Full wwPDB EM Validation Report

Jun 12, 2024 – 10:48 AM JST

PDB ID	:	8JUT
EMDB ID	:	EMD-36663
Title	:	rat megalin RAP complex
Authors	:	Goto, S.; Tsutsumi, A.; Lee, Y.; Hosojima, M.; Kabasawa, H.; Komochi, K.; Yun-san, L.; Nagatoshi, S.; Tsumoto, K.; Nishizawa, T.; Kikkawa, M.; Saito, A.
Deposited on	:	2023-06-27
Resolution	:	4.20 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 (i)) were used in the production of this report:

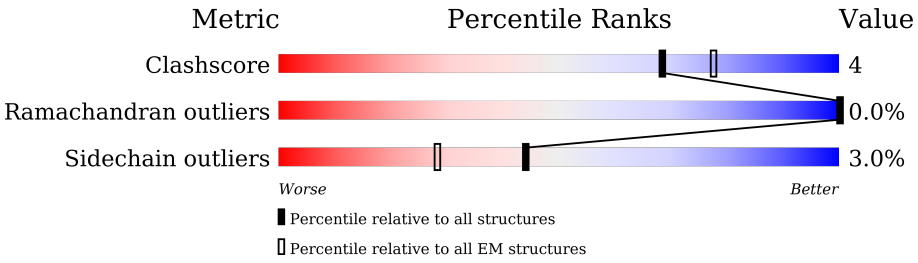
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance

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

The reported resolution of this entry is 4.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



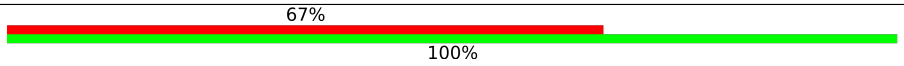
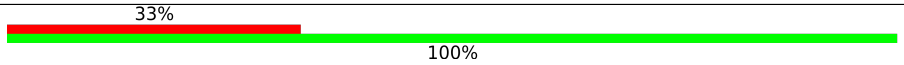
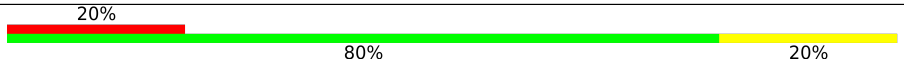
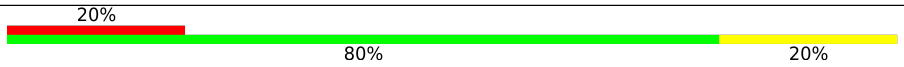
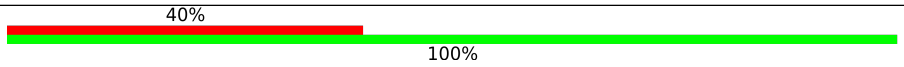
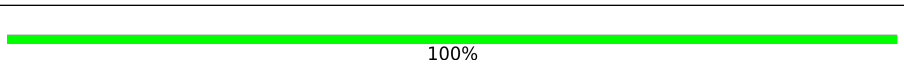
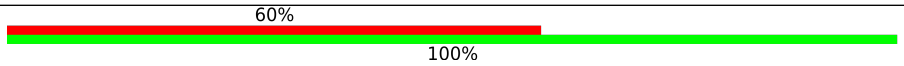
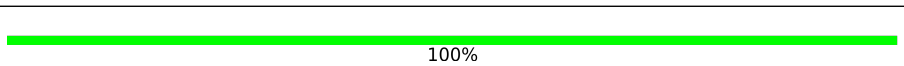
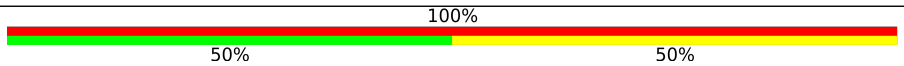
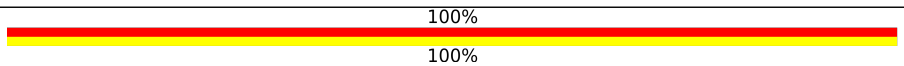
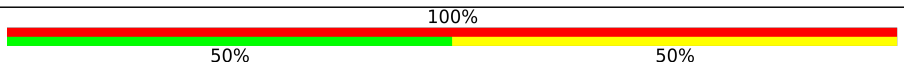
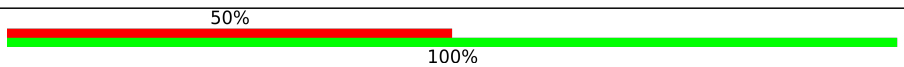
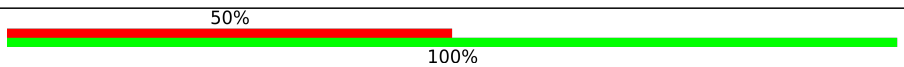
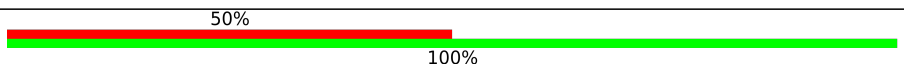
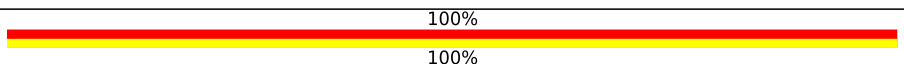
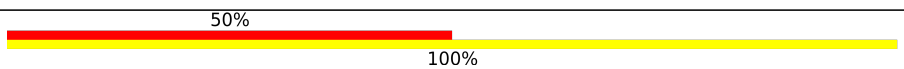
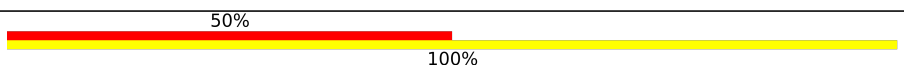
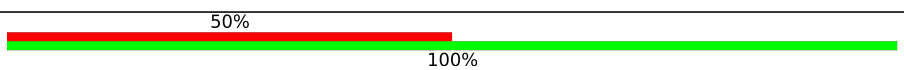
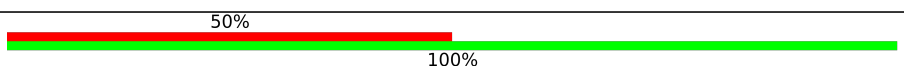
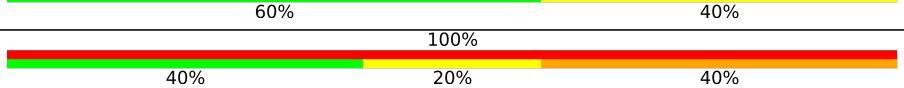
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	4660	34% 82% 10% 8%
1	B	4660	32% 82% 10% 8%
2	C	360	47% 39% 10% 51%
2	D	360	48% 38% 11% 51%
3	G	6	100% 100%
3	N	6	100% 100%
4	H	5	20% 100%
4	O	5	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	I	6	
5	P	6	
6	J	3	
6	Q	3	
7	K	5	
7	R	5	
8	L	5	
8	M	5	
8	S	5	
8	T	5	
9	E	2	
9	V	2	
9	X	2	
9	Y	2	
9	a	2	
9	d	2	
9	n	2	
9	q	2	
9	s	2	
9	t	2	
9	v	2	
9	x	2	
9	y	2	
10	1	5	
10	4	5	

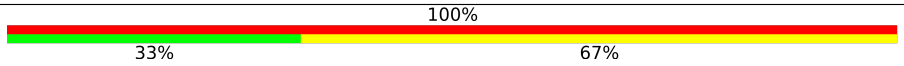
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
10	5	5	80% 60% 40%
10	9	5	100% 80% 20%
10	F	5	100% 80% 20%
10	Z	5	60% 60% 40%
10	b	5	20% 80% 20%
10	g	5	60% 60% 40%
10	j	5	80% 60% 40%
10	k	5	80% 40% 60%
10	l	5	100% 60% 40%
10	u	5	80% 80% 20%
11	U	5	60% 20% 60% 20%
12	2	3	67% 100%
12	3	3	67% 67% 33%
12	W	3	33% 33% 33% 33%
12	e	3	100% 67% 33%
12	f	3	67% 67% 33%
12	h	3	100% 100%
12	i	3	67% 33% 67%
12	m	3	100% 33% 67%
12	p	3	33% 67% 33%
12	r	3	33% 67% 33%
13	8	2	100% 100%
13	c	2	50% 100%
13	o	2	100% 100%
14	6	5	100% 40% 60%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
14	w	5	
15	z	3	
16	0	3	
16	7	3	

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 73258 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 LDL receptor related protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4308	Total	C	N	O	S	0	0
			33638	20708	5950	6605	375		
1	B	4308	Total	C	N	O	S	0	0
			33636	20706	5950	6605	375		

- Molecule 2 is a protein called Alpha-2-macroglobulin receptor-associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	177	Total	C	N	O	S	0	0
			1494	944	273	276	1		
2	D	177	Total	C	N	O	S	0	0
			1494	944	273	276	1		

- Molecule 3 is a protein called unclear peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	6	Total	C	N	O	0	0
			30	18	6	6		
3	N	6	Total	C	N	O	0	0
			30	18	6	6		

- Molecule 4 is a protein called unclear peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	H	5	Total	C	N	O	0	0
			28	16	6	6		
4	O	5	Total	C	N	O	0	0
			28	16	6	6		

- Molecule 5 is a protein called unclear peptide.

Mol	Chain	Residues	Atoms	AltConf	Trace
5	I	6	Total C N O 33 21 6 6	0	0
5	P	6	Total C N O 33 21 6 6	0	0

- Molecule 6 is a protein called unclear peptide.

Mol	Chain	Residues	Atoms	AltConf	Trace
6	J	3	Total C N O S 16 9 3 3 1	0	0
6	Q	3	Total C N O S 16 9 3 3 1	0	0

- Molecule 7 is a protein called unclear peptide.

Mol	Chain	Residues	Atoms	AltConf	Trace
7	K	5	Total C N O 33 19 5 9	0	0
7	R	5	Total C N O 33 19 5 9	0	0

- Molecule 8 is a protein called unclear peptide.

Mol	Chain	Residues	Atoms	AltConf	Trace
8	L	5	Total C N O 28 16 6 6	0	0
8	M	5	Total C N O 28 16 6 6	0	0
8	S	5	Total C N O 28 16 6 6	0	0
8	T	5	Total C N O 28 16 6 6	0	0

- Molecule 9 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

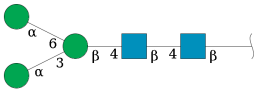
Mol	Chain	Residues	Atoms	AltConf	Trace
9	E	2	Total C N O 28 16 2 10	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
9	V	2	Total	C	N	O	0	0
			28	16	2	10		
9	X	2	Total	C	N	O	0	0
			28	16	2	10		
9	Y	2	Total	C	N	O	0	0
			28	16	2	10		
9	a	2	Total	C	N	O	0	0
			28	16	2	10		
9	d	2	Total	C	N	O	0	0
			28	16	2	10		
9	n	2	Total	C	N	O	0	0
			28	16	2	10		
9	q	2	Total	C	N	O	0	0
			28	16	2	10		
9	s	2	Total	C	N	O	0	0
			28	16	2	10		
9	t	2	Total	C	N	O	0	0
			28	16	2	10		
9	v	2	Total	C	N	O	0	0
			28	16	2	10		
9	x	2	Total	C	N	O	0	0
			28	16	2	10		
9	y	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



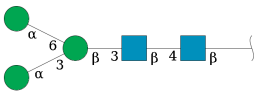
Mol	Chain	Residues	Atoms				AltConf	Trace
10	F	5	Total	C	N	O	0	0
			61	34	2	25		
10	Z	5	Total	C	N	O	0	0
			61	34	2	25		
10	b	5	Total	C	N	O	0	0
			61	34	2	25		
10	g	5	Total	C	N	O	0	0
			61	34	2	25		

Continued on next page...

Continued from previous page...

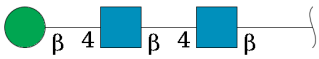
Mol	Chain	Residues	Atoms				AltConf	Trace
10	j	5	Total	C	N	O	0	0
			61	34	2	25		
10	k	5	Total	C	N	O	0	0
			61	34	2	25		
10	l	5	Total	C	N	O	0	0
			61	34	2	25		
10	u	5	Total	C	N	O	0	0
			61	34	2	25		
10	1	5	Total	C	N	O	0	0
			61	34	2	25		
10	4	5	Total	C	N	O	0	0
			61	34	2	25		
10	5	5	Total	C	N	O	0	0
			61	34	2	25		
10	9	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
11	U	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 12 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
12	W	3	Total	C	N	O	0	0
			39	22	2	15		
12	e	3	Total	C	N	O	0	0
			39	22	2	15		

Continued on next page...

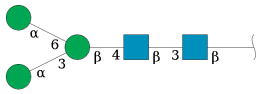
Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
12	f	3	Total	C	N	O	0	0
			39	22	2	15		
12	h	3	Total	C	N	O	0	0
			39	22	2	15		
12	i	3	Total	C	N	O	0	0
			39	22	2	15		
12	m	3	Total	C	N	O	0	0
			39	22	2	15		
12	p	3	Total	C	N	O	0	0
			39	22	2	15		
12	r	3	Total	C	N	O	0	0
			39	22	2	15		
12	2	3	Total	C	N	O	0	0
			39	22	2	15		
12	3	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 13 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.

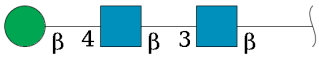
Mol	Chain	Residues	Atoms				AltConf	Trace
13	c	2	Total	C	N	O	0	0
			28	16	2	10		
13	o	2	Total	C	N	O	0	0
			28	16	2	10		
13	8	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 14 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



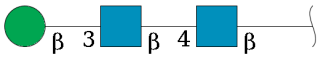
Mol	Chain	Residues	Atoms				AltConf	Trace
14	w	5	Total	C	N	O	0	0
			61	34	2	25		
14	6	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 15 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



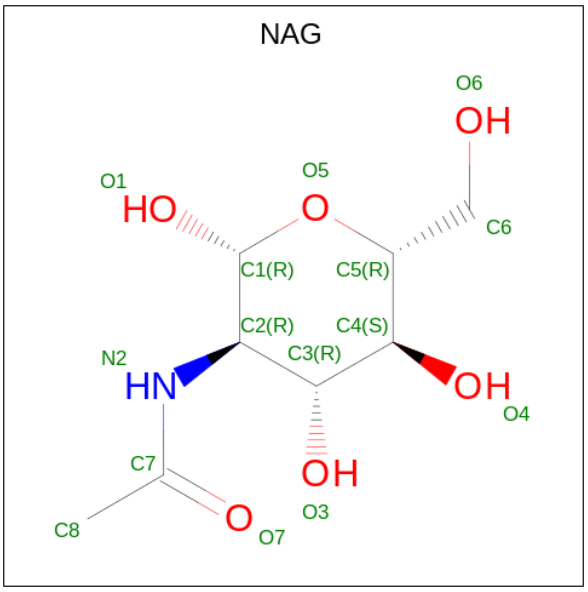
Mol	Chain	Residues	Atoms				AltConf	Trace
15	z	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 16 is an oligosaccharide called beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
16	0	3	Total	C	N	O	0	0
			39	22	2	15		
16	7	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 17 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



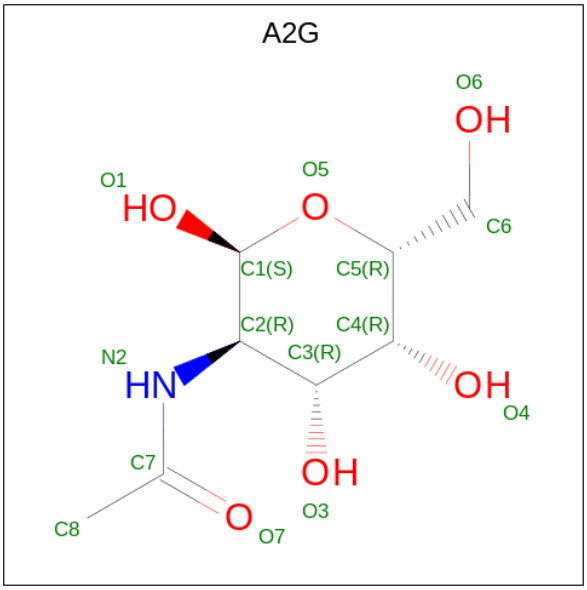
Mol	Chain	Residues	Atoms	AltConf
17	A	1	Total C N O 14 8 1 5	0
17	A	1	Total C N O 14 8 1 5	0
17	A	1	Total C N O 14 8 1 5	0
17	A	1	Total C N O 14 8 1 5	0
17	A	1	Total C N O 14 8 1 5	0
17	A	1	Total C N O 14 8 1 5	0
17	A	1	Total C N O 14 8 1 5	0
17	A	1	Total C N O 14 8 1 5	0
17	A	1	Total C N O 14 8 1 5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

Continued on next page...

Continued from previous page...

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

- Molecule 18 is 2-acetamido-2-deoxy-alpha-D-galactopyranose (three-letter code: A2G) (formula: $C_8H_{15}NO_6$).



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

Continued on next page...

Continued from previous page...

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

- Molecule 19 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
19	A	44	Total Ca 44 44	0
19	B	44	Total Ca 44 44	0

- Molecule 20 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

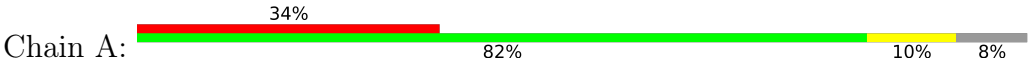
Mol	Chain	Residues	Atoms	AltConf
20	A	1	Total Ni 1 1	0
20	B	1	Total Ni 1 1	0

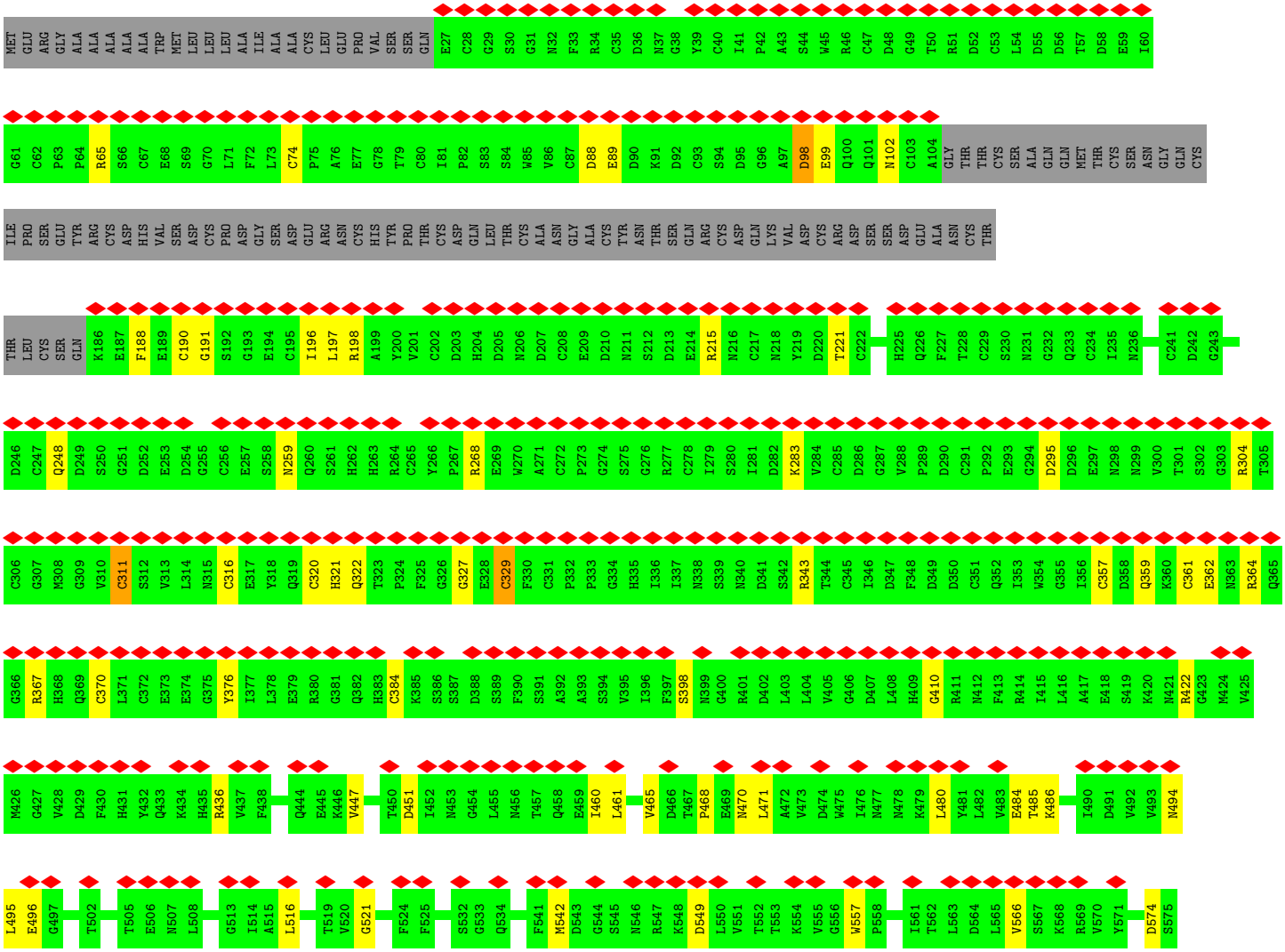
3 Residue-property plots (i)

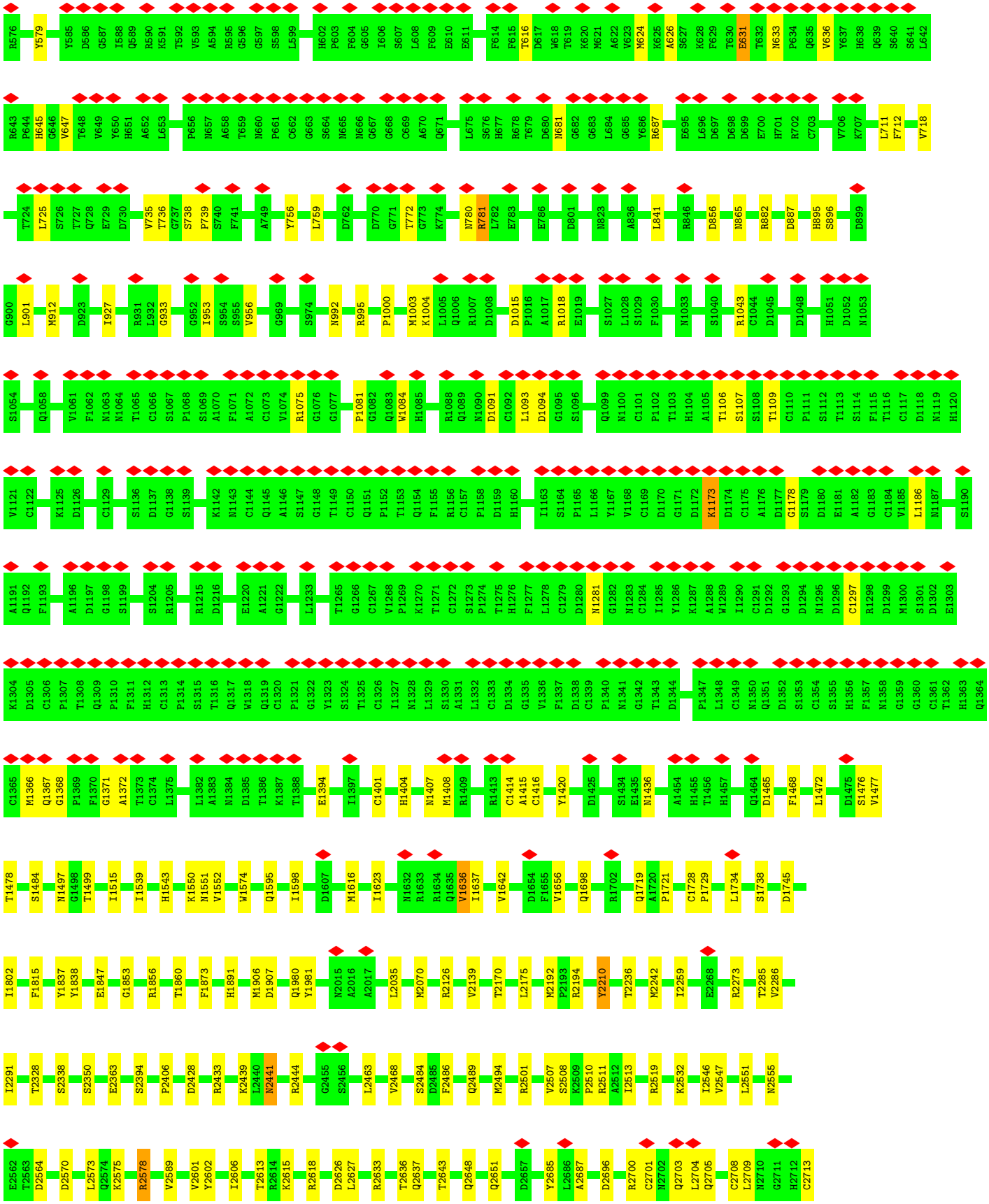
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: LDL receptor related protein 2

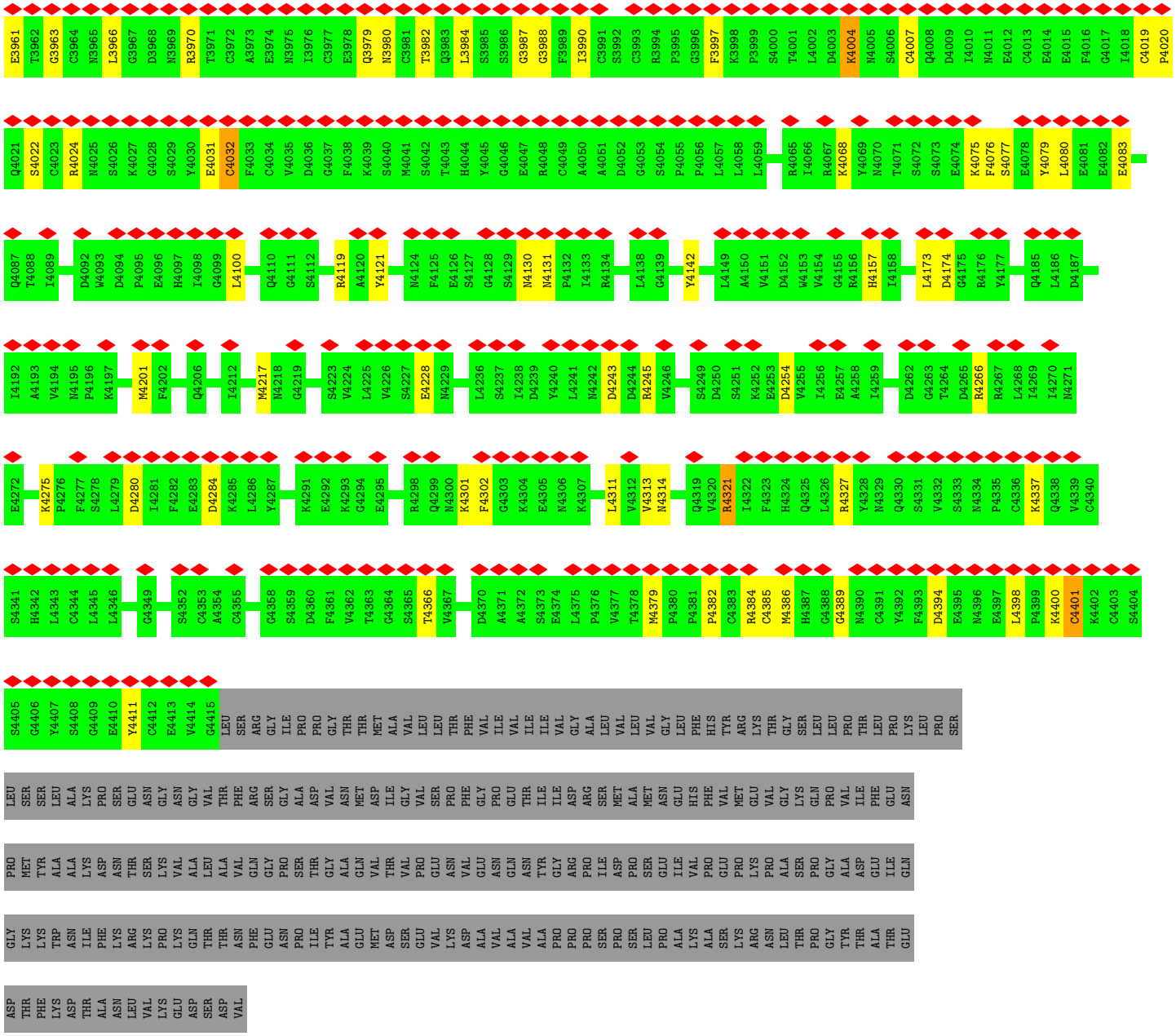
Chain A:





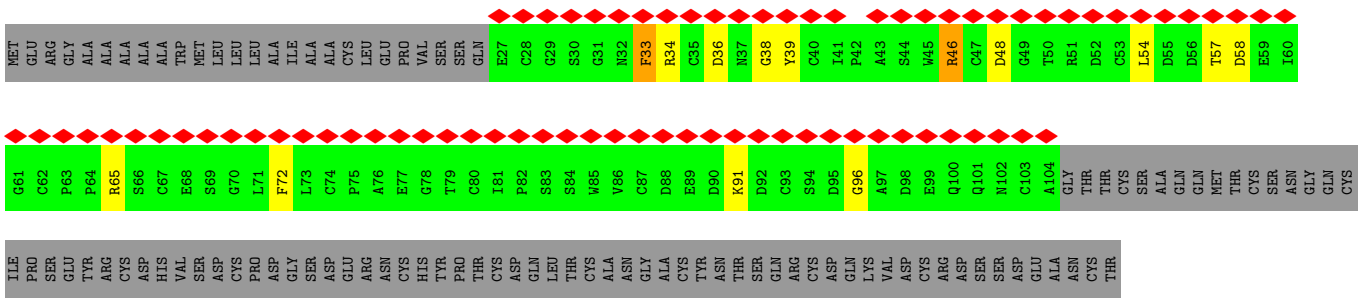

R576 Y579 Y585 D586 G587 I588 Q589 R590 K591 T592 V593 A594 R595 G596 G597 S598 L599 H602 P603 F604 G605 I606 S607 L608 F609 E610 E611 F614 F615 T616 D617 W618 T619 K620 M621 A622 V623 M624 K625 A626 S627 K628 F629 T630 E631 T632 N633 P634 Q635 V636 Y637 H638 Q639 S640 S641 L642
R643 P644 H645 G646 V647 T648 V649 Y650 H651 A652 L653 P656 N657 A658 T659 N660 P661 C662 G663 S664 N665 N666 G667 G668 C669 A670 Q671 L675 S676 H677 R678 T679 D680 N681 G682 G683 L684 G685 Y686 R687 E695 L696 D697 D698 D699 E700 H701 R702 C703 V706 K707 L711 F712 V718
T724 L725 S726 T727 Q728 E729 D730 V735 T736 G737 S738 P739 S740 F741 A749 Y756 L759 D762 D770 G771 T772 G773 K774 N780 R781 L782 E783 E786 D801 N823 A836 L841 R846 D856 N865 R882 D887 H895 S896 D899
G900 L901 M912 D923 I927 R931 L932 G933 G952 I953 S954 S955 V956 G969 S974 N992 R995 P1000 M1003 K1004 L1005 Q1006 R1007 D1008 D1015 P1016 A1017 R1018 E1019 S1027 L1028 S1029 F1030 N1033 S1040 R1043 C1044 D1045 D1048 H1051 D1052 N1053
S1054 Q1058 V1061 F1062 N1063 N1064 T1065 C1066 S1067 P1068 S1069 A1070 F1071 A1072 C1073 V1074 R1075 G1076 G1077 P1081 G1082 Q1083 W1084 H1085 R1088 Q1089 N1090 D1091 C1092 L1093 D1094 G1095 S1096 Q1099 N1100 C1101 P1102 T1103 H1104 A1105 T1106 S1107 S1108 T1109 C1110 P1111 S1112 T1113 S1114 F1115 T1116 C1117 D1118 N1119 H1120
V1121 C1122 K1125 D1126 C1129 S1136 D1137 G1138 S1139 K1142 N1143 C1144 Q1145 A1146 S1147 G1148 T1149 C1150 Q1151 P1152 T1153 Q1154 F1155 R1156 C1157 P1158 D1159 H1160 I1163 S1164 P1165 L1166 Y1167 V1168 C1169 D1170 G1171 D1172 K1173 D1174 C1175 A1176 D1177 G1178 S1179 D1180 E1181 A1182 G1183 C1184 V1185 L1186 N1187 S1190
A1191 Q1192 F1193 A1196 D1197 G1198 S1199 S1204 R1205 R1215 D1216 E1220 A1221 G1222 L1233 T1265 G1266 C1267 V1268 P1269 K1270 T1271 C1272 S1273 P1274 T1275 H1276 F1277 L1278 C1279 D1280 N1281 G1282 N1283 C1284 I1285 Y1286 K1287 A1288 W1289 I1290 C1291 D1292 G1293 D1294 N1295 D1296 C1297 R1298 D1299 M1300 S1301 D1302 E1303
K1304 D1305 C1306 P1307 T1308 Q1309 P1310 F1311 H1312 C1313 P1314 S1315 T1316 Q1317 W1318 Q1319 C1320 P1321 G1322 Y1323 S1324 T1325 C1326 I1327 N1328 L1329 S1330 A1331 L1332 C1333 D1334 G1335 V1336 F1337 D1338 C1339 P1340 N1341 G1342 T1343 D1344 P1347 L1348 C1349 N1350 Q1361 D1362 S1353 C1354 S1355 H1356 F1357 N1368 G1359 G1360 C1361 T1362 H1363 Q1364
C1365 M1366 Q1367 G1368 P1369 F1370 G1371 A1372 T1373 C1374 L1375 L1382 A1383 N1384 D1385 T1386 K1387 T1388 E1394 I1397 C1401 H1404 N1407 M1408 R1409 R1413 C1414 A1415 C1416 Y1420 D1425 S1434 E1435 N1436 A1454 H1455 T1456 H1457 Q1464 D1465 F1468 L1472 D1475 S1476 V1477
T1478 S1484 N1497 G1498 T1499 I1515 I1539 H1543 K1550 N1551 V1552 W1574 Q1595 I1598 D1607 M1616 I1623 N1632 R1633 R1634 Q1635 V1636 I1637 V1642 D1654 F1655 V1656 Q1698 R1702 Q1719 A1720 P1721 C1728 P1729 L1734 S1738 D1745
I1802 F1815 Y1837 Y1838 E1847 G1853 R1856 T1860 F1873 H1891 M1906 D1907 Q1980 Y1981 N2015 A2016 A2017 L2035 M2070 R2126 V2139 T2170 L2175 M2192 P2193 R2194 Y2210 T2236 M2242 I2259 E2268 R2273 T2285 V2286
I2291 T2328 S2338 S2350 E2363 S2394 P2406 D2428 R2433 K2439 L2440 N2441 R2444 G2455 S2456 L2463 V2468 S2484 D2485 F2486 Q2489 M2494 R2501 V2507 S2508 K2509 P2510 R2511 A2512 I2513 R2519 K2532 I2546 V2547 L2551 N2555
E2562 T2563 D2564 D2570 L2573 Q2574 K2575 R2578 V2589 V2601 Y2602 I2606 T2613 R2614 K2615 R2618 D2626 L2627 R2633 T2636 Q2637 T2643 Q2648 Q2651 D2657 Y2685 L2686 A2687 D2696 R2700 C2701 N2702 Q2703 L2704 Q2705 C2708 L2709 N2710 G2711 H2712 C2713

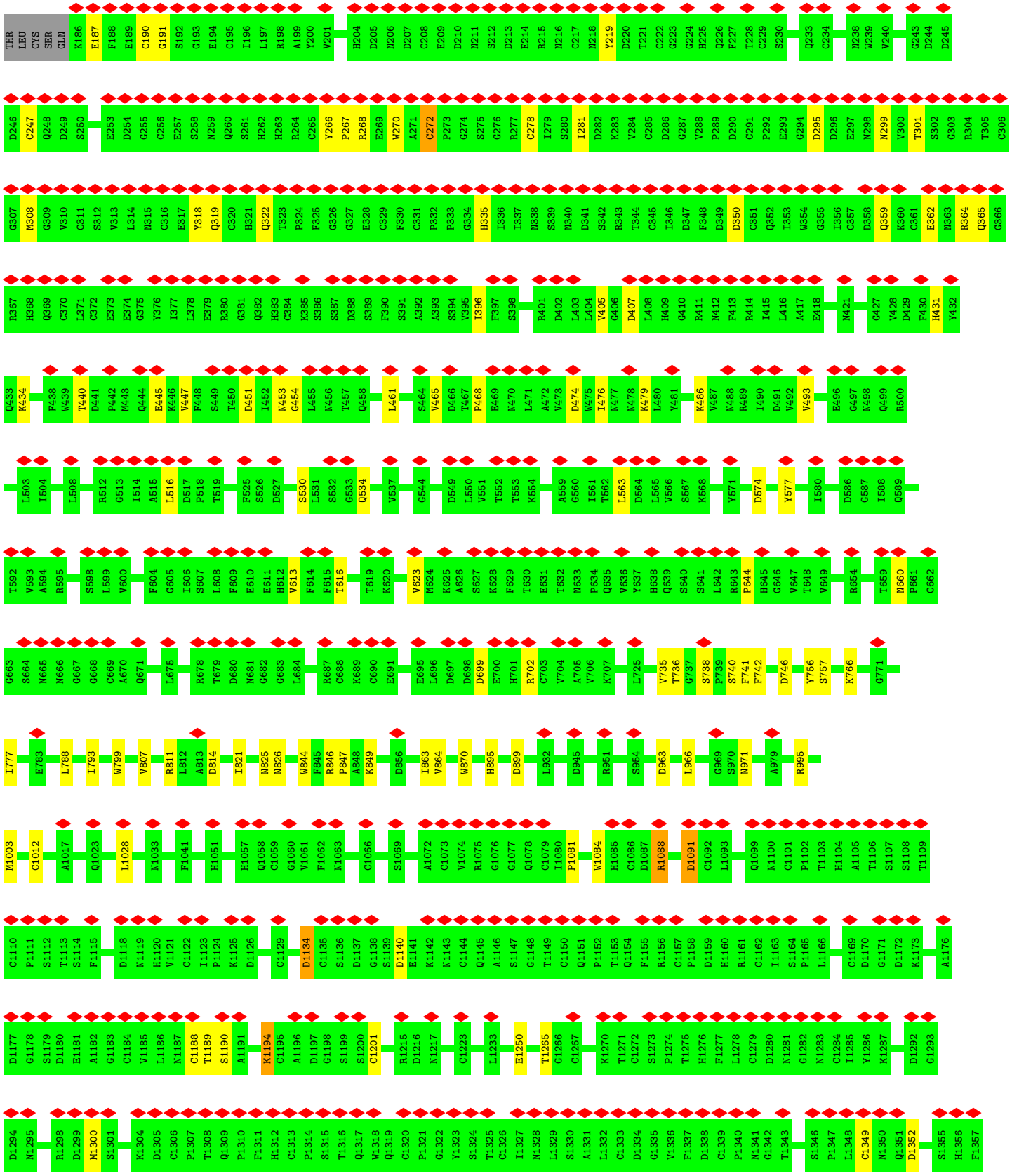

Q2716 N2722 G2727 S2730 F2739 G2775 R2779 N2780 C2781 N2782 S2783 T2784 T2785 E2786 F2787 T2788 C2789 S2790 N2791 G2792 R2793 C2794 I2795 P2796 L2797 S2798 Y2799 V2800 C2801 N2802 G2803 I2804 N2805 N2806 C2807 H2808 D2809 N2810 D2811 D2814 E2815 K2816 N2817 C2818 P2819 P2820 H2821 T2822 C2823 P2824 P2825 D2826
F2827 T2828 K2829 C2830 Q2831 T2832 T2833 N2834 I2835 C2836 V2837 P2838 R2839 A2840 F2841 L2842 C2843 D2844 G2845 D2846 N2847 D2848 C2849 G2850 D2851 G2852 S2853 D2854 E2855 N2856 P2857 I2858 Y2859 C2860 A2861 S2862 H2863 T2864 C2865 R2866 S2867 N2868 E2869 F2870 Q2871 C2872 L2873 S2874 P2875 Q2876 R2877 C2878 I2879 P2880 S2881 Y2882 W2883 F2884 C2885 D2886
G2887 E2888 A2889 D2890 C2891 A2892 D2893 G2894 S2895 D2896 D2899 T2900 C2901 G2902 H2903 S2904 V2905 N2906 T2907 C2908 R2909 A2910 S2911 Q2912 F2913 Q2914 C2915 D2916 N2917 G2918 R2919 S2922 G2923 N2924 C2927 D2928 G2929 D2930 N2931 D2932 C2933 G2934 D2935 D2938 E2939 D2940 Q2941 R2942 H2943 H2944 C2945 E2946 L2947 Q2948 N2949 C2950
S2951 S2952 T2953 Q2954 F2955 V2958 N2959 S2960 R2961 P2962 P2963 N2964 R2965 R2966 C2967 I2968 P2969 Q2970 Y2971 W2972 V2973 G2976 D2977 C2980 S2981 D2982 A2983 L2984 L2987 Q2988 N2989 C2990 T2991 M2992 R2993 T2994 C2995 S2996 A2997 G2998 E2999 F3000 S3001 C3002 A3003 N3004 G3005 R3006 R3009 Q3010 S3011 F3012 R3013 C3014 D3015
R3016 R3017 D3022 Y3023 E3026 R3027 G3028 C3029 S3030 Y3031 P3032 N3037 Q3038 F3039 Q3042 N3043 G3044 R3045 R3049 V3052 C3053 D3054 E3055 D3056 N3057 D3058 C3059 G3060 S3063 D3064 E3065 Q3066 E3067 H3068 L3069 C3070 H3071 T3072 P3073 E3074 P3075 T3076 C3077 P3078 L3079 H3080 Q3081 F3082 R3083 C3084 D3085 N3086 G3087
H3088 C3089 I3090 E3091 M3092 G3093 R3094 V3095 C3096 N3097 H3098 V3099 D3100 D3101 C3102 S3103 D3104 N3105 S3106 D3107 E3108 K3109 G3110 C3111 G3112 I3113 N3114 E3115 C3116 L3117 D3118 S3119 S3120 I3121 S3122 R3123 C3124 D3125 H3126 N3127 C3128 T3129 D3130 T3131 I3132 T3133 S3134 F3135 Y3136 C3137 K3144 L3145 M3146 S3147 D3148 K3149 R3150 S3151 C3152
I3155 C3158 K3159 E3160 V3173 D3189 G3190 K3191 S3206 R3212 S3220 L3228 V3231 E3249 N3262 R3270 L3271 R3272 E3275 S3276 L3277 D3280 S3283 C3295 L3296 G3303 M3308 H3312 D3315 A3316 R3326 H3345 D3375 N3378 D3406
L3415 T3416 I3417 D3420 T3421 V3422 T3425 D3426 T3431 N3448 T3449 T3450 H3451 K3452 P3453 T3473 N3474 N3475 G3476 G3477 C3478 S3479 H3480 L3481 C3482 L3483 D3497 D3498 T3501 V3502 Q3503 L3504 R3505 D3506 R3507 T3508 L3509 M3513 S3516 N3523 N3524 E3525 I3530 C3534 K3538
S3541 D3542 G3543 S3544 D3545 E3546 P3547 D3548 L3549 C3550 P3551 H3552 R3553 F3554 C3555 R3556 L3557 G3558 Q3559 C3562 R3563 D3564 G3565 N3566 Q3571 A3572 L3573 A3576 R3577 Q3578 D3579 C3580 A3581 D3582 R3588 V3589 L3590 C3591 E3592 H3593 H3594 R3595 C3596 E3597 S3598 N3599 A3604 I3609 Q3614 C3615 D3616 S3617 V3618
N3619 D3620 C3621 L3622 D3623 D3626 E3627 D3628 T3629 S3630 S3634 C3637 R3638 K3643 C3644 N3645 K3655 N3660 S3666 D3671 E3672 T3675 A3676 A3677 Y3678 N3679 C3680 D3681 N3682 H3683 S3687 C3688 K3689 R3693 C3694 I3695 D3705 R3708 Q3714 S3718 V3719 P3720 C3721 H3722 P3723
D3726 A3730 N3731 H3732 P3736 W3739 D3745 D3746 C3747 G3748 N3755 C3756 V3757 P3758 R3759 E3760 E3765 A3769 Q3782 E3783 N3784 G3787 R3793 E3796 M3797 K3798 H3801 T3808 S3809 G3810 H3811 C3812 V3813 P3814 L3817 A3818 C3819 D3820 G3821 L3826 C3834 P3835 T3836
R3837 F3838 P3839 N3840 G3841 C3844 P3845 A3846 A3847 M3848 F3849 E3850 C3851 K3852 N3853 H3854 I3857 F3860 W3861 I3862 C3863 E3866 N3867 D3868 C3869 V3870 D3871 G3872 S3873 D3874 E3875 E3876 I3877 H3878 L3879 C3880 F3881 N3882 I3883 P3884 C3885 E3886 S3887 P3888 Q3889 R3890 F3891 R3892 C3893 D3894 N3895 S3896 R3897 C3898 V3899 Y3900
G3901 H3902 Q3903 L3904 C3905 N3906 G3907 V3908 D3909 D3910 C3911 G3912 D3913 G3914 S3915 D3916 E3917 K3918 E3919 E3920 H3921 C3922 R3923 K3924 P3925 T3926 H3927 K3928 P3929 C3930 T3931 D3932 T3933 E3934 Y3935 K3936 C3937 S3938 N3939 G3940 N3941 C3942 I3943 S3944 Q3945 H3946 Y3947 V3948 C3949 D3950 N3951 V3952 N3953 D3954 C3955 G3956 D3957 L3958 S3959 D3960

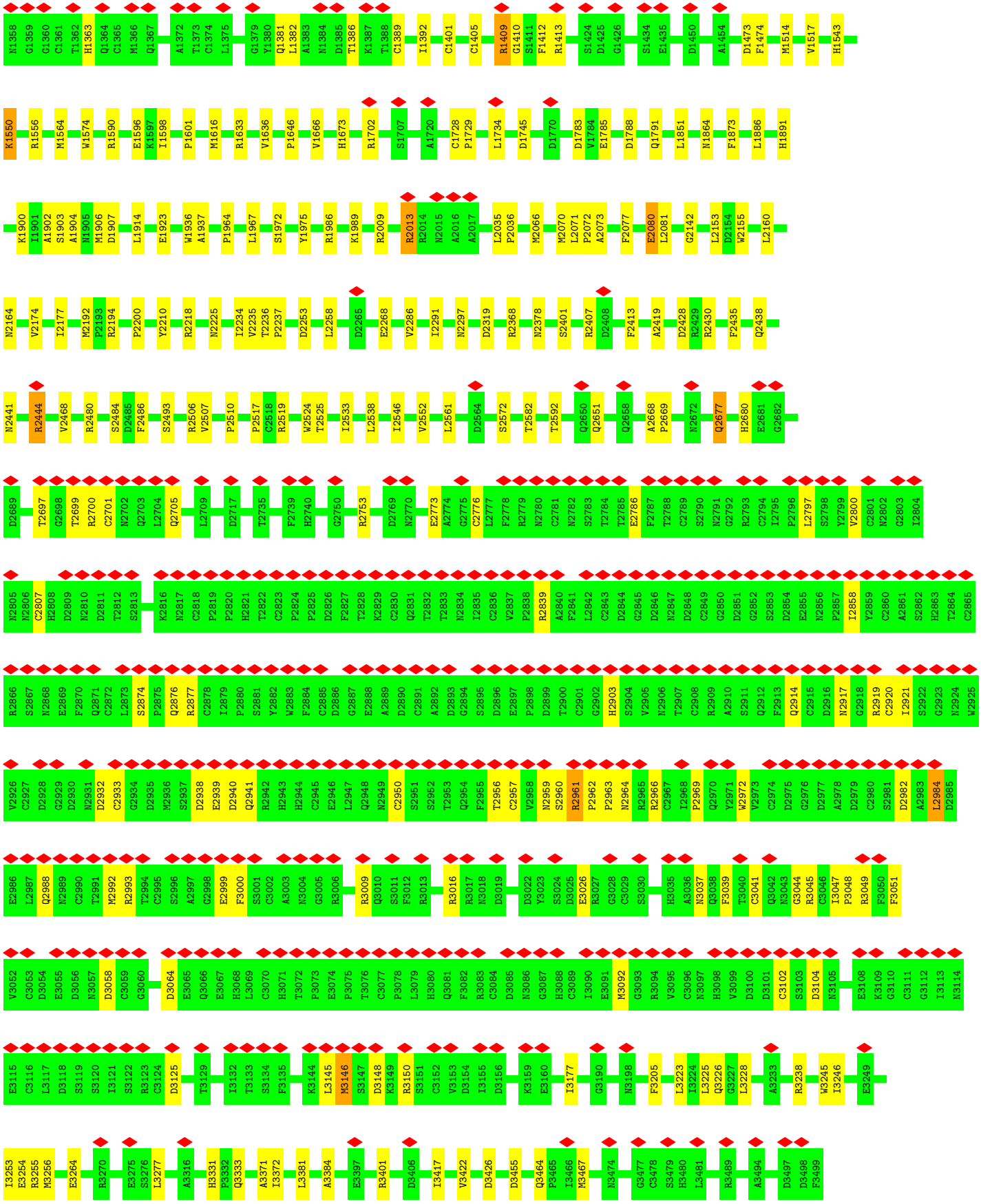


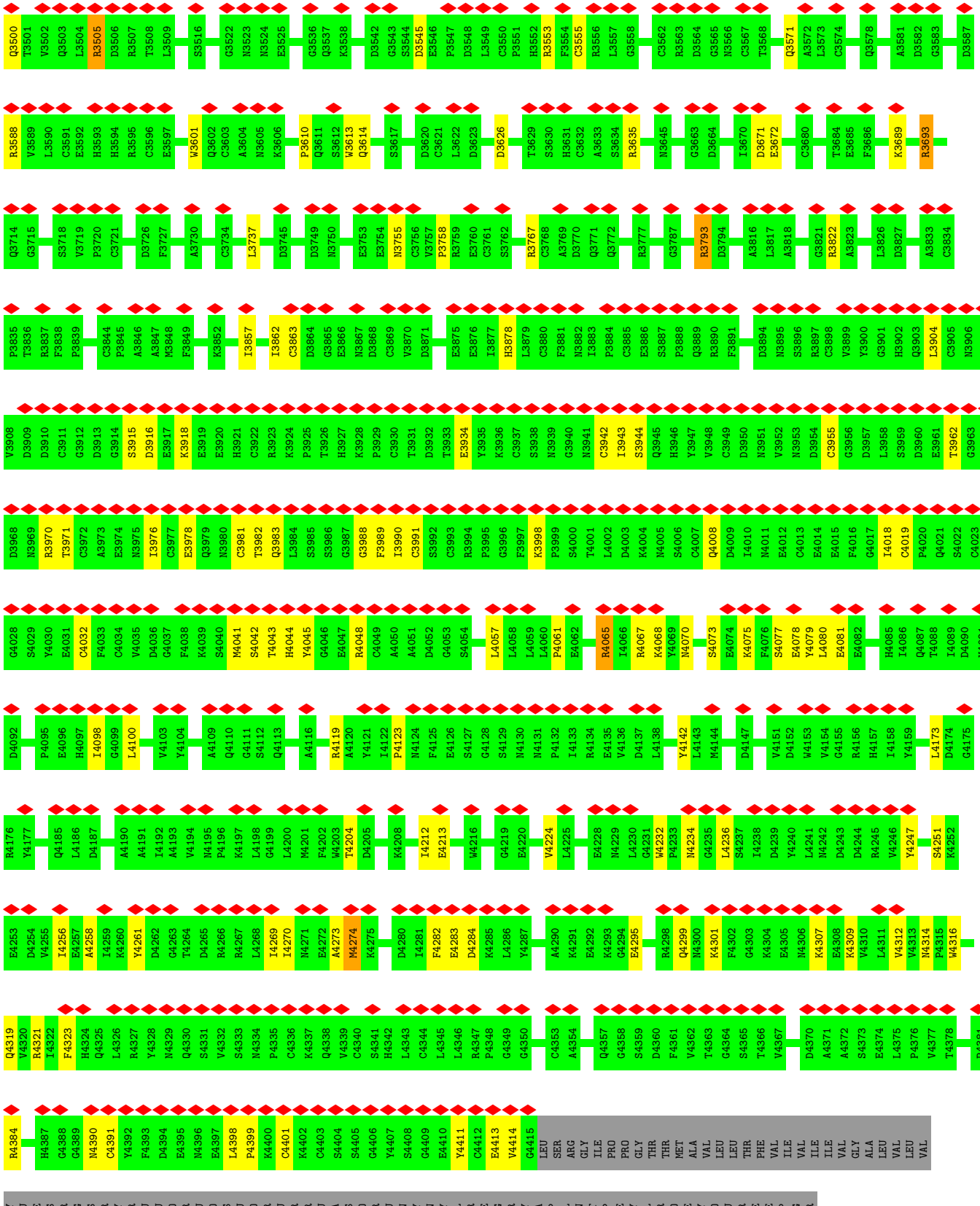
• Molecule 1: LDL receptor related protein 2

