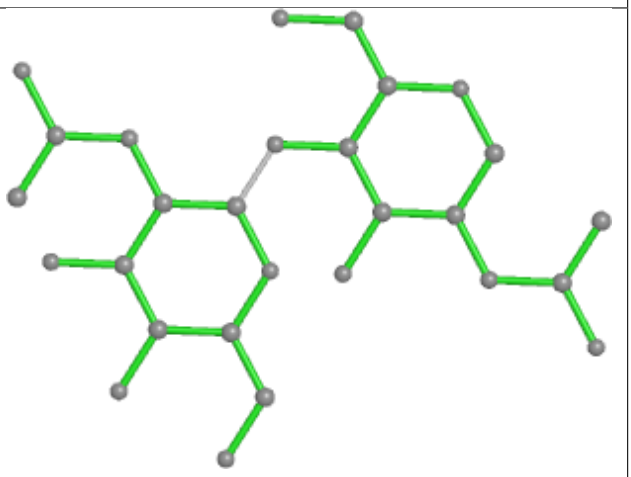
Rings

Oligosaccharide Chain E	
 Bond lengths	 Bond angles
 Torsions	 Rings

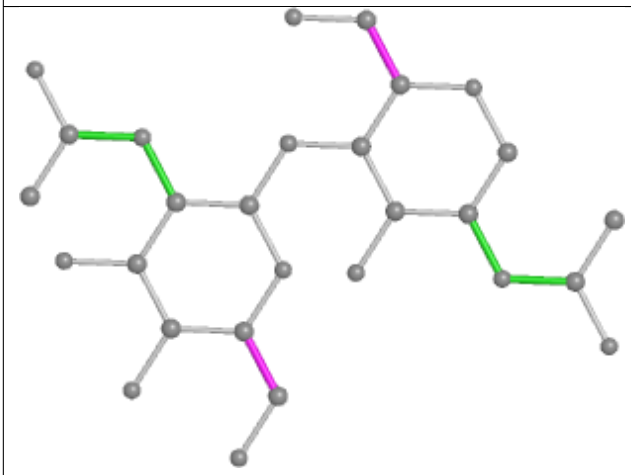
Oligosaccharide Chain F



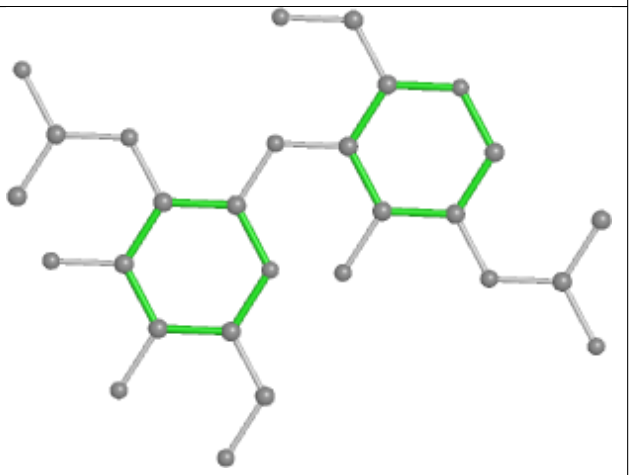
Bond lengths



Bond angles

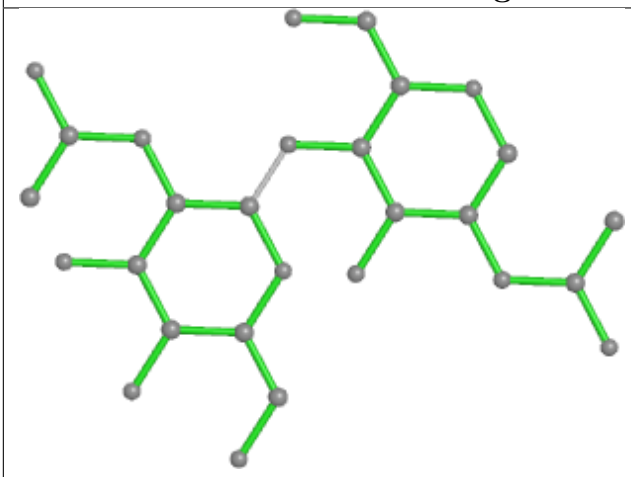


Torsions

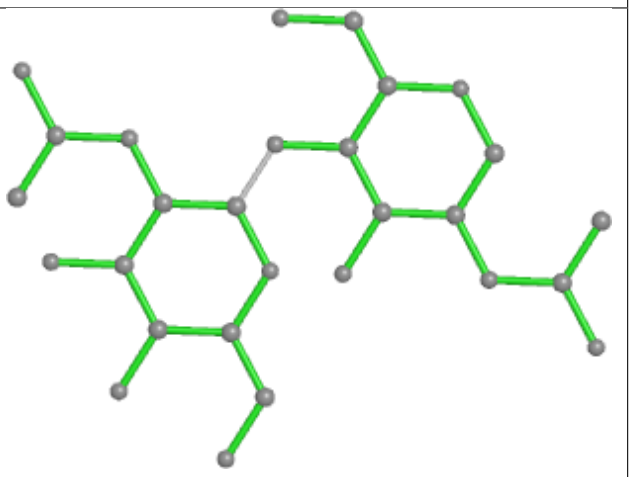


Rings

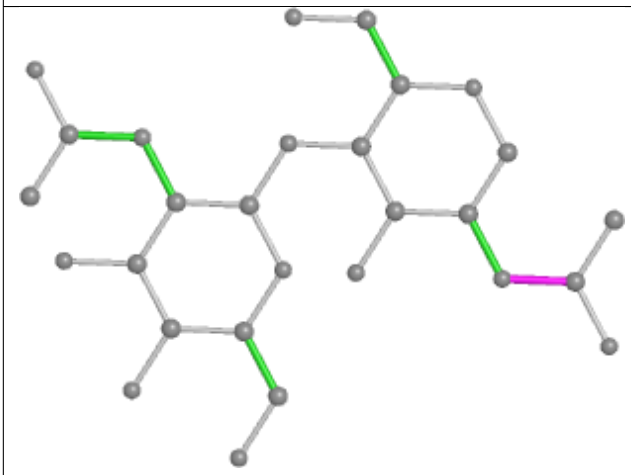
Oligosaccharide Chain G



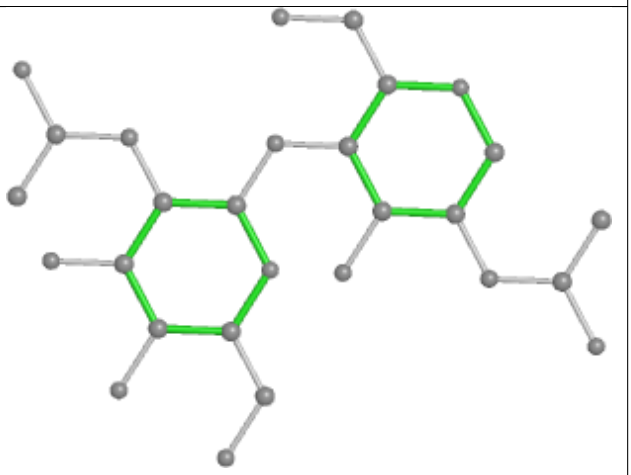
Bond lengths



Bond angles

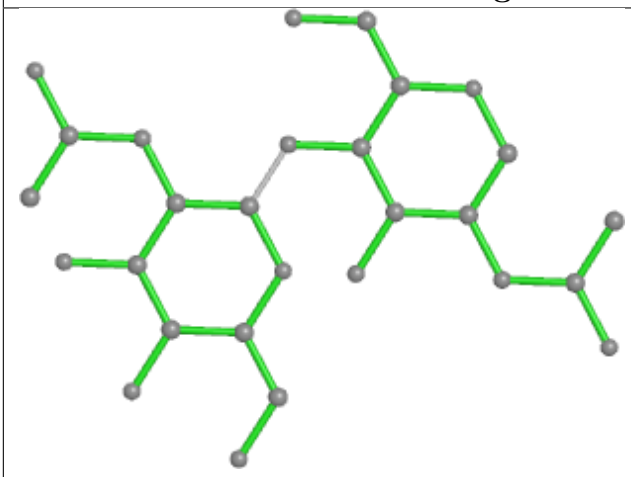


Torsions

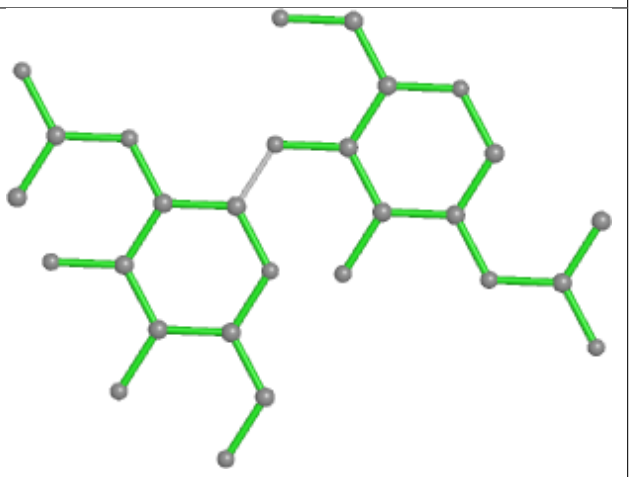


Rings

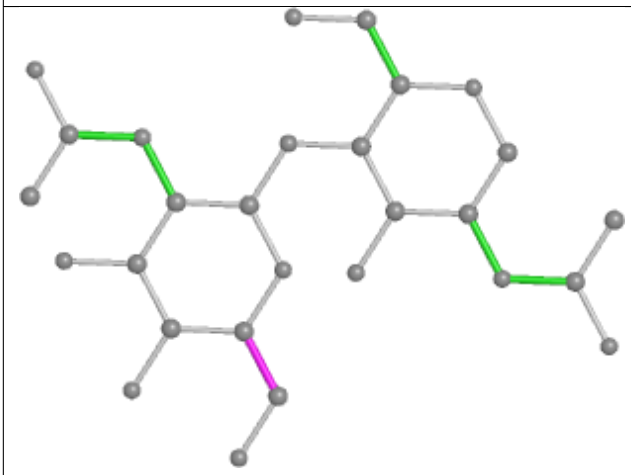
Oligosaccharide Chain H



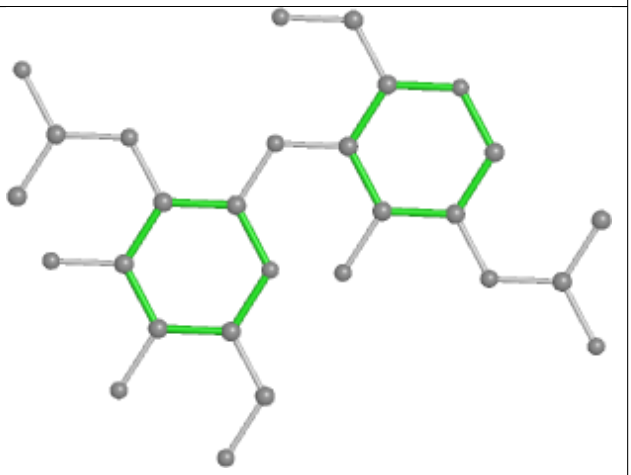
Bond lengths



Bond angles

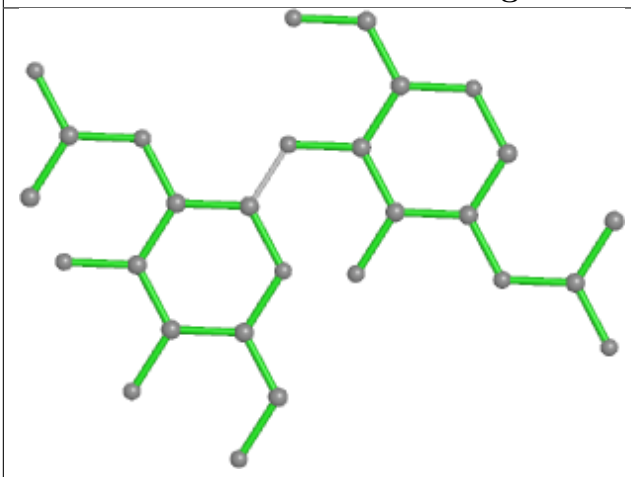


Torsions

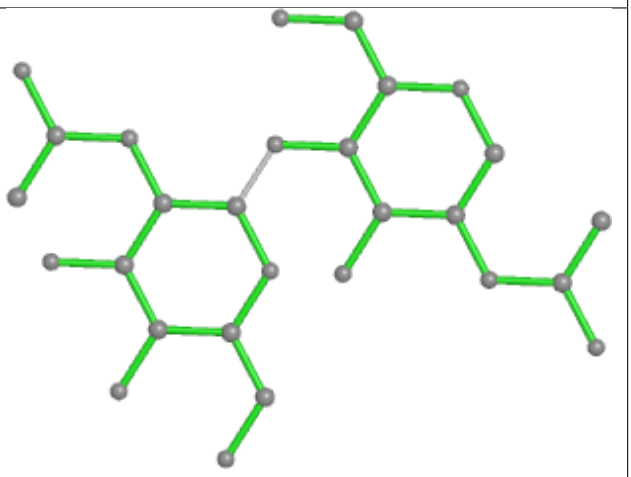


Rings

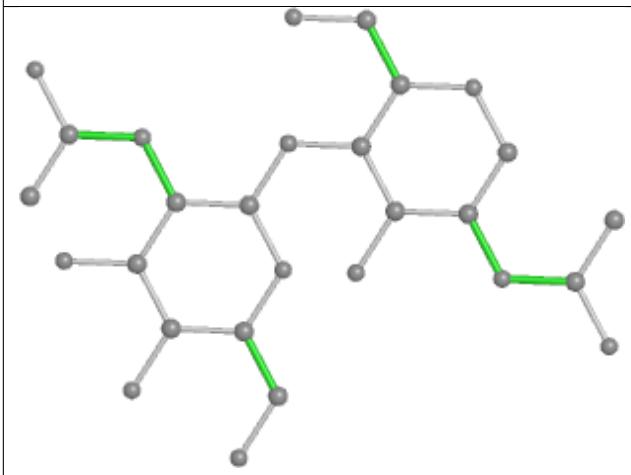
Oligosaccharide Chain I



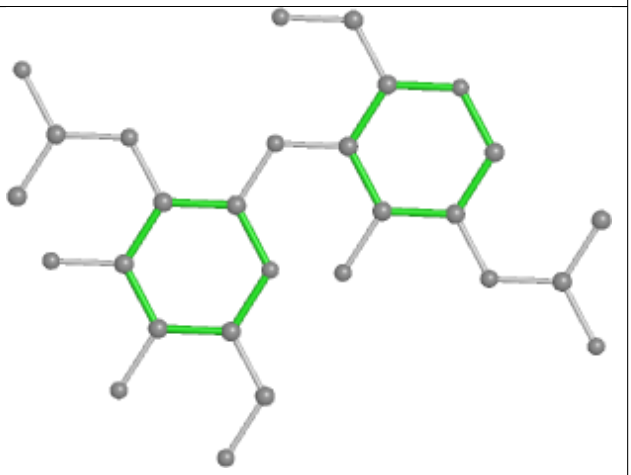
Bond lengths



Bond angles

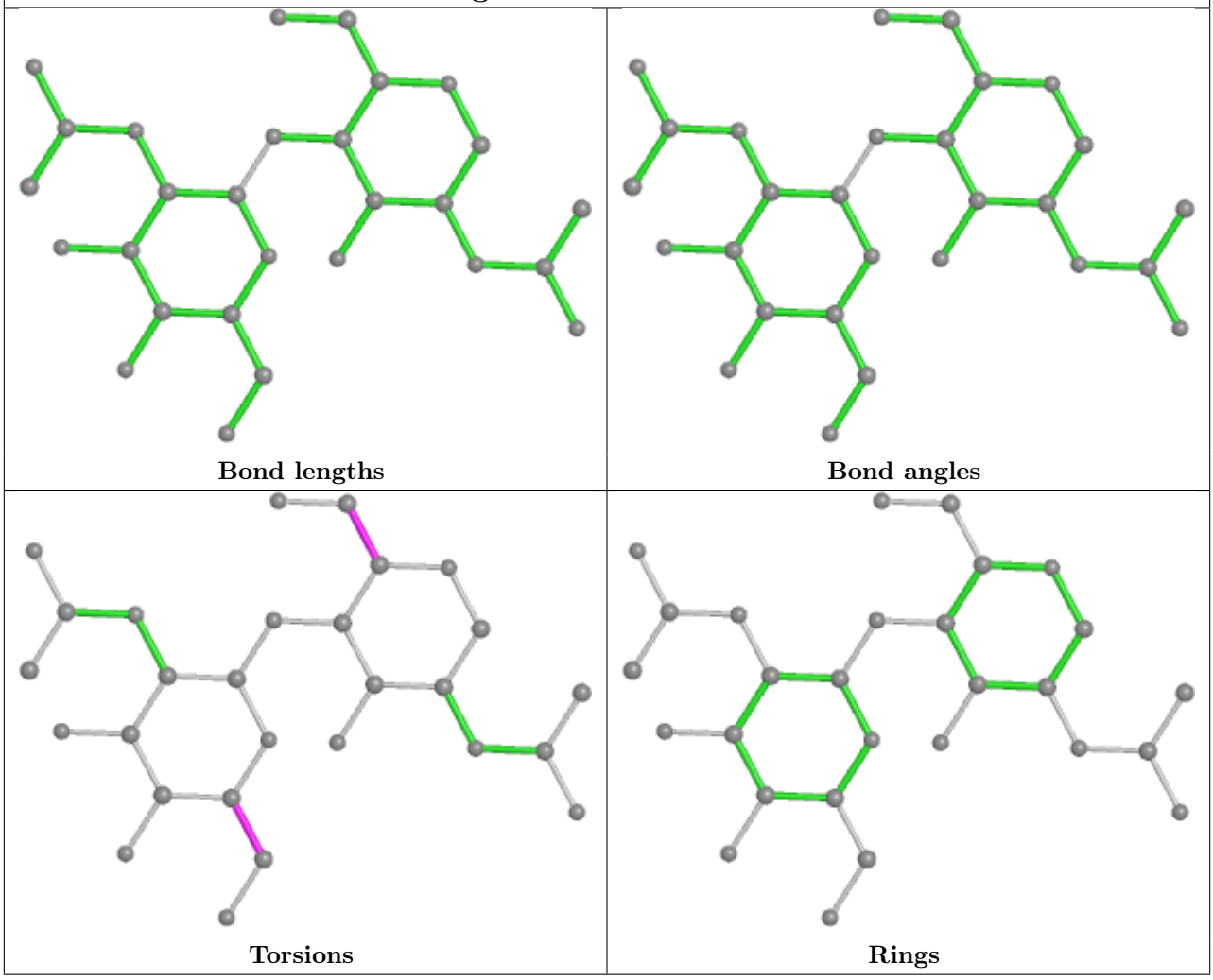


Torsions



Rings

Oligosaccharide Chain J



5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 6 are monoatomic - leaving 14 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	$\#\|Z\| > 2$
3	NAG	A	2804	1	14,14,15	0.29	0	17,19,21	0.53	0
3	NAG	B	2801	1	14,14,15	0.33	0	17,19,21	0.36	0
3	NAG	B	2802	1	14,14,15	0.15	0	17,19,21	0.44	0
3	NAG	B	2807	1	14,14,15	0.32	0	17,19,21	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	A	2807	1	14,14,15	0.32	0	17,19,21	0.44	0
3	NAG	B	2805	1	14,14,15	0.25	0	17,19,21	0.41	0
3	NAG	A	2805	1	14,14,15	0.25	0	17,19,21	0.41	0
3	NAG	A	2802	1	14,14,15	0.15	0	17,19,21	0.44	0
3	NAG	B	2803	1	14,14,15	0.39	0	17,19,21	1.42	2 (11%)
3	NAG	A	2803	1	14,14,15	0.39	0	17,19,21	1.41	2 (11%)
3	NAG	A	2801	1	14,14,15	0.31	0	17,19,21	0.36	0
