Full wwPDB EM Validation Report ⓘ

Jun 12, 2024 – 10:27 AM JST

PDB ID	:	8JX8
EMDB ID	:	EMD-36692
Title	:	rat megalin head
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	:	2023-06-30
Resolution	:	3.30 Å(reported)
Based on initial model	:	.

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 ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

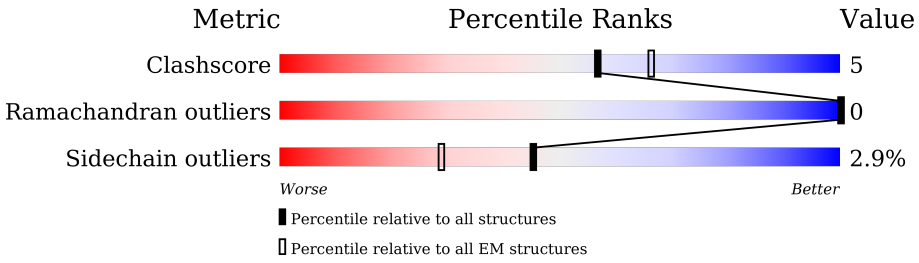
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (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 3.30 Å.

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



Metric	Whole archive (#Entries)	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	26% 5% 69%
1	B	4660	26% 69%
2	C	6	67% 33%
2	I	6	83% 17%
3	D	3	33% 100%
3	J	3	100%
4	G	5	20% 60% 40%
4	K	5	80% 20%

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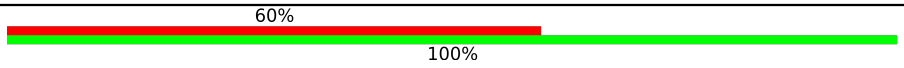
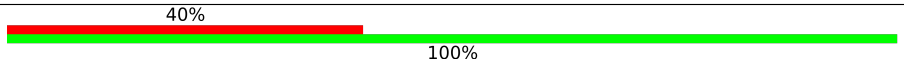
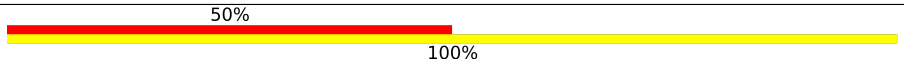
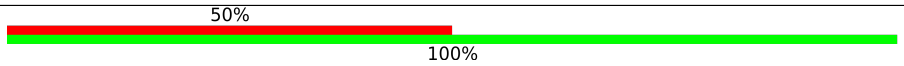
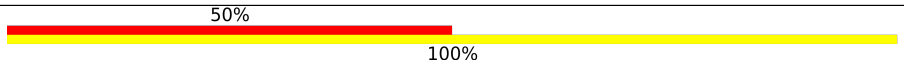
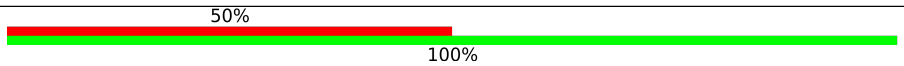
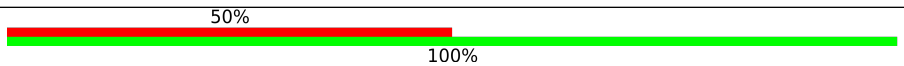
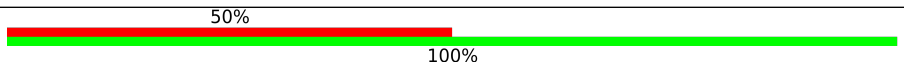
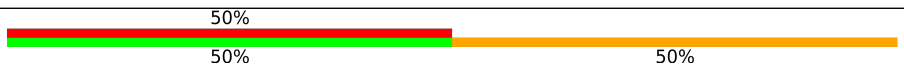
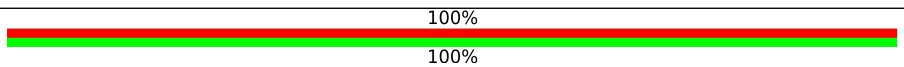
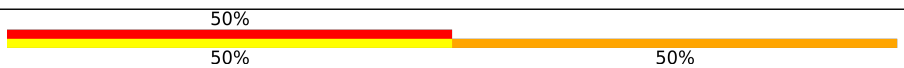
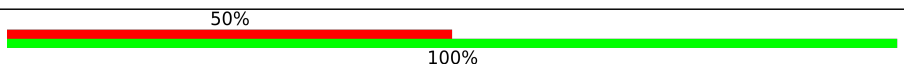
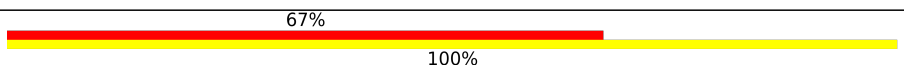
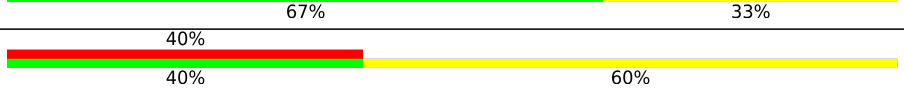
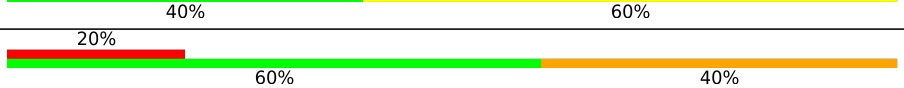
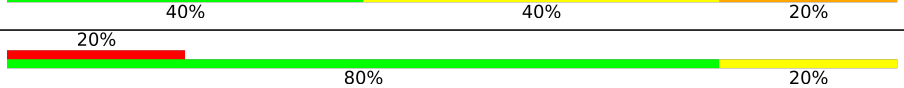
Mol	Chain	Length	Quality of chain
5	H	5	
5	L	5	
6	E	2	
6	M	2	
6	N	2	
6	P	2	
6	R	2	
6	S	2	
6	T	2	
6	V	2	
6	W	2	
6	Y	2	
6	a	2	
6	b	2	
7	F	3	
7	U	3	
8	O	5	
8	Q	5	
8	X	5	
8	Z	5	

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 23459 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	1436	Total	C	N	O	S	0	0
			11221	7043	1967	2133	78		
1	B	1434	Total	C	N	O	S	0	0
			11208	7035	1965	2131	77		

- Molecule 2 is a protein called unclear peptide.

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

- Molecule 3 is a protein called unclear peptide.

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

- Molecule 4 is a protein called unclear peptide.

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

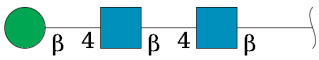
- Molecule 5 is a protein called unclear peptide.

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

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

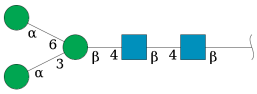
Mol	Chain	Residues	Atoms	AltConf	Trace
6	E	2	Total C N O 28 16 2 10	0	0
6	M	2	Total C N O 28 16 2 10	0	0
6	N	2	Total C N O 28 16 2 10	0	0
6	P	2	Total C N O 28 16 2 10	0	0
6	R	2	Total C N O 28 16 2 10	0	0
6	S	2	Total C N O 28 16 2 10	0	0
6	T	2	Total C N O 28 16 2 10	0	0
6	V	2	Total C N O 28 16 2 10	0	0
6	W	2	Total C N O 28 16 2 10	0	0
6	Y	2	Total C N O 28 16 2 10	0	0
6	a	2	Total C N O 28 16 2 10	0	0
6	b	2	Total C N O 28 16 2 10	0	0

- Molecule 7 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.



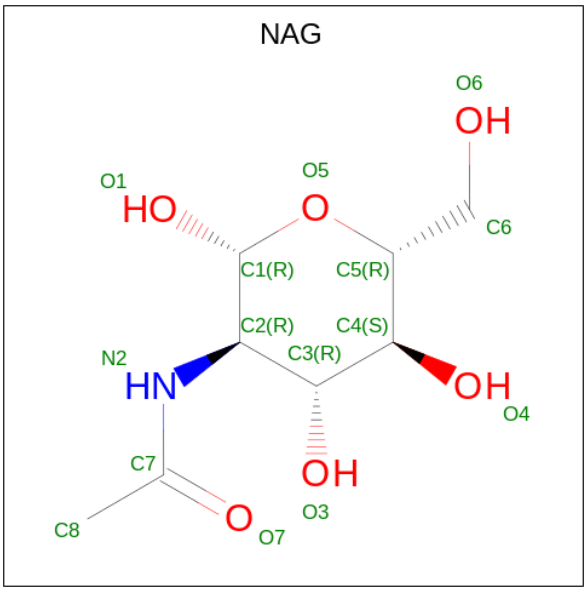
Mol	Chain	Residues	Atoms				AltConf	Trace
7	F	3	Total	C	N	O	0	0
			39	22	2	15		
7	U	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 8 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.



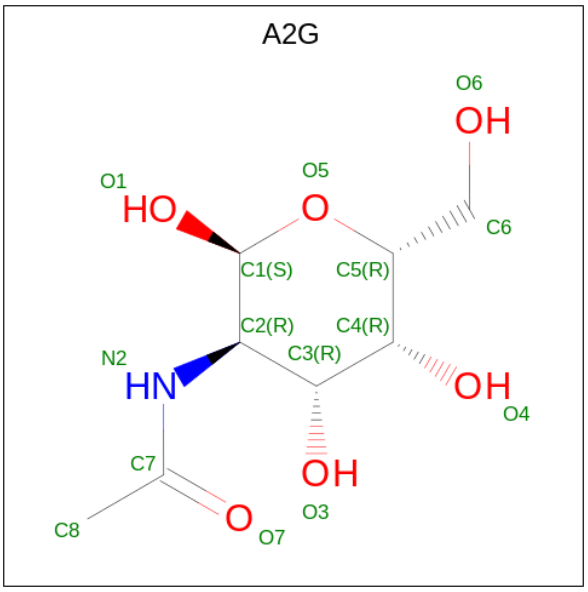
Mol	Chain	Residues	Atoms				AltConf	Trace
8	O	5	Total	C	N	O	0	0
			61	34	2	25		
8	Q	5	Total	C	N	O	0	0
			61	34	2	25		
8	X	5	Total	C	N	O	0	0
			61	34	2	25		
8	Z	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 10 is 2-acetamido-2-deoxy-alpha-D-galactopyranose (three-letter code: A2G) (formula: $C_8H_{15}NO_6$).