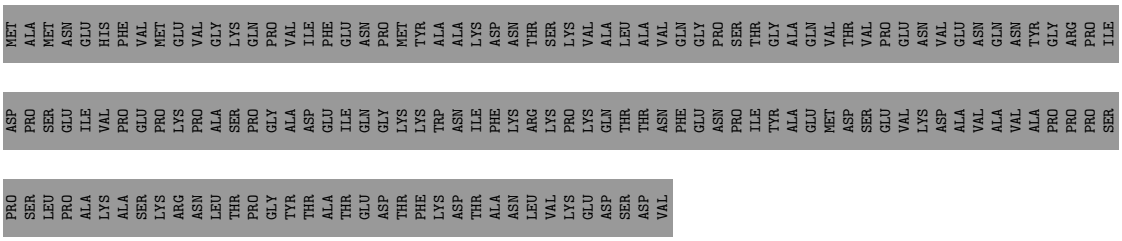
Chain B:




THR LEU CYS SER GLN K186 E187 F188 E189 C190 G191 S192 G193 E194 C195 I196 L197 R198 A199 Y200 V201 H204 D205 N206 D207 C208 E209 D210 N211 S212 D213 E214 R215 N216 C217 N218 Y219 D220 T221 C222 G223 G224 H225 Q226 F227 T228 C229 S230 Q233 C234 N238 W239 V240 G243 D244 D245
D246 C247 Q248 D249 S250 E253 D254 G255 C256 E257 S258 N259 Q260 S261 H262 H263 R264 C265 Y266 P267 R268 E269 W270 A271 C272 P273 G274 S275 G276 R277 C278 I279 S280 I281 D282 K283 V284 C285 D286 C287 V288 P289 D290 C291 P292 E293 C294 D295 D296 E297 N298 N299 Y300 T301 S302 G303 R304 T305 C306
G307 M308 G309 V310 C311 S312 V313 L314 N315 C316 E317 Y318 Q319 C320 H321 Q322 T323 P324 F325 G326 G327 E328 C329 F330 C331 P332 P333 G334 H335 I336 I337 N338 S339 N340 D341 S342 R343 T344 C345 I346 D347 F348 D349 D350 C351 Q352 I353 W354 G355 I356 C357 D358 Q359 K360 C361 E362 N363 R364 Q365 G366
R367 H368 Q369 C370 L371 C372 E373 E374 G375 Y376 I377 L378 E379 R380 G381 Q382 H383 C384 K385 S386 S387 D388 S389 F390 S391 A392 A393 S394 V395 I396 F397 S398 R401 D402 L403 L404 V405 G406 D407 L408 H409 G410 R411 N412 F413 R414 I415 L416 A417 E418 N421 G427 V428 D429 F430 H431 Y432
Q433 K434 F438 W439 T440 D441 P442 M443 Q444 E445 K446 V447 F448 S449 T450 D451 I452 N453 G454 L455 N456 T457 Q458 L461 S464 V465 D466 T467 P468 E469 N470 L471 A472 V473 D474 W475 I476 N477 N478 K479 L480 Y481 K486 V487 N488 R489 I490 D491 V492 V493 E496 G497 N498 Q499 R500
L503 I504 L508 R512 G513 I514 A515 L516 D517 P518 T519 F525 S526 D527 S530 L531 S532 G533 Q534 V537 G544 D549 L550 V551 T552 T553 K554 A559 G560 I561 T562 L563 D564 L565 V566 S567 K568 Y571 D574 Y577 I580 D586 G587 I588 Q589
T592 V593 A594 R595 S598 L599 V600 F604 G605 I606 S607 L608 F609 E610 E611 H612 V613 F614 F615 T616 T619 K620 V623 M624 K625 A626 S627 K628 F629 T630 E631 T632 N633 P634 Q635 V636 Y637 H638 Q639 S640 S641 L642 R643 P644 H645 G646 V647 T648 V649 R654 T659 N660 P661 C662
G663 S664 N665 N666 G667 G668 C669 A670 Q671 L675 R678 T679 D680 N681 G682 G683 L684 R687 C688 K689 C690 E691 E695 L696 D697 D698 D699 E700 H701 R702 C703 V704 A705 V706 K707 L725 V735 T736 G737 S738 P739 S740 F741 F742 D746 Y756 S757 K766 G771
I777 E783 L788 I793 W799 V807 R811 L812 A813 D814 I821 N825 N826 W844 F845 R846 P847 A848 K849 D856 I863 V864 W870 H895 D899 L932 D945 R951 S954 D963 L966 G969 S970 N971 A979 R995
M1003 C1012 A1017 Q1023 L1028 N1033 F1041 H1051 H1057 Q1058 C1059 G1060 V1061 F1062 N1063 C1066 S1069 A1072 C1073 V1074 R1075 G1076 G1077 Q1078 C1079 I1080 P1081 W1084 H1085 C1086 D1087 R1088 D1091 C1092 L1093 Q1099 N1100 C1101 P1102 T1103 H1104 A1105 T1106 S1107 S1108 T1109
C1110 P1111 S1112 T1113 S1114 F1115 D1118 N1119 H1120 V1121 C1122 I1123 P1124 K1125 D1126 C1129 D1134 C1135 S1136 D1137 G1138 S1139 D1140 E1141 K1142 N1143 C1144 Q1145 A1146 S1147 G1148 T1149 C1150 Q1151 P1152 T1153 Q1154 F1155 R1156 C1157 P1158 D1159 H1160 R1161 C1162 I1163 S1164 P1165 L1166 C1169 D1170 G1171 D1172 K1173 A1176
D1177 G1178 S1179 D1180 E1181 A1182 G1183 C1184 V1185 L1186 N1187 C1188 T1189 S1190 A1191 K1194 C1195 A1196 D1197 G1198 S1199 S1200 C1201 R1215 D1216 N1217 C1223 L1233 E1250 T1265 G1266 C1267 K1270 T1271 C1272 S1273 P1274 T1275 H1276 F1277 L1278 C1279 D1280 N1281 G1282 N1283 C1284 I1285 Y1286 K1287 D1292 G1293
D1294 N1295 R1298 D1299 M1300 S1301 K1304 D1305 C1306 P1307 T1308 Q1309 P1310 F1311 H1312 C1313 P1314 S1315 T1316 Q1317 W1318 Q1319 C1320 P1321 G1322 Y1323 S1324 T1325 C1326 I1327 N1328 L1329 S1330 A1331 L1332 C1333 D1334 G1335 V1336 F1337 D1338 C1339 P1340 N1341 G1342 T1343 S1346 P1347 L1348 C1349 N1350 Q1351 D1352 S1355 H1356 F1357

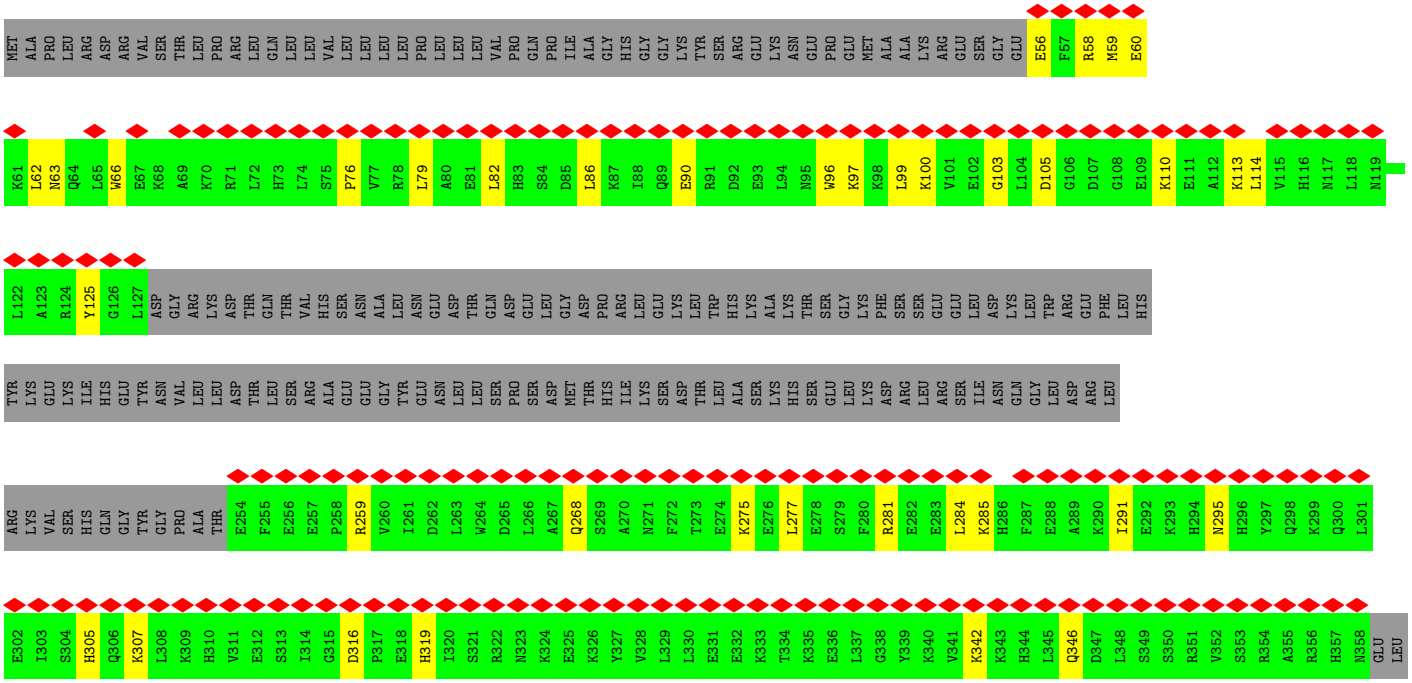

N1358 G1359 G1360 C1361 T1362 H1363 Q1364 C1365 M1366 Q1367 A1372 T1373 C1374 L1375 G1379 Y1380 Q1381 L1382 A1383 N1384 D1385 T1386 K1387 T1388 C1389 I1392 C1401 C1405 R1409 G1410 S1411 F1412 R1413 S1424 D1425 G1426 S1434 E1435 D1450 A1454 D1473 F1474 M1514 V1517 H1543
K1550 R1556 M1564 W1574 R1590 E1596 K1597 I1598 P1601 M1616 R1633 V1636 P1646 V1666 H1673 R1702 S1707 A1720 C1728 P1729 L1734 D1745 D1770 D1783 V1784 E1785 D1788 Q1791 L1851 N1864 F1873 L1886 H1891
K1900 I1901 A1902 S1903 A1904 N1905 M1906 D1907 L1914 E1923 W1936 A1937 P1964 L1967 S1972 Y1975 R1986 K1989 R2009 R2013 R2014 N2015 A2016 A2017 L2035 P2036 M2066 M2070 L2071 P2072 A2073 F2077 E2080 L2081 C2142 L2153 D2154 W2155 L2160
N2164 V2174 I2177 M2192 P2193 R2194 P2200 Y2210 R2218 N2225 I2234 V2235 T2236 P2237 D2253 L2258 D2265 E2268 V2286 I2291 N2297 D2319 R2368 N2378 S2401 R2407 D2408 F2413 A2419 D2428 R2429 R2430 F2435 Q2438
N2441 R2444 V2468 R2480 S2484 D2485 F2486 S2493 R2506 V2507 P2510 P2517 C2518 R2519 W2524 T2525 I2533 L2538 I2546 V2552 L2561 D2564 S2572 T2582 T2592 Q2650 Q2651 Q2658 A2668 P2669 N2672 Q2677 H2680 E2681 G2682
D2689 T2697 G2698 T2699 R2700 C2701 N2702 Q2703 L2704 Q2705 L2709 D2717 T2735 F2739 H2740 G2750 R2753 D2769 N2770 E2773 A2774 G2775 C2776 L2777 F2778 R2779 N2780 C2781 N2782 S2783 T2784 T2785 E2786 F2787 T2788 C2789 S2790 N2791 G2792 R2793 C2794 I2795 P2796 L2797 S2798 Y2799 V2800 C2801 N2802 G2803 I2804
N2805 N2806 C2807 H2808 D2809 N2810 D2811 T2812 S2813 K2816 N2817 C2818 P2819 P2820 H2821 T2822 C2823 P2824 P2825 D2826 F2827 T2828 K2829 C2830 Q2831 T2832 T2833 N2834 I2835 C2836 V2837 P2838 R2839 A2840 F2841 L2842 C2843 D2844 G2845 D2846 N2847 D2848 C2849 G2850 D2851 G2852 S2853 D2854 E2855 N2856 P2857 I2858 Y2859 C2860 A2861 S2862 H2863 T2864 C2865
R2866 S2867 N2868 E2869 P2870 Q2871 C2872 L2873 S2874 P2875 Q2876 R2877 C2878 I2879 P2880 S2881 Y2882 W2883 F2884 C2885 D2886 G2887 E2888 A2889 D2890 C2891 A2892 D2893 G2894 S2895 D2896 E2897 P2898 D2899 T2900 C2901 G2902 H2903 S2904 V2905 N2906 T2907 C2908 R2909 A2910 S2911 Q2912 F2913 Q2914 C2915 D2916 N2917 G2918 R2919 C2920 I2921 S2922 G2923 N2924 W2925
V2926 C2927 D2928 G2929 D2930 N2931 D2932 C2933 G2934 D2935 M2936 S2937 D2938 E2939 D2940 Q2941 R2942 H2943 H2944 C2945 E2946 L2947 Q2948 N2949 C2950 S2951 S2952 T2953 Q2954 F2955 T2956 C2957 V2958 N2959 S2960 R2961 P2962 P2963 N2964 R2965 R2966 C2967 I2968 P2969 Q2970 Y2971 W2972 V2973 C2974 D2975 G2976 D2977 A2978 D2979 C2980 S2981 D2982 A2983 L2984 D2985
E2986 L2987 Q2988 N2989 C2990 T2991 M2992 R2993 T2994 C2995 S2996 A2997 G2998 E2999 F3000 S3001 C3002 A3003 N3004 G3005 R3006 R3009 Q3010 S3011 F3012 R3013 R3016 R3017 N3018 D3019 D3022 Y3023 S3024 D3025 E3026 R3027 G3028 C3029 S3030 H3035 A3036 N3037 Q3038 F3039 T3040 C3041 Q3042 N3043 G3044 R3045 C3046 I3047 P3048 R3049 F3050 F3051
V3052 C3053 D3054 E3055 D3056 N3057 D3058 C3059 G3060 D3064 E3065 Q3066 E3067 H3068 L3069 C3070 H3071 T3072 P3073 E3074 P3075 T3076 C3077 P3078 L3079 H3080 Q3081 F3082 R3083 C3084 D3085 N3086 G3087 H3088 C3089 I3090 E3091 M3092 G3093 R3094 V3095 C3096 N3097 H3098 V3099 D3100 D3101 C3102 S3103 D3104 N3105 E3108 K3109 G3110 C3111 G3112 I3113 N3114
E3115 C3116 L3117 D3118 S3119 S3120 I3121 S3122 R3123 C3124 D3125 T3129 I3132 T3133 S3134 F3135 K3144 L3145 M3146 S3147 D3148 K3149 R3150 S3151 C3152 V3153 D3154 I3155 D3156 K3159 E3160 I3177 G3190 N3198 F3205 L3223 I3224 L3225 Q3226 G3227 L3228 A3233 R3238 W3245 I3246 E3249
I3253 E3254 R3255 M3256 E3264 R3270 E3275 S3276 L3277 A3316 H3331 P3332 Q3333 A3371 I3372 L3381 A3384 E3397 R3401 D3406 I3417 V3422 D3426 D3455 Q3464 P3465 I3466 M3467 N3474 G3477 C3478 S3479 H3480 L3481 R3489 A3494 D3497 D3498 F3499


Q3500 T3501 V3502 Q3503 L3504 R3505 D3506 R3507 T3508 L3509 S3516 G3522 N3523 N3524 E3525 G3536 Q3537 K3538 D3542 G3543 S3544 D3545 E3546 P3547 D3548 L3549 C3550 P3551 H3552 R3553 F3554 C3555 R3556 L3557 G3558 C3562 R3563 D3564 G3565 N3566 C3567 T3568 Q3571 A3572 L3573 C3574 Q3578 A3581 D3582 G3583 D3587
R3588 V3589 L3590 C3591 E3592 H3593 H3594 R3595 C3596 E3597 W3601 Q3602 C3603 A3604 N3605 K3606 P3610 Q3611 S3612 W3613 Q3614 S3617 D3620 C3621 L3622 D3623 D3626 T3629 S3630 H3631 C3632 A3633 S3634 R3635 N3645 G3663 D3664 I3670 D3671 E3672 C3680 T3684 E3685 F3686 K3689 R3693
Q3714 G3715 S3718 V3719 P3720 C3721 D3726 F3727 A3730 C3734 L3737 D3745 D3749 N3750 E3753 E3754 N3755 C3756 V3757 P3758 R3759 E3760 C3761 S3762 R3767 C3768 A3769 D3770 Q3771 Q3772 R3777 G3787 R3793 D3794 A3816 L3817 A3818 G3821 R3822 A3823 L3826 D3827 A3833 C3834
P3835 T3836 R3837 F3838 P3839 C3844 P3845 A3846 A3847 M3848 F3849 K3852 I3857 I3862 C3863 D3864 G3865 E3866 N3867 D3868 C3869 V3870 D3871 E3875 E3876 I3877 H3878 L3879 C3880 F3881 N3882 I3883 P3884 C3885 E3886 S3887 P3888 Q3889 R3890 F3891 D3894 N3895 S3896 R3897 C3898 V3899 Y3900 G3901 H3902 Q3903 L3904 C3905 N3906 G3907
V3908 D3909 D3910 C3911 G3912 D3913 G3914 S3915 D3916 E3917 K3918 E3919 E3920 H3921 C3922 R3923 K3924 P3925 T3926 H3927 K3928 P3929 C3930 T3931 D3932 T3933 E3934 Y3935 K3936 C3937 S3938 N3939 G3940 N3941 C3942 I3943 S3944 Q3945 H3946 Y3947 V3948 C3949 D3950 N3951 V3952 N3953 D3954 C3955 G3956 D3957 L3958 S3959 D3960 E3961 T3962 G3963 C3964 N3965 L3966 G3967
D3968 N3969 R3970 T3971 C3972 A3973 E3974 N3975 I3976 C3977 E3978 Q3979 N3980 C3981 T3982 Q3983 L3984 S3985 S3986 G3987 G3988 F3989 I3990 C3991 S3992 C3993 R3994 P3995 G3996 F3997 K3998 P3999 S4000 T4001 L4002 D4003 K4004 N4005 S4006 C4007 Q4008 D4009 I4010 N4011 E4012 C4013 E4014 E4015 F4016 G4017 I4018 C4019 P4020 Q4021 S4022 C4023 R4024 N4025 S4026 K4027
G4028 S4029 Y4030 E4031 C4032 F4033 C4034 V4035 D4036 G4037 F4038 K4039 S4040 M4041 S4042 T4043 H4044 Y4045 G4046 E4047 R4048 C4049 A4050 A4051 D4052 G4053 S4054 L4057 L4058 L4059 L4060 P4061 E4062 R4065 I4066 R4067 K4068 Y4069 N4070 S4073 E4074 K4075 F4076 S4077 E4078 Y4079 L4080 E4081 E4082 H4085 I4086 Q4087 T4088 I4089 D4090 Y4091
D4092 P4095 E4096 H4097 I4098 G4099 L4100 V4103 Y4104 A4109 Q4110 G4111 S4112 Q4113 A4116 R4119 A4120 Y4121 I4122 P4123 N4124 F4125 E4126 S4127 G4128 S4129 N4130 N4131 P4132 I4133 R4134 E4135 V4136 D4137 L4138 Y4142 L4143 M4144 D4147 V4151 D4152 W4153 V4154 G4155 R4156 H4157 I4158 Y4159 L4173 D4174 G4175
R4176 Y4177 Q4185 L4186 D4187 A4190 A4191 I4192 A4193 V4194 N4195 P4196 K4197 L4198 G4199 L4200 M4201 F4202 W4203 T4204 D4205 K4208 I4212 E4213 W4216 G4219 E4220 V4224 L4225 E4228 N4229 L4230 G4231 W4232 P4233 M4234 G4235 L4236 S4237 I4238 D4239 Y4240 L4241 N4242 D4243 D4244 R4245 V4246 Y4247 S4251 K4252
E4253 D4254 V4255 I4256 E4257 A4258 I4259 K4260 Y4261 D4262 G4263 T4264 D4265 R4266 R4267 L4268 I4269 I4270 N4271 E4272 A4273 M4274 K4275 D4280 I4281 F4282 E4283 D4284 K4285 L4286 Y4287 A4290 K4291 E4292 K4293 G4294 E4295 R4298 Q4299 N4300 K4301 F4302 G4303 K4304 E4305 N4306 K4307 E4308 K4309 V4310 L4311 V4312 V4313 N4314 P4315 W4316
Q4319 V4320 R4321 I4322 F4323 H4324 Q4325 L4326 R4327 Y4328 N4329 Q4330 S4331 V4332 S4333 N4334 P4335 C4336 K4337 Q4338 A4339 C4340 S4341 H4342 L4343 C4344 L4345 L4346 R4347 P4348 G4349 G4350 C4353 A4354 Q4357 G4358 S4359 D4360 F4361 V4362 T4363 G4364 S4365 T4366 V4367 D4370 A4371 A4372 S4373 E4374 L4375 P4376 V4377 T4378 P4381
R4384 H4387 G4388 G4389 N4390 C4391 Y4392 F4393 D4394 E4395 N4396 E4397 L4398 P4399 K4400 C4401 K4402 C4403 S4404 S4405 G4406 Y4407 S4408 G4409 E4410 Y4411 C4412 E4413 V4414 G4415
LEU SER ARG GLY ILE PRO PRO GLY THR THR MET ALA VAL LEU LEU THR PHE VAL ILE VAL ILE ILE VAL GLY ALA LEU VAL LEU VAL
GLY LEU PHE HIS TYR ARG LYS THR GLY SER LEU LEU PRO THR LEU PRO LYS LEU PRO SER LEU SER SER LEU ALA LYS PRO SER GLU ASN GLY ASN GLY VAL THR PHE ARG SER GLY ALA ASP VAL ASN MET ASP ILE GLY VAL SER PRO PHE GLY PRO GLU THR ILE ILE ASP ARG SER



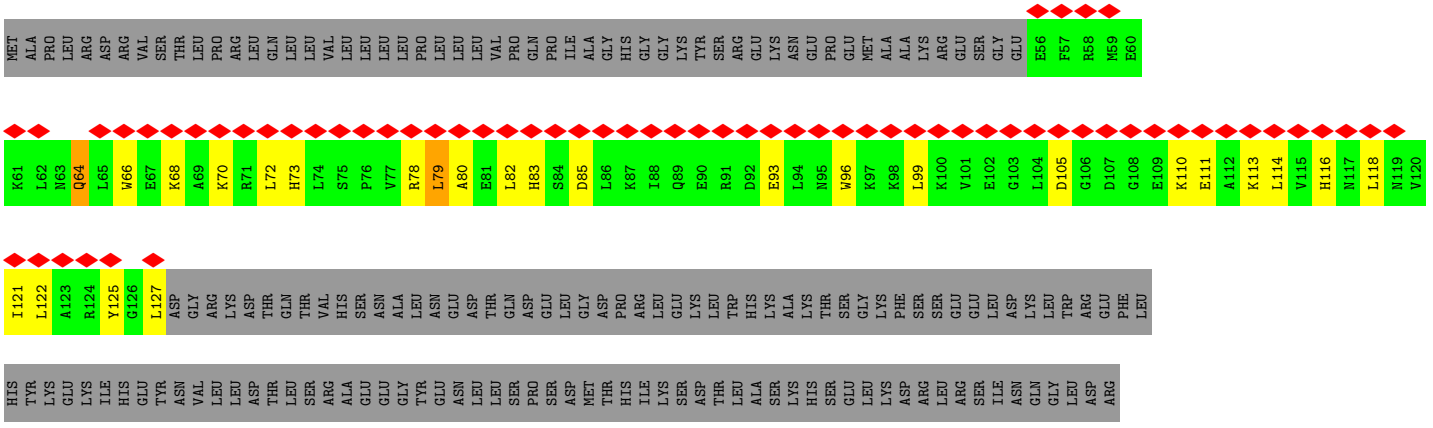
• Molecule 2: Alpha-2-macroglobulin receptor-associated protein

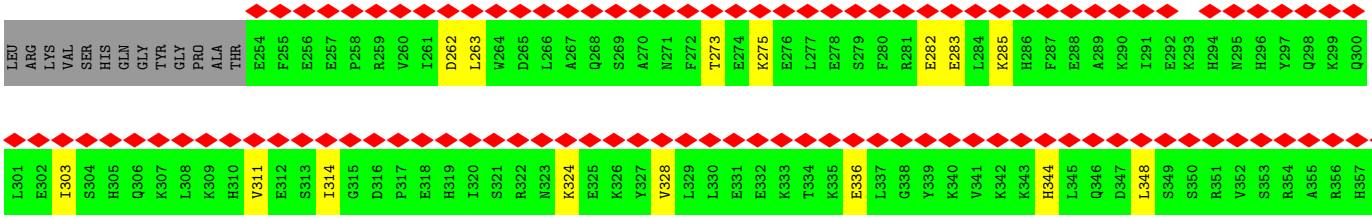
Chain C:



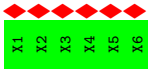
• Molecule 2: Alpha-2-macroglobulin receptor-associated protein

Chain D:

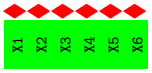




• Molecule 3: unclear peptide



• Molecule 3: unclear peptide

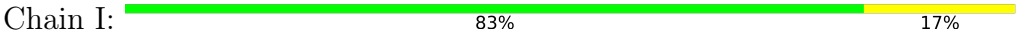


• Molecule 4: unclear peptide

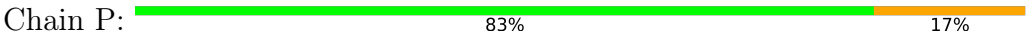
• Molecule 4: unclear peptide

There are no outlier residues recorded for this chain.

• Molecule 5: unclear peptide



• Molecule 5: unclear peptide

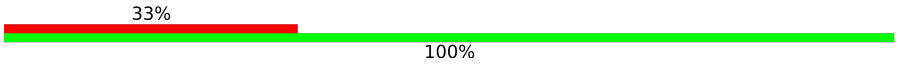


• Molecule 6: unclear peptide

Chain J:

• Molecule 6: unclear peptide

Chain Q:

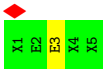


• Molecule 7: unclear peptide

Chain K:

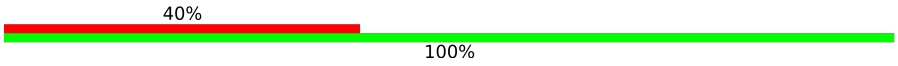
• Molecule 7: unclear peptide

Chain R:



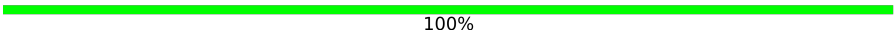
• Molecule 8: unclear peptide

Chain L:



• Molecule 8: unclear peptide

Chain M:



There are no outlier residues recorded for this chain.

• Molecule 8: unclear peptide

Chain S:

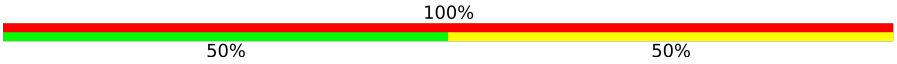
• Molecule 8: unclear peptide

Chain T:

There are no outlier residues recorded for this chain.

• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

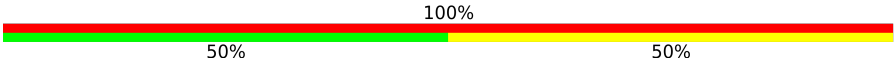


• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:

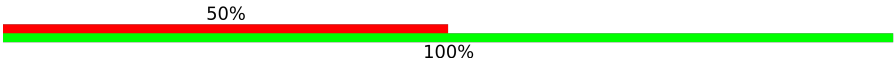
• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:



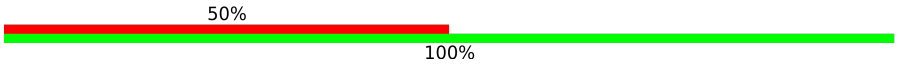
• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:



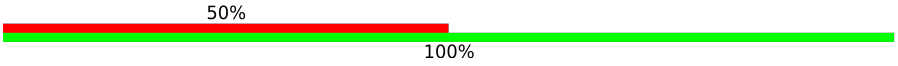
• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:



• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:

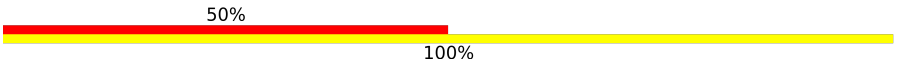


• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain n:

• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain q:



• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain s:

• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

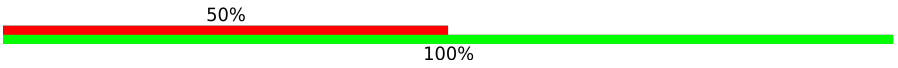
Chain t:

• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain v:

• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain x:

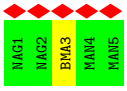


• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain y:

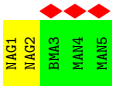
• Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



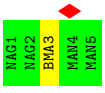
• Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:



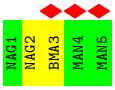
• Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:



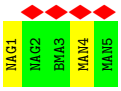
• Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:



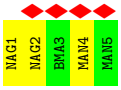
• Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:



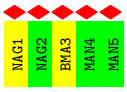
• Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k:



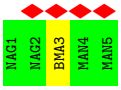
• Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l:



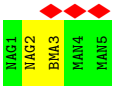
• Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain u:



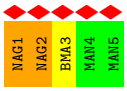
• Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 1:



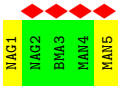
• Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 4:



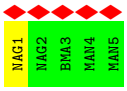
• Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 5:



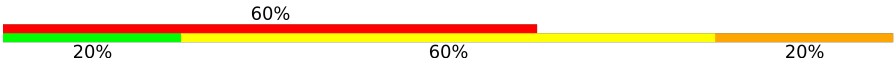
• Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

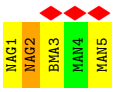
Chain 9:



• Molecule 11: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

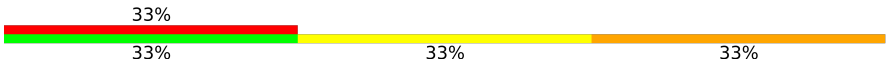
Chain U:





• Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:



• Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:

• Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:

• Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

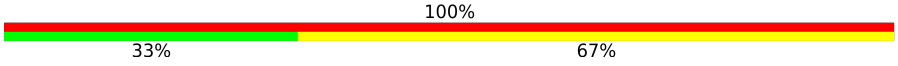
Chain h:

• Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i:

• Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m:



• Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p:

• Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain r:

• Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

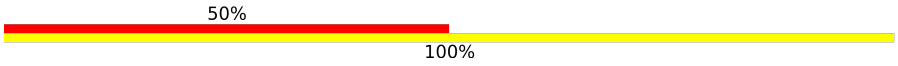
Chain 2:

• Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 3:

• Molecule 13: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:

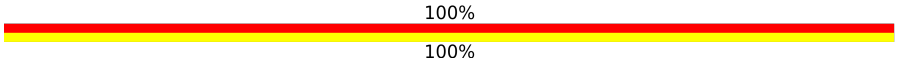


• Molecule 13: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain o:

• Molecule 13: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 8:

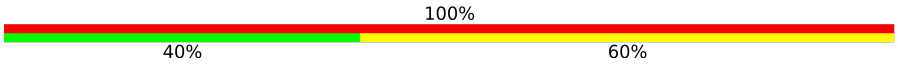


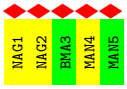
• Molecule 14: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain w:

• Molecule 14: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

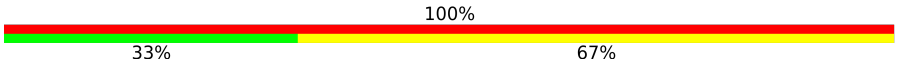
Chain 6:





• Molecule 15: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain z:

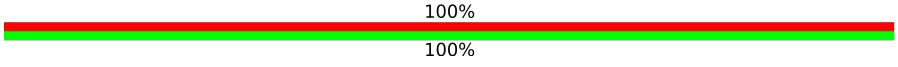


• Molecule 16: beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 0:

• Molecule 16: beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 7:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	67775	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.150	Depositor
Minimum map value	-0.078	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0242	Depositor
Map size (Å)	366.86002, 366.86002, 366.86002	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.411, 1.411, 1.411	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NI, MAN, A2G, BMA, NAG, CA

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	0.32	0/34456	0.58	5/46804 (0.0%)
1	B	0.63	0/34454	0.67	5/46801 (0.0%)
2	C	0.64	0/1521	0.60	0/2033
2	D	0.63	0/1521	0.62	0/2033
4	H	0.68	0/7	0.49	0/8
4	O	0.82	0/7	0.68	0/8
5	I	0.67	0/7	0.63	0/8
5	P	0.68	0/7	0.88	0/8
6	J	1.03	0/5	0.57	0/5
6	Q	1.03	0/5	0.38	0/5
7	K	0.95	0/17	0.64	0/21
7	R	0.65	0/17	0.48	0/21
8	L	0.57	0/7	0.62	0/8
8	M	0.64	0/7	0.52	0/8
8	S	0.93	0/7	0.59	0/8
8	T	0.58	0/7	0.54	0/8
All	All	0.51	0/72052	0.63	10/97787 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	2
All	All	0	6

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	4327	ARG	NE-CZ-NH2	7.00	123.80	120.30
1	B	3693	ARG	NE-CZ-NH2	6.85	123.73	120.30
1	B	2218	ARG	NE-CZ-NH2	6.74	123.67	120.30
1	B	364	ARG	NE-CZ-NH2	6.62	123.61	120.30
1	B	2919	ARG	NE-CZ-NH2	6.32	123.46	120.30
1	A	4245	ARG	NE-CZ-NH1	-5.59	117.50	120.30
1	A	2919	ARG	NE-CZ-NH2	5.43	123.02	120.30
1	A	4327	ARG	NE-CZ-NH1	-5.28	117.66	120.30
1	A	4245	ARG	NE-CZ-NH2	5.18	122.89	120.30
1	B	2368	ARG	NE-CZ-NH2	5.14	122.87	120.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1043	ARG	Sidechain
1	A	3212	ARG	Sidechain
1	A	4321	ARG	Sidechain
1	A	781	ARG	Sidechain
1	B	2877	ARG	Sidechain
1	B	3693	ARG	Sidechain

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	33638	0	31021	237	0
1	B	33636	0	31021	245	0
2	C	1494	0	1505	22	0
2	D	1494	0	1505	26	0
3	G	30	0	8	0	0
3	N	30	0	8	0	0
4	H	28	0	12	0	0
4	O	28	0	12	0	0
5	I	33	0	18	5	0
5	P	33	0	18	1	0
6	J	16	0	8	0	0
6	Q	16	0	8	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	K	33	0	18	1	0
7	R	33	0	17	0	0
8	L	28	0	12	0	0
8	M	28	0	12	0	0
8	S	28	0	12	0	0
8	T	28	0	12	0	0
9	E	28	0	25	0	0
9	V	28	0	25	0	0
9	X	28	0	25	1	0
9	Y	28	0	25	0	0
9	a	28	0	25	0	0
9	d	28	0	25	0	0
9	n	28	0	25	0	0
9	q	28	0	25	0	0
9	s	28	0	25	0	0
9	t	28	0	25	0	0
9	v	28	0	25	0	0
9	x	28	0	25	0	0
9	y	28	0	25	0	0
10	1	61	0	52	0	0
10	4	61	0	52	1	0
10	5	61	0	52	0	0
10	9	61	0	52	0	0
10	F	61	0	52	0	0
10	Z	61	0	52	0	0
10	b	61	0	52	0	0
10	g	61	0	52	0	0
10	j	61	0	52	0	0
10	k	61	0	52	0	0
10	l	61	0	52	0	0
10	u	61	0	52	0	0
11	U	61	0	52	2	0
12	2	39	0	34	0	0
12	3	39	0	34	0	0
12	W	39	0	34	1	0
12	e	39	0	34	0	0
12	f	39	0	34	0	0
12	h	39	0	34	0	0
12	i	39	0	34	0	0
12	m	39	0	34	0	0
12	p	39	0	34	0	0
12	r	39	0	34	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	8	28	0	25	0	0
13	c	28	0	25	0	0
13	o	28	0	25	0	0
14	6	61	0	52	1	0
14	w	61	0	52	0	0
15	z	39	0	34	0	0
16	0	39	0	34	0	0
16	7	39	0	34	0	0
17	A	154	0	143	2	0
17	B	154	0	143	0	0
18	A	168	0	144	0	0
18	B	168	0	144	0	0
19	A	44	0	0	0	0
19	B	44	0	0	0	0
20	A	1	0	0	0	0
20	B	1	0	0	0	0
All	All	73258	0	67423	526	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 4.