3	NAG	B	2806	1	14,14,15	0.29	0	17,19,21	0.39	0
3	NAG	A	2806	1	14,14,15	0.29	0	17,19,21	0.39	0
3	NAG	B	2804	1	14,14,15	0.30	0	17,19,21	0.53	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	2804	1	-	3/6/23/26	0/1/1/1
3	NAG	B	2801	1	-	2/6/23/26	0/1/1/1
3	NAG	B	2802	1	-	2/6/23/26	0/1/1/1
3	NAG	B	2807	1	-	1/6/23/26	0/1/1/1
3	NAG	A	2807	1	-	1/6/23/26	0/1/1/1
3	NAG	B	2805	1	-	2/6/23/26	0/1/1/1
3	NAG	A	2805	1	-	2/6/23/26	0/1/1/1
3	NAG	A	2802	1	-	2/6/23/26	0/1/1/1
3	NAG	B	2803	1	-	5/6/23/26	0/1/1/1
3	NAG	A	2803	1	-	5/6/23/26	0/1/1/1
3	NAG	A	2801	1	-	2/6/23/26	0/1/1/1
3	NAG	B	2806	1	-	1/6/23/26	0/1/1/1
3	NAG	A	2806	1	-	1/6/23/26	0/1/1/1
3	NAG	B	2804	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	2803	NAG	C2-N2-C7	4.33	129.07	122.90
3	A	2803	NAG	C2-N2-C7	4.32	129.05	122.90
3	B	2803	NAG	C1-O5-C5	2.80	115.98	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2803	NAG	C1-O5-C5	2.78	115.96	112.19

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2803	NAG	O5-C5-C6-O6
3	B	2803	NAG	O5-C5-C6-O6
3	A	2803	NAG	C4-C5-C6-O6
3	B	2803	NAG	C4-C5-C6-O6
3	A	2802	NAG	O5-C5-C6-O6
3	B	2802	NAG	O5-C5-C6-O6
3	A	2802	NAG	C4-C5-C6-O6
3	B	2802	NAG	C4-C5-C6-O6
3	A	2803	NAG	C8-C7-N2-C2
3	A	2803	NAG	O7-C7-N2-C2
3	A	2804	NAG	C8-C7-N2-C2
3	A	2804	NAG	O7-C7-N2-C2
3	B	2803	NAG	C8-C7-N2-C2
3	B	2803	NAG	O7-C7-N2-C2
3	B	2804	NAG	C8-C7-N2-C2
3	B	2804	NAG	O7-C7-N2-C2
3	A	2801	NAG	O5-C5-C6-O6
3	B	2801	NAG	O5-C5-C6-O6
3	A	2801	NAG	C4-C5-C6-O6
3	B	2801	NAG	C4-C5-C6-O6
3	A	2807	NAG	O5-C5-C6-O6
3	B	2807	NAG	O5-C5-C6-O6
3	A	2804	NAG	C4-C5-C6-O6
3	B	2804	NAG	C4-C5-C6-O6
3	A	2806	NAG	C4-C5-C6-O6
3	B	2806	NAG	C4-C5-C6-O6
3	A	2803	NAG	C3-C2-N2-C7
3	B	2803	NAG	C3-C2-N2-C7
3	B	2805	NAG	C4-C5-C6-O6
3	A	2805	NAG	C4-C5-C6-O6
3	A	2805	NAG	O5-C5-C6-O6
3	B	2805	NAG	O5-C5-C6-O6

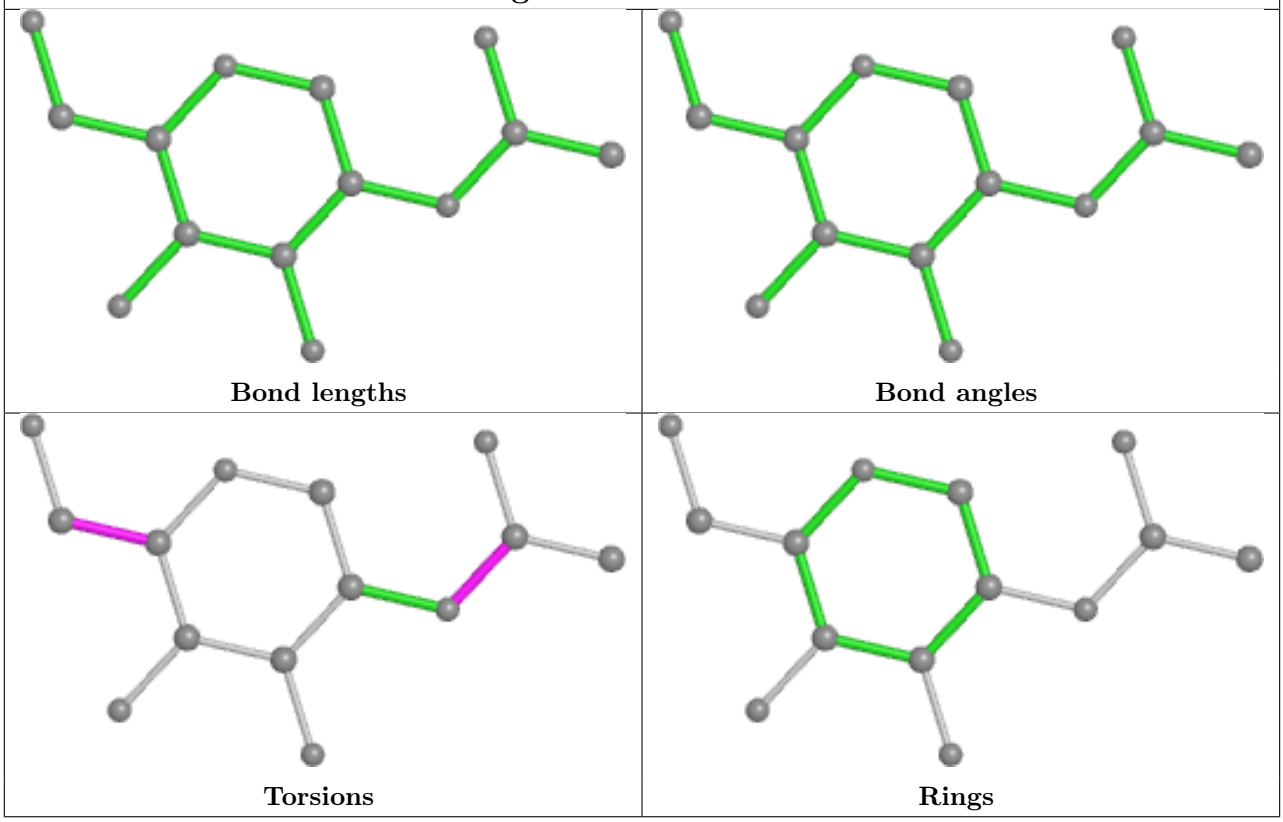
There are no ring outliers.