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

- Molecule 11 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
11	A	5	Total Ca 5 5	0
11	B	5	Total Ca 5 5	0

- Molecule 12 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

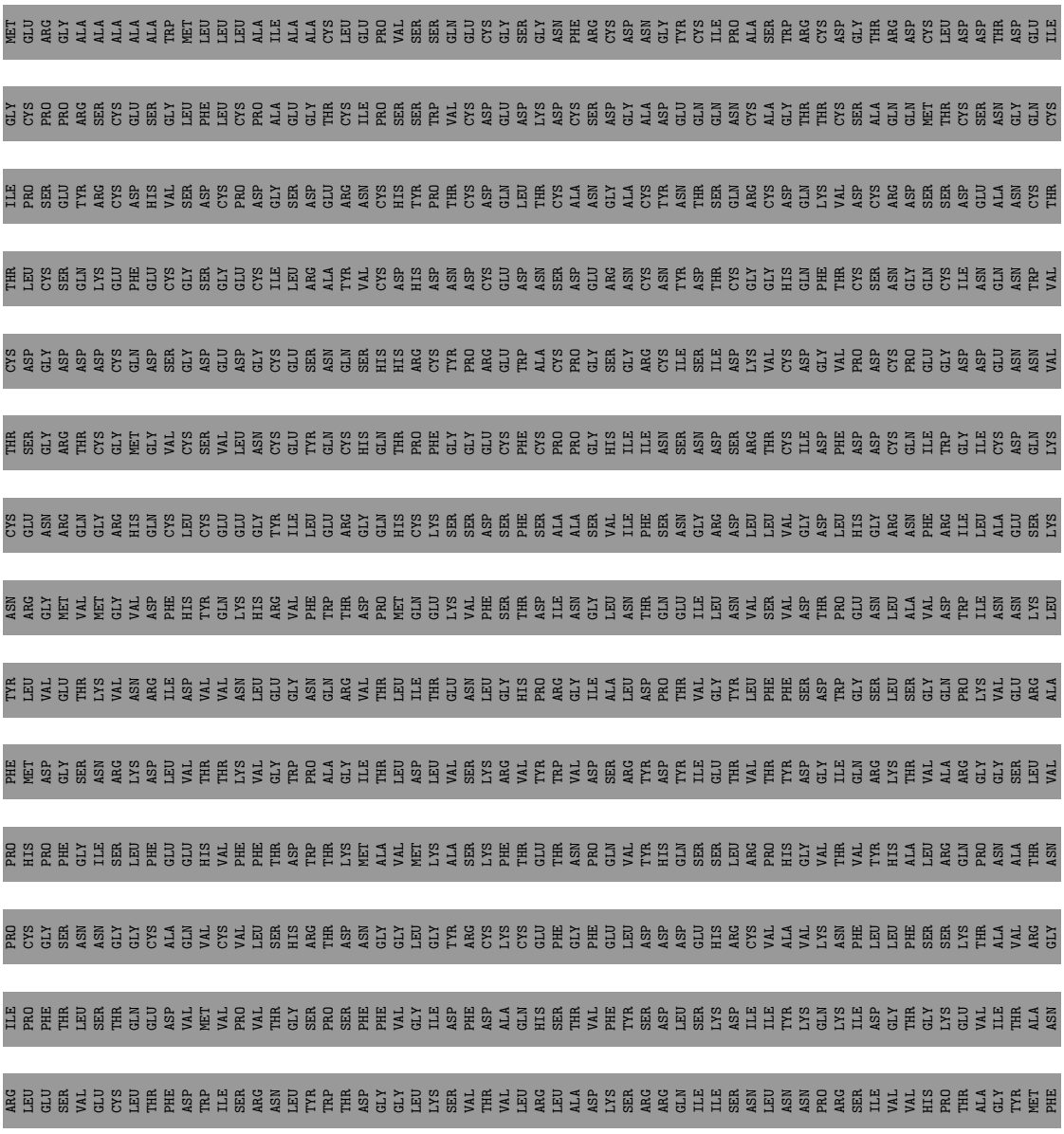
Mol	Chain	Residues	Atoms	AltConf
12	A	1	Total Ni 1 1	0
12	B	1	Total Ni 1 1	0

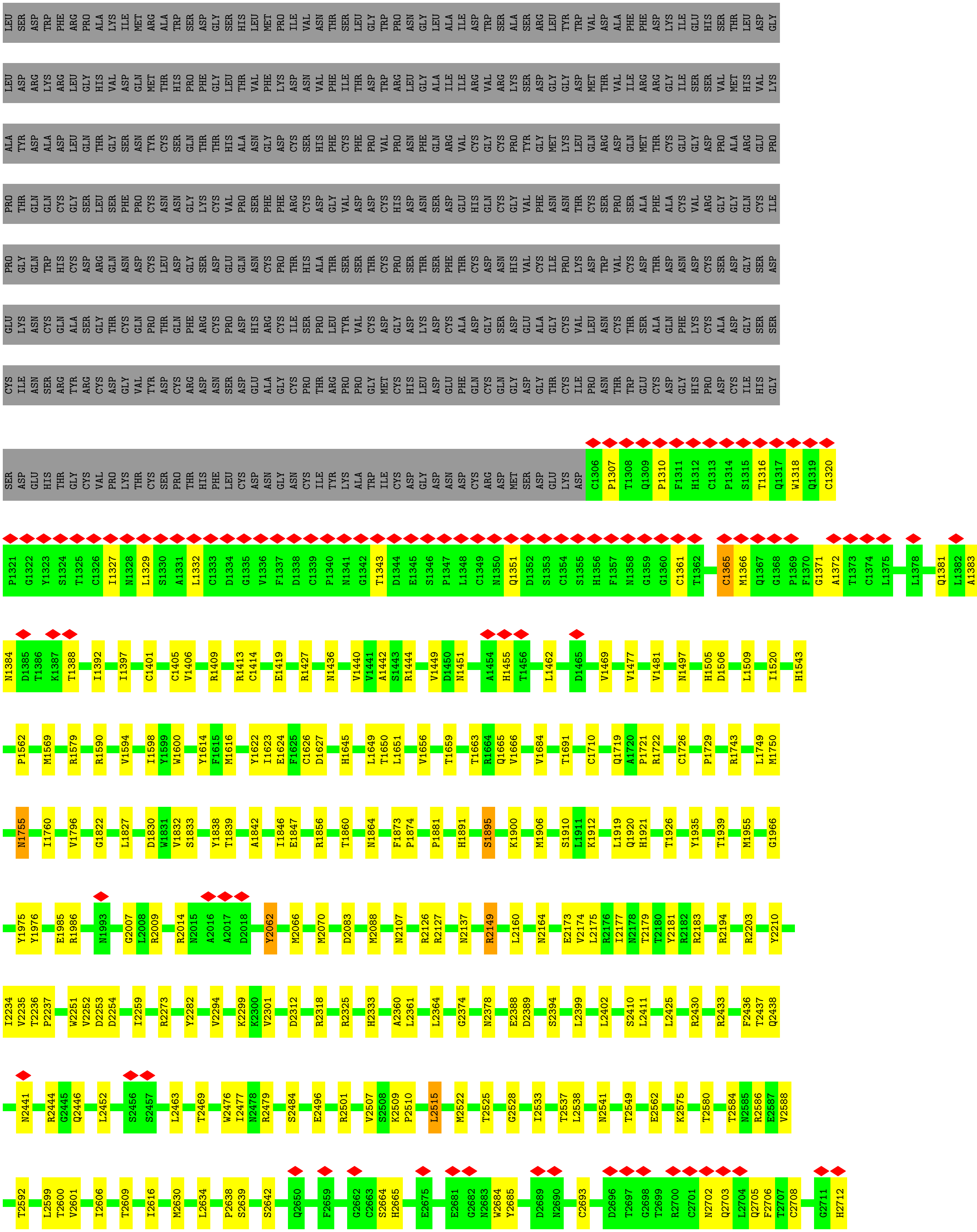
3 Residue-property plots (i)

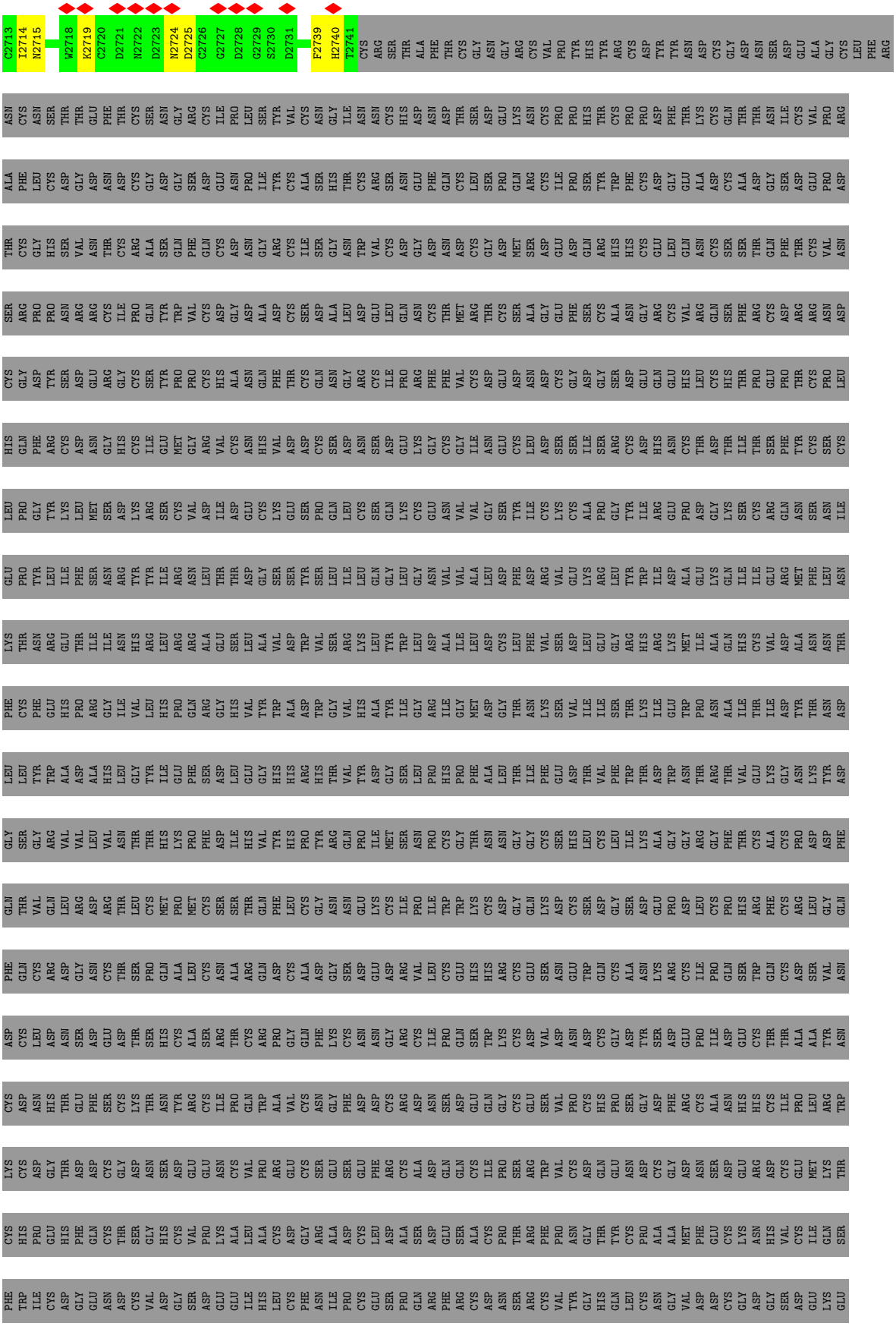
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