All (526) 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:3505:ARG:H	1:B:3505:ARG:HD3	1.38	0.90
1:A:3015:ASP:HB2	1:A:3017:ARG:NH2	1.90	0.87
1:A:2786:GLU:HG2	1:A:2788:THR:H	1.43	0.82
1:A:2708:CYS:SG	1:A:2730:SER:OG	2.40	0.79
1:A:3963:GLY:HA2	1:A:4004:LYS:HE2	1.65	0.79
1:B:4073:SER:HB3	1:B:4075:LYS:HG3	1.64	0.79
1:A:1574:TRP:CE3	5:I:3:LEU:HD23	2.20	0.77
1:A:1173:LYS:HD2	1:A:1178:GLY:HA2	1.69	0.74
1:A:4131:ASN:HD21	1:A:4385:CYS:HB2	1.54	0.73
1:B:1900:LYS:HE2	1:B:1902:ALA:HB2	1.70	0.72
1:B:3983:GLN:NE2	1:B:3988:GLY:O	2.23	0.71
1:A:3431:THR:HG22	1:A:3448:ASN:HB3	1.72	0.71
1:B:4282:PHE:O	1:B:4283:GLU:HG3	1.91	0.70
1:B:4041:MET:SD	1:B:4042:SER:N	2.65	0.70
1:A:4313:VAL:O	1:A:4314:ASN:ND2	2.24	0.69
1:A:3937:CYS:SG	1:A:3938:SER:N	2.65	0.69
1:B:2507:VAL:HG21	1:B:2524:TRP:HE1	1.57	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3675:THR:HG23	1:A:3677:ALA:H	1.57	0.69
1:B:1003:MET:HG2	1:B:1012:CYS:HB3	1.74	0.69
1:B:2959:ASN:ND2	1:B:2982:ASP:OD2	2.26	0.68
1:A:320:CYS:HA	1:A:329:CYS:HB2	1.75	0.68
1:A:4398:LEU:O	1:A:4400:LYS:NZ	2.23	0.68
1:B:2651:GLN:N	1:B:2651:GLN:OE1	2.27	0.68
14:6:1:NAG:O4	14:6:2:NAG:N2	2.25	0.67
1:B:3943:ILE:HG13	1:B:3955:CYS:HB3	1.75	0.67
2:C:99:LEU:O	2:C:103:GLY:N	2.29	0.66
1:A:1574:TRP:CE3	5:I:3:LEU:CD2	2.79	0.66
1:A:3814:PRO:HG2	1:A:3817:LEU:HD13	1.76	0.66
1:B:4269:ILE:HG22	1:B:4270:ILE:HG12	1.76	0.66
1:B:2939:GLU:HG2	1:B:2941:GLN:H	1.60	0.65
1:B:3372:ILE:HD11	1:B:3381:LEU:HD11	1.80	0.64
2:D:96:TRP:HB2	2:D:110:LYS:HG3	1.79	0.64
1:B:1382:LEU:HD12	1:B:1386:THR:HA	1.79	0.64
1:A:912:MET:HE1	1:A:927:ILE:HG21	1.80	0.64
1:A:2463:LEU:HD11	1:A:2501:ARG:HD2	1.79	0.64
1:A:3876:GLU:OE1	1:A:3876:GLU:N	2.31	0.64
1:A:4100:LEU:HD11	1:A:4384:ARG:HG2	1.79	0.63
1:B:574:ASP:OD1	1:B:577:TYR:N	2.23	0.63
2:D:122:LEU:HD22	2:D:127:LEU:HD22	1.79	0.63
1:B:4204:THR:HG22	1:B:4212:ILE:HG12	1.79	0.63
1:A:1719:GLN:HG3	1:A:1721:PRO:HD2	1.81	0.63
1:A:1574:TRP:CZ3	5:I:3:LEU:HD23	2.34	0.63
1:A:2954:GLN:HA	1:A:2969:PRO:HA	1.79	0.63
1:B:811:ARG:NH2	1:B:814:ASP:OD1	2.31	0.63
2:D:79:LEU:HA	2:D:82:LEU:HD12	1.81	0.63
1:A:882:ARG:HE	1:A:895:HIS:HD2	1.46	0.62
1:A:3295:CYS:SG	1:A:3296:LEU:N	2.72	0.62
1:A:2705:GLN:HB3	1:A:2713:CYS:HB3	1.80	0.62
1:A:1550:LYS:O	1:A:1552:VAL:HG23	2.00	0.61
1:A:1281:ASN:ND2	1:A:1297:CYS:O	2.32	0.61
2:D:282:GLU:HA	2:D:285:LYS:HZ3	1.66	0.61
1:A:1595:GLN:HA	1:A:1598:ILE:HD11	1.82	0.61
1:B:863:ILE:HG22	1:B:864:VAL:HG23	1.82	0.60
1:B:616:THR:HG22	1:B:623:VAL:HG22	1.83	0.60
1:A:2795:ILE:HD11	1:A:2800:VAL:HG12	1.84	0.60
1:A:2546:ILE:HG22	1:A:2547:VAL:HG13	1.82	0.60
1:A:1574:TRP:CD2	5:I:3:LEU:HD23	2.37	0.60
1:A:4068:LYS:HB2	1:A:4077:SER:HB2	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3862:ILE:HG13	1:B:3863:CYS:SG	2.41	0.60
2:C:291:ILE:O	2:C:295:ASN:ND2	2.35	0.60
1:B:2933:CYS:HB2	1:B:2938:ASP:HB3	1.83	0.60
1:A:3017:ARG:HD3	1:A:3017:ARG:N	2.17	0.60
1:B:465:VAL:HG12	1:B:465:VAL:O	2.02	0.59
1:B:4295:GLU:N	1:B:4295:GLU:OE1	2.35	0.59
1:A:1551:ASN:OD1	9:X:1:NAG:N2	2.35	0.59
1:A:2809:ASP:OD1	1:A:2811:ASP:N	2.35	0.59
1:A:2648:GLN:HB3	1:A:2651:GLN:HE21	1.68	0.59
1:B:1088:ARG:HB3	1:B:1088:ARG:HH21	1.67	0.59
2:C:56:GLU:OE1	2:C:66:TRP:NE1	2.36	0.59
1:B:451:ASP:OD2	1:B:453:ASN:ND2	2.36	0.59
1:B:36:ASP:HB2	1:B:57:THR:HG21	1.84	0.58
1:B:4100:LEU:HD11	1:B:4384:ARG:HG2	1.83	0.58
2:D:111:GLU:O	2:D:114:LEU:HG	2.01	0.58
1:A:3082:PHE:CD2	1:A:3095:VAL:HG21	2.39	0.58
1:B:431:HIS:HD2	1:B:434:LYS:H	1.50	0.58
1:A:2192:MET:HG3	1:A:2192:MET:O	2.04	0.58
1:B:2210:TYR:HB2	1:B:2236:THR:HA	1.85	0.58
1:A:1367:GLN:NE2	1:A:1371:GLY:O	2.31	0.58
2:C:59:MET:O	2:C:63:ASN:ND2	2.26	0.58
1:B:3016:ARG:HD3	1:B:3045:ARG:HD2	1.85	0.58
2:D:72:LEU:O	2:D:73:HIS:ND1	2.37	0.58
1:A:3982:THR:HB	1:A:3990:ILE:HG23	1.86	0.58
1:A:3984:LEU:HD13	1:A:3987:GLY:HA3	1.85	0.58
1:A:4119:ARG:NH2	1:A:4173:LEU:O	2.36	0.58
1:B:766:LYS:HD3	1:B:777:ILE:HD11	1.86	0.58
1:B:2525:THR:HG22	1:B:2533:ILE:HD12	1.86	0.58
1:A:1497:ASN:OD1	12:W:1:NAG:N2	2.37	0.58
1:A:1574:TRP:CD2	5:I:3:LEU:CD2	2.86	0.58
1:A:738:SER:OG	1:A:739:PRO:HD3	2.03	0.57
1:A:2972:TRP:CZ2	2:D:127:LEU:HD21	2.39	0.57
1:B:268:ARG:HG3	1:B:281:ILE:HG12	1.86	0.57
1:B:2070:MET:HG3	1:B:2072:PRO:HD2	1.86	0.57
1:B:3064:ASP:OD1	1:B:3064:ASP:N	2.33	0.57
1:B:1923:GLU:HB2	1:B:1937:ALA:HB3	1.86	0.57
10:4:1:NAG:H83	10:4:2:NAG:H83	1.85	0.57
1:B:1864:ASN:ND2	1:B:2319:ASP:OD1	2.37	0.57
2:C:281:ARG:O	2:C:285:LYS:HG2	2.05	0.57
1:A:3144:LYS:HB3	1:A:3155:ILE:HD11	1.86	0.57
1:B:2950:CYS:HB3	1:B:2956:THR:HB	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:281:ARG:HA	2:C:284:LEU:HD12	1.87	0.57
1:A:321:HIS:CD2	1:A:322:GLN:H	2.22	0.56
1:B:1937:ALA:HB1	1:B:1964:PRO:HG2	1.87	0.56
1:A:2484:SER:HB3	1:A:2513:ILE:HD11	1.86	0.56
1:B:3225:LEU:HD13	1:B:3256:MET:HE1	1.87	0.56
1:A:3295:CYS:SG	1:A:3308:MET:HG2	2.45	0.56
1:A:4254:ASP:HB2	1:A:4275:LYS:H	1.71	0.56
1:B:486:LYS:HG2	1:B:736:THR:HG21	1.87	0.56
1:B:616:THR:HB	1:B:644:PRO:HB2	1.88	0.56
1:B:4295:GLU:HG3	1:B:4312:VAL:HG13	1.87	0.56
1:A:295:ASP:OD1	1:A:304:ARG:NH1	2.38	0.56
1:B:3016:ARG:NE	1:B:3044:GLY:O	2.38	0.56
1:B:2959:ASN:O	1:B:2961:ARG:NH1	2.39	0.56
1:B:4098:ILE:O	1:B:4384:ARG:NH1	2.38	0.56
1:A:3066:GLN:HE21	1:A:3069:LEU:H	1.54	0.56
1:B:4398:LEU:HD23	1:B:4399:PRO:HD2	1.88	0.56
1:A:1853:GLY:O	1:A:1856:ARG:NH1	2.30	0.56
1:B:3981:CYS:SG	1:B:3982:THR:N	2.78	0.56
1:A:3693:ARG:HH22	1:A:3708:ARG:HG2	1.70	0.55
1:B:272:CYS:HB2	1:B:295:ASP:HB3	1.88	0.55
1:B:3976:ILE:HG12	1:B:3989:PHE:HE2	1.70	0.55
1:B:3048:PRO:HD2	1:B:3051:PHE:HE1	1.71	0.55
1:A:486:LYS:HG2	1:A:736:THR:HG21	1.87	0.55
1:B:3026:GLU:HA	1:B:3026:GLU:OE1	2.07	0.55
1:A:712:PHE:CE1	1:A:953:ILE:HD11	2.41	0.55
1:A:3617:SER:N	1:A:3627:GLU:OE1	2.39	0.55
1:A:3425:THR:HB	1:A:3453:PRO:HG2	1.88	0.55
1:A:2285:THR:HG21	1:A:2328:THR:HA	1.89	0.54
1:B:1473:ASP:OD1	1:B:1474:PHE:N	2.40	0.54
1:B:4204:THR:HG23	1:B:4236:LEU:HD22	1.88	0.54
1:A:616:THR:HG23	1:A:647:VAL:HG23	1.89	0.54
1:A:2139:VAL:HG22	1:A:2175:LEU:HD13	1.88	0.54
1:B:2081:LEU:H	1:B:2081:LEU:HD22	1.72	0.54
1:B:4256:ILE:HB	1:B:4270:ILE:HB	1.89	0.54
1:B:3146:MET:SD	1:B:3146:MET:N	2.80	0.54
1:B:190:CYS:SG	1:B:191:GLY:N	2.81	0.54
1:B:1088:ARG:HB3	1:B:1088:ARG:NH2	2.22	0.54
1:B:2999:GLU:HA	1:B:3009:ARG:HA	1.89	0.54
2:D:283:GLU:HG2	2:D:348:LEU:HD21	1.88	0.54
1:B:4390:ASN:O	1:B:4401:CYS:HB2	2.08	0.54
1:A:3760:GLU:OE1	1:A:3760:GLU:N	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4130:ASN:HB2	1:A:4389:GLY:O	2.08	0.54
1:A:1636:VAL:HG23	1:A:1637:ILE:HG13	1.90	0.54
1:B:2192:MET:O	1:B:2192:MET:HG3	2.08	0.54
1:A:557:TRP:N	1:A:574:ASP:OD1	2.41	0.53
1:A:3949:CYS:SG	1:A:3990:ILE:HB	2.48	0.53
1:B:3145:LEU:HD22	1:B:3146:MET:H	1.73	0.53
2:D:113:LYS:HA	2:D:116:HIS:CD2	2.42	0.53
1:B:2080:GLU:O	1:B:2080:GLU:HG3	2.08	0.53
1:A:321:HIS:HD2	1:A:322:GLN:H	1.57	0.53
1:A:3090:ILE:HG12	1:A:3094:ARG:HG3	1.91	0.53
2:C:62:LEU:HG	2:C:86:LEU:HD22	1.89	0.53
1:A:2468:VAL:HG12	1:A:2486:PHE:HB3	1.90	0.53
1:B:1598:ILE:HD11	1:B:1601:PRO:HB3	1.88	0.53
1:B:1550:LYS:O	1:B:1590:ARG:NH2	2.38	0.53
1:B:4391:CYS:HA	1:B:4401:CYS:HB2	1.90	0.53
1:A:1497:ASN:OD1	1:A:1499:THR:OG1	2.22	0.53
1:A:2484:SER:HB2	1:A:2510:PRO:HB2	1.90	0.53
1:A:1394:GLU:OE1	1:A:1407:ASN:ND2	2.35	0.53
1:A:4131:ASN:ND2	1:A:4385:CYS:HB2	2.20	0.53
1:A:3504:LEU:HG	1:A:3505:ARG:H	1.74	0.52
1:B:2903:HIS:CD2	1:B:2917:ASN:HD22	2.27	0.52
1:B:4314:ASN:OD1	1:B:4314:ASN:N	2.41	0.52
1:A:2954:GLN:HG2	1:A:2969:PRO:HA	1.91	0.52
1:B:3238:ARG:NH2	1:B:3464:GLN:O	2.43	0.52
1:A:2601:VAL:HB	1:A:2606:ILE:HG22	1.90	0.52
1:A:4024:ARG:N	1:A:4031:GLU:O	2.41	0.52
1:A:4228:GLU:O	1:A:4266:ARG:NH2	2.29	0.52
1:A:1004:LYS:HD2	1:A:1015:ASP:HB2	1.92	0.52
1:B:2697:THR:HG23	1:B:2699:THR:H	1.74	0.52
1:A:3564:ASP:OD2	1:A:3582:ASP:HB2	2.09	0.52
1:A:2194:ARG:HG3	1:A:2210:TYR:CZ	2.45	0.52
1:B:1543:HIS:HB3	1:B:1729:PRO:HG3	1.91	0.52
1:B:3371:ALA:HB3	1:B:3384:ALA:HB3	1.92	0.52
1:A:616:THR:HG23	1:A:647:VAL:CG2	2.39	0.52
1:A:1416:CYS:SG	1:A:1420:TYR:HB2	2.50	0.52
1:B:3978:GLU:OE1	1:B:3978:GLU:N	2.43	0.52
1:B:4299:GLN:NE2	1:B:4307:LYS:HG3	2.25	0.52
1:A:359:GLN:HE21	1:A:566:VAL:HG21	1.73	0.52
1:B:963:ASP:HB3	1:B:966:LEU:HD23	1.92	0.52
1:B:3915:SER:HA	1:B:3918:LYS:HG3	1.92	0.52
1:A:2797:LEU:O	1:A:2798:SER:HB3	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:807:VAL:HG13	1:B:821:ILE:HB	1.93	0.51
1:B:2468:VAL:HG23	1:B:2486:PHE:HB3	1.92	0.51
1:A:3597:GLU:OE1	1:A:3597:GLU:N	2.37	0.51
1:A:3886:GLU:HG3	1:A:3888:PRO:HD2	1.91	0.51
1:A:1980:GLN:O	1:A:1981:TYR:HB2	2.10	0.51
1:B:735:VAL:HG11	1:B:756:TYR:CZ	2.45	0.51
1:B:825:ASN:O	1:B:826:ASN:ND2	2.43	0.51
1:A:1802:ILE:HG23	1:A:1815:PHE:HB3	1.93	0.51
1:A:2955:PHE:HB2	1:A:2970:GLN:HE22	1.75	0.51
1:B:3246:ILE:HG12	1:B:3253:ILE:HG12	1.92	0.51
1:B:3671:ASP:OD1	1:B:3672:GLU:N	2.43	0.51
2:D:64:GLN:HG2	2:D:68:LYS:HD2	1.92	0.51
1:B:1081:PRO:HD2	1:B:1084:TRP:CE3	2.45	0.51
1:B:1574:TRP:CD2	5:P:3:LEU:HD13	2.46	0.51
1:A:2960:SER:O	1:A:2961:ARG:NH2	2.43	0.51
1:A:3966:LEU:O	1:A:3970:ARG:NH1	2.44	0.51
1:B:2210:TYR:CB	1:B:2236:THR:HA	2.41	0.51
1:A:3015:ASP:HB2	1:A:3017:ARG:HH22	1.72	0.50
1:B:2441:ASN:OD1	1:B:2444:ARG:N	2.41	0.50
1:B:3039:PHE:N	1:B:3047:ILE:O	2.44	0.50
1:B:407:ASP:OD1	1:B:407:ASP:N	2.44	0.50
1:B:4299:GLN:HE21	1:B:4307:LYS:HG3	1.75	0.50
1:A:2547:VAL:HG23	1:A:2551:LEU:HD11	1.93	0.50
1:B:3125:ASP:OD1	1:B:3125:ASP:N	2.45	0.50
1:B:3331:HIS:CE1	1:B:3333:GLN:HB3	2.46	0.50
1:A:1000:PRO:HD2	1:A:1003:MET:HE3	1.93	0.50
1:A:2441:ASN:HD21	1:A:2444:ARG:HD3	1.75	0.50
1:B:4234:ASN:HD21	1:B:4251:SER:HB3	1.77	0.50
1:A:471:LEU:HD11	1:A:480:LEU:HD21	1.94	0.50
1:A:1404:HIS:HB2	1:A:1415:ALA:HB3	1.93	0.50
1:B:4078:GLU:OE1	1:B:4078:GLU:HA	2.12	0.50
1:A:447:VAL:O	1:A:460:ILE:N	2.41	0.49
1:B:461:LEU:HB3	1:B:465:VAL:HG21	1.95	0.49
1:B:1363:HIS:ND1	1:B:1389:CYS:SG	2.86	0.49
1:A:436:ARG:NH2	1:A:451:ASP:OD1	2.43	0.49
1:A:460:ILE:HD12	1:A:496:GLU:HA	1.95	0.49
1:A:4079:TYR:HD2	1:A:4080:LEU:H	1.61	0.49
2:C:113:LYS:HG2	2:C:114:LEU:HD23	1.93	0.49
2:D:99:LEU:HB3	2:D:105:ASP:HB2	1.95	0.49
1:A:2519:ARG:NH1	1:A:2564:ASP:OD1	2.46	0.49
1:B:1140:ASP:OD1	1:B:1140:ASP:N	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:CYS:SG	1:A:191:GLY:N	2.86	0.49
1:A:953:ILE:HG23	1:A:956:VAL:HB	1.94	0.49
1:A:3849:PHE:HB3	1:A:3857:ILE:HG23	1.94	0.49
1:A:3863:CYS:O	1:A:3890:ARG:NH1	2.45	0.49
1:A:3128:CYS:SG	1:A:3129:THR:N	2.85	0.49
1:A:3616:ASP:N	1:A:3627:GLU:OE1	2.46	0.49
1:B:2480:ARG:NH2	1:B:2493:SER:OG	2.46	0.49
2:D:78:ARG:HG3	2:D:125:TYR:HD1	1.78	0.49
1:A:1907:ASP:HA	1:A:2035:LEU:HD13	1.94	0.49
1:A:4337:LYS:NZ	1:B:48:ASP:OD2	2.33	0.49
1:B:2268:GLU:HA	1:B:2268:GLU:OE1	2.13	0.49
1:B:4098:ILE:HG23	1:B:4384:ARG:HH11	1.76	0.49
1:B:4314:ASN:ND2	1:B:4316:TRP:HB2	2.28	0.49
1:A:1075:ARG:HD2	1:A:1094:ASP:CB	2.43	0.48
1:A:321:HIS:HD2	1:A:322:GLN:HG2	1.78	0.48
1:B:2194:ARG:HG3	1:B:2210:TYR:CZ	2.48	0.48
1:A:2511:ARG:NH2	1:A:2555:ASN:OD1	2.45	0.48
1:A:484:GLU:OE1	1:A:486:LYS:N	2.46	0.48
1:A:4394:ASP:N	1:A:4400:LYS:HZ1	2.12	0.48
1:B:91:LYS:HD2	1:B:96:GLY:HA3	1.95	0.48
1:B:396:ILE:HG22	1:B:405:VAL:HG22	1.94	0.48
1:B:2969:PRO:HD2	1:B:2972:TRP:CD2	2.48	0.48
1:B:4043:THR:HG22	1:B:4044:HIS:H	1.77	0.48
1:A:494:ASN:OD1	1:A:495:LEU:N	2.47	0.48
1:B:2070:MET:HG2	1:B:2073:ALA:O	2.14	0.48
1:B:2234:ILE:HD11	1:B:2237:PRO:HG3	1.96	0.48
1:B:2921:ILE:HD11	1:B:2938:ASP:HB2	1.96	0.48
2:C:96:TRP:HA	2:C:110:LYS:HZ3	1.79	0.48
1:B:1903:SER:HB3	1:B:1914:LEU:HD11	1.95	0.48
1:B:2957:CYS:HB3	1:B:2984:LEU:HD11	1.96	0.48
1:A:1477:VAL:HG23	1:A:1478:THR:HG23	1.96	0.48
1:A:3135:PHE:CD1	1:A:3135:PHE:C	2.88	0.48
1:B:1514:MET:HG3	1:B:1556:ARG:O	2.14	0.48
1:B:793:ILE:HG21	1:B:971:ASN:OD1	2.14	0.47
1:B:3048:PRO:HD2	1:B:3051:PHE:CE1	2.49	0.47
1:A:197:LEU:H	1:A:197:LEU:HD22	1.79	0.47
1:B:3051:PHE:HB3	1:B:3058:ASP:OD2	2.14	0.47
1:A:98:ASP:OD1	1:A:98:ASP:N	2.42	0.47
1:B:788:LEU:HD13	1:B:799:TRP:HB3	1.95	0.47
1:A:1543:HIS:HB3	1:A:1729:PRO:HG3	1.95	0.47
1:A:1873:PHE:HB3	1:A:1891:HIS:HB2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:846:ARG:HB3	1:B:847:PRO:HD3	1.97	0.47
1:B:2984:LEU:O	1:B:2988:GLN:HG2	2.13	0.47
2:D:110:LYS:O	2:D:114:LEU:HD23	2.14	0.47
1:A:311:CYS:HB2	1:A:327:GLY:HA3	1.96	0.47
1:A:3417:ILE:CD1	1:A:3422:VAL:HG12	2.45	0.47
1:B:699:ASP:OD2	1:B:702:ARG:NH2	2.47	0.47
1:B:1596:GLU:O	1:B:1633:ARG:NH2	2.32	0.47
1:B:299:ASN:OD1	1:B:301:THR:OG1	2.31	0.47
1:B:1381:GLN:HB3	1:B:1392:ILE:HD11	1.96	0.47
1:B:4247:TYR:CD2	1:B:4258:ALA:HB2	2.49	0.47
1:A:2972:TRP:CH2	2:D:127:LEU:HD21	2.50	0.47
1:B:1188:CYS:HB2	1:B:1194:LYS:HE2	1.97	0.47
1:B:1412:PHE:O	1:B:1413:ARG:NH2	2.48	0.47
1:B:1616:MET:CE	1:B:1646:PRO:HB2	2.45	0.47
1:B:3758:PRO:HB2	1:B:3767:ARG:NH1	2.30	0.47
1:B:4068:LYS:HB2	1:B:4077:SER:OG	2.15	0.47
1:B:4070:ASN:HD22	1:B:4073:SER:HB2	1.79	0.47
1:B:2160:LEU:HB2	1:B:2177:ILE:HD11	1.96	0.47
1:A:2519:ARG:HH21	1:A:2519:ARG:HG3	1.80	0.47
1:A:2210:TYR:OH	7:K:2:GLU:OE2	2.28	0.47
1:B:1785:GLU:OE2	1:B:2009:ARG:NH2	2.48	0.47
1:A:460:ILE:HG22	1:A:461:LEU:HG	1.97	0.46
1:A:484:GLU:OE1	1:A:485:THR:N	2.49	0.46
1:A:2602:TYR:HB2	1:A:2643:THR:HG21	1.96	0.46
1:B:34:ARG:NE	1:B:38:GLY:HA2	2.30	0.46
1:B:3553:ARG:NH2	1:B:3555:CYS:HB2	2.30	0.46
1:B:3758:PRO:HB2	1:B:3767:ARG:HH11	1.80	0.46
1:A:3930:CYS:N	1:A:3942:CYS:SG	2.89	0.46
1:A:4080:LEU:HD21	1:A:4083:GLU:HG3	1.96	0.46
1:A:3949:CYS:HA	1:A:3961:GLU:HG3	1.97	0.46
1:A:4022:SER:O	1:A:4032:CYS:HB2	2.15	0.46
1:A:4142:TYR:HB3	1:B:3793:ARG:HB2	1.96	0.46
1:A:4301:LYS:HE3	1:A:4302:PHE:CZ	2.51	0.46
1:B:1907:ASP:HA	1:B:2035:LEU:HD13	1.97	0.46
1:B:3102:CYS:HB3	1:B:3104:ASP:OD1	2.16	0.46
1:B:1734:LEU:HD12	1:B:1734:LEU:HA	1.82	0.46
1:A:2703:GLN:HE21	1:A:2704:LEU:HG	1.80	0.46
1:A:735:VAL:HG11	1:A:756:TYR:CZ	2.51	0.46
1:A:1476:SER:HB3	1:A:1698:GLN:HG3	1.97	0.46
1:A:2573:LEU:HB3	1:A:2575:LYS:HE2	1.98	0.46
1:A:3721:CYS:HB3	1:A:3726:ASP:HB2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1409:ARG:HG3	1:B:1410:GLY:N	2.30	0.46
1:B:2419:ALA:O	1:B:2438:GLN:NE2	2.45	0.46
1:A:465:VAL:O	1:A:468:PRO:HD3	2.15	0.46
1:A:2286:VAL:HG22	1:A:2291:ILE:HG22	1.97	0.46
1:B:33:PHE:CD2	1:B:46:ARG:HG3	2.51	0.46
1:B:3041:CYS:SG	1:B:3045:ARG:HB2	2.56	0.46
1:A:316:CYS:HB3	1:A:343:ARG:HA	1.98	0.45
1:A:3280:ASP:OD2	1:A:3283:SER:N	2.36	0.45
1:A:3449:THR:OG1	1:A:3451:HIS:O	2.34	0.45
1:B:844:TRP:HB2	1:B:870:TRP:HA	1.98	0.45
1:B:1596:GLU:HA	1:B:1596:GLU:OE1	2.16	0.45
1:B:2932:ASP:HB2	1:B:2938:ASP:CG	2.35	0.45
1:B:3417:ILE:CD1	1:B:3422:VAL:HG12	2.46	0.45
1:A:1734:LEU:HD11	1:A:1738:SER:HA	1.98	0.45
1:A:2685:TYR:CE2	1:A:2687:ALA:HB2	2.51	0.45
1:A:3125:ASP:HB2	1:A:3151:SER:HA	1.98	0.45
1:B:4018:ILE:HG22	1:B:4019:CYS:SG	2.56	0.45
1:B:4065:ARG:HD2	1:B:4067:ARG:HD3	1.98	0.45
1:A:422:ARG:HH11	1:A:1091:ASP:CG	2.20	0.45
1:A:3984:LEU:HB3	1:A:3988:GLY:N	2.32	0.45
1:B:1788:ASP:OD2	1:B:2013:ARG:HA	2.16	0.45
1:A:1847:GLU:HB3	1:A:1860:THR:HA	1.99	0.45
1:A:2210:TYR:HB2	1:A:2236:THR:HA	1.98	0.45
1:A:2613:THR:O	1:A:2615:LYS:N	2.50	0.45
1:B:2253:ASP:HB3	1:B:2258:LEU:HD23	1.99	0.45
1:B:3916:ASP:OD1	1:B:3916:ASP:N	2.50	0.45
1:B:757:SER:HB3	1:B:788:LEU:HD21	1.98	0.45
2:D:311:VAL:HA	2:D:314:ILE:HD12	1.97	0.45
1:A:1837:TYR:CZ	1:A:1906:MET:HG2	2.52	0.45
1:B:318:TYR:CD2	1:B:319:GLN:HG2	2.52	0.45
1:B:1564:MET:HE1	1:B:1702:ARG:HE	1.82	0.45
1:B:2797:LEU:O	1:B:2800:VAL:HG22	2.17	0.45
1:B:4384:ARG:HD3	1:B:4411:TYR:CE2	2.52	0.45
1:A:1075:ARG:HD2	1:A:1094:ASP:HB2	1.98	0.45
1:B:266:TYR:HB3	1:B:267:PRO:HD2	1.99	0.45
1:A:321:HIS:CD2	1:A:322:GLN:HG2	2.53	0.45
1:A:1106:THR:HG22	1:A:1107:SER:H	1.81	0.45
1:B:2592:THR:HG22	1:B:2592:THR:O	2.16	0.45
1:B:4295:GLU:HG2	1:B:4309:LYS:HE2	1.99	0.45
2:D:85:ASP:HB3	2:D:121:ILE:HD11	1.99	0.45
1:A:1539:ILE:HD12	1:A:1539:ILE:HA	1.86	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:440:THR:HB	1:B:468:PRO:HG2	1.98	0.44
1:B:1091:ASP:OD1	1:B:1091:ASP:N	2.50	0.44
1:B:2506:ARG:HH21	1:B:2506:ARG:HB3	1.81	0.44
2:C:58:ARG:N	2:C:90:GLU:OE1	2.50	0.44
1:A:89:GLU:N	1:A:99:GLU:OE1	2.50	0.44
1:A:461:LEU:HB3	1:A:465:VAL:HG21	2.00	0.44
1:A:1368:GLY:H	1:A:1372:ALA:HA	1.82	0.44
1:A:3562:CYS:SG	1:A:3566:ASN:HB2	2.57	0.44
1:B:4079:TYR:CG	1:B:4080:LEU:N	2.85	0.44
1:A:1484:SER:HB3	1:A:1515:ILE:HD11	1.99	0.44
1:A:2406:PRO:HG2	1:A:2618:ARG:HH11	1.82	0.44
1:A:2489:GLN:NE2	1:A:2508:SER:O	2.49	0.44
1:A:3146:MET:HG2	1:A:3147:SER:N	2.32	0.44
1:B:474:ASP:HB3	1:B:479:LYS:HB2	1.99	0.44
2:D:118:LEU:O	2:D:122:LEU:HG	2.18	0.44
1:A:687:ARG:HH22	2:C:275:LYS:HE3	1.82	0.44
1:A:3228:LEU:HD13	1:A:3231:VAL:HG21	2.00	0.44
1:B:4100:LEU:HD23	1:B:4123:PRO:HA	1.99	0.44
2:D:273:THR:HG22	2:D:275:LYS:H	1.82	0.44
1:A:3115:GLU:HB2	1:A:3135:PHE:HD2	1.81	0.44
1:A:98:ASP:HA	1:A:102:ASN:ND2	2.33	0.44
1:A:1109:THR:HG23	1:A:1109:THR:O	2.17	0.44
1:B:3223:LEU:HD11	1:B:3226:GLN:HB3	1.99	0.44
1:B:4019:CYS:HB3	1:B:4032:CYS:HB3	1.94	0.44
1:A:3626:ASP:OD1	1:A:3626:ASP:N	2.51	0.44
1:A:3887:SER:N	1:A:3888:PRO:HD2	2.33	0.44
2:D:66:TRP:CZ2	2:D:70:LYS:NZ	2.84	0.44
1:B:308:MET:HG3	1:B:322:GLN:HB3	2.00	0.44
1:B:2962:PRO:N	1:B:2963:PRO:HD2	2.32	0.44
1:B:3626:ASP:OD1	1:B:3626:ASP:N	2.50	0.44
1:B:3962:THR:N	1:B:3990:ILE:HD11	2.32	0.44
1:B:270:TRP:CH2	1:B:272:CYS:HA	2.53	0.43
1:B:1972:SER:HA	1:B:1989:LYS:HD2	2.00	0.43
1:B:2286:VAL:HG22	1:B:2291:ILE:HG22	2.00	0.43
1:A:718:VAL:HB	1:A:735:VAL:HB	2.00	0.43
1:A:2787:PHE:CZ	1:A:2814:ASP:HA	2.53	0.43
1:A:3081:GLN:HB3	1:A:3089:CYS:SG	2.58	0.43
1:B:1616:MET:HE3	1:B:1646:PRO:HB2	1.99	0.43
2:C:76:PRO:HA	2:C:79:LEU:HB3	2.01	0.43
2:C:82:LEU:HD13	2:C:125:TYR:CE2	2.53	0.43
1:A:626:ALA:HB1	1:A:631:GLU:HG2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3671:ASP:OD1	1:B:3671:ASP:C	2.57	0.43
2:C:316:ASP:HB3	2:C:319:HIS:HB2	2.00	0.43
1:A:364:ARG:O	1:A:367:ARG:HD3	2.19	0.43
1:A:1616:MET:HG2	1:A:1623:ILE:HG12	2.00	0.43
1:B:1873:PHE:HB3	1:B:1891:HIS:HB2	1.99	0.43
1:B:2507:VAL:HG21	1:B:2524:TRP:NE1	2.30	0.43
1:B:2773:GLU:HA	1:B:2776:CYS:SG	2.59	0.43
1:A:188:PHE:O	1:A:196:ILE:N	2.52	0.43
1:A:780:ASN:OD1	1:A:781:ARG:HG2	2.19	0.43
1:A:1734:LEU:CD1	1:A:1738:SER:HA	2.49	0.43
1:A:3793:ARG:NH1	1:B:4142:TYR:O	2.52	0.43
1:B:2484:SER:HB2	1:B:2510:PRO:HG2	2.01	0.43
1:B:2561:LEU:HD12	1:B:2561:LEU:HA	1.87	0.43
1:B:3037:ASN:O	1:B:3049:ARG:HG2	2.18	0.43
1:B:3225:LEU:HD23	1:B:3228:LEU:HD11	2.01	0.43
1:B:3255:ARG:NE	1:B:3264:GLU:OE2	2.36	0.43
1:B:3857:ILE:HD12	1:B:3857:ILE:O	2.17	0.43
2:D:96:TRP:HE3	2:D:110:LYS:HB3	1.84	0.43
1:A:1186:LEU:HD12	1:A:1186:LEU:O	2.19	0.43
1:A:2636:THR:HG22	1:A:2637:GLN:N	2.33	0.43
1:A:2787:PHE:O	1:A:2788:THR:OG1	2.29	0.43
1:B:1265:THR:HG21	1:B:3177:ILE:HD11	2.00	0.43
1:B:3610:PRO:HG2	1:B:3613:TRP:CD2	2.54	0.43
2:C:97:LYS:O	2:C:100:LYS:N	2.50	0.43
1:A:1623:ILE:HD12	1:A:1637:ILE:HD12	2.00	0.43
1:B:451:ASP:HB3	1:B:454:GLY:O	2.19	0.43
2:C:59:MET:SD	2:C:60:GLU:N	2.91	0.43
1:A:3722:HIS:CG	1:A:3723:PRO:HD2	2.54	0.43
1:B:461:LEU:HD11	1:B:493:VAL:HG11	2.00	0.43
1:A:3980:ASN:OD1	17:A:4710:NAG:N2	2.52	0.43
1:B:2401:SER:HB2	1:B:2413:PHE:CZ	2.54	0.43
1:B:2939:GLU:HG2	1:B:2940:ASP:N	2.33	0.43
1:B:3016:ARG:HB2	1:B:3016:ARG:NH2	2.33	0.43
2:D:80:ALA:O	2:D:83:HIS:ND1	2.48	0.43
2:D:303:ILE:HD13	2:D:303:ILE:HA	1.95	0.43
1:A:865:ASN:N	1:A:865:ASN:OD1	2.50	0.42
1:A:2578:ARG:HD2	1:A:2589:VAL:HG22	2.00	0.42
1:B:2960:SER:HB3	1:B:2964:ASN:HB3	2.01	0.42
1:B:3904:LEU:HD12	1:B:3916:ASP:HA	2.00	0.42
1:A:2428:ASP:HB3	1:A:2433:ARG:HG2	2.01	0.42
1:B:2546:ILE:HD12	1:B:2582:THR:HA	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:865:ASN:HD22	11:U:1:NAG:C7	2.32	0.42
1:A:1838:TYR:CZ	1:A:1847:GLU:HG3	2.54	0.42
1:A:2259:ILE:HB	1:A:2273:ARG:HB2	2.01	0.42
1:A:3052:VAL:HG12	1:A:3053:CYS:SG	2.59	0.42
1:B:1189:THR:OG1	1:B:1190:SER:N	2.52	0.42
1:B:4065:ARG:HD3	1:B:4081:GLU:OE2	2.19	0.42
1:A:2810:ASN:HB2	17:A:4707:NAG:O5	2.19	0.42
1:B:740:SER:HB2	1:B:742:PHE:CE2	2.55	0.42
2:D:96:TRP:CH2	2:D:111:GLU:HB2	2.54	0.42
1:B:1906:MET:SD	1:B:2036:PRO:HG2	2.59	0.42
1:B:4284:ASP:HA	1:B:4301:LYS:HE2	2.01	0.42
1:A:521:GLY:C	1:A:542:MET:HG3	2.40	0.42
1:B:1886:LEU:N	1:B:1904:ALA:O	2.45	0.42
1:B:2235:VAL:HG12	1:B:2236:THR:HG23	2.02	0.42
1:B:2699:THR:O	1:B:2700:ARG:HD3	2.20	0.42
1:B:2914:GLN:HA	1:B:2920:CYS:HB3	2.02	0.42
2:C:97:LYS:O	2:C:97:LYS:HD2	2.20	0.42
2:D:262:ASP:OD1	2:D:263:LEU:N	2.53	0.42
1:A:376:TYR:HB3	1:A:384:CYS:HB3	2.02	0.42
1:A:3015:ASP:HB2	1:A:3017:ARG:CZ	2.46	0.42
1:B:2668:ALA:HB2	1:B:2677:GLN:HE22	1.84	0.42
1:A:3275:GLU:OE1	1:A:3326:ARG:NE	2.45	0.42
1:A:3997:PHE:HB3	1:A:4007:CYS:HB3	2.02	0.42
1:B:431:HIS:CD2	1:B:434:LYS:H	2.33	0.42
1:B:2517:PRO:HA	1:B:2538:LEU:HD11	2.01	0.42
1:B:4061:PRO:HD2	1:B:4319:GLN:O	2.20	0.42
2:D:324:LYS:O	2:D:328:VAL:HG13	2.20	0.42
1:B:445:GLU:OE2	1:B:738:SER:OG	2.28	0.42
1:B:4213:GLU:HG2	1:B:4224:VAL:HG12	2.02	0.42
1:B:4234:ASN:HD21	1:B:4251:SER:CB	2.32	0.42
1:A:361:CYS:SG	1:A:362:GLU:N	2.93	0.41
1:A:4076:PHE:HZ	1:A:4311:LEU:HD13	1.85	0.41
1:B:2538:LEU:HD12	1:B:2669:PRO:O	2.20	0.41
1:B:2701:CYS:SG	1:B:2705:GLN:HB2	2.60	0.41
1:B:3245:TRP:CE2	1:B:3254:GLU:HB2	2.55	0.41
1:B:3981:CYS:HA	1:B:3991:CYS:HA	2.00	0.41
2:C:82:LEU:HD22	2:C:125:TYR:CD1	2.55	0.41
1:A:896:SER:OG	1:A:901:LEU:O	2.23	0.41
1:A:1081:PRO:HD2	1:A:1084:TRP:CE3	2.55	0.41
1:A:4121:TYR:CD2	1:A:4382:PRO:HB3	2.55	0.41
1:B:3998:LYS:O	1:B:4008:GLN:HG3	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1401:CYS:HB3	1:A:1414:CYS:HB3	1.98	0.41
1:A:3609:ILE:HD12	1:A:3609:ILE:O	2.18	0.41
1:B:3205:PHE:HA	1:B:3455:ASP:O	2.21	0.41
1:A:882:ARG:HE	1:A:895:HIS:CD2	2.32	0.41
1:A:2350:SER:O	1:A:2350:SER:OG	2.34	0.41
1:A:3736:PRO:HD2	1:A:3739:TRP:CE3	2.55	0.41
1:B:3601:TRP:CD2	1:B:3614:GLN:NE2	2.89	0.41
1:A:357:CYS:HB3	1:A:370:CYS:HB3	1.89	0.41
1:A:398:SER:HB3	1:A:645:HIS:O	2.20	0.41
1:A:1642:VAL:HA	1:B:2592:THR:HG21	2.02	0.41
1:B:4314:ASN:HD22	1:B:4316:TRP:HB2	1.84	0.41
1:A:88:ASP:N	1:A:99:GLU:OE1	2.50	0.41
1:A:631:GLU:OE1	1:A:633:ASN:N	2.49	0.41
1:A:933:GLY:O	1:A:953:ILE:HG22	2.20	0.41
1:B:2155:TRP:CH2	1:B:2200:PRO:HD2	2.55	0.41
1:B:2428:ASP:HB2	1:B:2435:PHE:HE2	1.85	0.41
1:A:2696:ASP:HA	1:A:2700:ARG:HH12	1.86	0.41
1:B:1975:TYR:CE2	1:B:1986:ARG:HD3	2.56	0.41
2:C:97:LYS:HD2	2:C:100:LYS:HB2	2.03	0.41
1:A:3672:GLU:O	1:A:3675:THR:HG22	2.21	0.41
1:A:3860:PHE:CE1	1:A:3861:TRP:CD1	3.09	0.41
1:B:476:ILE:HG22	1:B:660:ASN:HB3	2.02	0.41
1:B:1134:ASP:OD1	1:B:1134:ASP:N	2.54	0.41
1:B:2552:VAL:HB	1:B:2572:SER:HB3	2.03	0.41
1:B:4413:GLU:OE1	1:B:4413:GLU:N	2.54	0.41
2:C:100:LYS:NZ	2:C:105:ASP:HB3	2.36	0.41
1:A:3417:ILE:HD13	1:A:3422:VAL:HG12	2.03	0.41
1:A:4019:CYS:SG	1:A:4020:PRO:HD2	2.60	0.41
1:B:54:LEU:HD13	1:B:54:LEU:HA	1.95	0.41
1:B:4232:TRP:N	1:B:4232:TRP:CD1	2.88	0.41
1:A:2618:ARG:O	1:A:2627:LEU:HA	2.21	0.40
1:A:2709:LEU:HD12	1:A:2730:SER:HB2	2.03	0.40
1:A:2970:GLN:NE2	1:A:2973:VAL:HG21	2.35	0.40
1:A:3759:ARG:HH22	1:A:3765:GLU:CD	2.24	0.40
1:A:3984:LEU:HD13	1:A:3987:GLY:CA	2.52	0.40
1:B:2066:MET:HG2	1:B:2077:PHE:O	2.20	0.40
1:B:2142:GLY:O	1:B:2164:ASN:ND2	2.54	0.40
1:B:3970:ARG:CZ	1:B:3976:ILE:HD13	2.51	0.40
2:C:96:TRP:HA	2:C:110:LYS:NZ	2.35	0.40
2:D:283:GLU:OE2	2:D:344:HIS:NE2	2.40	0.40
11:U:1:NAG:H61	11:U:2:NAG:H82	3.70	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1401:CYS:HB3	1:B:1405:CYS:HB2	2.04	0.40
1:B:3246:ILE:HD11	1:B:3277:LEU:HB3	2.04	0.40
1:B:3934:GLU:HA	1:B:3944:SER:HA	2.02	0.40
1:B:4413:GLU:HG2	1:B:4414:VAL:HG13	2.03	0.40
2:C:97:LYS:HA	2:C:100:LYS:HG2	2.04	0.40
1:A:359:GLN:OE1	1:A:384:CYS:HB2	2.20	0.40
1:A:624:MET:HE3	1:A:636:VAL:HA	2.03	0.40
1:A:3479:SER:HG	1:A:3480:HIS:CE1	2.34	0.40
1:A:4401:CYS:HB2	1:A:4411:TYR:HA	2.03	0.40
1:B:2071:LEU:HB2	1:B:2072:PRO:HD3	2.02	0.40
1:B:4057:LEU:HD12	1:B:4323:PHE:HD2	1.87	0.40
1:A:3553:ARG:NH1	1:A:3559:GLN:O	2.53	0.40
1:B:447:VAL:HG23	1:B:465:VAL:HG11	2.03	0.40
1:B:4273:ALA:O	1:B:4274:MET:HG2	2.21	0.40
1:A:1173:LYS:CD	1:A:1178:GLY:HA2	2.47	0.40
1:B:4057:LEU:HB2	1:B:4323:PHE:HB3	2.03	0.40
1:B:4119:ARG:HH11	1:B:4173:LEU:C	2.23	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	4304/4660 (92%)	3983 (92%)	319 (7%)	2 (0%)	100	100
1	B	4304/4660 (92%)	3994 (93%)	308 (7%)	2 (0%)	100	100
2	C	173/360 (48%)	170 (98%)	3 (2%)	0	100	100
2	D	173/360 (48%)	171 (99%)	2 (1%)	0	100	100
4	H	1/5 (20%)	1 (100%)	0	0	100	100
4	O	1/5 (20%)	1 (100%)	0	0	100	100
5	I	1/6 (17%)	1 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	P	1/6 (17%)	1 (100%)	0	0	100	100
6	J	1/3 (33%)	0	1 (100%)	0	100	100
6	Q	1/3 (33%)	1 (100%)	0	0	100	100
7	K	2/5 (40%)	0	2 (100%)	0	100	100
7	R	2/5 (40%)	2 (100%)	0	0	100	100
8	L	1/5 (20%)	0	1 (100%)	0	100	100
8	M	1/5 (20%)	1 (100%)	0	0	100	100
8	S	1/5 (20%)	0	1 (100%)	0	100	100
8	T	1/5 (20%)	1 (100%)	0	0	100	100
All	All	8968/10098 (89%)	8327 (93%)	637 (7%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2874	SER
1	A	2874	SER
1	B	2858	ILE
1	A	410	GLY

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	3791/4089 (93%)	3672 (97%)	119 (3%)	40	62
1	B	3790/4089 (93%)	3688 (97%)	102 (3%)	44	66
2	C	163/326 (50%)	156 (96%)	7 (4%)	29	55
2	D	163/326 (50%)	159 (98%)	4 (2%)	47	68
4	H	1/1 (100%)	1 (100%)	0	100	100
4	O	1/1 (100%)	1 (100%)	0	100	100
5	I	1/1 (100%)	1 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	P	1/1 (100%)	0	1 (100%)	0 0
6	J	1/1 (100%)	1 (100%)	0	100 100
6	Q	1/1 (100%)	1 (100%)	0	100 100
7	K	2/2 (100%)	2 (100%)	0	100 100
7	R	2/2 (100%)	1 (50%)	1 (50%)	0 0
8	L	1/1 (100%)	1 (100%)	0	100 100
8	M	1/1 (100%)	1 (100%)	0	100 100
8	S	1/1 (100%)	1 (100%)	0	100 100
8	T	1/1 (100%)	1 (100%)	0	100 100
All	All	7921/8844 (90%)	7687 (97%)	234 (3%)	44 63

All (234) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	ARG
1	A	74	CYS
1	A	98	ASP
1	A	198	ARG
1	A	215	ARG
1	A	221	THR
1	A	248	GLN
1	A	259	ASN
1	A	268	ARG
1	A	283	LYS
1	A	311	CYS
1	A	329	CYS
1	A	470	ASN
1	A	516	LEU
1	A	549	ASP
1	A	579	TYR
1	A	631	GLU
1	A	681	ASN
1	A	711	LEU
1	A	725	LEU
1	A	759	LEU
1	A	772	THR
1	A	841	LEU
1	A	856	ASP
1	A	887	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	992	ASN
1	A	995	ARG
1	A	1018	ARG
1	A	1093	LEU
1	A	1173	LYS
1	A	1366	MET
1	A	1408	MET
1	A	1436	ASN
1	A	1465	ASP
1	A	1468	PHE
1	A	1472	LEU
1	A	1636	VAL
1	A	1656	VAL
1	A	1728	CYS
1	A	1745	ASP
1	A	2070	MET
1	A	2126	ARG
1	A	2170	THR
1	A	2210	TYR
1	A	2242	MET
1	A	2338	SER
1	A	2363	GLU
1	A	2394	SER
1	A	2439	LYS
1	A	2441	ASN
1	A	2494	MET
1	A	2507	VAL
1	A	2532	LYS
1	A	2570	ASP
1	A	2578	ARG
1	A	2626	ASP
1	A	2633	ARG
1	A	2701	CYS
1	A	2722	ASN
1	A	2781	CYS
1	A	2823	CYS
1	A	2835	ILE
1	A	2849	CYS
1	A	2856	ASN
1	A	2868	ASN
1	A	2914	GLN
1	A	2919	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2924	ASN
1	A	2927	CYS
1	A	2938	ASP
1	A	2971	TYR
1	A	3012	PHE
1	A	3017	ARG
1	A	3027	ARG
1	A	3086	ASN
1	A	3092	MET
1	A	3096	CYS
1	A	3106	SER
1	A	3135	PHE
1	A	3146	MET
1	A	3150	ARG
1	A	3206	SER
1	A	3212	ARG
1	A	3220	SER
1	A	3262	ASN
1	A	3277	LEU
1	A	3375	ASP
1	A	3378	ASN
1	A	3415	LEU
1	A	3449	THR
1	A	3450	THR
1	A	3509	LEU
1	A	3549	LEU
1	A	3578	GLN
1	A	3782	GLN
1	A	3784	ASN
1	A	3793	ARG
1	A	3797	MET
1	A	3812	CYS
1	A	3826	LEU
1	A	3874	ASP
1	A	3922	CYS
1	A	3924	LYS
1	A	3979	GLN
1	A	4004	LYS
1	A	4032	CYS
1	A	4075	LYS
1	A	4157	HIS
1	A	4174	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	4201	MET
1	A	4217	MET
1	A	4243	ASP
1	A	4280	ASP
1	A	4284	ASP
1	A	4321	ARG
1	A	4366	THR
1	A	4379	MET
1	A	4386	MET
1	A	4401	CYS
1	B	33	PHE
1	B	39	TYR
1	B	46	ARG
1	B	58	ASP
1	B	65	ARG
1	B	72	PHE
1	B	187	GLU
1	B	219	TYR
1	B	247	CYS
1	B	272	CYS
1	B	278	CYS
1	B	335	HIS
1	B	350	ASP
1	B	359	GLN
1	B	362	GLU
1	B	365	GLN
1	B	516	LEU
1	B	530	SER
1	B	534	GLN
1	B	563	LEU
1	B	613	VAL
1	B	741	PHE
1	B	746	ASP
1	B	849	LYS
1	B	895	HIS
1	B	899	ASP
1	B	995	ARG
1	B	1028	LEU
1	B	1088	ARG
1	B	1091	ASP
1	B	1134	ASP
1	B	1194	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1201	CYS
1	B	1250	GLU
1	B	1300	MET
1	B	1349	CYS
1	B	1352	ASP
1	B	1409	ARG
1	B	1517	VAL
1	B	1550	LYS
1	B	1636	VAL
1	B	1666	VAL
1	B	1673	HIS
1	B	1728	CYS
1	B	1745	ASP
1	B	1783	ASP
1	B	1791	GLN
1	B	1851	LEU
1	B	1936	TRP
1	B	1967	LEU
1	B	2013	ARG
1	B	2080	GLU
1	B	2153	LEU
1	B	2174	VAL
1	B	2225	ASN
1	B	2297	ASN
1	B	2378	ASN
1	B	2407	ARG
1	B	2430	ARG
1	B	2444	ARG
1	B	2519	ARG
1	B	2677	GLN
1	B	2680	HIS
1	B	2753	ARG
1	B	2786	GLU
1	B	2807	CYS
1	B	2839	ARG
1	B	2876	GLN
1	B	2961	ARG
1	B	2966	ARG
1	B	2984	LEU
1	B	2992	MET
1	B	2993	ARG
1	B	3000	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	3092	MET
1	B	3146	MET
1	B	3148	ASP
1	B	3150	ARG
1	B	3401	ARG
1	B	3426	ASP
1	B	3467	MET
1	B	3500	GLN
1	B	3505	ARG
1	B	3545	ASP
1	B	3571	GLN
1	B	3588	ARG
1	B	3635	ARG
1	B	3689	LYS
1	B	3737	LEU
1	B	3755	ASN
1	B	3793	ARG
1	B	3822	ARG
1	B	3878	HIS
1	B	3942	CYS
1	B	3965	ASN
1	B	3971	THR
1	B	4045	TYR
1	B	4048	ARG
1	B	4065	ARG
1	B	4261	TYR
1	B	4274	MET
1	B	4321	ARG
2	C	259	ARG
2	C	268	GLN
2	C	277	LEU
2	C	305	HIS
2	C	307	LYS
2	C	342	LYS
2	C	346	GLN
2	D	64	GLN
2	D	79	LEU
2	D	93	GLU
2	D	336	GLU
5	P	3	LEU
7	R	3	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	ASN
1	A	321	HIS
1	A	382	GLN
1	A	412	ASN
1	A	444	GLN
1	A	456	ASN
1	A	639	GLN
1	A	681	ASN
1	A	895	HIS
1	A	985	HIS
1	A	992	ASN
1	A	1058	GLN
1	A	1254	HIS
1	A	1393	ASN
1	A	1891	HIS
1	A	1920	GLN
1	A	1921	HIS
1	A	1963	HIS
1	A	2001	ASN
1	A	2489	GLN
1	A	2595	HIS
1	A	2651	GLN
1	A	2703	GLN
1	A	2808	HIS
1	A	3066	GLN
1	A	3262	ASN
1	A	3523	ASN
1	A	3878	HIS
1	A	3941	ASN
1	A	4221	HIS
1	A	4314	ASN
1	B	315	ASN
1	B	412	ASN
1	B	431	HIS
1	B	826	ASN
1	B	1033	ASN
1	B	1192	GLN
1	B	1283	ASN
1	B	1891	HIS
1	B	1980	GLN
1	B	2212	GLN
1	B	2297	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	2378	ASN
1	B	2414	GLN
1	B	2500	ASN
1	B	2710	ASN
1	B	2903	HIS
1	B	3336	HIS
1	B	3378	ASN
1	B	4008	GLN
1	B	4131	ASN
1	B	4234	ASN
2	C	295	ASN
2	D	268	GLN
2	D	294	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