2 monomers are involved in 2 short contacts:

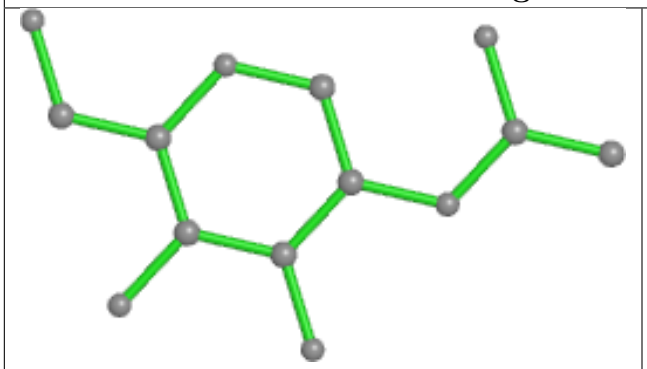
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2803	NAG	1	0
3	A	2803	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

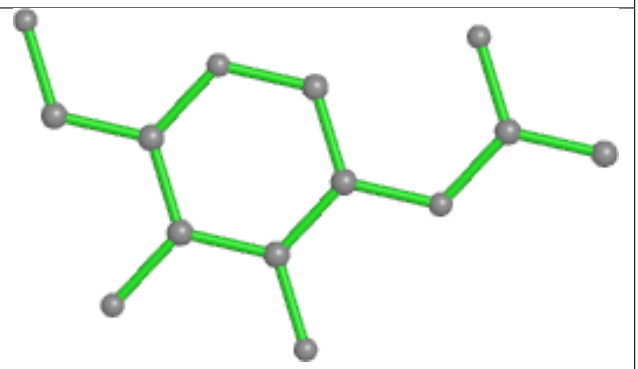
Ligand NAG A 2804



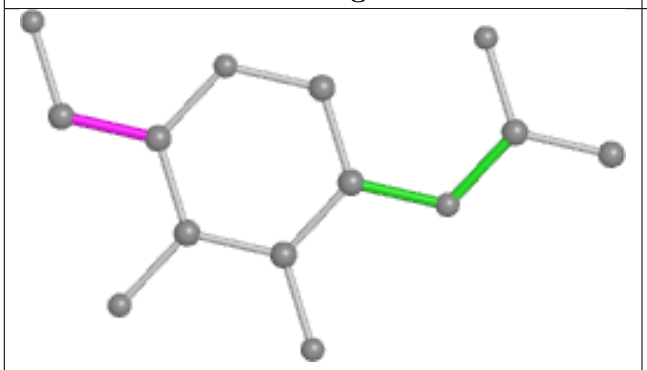
Ligand NAG B 2801



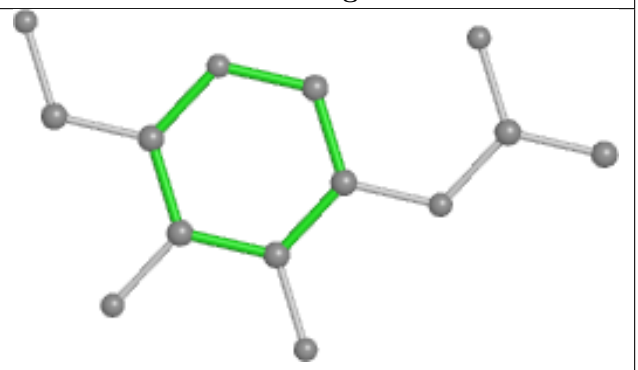
Bond lengths



Bond angles

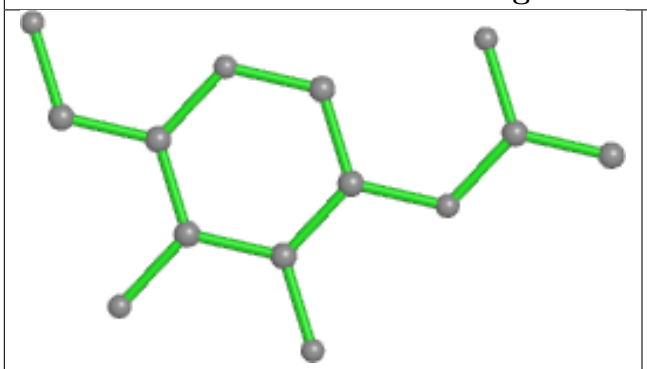


Torsions

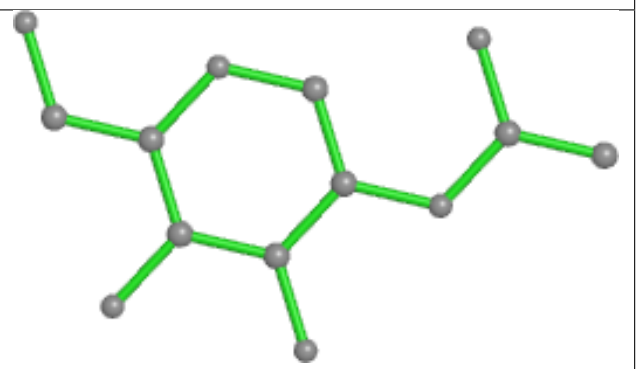


Rings

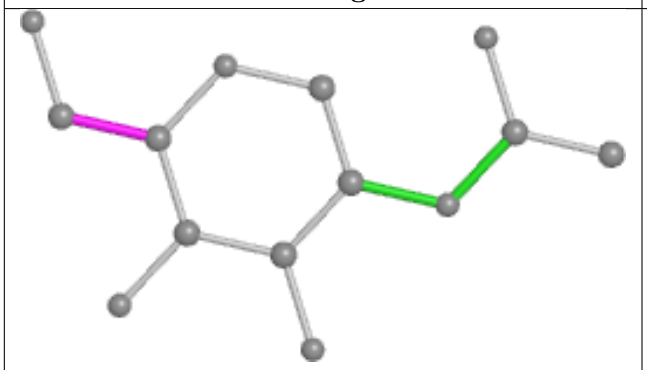
Ligand NAG B 2802



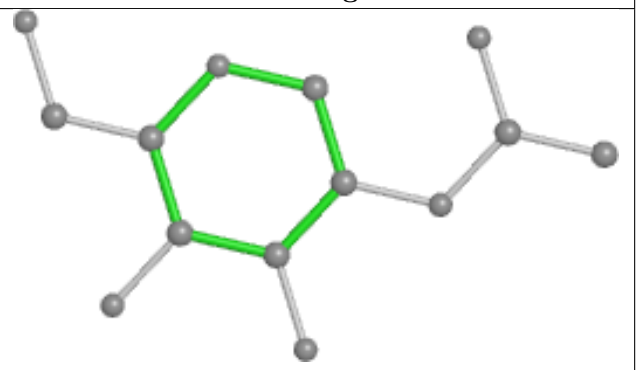
Bond lengths



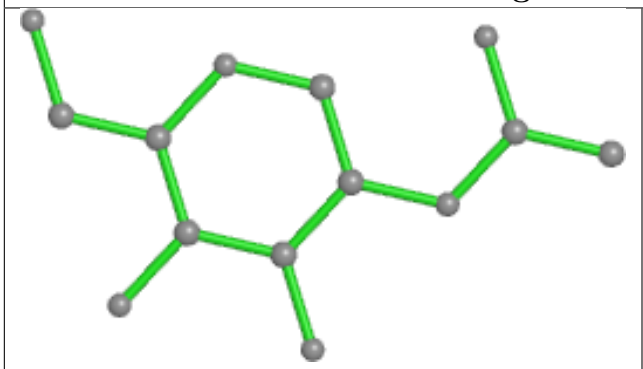
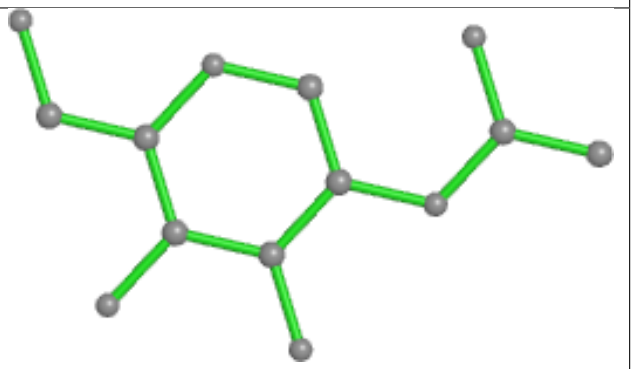
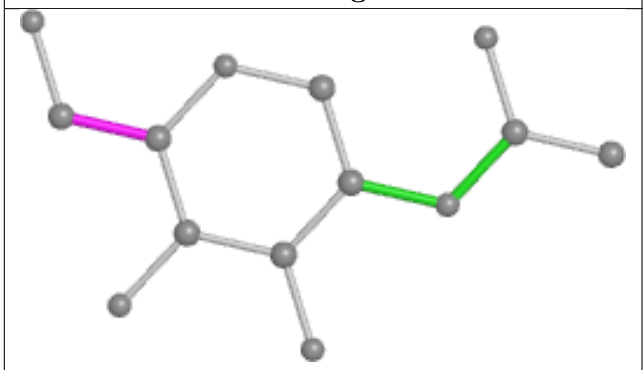
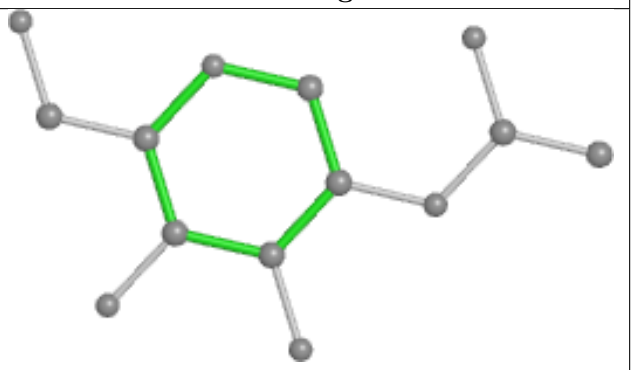
Bond angles