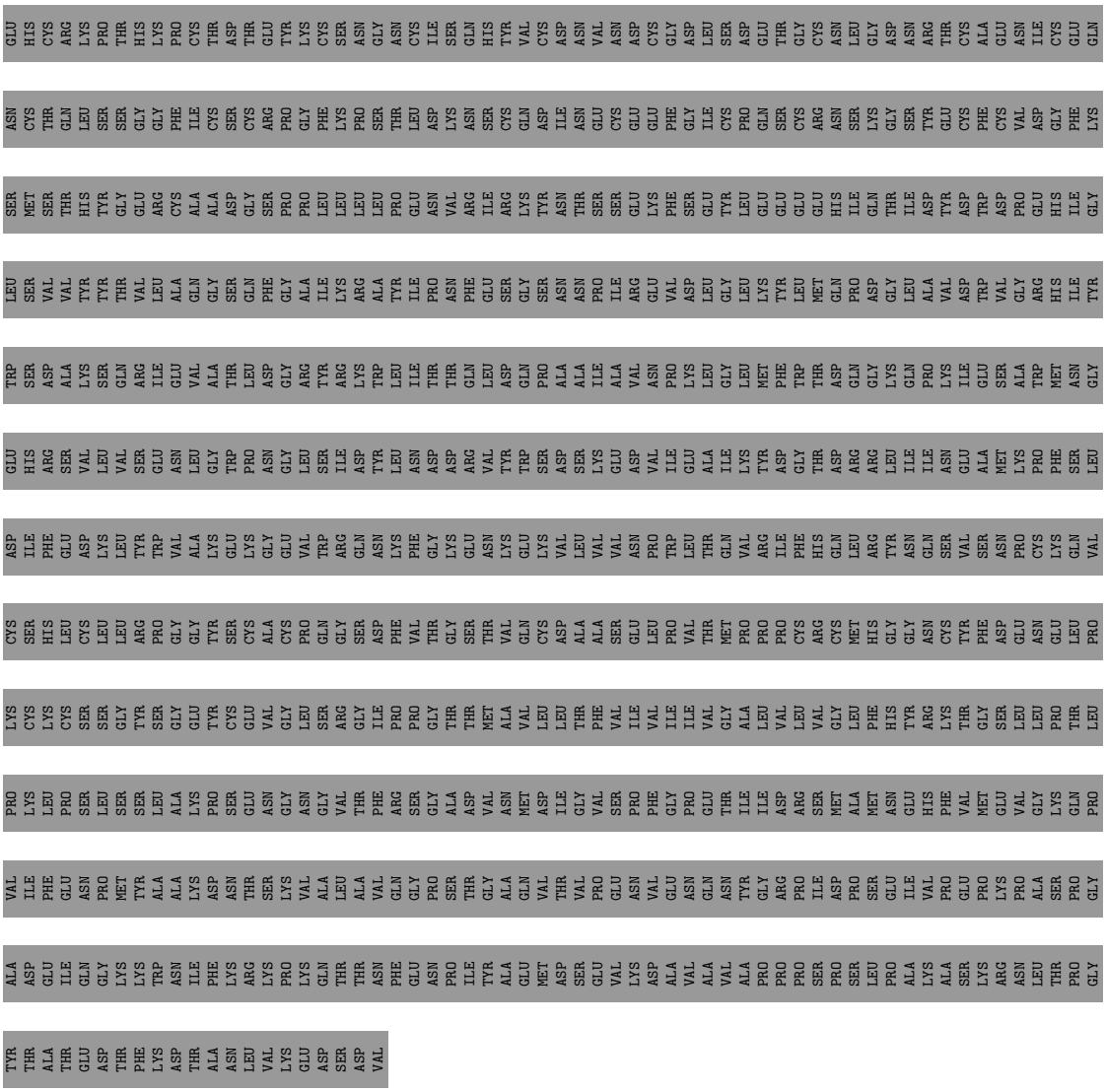
- Molecule 1: LDL receptor related protein 2

Chain A:



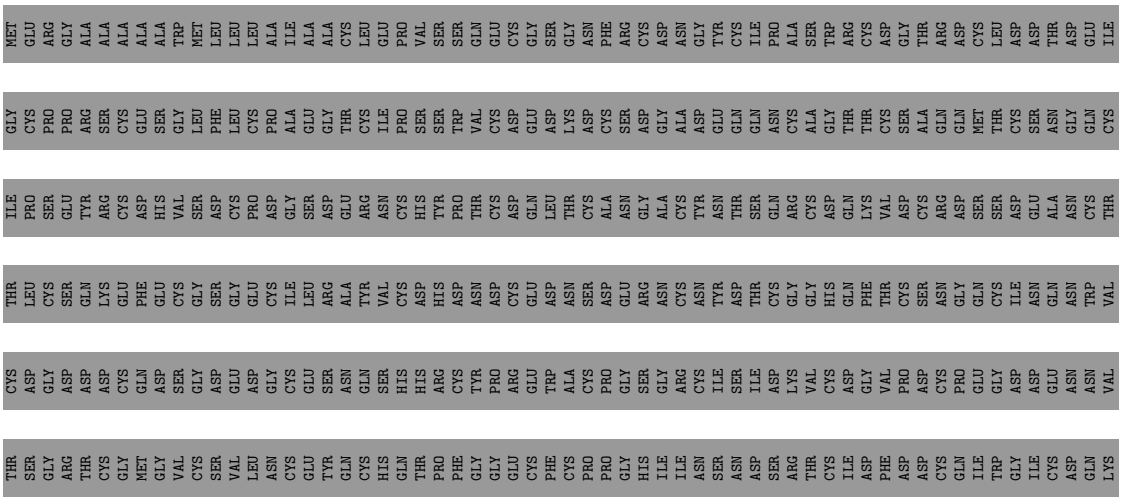

LEU SER ASP TRP PHE ARG PRO ALA LYS ILE MET ARG ALA TRP SER ASP GLY SER HIS LEU MET PRO ILE VAL ASN THR SER LEU GLY TRP PRO ASN GLY LEU ALA ILE ASP TRP SER ALA SER ARG LEU TYR TRP VAL ASP ALA PHE PHE ASP LYS ILE GLU HIS SER THR LEU ASP GLY
LEU ASP ARG LYS ARG LEU GLY HIS VAL ASP GLN MET THR HIS PRO PHE GLY LEU THR VAL PHE LYS ASP ASN VAL PHE ILE THR ASP TRP ARG LEU GLY ALA ILE ILE ARG VAL ARG LYS SER ASP GLY GLY ASP MET THR VAL ILE ARG ARG GLY ILE SER SER VAL MET HIS VAL LYS
ALA TYR ASP ALA ASP LEU GLN THR GLY SER ASN TYR CYS SER GLN THR THR HIS ALA ASN GLY ASP CYS SER HIS PHE CYS PHE PRO VAL PRO ASN PHE GLN ARG VAL CYS GLY CYS PRO TYR GLY MET LYS LEU GLN ARG ASP GLN MET THR CYS GLU GLY ASP PRO ALA ARG GLU PRO
PRO THR GLN GLN CYS GLY SER LEU SER PHE PRO CYS ASN ASN GLY LYS CYS VAL PRO SER PHE PHE ARG CYS ASP GLY VAL ASP ASP CYS HIS ASP ASN SER ASP GLU HIS GLN CYS GLY VAL PHE ASN ASN THR CYS SER PRO SER ALA PHE ALA CYS VAL ARG GLY GLY GLN CYS ILE
PRO GLY GLN TRP HIS CYS ASP ARG GLN ASN ASP CYS LEU ASP ASP GLY SER ASP GLU GLN ASN CYS PRO THR HIS ALA THR SER SER THR CYS PRO SER THR SER PHE THR CYS ASP ASN HIS VAL CYS ILE PRO LYS ASP TRP VAL CYS ASP THR ASP ASN ASP CYS SER ASP GLY SER ASP
GLU LYS ASN CYS GLN ALA SER GLY THR CYS GLN PRO THR GLN PHE ARG CYS PRO ASP HIS ARG CYS ILE SER PRO LEU TYR VAL CYS ASP GLY ASP LYS ASP CYS ALA ASP GLY SER ASP GLU ALA GLY CYS VAL LEU ASN CYS THR SER ALA GLN PHE LYS CYS ALA ASP GLY SER SER
CYS ILE ASN SER ARG TYR ARG CYS ASP GLY VAL TYR ASP CYS ARG ASP ASN SER ASP GLU ALA GLY CYS PRO THR ARG PRO PRO GLY MET CYS HIS LEU ASP GLU PHE GLN CYS GLN GLY ASP GLY THR CYS ILE PRO ASN THR TRP GLU CYS ASP GLY HIS PRO ASP CYS ILE HIS GLY
SER ASP GLU HIS THR GLY CYS VAL PRO LYS THR CYS SER PRO THR HIS PHE LEU CYS ASP ASN GLY ASN CYS ILE TYR LYS ALA TRP ILE CYS ASP GLY ASP ASN ASP CYS ARG ASP MET SER ASP GLU LYS ASP 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 E1345 S1346 P1347 L1348 C1349 N1350 Q1351 D1352 S1353 C1354 S1355 H1356 F1357 N1358 G1359 G1360 C1361 T1362 C1365 M1366 Q1367 G1368 P1369 F1370 G1371 A1372 T1373 C1374 L1375 L1378 Q1381 L1382 A1383
N1384 D1385 T1386 K1387 T1388 I1392 I1397 C1401 C1405 V1406 R1409 R1413 C1414 E1419 R1427 N1436 V1440 V1441 A1442 S1443 R1444 V1449 D1450 N1451 A1454 H1455 T1456 L1462 D1465 V1469 V1477 V1481 N1497 H1505 D1506 L1509 I1520 H1543
P1562 M1569 R1579 R1590 V1594 I1598 Y1599 W1600 Y1614 F1615 M1616 Y1622 I1623 E1624 F1625 C1626 D1627 H1645 L1649 T1650 L1651 V1656 T1659 T1663 R1664 Q1665 V1666 V1684 T1691 C1710 Q1719 A1720 P1721 R1722 C1726 P1729 R1743 L1749 M1750
N1755 I1760 V1796 G1822 L1827 D1830 W1831 V1832 S1833 Y1838 T1839 A1842 I1846 E1847 R1856 T1860 N1864 F1873 P1874 P1881 H1891 S1895 K1900 M1906 S1910 L1911 K1912 L1919 Q1920 H1921 T1926 Y1935 T1939 M1955 G1966
Y1975 Y1976 E1985 R1986 N1993 G2007 L2008 R2009 R2014 N2015 A2016 A2017 D2018 Y2062 M2066 M2070 D2083 M2088 N2107 R2126 R2127 N2137 R2149 L2160 N2164 E2173 V2174 L2175 R2176 I2177 N2178 T2179 T2180 Y2181 R2182 R2183 R2194 R2203 Y2210
I2234 V2235 T2236 P2237 W2251 V2252 D2253 D2254 I2259 R2273 Y2282 V2294 K2299 K2300 V2301 D2312 R2318 R2325 H2333 A2360 L2361 L2364 G2374 N2378 E2388 D2389 S2394 L2399 L2402 S2410 L2411 L2425 R2430 R2433 F2436 T2437 Q2438
N2441 R2444 G2445 Q2446 L2452 S2456 S2457 L2463 T2469 W2476 I2477 N2478 R2479 S2484 E2496 R2501 V2507 S2508 K2509 P2510 L2515 M2522 T2525 G2528 I2533 T2537 L2538 N2541 T2549 E2562 K2575 T2580 T2584 N2585 R2586 E2587 V2588
T2592 L2599 T2600 V2601 I2606 T2609 I2616 M2630 L2634 P2638 S2639 S2642 Q2650 F2659 G2662 C2663 S2664 H2665 E2675 E2681 G2682 N2683 W2684 Y2685 D2689 N2690 C2693 D2696 T2697 G2698 T2699 R2700 C2701 N2702 Q2703 L2704 Q2705 F2706 T2707 C2708 G2711 H2712