146 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	$\#\|Z\| > 2$
16	NAG	0	1	1,16	14,14,15	0.49	0	17,19,21	1.42	1 (5%)
16	NAG	0	2	16	14,14,15	0.38	0	17,19,21	1.41	3 (17%)
16	BMA	0	3	16	11,11,12	0.32	0	15,15,17	0.54	0
10	NAG	1	1	10,1	14,14,15	0.49	0	17,19,21	0.86	0
10	NAG	1	2	10	14,14,15	0.43	0	17,19,21	0.66	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	BMA	1	3	10	11,11,12	0.27	0	15,15,17	0.90	1 (6%)
10	MAN	1	4	10	11,11,12	0.30	0	15,15,17	0.69	0
10	MAN	1	5	10	11,11,12	0.29	0	15,15,17	0.60	0
12	NAG	2	1	12,1	14,14,15	0.89	0	17,19,21	1.52	5 (29%)
12	NAG	2	2	12	14,14,15	1.18	2 (14%)	17,19,21	1.04	1 (5%)
12	BMA	2	3	12	11,11,12	1.07	2 (18%)	15,15,17	1.00	1 (6%)
12	NAG	3	1	12,1	14,14,15	0.44	0	17,19,21	0.53	0
12	NAG	3	2	12	14,14,15	0.47	0	17,19,21	0.59	0
12	BMA	3	3	12	11,11,12	0.79	0	15,15,17	0.85	1 (6%)
10	NAG	4	1	10,1	14,14,15	0.41	0	17,19,21	0.99	1 (5%)
10	NAG	4	2	10	14,14,15	0.45	0	17,19,21	1.06	1 (5%)
10	BMA	4	3	10	11,11,12	0.31	0	15,15,17	1.04	2 (13%)
10	MAN	4	4	10	11,11,12	0.30	0	15,15,17	0.54	0
10	MAN	4	5	10	11,11,12	0.34	0	15,15,17	0.55	0
10	NAG	5	1	10,1	14,14,15	0.49	0	17,19,21	0.89	1 (5%)
10	NAG	5	2	10	14,14,15	0.46	0	17,19,21	0.38	0
10	BMA	5	3	10	11,11,12	0.34	0	15,15,17	0.69	0
10	MAN	5	4	10	11,11,12	0.27	0	15,15,17	0.62	0
10	MAN	5	5	10	11,11,12	0.22	0	15,15,17	0.66	1 (6%)
14	NAG	6	1	14,1	14,14,15	0.44	0	17,19,21	0.77	0
14	NAG	6	2	14	14,14,15	0.44	0	17,19,21	0.86	0
14	BMA	6	3	14	11,11,12	0.39	0	15,15,17	1.04	0
14	MAN	6	4	14	11,11,12	0.27	0	15,15,17	0.88	2 (13%)
14	MAN	6	5	14	11,11,12	0.31	0	15,15,17	0.62	0
16	NAG	7	1	1,16	14,14,15	0.43	0	17,19,21	0.50	0
16	NAG	7	2	16	14,14,15	0.44	0	17,19,21	0.41	0
16	BMA	7	3	16	11,11,12	0.23	0	15,15,17	0.66	0
13	NAG	8	1	13,1	14,14,15	0.68	0	17,19,21	1.36	2 (11%)
13	NAG	8	2	13	14,14,15	0.58	0	17,19,21	0.94	1 (5%)
10	NAG	9	1	10,1	14,14,15	0.39	0	17,19,21	0.82	1 (5%)
10	NAG	9	2	10	14,14,15	0.40	0	17,19,21	0.47	0
10	BMA	9	3	10	11,11,12	0.27	0	15,15,17	0.71	0
10	MAN	9	4	10	11,11,12	0.27	0	15,15,17	0.65	0
10	MAN	9	5	10	11,11,12	0.26	0	15,15,17	0.54	0
9	NAG	E	1	1,9	14,14,15	0.40	0	17,19,21	0.99	1 (5%)
9	NAG	E	2	9	14,14,15	0.38	0	17,19,21	0.53	0
10	NAG	F	1	10,1	14,14,15	0.40	0	17,19,21	0.53	0
10	NAG	F	2	10	14,14,15	0.40	0	17,19,21	0.36	0
10	BMA	F	3	10	11,11,12	0.27	0	15,15,17	0.70	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	MAN	F	4	10	11,11,12	0.34	0	15,15,17	0.58	0
10	MAN	F	5	10	11,11,12	0.22	0	15,15,17	0.62	0
11	NAG	U	1	11,1	14,14,15	0.41	0	17,19,21	0.56	0
11	NAG	U	2	11	14,14,15	0.49	0	17,19,21	1.77	4 (23%)
11	BMA	U	3	11	11,11,12	0.59	0	15,15,17	1.02	1 (6%)
11	MAN	U	4	11	11,11,12	0.30	0	15,15,17	0.69	0
11	MAN	U	5	11	11,11,12	0.36	0	15,15,17	0.79	2 (13%)
9	NAG	V	1	1,9	14,14,15	0.51	0	17,19,21	1.29	2 (11%)
9	NAG	V	2	9	14,14,15	0.52	0	17,19,21	0.88	1 (5%)
12	NAG	W	1	12,1	14,14,15	0.42	0	17,19,21	0.72	1 (5%)
12	NAG	W	2	12	14,14,15	0.41	0	17,19,21	0.83	1 (5%)
12	BMA	W	3	12	11,11,12	0.35	0	15,15,17	0.70	0
9	NAG	X	1	1,9	14,14,15	0.42	0	17,19,21	0.60	0
9	NAG	X	2	9	14,14,15	0.42	0	17,19,21	0.60	0
9	NAG	Y	1	1,9	14,14,15	0.39	0	17,19,21	0.41	0
9	NAG	Y	2	9	14,14,15	0.40	0	17,19,21	0.69	0
10	NAG	Z	1	10,1	14,14,15	0.46	0	17,19,21	1.32	1 (5%)
10	NAG	Z	2	10	14,14,15	0.38	0	17,19,21	1.18	2 (11%)
10	BMA	Z	3	10	11,11,12	0.33	0	15,15,17	0.66	0
10	MAN	Z	4	10	11,11,12	0.28	0	15,15,17	0.50	0
10	MAN	Z	5	10	11,11,12	0.24	0	15,15,17	0.56	0
9	NAG	a	1	1,9	14,14,15	0.40	0	17,19,21	0.71	0
9	NAG	a	2	9	14,14,15	0.40	0	17,19,21	0.35	0
10	NAG	b	1	10,1	14,14,15	0.41	0	17,19,21	0.41	0
10	NAG	b	2	10	14,14,15	0.40	0	17,19,21	0.42	0
10	BMA	b	3	10	11,11,12	0.34	0	15,15,17	0.83	1 (6%)
10	MAN	b	4	10	11,11,12	0.28	0	15,15,17	0.67	0
10	MAN	b	5	10	11,11,12	0.23	0	15,15,17	0.54	0
13	NAG	c	1	13,1	14,14,15	0.51	0	17,19,21	0.85	1 (5%)
13	NAG	c	2	13	14,14,15	0.53	0	17,19,21	1.07	1 (5%)
9	NAG	d	1	1,9	14,14,15	0.40	0	17,19,21	0.62	0
9	NAG	d	2	9	14,14,15	0.39	0	17,19,21	0.50	0
12	NAG	e	1	12,1	14,14,15	0.41	0	17,19,21	0.39	0
12	NAG	e	2	12	14,14,15	0.42	0	17,19,21	0.58	0
12	BMA	e	3	12	11,11,12	0.32	0	15,15,17	0.79	1 (6%)
12	NAG	f	1	12,1	14,14,15	0.42	0	17,19,21	0.45	0
12	NAG	f	2	12	14,14,15	0.42	0	17,19,21	0.54	0
12	BMA	f	3	12	11,11,12	0.22	0	15,15,17	0.63	1 (6%)
10	NAG	g	1	10,1	14,14,15	0.46	0	17,19,21	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	NAG	g	2	10	14,14,15	0.39	0	17,19,21	0.71	1 (5%)
10	BMA	g	3	10	11,11,12	0.40	0	15,15,17	0.79	1 (6%)
10	MAN	g	4	10	11,11,12	0.30	0	15,15,17	0.58	0
10	MAN	g	5	10	11,11,12	0.27	0	15,15,17	0.64	0
12	NAG	h	1	12,1	14,14,15	0.41	0	17,19,21	0.70	0
12	NAG	h	2	12	14,14,15	0.43	0	17,19,21	0.49	0
12	BMA	h	3	12	11,11,12	0.29	0	15,15,17	0.57	0
12	NAG	i	1	12,1	14,14,15	0.47	0	17,19,21	0.80	0
12	NAG	i	2	12	14,14,15	0.47	0	17,19,21	0.95	1 (5%)
12	BMA	i	3	12	11,11,12	0.62	0	15,15,17	0.84	1 (6%)
10	NAG	j	1	10,1	14,14,15	0.40	0	17,19,21	1.30	3 (17%)
10	NAG	j	2	10	14,14,15	0.41	0	17,19,21	0.38	0
10	BMA	j	3	10	11,11,12	0.55	0	15,15,17	0.79	0
10	MAN	j	4	10	11,11,12	0.50	0	15,15,17	0.88	1 (6%)
10	MAN	j	5	10	11,11,12	0.38	0	15,15,17	0.65	0
10	NAG	k	1	10,1	14,14,15	0.44	0	17,19,21	0.89	1 (5%)
10	NAG	k	2	10	14,14,15	0.49	0	17,19,21	1.11	2 (11%)
10	BMA	k	3	10	11,11,12	0.26	0	15,15,17	0.64	0
10	MAN	k	4	10	11,11,12	0.31	0	15,15,17	0.93	2 (13%)
10	MAN	k	5	10	11,11,12	0.33	0	15,15,17	0.56	0
10	NAG	l	1	10,1	14,14,15	0.39	0	17,19,21	0.71	1 (5%)
10	NAG	l	2	10	14,14,15	0.43	0	17,19,21	0.37	0
10	BMA	l	3	10	11,11,12	0.34	0	15,15,17	1.21	2 (13%)
10	MAN	l	4	10	11,11,12	0.29	0	15,15,17	0.70	0
10	MAN	l	5	10	11,11,12	0.33	0	15,15,17	0.53	0
12	NAG	m	1	12,1	14,14,15	1.07	1 (7%)	17,19,21	1.19	1 (5%)
12	NAG	m	2	12	14,14,15	0.42	0	17,19,21	0.70	1 (5%)
12	BMA	m	3	12	11,11,12	0.28	0	15,15,17	0.61	0
9	NAG	n	1	1,9	14,14,15	0.53	0	17,19,21	1.01	1 (5%)
9	NAG	n	2	9	14,14,15	0.54	0	17,19,21	0.88	1 (5%)
13	NAG	o	1	13,1	14,14,15	0.40	0	17,19,21	0.82	0
13	NAG	o	2	13	14,14,15	0.41	0	17,19,21	0.41	0
12	NAG	p	1	12,1	14,14,15	0.42	0	17,19,21	0.71	0
12	NAG	p	2	12	14,14,15	0.40	0	17,19,21	0.82	1 (5%)
12	BMA	p	3	12	11,11,12	0.26	0	15,15,17	0.67	0
9	NAG	q	1	1,9	14,14,15	1.13	1 (7%)	17,19,21	1.14	1 (5%)
9	NAG	q	2	9	14,14,15	0.92	1 (7%)	17,19,21	1.07	1 (5%)
12	NAG	r	1	12,1	14,14,15	0.42	0	17,19,21	0.82	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	NAG	r	2	12	14,14,15	0.41	0	17,19,21	0.57	0
12	BMA	r	3	12	11,11,12	0.30	0	15,15,17	0.66	0
9	NAG	s	1	1,9	14,14,15	0.44	0	17,19,21	1.02	2 (11%)
9	NAG	s	2	9	14,14,15	0.40	0	17,19,21	0.61	0
9	NAG	t	1	1,9	14,14,15	0.98	0	17,19,21	1.55	3 (17%)
9	NAG	t	2	9	14,14,15	1.08	1 (7%)	17,19,21	1.53	1 (5%)
10	NAG	u	1	10,1	14,14,15	0.48	0	17,19,21	0.56	0
10	NAG	u	2	10	14,14,15	0.45	0	17,19,21	0.70	0
10	BMA	u	3	10	11,11,12	0.40	0	15,15,17	0.72	1 (6%)
10	MAN	u	4	10	11,11,12	0.24	0	15,15,17	0.60	0
10	MAN	u	5	10	11,11,12	0.27	0	15,15,17	0.64	0
9	NAG	v	1	1,9	14,14,15	0.45	0	17,19,21	0.49	0
9	NAG	v	2	9	14,14,15	0.39	0	17,19,21	0.39	0
14	NAG	w	1	14,1	14,14,15	0.52	0	17,19,21	1.20	2 (11%)
14	NAG	w	2	14	14,14,15	0.46	0	17,19,21	1.34	3 (17%)
14	BMA	w	3	14	11,11,12	0.42	0	15,15,17	0.66	0
14	MAN	w	4	14	11,11,12	0.29	0	15,15,17	0.62	0
14	MAN	w	5	14	11,11,12	0.27	0	15,15,17	0.57	0
9	NAG	x	1	1,9	14,14,15	0.51	0	17,19,21	0.85	0
9	NAG	x	2	9	14,14,15	0.40	0	17,19,21	0.69	0
9	NAG	y	1	1,9	14,14,15	0.41	0	17,19,21	0.67	1 (5%)
9	NAG	y	2	9	14,14,15	0.41	0	17,19,21	0.43	0
15	NAG	z	1	15,1	14,14,15	0.54	0	17,19,21	0.82	1 (5%)
15	NAG	z	2	15	14,14,15	0.39	0	17,19,21	1.29	2 (11%)
15	BMA	z	3	15	11,11,12	0.37	0	15,15,17	0.69	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
16	NAG	0	1	1,16	-	2/6/23/26	0/1/1/1
16	NAG	0	2	16	-	0/6/23/26	0/1/1/1
16	BMA	0	3	16	-	0/2/19/22	0/1/1/1
10	NAG	1	1	10,1	-	0/6/23/26	0/1/1/1
10	NAG	1	2	10	-	0/6/23/26	0/1/1/1
10	BMA	1	3	10	-	2/2/19/22	0/1/1/1
10	MAN	1	4	10	-	0/2/19/22	0/1/1/1
10	MAN	1	5	10	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAG	2	1	12,1	-	1/6/23/26	0/1/1/1
12	NAG	2	2	12	-	1/6/23/26	0/1/1/1
12	BMA	2	3	12	-	0/2/19/22	0/1/1/1
12	NAG	3	1	12,1	-	0/6/23/26	0/1/1/1
12	NAG	3	2	12	-	0/6/23/26	0/1/1/1
12	BMA	3	3	12	-	0/2/19/22	0/1/1/1
10	NAG	4	1	10,1	-	6/6/23/26	0/1/1/1
10	NAG	4	2	10	-	5/6/23/26	0/1/1/1
10	BMA	4	3	10	-	2/2/19/22	0/1/1/1
10	MAN	4	4	10	-	0/2/19/22	0/1/1/1
10	MAN	4	5	10	-	0/2/19/22	0/1/1/1
10	NAG	5	1	10,1	-	1/6/23/26	0/1/1/1
10	NAG	5	2	10	-	0/6/23/26	0/1/1/1
10	BMA	5	3	10	-	2/2/19/22	0/1/1/1
10	MAN	5	4	10	-	0/2/19/22	0/1/1/1
10	MAN	5	5	10	-	0/2/19/22	0/1/1/1
14	NAG	6	1	14,1	-	2/6/23/26	0/1/1/1
14	NAG	6	2	14	-	4/6/23/26	0/1/1/1
14	BMA	6	3	14	-	0/2/19/22	0/1/1/1
14	MAN	6	4	14	-	1/2/19/22	0/1/1/1
14	MAN	6	5	14	-	1/2/19/22	0/1/1/1
16	NAG	7	1	1,16	-	0/6/23/26	0/1/1/1
16	NAG	7	2	16	-	3/6/23/26	0/1/1/1
16	BMA	7	3	16	-	0/2/19/22	0/1/1/1
13	NAG	8	1	13,1	-	1/6/23/26	0/1/1/1
13	NAG	8	2	13	-	2/6/23/26	0/1/1/1
10	NAG	9	1	10,1	-	2/6/23/26	0/1/1/1
10	NAG	9	2	10	-	0/6/23/26	0/1/1/1
10	BMA	9	3	10	-	2/2/19/22	0/1/1/1
10	MAN	9	4	10	-	0/2/19/22	0/1/1/1
10	MAN	9	5	10	-	0/2/19/22	0/1/1/1
9	NAG	E	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	E	2	9	-	0/6/23/26	0/1/1/1
10	NAG	F	1	10,1	-	0/6/23/26	0/1/1/1
10	NAG	F	2	10	-	0/6/23/26	0/1/1/1
10	BMA	F	3	10	-	0/2/19/22	0/1/1/1
10	MAN	F	4	10	-	0/2/19/22	0/1/1/1
10	MAN	F	5	10	-	0/2/19/22	0/1/1/1
11	NAG	U	1	11,1	-	0/6/23/26	0/1/1/1
11	NAG	U	2	11	-	4/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	BMA	U	3	11	-	1/2/19/22	0/1/1/1
11	MAN	U	4	11	-	0/2/19/22	0/1/1/1
11	MAN	U	5	11	-	1/2/19/22	0/1/1/1
9	NAG	V	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	V	2	9	-	0/6/23/26	0/1/1/1
12	NAG	W	1	12,1	-	0/6/23/26	0/1/1/1
12	NAG	W	2	12	-	2/6/23/26	0/1/1/1
12	BMA	W	3	12	-	0/2/19/22	0/1/1/1
9	NAG	X	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	X	2	9	-	1/6/23/26	0/1/1/1
9	NAG	Y	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	Y	2	9	-	3/6/23/26	0/1/1/1
10	NAG	Z	1	10,1	-	0/6/23/26	0/1/1/1
10	NAG	Z	2	10	-	0/6/23/26	0/1/1/1
10	BMA	Z	3	10	-	0/2/19/22	0/1/1/1
10	MAN	Z	4	10	-	0/2/19/22	0/1/1/1
10	MAN	Z	5	10	-	0/2/19/22	0/1/1/1
9	NAG	a	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	a	2	9	-	0/6/23/26	0/1/1/1
10	NAG	b	1	10,1	-	0/6/23/26	0/1/1/1
10	NAG	b	2	10	-	1/6/23/26	0/1/1/1
10	BMA	b	3	10	-	0/2/19/22	0/1/1/1
10	MAN	b	4	10	-	0/2/19/22	0/1/1/1
10	MAN	b	5	10	-	0/2/19/22	0/1/1/1
13	NAG	c	1	13,1	-	0/6/23/26	0/1/1/1
13	NAG	c	2	13	-	1/6/23/26	0/1/1/1
9	NAG	d	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	d	2	9	-	0/6/23/26	0/1/1/1
12	NAG	e	1	12,1	-	2/6/23/26	0/1/1/1
12	NAG	e	2	12	-	2/6/23/26	0/1/1/1
12	BMA	e	3	12	-	0/2/19/22	0/1/1/1
12	NAG	f	1	12,1	-	0/6/23/26	0/1/1/1
12	NAG	f	2	12	-	0/6/23/26	0/1/1/1
12	BMA	f	3	12	-	0/2/19/22	0/1/1/1
10	NAG	g	1	10,1	-	0/6/23/26	0/1/1/1
10	NAG	g	2	10	-	0/6/23/26	0/1/1/1
10	BMA	g	3	10	-	0/2/19/22	0/1/1/1
10	MAN	g	4	10	-	0/2/19/22	0/1/1/1
10	MAN	g	5	10	-	1/2/19/22	0/1/1/1
12	NAG	h	1	12,1	-	3/6/23/26	0/1/1/1
12	NAG	h	2	12	-	4/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	BMA	h	3	12	-	0/2/19/22	0/1/1/1
12	NAG	i	1	12,1	-	0/6/23/26	0/1/1/1
12	NAG	i	2	12	-	0/6/23/26	0/1/1/1
12	BMA	i	3	12	-	0/2/19/22	0/1/1/1
10	NAG	j	1	10,1	-	3/6/23/26	0/1/1/1
10	NAG	j	2	10	-	4/6/23/26	0/1/1/1
10	BMA	j	3	10	-	2/2/19/22	0/1/1/1
10	MAN	j	4	10	-	0/2/19/22	0/1/1/1
10	MAN	j	5	10	-	1/2/19/22	0/1/1/1
10	NAG	k	1	10,1	-	0/6/23/26	0/1/1/1
10	NAG	k	2	10	-	0/6/23/26	0/1/1/1
10	BMA	k	3	10	-	0/2/19/22	0/1/1/1
10	MAN	k	4	10	-	0/2/19/22	0/1/1/1
10	MAN	k	5	10	-	0/2/19/22	0/1/1/1
10	NAG	l	1	10,1	-	2/6/23/26	0/1/1/1
10	NAG	l	2	10	-	0/6/23/26	0/1/1/1
10	BMA	l	3	10	-	0/2/19/22	0/1/1/1
10	MAN	l	4	10	-	1/2/19/22	0/1/1/1
10	MAN	l	5	10	-	1/2/19/22	0/1/1/1
12	NAG	m	1	12,1	-	2/6/23/26	0/1/1/1
12	NAG	m	2	12	-	2/6/23/26	0/1/1/1
12	BMA	m	3	12	-	0/2/19/22	0/1/1/1
9	NAG	n	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	n	2	9	-	1/6/23/26	0/1/1/1
13	NAG	o	1	13,1	-	0/6/23/26	0/1/1/1
13	NAG	o	2	13	-	2/6/23/26	0/1/1/1
12	NAG	p	1	12,1	-	2/6/23/26	0/1/1/1
12	NAG	p	2	12	-	0/6/23/26	0/1/1/1
12	BMA	p	3	12	-	0/2/19/22	0/1/1/1
9	NAG	q	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	q	2	9	-	0/6/23/26	0/1/1/1
12	NAG	r	1	12,1	-	0/6/23/26	0/1/1/1
12	NAG	r	2	12	-	3/6/23/26	0/1/1/1
12	BMA	r	3	12	-	1/2/19/22	0/1/1/1
9	NAG	s	1	1,9	-	1/6/23/26	0/1/1/1
9	NAG	s	2	9	-	0/6/23/26	0/1/1/1
9	NAG	t	1	1,9	-	1/6/23/26	0/1/1/1
9	NAG	t	2	9	-	0/6/23/26	0/1/1/1
10	NAG	u	1	10,1	-	1/6/23/26	0/1/1/1
10	NAG	u	2	10	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	BMA	u	3	10	-	2/2/19/22	0/1/1/1
10	MAN	u	4	10	-	0/2/19/22	0/1/1/1
10	MAN	u	5	10	-	0/2/19/22	0/1/1/1
9	NAG	v	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	v	2	9	-	0/6/23/26	0/1/1/1
14	NAG	w	1	14,1	-	4/6/23/26	0/1/1/1
14	NAG	w	2	14	-	3/6/23/26	0/1/1/1
14	BMA	w	3	14	-	0/2/19/22	0/1/1/1
14	MAN	w	4	14	-	1/2/19/22	0/1/1/1
14	MAN	w	5	14	-	1/2/19/22	0/1/1/1
9	NAG	x	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	x	2	9	-	3/6/23/26	0/1/1/1
9	NAG	y	1	1,9	-	3/6/23/26	0/1/1/1
9	NAG	y	2	9	-	1/6/23/26	0/1/1/1
15	NAG	z	1	15,1	-	2/6/23/26	0/1/1/1
15	NAG	z	2	15	-	1/6/23/26	0/1/1/1
15	BMA	z	3	15	-	1/2/19/22	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	m	1	NAG	O5-C5	2.57	1.48	1.43
9	q	1	NAG	O5-C5	2.45	1.48	1.43
9	t	2	NAG	C1-C2	2.36	1.55	1.52
12	2	2	NAG	O5-C5	2.31	1.48	1.43
9	q	2	NAG	O5-C5	2.23	1.48	1.43
12	2	3	BMA	O5-C5	2.18	1.47	1.43
12	2	3	BMA	O5-C1	2.06	1.47	1.43
12	2	2	NAG	C1-C2	2.05	1.55	1.52

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	0	1	NAG	C1-O5-C5	5.01	118.98	112.19
9	t	2	NAG	C1-O5-C5	4.88	118.80	112.19
11	U	2	NAG	C4-C3-C2	4.72	117.93	111.02
9	t	1	NAG	C4-C3-C2	4.47	117.57	111.02
15	z	2	NAG	O5-C1-C2	-4.16	104.72	111.29
13	8	1	NAG	O5-C1-C2	4.00	117.60	111.29
10	Z	1	NAG	O5-C1-C2	-3.76	105.36	111.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	w	2	NAG	O5-C1-C2	-3.67	105.49	111.29
10	Z	2	NAG	C1-O5-C5	3.51	116.95	112.19
16	0	2	NAG	O5-C1-C2	3.43	116.70	111.29
9	V	1	NAG	C1-O5-C5	3.38	116.77	112.19
14	w	1	NAG	C4-C3-C2	3.33	115.89	111.02
9	E	1	NAG	O5-C1-C2	-3.32	106.04	111.29
9	n	1	NAG	C1-C2-N2	3.32	116.16	110.49
10	j	1	NAG	O5-C1-C2	-3.16	106.30	111.29
11	U	2	NAG	C3-C4-C5	3.15	115.86	110.24
10	l	3	BMA	C1-C2-C3	3.08	113.46	109.67
13	c	2	NAG	C1-O5-C5	3.08	116.37	112.19
9	q	2	NAG	O5-C1-C2	-3.03	106.51	111.29
12	m	1	NAG	C1-O5-C5	2.94	116.18	112.19
12	2	1	NAG	C3-C4-C5	2.93	115.47	110.24
10	1	3	BMA	C1-C2-C3	2.91	113.24	109.67
10	j	4	MAN	C1-O5-C5	2.90	116.12	112.19
9	V	2	NAG	C1-O5-C5	2.89	116.11	112.19
11	U	2	NAG	O5-C1-C2	-2.88	106.74	111.29
9	q	1	NAG	C1-O5-C5	2.85	116.05	112.19
9	V	1	NAG	O5-C1-C2	2.82	115.75	111.29
10	4	1	NAG	C1-O5-C5	2.78	115.96	112.19
12	i	2	NAG	C1-O5-C5	2.75	115.92	112.19
10	k	1	NAG	C1-O5-C5	2.74	115.91	112.19
12	2	3	BMA	C1-O5-C5	2.70	115.85	112.19
9	t	1	NAG	C1-C2-N2	2.70	115.10	110.49
16	0	2	NAG	O3-C3-C2	-2.69	103.89	109.47
10	k	4	MAN	C1-C2-C3	2.62	112.89	109.67
11	U	3	BMA	O5-C1-C2	-2.61	106.75	110.77
10	4	3	BMA	C1-C2-C3	2.60	112.86	109.67
10	4	2	NAG	C1-O5-C5	2.59	115.71	112.19
12	i	3	BMA	C1-O5-C5	2.56	115.66	112.19
13	8	2	NAG	C1-C2-N2	2.52	114.79	110.49
12	2	1	NAG	C4-C3-C2	2.51	114.69	111.02
13	8	1	NAG	C1-O5-C5	2.46	115.52	112.19
10	4	3	BMA	C1-O5-C5	2.45	115.52	112.19
9	s	1	NAG	O5-C1-C2	2.44	115.14	111.29
12	e	3	BMA	C1-C2-C3	2.44	112.66	109.67
10	l	1	NAG	C1-O5-C5	2.43	115.49	112.19
12	2	1	NAG	C1-C2-N2	2.42	114.62	110.49
11	U	2	NAG	O3-C3-C2	-2.38	104.55	109.47
10	j	1	NAG	C3-C4-C5	2.36	114.45	110.24
14	w	1	NAG	C3-C4-C5	2.35	114.43	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	3	3	BMA	C1-O5-C5	2.32	115.34	112.19
12	2	1	NAG	C2-N2-C7	2.31	126.19	122.90
10	k	2	NAG	C1-O5-C5	2.31	115.32	112.19
12	2	2	NAG	C1-O5-C5	2.29	115.30	112.19
9	t	1	NAG	O5-C1-C2	-2.29	107.67	111.29
13	c	1	NAG	C4-C3-C2	2.29	114.37	111.02
10	F	3	BMA	C1-C2-C3	2.27	112.46	109.67
10	b	3	BMA	C1-C2-C3	2.25	112.44	109.67
10	k	2	NAG	O3-C3-C2	2.24	114.11	109.47
14	6	4	MAN	C1-O5-C5	2.24	115.23	112.19
10	5	1	NAG	C1-C2-N2	2.24	114.32	110.49
10	9	1	NAG	C1-C2-N2	2.23	114.30	110.49
14	w	2	NAG	C1-O5-C5	-2.22	109.19	112.19
12	r	1	NAG	O5-C1-C2	-2.20	107.82	111.29
12	2	1	NAG	O4-C4-C3	-2.19	105.28	110.35
12	p	2	NAG	C1-C2-N2	2.19	114.23	110.49
10	l	3	BMA	O3-C3-C2	-2.18	105.81	109.99
12	W	1	NAG	C1-O5-C5	2.18	115.15	112.19
10	k	4	MAN	C1-O5-C5	2.17	115.13	112.19
14	6	4	MAN	C1-C2-C3	2.16	112.31	109.67
10	g	3	BMA	C1-C2-C3	2.13	112.29	109.67
15	z	2	NAG	C1-C2-N2	2.12	114.12	110.49
12	m	2	NAG	O5-C1-C2	-2.12	107.94	111.29
10	Z	2	NAG	C4-C3-C2	-2.11	107.93	111.02
11	U	5	MAN	C1-O5-C5	2.10	115.04	112.19
12	W	2	NAG	O5-C1-C2	-2.10	107.98	111.29
15	z	1	NAG	O4-C4-C5	-2.09	104.10	109.30
10	j	1	NAG	C4-C3-C2	2.08	114.07	111.02
9	n	2	NAG	C1-C2-N2	2.08	114.04	110.49
14	w	2	NAG	C3-C4-C5	2.08	113.95	110.24
10	u	3	BMA	C1-C2-C3	2.05	112.19	109.67
10	g	2	NAG	C1-O5-C5	2.05	114.97	112.19
16	0	2	NAG	C2-N2-C7	-2.05	119.99	122.90
10	5	5	MAN	C1-C2-C3	2.04	112.17	109.67
12	f	3	BMA	C1-C2-C3	2.04	112.17	109.67
11	U	5	MAN	C1-C2-C3	2.03	112.17	109.67
9	y	1	NAG	C1-C2-N2	2.03	113.96	110.49
10	1	2	NAG	O5-C1-C2	-2.03	108.08	111.29
9	s	1	NAG	C1-O5-C5	2.02	114.92	112.19

There are no chirality outliers.

All (124) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	4	1	NAG	C1-C2-N2-C7
12	h	1	NAG	C3-C2-N2-C7
12	h	1	NAG	C8-C7-N2-C2
12	h	1	NAG	O7-C7-N2-C2
14	w	1	NAG	C1-C2-N2-C7
14	w	1	NAG	C8-C7-N2-C2
14	w	1	NAG	O7-C7-N2-C2
14	6	2	NAG	C8-C7-N2-C2
14	6	2	NAG	O7-C7-N2-C2
16	7	2	NAG	C8-C7-N2-C2
16	7	2	NAG	O7-C7-N2-C2
10	4	1	NAG	C8-C7-N2-C2
14	6	1	NAG	C8-C7-N2-C2
14	6	1	NAG	O7-C7-N2-C2
10	u	3	BMA	O5-C5-C6-O6
9	x	2	NAG	C8-C7-N2-C2
9	y	1	NAG	C8-C7-N2-C2
9	y	1	NAG	O7-C7-N2-C2
10	4	1	NAG	O7-C7-N2-C2
10	9	1	NAG	C8-C7-N2-C2
13	o	2	NAG	C8-C7-N2-C2
15	z	1	NAG	C8-C7-N2-C2
10	j	2	NAG	O5-C5-C6-O6
11	U	2	NAG	C8-C7-N2-C2
15	z	1	NAG	O7-C7-N2-C2
11	U	2	NAG	O5-C5-C6-O6
10	j	1	NAG	C1-C2-N2-C7
12	h	2	NAG	C1-C2-N2-C7
16	7	2	NAG	C1-C2-N2-C7
10	u	3	BMA	C4-C5-C6-O6
9	x	2	NAG	O7-C7-N2-C2
10	l	1	NAG	C8-C7-N2-C2
10	9	1	NAG	O7-C7-N2-C2
11	U	2	NAG	O7-C7-N2-C2
12	W	2	NAG	C8-C7-N2-C2
12	h	2	NAG	C8-C7-N2-C2
13	o	2	NAG	O7-C7-N2-C2
11	U	2	NAG	C4-C5-C6-O6
9	x	2	NAG	C1-C2-N2-C7
9	y	1	NAG	C1-C2-N2-C7
12	h	2	NAG	O7-C7-N2-C2
14	6	2	NAG	C1-C2-N2-C7
10	4	3	BMA	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	j	2	NAG	C4-C5-C6-O6
10	l	1	NAG	O7-C7-N2-C2
12	p	1	NAG	C8-C7-N2-C2
16	0	1	NAG	C8-C7-N2-C2
10	j	1	NAG	O5-C5-C6-O6
14	w	1	NAG	O5-C5-C6-O6
10	4	2	NAG	C4-C5-C6-O6
12	m	1	NAG	O5-C5-C6-O6
12	2	1	NAG	C1-C2-N2-C7
10	4	3	BMA	C4-C5-C6-O6
10	b	2	NAG	O5-C5-C6-O6
11	U	3	BMA	O5-C5-C6-O6
10	9	3	BMA	O5-C5-C6-O6
14	6	4	MAN	O5-C5-C6-O6
14	w	2	NAG	C1-C2-N2-C7
12	m	2	NAG	C8-C7-N2-C2
12	W	2	NAG	O7-C7-N2-C2
12	p	1	NAG	O7-C7-N2-C2
9	Y	2	NAG	C1-C2-N2-C7
14	w	4	MAN	O5-C5-C6-O6
12	r	3	BMA	O5-C5-C6-O6
9	Y	2	NAG	C8-C7-N2-C2
16	0	1	NAG	O7-C7-N2-C2
9	y	2	NAG	O5-C5-C6-O6
10	l	4	MAN	O5-C5-C6-O6
10	j	5	MAN	O5-C5-C6-O6
10	l	5	MAN	O5-C5-C6-O6
10	g	5	MAN	O5-C5-C6-O6
9	s	1	NAG	C8-C7-N2-C2
14	6	5	MAN	O5-C5-C6-O6
11	U	5	MAN	O5-C5-C6-O6
14	w	5	MAN	O5-C5-C6-O6
9	X	2	NAG	O5-C5-C6-O6
10	j	2	NAG	C1-C2-N2-C7
12	r	2	NAG	O5-C5-C6-O6
14	w	2	NAG	O5-C5-C6-O6
10	j	1	NAG	C3-C2-N2-C7
14	6	2	NAG	C3-C2-N2-C7
10	1	3	BMA	C4-C5-C6-O6
12	2	2	NAG	C1-C2-N2-C7
9	v	1	NAG	C8-C7-N2-C2
12	e	1	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	1	3	BMA	O5-C5-C6-O6
10	4	2	NAG	O5-C5-C6-O6
10	5	3	BMA	C4-C5-C6-O6
9	Y	2	NAG	O7-C7-N2-C2
12	m	2	NAG	O7-C7-N2-C2
12	r	2	NAG	C8-C7-N2-C2
12	e	2	NAG	C8-C7-N2-C2
15	z	3	BMA	O5-C5-C6-O6
10	u	2	NAG	C8-C7-N2-C2
9	v	1	NAG	O7-C7-N2-C2
10	5	3	BMA	O5-C5-C6-O6
12	e	1	NAG	O5-C5-C6-O6
10	j	3	BMA	C4-C5-C6-O6
9	t	1	NAG	C3-C2-N2-C7
10	4	1	NAG	C3-C2-N2-C7
10	4	2	NAG	C3-C2-N2-C7
12	h	2	NAG	C3-C2-N2-C7
10	u	2	NAG	O7-C7-N2-C2
12	e	2	NAG	O7-C7-N2-C2
9	n	2	NAG	C1-C2-N2-C7
9	X	1	NAG	C8-C7-N2-C2
12	r	2	NAG	O7-C7-N2-C2
10	u	1	NAG	C8-C7-N2-C2
10	9	3	BMA	C4-C5-C6-O6
10	j	3	BMA	O5-C5-C6-O6
10	4	2	NAG	O7-C7-N2-C2
10	4	2	NAG	C8-C7-N2-C2
12	m	1	NAG	C4-C5-C6-O6
10	4	1	NAG	O5-C5-C6-O6
13	8	2	NAG	C1-C2-N2-C7
9	X	1	NAG	O7-C7-N2-C2
10	4	1	NAG	C4-C5-C6-O6
10	j	2	NAG	C3-C2-N2-C7
10	5	1	NAG	C3-C2-N2-C7
13	8	1	NAG	C3-C2-N2-C7
13	8	2	NAG	C3-C2-N2-C7
14	w	2	NAG	C3-C2-N2-C7
15	z	2	NAG	C3-C2-N2-C7
13	c	2	NAG	C4-C5-C6-O6

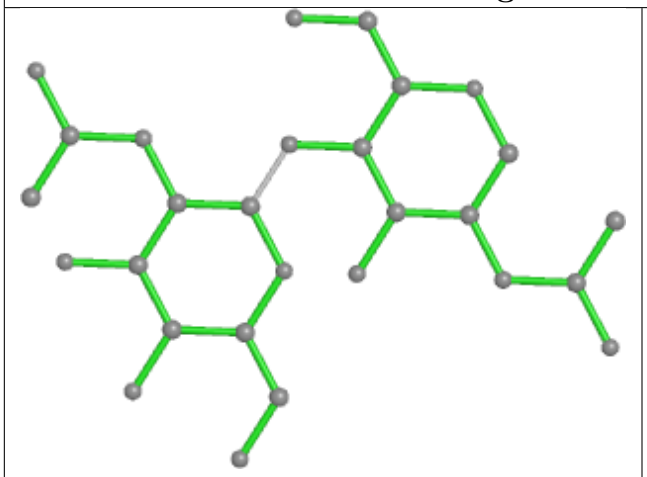
There are no ring outliers.

8 monomers are involved in 6 short contacts:

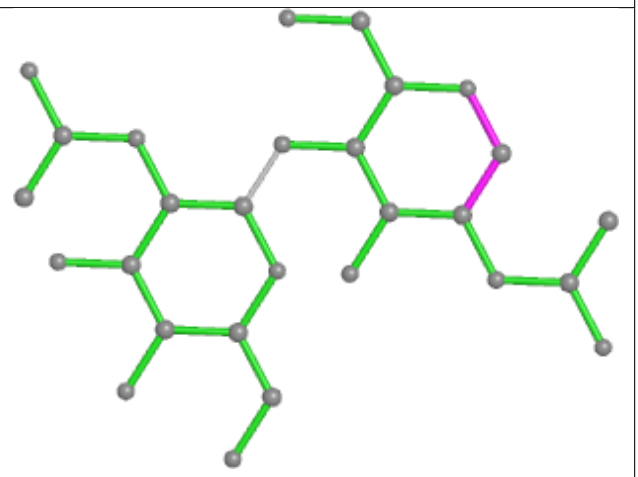
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	U	1	NAG	2	0
11	U	2	NAG	1	0
14	6	2	NAG	1	0
9	X	1	NAG	1	0
14	6	1	NAG	1	0
12	W	1	NAG	1	0
10	4	1	NAG	1	0
10	4	2	NAG	1	0