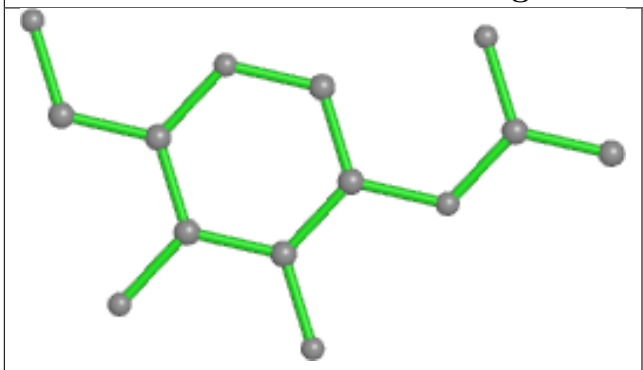
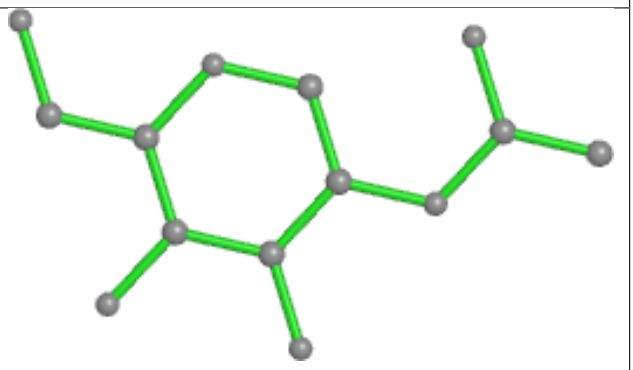
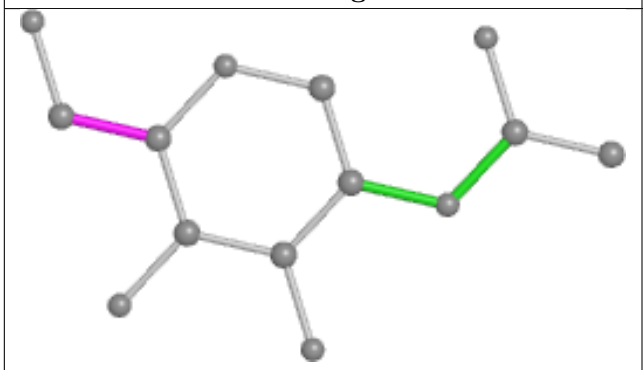
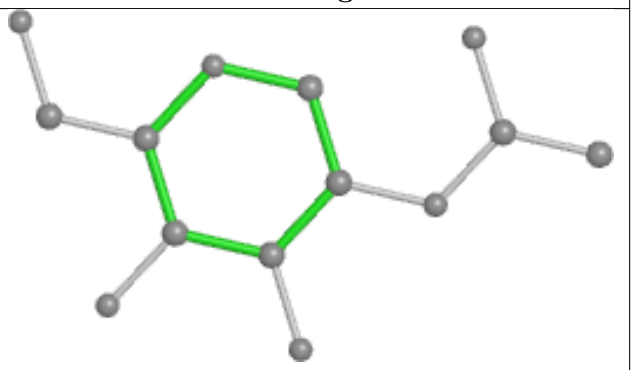


Torsions

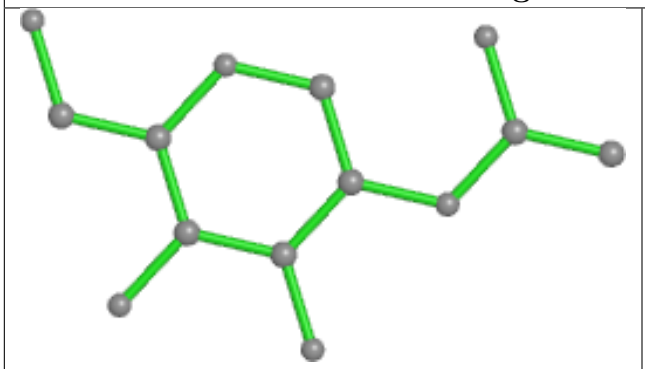


Rings

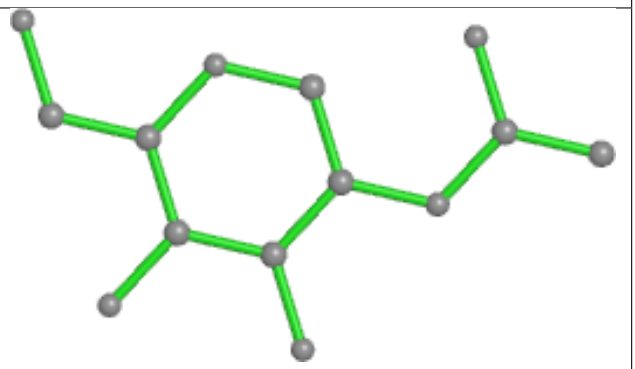
Ligand NAG B 2807	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 2807	
 Bond lengths	 Bond angles
 Torsions	 Rings

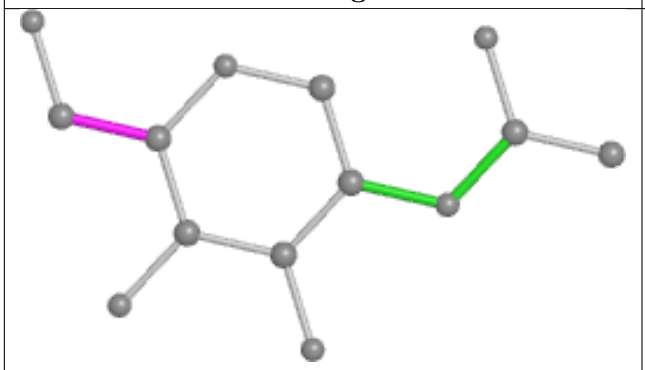
Ligand NAG B 2805



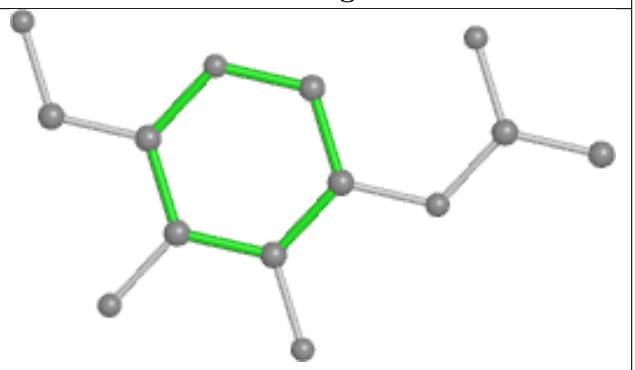
Bond lengths



Bond angles

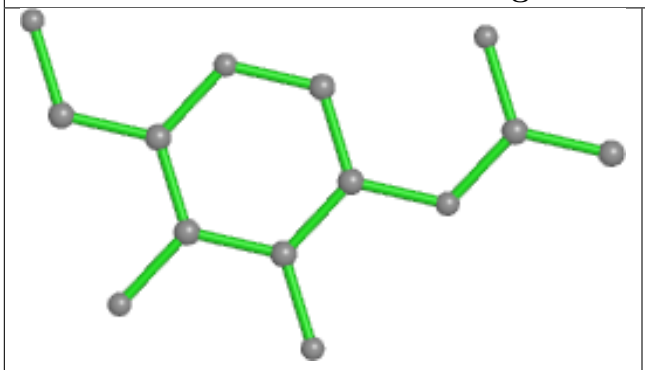


Torsions

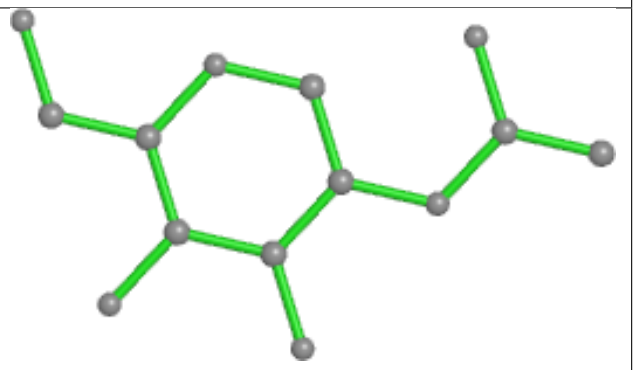


Rings

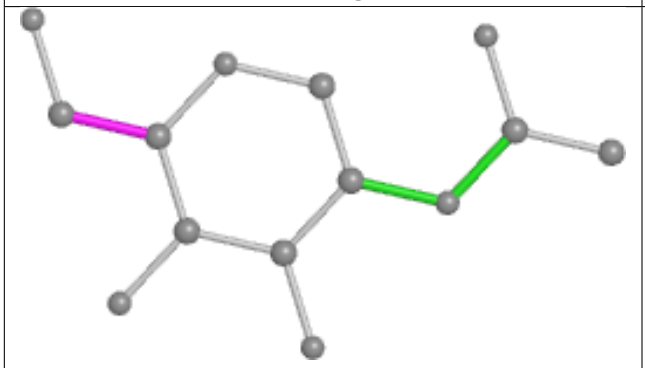
Ligand NAG A 2805



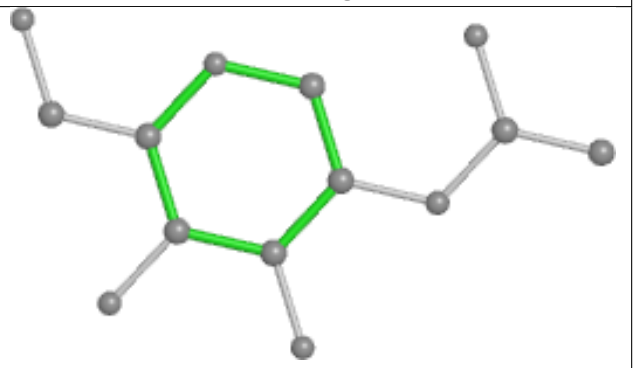
Bond lengths



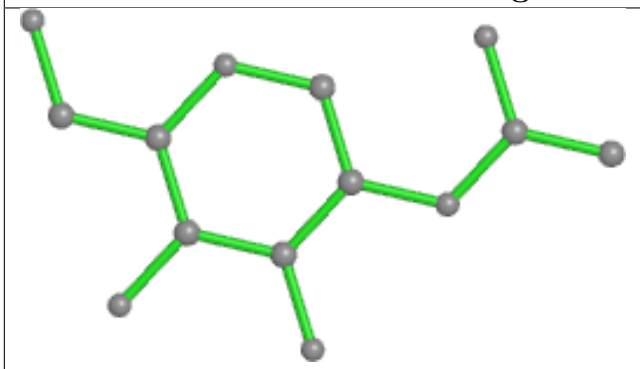
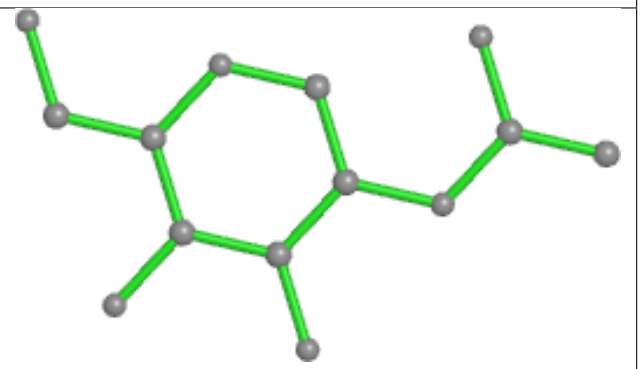
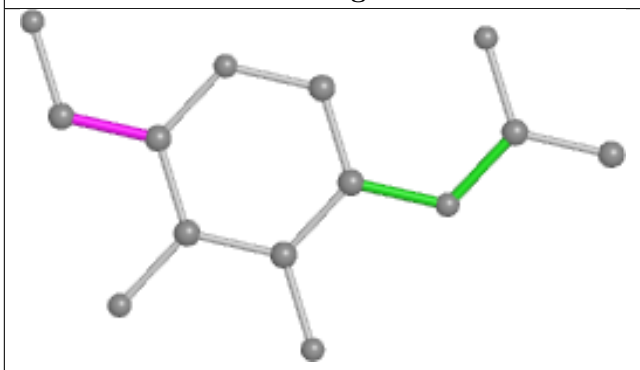
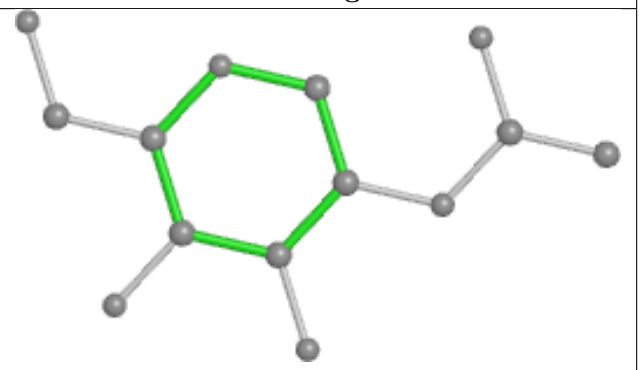
Bond angles