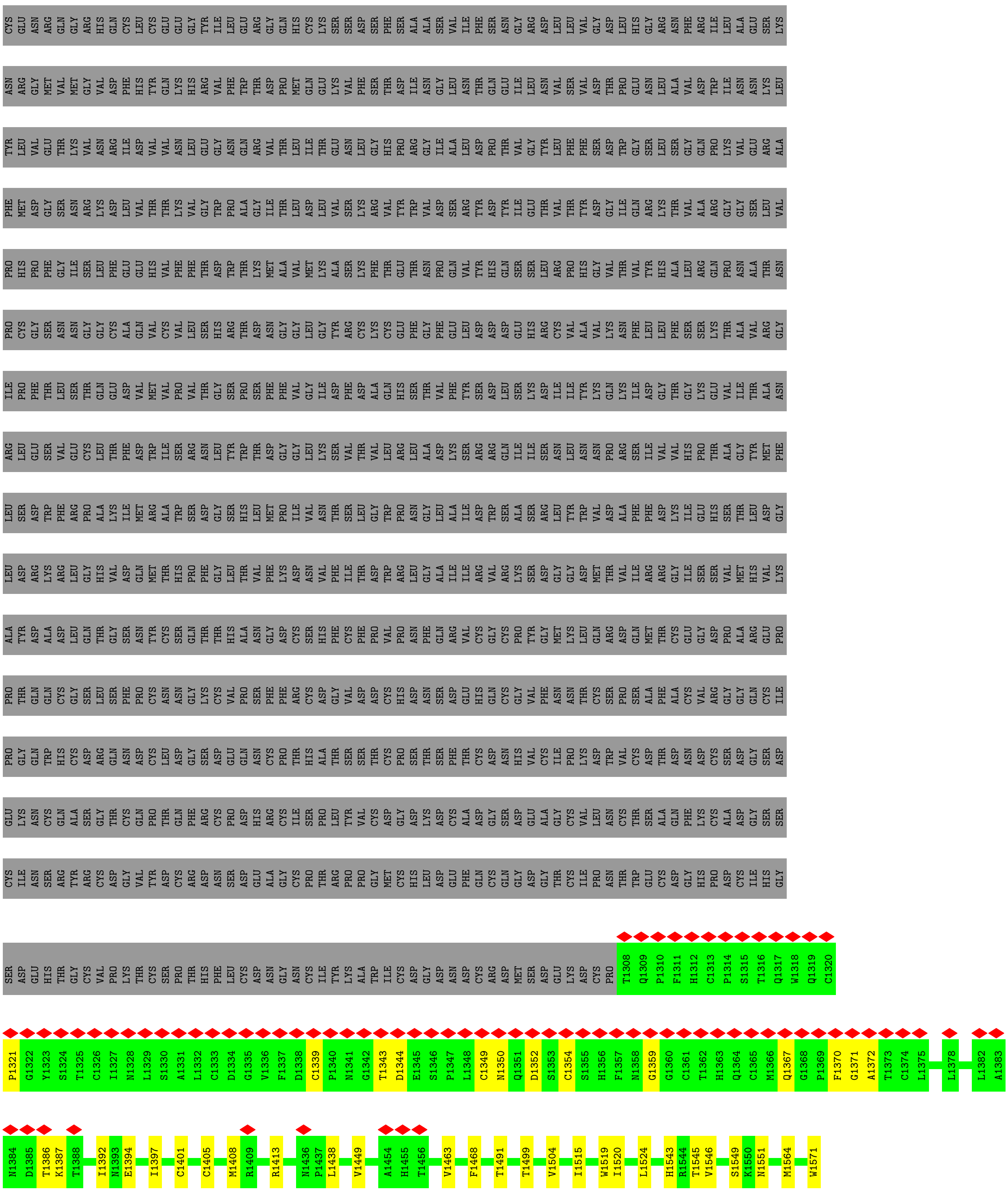

C2713 I2714 N2715 W2718 K2719 C2720 D2721 N2722 D2723 N2724 D2725 C2726 G2727 D2728 G2729 S2730 D2731 F2739 H2740 T2741



• Molecule 1: LDL receptor related protein 2

Chain B:

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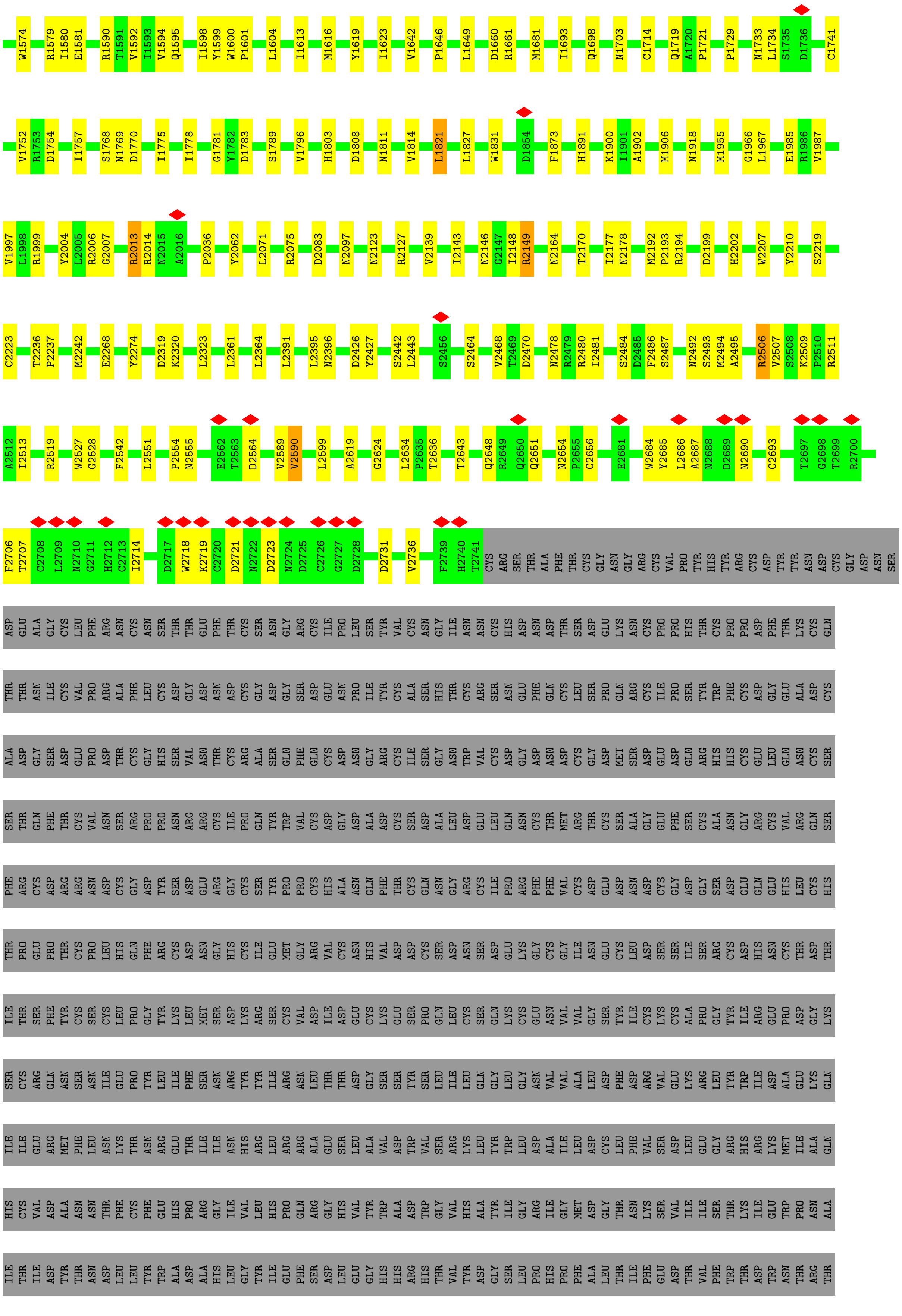
ASN ARG GLY MET VAL MET GLY VAL ASP PHE HIS TYR GLN LYS HIS ARG VAL PHE TRP THR ASP PRO MET GLN GLU LYS VAL PHE SER THR ASP ILE ASN GLY LEU ASN THR GLN GLU ILE LEU ASN VAL SER VAL ASP THR PRO GLU ASN LEU ALA VAL ASP TRP ILE ASN ASN LYS LEU
TYR LEU VAL GLU THR LYS VAL ASN ARG ILE ASP VAL VAL ASN LEU GLU GLY ASN GLN ARG VAL THR LEU ILE THR GLU ASN LEU GLY HIS PRO ARG GLY ILE ALA LEU ASP PRO THR VAL GLY TYR LEU PHE PHE SER ASP TRP GLY SER LEU SER GLY GLN PRO LYS VAL GLU ARG ALA
PHE MET ASP GLY SER ASN ARG LYS ASP LEU VAL THR THR LYS VAL GLY TRP PRO ALA GLY ILE THR LEU ASP LEU VAL SER LYS ARG VAL TYR TRP VAL ASP SER ARG TYR ASP TYR ILE GLU THR VAL THR TYR ASP GLY ILE GLN ARG LYS THR VAL ALA ARG GLY GLY SER LEU VAL
PRO HIS PRO PHE GLY ILE SER LEU PHE GLU GLU HIS VAL PHE PHE THR ASP TRP THR LYS MET ALA VAL MET LYS ALA SER LYS PHE THR GLU THR ASN PRO GLN VAL TYR HIS GLN SER SER LEU ARG PRO HIS GLY VAL THR VAL TYR HIS ALA LEU ARG GLN PRO ASN ALA THR ASN
PRO CYS GLY SER ASN ASN GLY GLY CYS ALA GLN VAL CYS VAL LEU SER HIS ARG THR ASP ASN GLY GLY LEU GLY TYR ARG CYS LYS CYS GLU PHE GLY PHE GLU LEU ASP ASP ASP GLU HIS ARG CYS VAL ALA VAL LYS ASN PHE LEU LEU PHE SER SER LYS THR ALA VAL ARG GLY
ILE PRO PHE THR LEU SER THR GLN GLU ASP VAL MET VAL PRO VAL THR GLY SER PRO SER PHE PHE VAL GLY ILE ASP PHE ASP ALA GLN HIS SER THR VAL PHE TYR SER ASP LEU SER LYS ASP ILE ILE TYR LYS GLN LYS ILE ASP GLY THR GLY LYS GLU VAL ILE THR ALA ASN
ARG LEU GLU SER VAL GLU CYS LEU THR PHE ASP TRP ILE SER ARG ASN LEU TYR TRP THR ASP GLY GLY LEU LYS SER VAL THR VAL LEU ARG LEU ALA ASP LYS SER ARG ARG GLN ILE ILE SER ASN LEU ASN ASN PRO ARG SER ILE VAL VAL HIS PRO THR ALA GLY TYR MET PHE
LEU SER ASP TRP PHE ARG PRO ALA LYS ILE MET ARG ALA TRP SER ASP GLY SER HIS LEU MET PRO ILE VAL ASN THR SER LEU GLY TRP PRO ASN GLY LEU ALA ILE ASP TRP SER ALA SER ARG LEU TYR TRP VAL ASP ALA PHE PHE ASP LYS ILE GLU HIS SER THR LEU ASP GLY
LEU ASP ARG LYS ARG LEU GLY HIS VAL ASP GLN MET THR HIS PRO PHE GLY LEU THR VAL PHE LYS ASP ASN VAL PHE ILE THR ASP TRP ARG LEU GLY ALA ILE ILE ARG VAL ARG LYS SER ASP GLY GLY ASP MET THR VAL ILE ARG ARG GLY ILE SER SER VAL MET HIS VAL LYS
ALA TYR ASP ALA ASP LEU GLN THR GLY SER ASN TYR CYS SER GLN THR THR HIS ALA ASN GLY ASP CYS SER HIS PHE CYS PHE PRO VAL PRO ASN PHE GLN ARG VAL CYS GLY CYS PRO TYR GLY MET LYS LEU GLN ARG ASP GLN MET THR CYS GLU GLY ASP PRO ALA ARG GLU PRO
PRO THR GLN GLN CYS GLY SER LEU SER PHE PRO CYS ASN ASN GLY LYS CYS VAL PRO SER PHE PHE ARG CYS ASP GLY VAL ASP ASP CYS HIS ASP ASN SER ASP GLU HIS GLN CYS GLY VAL PHE ASN ASN THR CYS SER PRO SER ALA PHE ALA CYS VAL ARG GLY GLY GLN CYS ILE
PRO GLY GLN TRP HIS CYS ASP ARG GLN ASN ASP CYS LEU ASP GLY SER ASP GLU GLN ASN CYS PRO THR HIS ALA THR SER SER THR CYS PRO SER THR SER PHE THR CYS ASP ASN HIS VAL CYS ILE PRO LYS ASP TRP VAL CYS ASP THR ASP ASN ASP CYS SER ASP GLY SER ASP
GLU LYS ASN CYS GLN ALA SER GLY THR CYS GLN PRO THR GLN PHE ARG CYS PRO ASP HIS ARG CYS ILE SER PRO LEU TYR VAL CYS ASP GLY ASP LYS ASP CYS ALA ASP GLY SER ASP GLU ALA GLY CYS VAL LEU ASN CYS THR SER ALA GLN PHE LYS CYS ALA ASP GLY SER SER
CYS ILE ASN SER ARG TYR ARG CYS ASP GLY VAL TYR ASP CYS ARG ASP ASN SER ASP GLU ALA GLY CYS PRO THR ARG PRO PRO GLY MET CYS HIS LEU ASP GLU PHE GLN CYS GLN GLY ASP GLY THR CYS ILE PRO ASN THR TRP GLU CYS ASP GLY HIS PRO ASP CYS ILE HIS GLY
SER ASP GLU HIS THR GLY CYS VAL PRO LYS THR CYS SER PRO THR HIS PHE LEU CYS ASP ASN GLY ASN CYS ILE TYR LYS ALA TRP ILE CYS ASP GLY ASP ASN ASP CYS ARG ASP MET SER ASP GLU LYS ASP CYS PRO 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 E1345 S1346 P1347 L1348 C1349 N1350 Q1351 D1352 S1353 C1354 S1355 H1356 F1357 N1358 G1359 G1360 C1361 T1362 H1363 Q1364 C1365 M1366 Q1367 G1368 P1369 F1370 G1371 A1372 T1373 C1374 L1375 L1378 L1382 A1383
N1384 D1385 T1386 K1387 T1388 I1392 N1393 E1394 I1397 C1401 C1405 M1408 R1409 R1413 N1436 P1437 L1438 V1449 A1454 H1455 T1456 V1463 F1468 T1491 T1499 V1504 I1515 W1519 I1520 L1524 H1543 R1544 T1545 V1546 S1549 K1550 N1551 M1564 W1571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V1752 R1753 D1754 I1757 S1768 N1769 D1770 I1775 I1778 G1781 Y1782 D1783 S1789 V1796 H1803 D1808 N1811 V1814 L1821 L1827 W1831 D1854 F1873 H1891 K1900 I1901 A1902 M1906 N1918 M1955 G1966 L1967 E1985 R1986 V1987
V1997 L1998 R1999 Y2004 L2005 R2006 G2007 R2013 R2014 N2015 A2016 P2036 Y2062 L2071 R2075 D2083 N2097 N2123 R2127 V2139 I2143 N2146 G2147 I2148 R2149 N2164 T2170 I2177 N2178 M2192 P2193 R2194 D2199 H2202 W2207 Y2210 S2219
C2223 T2236 P2237 M2242 E2268 Y2274 D2319 K2320 L2323 L2361 L2364 L2391 L2395 N2396 D2426 Y2427 S2442 L2443 S2456 S2464 V2468 T2469 D2470 N2478 R2479 R2480 I2481 S2484 D2485 F2486 S2487 N2492 S2493 M2494 A2495 R2506 V2507 S2508 K2509 P2510 R2511
A2512 I2513 R2519 W2527 G2528 F2542 L2551 P2554 N2555 E2562 T2563 D2564 V2589 V2590 L2599 A2619 G2624 L2634 P2635 T2636 T2643 Q2648 R2649 Q2650 Q2651 N2654 P2655 C2656 E2681 W2684 Y2685 L2686 A2687 N2688 D2689 N2690 C2693 T2697 G2698 T2699 R2700
F2706 T2707 C2708 L2709 N2710 G2711 H2712 C2713 I2714 D2717 W2718 K2719 C2720 D2721 N2722 D2723 N2724 D2725 C2726 G2727 D2728 D2731 V2736 F2739 H2740 T2741 CYS ARG SER THR ALA PHE THR CYS GLY ASN GLY ARG CYS VAL PRO TYR HIS TYR ARG CYS ASP TYR TYR ASN ASP CYS GLY ASP ASN SER
ASP GLU ALA GLY CYS LEU PHE ARG ASN CYS ASN SER THR THR GLU PHE THR CYS SER ASN GLY ARG CYS ILE PRO LEU SER TYR VAL CYS ASN GLY ILE ASN ASN CYS HIS ASP ASN ASP THR SER ASP GLU LYS ASN CYS PRO PRO HIS THR CYS PRO PRO ASP PHE THR LYS CYS GLN
THR THR ASN ILE CYS VAL PRO ARG ALA PHE LEU CYS ASP GLY ASP ASN ASP CYS GLY ASP GLY SER ASP GLU ASN PRO ILE TYR CYS ALA SER HIS THR CYS ARG SER ASN GLU PHE GLN CYS LEU SER PRO GLN ARG CYS ILE PRO SER TYR TRP PHE CYS ASP GLY GLU ALA ASP CYS
ALA ASP GLY SER ASP GLU PRO ASP THR CYS GLY HIS SER VAL ASN THR CYS ARG ALA SER GLN PHE GLN CYS ASP ASN GLY ARG CYS ILE SER GLY ASN TRP VAL CYS ASP GLY ASP ASN ASP CYS GLY ASP MET SER ASP GLU ASP GLN ARG HIS HIS CYS GLU LEU GLN ASN CYS SER
SER THR GLN PHE THR CYS VAL ASN SER ARG PRO PRO ASN ARG ARG CYS ILE PRO GLN TYR TRP VAL CYS ASP GLY ASP ALA ASP CYS SER ASP ALA LEU ASP GLU LEU GLN ASN CYS THR MET ARG THR CYS SER ALA GLY GLU PHE SER CYS ALA ASN GLY ARG CYS VAL ARG GLN SER
PHE ARG CYS ASP ARG ARG ASN ASP CYS GLY ASP TYR SER ASP GLU ARG GLY CYS SER TYR PRO PRO CYS HIS ALA ASN GLN PHE THR CYS GLN ASN GLY ARG CYS ILE PRO ARG PHE PHE VAL CYS ASP GLU ASP ASN ASP CYS GLY ASP GLY SER ASP GLU GLN GLU HIS LEU CYS HIS
THR PRO GLU PRO THR CYS PRO LEU HIS GLN PHE ARG CYS ASP ASN GLY HIS CYS ILE GLU MET GLY ARG VAL CYS ASN HIS VAL ASP ASP CYS SER ASP ASN SER ASP GLU LYS GLY CYS GLY ILE ASN GLU CYS LEU ASP SER SER ILE SER ARG CYS ASP HIS ASN CYS THR ASP THR
ILE THR SER PHE TYR CYS SER CYS LEU PRO GLY TYR LYS LEU MET SER ASP LYS ARG SER CYS VAL ASP ILE ASP GLU CYS LYS GLU SER PRO GLN LEU CYS SER GLN LYS CYS GLU ASN VAL VAL GLY SER TYR ILE CYS LYS CYS ALA PRO GLY TYR ILE ARG GLU PRO ASP GLY LYS
SER CYS ARG GLN ASN SER ASN ILE GLU PRO TYR LEU ILE PHE SER ASN ARG TYR TYR ILE ARG ASN LEU THR THR ASP GLY SER SER TYR SER LEU ILE LEU GLN GLY LEU GLY ASN VAL VAL ALA LEU ASP PHE ASP ARG VAL GLU LYS ARG LEU TYR TRP ILE ASP ALA GLU LYS GLN
ILE ILE GLU ARG MET PHE LEU ASN LYS THR ASN ARG GLU THR ILE ILE ASN HIS ARG LEU ARG ARG ALA GLU SER LEU ALA VAL ASP TRP VAL SER ARG LYS LEU TYR TRP LEU ASP ALA ILE LEU ASP CYS LEU PHE VAL SER ASP LEU GLU GLY ARG HIS ARG LYS MET ILE ALA GLN
HIS CYS VAL ASP ALA ASN ASN THR PHE CYS PHE GLU HIS PRO ARG GLY ILE VAL LEU HIS PRO GLN ARG GLY HIS VAL TYR TRP ALA ASP TRP GLY VAL HIS ALA TYR ILE GLY ARG ILE GLY MET ASP GLY THR ASN LYS SER VAL ILE ILE SER THR LYS ILE GLU TRP PRO ASN ALA
ILE THR ILE ASP TYR THR ASN ASP LEU LEU TYR TRP ALA ASP ALA HIS LEU GLY TYR ILE GLU PHE SER ASP LEU GLU GLY HIS HIS ARG HIS THR VAL TYR ASP GLY SER LEU PRO HIS PRO PHE ALA LEU THR ILE PHE GLU ASP THR VAL PHE TRP THR ASP TRP ASN THR ARG THR