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

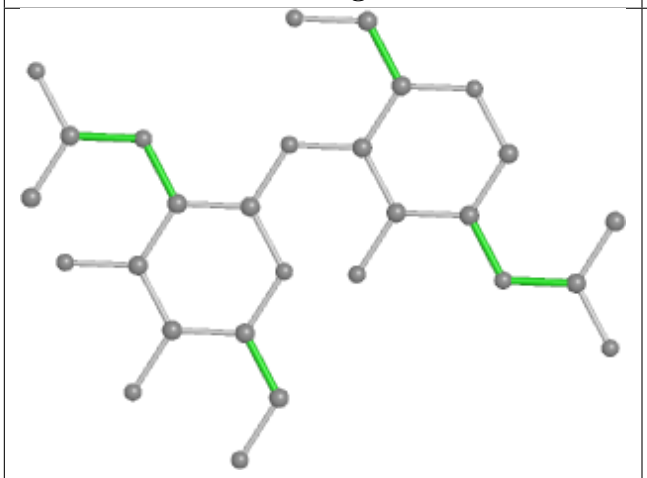
Oligosaccharide Chain E



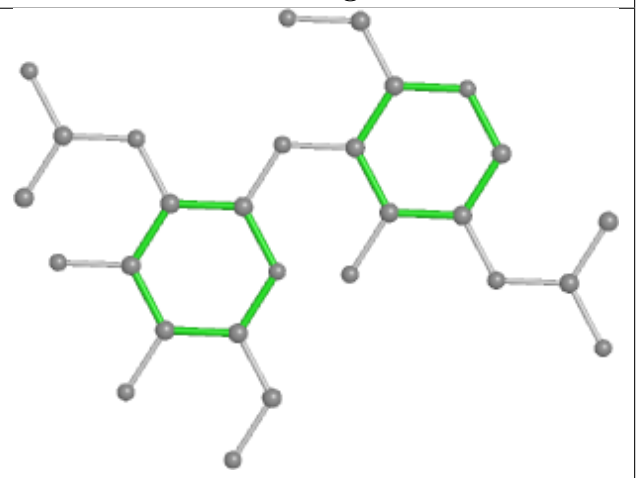
Bond lengths



Bond angles

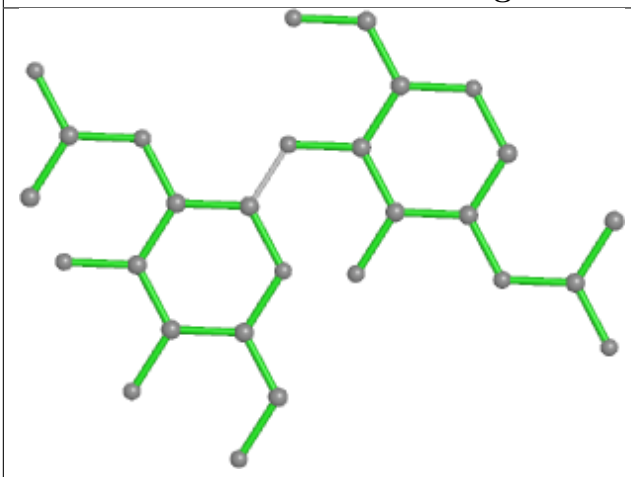


Torsions

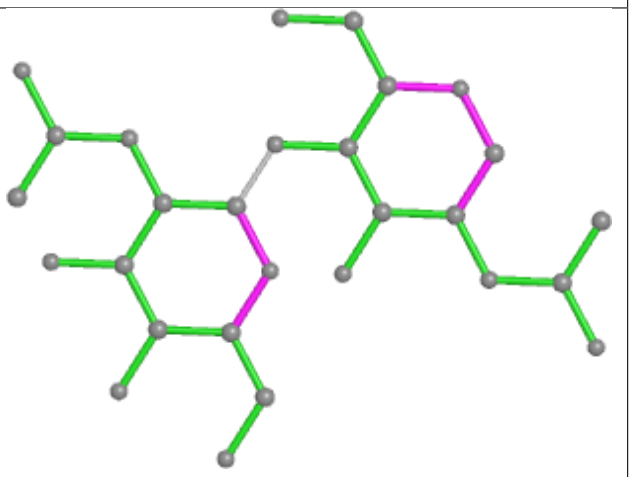


Rings

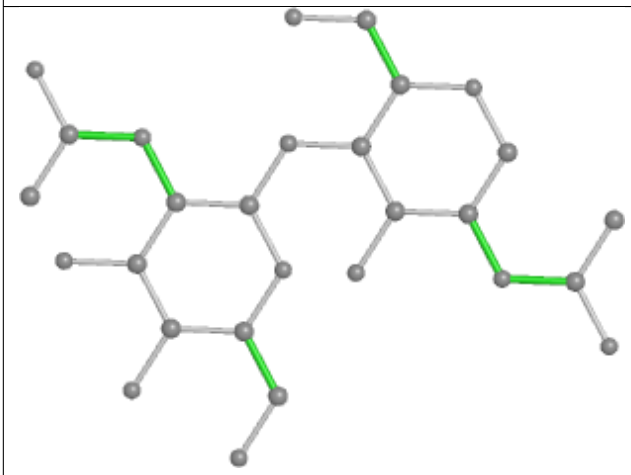
Oligosaccharide Chain V



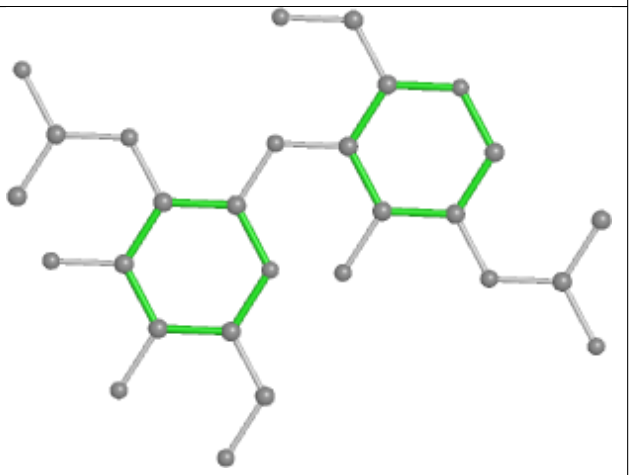
Bond lengths



Bond angles

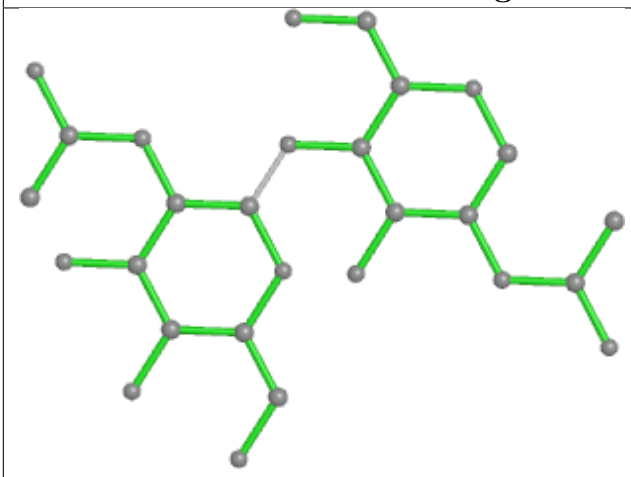


Torsions

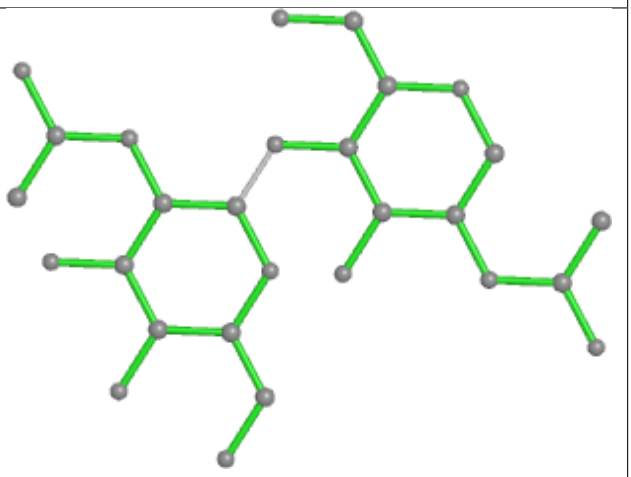


Rings

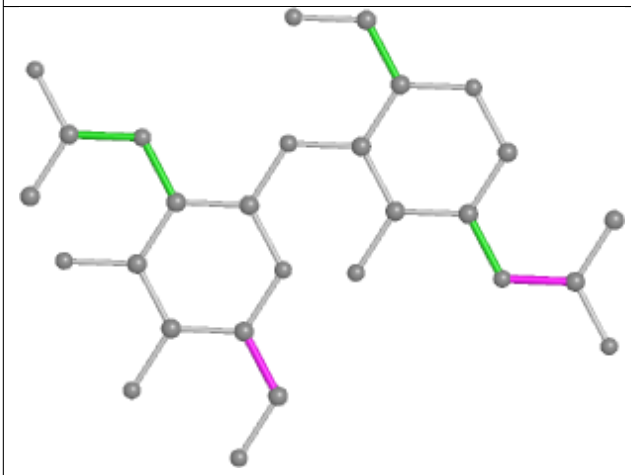
Oligosaccharide Chain X



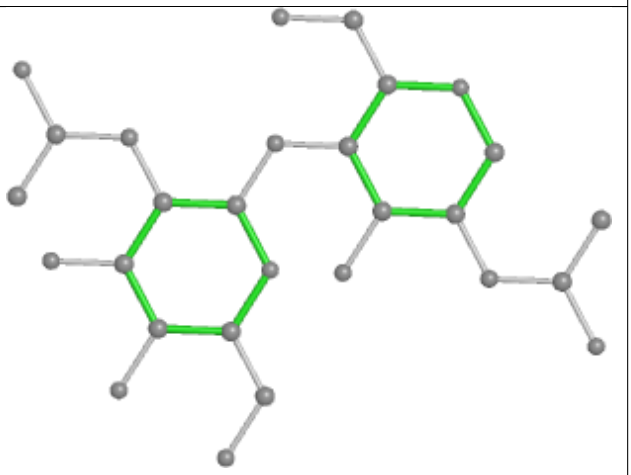
Bond lengths



Bond angles

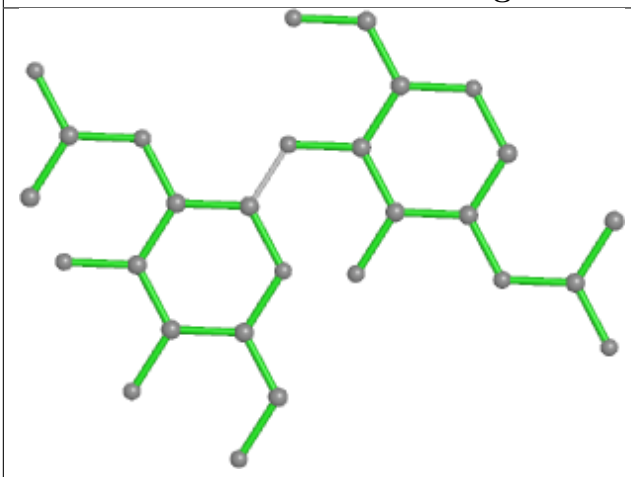


Torsions

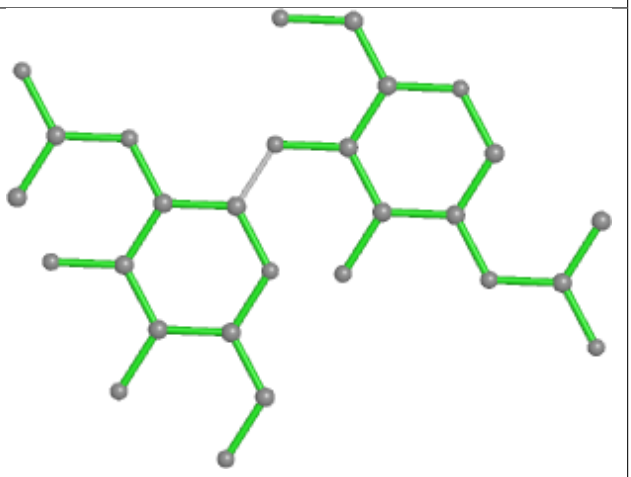


Rings

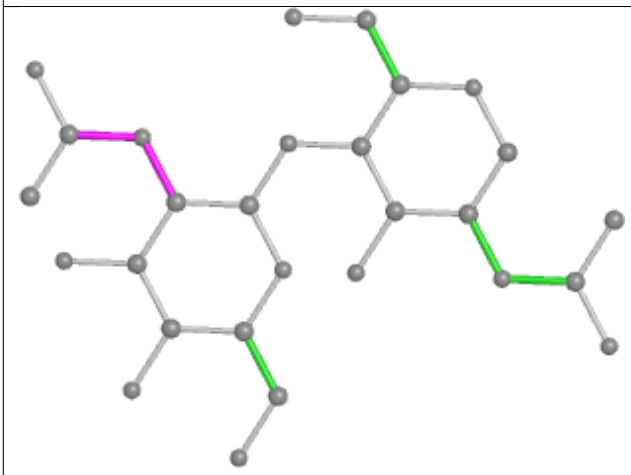
Oligosaccharide Chain Y



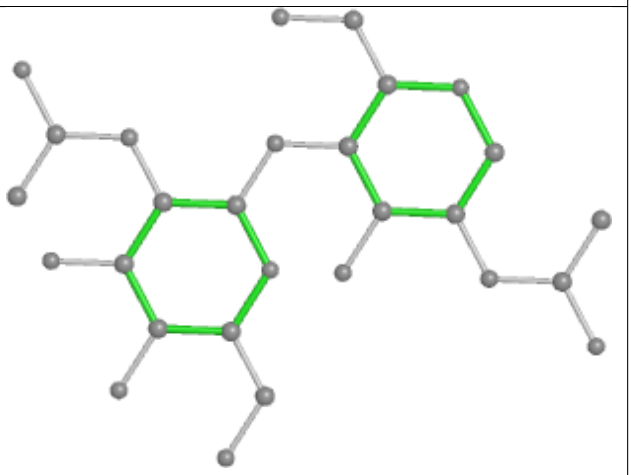
Bond lengths



Bond angles

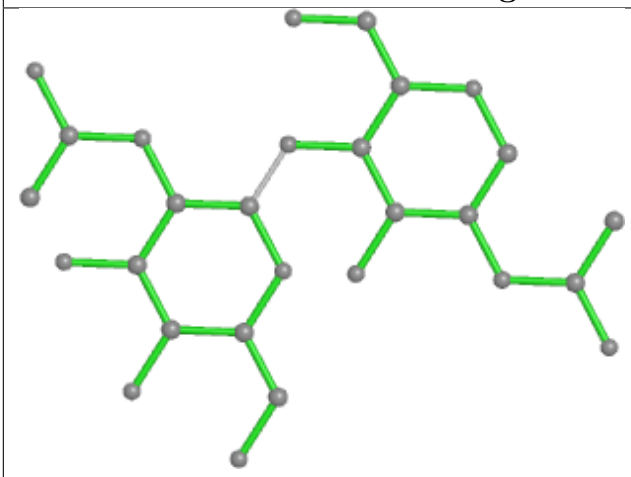


Torsions

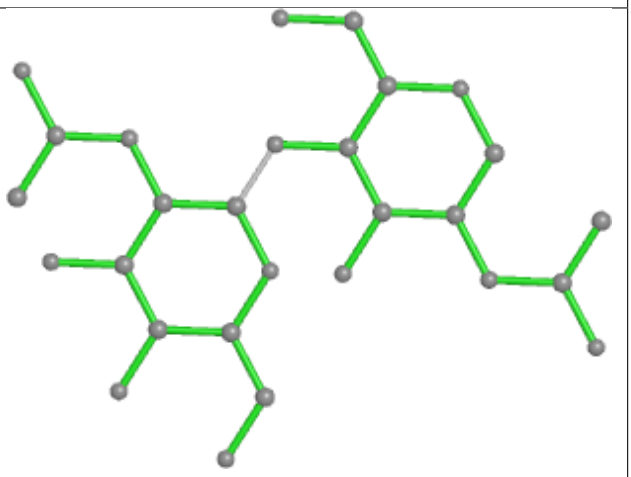


Rings

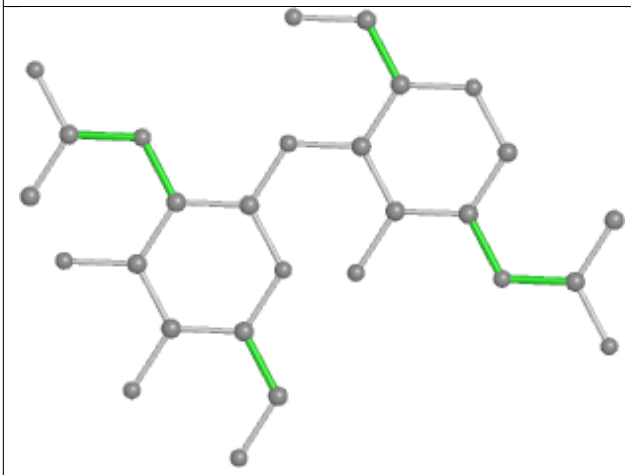
Oligosaccharide Chain a



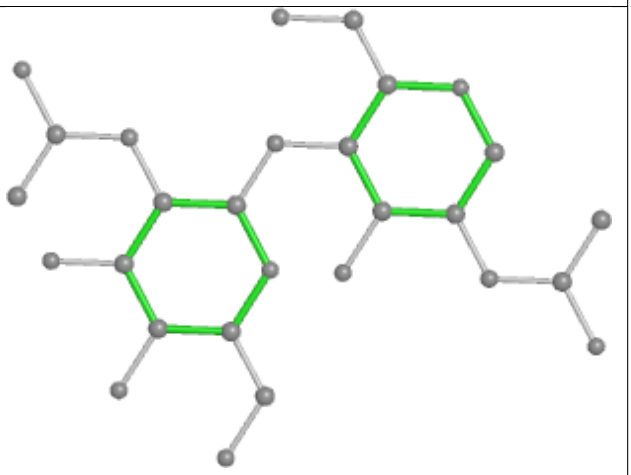
Bond lengths



Bond angles

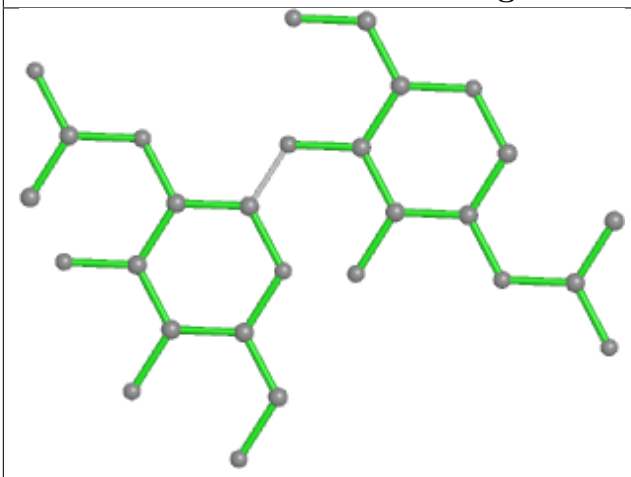


Torsions

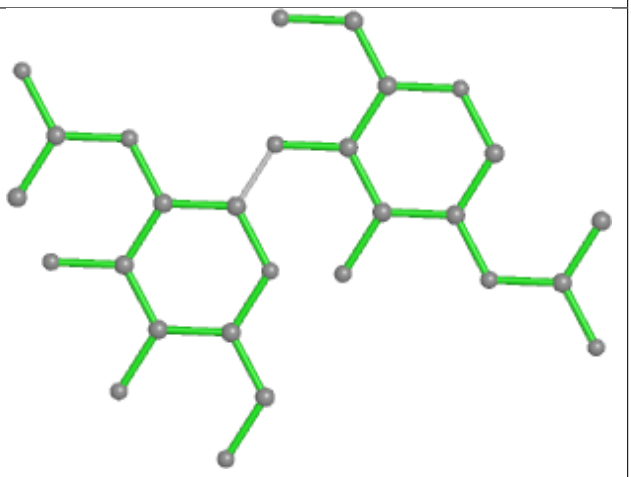


Rings

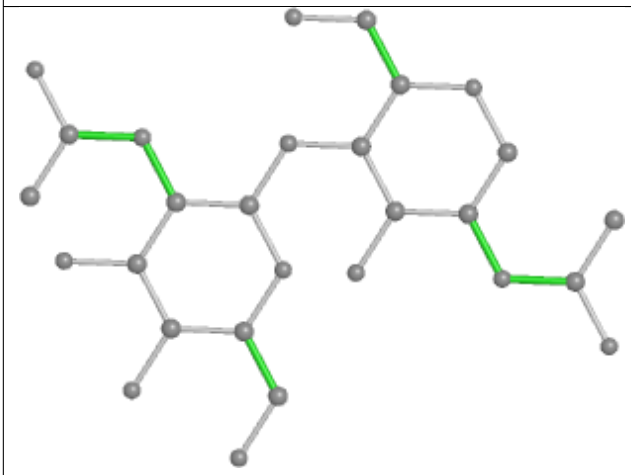
Oligosaccharide Chain d



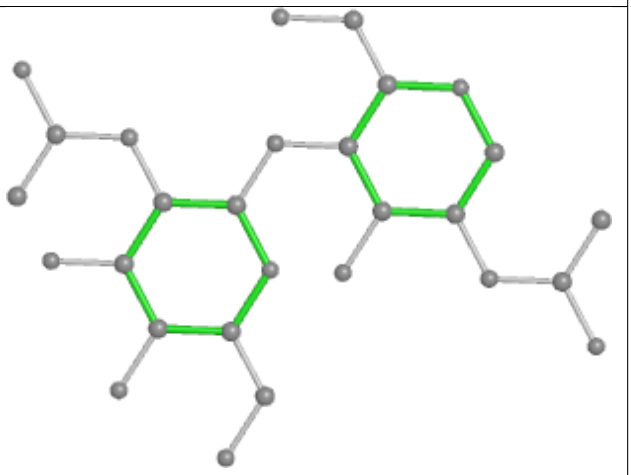
Bond lengths



Bond angles

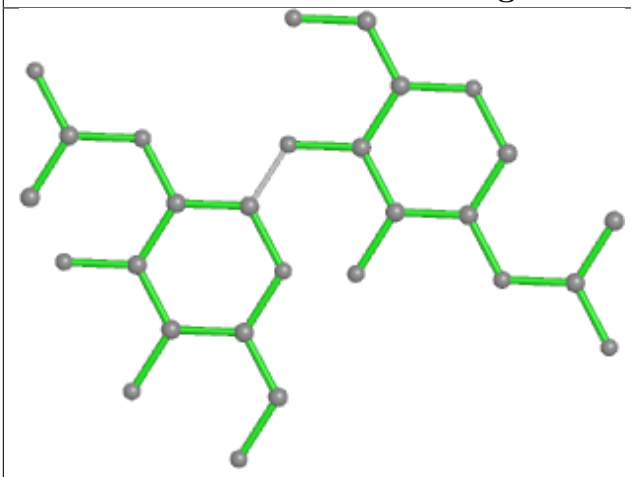


Torsions

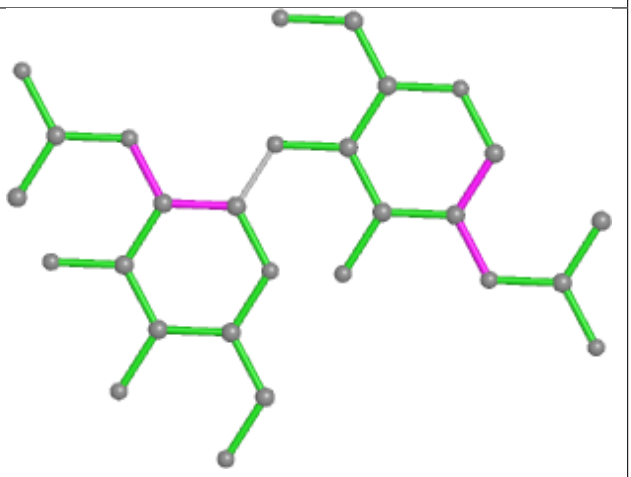


Rings

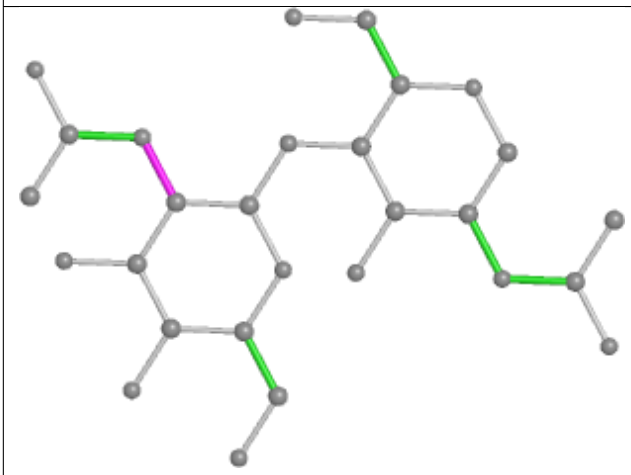
Oligosaccharide Chain n



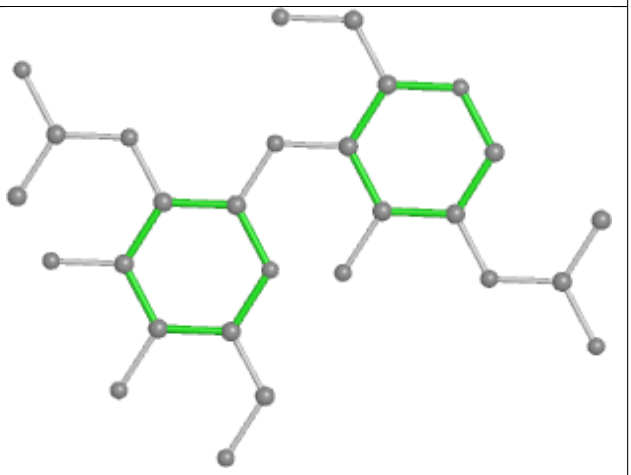
Bond lengths



Bond angles

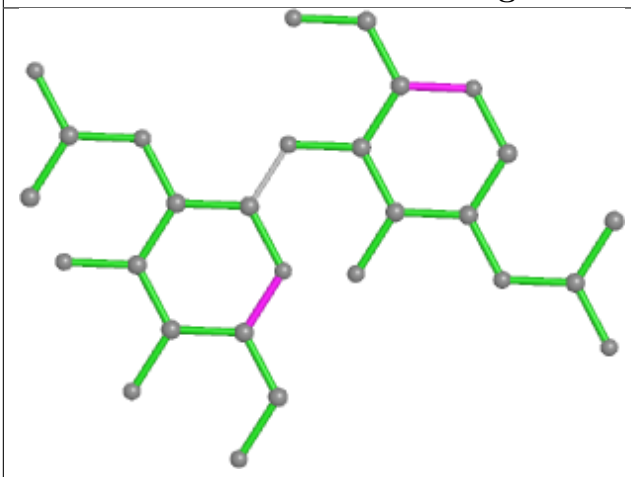


Torsions

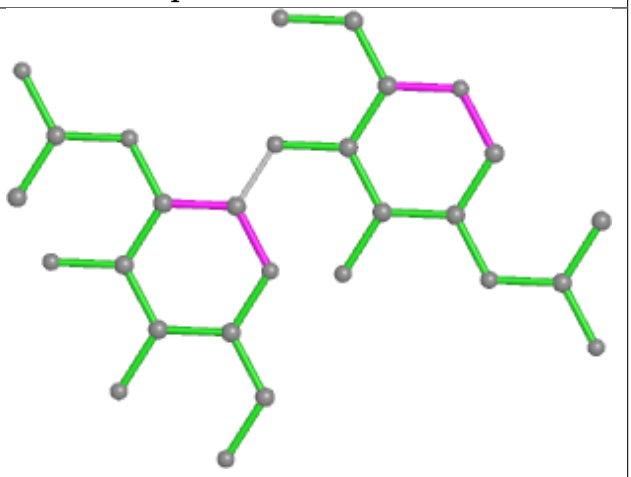


Rings

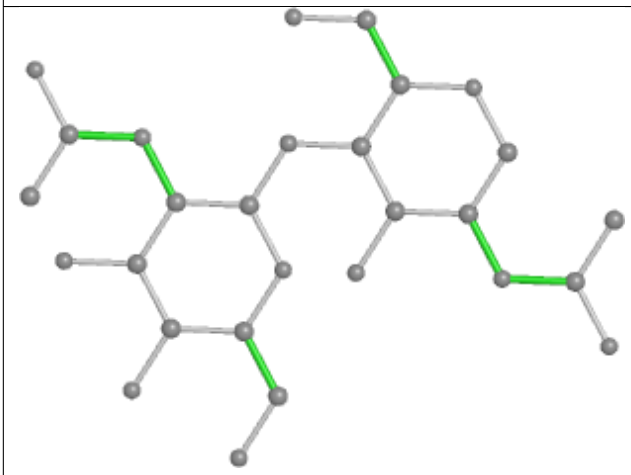
Oligosaccharide Chain q



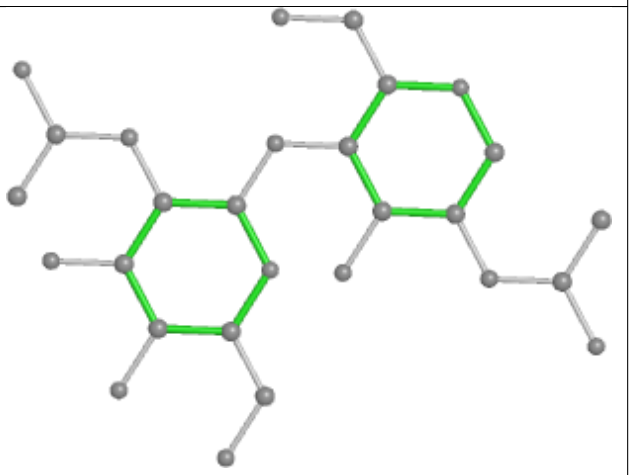
Bond lengths



Bond angles

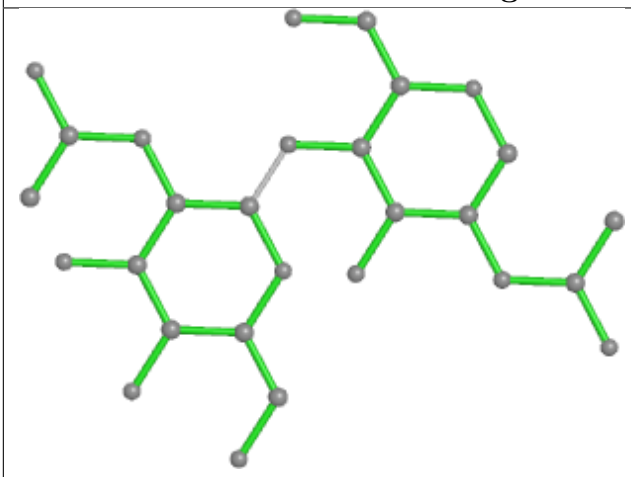


Torsions

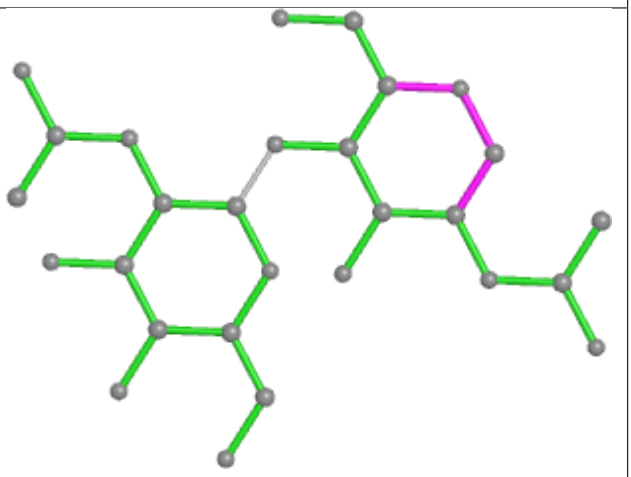


Rings

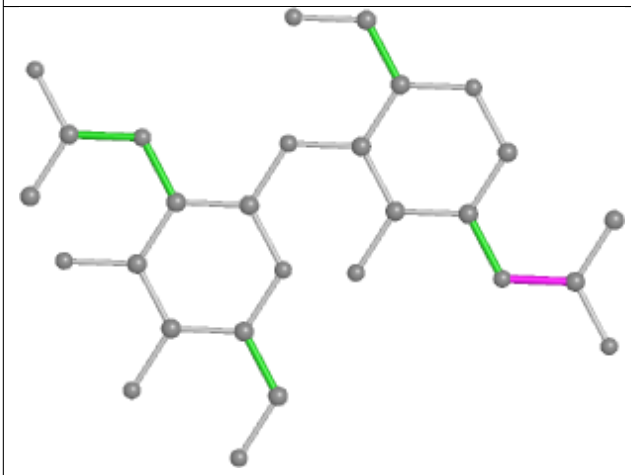
Oligosaccharide Chain s



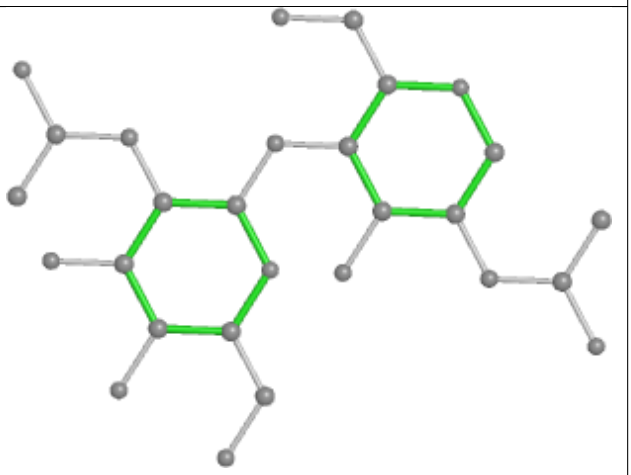
Bond lengths



Bond angles

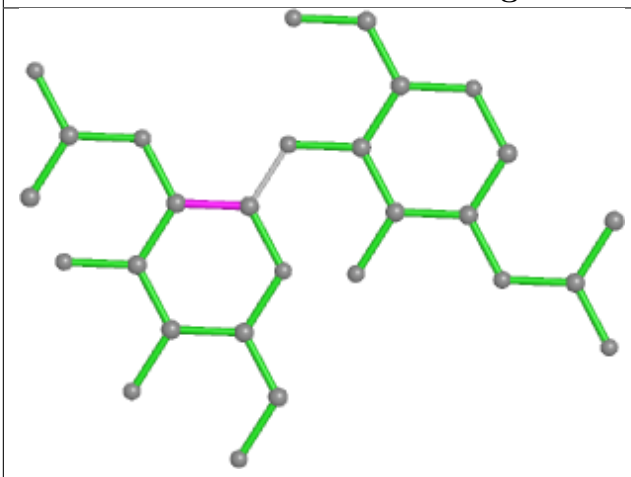


Torsions

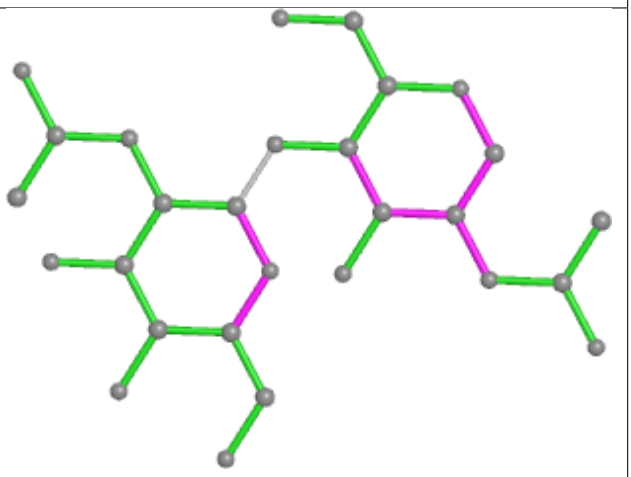


Rings

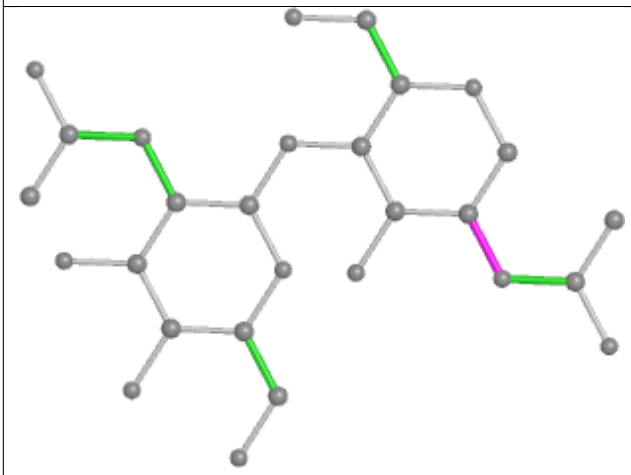
Oligosaccharide Chain t



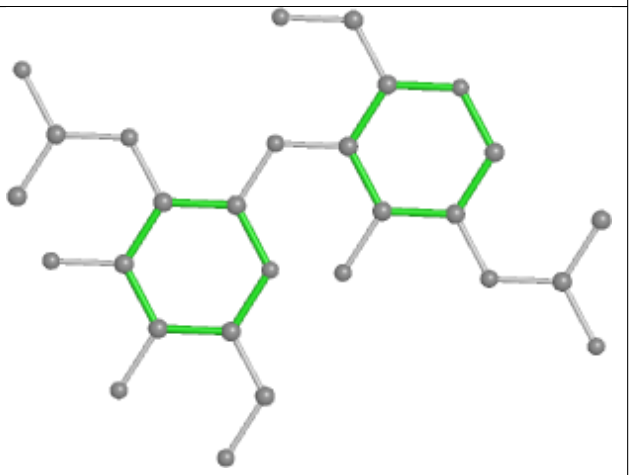
Bond lengths



Bond angles

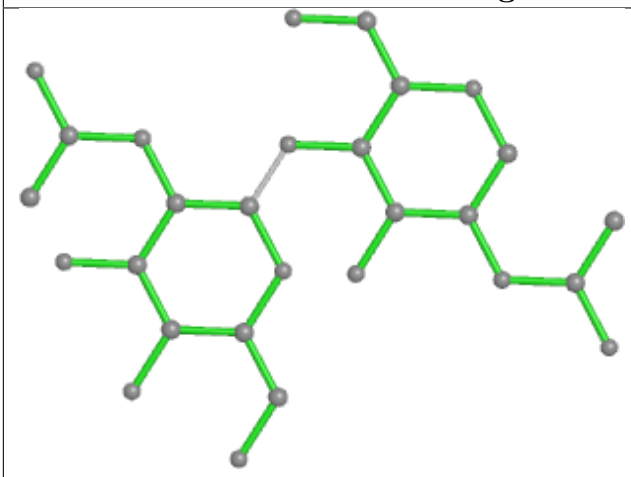


Torsions

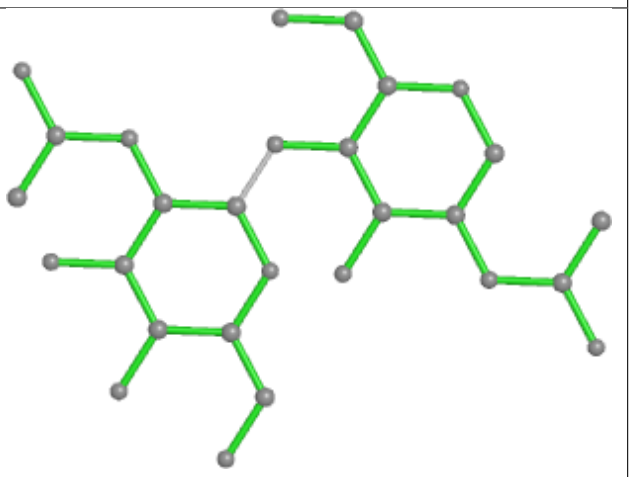


Rings

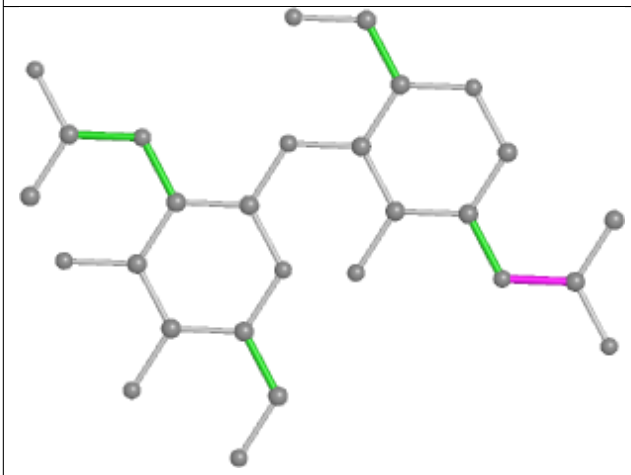
Oligosaccharide Chain v



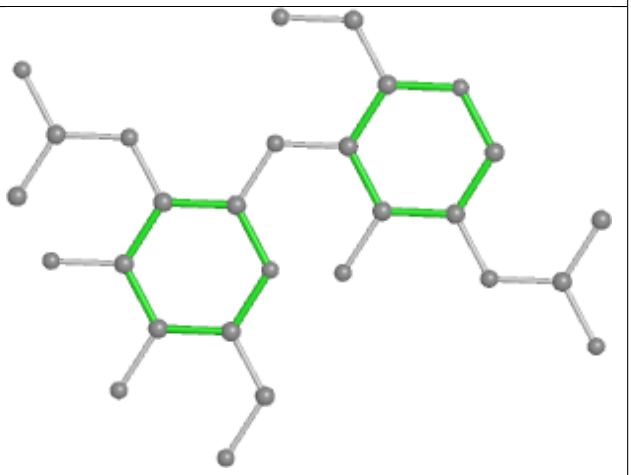
Bond lengths



Bond angles

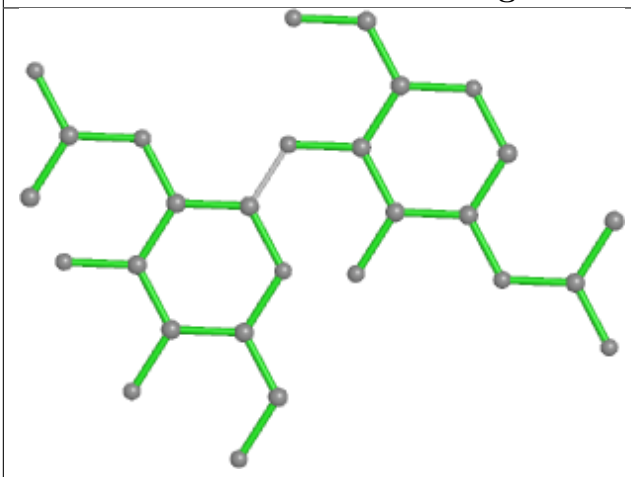


Torsions

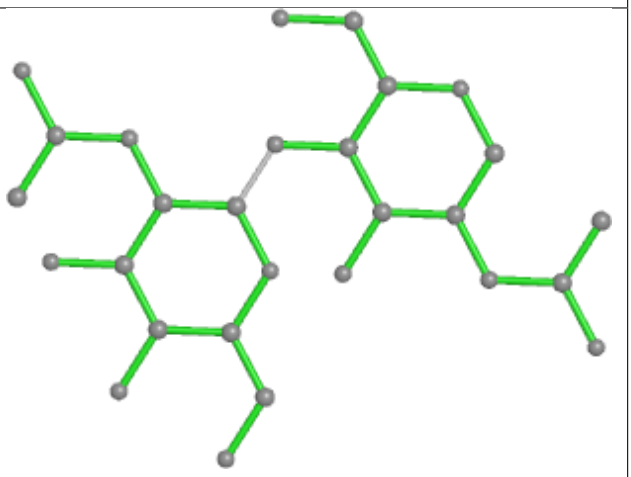


Rings

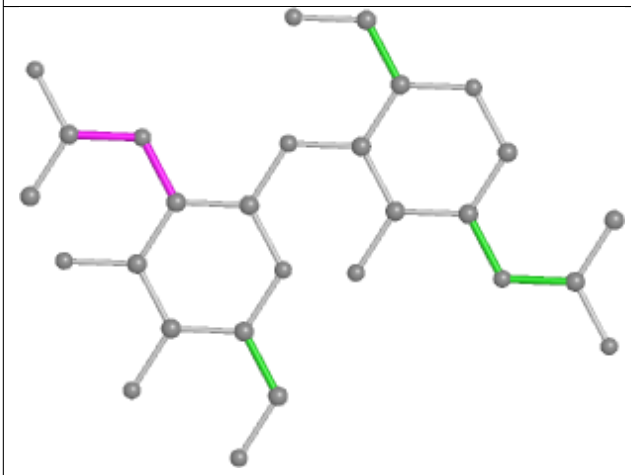
Oligosaccharide Chain x



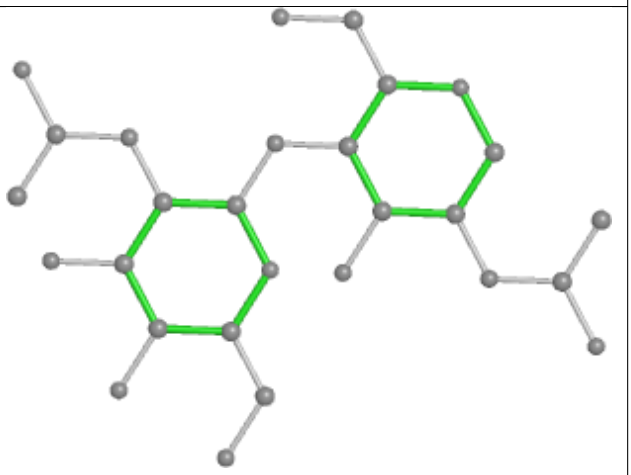
Bond lengths



Bond angles

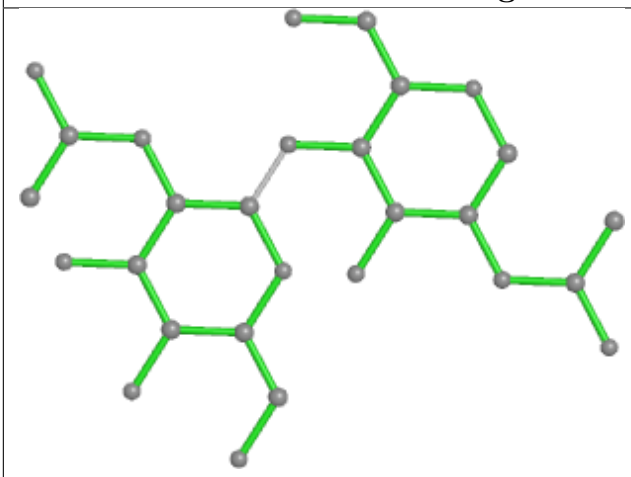


Torsions

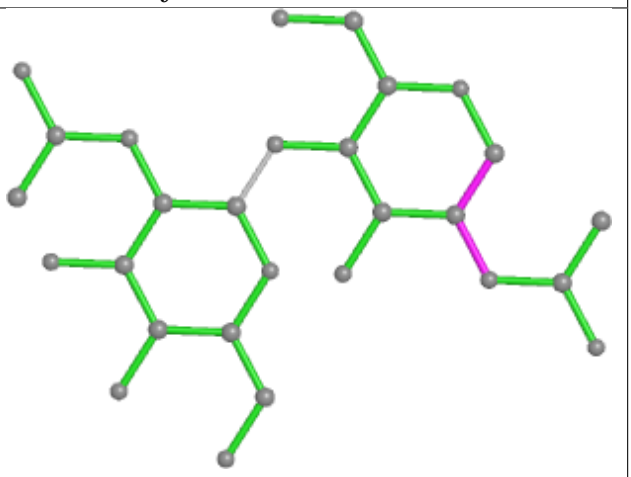


Rings

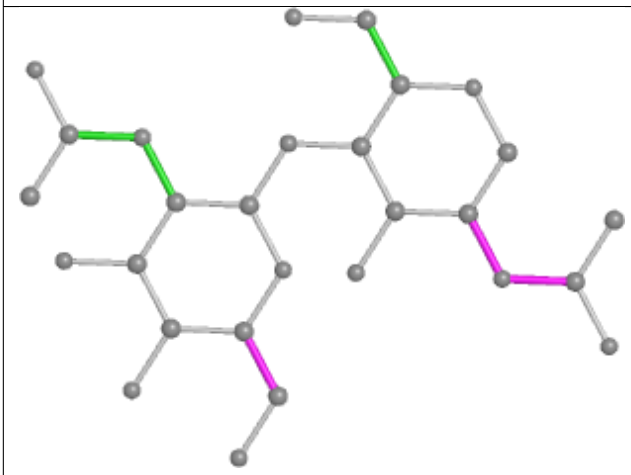
Oligosaccharide Chain y



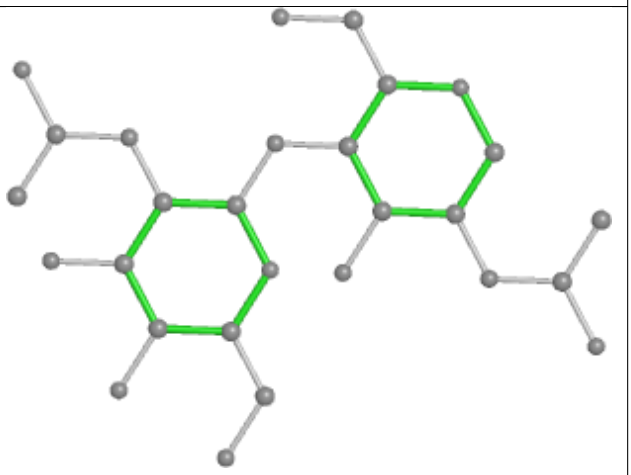
Bond lengths



Bond angles

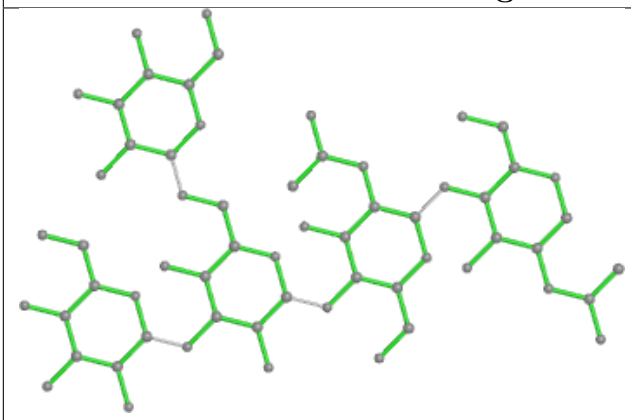


Torsions

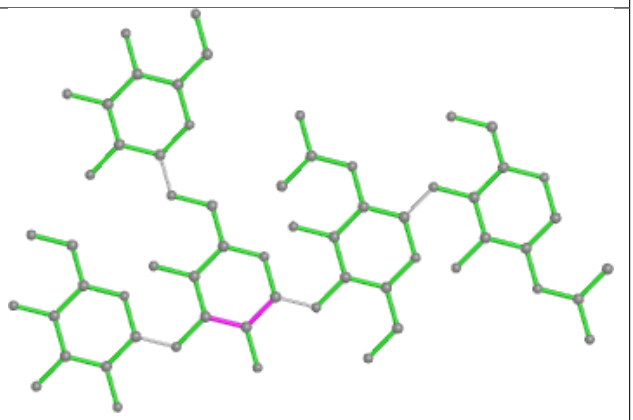


Rings

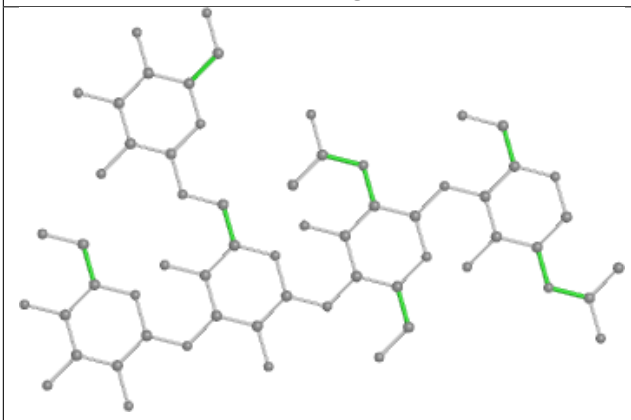
Oligosaccharide Chain F



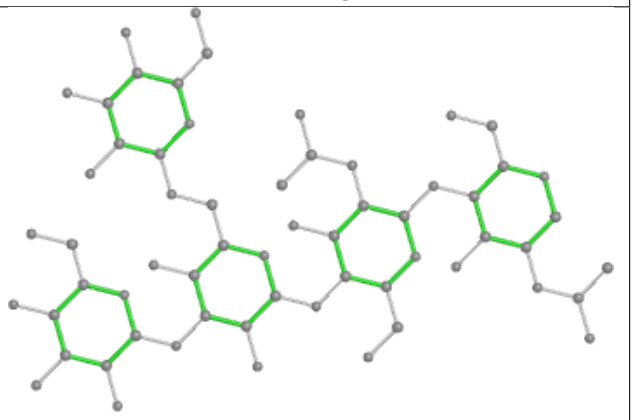
Bond lengths



Bond angles

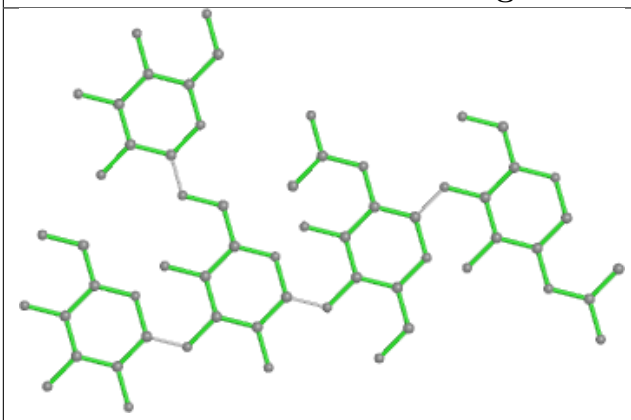


Torsions

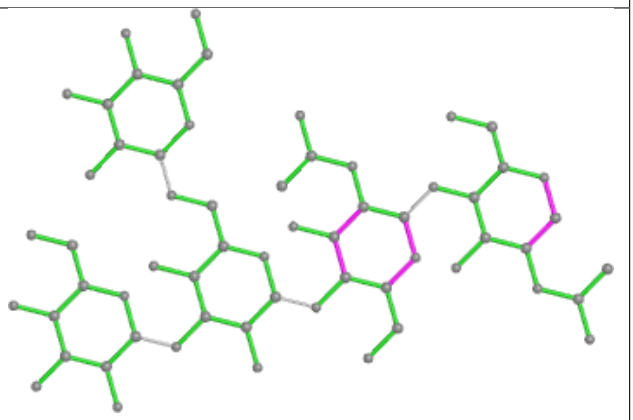


Rings

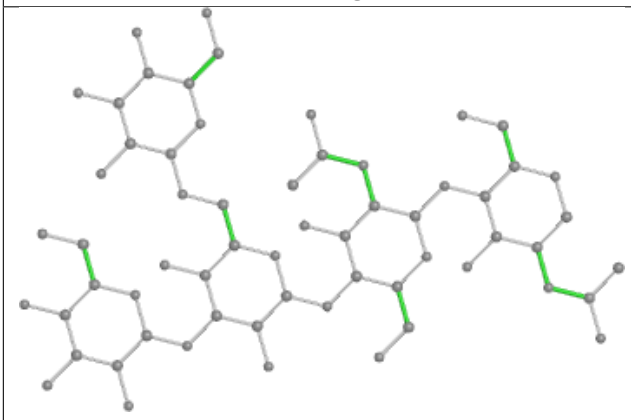
Oligosaccharide Chain Z



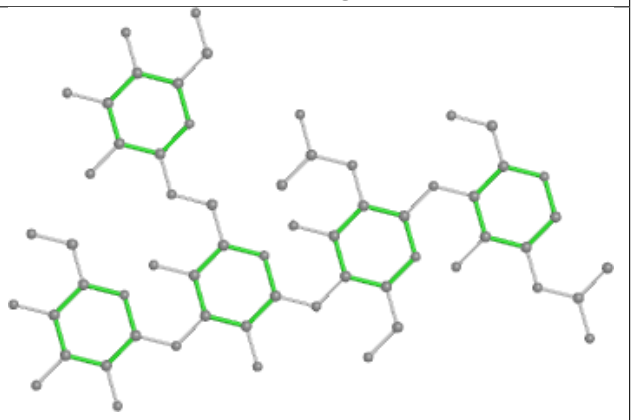
Bond lengths



Bond angles

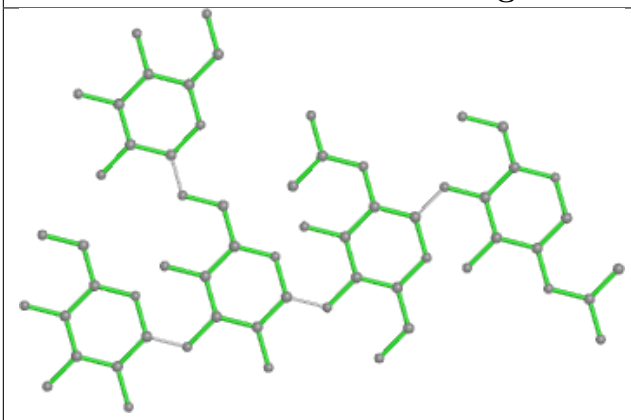


Torsions

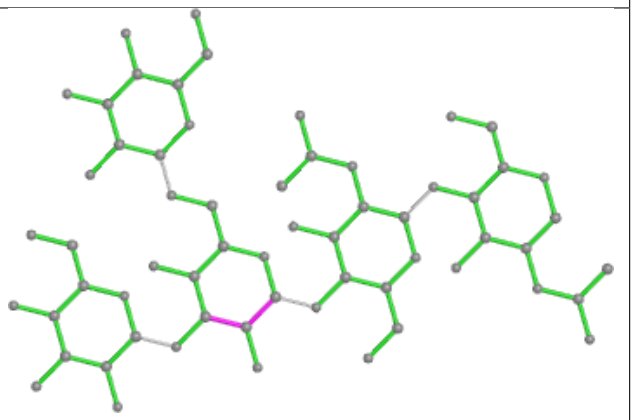


Rings

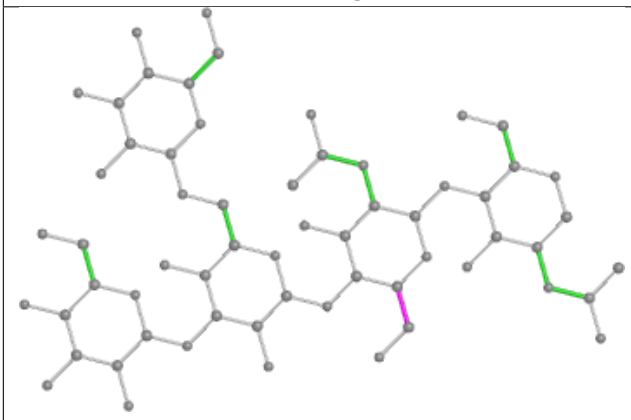
Oligosaccharide Chain b



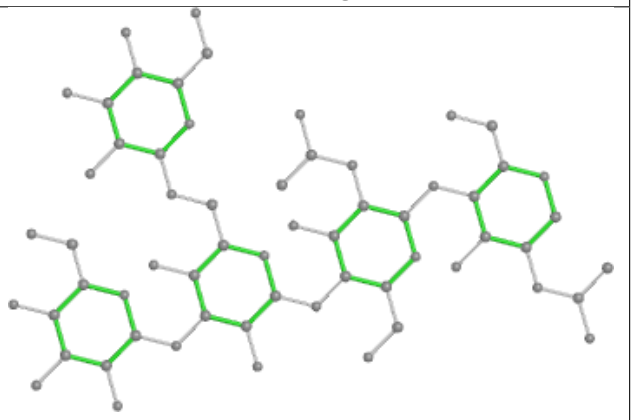
Bond lengths



Bond angles

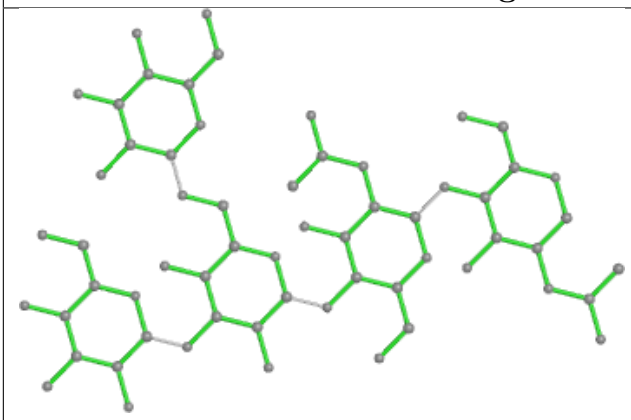


Torsions

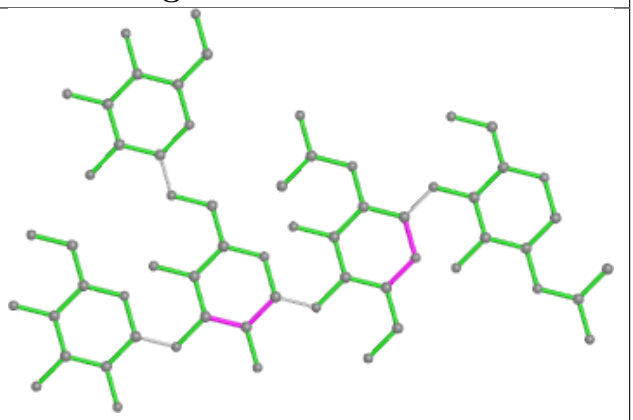


Rings

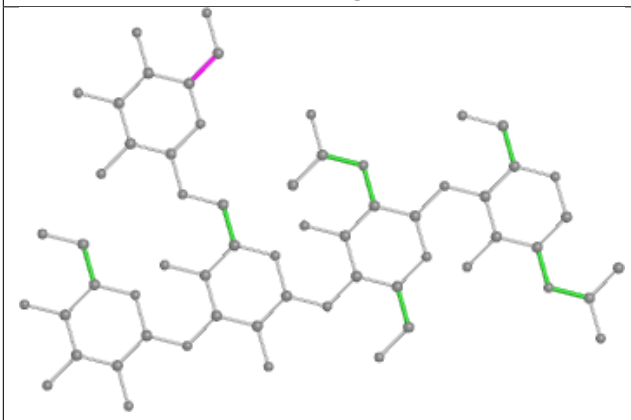
Oligosaccharide Chain g



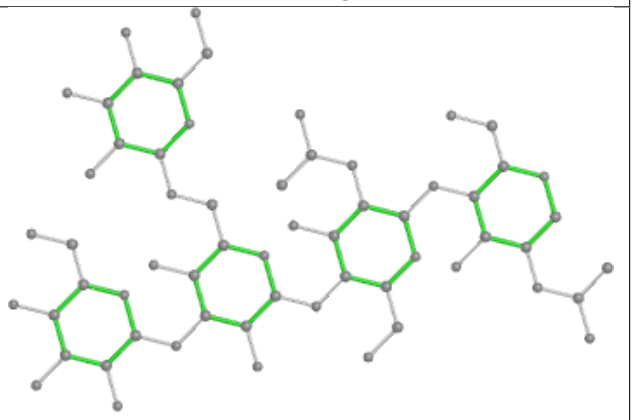
Bond lengths



Bond angles

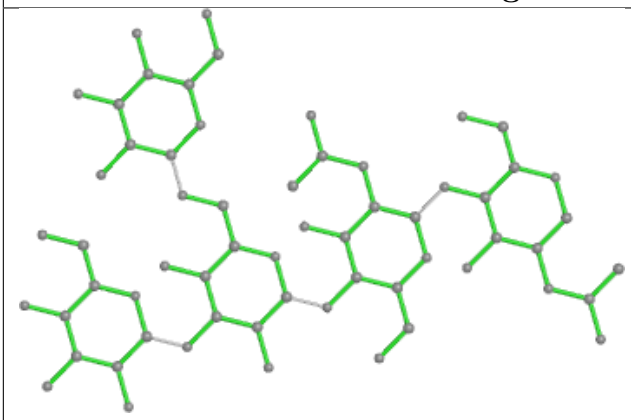


Torsions

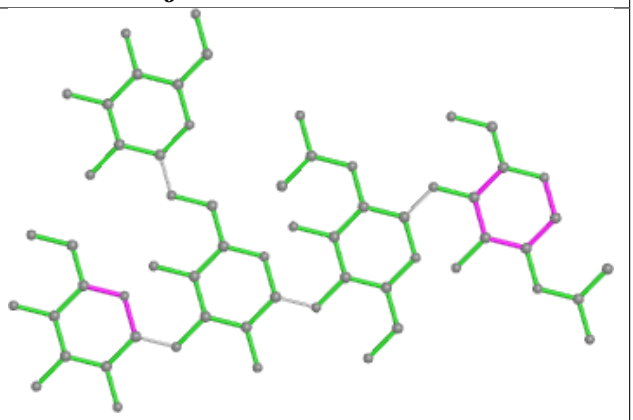


Rings

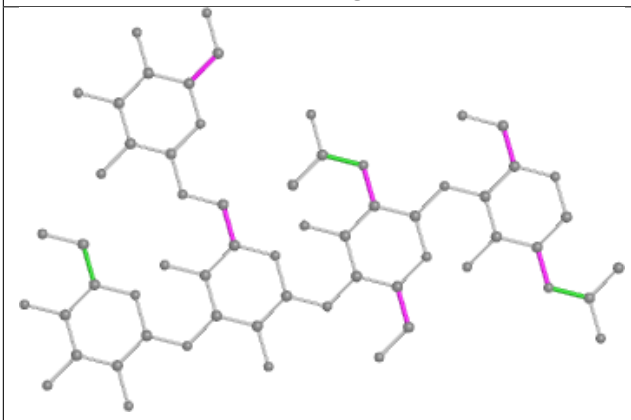
Oligosaccharide Chain j



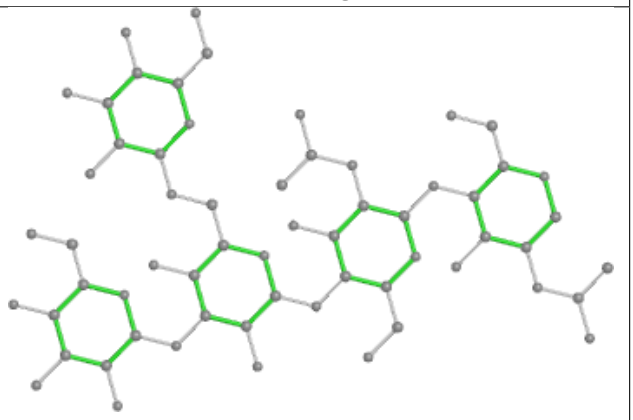
Bond lengths



Bond angles

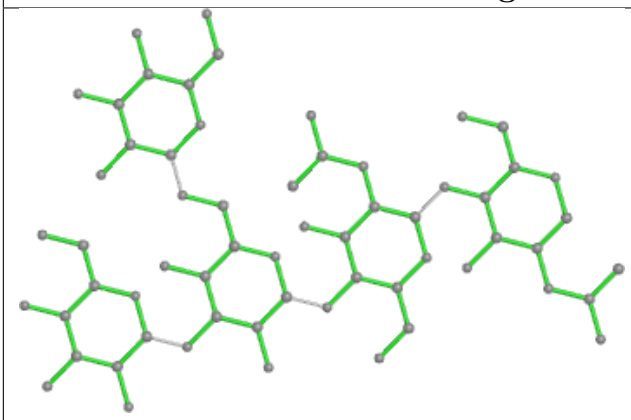


Torsions

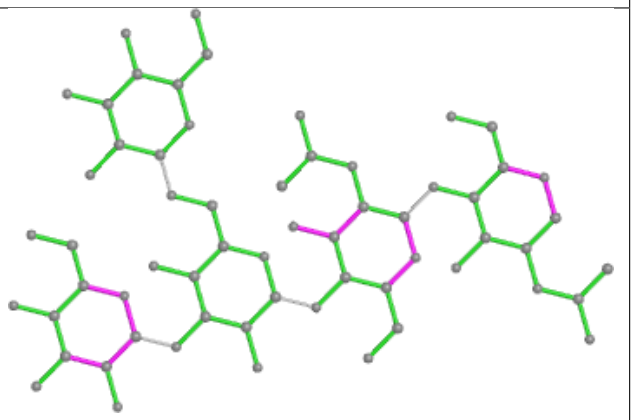


Rings

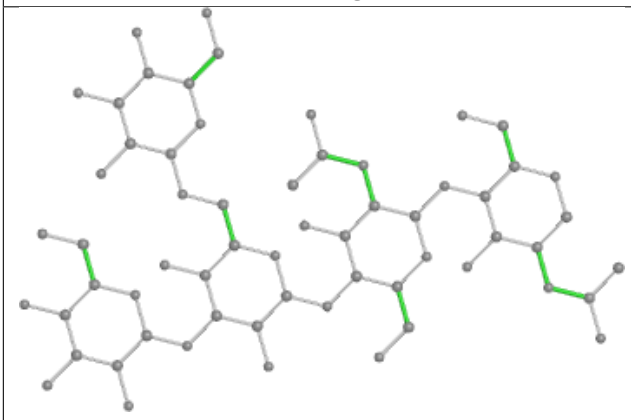
Oligosaccharide Chain k



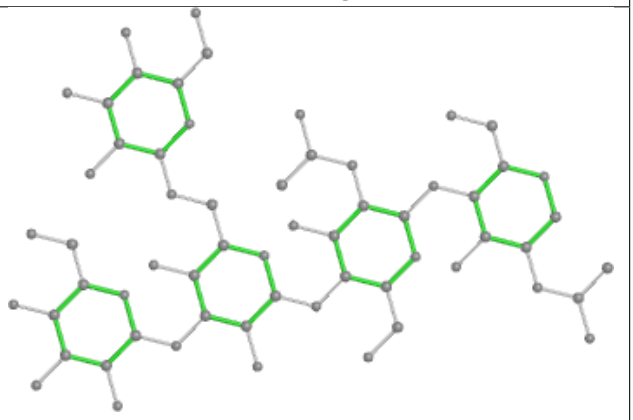
Bond lengths



Bond angles

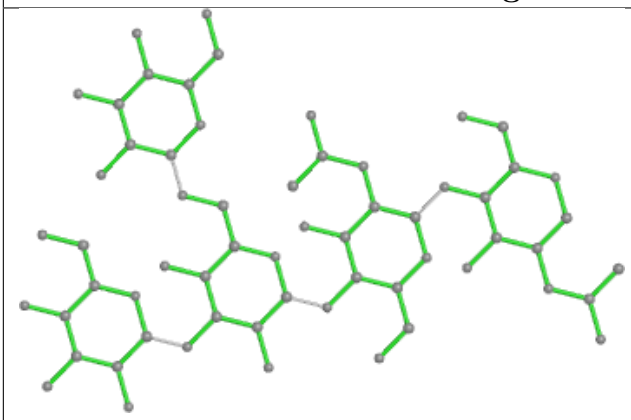


Torsions

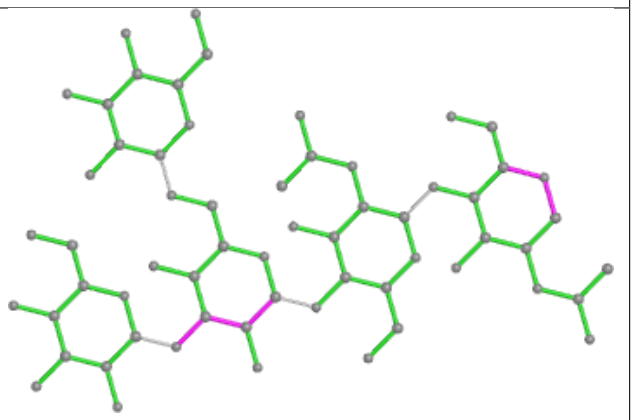


Rings

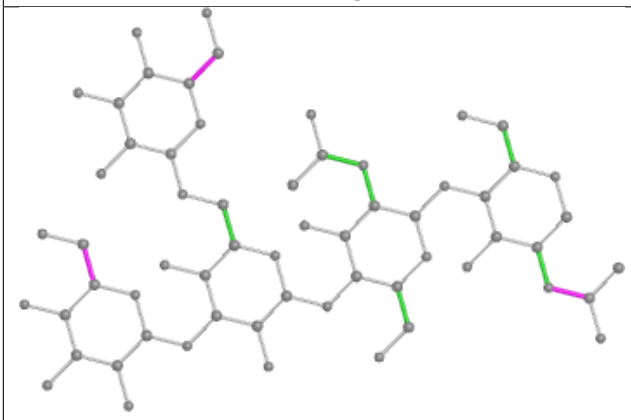
Oligosaccharide Chain l



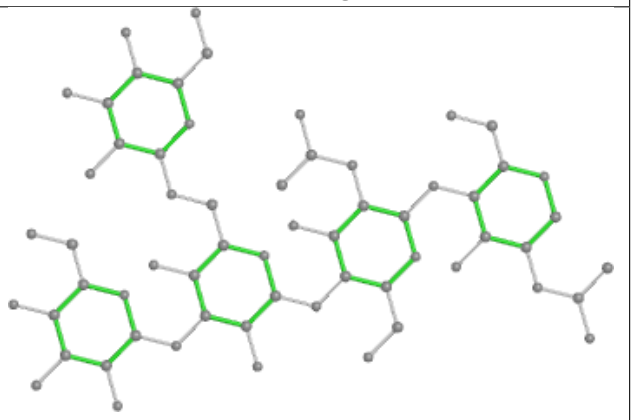
Bond lengths



Bond angles

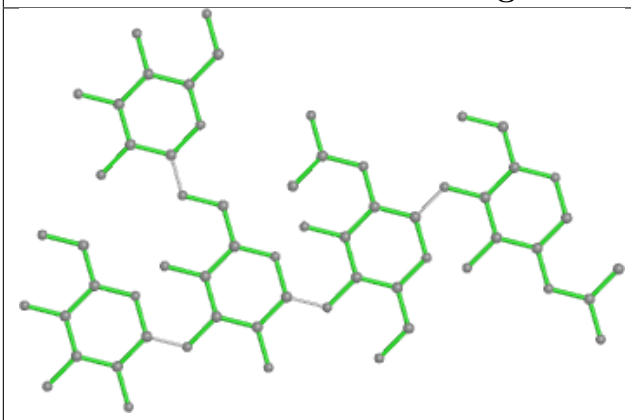


Torsions

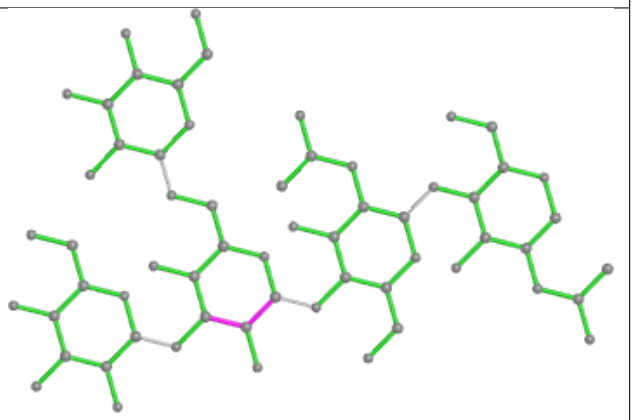


Rings

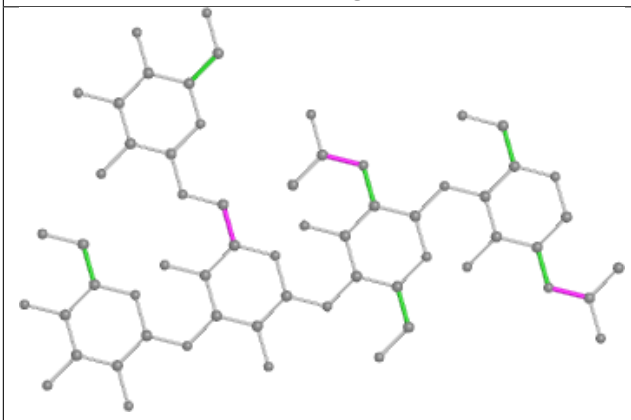
Oligosaccharide Chain u



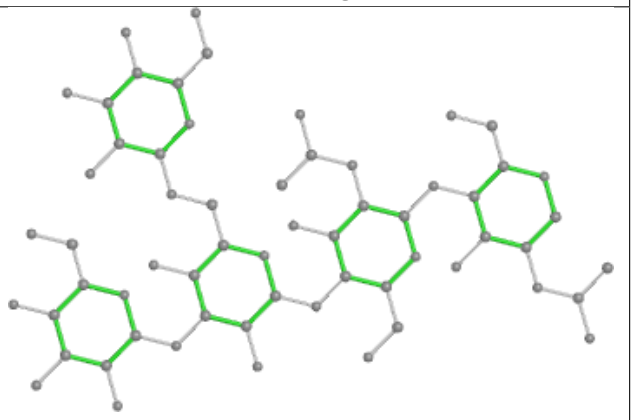
Bond lengths



Bond angles

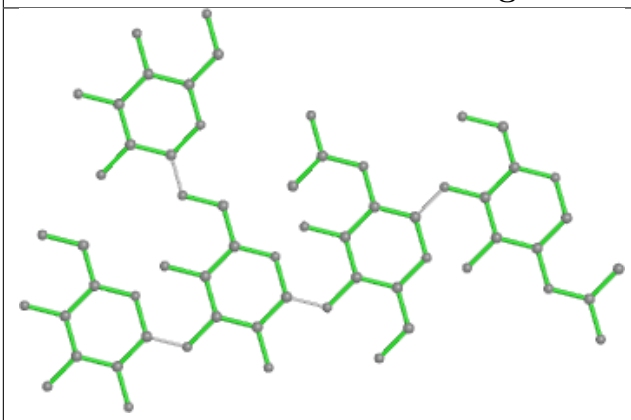


Torsions

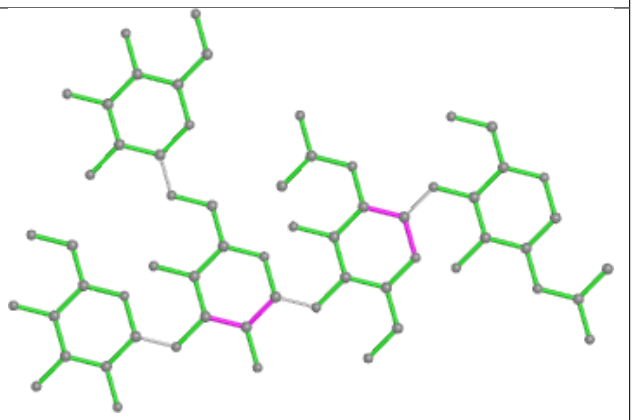


Rings

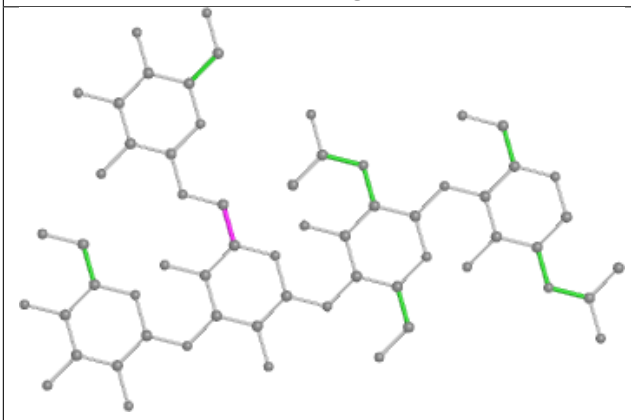
Oligosaccharide Chain 1



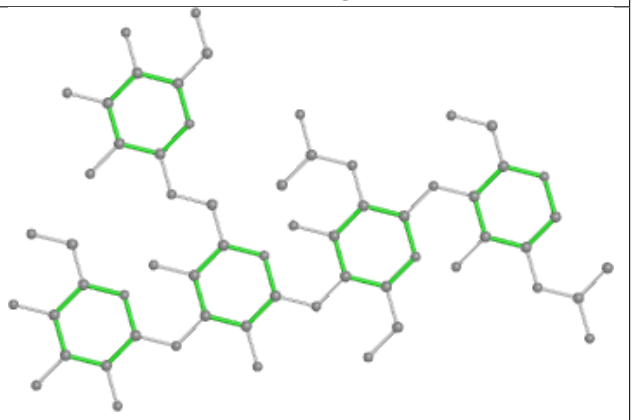
Bond lengths



Bond angles

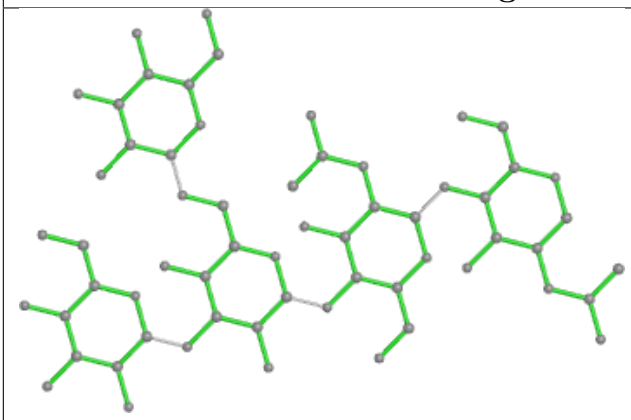


Torsions

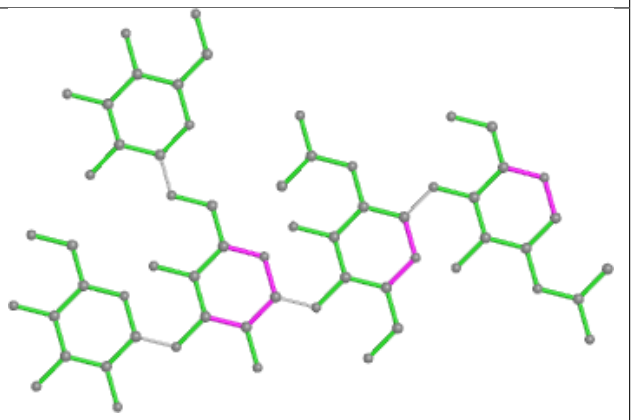


Rings

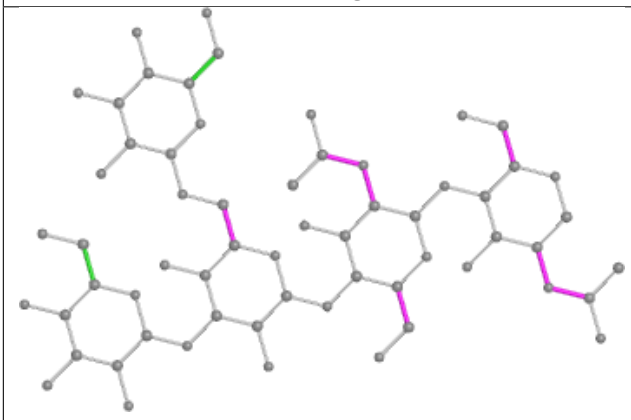
Oligosaccharide Chain 4



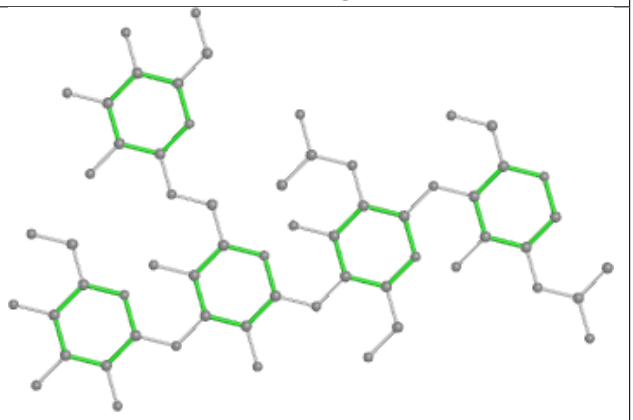
Bond lengths



Bond angles

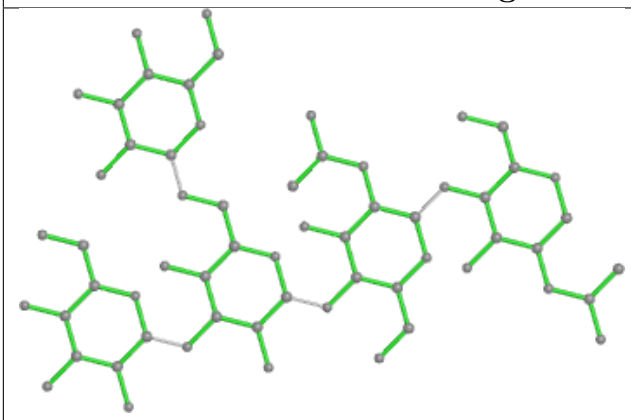


Torsions

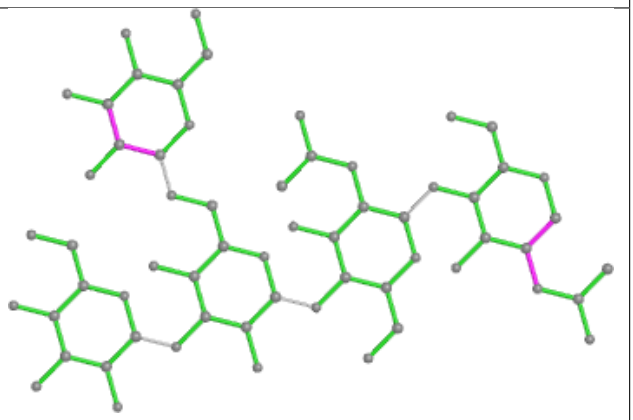


Rings

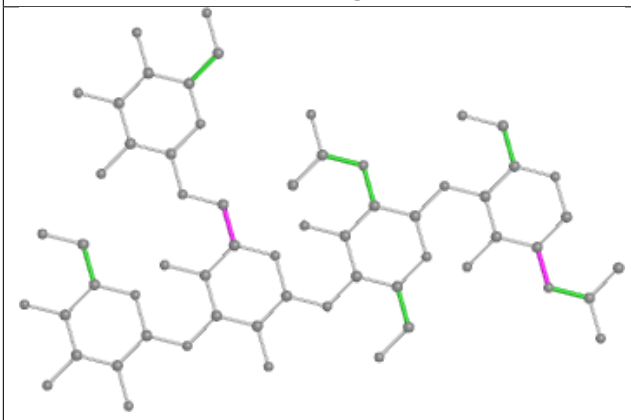
Oligosaccharide Chain 5



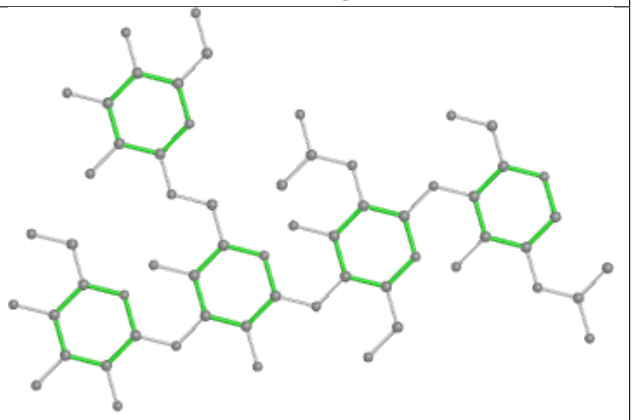
Bond lengths



Bond angles

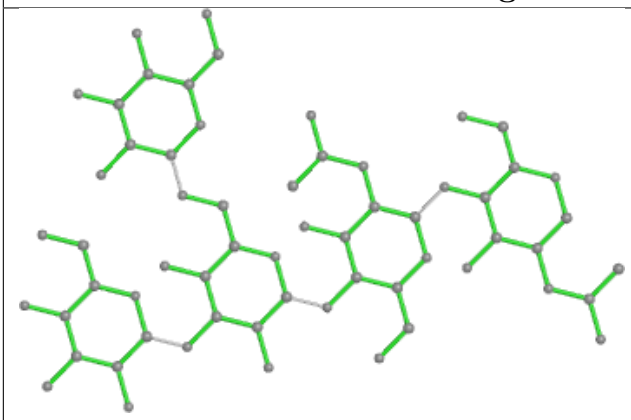


Torsions

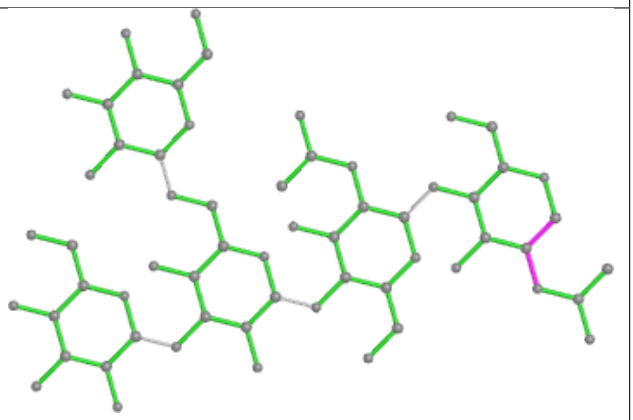


Rings

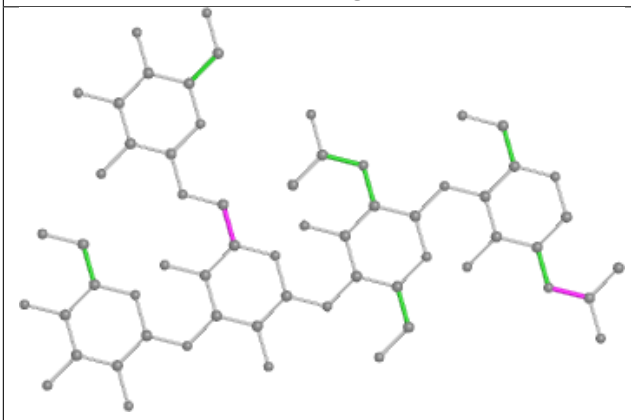
Oligosaccharide Chain 9



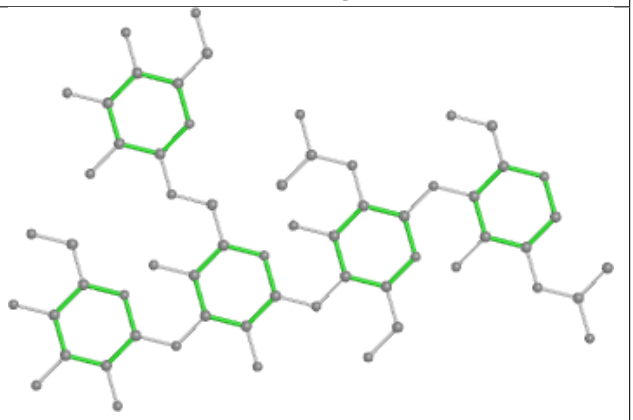
Bond lengths



Bond angles

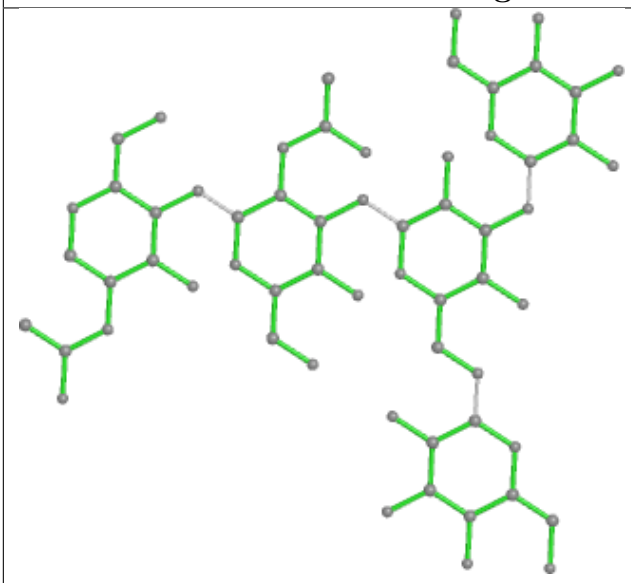


Torsions

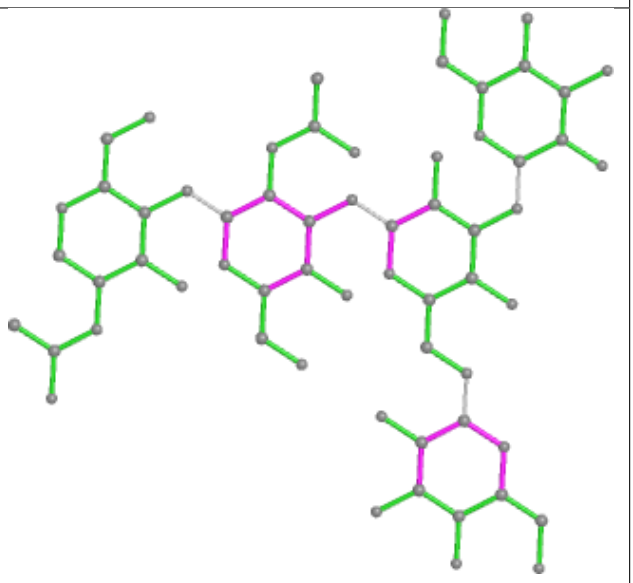


Rings