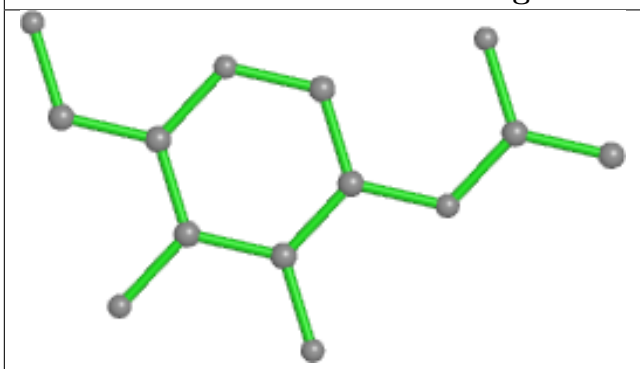
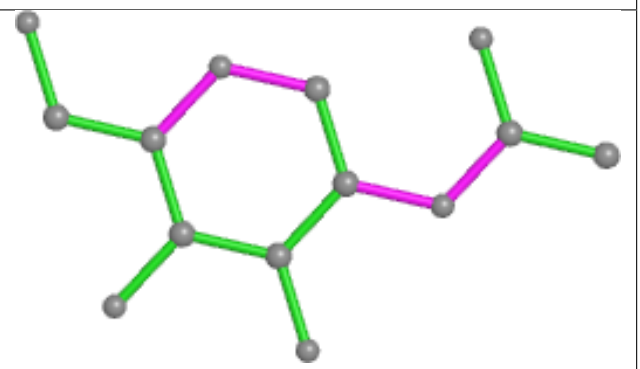
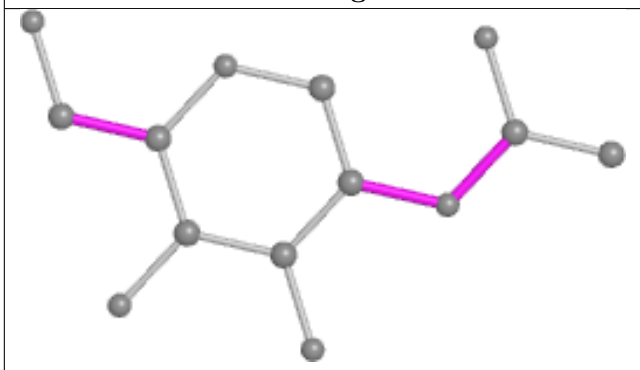
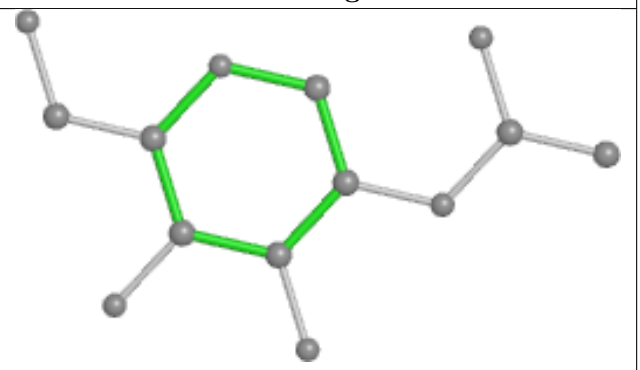


Torsions

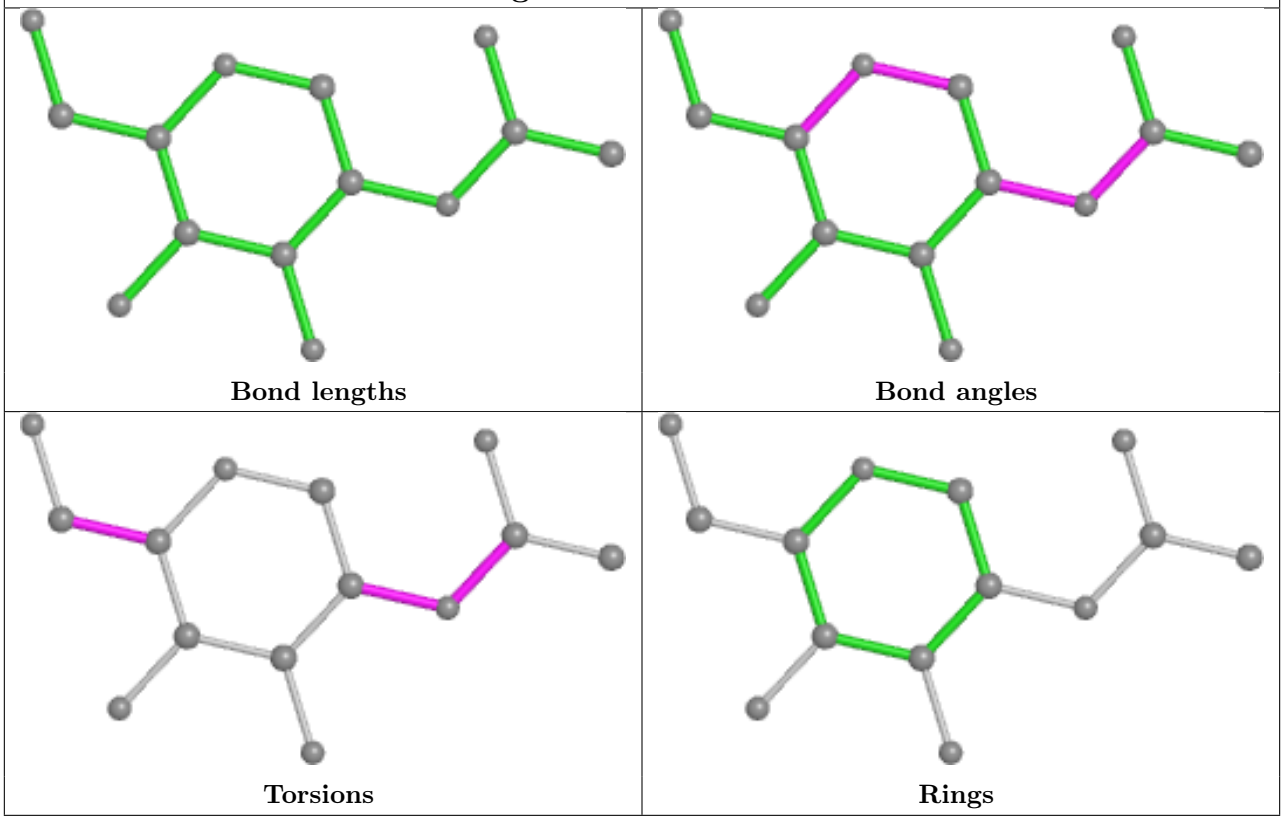


Rings

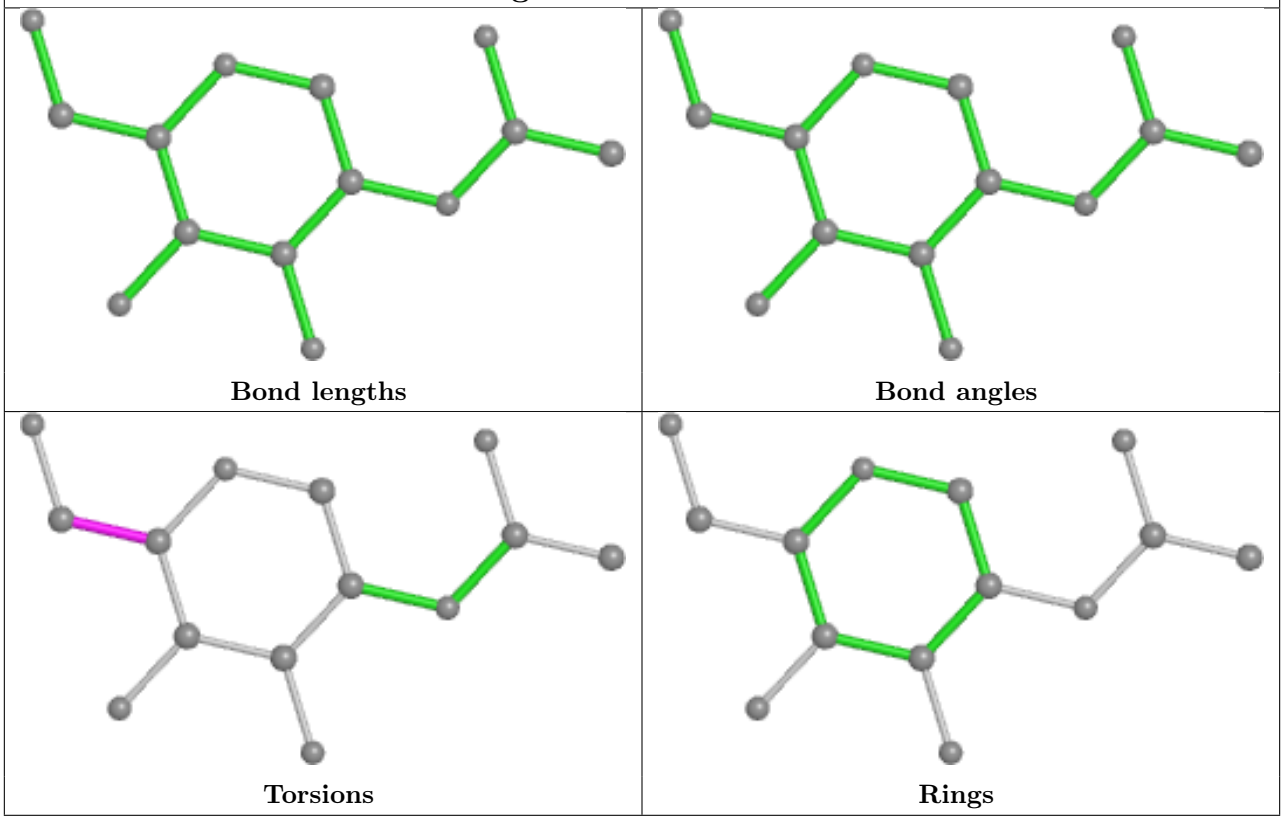
Ligand NAG A 2802	
 Bond lengths	 Bond angles
 Torsions	 Rings

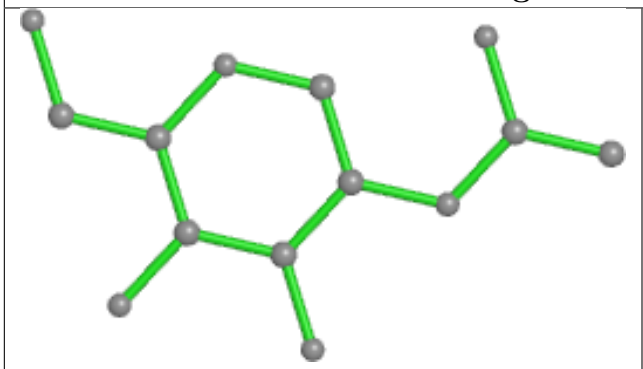
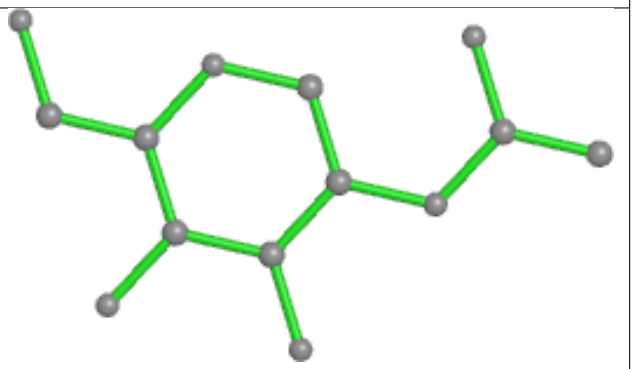
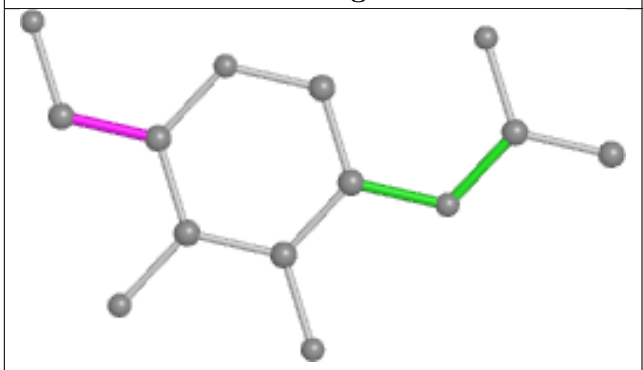
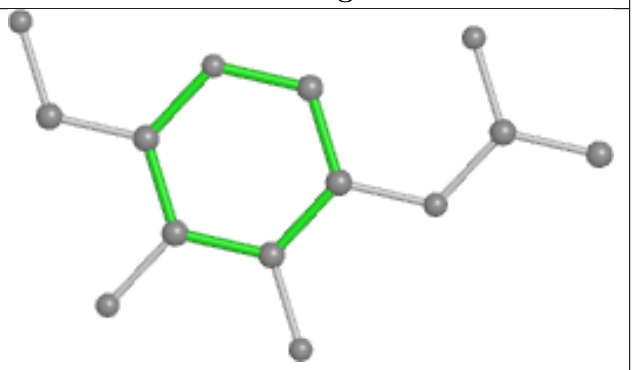
Ligand NAG B 2803	
 Bond lengths	 Bond angles
 Torsions	 Rings