VAL GLU LYS GLY ASN LYS TYR ASP GLY SER GLY ARG VAL VAL LEU VAL ASN THR THR HIS LYS PRO PHE ASP ILE HIS VAL TYR HIS PRO TYR ARG GLN PRO ILE MET SER ASN PRO CYS GLY THR ASN ASN GLY GLY CYS SER HIS LEU CYS LEU ILE LYS ALA GLY GLY ARG GLY PHE

THR CYS ALA CYS PRO ASP ASP PHE GLN THR VAL GLN LEU ARG ASP ARG THR LEU CYS MET PRO MET CYS SER SER THR GLN PHE LEU CYS GLY ASN ASN GLU LYS CYS ILE PRO ILE TRP TRP LYS CYS ASP GLY GLN LYS ASP CYS SER ASP GLY SER ASP GLU PRO ASP LEU CYS PRO

HIS ARG PHE CYS ARG LEU GLY GLN PHE GLN CYS ARG ASP GLY ASN CYS THR SER PRO GLN ALA LEU CYS ASN ALA ARG GLN ASP CYS ALA ASP GLY SER ASP GLU ASP ARG VAL LEU CYS GLU HIS HIS ARG CYS GLU SER ASN GLU TRP GLN CYS ALA ASN LYS ARG CYS ILE PRO GLN

SER TRP GLN CYS ASP SER VAL ASN ASP CYS LEU ASP ASN SER ASP GLU ASP THR SER HIS CYS ALA SER ARG THR CYS ARG PRO GLY GLN PHE LYS CYS ASN ASN GLY ARG CYS ILE PRO GLN SER TRP LYS CYS ASP VAL ASP ASN ASP CYS GLY ASP TYR SER ASP GLU PRO ILE ASP

GLU CYS THR THR ALA ALA TYR ASN CYS ASP ASN HIS THR GLU PHE SER CYS LYS THR ASN TYR ARG CYS ILE PRO GLN TRP ALA VAL CYS ASN GLY PHE ASP ASP CYS ARG ASP ASN SER ASP GLU GLN GLY CYS GLU SER VAL PRO CYS HIS PRO SER GLY ASP PHE ARG CYS ALA ASN

HIS HIS CYS ILE PRO LEU ARG TRP LYS CYS ASP GLY THR ASP ASP CYS GLY ASP ASN SER ASP GLU GLU ASN CYS VAL PRO ARG GLU CYS SER GLU SER GLU PHE ARG CYS ALA ASP GLN GLN CYS ILE PRO SER ARG TRP VAL CYS ASP GLN GLU ASN ASP CYS GLY ASP ASN SER ASP

GLU ARG ASP CYS GLU MET LYS THR CYS HIS PRO GLU HIS PHE GLN CYS THR SER GLY HIS CYS VAL PRO LYS ALA LEU ALA CYS ASP GLY ARG ALA ASP CYS LEU ASP ALA SER ASP GLU SER ALA CYS PRO THR ARG PHE PRO ASN GLY THR TYR CYS PRO ALA ALA MET PHE GLU CYS

LYS ASN HIS VAL CYS ILE GLN SER PHE TRP ILE CYS ASP GLY GLU ASN ASP CYS VAL ASP GLY SER ASP GLU GLU ILE HIS LEU CYS PHE ASN ILE PRO CYS GLU SER PRO GLN ARG PHE ARG CYS ASP ASN SER ARG CYS VAL TYR GLY HIS GLN LEU CYS ASN GLY VAL ASP ASP CYS

GLY ASP GLY SER ASP GLU LYS GLU GLU HIS CYS ARG LYS PRO THR HIS LYS PRO CYS THR ASP THR GLU TYR LYS CYS SER ASN GLY ASN CYS ILE SER GLN HIS TYR VAL CYS ASP ASN VAL ASN ASP CYS GLY ASP LEU SER ASP GLU THR GLY CYS ASN LEU GLY ASP ASN ARG THR

CYS ALA GLU ASN ILE CYS GLU GLN ASN CYS THR GLN LEU SER SER GLY GLY PHE ILE CYS SER CYS ARG PRO GLY PHE LYS PRO SER THR LEU ASP LYS ASN SER CYS GLN ASP ILE ASN GLU CYS GLU GLU PHE GLY ILE CYS PRO GLN SER CYS ARG ASN SER LYS GLY SER TYR GLU