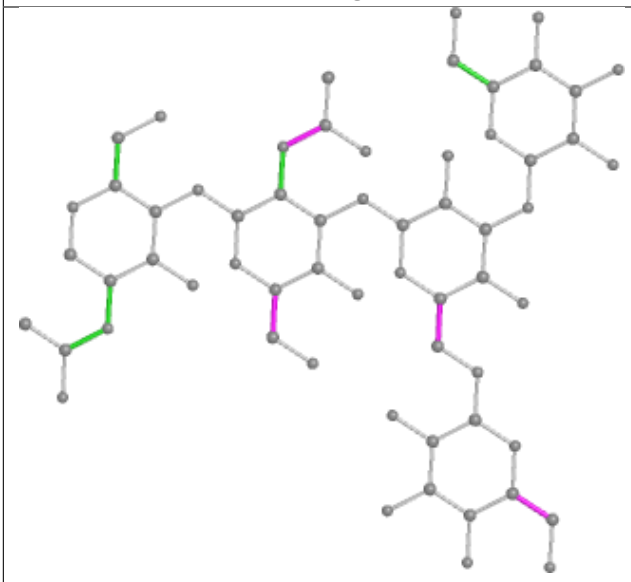
Oligosaccharide Chain U



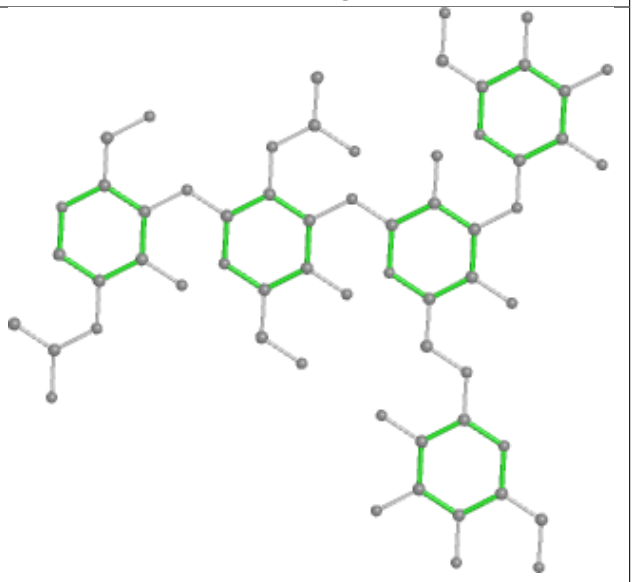
Bond lengths



Bond angles

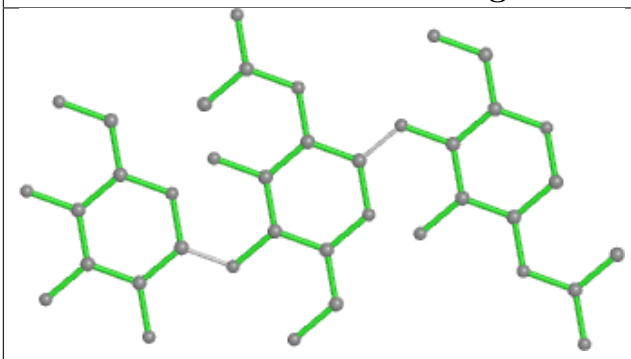


Torsions

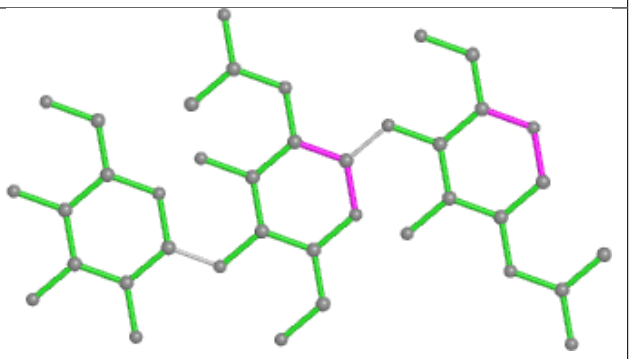


Rings

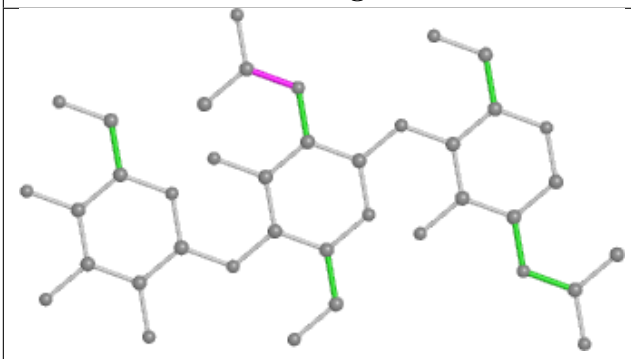
Oligosaccharide Chain W



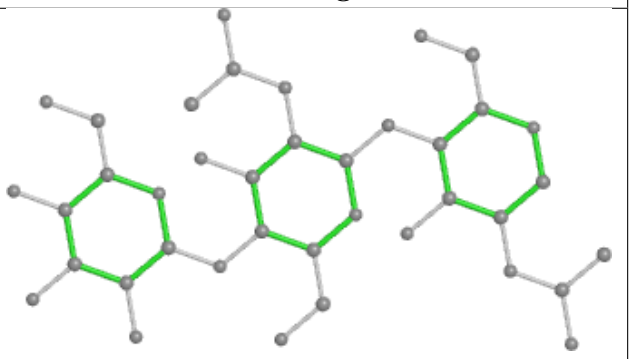
Bond lengths



Bond angles

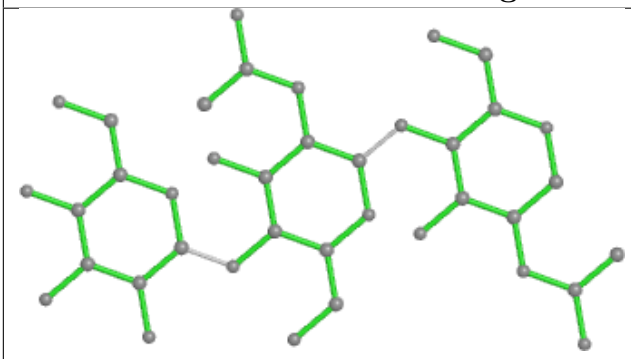


Torsions

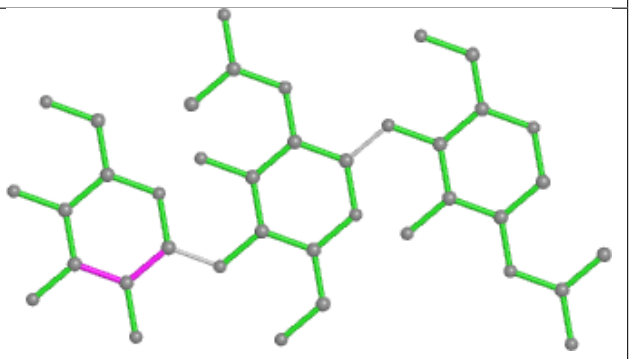


Rings

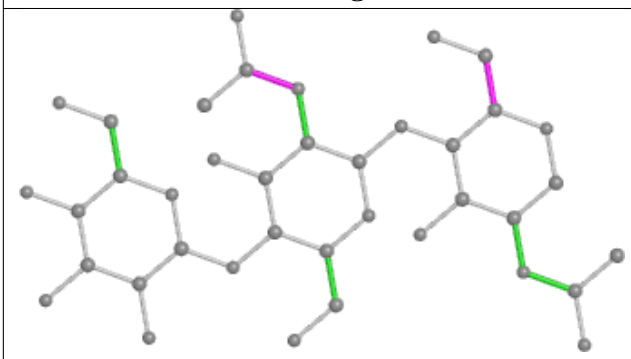
Oligosaccharide Chain e



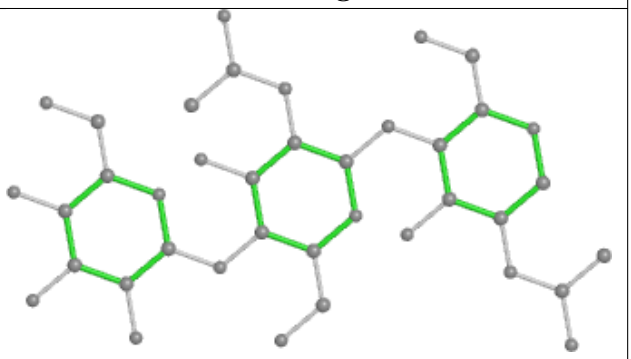
Bond lengths



Bond angles

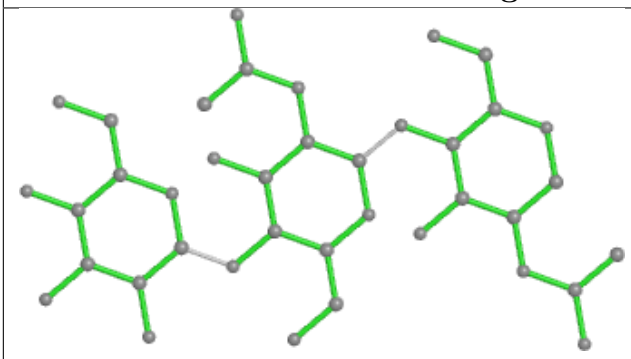


Torsions

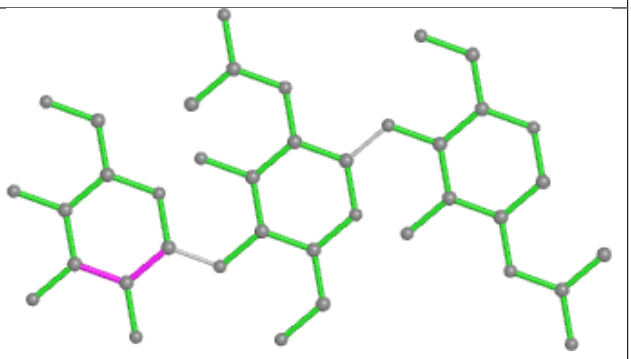


Rings

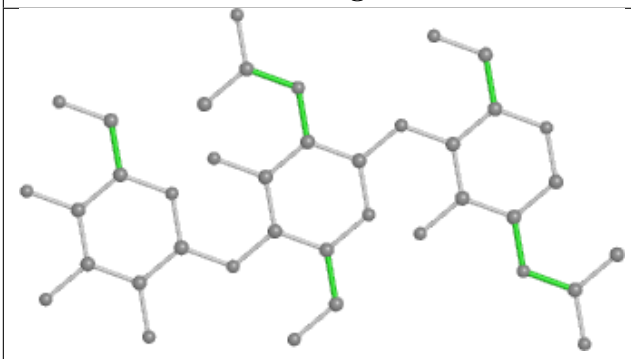
Oligosaccharide Chain f



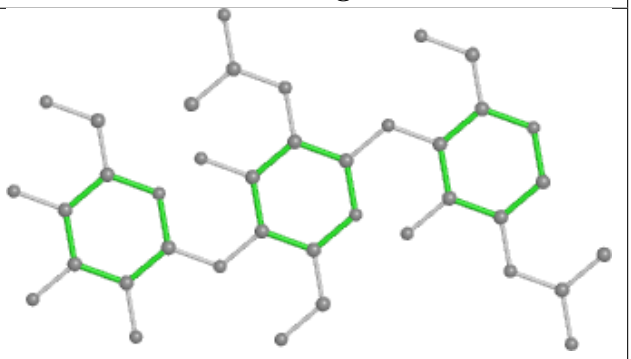
Bond lengths



Bond angles

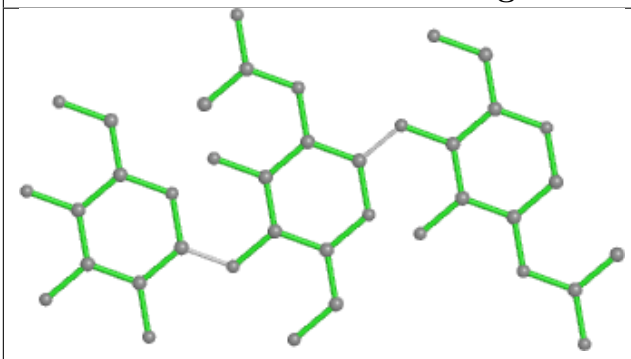


Torsions

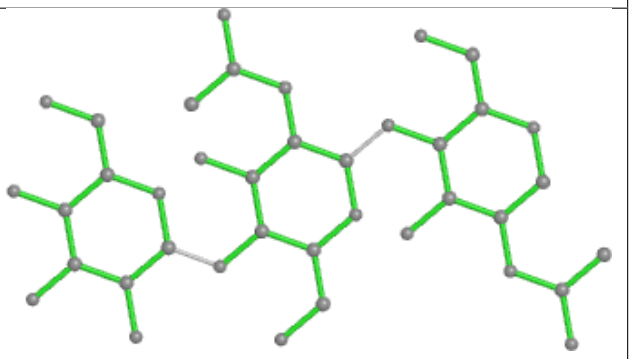


Rings

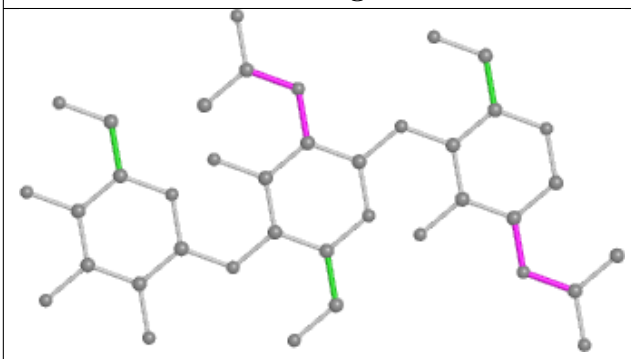
Oligosaccharide Chain h



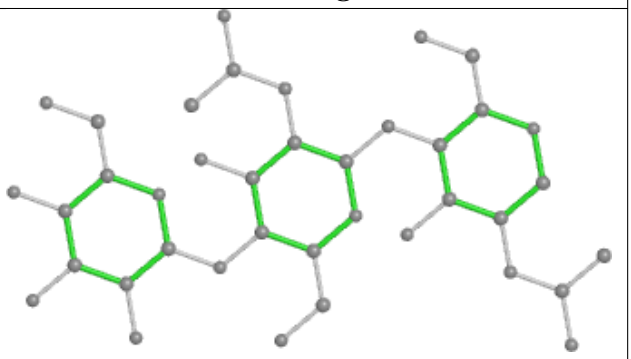
Bond lengths



Bond angles

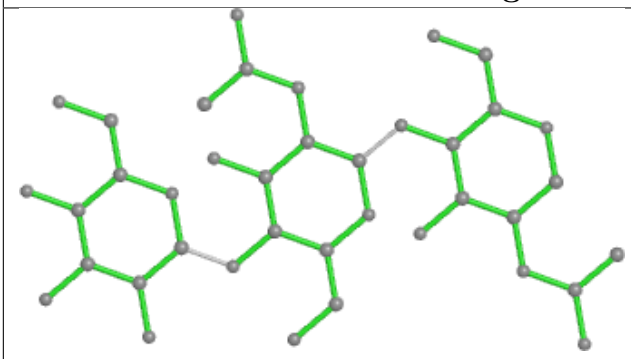


Torsions

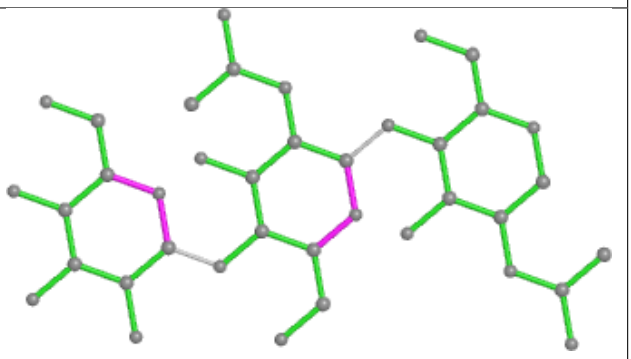


Rings

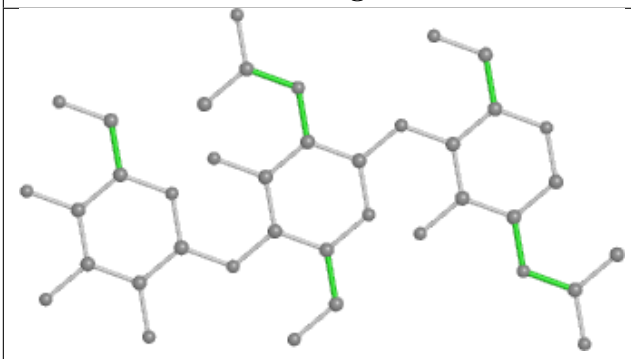
Oligosaccharide Chain i



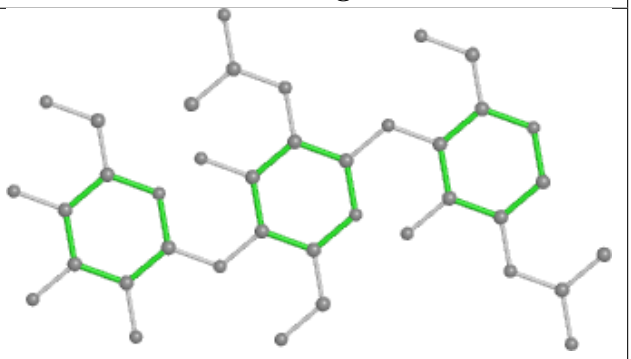
Bond lengths



Bond angles

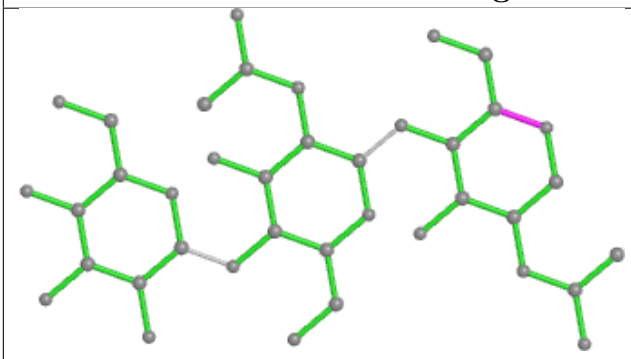


Torsions

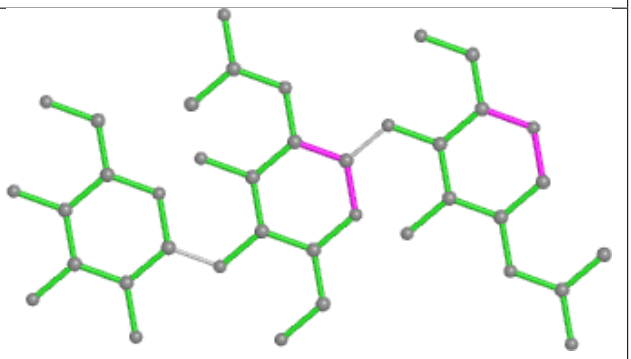


Rings

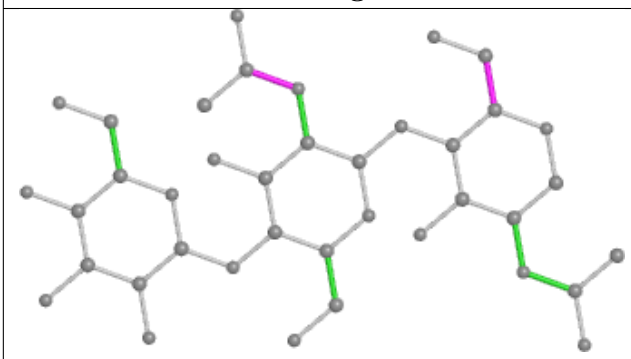
Oligosaccharide Chain m



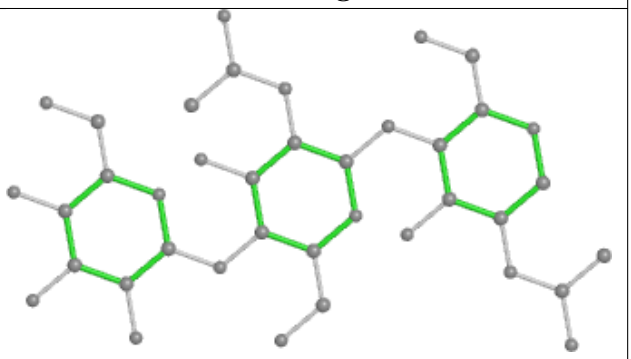
Bond lengths



Bond angles

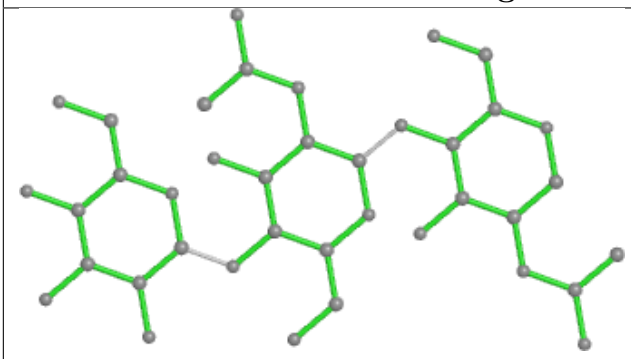


Torsions

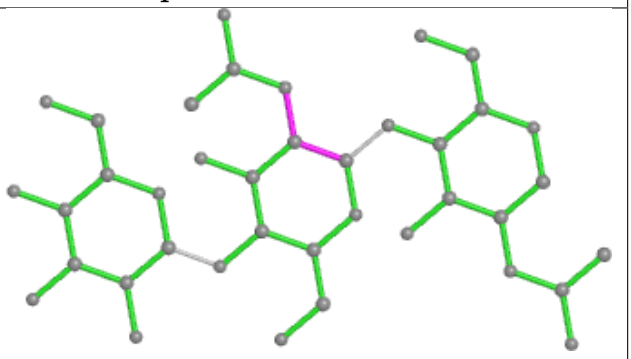


Rings

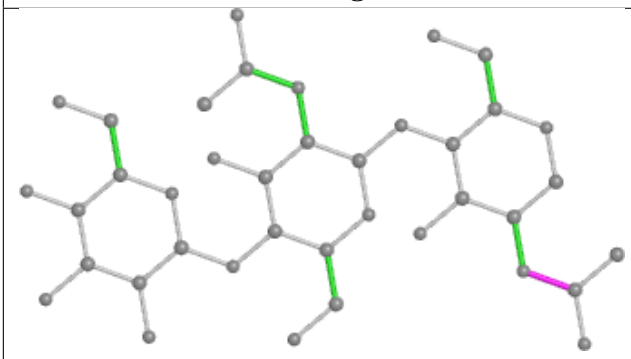
Oligosaccharide Chain p



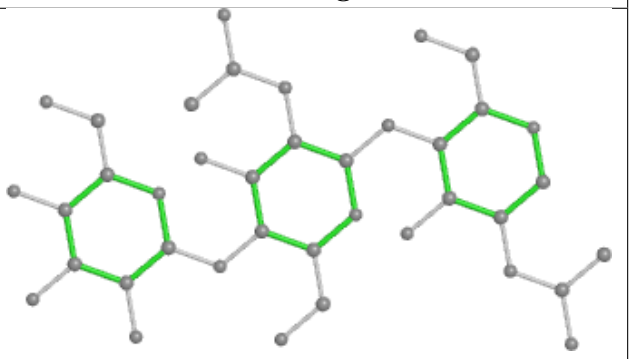
Bond lengths



Bond angles

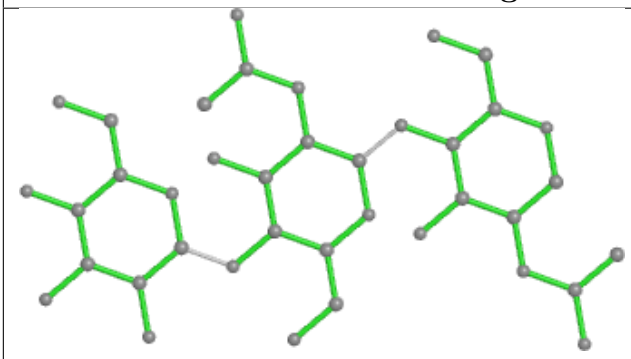


Torsions

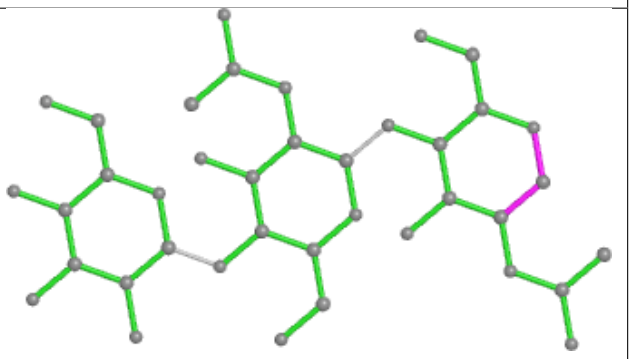


Rings

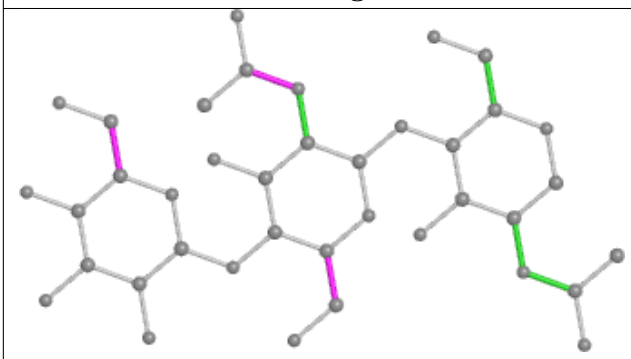
Oligosaccharide Chain r



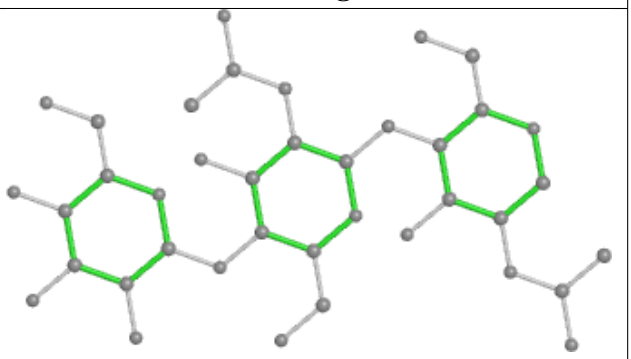
Bond lengths



Bond angles

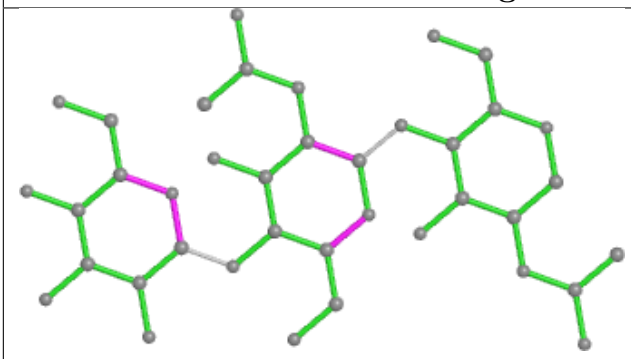


Torsions

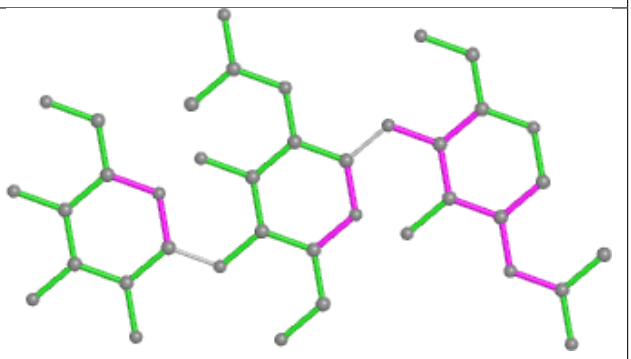


Rings

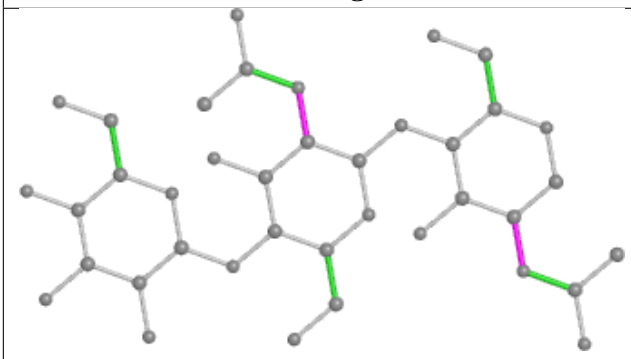
Oligosaccharide Chain 2



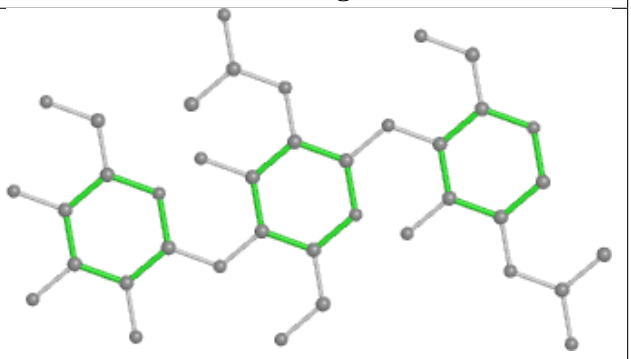
Bond lengths



Bond angles

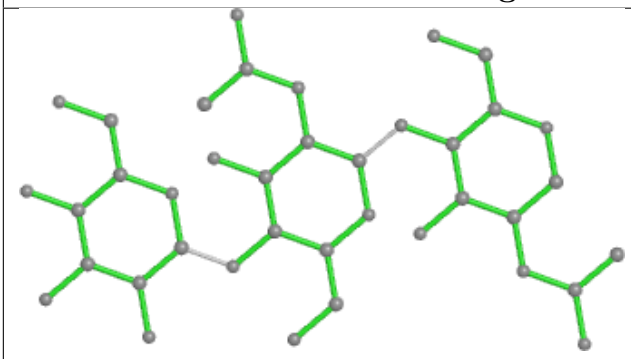


Torsions

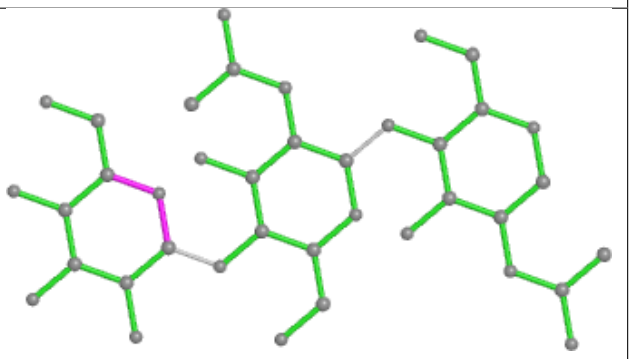


Rings

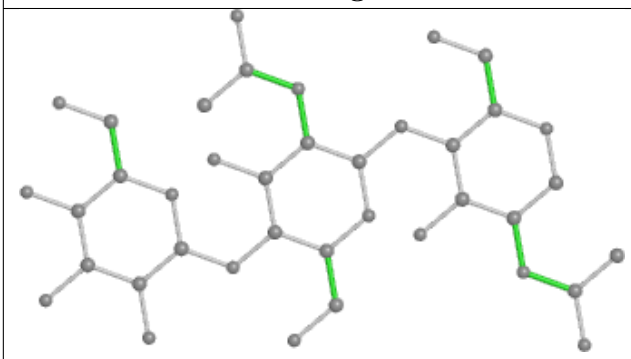
Oligosaccharide Chain 3



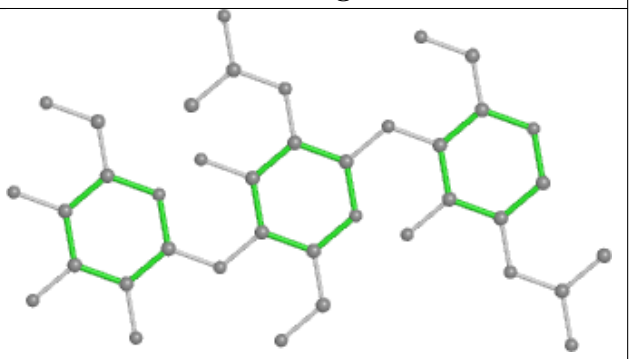
Bond lengths



Bond angles

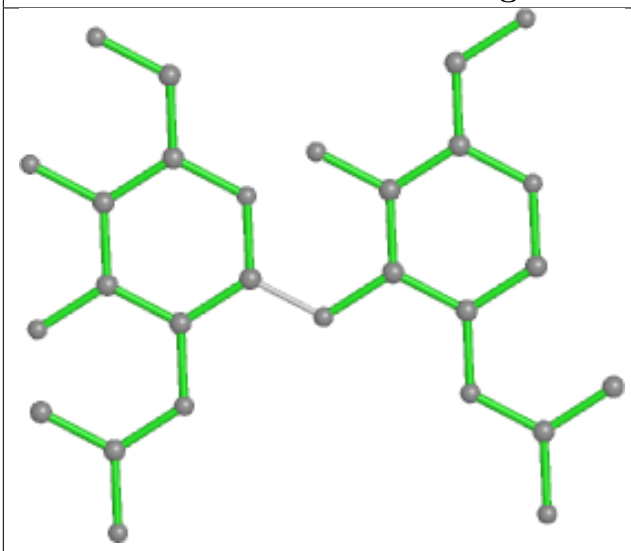


Torsions

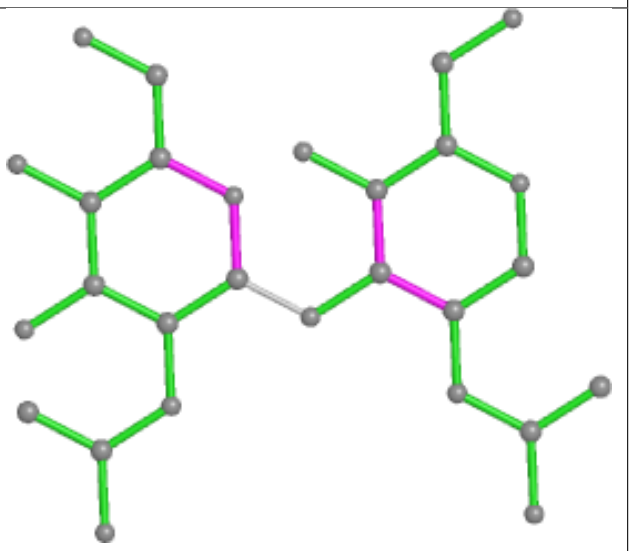


Rings

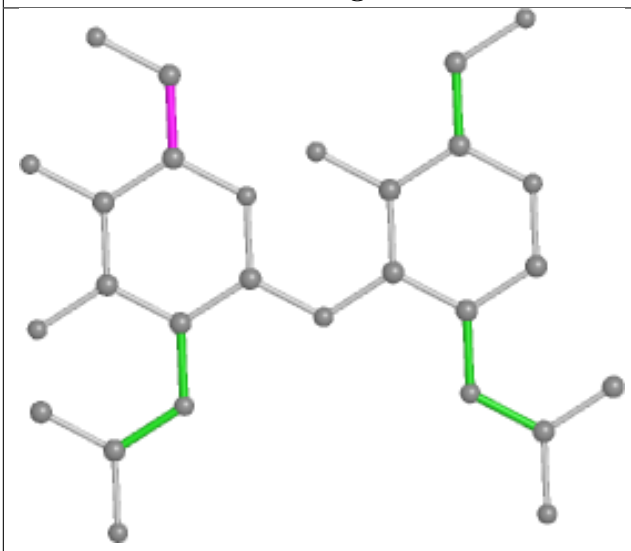
Oligosaccharide Chain c



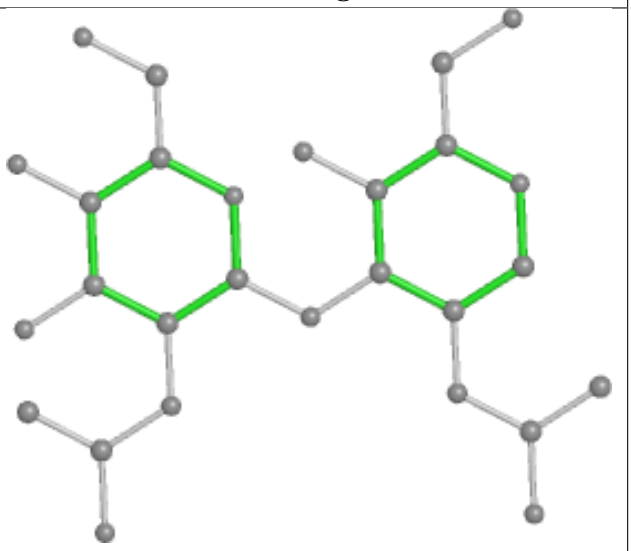
Bond lengths



Bond angles

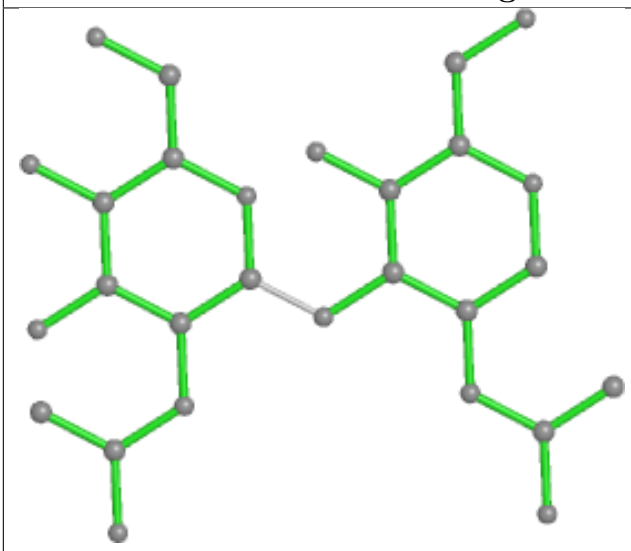


Torsions

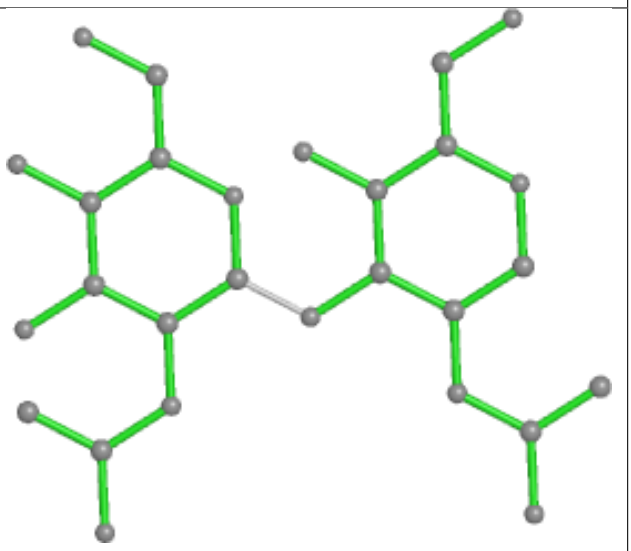


Rings

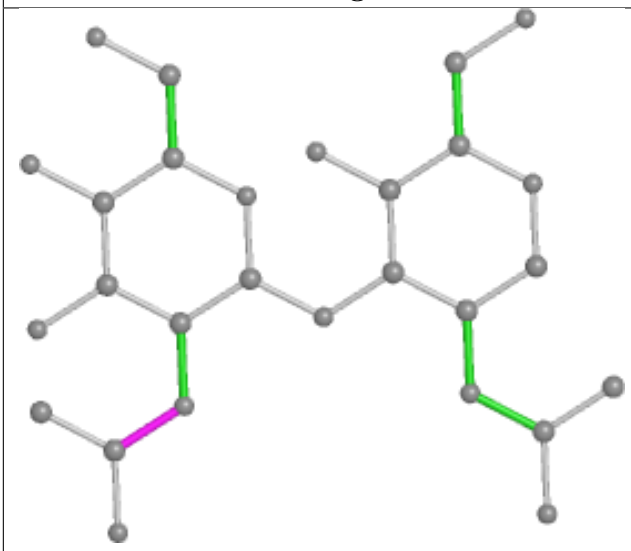
Oligosaccharide Chain o



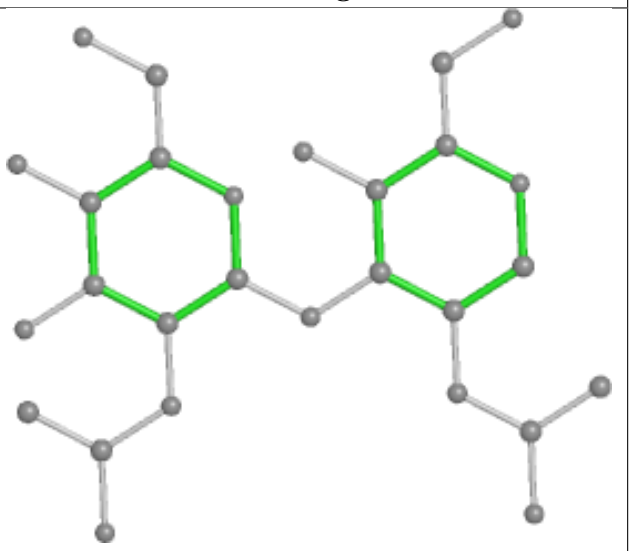
Bond lengths



Bond angles

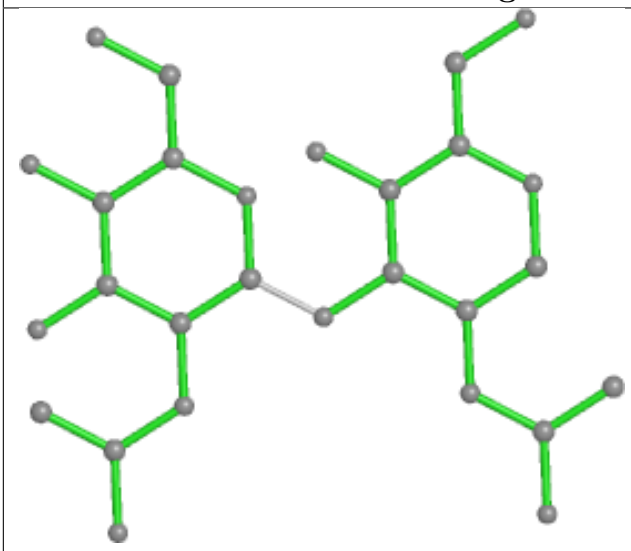


Torsions

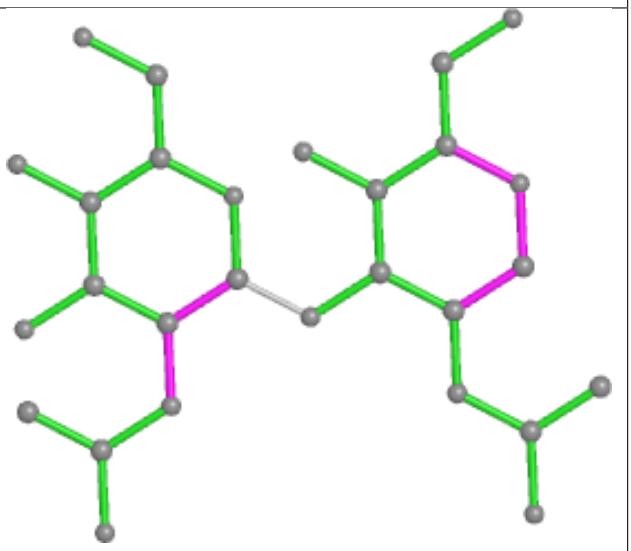


Rings

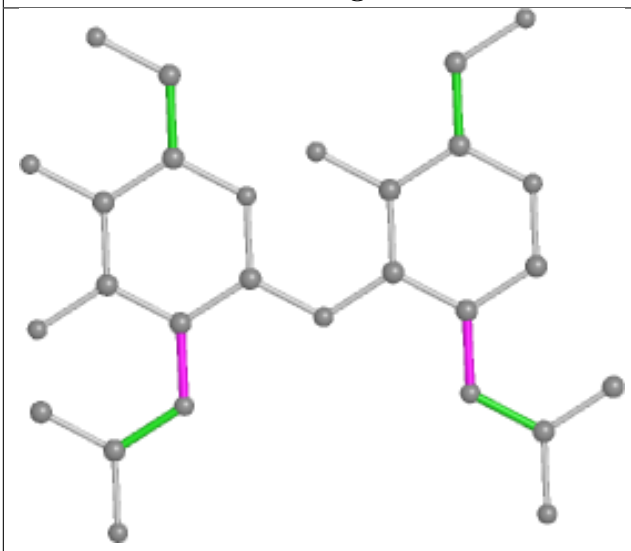
Oligosaccharide Chain 8



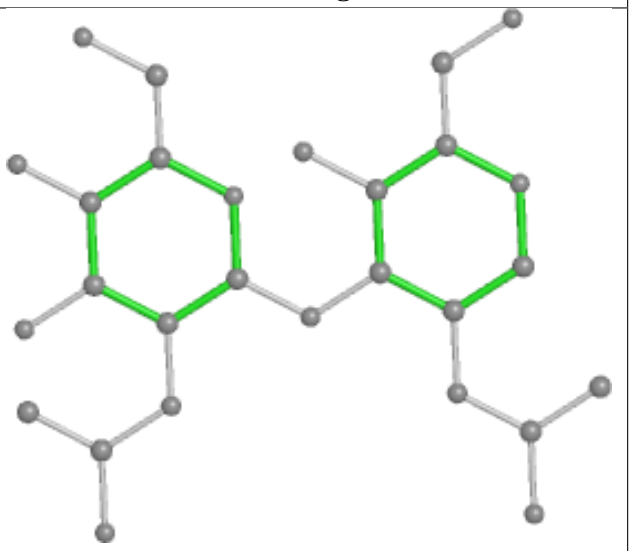
Bond lengths



Bond angles

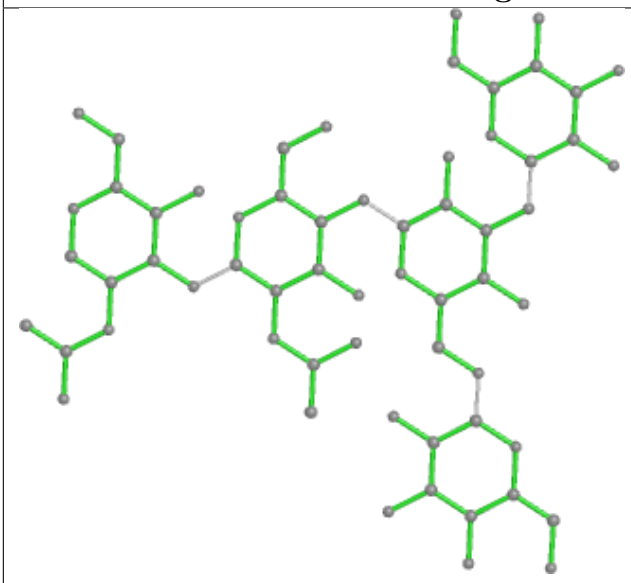


Torsions

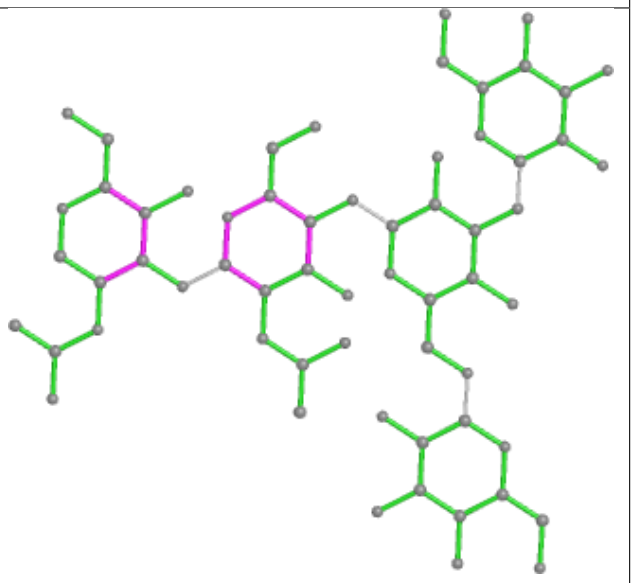


Rings

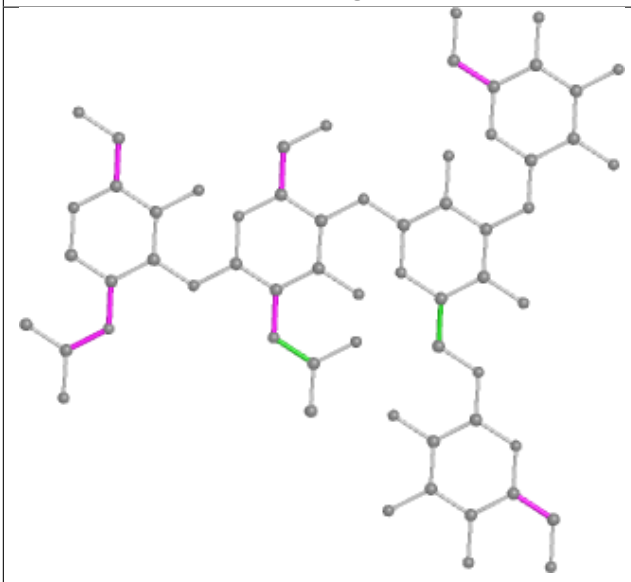
Oligosaccharide Chain w



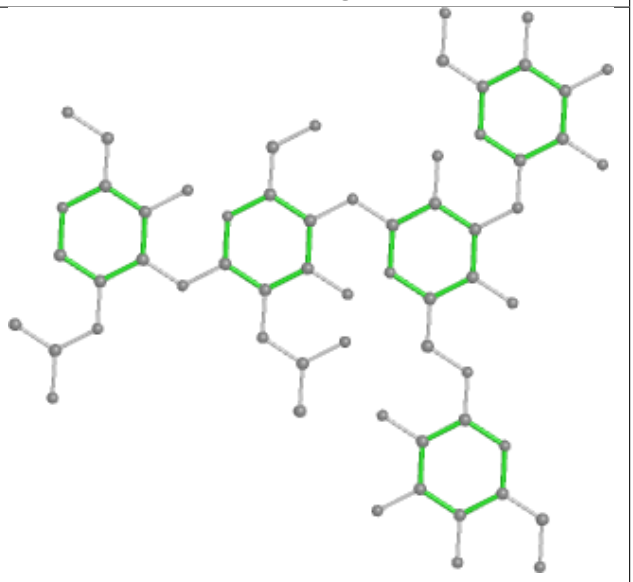
Bond lengths



Bond angles

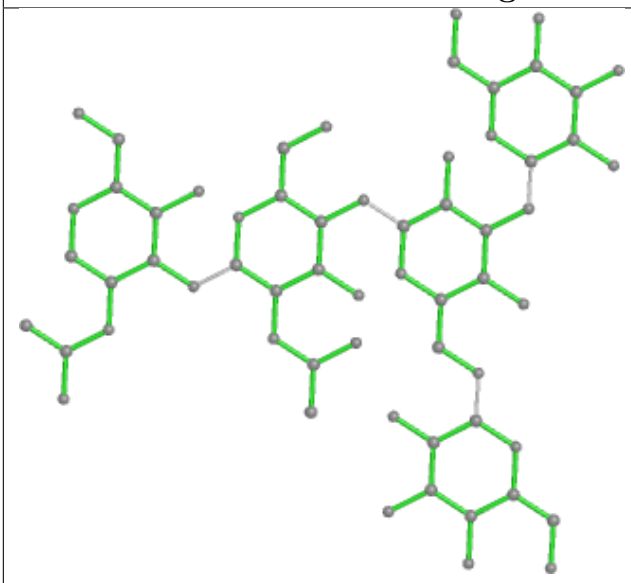


Torsions

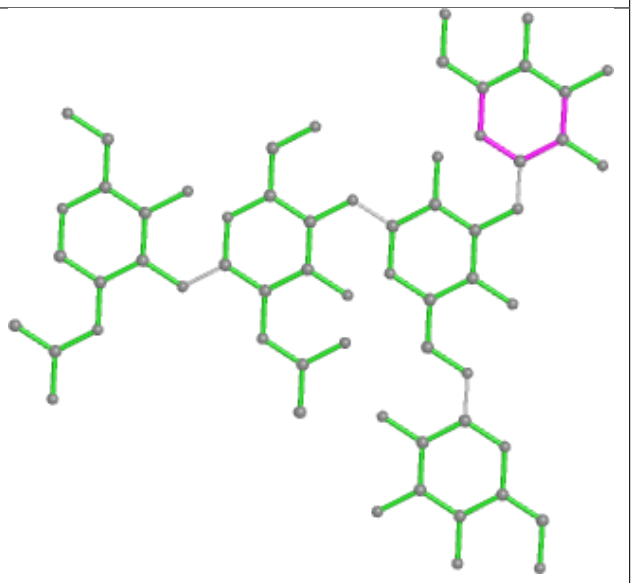


Rings

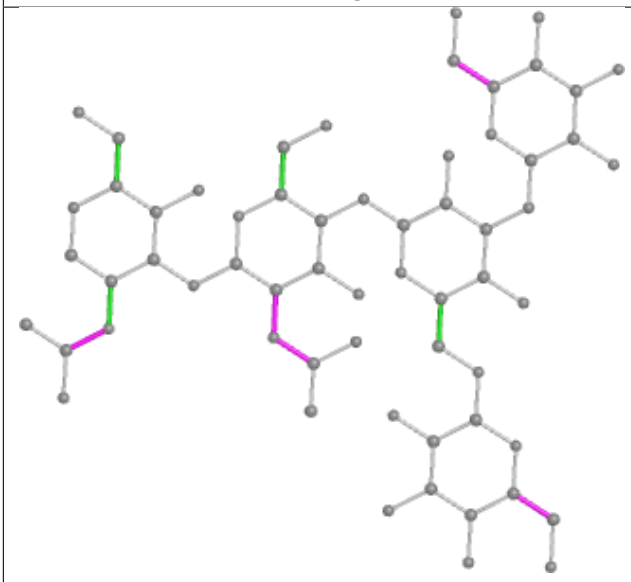
Oligosaccharide Chain 6



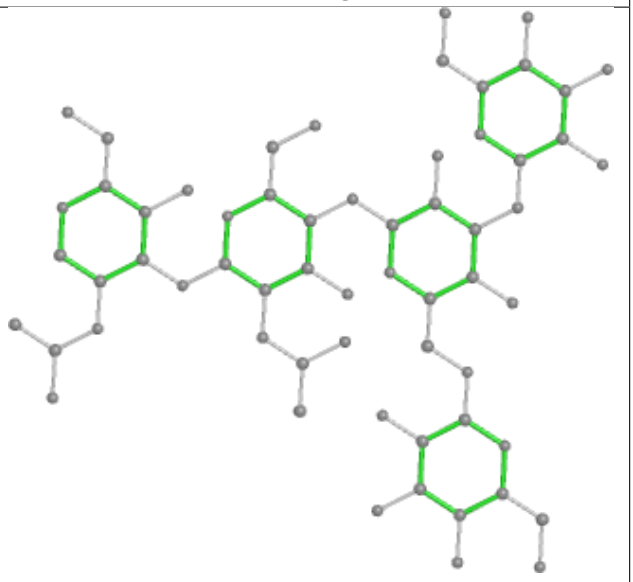
Bond lengths



Bond angles

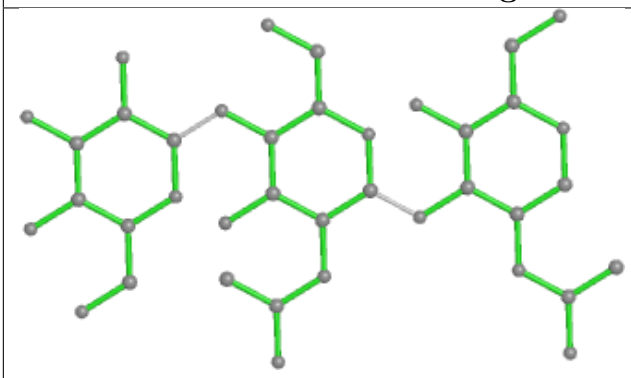


Torsions

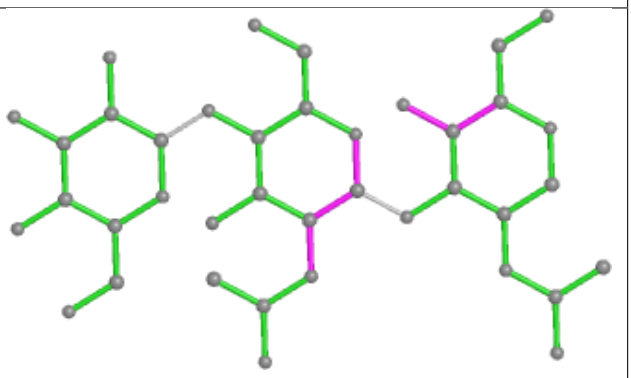


Rings

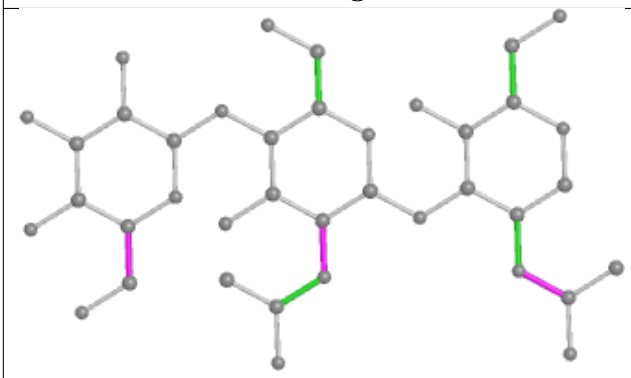
Oligosaccharide Chain z



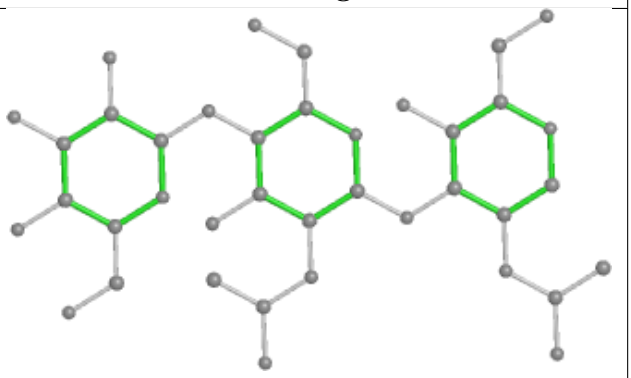
Bond lengths



Bond angles

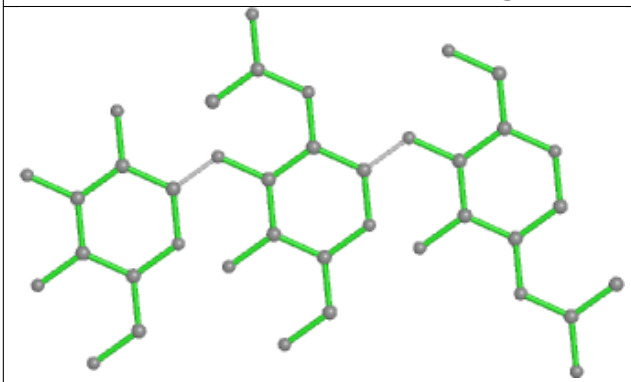


Torsions

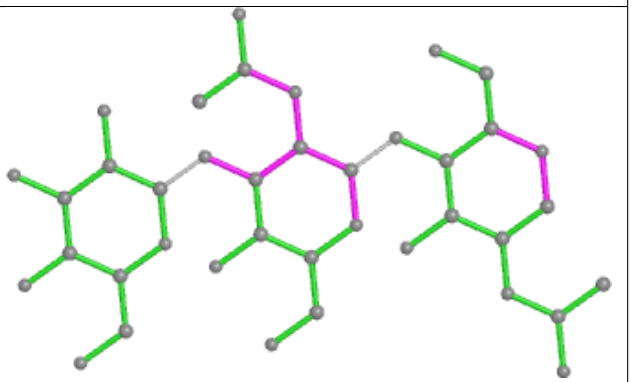


Rings

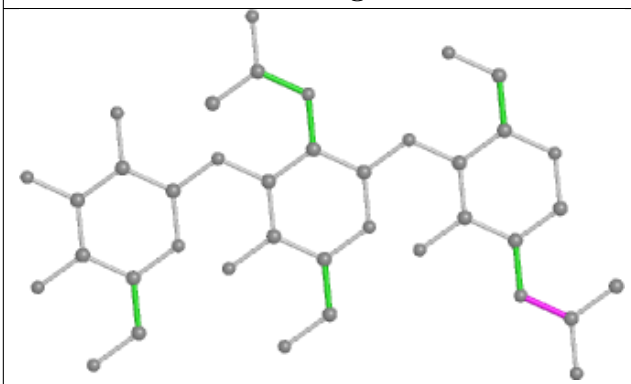
Oligosaccharide Chain 0



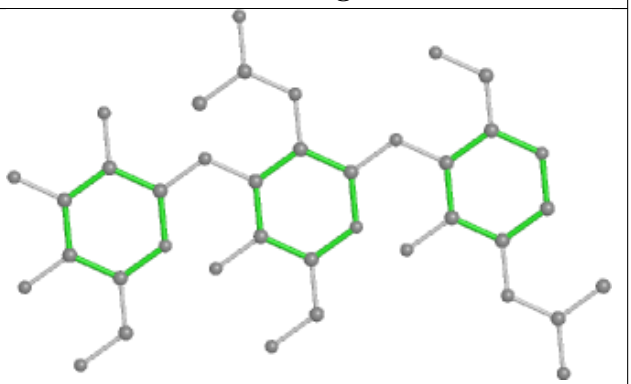
Bond lengths



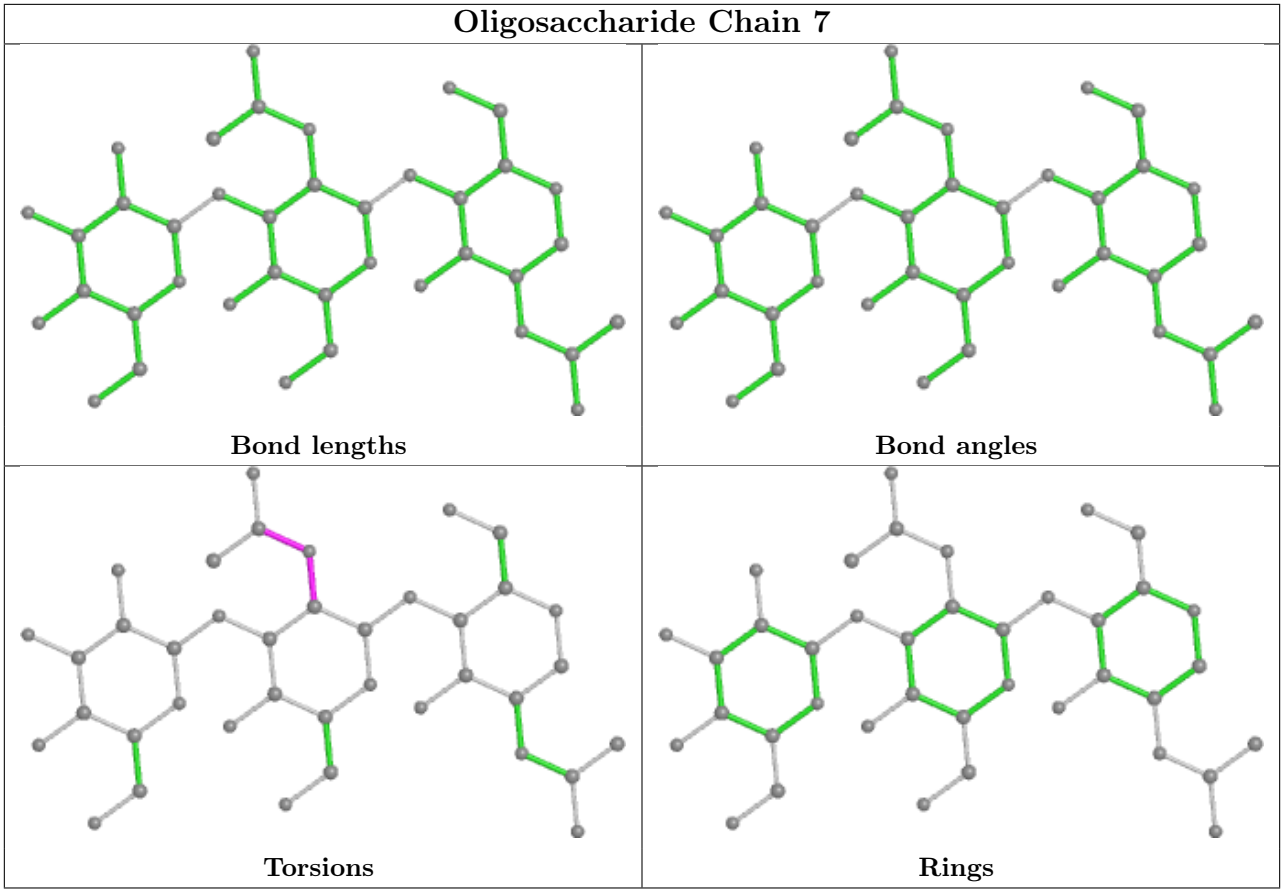
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 136 ligands modelled in this entry, 90 are monoatomic - leaving 46 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	$\#\|Z\| > 2$
17	NAG	B	4707	1	14,14,15	0.46	0	17,19,21	0.93	1 (5%)
18	A2G	B	4718	1	14,14,15	0.50	0	17,19,21	0.88	0
18	A2G	B	4719	1	14,14,15	0.39	0	17,19,21	1.07	1 (5%)
18	A2G	A	4720	1	14,14,15	0.46	0	17,19,21	0.51	0
18	A2G	B	4713	1	14,14,15	0.52	0	17,19,21	0.65	0
18	A2G	A	4721	1	14,14,15	0.52	0	17,19,21	1.02	1 (5%)
18	A2G	B	4715	1	14,14,15	0.45	0	17,19,21	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	A2G	A	4718	1	14,14,15	0.52	0	17,19,21	1.56	3 (17%)
18	A2G	B	4721	1	14,14,15	0.53	0	17,19,21	1.07	2 (11%)
17	NAG	B	4703	1	14,14,15	0.40	0	17,19,21	0.41	0
18	A2G	A	4714	1	14,14,15	0.48	0	17,19,21	0.91	1 (5%)
18	A2G	A	4722	1	14,14,15	0.51	0	17,19,21	1.55	3 (17%)
17	NAG	A	4701	1	14,14,15	0.41	0	17,19,21	0.65	0
17	NAG	A	4710	1	14,14,15	0.40	0	17,19,21	0.59	0
17	NAG	A	4703	1	14,14,15	0.39	0	17,19,21	0.42	0
17	NAG	B	4705	1	14,14,15	0.40	0	17,19,21	0.69	0
17	NAG	B	4706	1	14,14,15	0.40	0	17,19,21	0.39	0
18	A2G	A	4713	1	14,14,15	0.56	0	17,19,21	0.58	0
17	NAG	A	4702	1	14,14,15	0.39	0	17,19,21	0.99	1 (5%)
18	A2G	A	4719	1	14,14,15	0.50	0	17,19,21	1.14	2 (11%)
18	A2G	B	4714	1	14,14,15	0.89	1 (7%)	17,19,21	0.86	1 (5%)
17	NAG	A	4707	1	14,14,15	0.40	0	17,19,21	1.36	4 (23%)
18	A2G	A	4716	1	14,14,15	0.99	1 (7%)	17,19,21	1.33	2 (11%)
18	A2G	B	4723	1	14,14,15	0.53	0	17,19,21	0.99	1 (5%)
18	A2G	A	4723	1	14,14,15	0.53	0	17,19,21	1.07	1 (5%)
17	NAG	B	4709	1	14,14,15	0.98	1 (7%)	17,19,21	0.92	1 (5%)
18	A2G	B	4712	1	14,14,15	0.46	0	17,19,21	1.41	4 (23%)
18	A2G	B	4716	1	14,14,15	0.51	0	17,19,21	1.11	2 (11%)
17	NAG	A	4711	1	14,14,15	0.39	0	17,19,21	1.19	2 (11%)
18	A2G	B	4717	1	14,14,15	0.38	0	17,19,21	0.76	0
18	A2G	A	4717	1	14,14,15	0.40	0	17,19,21	0.64	0