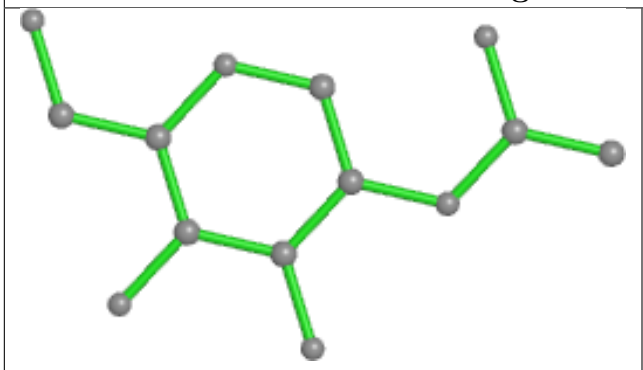
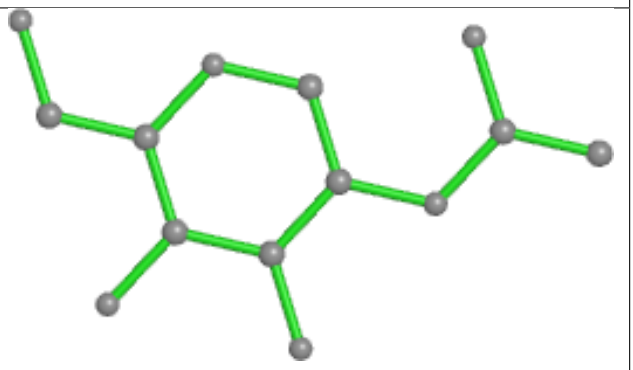
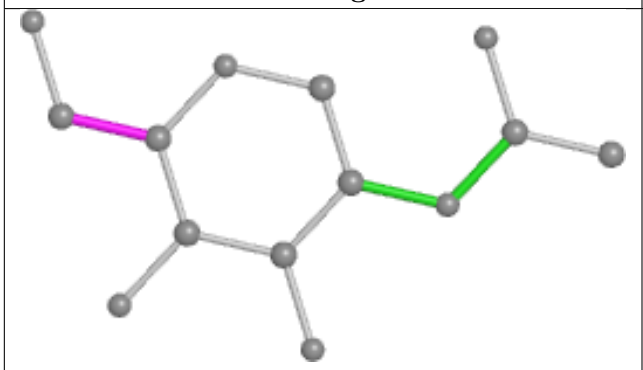
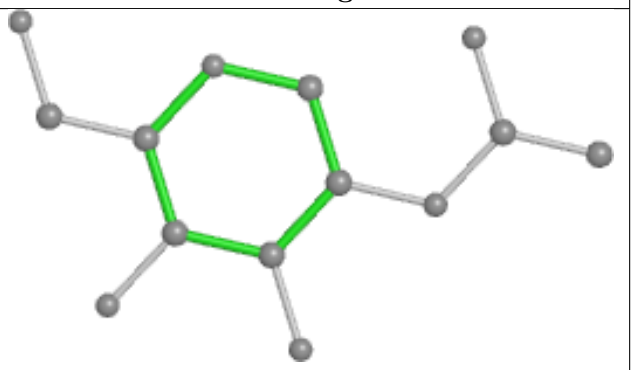
Ligand NAG A 2803

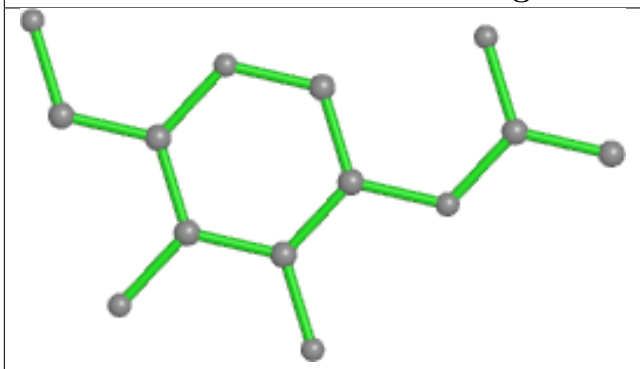
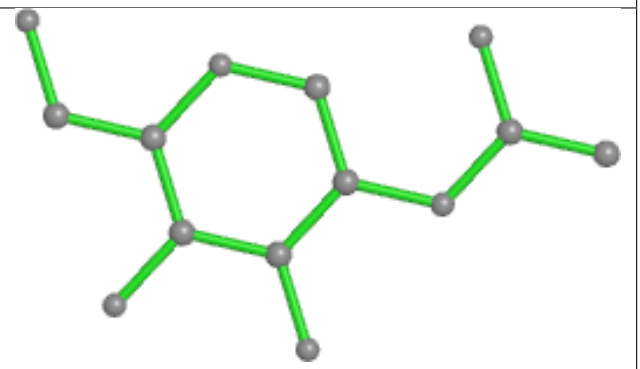
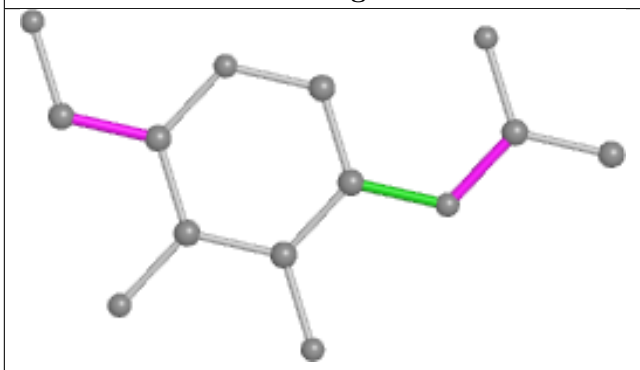
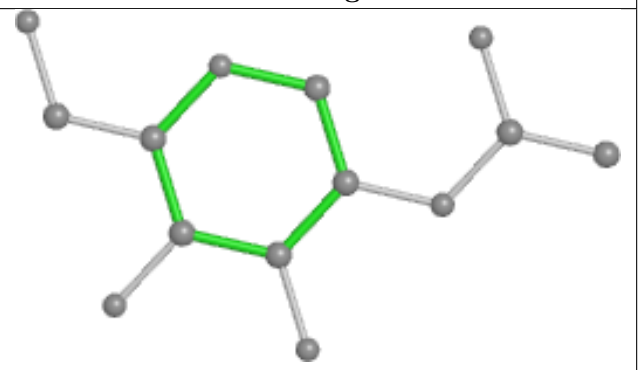


Ligand NAG A 2801



Ligand NAG B 2806	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 2806	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG B 2804	
 Bond lengths	 Bond angles
 Torsions	 Rings

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.

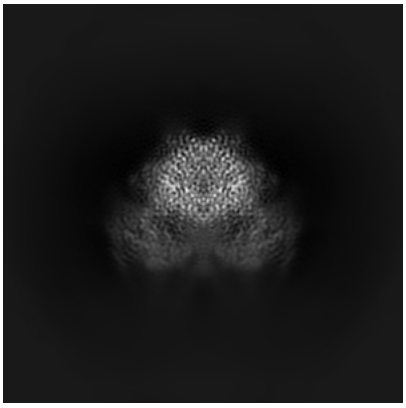
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-12125. These allow visual inspection of the internal detail of the map and identification of artifacts.

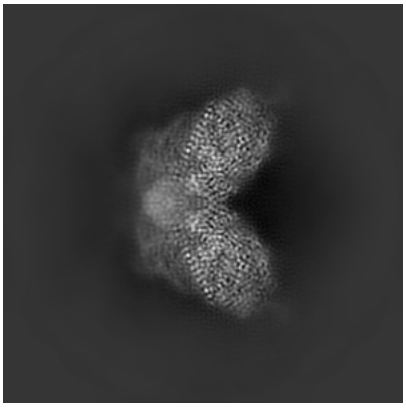
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

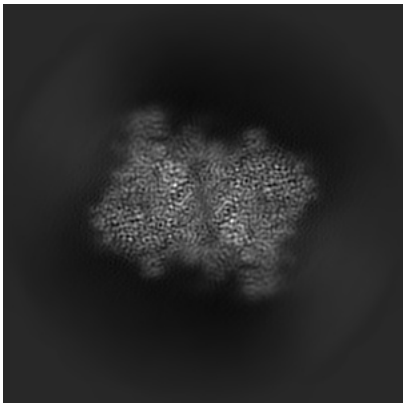
6.1.1 Primary map



X



Y

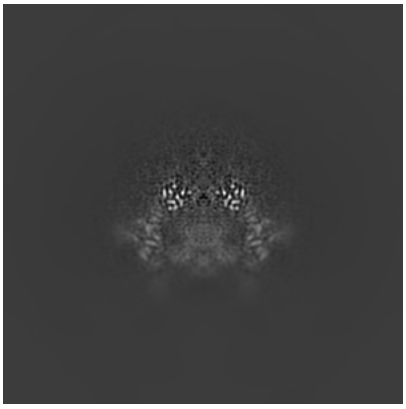


Z

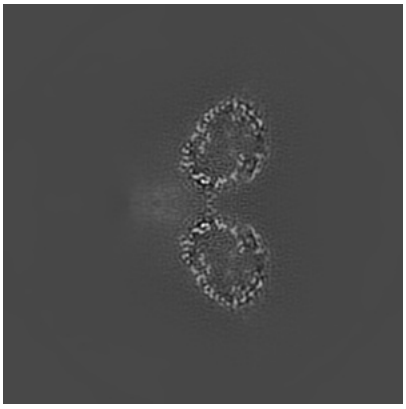
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

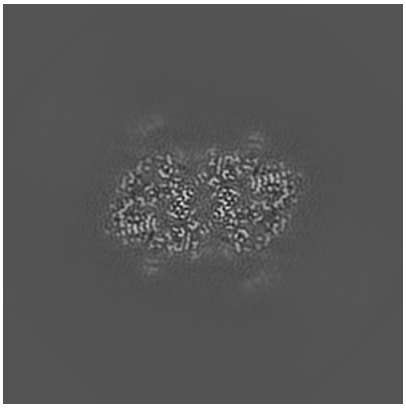
6.2.1 Primary map



X Index: 180



Y Index: 180

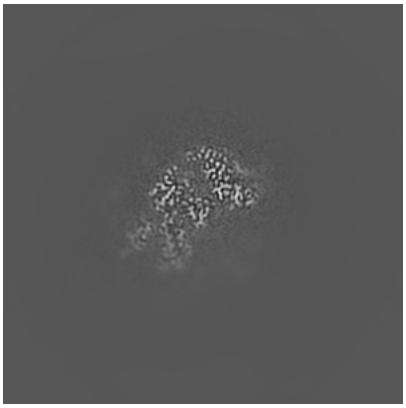


Z Index: 180

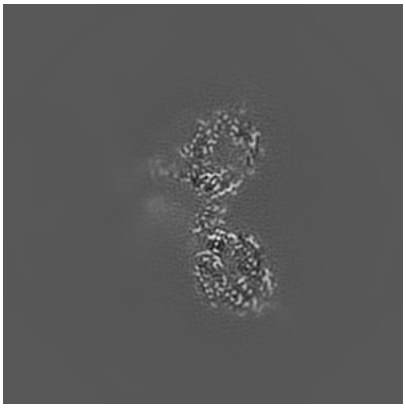
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

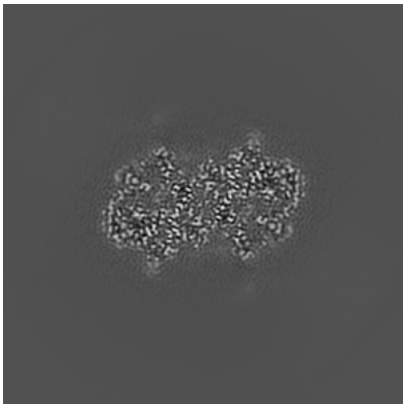
6.3.1 Primary map



X Index: 210



Y Index: 165



Z Index: 186

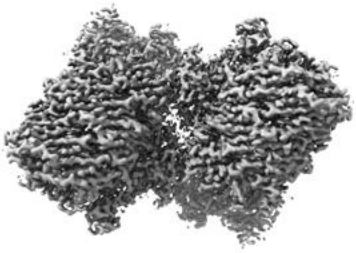
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.028. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

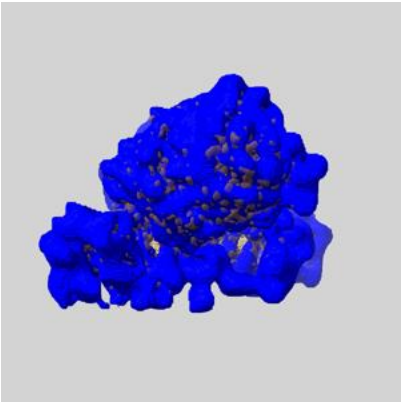
6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

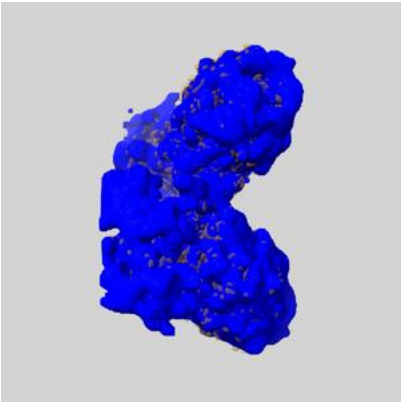
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