CYS PHE CYS VAL ASP GLY PHE LYS SER MET SER THR HIS TYR GLY GLU ARG CYS ALA ALA ASP GLY SER PRO PRO LEU LEU LEU LEU PRO GLU ASN VAL ARG ILE ARG LYS TYR ASN THR SER SER GLU LYS PHE SER GLU TYR LEU GLU GLU GLU GLU HIS ILE GLN THR ILE ASP TYR

ASP TRP ASP PRO GLU HIS ILE GLY LEU SER VAL VAL TYR TYR THR VAL LEU ALA GLN GLY SER GLN PHE GLY ALA ILE LYS ARG ALA TYR ILE PRO ASN PHE GLU SER GLY SER ASN ASN PRO ILE ARG GLU VAL ASP LEU GLY LEU LYS TYR LEU MET GLN PRO ASP GLY LEU ALA VAL

ASP TRP VAL GLY ARG HIS ILE TYR TRP SER ASP ALA LYS SER GLN ARG ILE GLU VAL ALA THR LEU ASP GLY ARG TYR ARG LYS TRP LEU ILE THR THR GLN LEU ASP GLN PRO ALA ALA ILE ALA VAL ASN PRO LYS LEU GLY LEU MET PHE TRP THR ASP GLN GLY LYS GLN PRO LYS

ILE GLU SER ALA TRP MET ASN GLY GLU HIS ARG SER VAL LEU VAL SER GLU ASN LEU GLY TRP PRO ASN GLY LEU SER ILE ASP TYR LEU ASN ASP ASP ARG VAL TYR TRP SER ASP SER LYS GLU ASP VAL ILE GLU ALA ILE LYS TYR ASP GLY THR ASP ARG ARG LEU ILE ILE ASN

GLU ALA MET LYS PRO PHE SER LEU ASP ILE PHE GLU ASP LYS LEU TYR TRP VAL ALA LYS GLU LYS GLY GLU VAL TRP ARG GLN ASN LYS PHE GLY LYS GLU ASN LYS GLU LYS VAL LEU VAL VAL ASN PRO TRP LEU THR GLN VAL ARG ILE PHE HIS GLN LEU ARG TYR ASN GLN SER

VAL SER ASN PRO CYS LYS GLN VAL CYS SER HIS LEU CYS LEU LEU ARG PRO GLY GLY TYR SER CYS ALA CYS PRO GLN GLY SER ASP PHE VAL THR GLY SER THR VAL GLN CYS ASP ALA ALA SER GLU LEU PRO VAL THR MET PRO PRO PRO CYS ARG CYS MET HIS GLY GLY ASN CYS

TYR PHE ASP GLU ASN GLU LEU PRO LYS CYS LYS CYS SER SER GLY TYR SER GLY GLU TYR CYS GLU VAL GLY 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 MET ALA MET ASN GLU HIS PHE

VAL MET GLU VAL GLY LYS GLN PRO VAL ILE PHE GLU ASN PRO MET TYR ALA ALA LYS ASP ASN THR SER LYS VAL ALA LEU ALA VAL GLN GLY PRO SER THR GLY ALA GLN VAL THR VAL PRO GLU ASN VAL GLU ASN GLN ASN TYR GLY ARG PRO ILE ASP PRO SER GLU ILE VAL PRO

GLU PRO LYS PRO ALA SER PRO GLY ALA ASP GLU ILE GLN GLY LYS LYS TRP ASN ILE PHE LYS ARG LYS PRO LYS GLN THR THR ASN PHE GLU ASN PRO ILE TYR ALA GLU MET ASP SER GLU VAL LYS ASP ALA VAL ALA VAL ALA PRO PRO PRO SER PRO SER LEU PRO ALA LYS ALA

• Molecule 2: unclear peptide

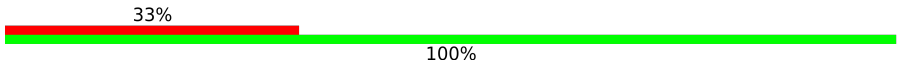
Chain C:

• Molecule 2: unclear peptide

Chain I:

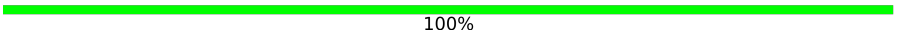
• Molecule 3: unclear peptide

Chain D:



• Molecule 3: unclear peptide

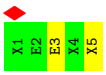
Chain J:



There are no outlier residues recorded for this chain.

• Molecule 4: unclear peptide

Chain G:



• Molecule 4: unclear peptide

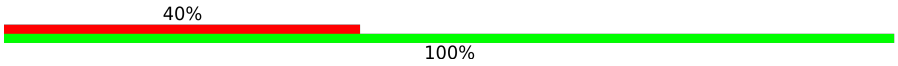
Chain K:

• Molecule 5: unclear peptide

Chain H:

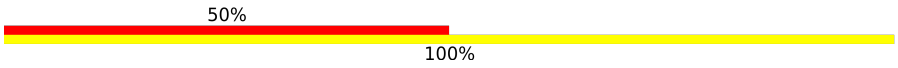
• Molecule 5: unclear peptide

Chain L:



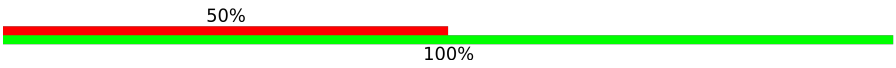
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



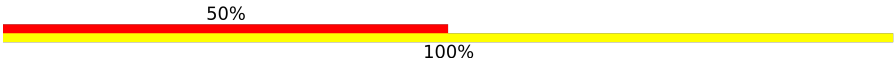
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



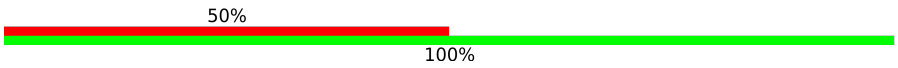
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:

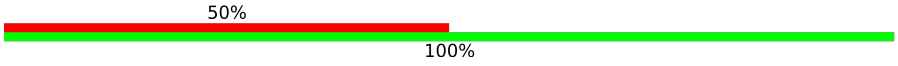


• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:

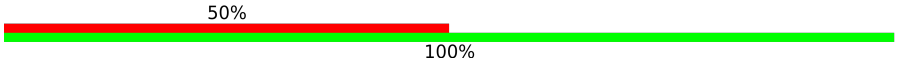
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:



• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:



• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

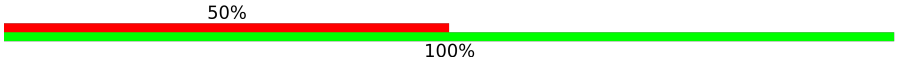
Chain W:

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:



• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:

• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

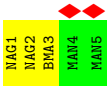
Chain F:

• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:

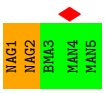
• Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



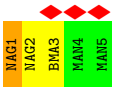
• Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



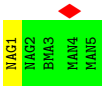
• Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:



• Molecule 8: 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:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	101096	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)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.278	Depositor
Minimum map value	-0.136	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0434	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: NAG, CA, MAN, NI, BMA, A2G

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	0.26	0/11504	0.52	0/15672
1	B	0.26	0/11490	0.52	0/15652
2	C	0.31	0/7	0.59	0/8
2	I	0.42	0/7	0.54	0/8
3	D	0.32	0/5	0.25	0/5
3	J	0.22	0/5	0.14	0/5
4	G	0.24	0/17	0.29	0/21
4	K	0.23	0/17	0.40	0/21
5	H	0.22	0/7	0.41	0/8
5	L	0.27	0/7	0.30	0/8
All	All	0.26	0/23066	0.52	0/31408

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11221	0	10723	121	0
1	B	11208	0	10709	113	0
2	C	33	0	18	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	33	0	18	2	0
3	D	16	0	8	0	0
3	J	16	0	8	0	0
4	G	33	0	19	1	0
4	K	33	0	18	1	0
5	H	28	0	12	0	0
5	L	28	0	12	0	0
6	E	28	0	25	0	0
6	M	28	0	25	0	0
6	N	28	0	25	0	0
6	P	28	0	25	0	0
6	R	28	0	25	0	0
6	S	28	0	25	0	0
6	T	28	0	25	0	0
6	V	28	0	25	1	0
6	W	28	0	25	0	0
6	Y	28	0	25	1	0
6	a	28	0	25	0	0
6	b	28	0	25	0	0
7	F	39	0	34	0	0
7	U	39	0	34	1	0
8	O	61	0	52	0	0
8	Q	61	0	52	2	0
8	X	61	0	52	1	0
8	Z	61	0	52	0	0
9	A	56	0	52	1	0
9	B	56	0	52	0	0
10	A	14	0	12	0	0
10	B	14	0	12	0	0
11	A	5	0	0	0	0
11	B	5	0	0	0	0
12	A	1	0	0	0	0
12	B	1	0	0	0	0
All	All	23459	0	22249	234	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 5.