17	NAG	B	4710	1	14,14,15	0.43	0	17,19,21	0.80	0
17	NAG	B	4711	1	14,14,15	0.43	0	17,19,21	0.67	0
17	NAG	B	4701	1	14,14,15	0.40	0	17,19,21	0.63	0
18	A2G	B	4720	1	14,14,15	0.49	0	17,19,21	0.85	1 (5%)
17	NAG	A	4706	1	14,14,15	0.38	0	17,19,21	0.79	1 (5%)
17	NAG	B	4704	1	14,14,15	0.90	0	17,19,21	0.98	0
17	NAG	A	4708	1	14,14,15	0.41	0	17,19,21	0.31	0
17	NAG	A	4709	1	14,14,15	0.41	0	17,19,21	0.30	0
17	NAG	A	4705	1	14,14,15	0.51	0	17,19,21	2.13	2 (11%)
18	A2G	B	4722	1	14,14,15	0.51	0	17,19,21	1.53	3 (17%)
17	NAG	B	4702	1	14,14,15	0.40	0	17,19,21	0.47	0
18	A2G	A	4712	1	14,14,15	0.47	0	17,19,21	1.73	3 (17%)
18	A2G	A	4715	1	14,14,15	0.50	0	17,19,21	1.37	1 (5%)
17	NAG	A	4704	1	14,14,15	0.53	0	17,19,21	1.13	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	NAG	B	4708	1	14,14,15	0.50	0	17,19,21	1.01	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	NAG	B	4707	1	-	0/6/23/26	0/1/1/1
18	A2G	B	4718	1	-	1/6/23/26	0/1/1/1
18	A2G	B	4719	1	-	1/6/23/26	0/1/1/1
18	A2G	A	4720	1	-	0/6/23/26	0/1/1/1
18	A2G	B	4713	1	-	0/6/23/26	0/1/1/1
18	A2G	A	4721	1	-	0/6/23/26	0/1/1/1
18	A2G	B	4715	1	-	0/6/23/26	0/1/1/1
18	A2G	A	4718	1	-	2/6/23/26	0/1/1/1
18	A2G	B	4721	1	-	1/6/23/26	0/1/1/1
17	NAG	B	4703	1	-	0/6/23/26	0/1/1/1
18	A2G	A	4714	1	-	0/6/23/26	0/1/1/1
18	A2G	A	4722	1	-	2/6/23/26	0/1/1/1
17	NAG	A	4701	1	-	0/6/23/26	0/1/1/1
17	NAG	A	4710	1	-	0/6/23/26	0/1/1/1
17	NAG	A	4703	1	-	0/6/23/26	0/1/1/1
17	NAG	B	4705	1	-	3/6/23/26	0/1/1/1
17	NAG	B	4706	1	-	0/6/23/26	0/1/1/1
18	A2G	A	4713	1	-	0/6/23/26	0/1/1/1
17	NAG	A	4702	1	-	0/6/23/26	0/1/1/1
18	A2G	A	4719	1	-	1/6/23/26	0/1/1/1
18	A2G	B	4714	1	-	1/6/23/26	0/1/1/1
17	NAG	A	4707	1	-	2/6/23/26	0/1/1/1
18	A2G	A	4716	1	-	1/6/23/26	0/1/1/1
18	A2G	B	4723	1	-	2/6/23/26	0/1/1/1
18	A2G	A	4723	1	-	0/6/23/26	0/1/1/1
17	NAG	B	4709	1	-	1/6/23/26	0/1/1/1
18	A2G	B	4712	1	-	2/6/23/26	0/1/1/1
18	A2G	B	4716	1	-	1/6/23/26	0/1/1/1
17	NAG	A	4711	1	-	0/6/23/26	0/1/1/1
18	A2G	B	4717	1	-	1/6/23/26	0/1/1/1
18	A2G	A	4717	1	-	0/6/23/26	0/1/1/1
17	NAG	B	4710	1	-	2/6/23/26	0/1/1/1
17	NAG	B	4711	1	-	4/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	NAG	B	4701	1	-	3/6/23/26	0/1/1/1
18	A2G	B	4720	1	-	0/6/23/26	0/1/1/1
17	NAG	A	4706	1	-	1/6/23/26	0/1/1/1
17	NAG	B	4704	1	-	0/6/23/26	0/1/1/1
17	NAG	A	4708	1	-	2/6/23/26	0/1/1/1
17	NAG	A	4709	1	-	2/6/23/26	0/1/1/1
17	NAG	A	4705	1	-	3/6/23/26	0/1/1/1
18	A2G	B	4722	1	-	1/6/23/26	0/1/1/1
17	NAG	B	4702	1	-	0/6/23/26	0/1/1/1
18	A2G	A	4712	1	-	2/6/23/26	0/1/1/1
18	A2G	A	4715	1	-	0/6/23/26	0/1/1/1
17	NAG	A	4704	1	-	2/6/23/26	0/1/1/1
17	NAG	B	4708	1	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	4709	NAG	O5-C5	2.43	1.48	1.43
18	A	4716	A2G	O5-C5	2.12	1.47	1.43
18	B	4714	A2G	O5-C5	2.07	1.47	1.43

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	4705	NAG	O5-C1-C2	6.32	121.26	111.29
17	A	4705	NAG	C1-O5-C5	5.74	119.97	112.19
18	A	4712	A2G	C1-C2-N2	4.51	118.19	110.49
18	A	4715	A2G	C1-C2-N2	4.21	117.67	110.49
18	A	4718	A2G	C2-N2-C7	4.01	128.61	122.90
18	B	4722	A2G	C2-N2-C7	3.88	128.43	122.90
18	A	4722	A2G	C2-N2-C7	3.78	128.29	122.90
18	A	4723	A2G	C1-C2-N2	3.76	116.92	110.49
18	A	4722	A2G	C1-C2-N2	3.75	116.89	110.49
17	A	4704	NAG	C1-O5-C5	3.74	117.26	112.19
18	A	4718	A2G	C1-C2-N2	3.74	116.88	110.49
18	B	4712	A2G	O5-C1-C2	3.48	116.79	111.29
17	A	4707	NAG	C1-O5-C5	3.43	116.84	112.19
18	A	4712	A2G	C2-N2-C7	3.42	127.77	122.90
17	A	4711	NAG	C1-O5-C5	3.32	116.69	112.19
18	A	4716	A2G	C2-N2-C7	3.22	127.48	122.90
17	A	4702	NAG	C1-O5-C5	3.03	116.30	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	4708	NAG	C1-O5-C5	2.99	116.24	112.19
18	B	4712	A2G	C1-O5-C5	-2.89	108.27	112.19
18	A	4712	A2G	O5-C1-C2	2.88	115.84	111.29
18	B	4719	A2G	O5-C1-C2	2.87	115.82	111.29
18	B	4722	A2G	C1-C2-N2	2.86	115.38	110.49
18	A	4719	A2G	O5-C1-C2	2.82	115.75	111.29
17	B	4709	NAG	C1-O5-C5	2.80	115.98	112.19
17	A	4711	NAG	O5-C1-C2	2.79	115.69	111.29
18	B	4716	A2G	C1-O5-C5	-2.78	108.43	112.19
18	A	4716	A2G	O5-C5-C6	2.73	111.48	107.20
18	A	4714	A2G	O5-C1-C2	2.71	115.57	111.29
18	A	4721	A2G	C1-C2-N2	2.56	114.87	110.49
18	B	4716	A2G	O5-C5-C6	2.47	111.07	107.20
18	B	4721	A2G	O5-C5-C6	2.44	111.02	107.20
17	B	4707	NAG	C1-O5-C5	2.41	115.45	112.19
18	B	4720	A2G	C1-O5-C5	-2.37	108.98	112.19
18	B	4712	A2G	O5-C5-C6	2.37	110.92	107.20
17	A	4707	NAG	O5-C1-C2	2.37	115.03	111.29
18	B	4723	A2G	C1-O5-C5	-2.32	109.05	112.19
18	B	4722	A2G	C1-O5-C5	-2.28	109.10	112.19
18	A	4718	A2G	O3-C3-C2	2.16	113.94	109.47
17	A	4706	NAG	C2-N2-C7	2.16	125.98	122.90
18	A	4722	A2G	O3-C3-C2	2.14	113.89	109.47
18	B	4721	A2G	C1-O5-C5	-2.12	109.33	112.19
18	B	4714	A2G	C1-O5-C5	2.02	114.93	112.19
18	B	4712	A2G	O3-C3-C2	2.02	113.64	109.47
18	A	4719	A2G	C1-O5-C5	-2.02	109.46	112.19
17	A	4707	NAG	O5-C5-C6	2.01	110.36	107.20
17	A	4707	NAG	C2-N2-C7	-2.00	120.05	122.90

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	A	4705	NAG	C3-C2-N2-C7
17	A	4705	NAG	C8-C7-N2-C2
17	A	4705	NAG	O7-C7-N2-C2
17	A	4708	NAG	C8-C7-N2-C2
17	A	4708	NAG	O7-C7-N2-C2
17	B	4711	NAG	C8-C7-N2-C2
17	B	4711	NAG	O7-C7-N2-C2
18	A	4718	A2G	C3-C2-N2-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	A	4722	A2G	C3-C2-N2-C7
17	A	4709	NAG	C8-C7-N2-C2
17	A	4709	NAG	O7-C7-N2-C2
17	B	4701	NAG	C8-C7-N2-C2
17	B	4705	NAG	C8-C7-N2-C2
17	B	4711	NAG	C1-C2-N2-C7
17	A	4707	NAG	O5-C5-C6-O6
17	B	4701	NAG	O7-C7-N2-C2
17	B	4705	NAG	O7-C7-N2-C2
18	B	4723	A2G	O5-C5-C6-O6
18	B	4716	A2G	O5-C5-C6-O6
17	B	4710	NAG	C4-C5-C6-O6
17	B	4701	NAG	C1-C2-N2-C7
17	B	4705	NAG	C1-C2-N2-C7
17	B	4711	NAG	O5-C5-C6-O6
17	A	4707	NAG	C4-C5-C6-O6
18	A	4719	A2G	C1-C2-N2-C7
18	B	4721	A2G	O5-C5-C6-O6
18	A	4722	A2G	O5-C5-C6-O6
18	B	4714	A2G	O5-C5-C6-O6
18	B	4718	A2G	O5-C5-C6-O6
18	B	4712	A2G	O5-C5-C6-O6
18	A	4712	A2G	C3-C2-N2-C7
18	B	4722	A2G	C3-C2-N2-C7
17	B	4710	NAG	O5-C5-C6-O6
18	B	4712	A2G	C1-C2-N2-C7
17	A	4704	NAG	C1-C2-N2-C7
17	A	4706	NAG	C3-C2-N2-C7
18	A	4716	A2G	C3-C2-N2-C7
17	B	4709	NAG	O5-C5-C6-O6
18	B	4719	A2G	C1-C2-N2-C7
18	B	4723	A2G	C4-C5-C6-O6
18	A	4712	A2G	C4-C5-C6-O6
18	B	4717	A2G	C4-C5-C6-O6
17	A	4704	NAG	C3-C2-N2-C7
18	A	4718	A2G	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	4710	NAG	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	4707	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.