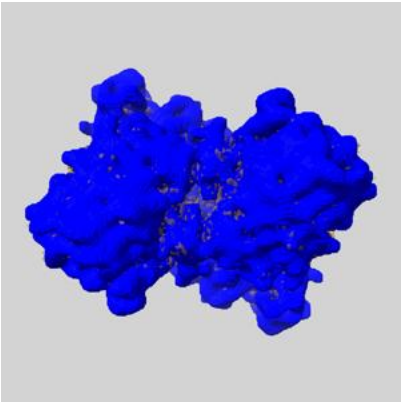
6.5.1 emd_12125_msk_1.map (i)



X



Y

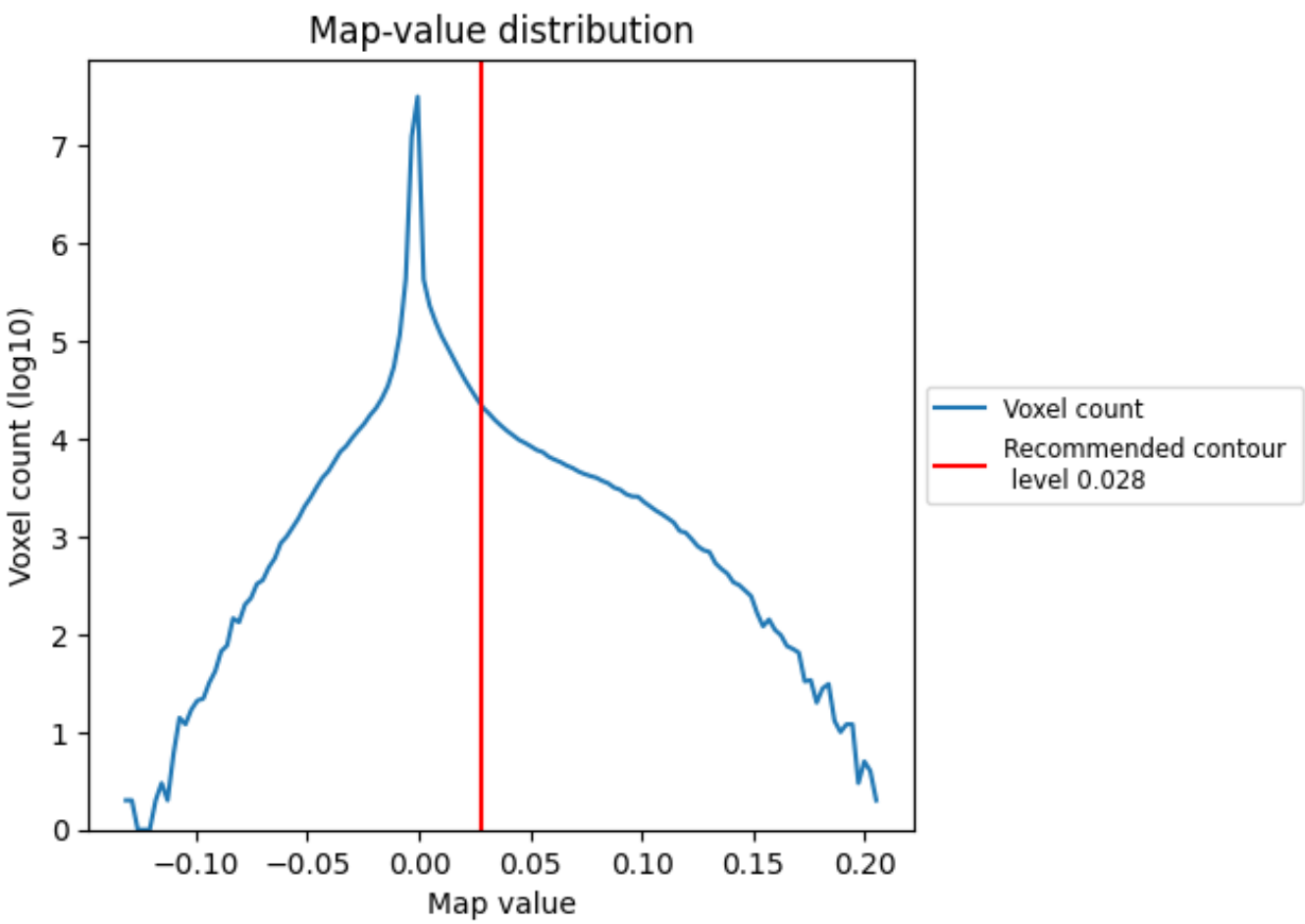


Z

7 Map analysis (i)

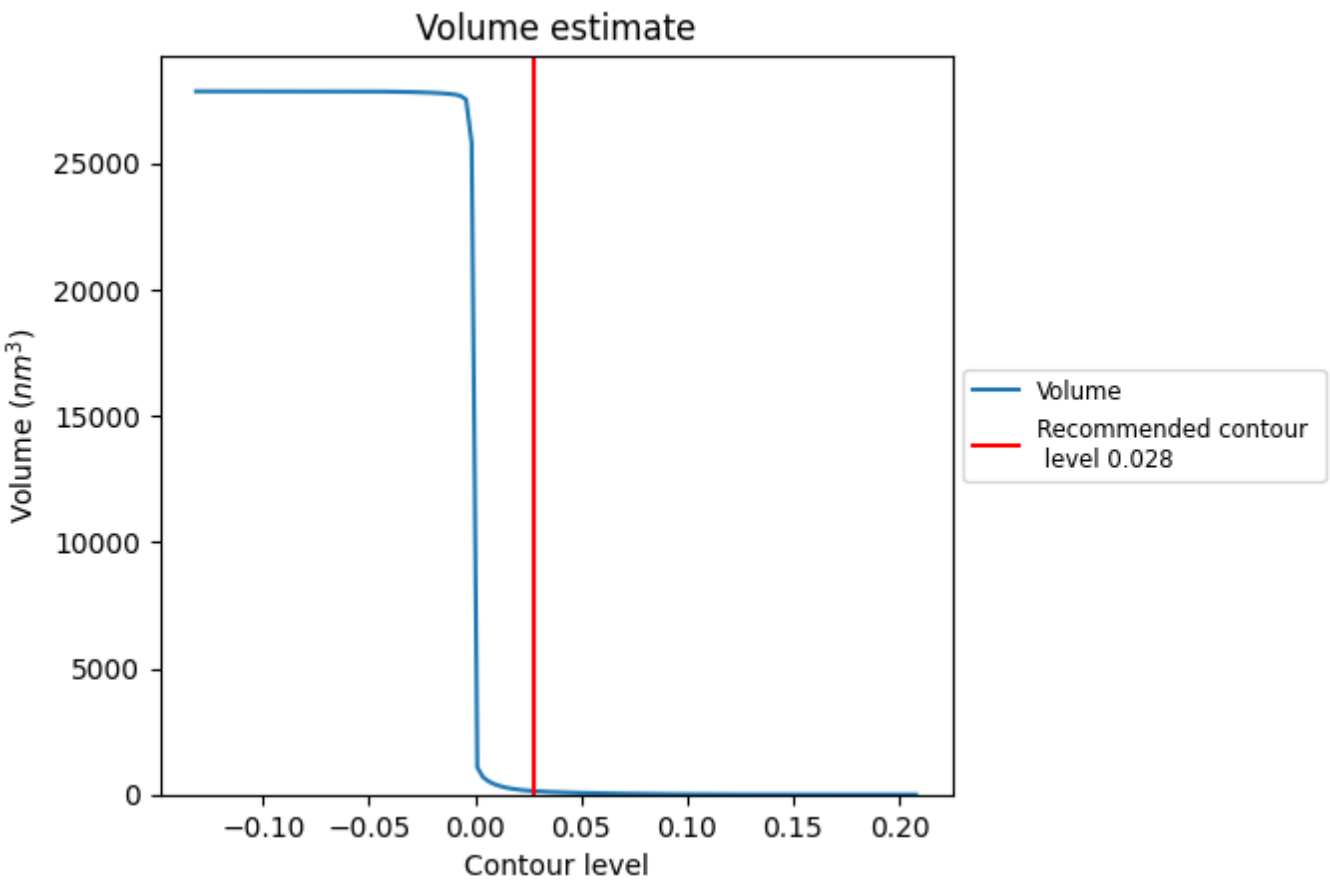
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

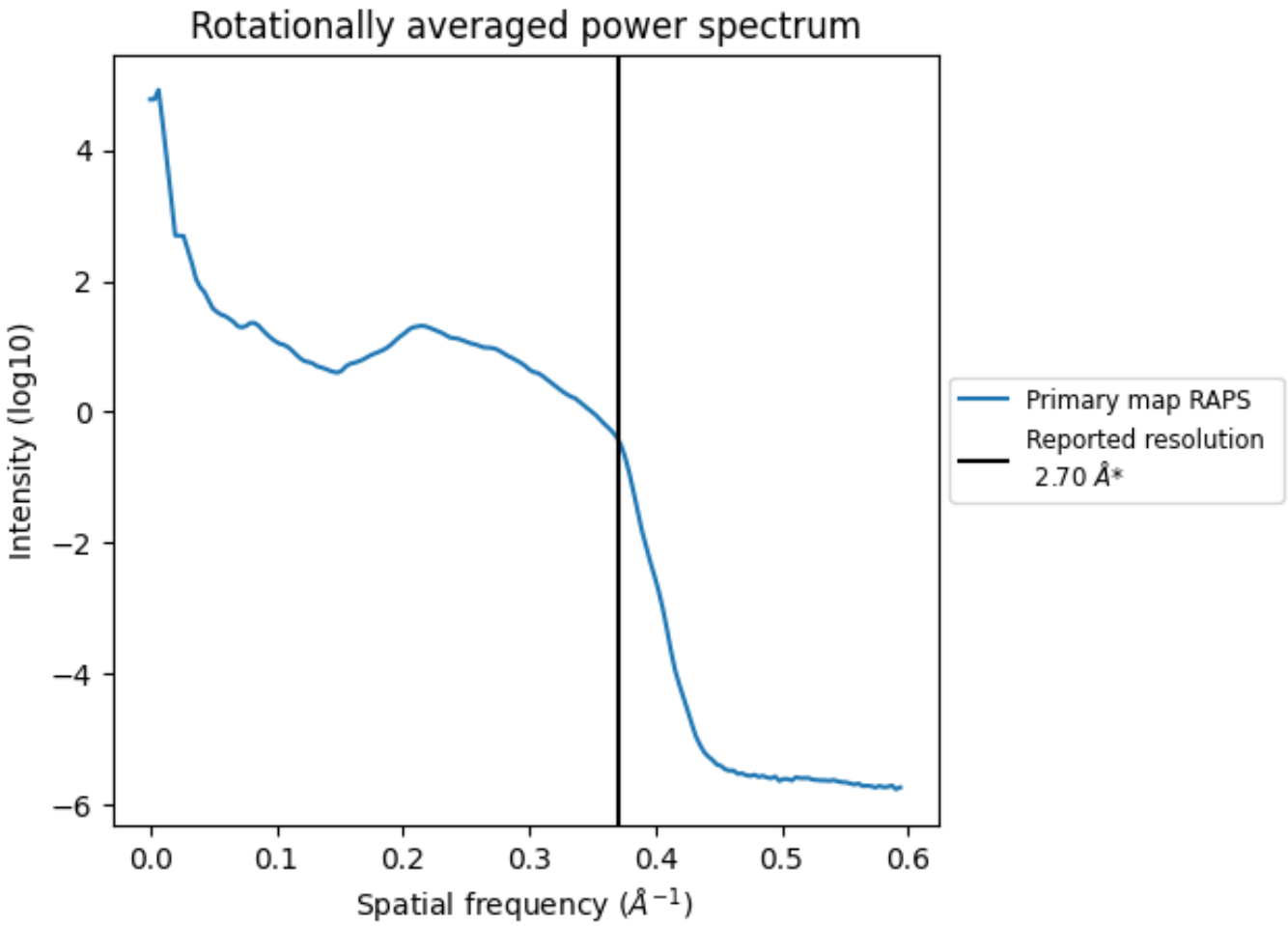
7.2 Volume estimate (i)



The volume at the recommended contour level is 137 nm^3; this corresponds to an approximate mass of 124 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