All (234) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1436:ASN:ND2	1:A:1451:ASN:OD1	2.25	0.70
1:A:2600:THR:HG21	1:A:2642:SER:HA	1.73	0.69
1:A:1383:ALA:HB3	1:A:1388:THR:HG23	1.77	0.67
1:A:1543:HIS:HB3	1:A:1729:PRO:HG3	1.76	0.67
1:A:1719:GLN:HG3	1:A:1721:PRO:HD2	1.76	0.66
1:A:1351:GLN:HB2	1:A:1371:GLY:HA3	1.77	0.66
1:B:1387:LYS:HE2	1:B:1387:LYS:HA	1.78	0.65
1:B:2149:ARG:HG2	1:B:2194:ARG:HD2	1.79	0.65
1:A:1659:THR:HG22	1:A:1666:VAL:HG22	1.78	0.63
1:B:1595:GLN:HA	1:B:1598:ILE:HD11	1.80	0.63
1:A:2179:THR:HG22	1:A:2181:TYR:H	1.64	0.63
1:A:1839:THR:HG22	1:A:1846:ILE:HG12	1.82	0.62
1:B:2170:THR:HG21	1:B:2192:MET:HA	1.82	0.61
1:A:1650:THR:HG21	1:A:1691:THR:HA	1.83	0.61
1:A:1966:GLY:HA3	1:A:2007:GLY:HA2	1.82	0.61
1:B:2714:ILE:HB	1:B:2718:TRP:HE3	1.65	0.60
1:A:2433:ARG:NH1	1:A:2496:GLU:OE2	2.33	0.60
1:A:2235:VAL:HG12	1:A:2236:THR:HG23	1.84	0.60
1:B:1321:PRO:HG2	1:B:1343:THR:HG21	1.83	0.60
1:A:2374:GLY:N	1:A:2411:LEU:O	2.34	0.60
1:B:1616:MET:CE	1:B:1646:PRO:HB2	2.33	0.59
1:A:2484:SER:HB3	1:A:2510:PRO:HB2	1.84	0.59
1:A:1520:ILE:HD12	1:A:1562:PRO:HB2	1.85	0.59
1:A:2441:ASN:HD21	1:A:2444:ARG:HD3	1.68	0.59
1:B:2210:TYR:HB2	1:B:2236:THR:HA	1.83	0.58
1:A:1397:ILE:HD12	1:A:1397:ILE:H	1.69	0.58
1:A:1318:TRP:N	1:A:1327:ILE:O	2.34	0.57
1:B:2146:ASN:O	1:B:2149:ARG:NH1	2.38	0.57
1:B:1408:MET:SD	1:B:1413:ARG:NH2	2.77	0.56
1:A:2149:ARG:HG2	1:A:2194:ARG:HD2	1.87	0.56
1:A:2609:THR:HG22	1:A:2616:ILE:HG12	1.86	0.56
1:A:1616:MET:HG2	1:A:1623:ILE:HG12	1.86	0.56
1:B:1352:ASP:O	1:B:1367:GLN:NE2	2.39	0.55
1:B:2426:ASP:OD1	1:B:2427:TYR:N	2.40	0.55
1:B:1769:ASN:OD1	1:B:1999:ARG:NH2	2.35	0.55
1:B:1616:MET:HG2	1:B:1623:ILE:HG12	1.89	0.55
1:A:1442:ALA:HB1	1:A:1469:VAL:HG13	1.88	0.55
1:A:1579:ARG:HA	1:A:1598:ILE:HD11	1.87	0.54
1:B:1519:TRP:HB3	1:B:1698:GLN:HE21	1.72	0.54
1:A:2525:THR:HG22	1:A:2533:ILE:HG12	1.90	0.54
1:B:1520:ILE:O	1:B:1703:ASN:ND2	2.41	0.54
1:B:1604:LEU:HD22	1:B:1613:ILE:HD11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1616:MET:HE3	1:B:1646:PRO:HB2	1.89	0.54
1:A:2592:THR:HG21	1:B:1642:VAL:HG12	1.90	0.54
1:B:1966:GLY:HA3	1:B:2007:GLY:HA2	1.90	0.54
1:B:1350:ASN:H	1:B:1371:GLY:HA3	1.73	0.53
1:B:1661:ARG:NH2	2:C:2:UNK:O	2.37	0.53
1:B:1900:LYS:HE2	1:B:1902:ALA:HB2	1.90	0.53
1:B:2481:ILE:HB	1:B:2494:MET:HG2	1.89	0.53
1:A:1307:PRO:HB2	1:A:1310:PRO:HG3	1.91	0.53
1:A:1895:SER:O	1:A:1895:SER:OG	2.26	0.53
1:A:2634:LEU:HD12	1:A:2638:PRO:HG3	1.91	0.53
1:B:1811:ASN:OD1	6:Y:1:NAG:N2	2.41	0.53
1:A:1440:VAL:HG22	1:A:1449:VAL:HG22	1.91	0.53
1:A:1649:LEU:HD11	1:A:1656:VAL:HB	1.91	0.52
1:B:1733:ASN:OD1	8:X:1:NAG:N2	2.42	0.52
1:B:1752:VAL:HG23	1:B:1757:ILE:HG12	1.92	0.52
1:B:1821:LEU:HD13	1:B:2075:ARG:HD2	1.92	0.52
1:A:1847:GLU:HB3	1:A:1860:THR:HA	1.92	0.52
1:A:1626:CYS:SG	1:A:1627:ASP:N	2.83	0.51
1:B:1545:THR:HB	1:B:1729:PRO:HA	1.92	0.51
1:B:1918:ASN:OD1	1:B:1918:ASN:N	2.44	0.51
1:A:2394:SER:OG	1:A:2639:SER:O	2.26	0.51
1:B:1580:ILE:HB	1:B:1594:VAL:HB	1.91	0.51
1:B:1499:THR:HG21	7:U:1:NAG:H82	1.92	0.51
1:B:2148:ILE:HD13	1:B:2164:ASN:HB3	1.93	0.51
1:B:2478:ASN:OD1	1:B:2480:ARG:HD3	2.11	0.51
1:B:1616:MET:SD	1:B:1649:LEU:HB3	2.51	0.51
1:B:2062:TYR:OH	1:B:2083:ASP:OD2	2.26	0.51
1:B:2511:ARG:HD2	1:B:2555:ASN:HA	1.92	0.51
1:A:2562:GLU:OE2	1:A:2562:GLU:N	2.44	0.50
1:A:1320:CYS:HB2	1:A:1343:THR:HB	1.93	0.50
1:A:1600:TRP:CD2	2:I:3:LEU:HD12	2.46	0.50
1:A:2234:ILE:HD11	1:A:2237:PRO:HB3	1.93	0.50
1:A:1594:VAL:HG12	1:A:1598:ILE:HD13	1.92	0.50
1:B:2319:ASP:OD1	1:B:2320:LYS:N	2.45	0.50
1:B:2268:GLU:OE1	1:B:2268:GLU:N	2.38	0.50
1:B:2361:LEU:HD12	1:B:2364:LEU:HD12	1.94	0.50
1:B:1551:ASN:HD22	6:V:1:NAG:C7	2.25	0.50
1:B:1600:TRP:CD2	2:C:3:LEU:HD22	2.47	0.50
1:A:2702:ASN:OD1	1:A:2703:GLN:N	2.38	0.50
1:A:2706:PHE:N	1:A:2714:ILE:O	2.45	0.50
1:A:1663:THR:HG23	1:A:1665:GLN:HG2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1838:TYR:CZ	1:A:1847:GLU:HG3	2.47	0.49
1:A:2580:THR:HG1	1:A:2584:THR:HG1	1.56	0.49
1:B:1438:LEU:HB3	1:B:1693:ILE:HB	1.94	0.49
1:A:2708:CYS:HB2	1:A:2712:HIS:O	2.12	0.49
1:B:1581:GLU:HG2	1:B:1592:VAL:HG22	1.94	0.49
1:A:1832:VAL:HG22	1:A:1881:PRO:HB3	1.94	0.49
1:A:2430:ARG:HB2	1:A:2479:ARG:HH12	1.78	0.49
1:A:2515:LEU:HA	1:A:2522:MET:HA	1.95	0.48
1:A:2549:THR:OG1	1:A:2586:ARG:NH1	2.46	0.48
1:A:1413:ARG:NH1	1:A:1413:ARG:HB2	2.27	0.48
1:A:1462:LEU:HD21	1:A:1481:VAL:HG11	1.95	0.48
1:A:2664:SER:HB2	1:A:2665:HIS:HD1	1.78	0.48
1:A:2325:ARG:NH1	4:K:3:GLU:OE1	2.47	0.48
1:B:1775:ILE:HG22	1:B:1778:ILE:HD11	1.95	0.48
1:A:1975:TYR:CE2	1:A:1986:ARG:HD3	2.49	0.48
1:B:2731:ASP:OD1	1:B:2731:ASP:N	2.44	0.48
1:A:2251:TRP:NE1	1:A:2253:ASP:OD2	2.43	0.47
1:B:2470:ASP:OD2	1:B:2511:ARG:NH1	2.47	0.47
1:A:1830:ASP:OD2	1:A:1833:SER:OG	2.23	0.47
1:B:2506:ARG:CZ	1:B:2506:ARG:HB3	2.44	0.47
1:B:1354:CYS:HA	1:B:1359:GLY:HA3	1.95	0.47
1:A:2062:TYR:OH	1:A:2083:ASP:OD2	2.24	0.47
1:A:2107:ASN:ND2	8:Q:1:NAG:O3	2.33	0.47
1:B:1574:TRP:HB3	1:B:1601:PRO:HD2	1.97	0.47
1:B:2494:MET:HG3	1:B:2495:ALA:O	2.14	0.47
1:A:1329:LEU:HA	1:A:1332:LEU:HG	1.95	0.47
1:B:1367:GLN:HA	1:B:1372:ALA:HA	1.97	0.47
1:B:2071:LEU:HD12	1:B:2323:LEU:HD22	1.97	0.46
1:B:2210:TYR:HB3	1:B:2237:PRO:HD2	1.97	0.46
1:B:2219:SER:OG	1:B:2223:CYS:HA	2.15	0.46
1:A:1710:CYS:HB3	1:A:1726:CYS:HB3	1.89	0.46
1:A:2160:LEU:HB2	1:A:2177:ILE:HD11	1.97	0.46
1:A:2210:TYR:HB2	1:A:2236:THR:HA	1.97	0.46
1:B:2013:ARG:HG3	1:B:2013:ARG:HH11	1.80	0.46
1:B:2509:LYS:HD2	1:B:2528:GLY:HA2	1.97	0.46
1:A:2437:THR:HB	1:A:2469:THR:HG23	1.96	0.46
1:B:1599:TYR:HB3	1:B:1619:TYR:HB3	1.98	0.46
1:A:2210:TYR:CB	1:A:2236:THR:HA	2.46	0.46
1:A:2294:VAL:HG12	1:A:2301:VAL:HG22	1.98	0.46
1:A:2705:GLN:HA	1:A:2715:ASN:HA	1.97	0.46
1:B:2551:LEU:HD13	1:B:2554:PRO:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2537:THR:OG1	1:A:2541:ASN:OD1	2.32	0.46
1:A:2438:GLN:OE1	1:A:2446:GLN:NE2	2.41	0.46
1:B:1752:VAL:HG11	1:B:1783:ASP:HA	1.98	0.46
1:A:1749:LEU:HD23	1:A:1760:ILE:HD11	1.97	0.46
1:B:2194:ARG:HG3	1:B:2210:TYR:CZ	2.51	0.46
1:A:1405:CYS:SG	1:A:1406:VAL:N	2.89	0.45
1:B:2468:VAL:HG23	1:B:2486:PHE:HB3	1.99	0.45
1:A:2601:VAL:HG22	1:A:2606:ILE:HG22	1.99	0.45
1:B:1386:THR:HG23	1:B:1387:LYS:HE3	1.97	0.45
1:B:2396:ASN:HB2	1:B:2636:THR:HG21	1.98	0.45
1:B:2097:ASN:HD21	4:G:5:UNK:H	1.65	0.45
1:B:2685:TYR:CE2	1:B:2687:ALA:HB2	2.51	0.45
1:B:2684:TRP:CE3	1:B:2693:CYS:HB3	2.52	0.45
1:A:2719:LYS:HE3	1:A:2740:HIS:NE2	2.32	0.45
1:B:1349:CYS:HA	1:B:1370:PHE:O	2.17	0.45
1:A:1316:THR:O	1:A:1329:LEU:HD23	2.17	0.44
1:A:1497:ASN:OD1	1:A:1497:ASN:O	2.35	0.44
1:A:2394:SER:HB3	1:A:2425:LEU:HD11	1.99	0.44
1:B:2589:VAL:HG13	1:B:2590:VAL:HG12	1.99	0.44
1:A:1409:ARG:HB3	1:A:1409:ARG:CZ	2.48	0.44
1:A:2183:ARG:NH2	1:A:2410:SER:OG	2.51	0.44
1:B:2391:LEU:HD23	1:B:2643:THR:HG22	1.99	0.44
1:A:1397:ILE:HD12	1:A:1397:ILE:N	2.32	0.44
1:B:2193:PRO:HB3	1:B:2207:TRP:CD1	2.52	0.44
1:B:2139:VAL:HG12	1:B:2143:ILE:HD11	2.00	0.44
1:A:1419:GLU:OE2	1:A:1419:GLU:N	2.41	0.44
1:B:2123:ASN:HB3	1:B:2143:ILE:HG21	1.99	0.44
1:B:1781:GLY:O	1:B:2006:ARG:HG2	2.18	0.43
1:B:2686:LEU:HB3	1:B:2690:ASN:HA	1.99	0.43
1:A:1506:ASP:OD1	1:A:1506:ASP:N	2.42	0.43
1:A:1856:ARG:HA	1:A:1856:ARG:HH11	1.84	0.43
1:A:2126:ARG:NH1	1:A:2137:ASN:OD1	2.51	0.43
1:A:1384:ASN:OD1	9:A:4701:NAG:N2	2.51	0.43
1:A:2252:VAL:HG12	1:A:2259:ILE:HG12	2.00	0.43
1:A:2378:ASN:OD1	1:A:2378:ASN:N	2.42	0.43
1:A:2714:ILE:HD12	1:A:2715:ASN:O	2.18	0.43
1:B:2484:SER:HB3	1:B:2513:ILE:HD11	2.00	0.43
1:B:2648:GLN:NE2	1:B:2651:GLN:OE1	2.51	0.43
1:B:1827:LEU:HD12	1:B:1827:LEU:HA	1.81	0.43
1:A:2599:LEU:HD11	1:A:2606:ILE:HB	2.01	0.43
1:B:2492:ASN:OD1	1:B:2492:ASN:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1361:CYS:SG	1:A:1365:CYS:HB2	2.59	0.43
1:B:2468:VAL:HG22	1:B:2487:SER:HB3	2.01	0.43
1:B:2395:LEU:HD13	1:B:2634:LEU:HD13	2.00	0.43
1:A:1444:ARG:O	1:A:1469:VAL:HG12	2.18	0.43
1:B:2480:ARG:NH2	1:B:2493:SER:OG	2.52	0.43
1:B:2654:ASN:OD1	1:B:2654:ASN:N	2.52	0.42
1:A:1351:GLN:HB3	1:A:1372:ALA:H	1.83	0.42
1:B:1519:TRP:CD2	1:B:1698:GLN:HG3	2.54	0.42
8:Q:1:NAG:H62	8:Q:2:NAG:H82	2.01	0.42
1:A:1381:GLN:HG2	1:A:1392:ILE:HD11	2.01	0.42
1:A:1839:THR:HG21	1:A:1874:PRO:HB2	2.00	0.42
1:A:2164:ASN:ND2	1:A:2173:GLU:OE2	2.52	0.42
1:B:1831:TRP:CD2	1:B:2014:ARG:HD2	2.55	0.42
1:A:1796:VAL:HG13	1:A:1827:LEU:HD11	2.01	0.42
1:B:1719:GLN:HG3	1:B:1721:PRO:HD2	2.01	0.42
1:B:1985:GLU:HG2	1:B:1997:VAL:HG22	2.02	0.42
1:A:1614:TYR:HB3	1:A:1649:LEU:HD21	2.02	0.42
1:B:1339:CYS:HB2	1:B:1344:ASP:HB2	2.00	0.42
1:A:2273:ARG:NH2	1:A:2312:ASP:O	2.49	0.42
1:A:2388:GLU:HG3	1:A:2389:ASP:H	1.85	0.42
1:B:2143:ILE:HD12	1:B:2148:ILE:HD11	2.02	0.42
1:A:1976:TYR:OH	1:A:1985:GLU:OE1	2.26	0.42
1:A:1743:ARG:NH1	1:A:1743:ARG:HB3	2.35	0.42
1:A:2724:ASN:OD1	1:A:2725:ASP:N	2.53	0.42
1:B:1392:ILE:HG13	1:B:1394:GLU:HG3	2.02	0.42
1:A:1921:HIS:CG	1:A:1939:THR:HB	2.55	0.41
1:B:1401:CYS:HB3	1:B:1405:CYS:HB2	2.01	0.41
1:B:1571:TRP:HH2	1:B:1590:ARG:HG3	1.85	0.41
1:B:2719:LYS:HE2	1:B:2719:LYS:HB3	1.90	0.41
1:A:1750:MET:HE2	1:A:2009:ARG:HB3	2.03	0.41
1:A:1755:ASN:ND2	1:A:1755:ASN:O	2.53	0.41
1:A:2684:TRP:CE3	1:A:2693:CYS:HB3	2.55	0.41
1:A:2399:LEU:HD22	1:A:2425:LEU:HD21	2.03	0.41
1:A:2538:LEU:HD12	1:A:2538:LEU:HA	1.85	0.41
1:B:1754:ASP:HB2	1:B:2004:TYR:HB3	2.03	0.41
1:A:2361:LEU:HD12	1:A:2364:LEU:HD22	2.01	0.41
1:B:1519:TRP:CE3	1:B:1698:GLN:NE2	2.88	0.41
1:A:1873:PHE:HB3	1:A:1891:HIS:HB2	2.01	0.41
1:A:2203:ARG:HD3	1:A:2360:ALA:HB1	2.03	0.41
1:B:1546:VAL:CG1	1:B:1549:SER:HB2	2.51	0.41
1:A:1926:THR:HG23	1:A:1935:TYR:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1543:HIS:HB3	1:B:1729:PRO:HG3	2.03	0.41
1:B:2442:SER:C	1:B:2443:LEU:HD23	2.40	0.41
1:A:2402:LEU:HD21	1:A:2630:MET:HB3	2.03	0.41
1:B:2527:TRP:HB3	1:B:2554:PRO:HD2	2.02	0.41
1:A:1505:HIS:HB3	1:A:1509:LEU:HD11	2.03	0.41
1:A:2436:PHE:HE2	1:A:2438:GLN:HE21	1.68	0.41
1:A:2463:LEU:HD21	1:A:2501:ARG:HD3	2.02	0.41
1:B:1491:THR:HG22	1:B:1504:VAL:HB	2.03	0.41
1:B:1515:ILE:HD11	1:B:1524:LEU:HD11	2.03	0.41
1:B:1734:LEU:HD12	1:B:1741:CYS:SG	2.61	0.41
1:B:1796:VAL:HG13	1:B:1827:LEU:HD22	2.03	0.41
1:B:1803:HIS:CE1	1:B:1814:VAL:HG12	2.55	0.41
1:B:1873:PHE:HB3	1:B:1891:HIS:HB2	2.03	0.41
1:B:2721:ASP:O	1:B:2723:ASP:N	2.54	0.41
1:B:1397:ILE:HD12	1:B:1397:ILE:H	1.85	0.41
1:A:1622:TYR:CD1	1:A:1624:GLU:HG3	2.57	0.40
1:A:2476:TRP:CD1	1:A:2477:ILE:HG23	2.56	0.40
1:B:1546:VAL:HG11	1:B:1549:SER:HB2	2.03	0.40
1:B:1906:MET:SD	1:B:2036:PRO:HG2	2.62	0.40
1:A:1822:GLY:HA3	1:A:1842:ALA:HB3	2.03	0.40
1:A:1920:GLN:HE21	1:A:1920:GLN:HB3	1.56	0.40
1:A:2509:LYS:HD2	1:A:2528:GLY:HA2	2.03	0.40
1:A:1645:HIS:HE1	2:I:3:LEU:HG	1.87	0.40
1:B:1768:SER:HB3	1:B:1770:ASP:OD2	2.21	0.40
1:A:1912:LYS:HE2	1:A:1912:LYS:HB2	1.90	0.40
1:B:2177:ILE:HG22	1:B:2178:ASN:OD1	2.21	0.40
1:B:2199:ASP:OD2	1:B:2202:HIS:ND1	2.46	0.40
1:B:2619:ALA:HB1	1:B:2624:GLY:HA2	2.03	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	1434/4660 (31%)	1338 (93%)	96 (7%)	0	100	100
1	B	1432/4660 (31%)	1366 (95%)	66 (5%)	0	100	100
2	C	1/6 (17%)	1 (100%)	0	0	100	100
2	I	1/6 (17%)	1 (100%)	0	0	100	100
3	D	1/3 (33%)	1 (100%)	0	0	100	100
3	J	1/3 (33%)	0	1 (100%)	0	100	100
4	G	2/5 (40%)	2 (100%)	0	0	100	100
4	K	2/5 (40%)	2 (100%)	0	0	100	100
5	H	1/5 (20%)	1 (100%)	0	0	100	100
5	L	1/5 (20%)	1 (100%)	0	0	100	100
All	All	2876/9358 (31%)	2713 (94%)	163 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1247/4089 (30%)	1206 (97%)	41 (3%)	38	66
1	B	1245/4089 (30%)	1214 (98%)	31 (2%)	47	72
2	C	1/1 (100%)	1 (100%)	0	100	100
2	I	1/1 (100%)	1 (100%)	0	100	100
3	D	1/1 (100%)	1 (100%)	0	100	100
3	J	1/1 (100%)	1 (100%)	0	100	100
4	G	2/2 (100%)	1 (50%)	1 (50%)	0	0
4	K	2/2 (100%)	2 (100%)	0	100	100
5	H	1/1 (100%)	1 (100%)	0	100	100
5	L	1/1 (100%)	1 (100%)	0	100	100
All	All	2502/8188 (31%)	2429 (97%)	73 (3%)	45	69