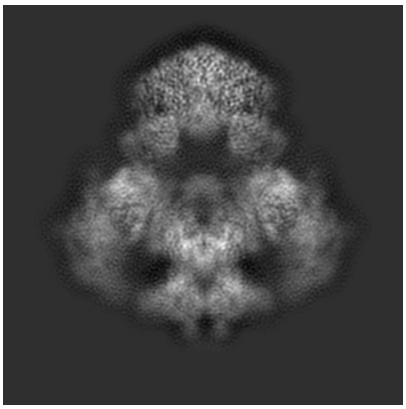
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-36663. These allow visual inspection of the internal detail of the map and identification of artifacts.

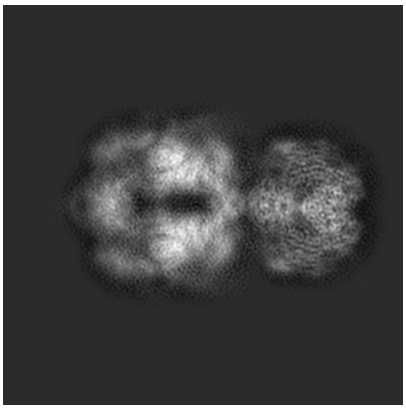
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

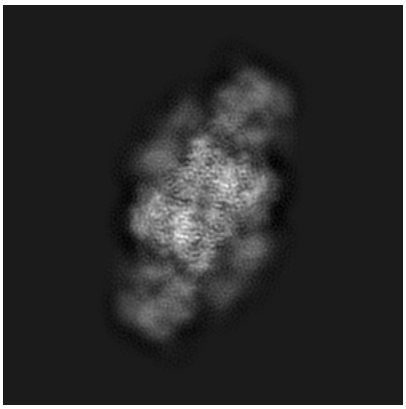
6.1.1 Primary map



X

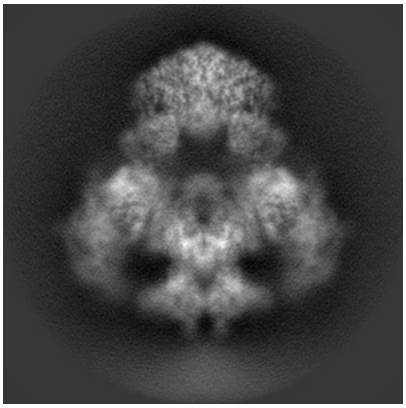


Y

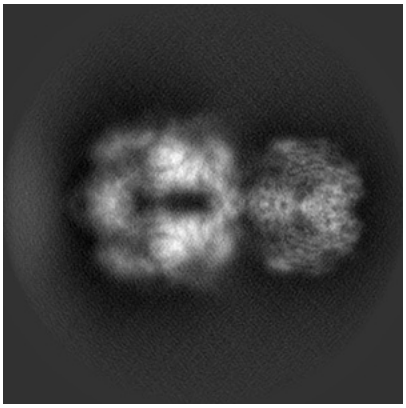


Z

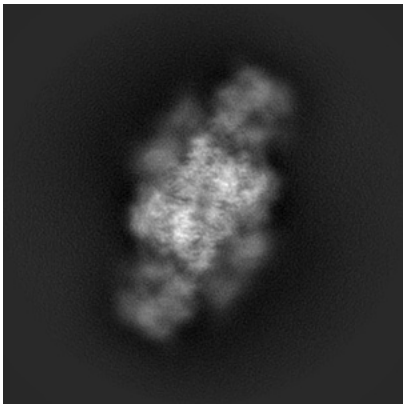
6.1.2 Raw map



X



Y

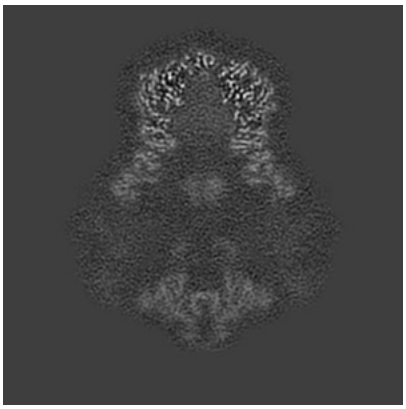


Z

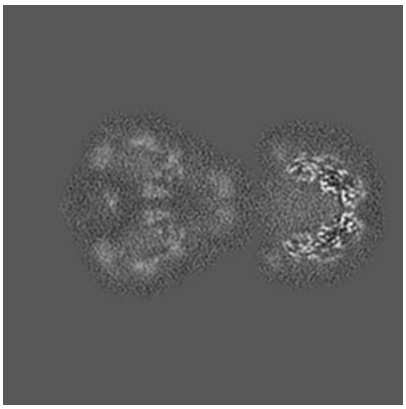
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

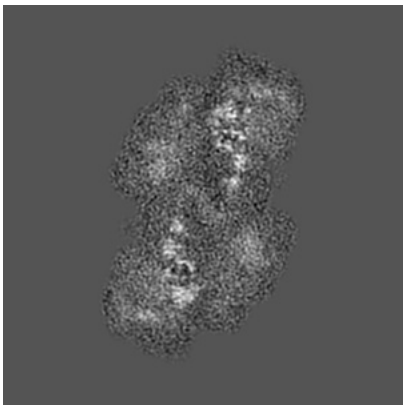
6.2.1 Primary map



X Index: 130

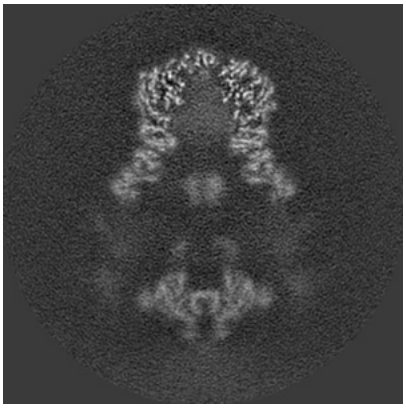


Y Index: 130

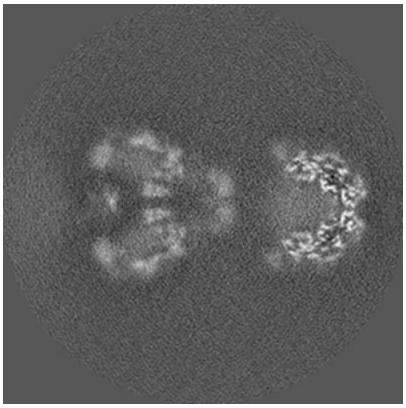


Z Index: 130

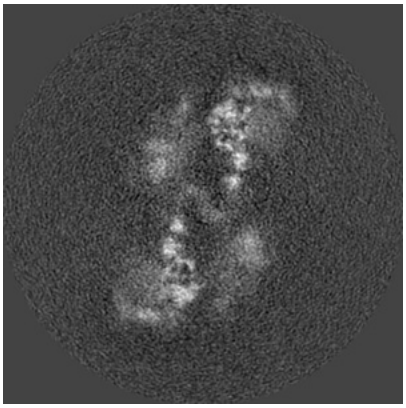
6.2.2 Raw map



X Index: 130



Y Index: 130

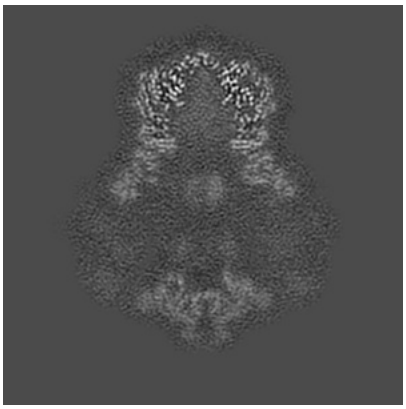


Z Index: 130

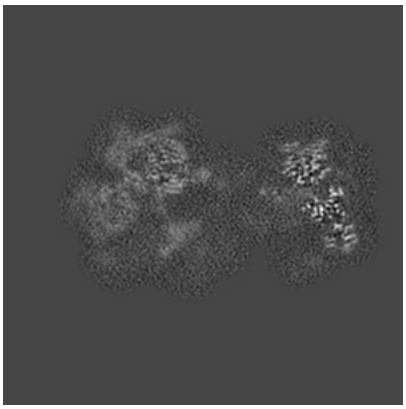
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

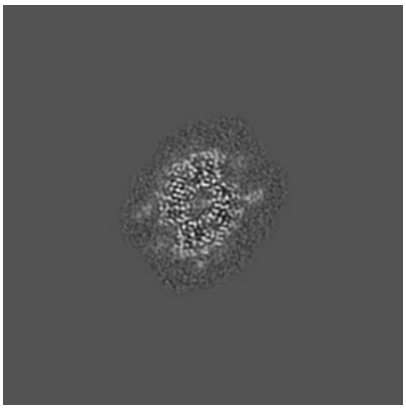
6.3.1 Primary map



X Index: 129

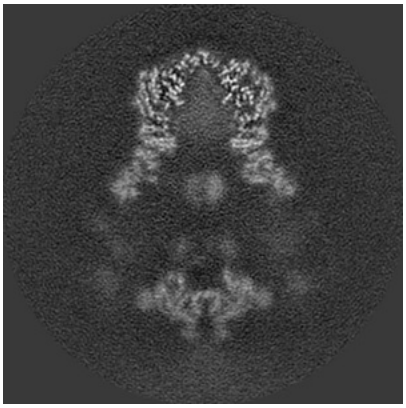


Y Index: 145

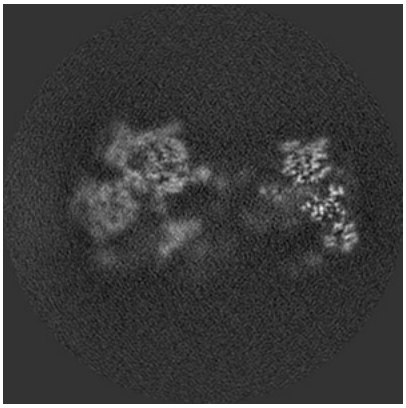


Z Index: 215

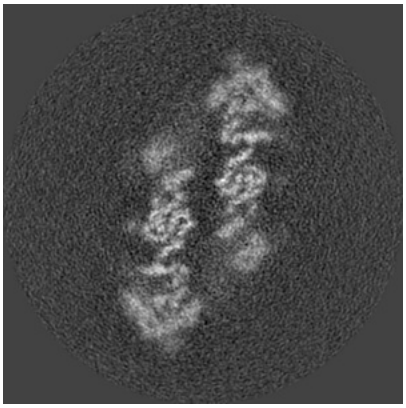
6.3.2 Raw map



X Index: 129



Y Index: 145

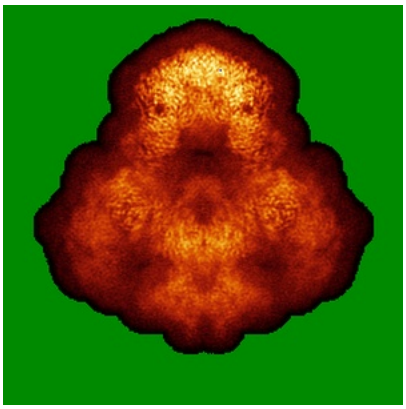


Z Index: 115

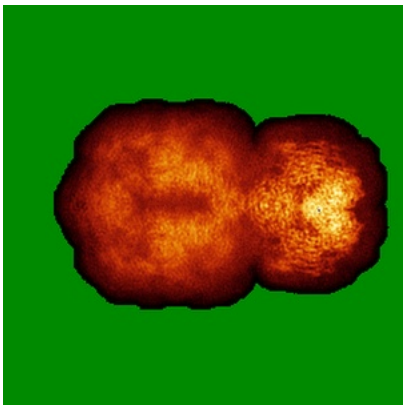
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

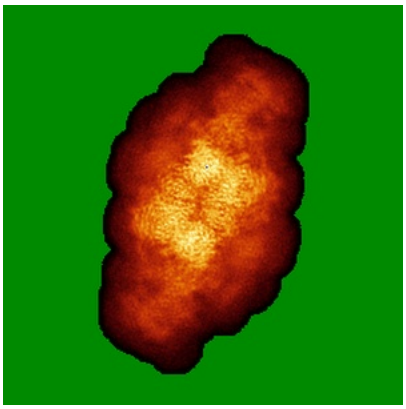
6.4.1 Primary map



X

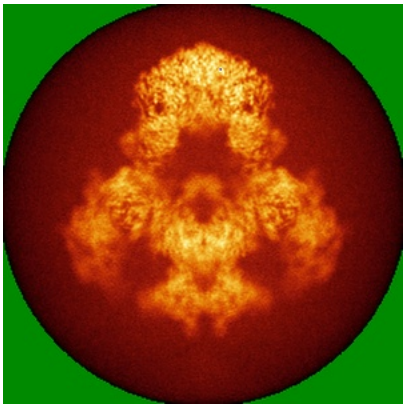


Y

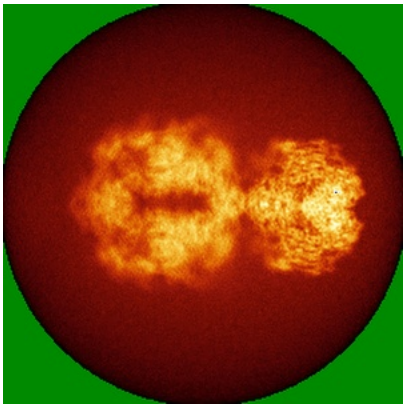


Z

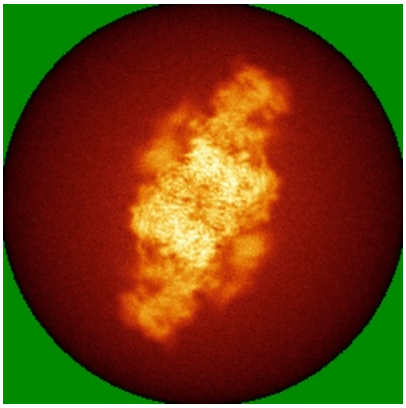
6.4.2 Raw map



X



Y

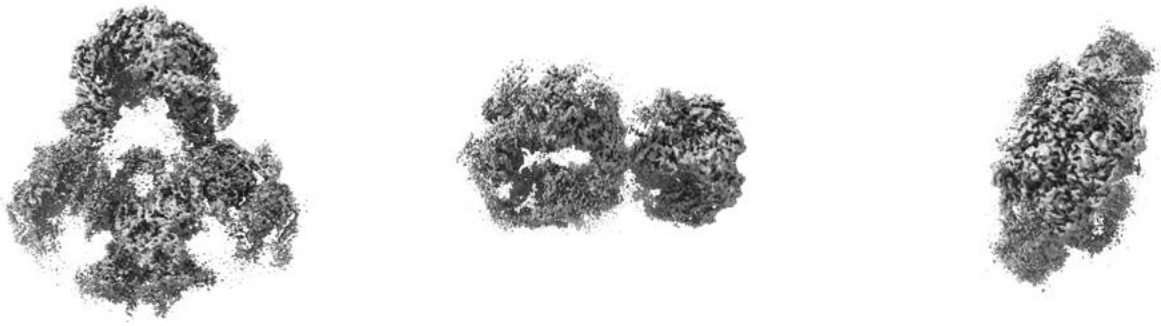


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

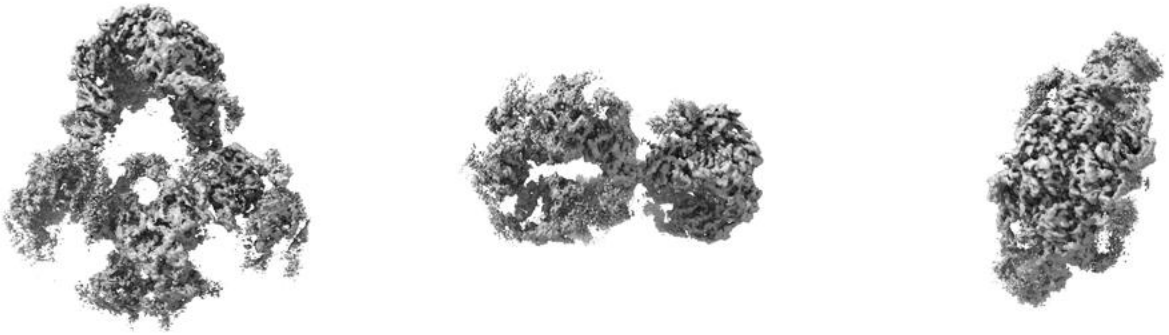
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0242. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

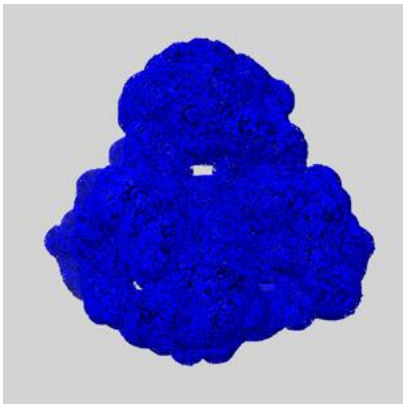
6.6 Mask visualisation

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

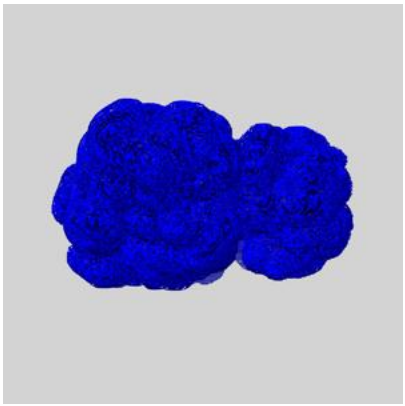
A mask typically either:

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

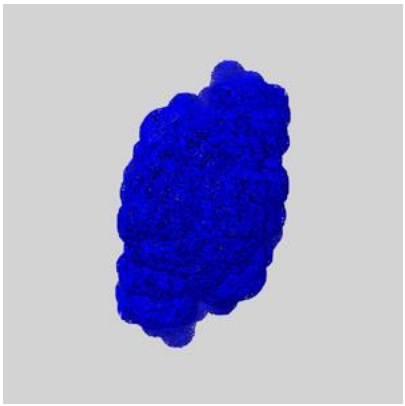
6.6.1 emd_36663_msk_1.map



X



Y

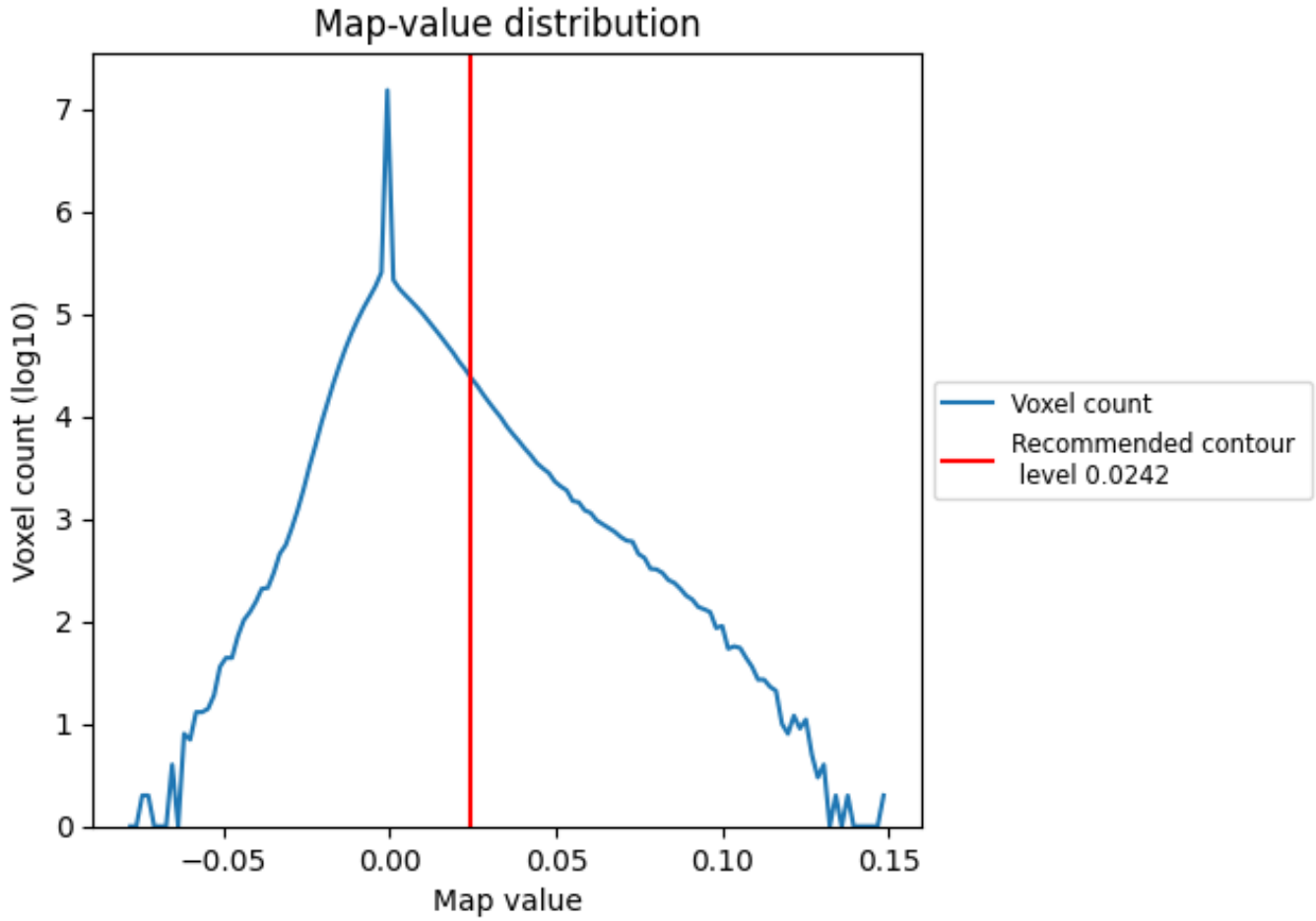


Z

7 Map analysis

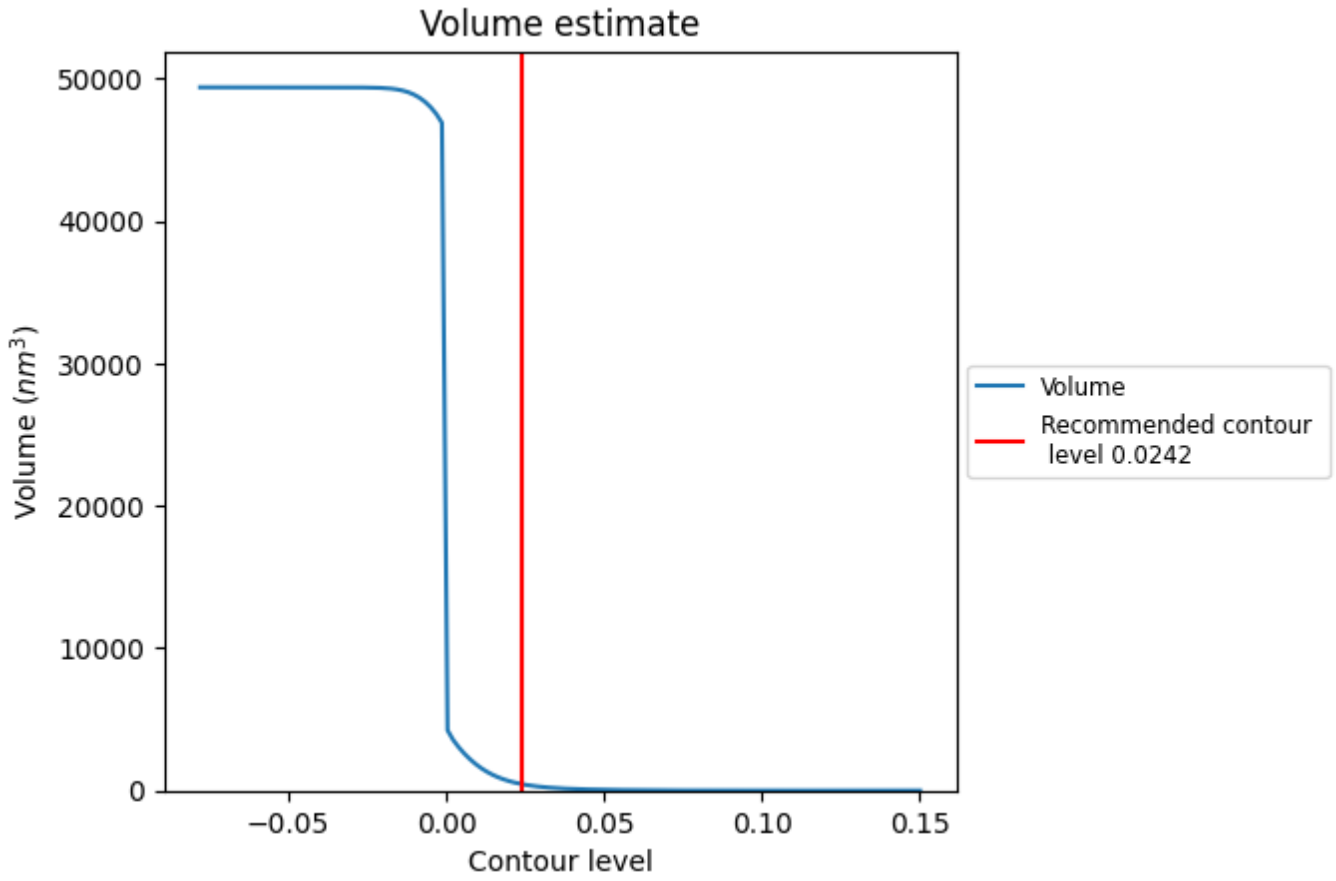
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

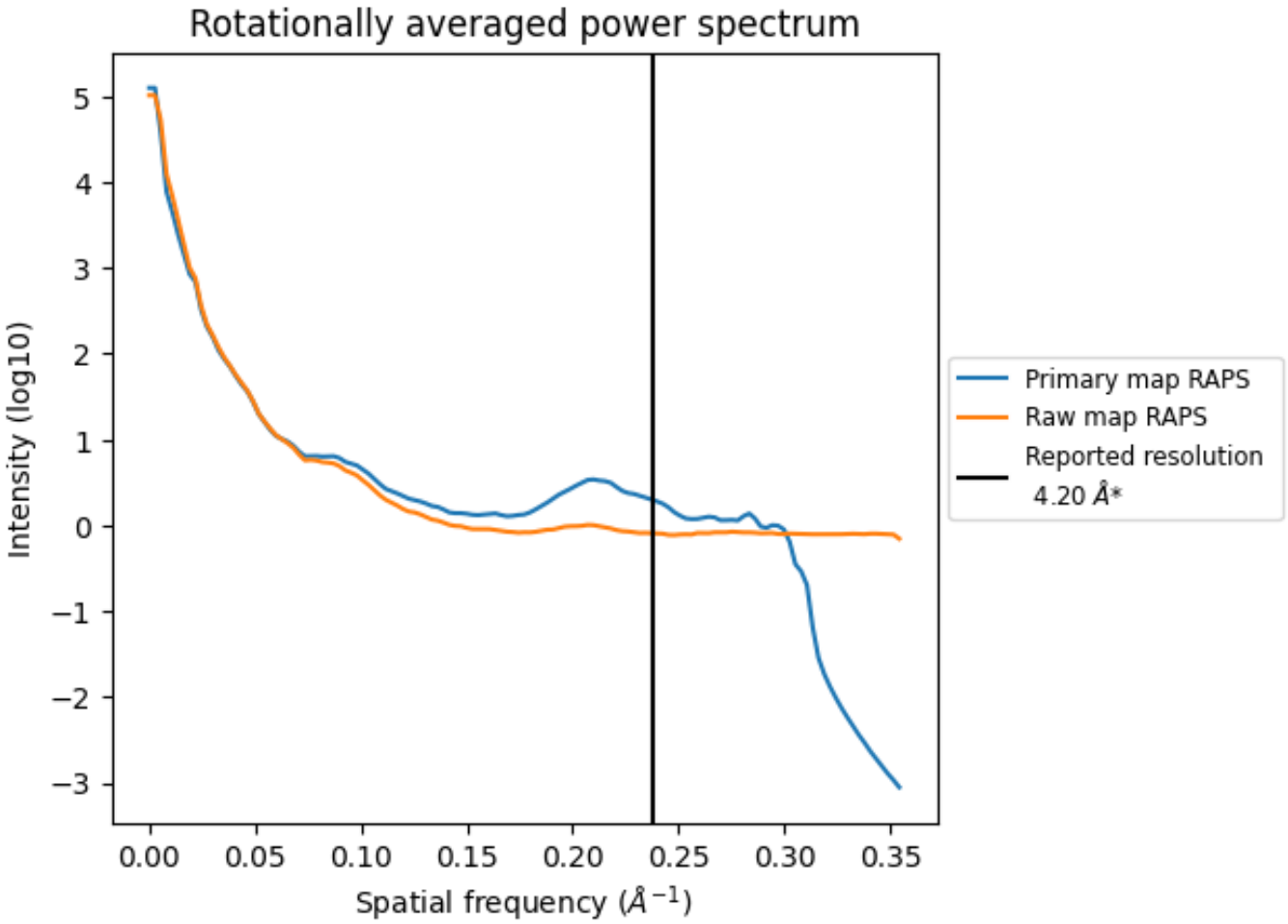
7.2 Volume estimate



The volume at the recommended contour level is 445 nm^3; this corresponds to an approximate mass of 402 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)

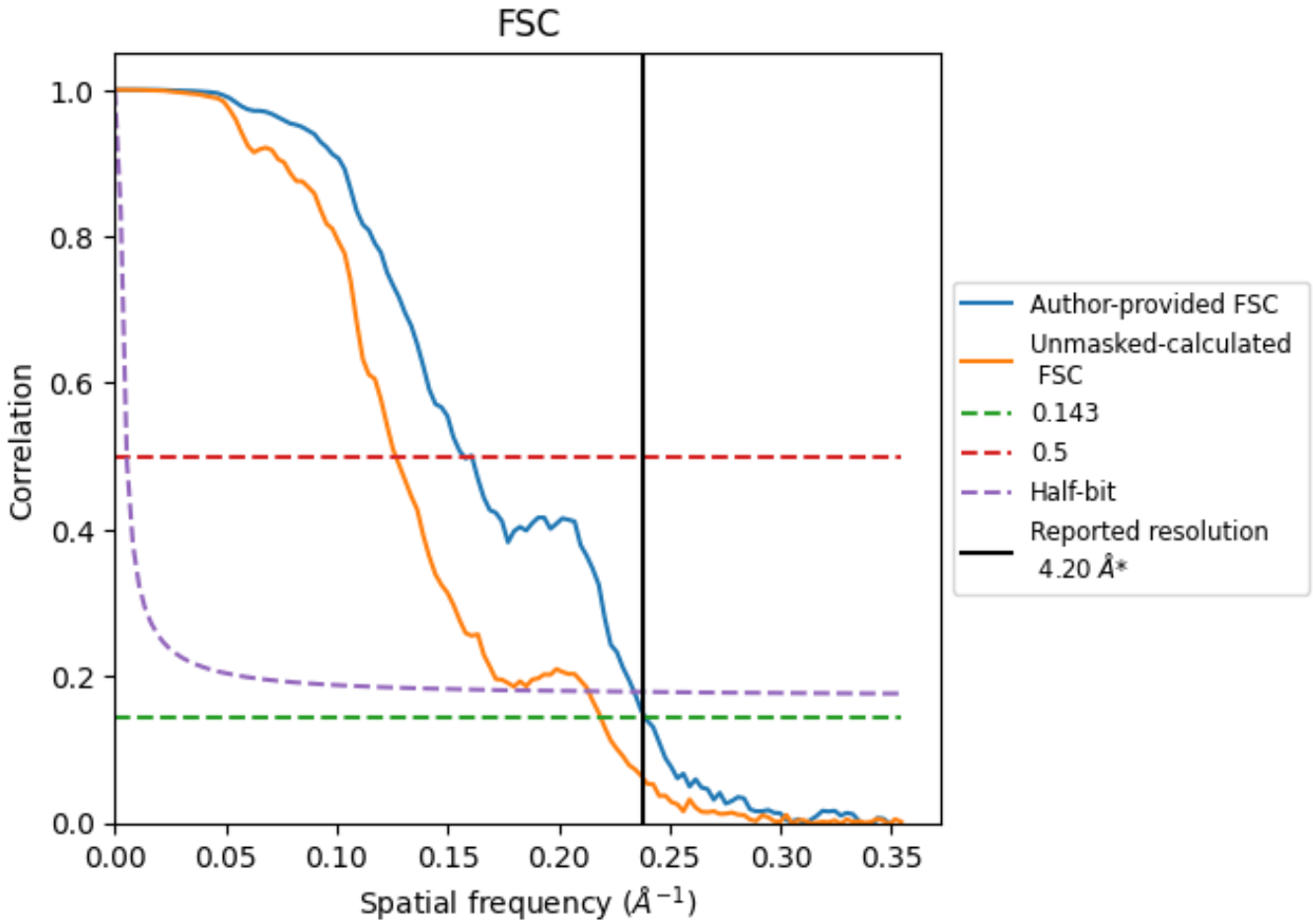


*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

8.2 Resolution estimates (i)

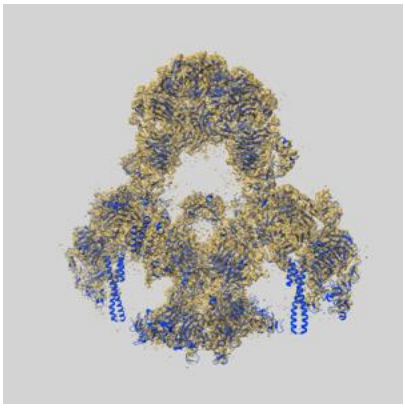
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.18	6.36	4.27
Unmasked-calculated*	4.57	7.90	4.69

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

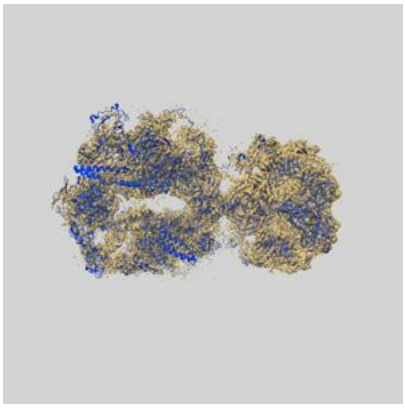
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-36663 and PDB model 8JUT. Per-residue inclusion information can be found in section 3 on page 16.

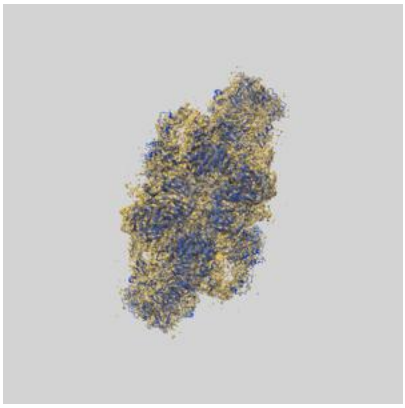
9.1 Map-model overlay



X



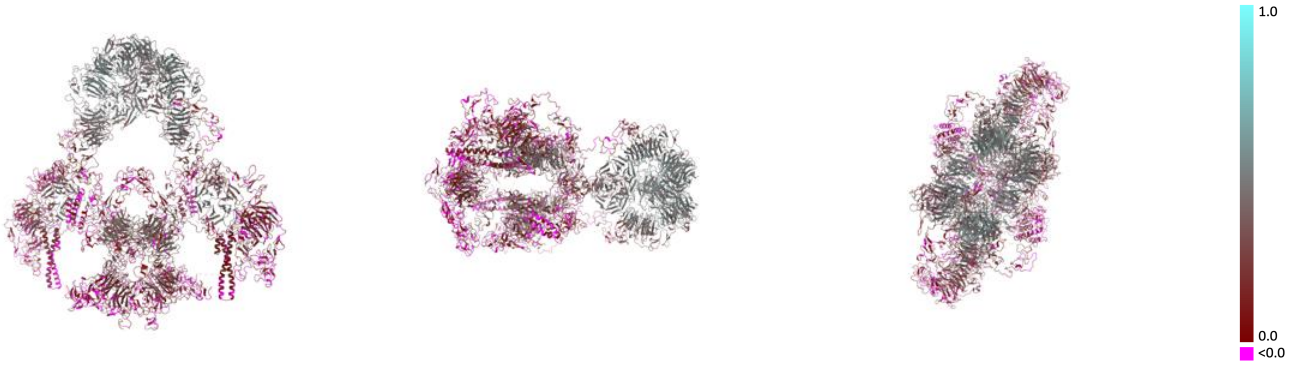
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0242 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.

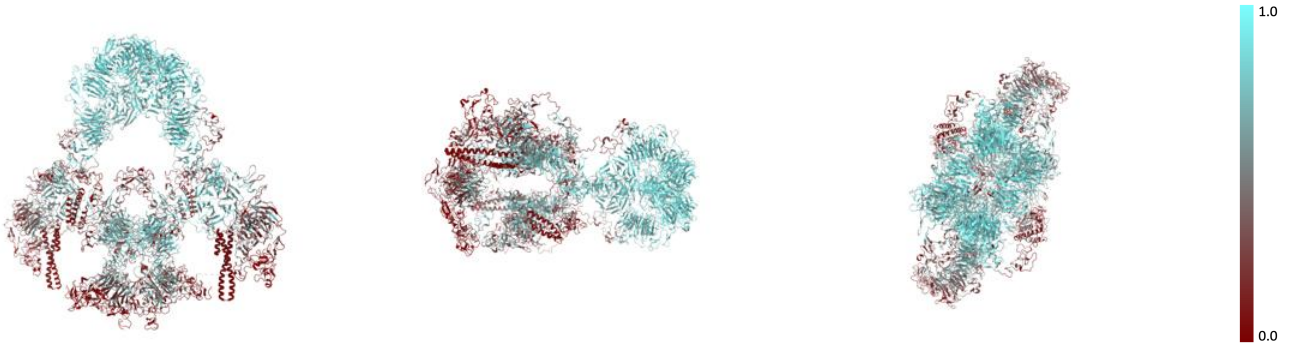
9.2 Q-score mapped to coordinate model



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.

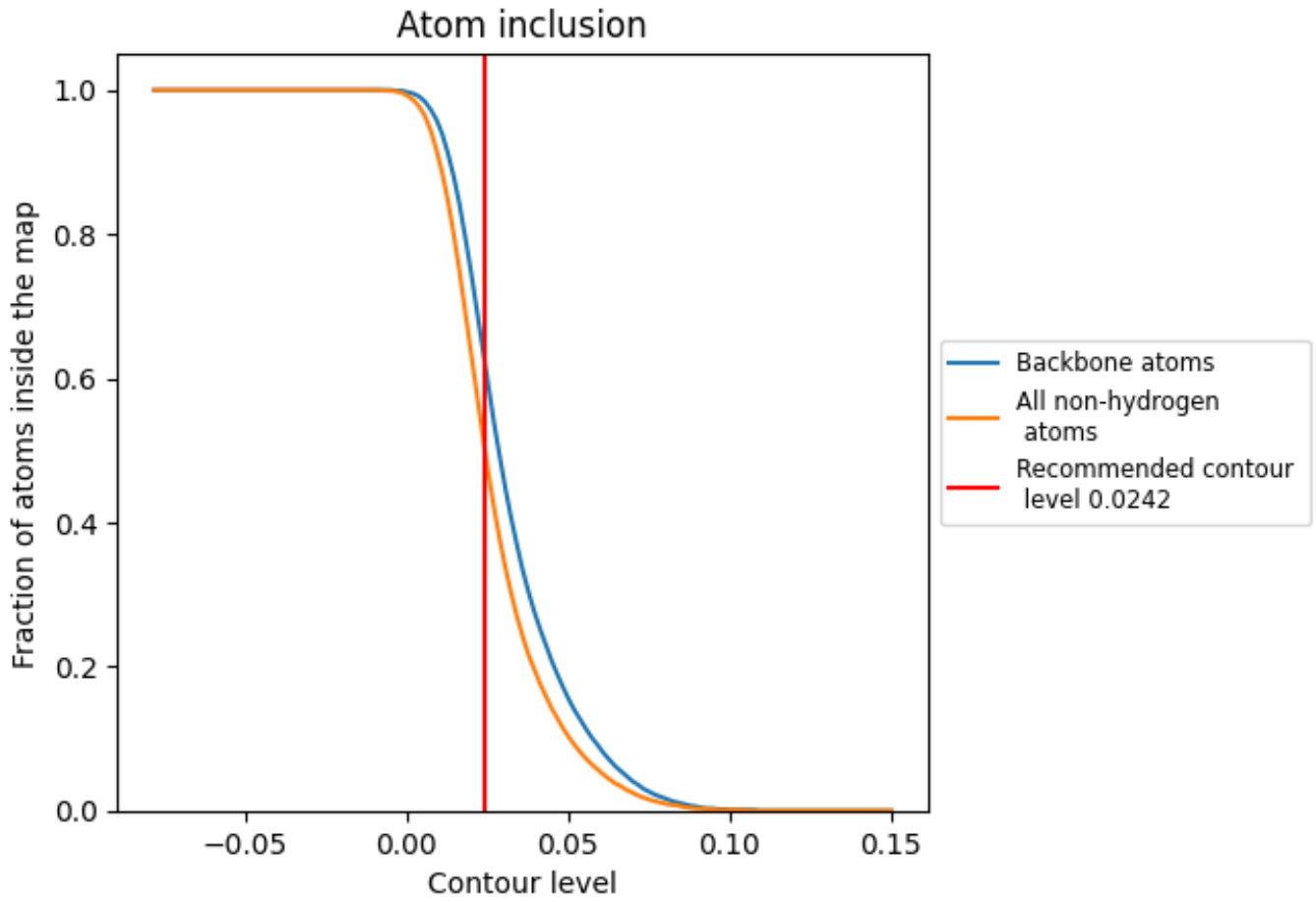
9.3 Atom inclusion mapped to coordinate model



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 (0.0242).

9.4 Atom inclusion (i)



At the recommended contour level, 63% of all backbone atoms, 50% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0242) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5050	0.2660
0	0.3850	0.2180
1	0.3440	0.2710
2	0.1540	0.3230
3	0.2050	0.1120
4	0.0820	0.1020
5	0.1640	0.1380
6	0.0000	0.0090
7	0.0260	0.1010
8	0.0000	-0.0760
9	0.0160	0.0770
A	0.5220	0.2700
B	0.5360	0.2830
C	0.1000	0.0690
D	0.0830	0.0740
E	0.0360	0.0950
F	0.0330	0.1270
G	0.1670	0.0860
H	0.6790	0.3580
I	0.8790	0.4280
J	0.4380	0.2380
K	0.5450	0.3920
L	0.5000	0.3310
M	0.7500	0.4240
N	0.2000	0.2410
O	0.8210	0.4120
P	0.8490	0.4680
Q	0.6250	0.2130
R	0.6360	0.4410
S	0.5360	0.3240
T	0.8570	0.4090
U	0.3610	0.2860
V	0.1790	0.0880
W	0.5130	0.3470
X	0.3570	0.1840

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Y	0.3570	0.2610
Z	0.3440	0.2510
a	0.3570	0.1800
b	0.7210	0.4070
c	0.4290	0.2360
d	0.3930	0.2950
e	0.2050	0.1320
f	0.4100	0.3070
g	0.3770	0.2160
h	0.1280	0.0990
i	0.2050	0.1630
j	0.1310	-0.0180
k	0.1310	0.1450
l	0.0160	0.0730
m	0.0260	0.1920
n	0.0710	-0.0280
o	0.0710	0.0970
p	0.5130	0.3370
q	0.4290	0.4120
r	0.5640	0.3000
s	0.6070	0.4470
t	0.4640	0.3800
u	0.2460	0.2960
v	0.3930	0.3110
w	0.7210	0.3990
x	0.4290	0.2300
y	0.4290	0.2700
z	0.1030	0.0360