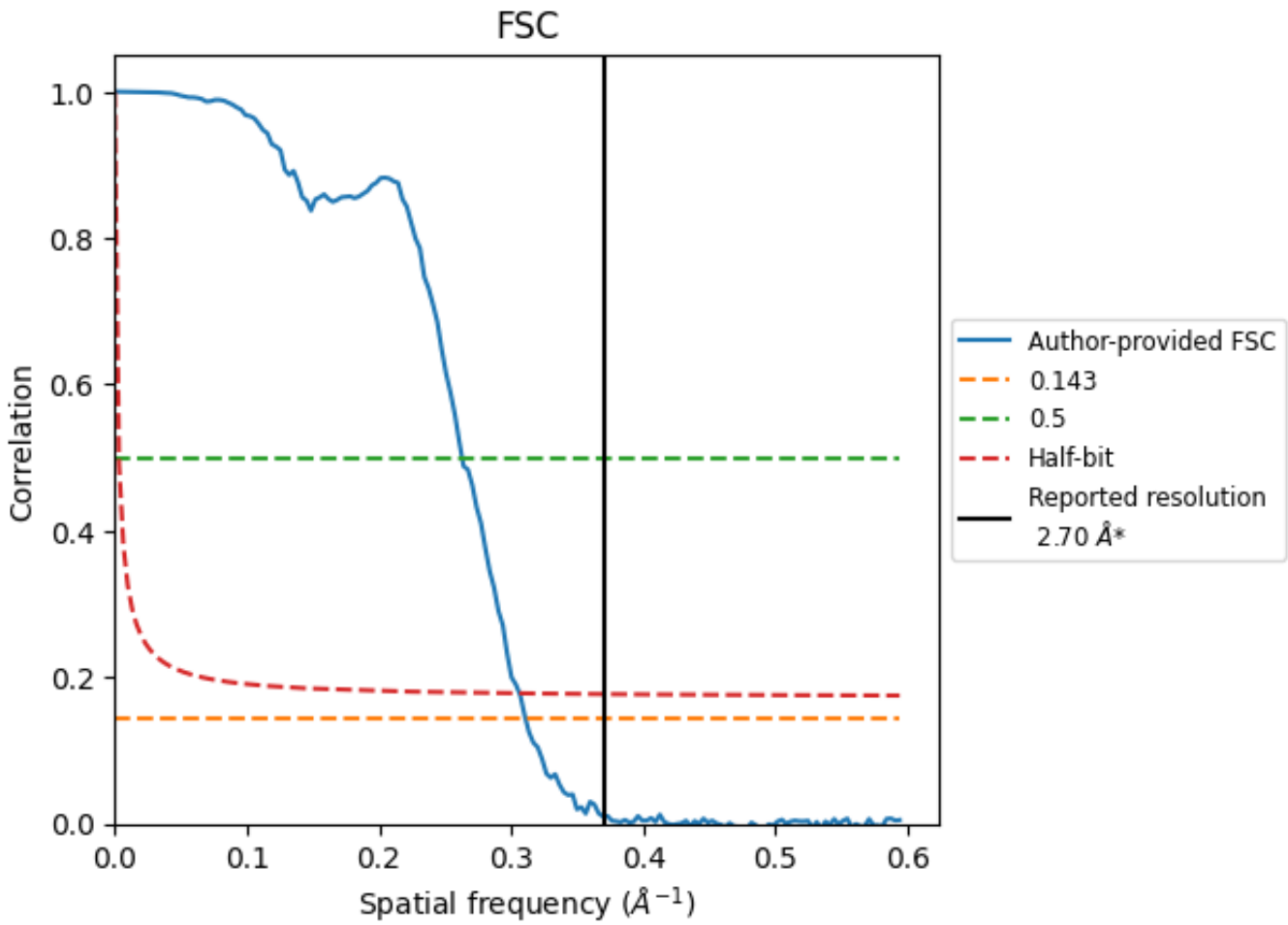


*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

8.2 Resolution estimates (i)

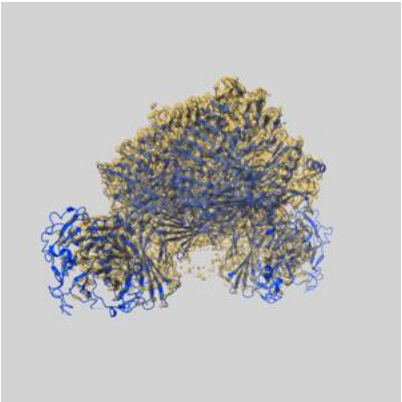
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	3.22	3.81	3.27
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.22 differs from the reported value 2.7 by more than 10 %

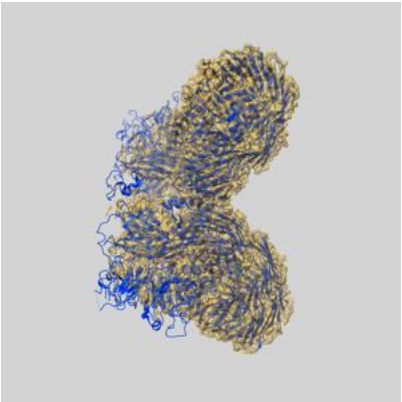
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-12125 and PDB model 7BAN. Per-residue inclusion information can be found in section 3 on page 7.

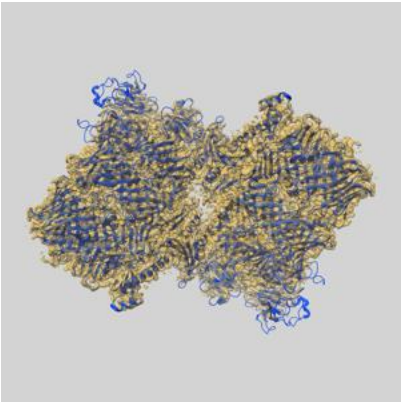
9.1 Map-model overlay (i)



X



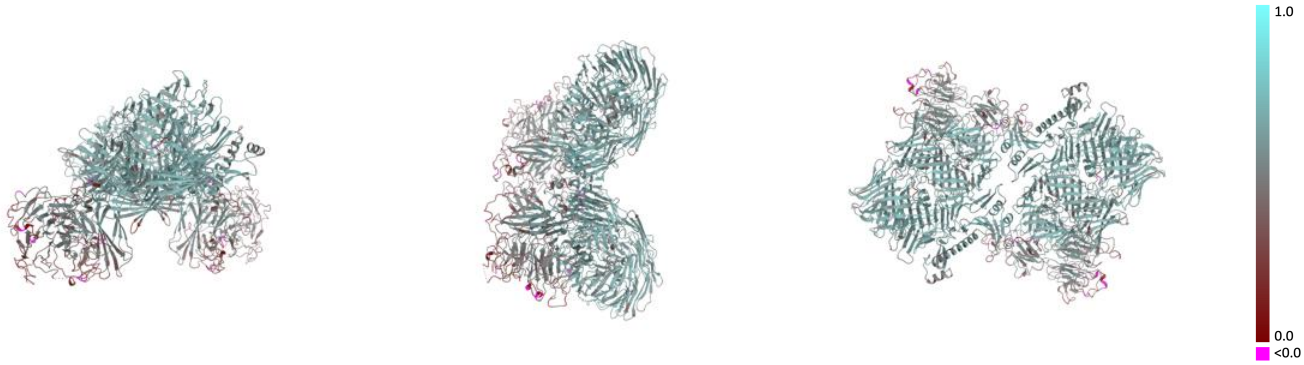
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.028 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

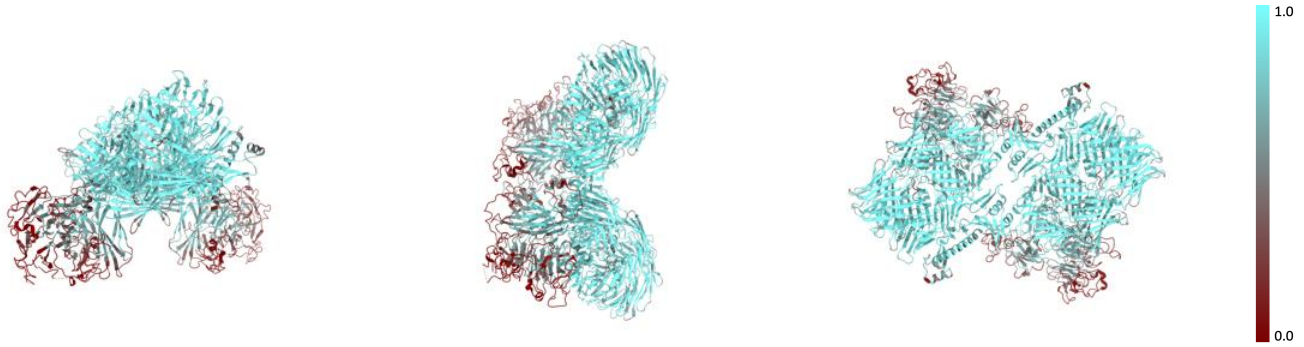
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

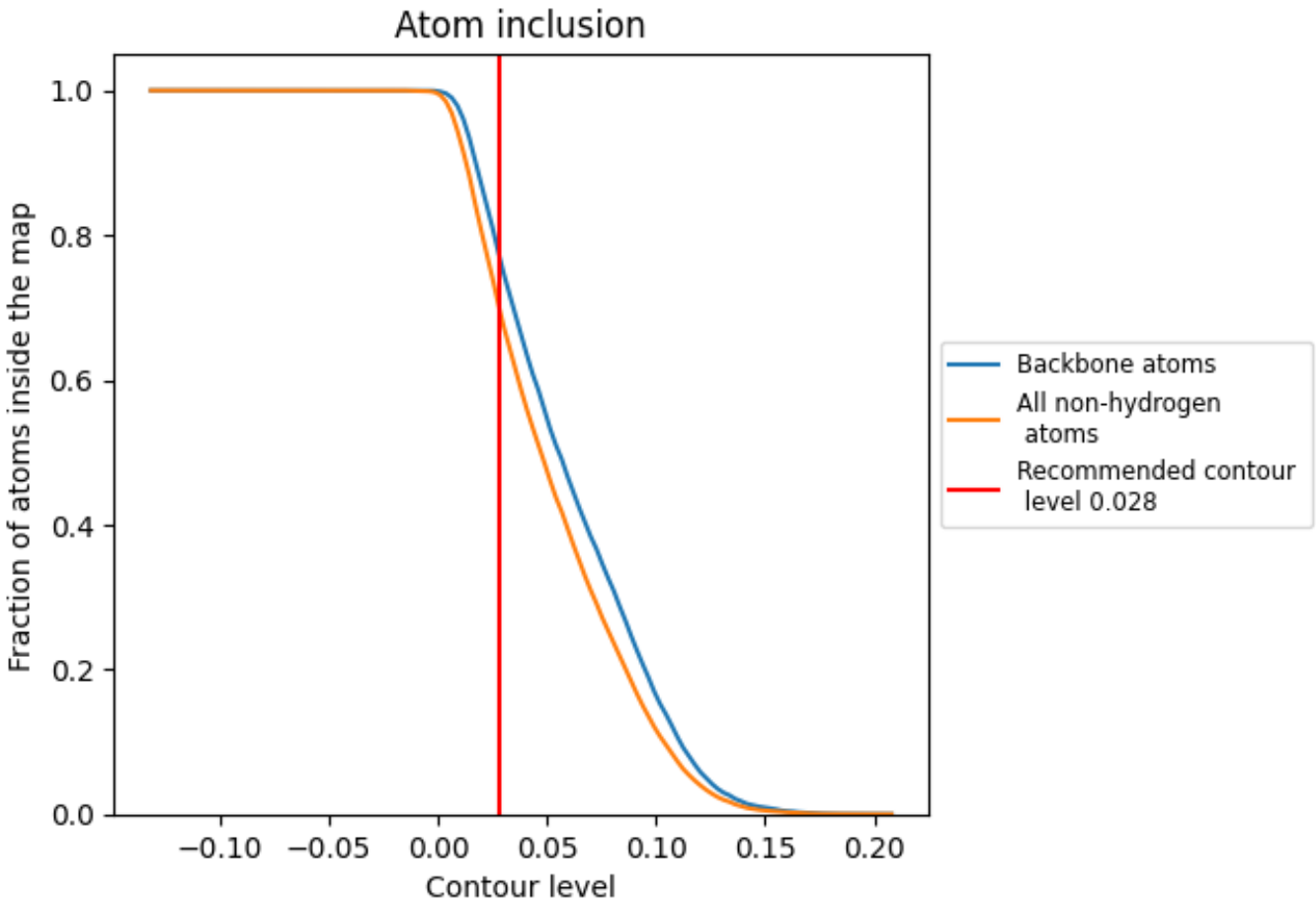
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.028).

9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.028) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7015	0.5360
A	0.7021	0.5360
B	0.7026	0.5370
C	0.7143	0.5510
D	0.7500	0.6100
E	0.7143	0.5620
F	0.1429	0.3530
G	0.7143	0.5450
H	0.7500	0.6030
I	0.7500	0.5530
J	0.1429	0.3670