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1365	CYS
1	A	1366	MET
1	A	1401	CYS
1	A	1414	CYS
1	A	1427	ARG
1	A	1455	HIS
1	A	1477	VAL
1	A	1569	MET
1	A	1590	ARG
1	A	1651	LEU
1	A	1684	VAL
1	A	1722	ARG
1	A	1755	ASN
1	A	1864	ASN
1	A	1895	SER
1	A	1900	LYS
1	A	1906	MET
1	A	1910	SER
1	A	1919	LEU
1	A	1955	MET
1	A	2014	ARG
1	A	2062	TYR
1	A	2066	MET
1	A	2070	MET
1	A	2088	MET
1	A	2127	ARG
1	A	2149	ARG
1	A	2174	VAL
1	A	2175	LEU
1	A	2254	ASP
1	A	2282	TYR
1	A	2299	LYS
1	A	2318	ARG
1	A	2333	HIS
1	A	2452	LEU
1	A	2507	VAL
1	A	2515	LEU
1	A	2575	LYS
1	A	2588	VAL
1	A	2685	TYR
1	A	2739	PHE
1	B	1449	VAL

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Mol	Chain	Res	Type
1	B	1463	VAL
1	B	1468	PHE
1	B	1564	MET
1	B	1579	ARG
1	B	1660	ASP
1	B	1681	MET
1	B	1714	CYS
1	B	1789	SER
1	B	1808	ASP
1	B	1821	LEU
1	B	1955	MET
1	B	1967	LEU
1	B	1987	VAL
1	B	2013	ARG
1	B	2127	ARG
1	B	2149	ARG
1	B	2242	MET
1	B	2274	TYR
1	B	2464	SER
1	B	2506	ARG
1	B	2507	VAL
1	B	2519	ARG
1	B	2542	PHE
1	B	2564	ASP
1	B	2590	VAL
1	B	2599	LEU
1	B	2656	CYS
1	B	2706	PHE
1	B	2707	THR
1	B	2736	VAL
4	G	3	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1458	ASN
1	A	1632	ASN
1	A	1645	HIS
1	A	1712	HIS
1	A	1755	ASN
1	A	1780	HIS
1	A	1864	ASN

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Mol	Chain	Res	Type
1	A	1920	GLN
1	A	2349	GLN
1	A	2356	HIS
1	A	2660	ASN
1	A	2710	ASN
1	A	2712	HIS
1	A	2715	ASN
1	B	1367	GLN
1	B	1576	HIS
1	B	1798	ASN
1	B	1993	ASN
1	B	2097	ASN
1	B	2710	ASN

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

50 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	$\#\|Z\| > 2$
6	NAG	E	1	6,1	14,14,15	0.35	0	17,19,21	0.89	1 (5%)
6	NAG	E	2	6	14,14,15	0.31	0	17,19,21	1.04	2 (11%)
7	NAG	F	1	7,1	14,14,15	0.45	0	17,19,21	1.46	4 (23%)
7	NAG	F	2	7	14,14,15	0.26	0	17,19,21	0.72	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	BMA	F	3	7	11,11,12	0.24	0	15,15,17	0.86	1 (6%)
6	NAG	M	1	6,1	14,14,15	0.32	0	17,19,21	0.62	0
6	NAG	M	2	6	14,14,15	0.30	0	17,19,21	0.74	0
6	NAG	N	1	6,1	14,14,15	0.34	0	17,19,21	1.18	2 (11%)
6	NAG	N	2	6	14,14,15	0.32	0	17,19,21	0.93	1 (5%)
8	NAG	O	1	8,1	14,14,15	0.33	0	17,19,21	1.50	2 (11%)
8	NAG	O	2	8	14,14,15	0.29	0	17,19,21	0.90	1 (5%)
8	BMA	O	3	8	11,11,12	0.23	0	15,15,17	0.97	1 (6%)
8	MAN	O	4	8	11,11,12	0.25	0	15,15,17	0.64	0
8	MAN	O	5	8	11,11,12	0.27	0	15,15,17	0.71	0
6	NAG	P	1	6,1	14,14,15	0.29	0	17,19,21	0.64	0
6	NAG	P	2	6	14,14,15	0.30	0	17,19,21	0.90	0
8	NAG	Q	1	8,1	14,14,15	0.35	0	17,19,21	0.87	1 (5%)
8	NAG	Q	2	8	14,14,15	0.29	0	17,19,21	0.72	1 (5%)
8	BMA	Q	3	8	11,11,12	0.21	0	15,15,17	0.79	0
8	MAN	Q	4	8	11,11,12	0.24	0	15,15,17	0.73	0
8	MAN	Q	5	8	11,11,12	0.21	0	15,15,17	0.65	0
6	NAG	R	1	6,1	14,14,15	0.29	0	17,19,21	0.71	0
6	NAG	R	2	6	14,14,15	0.31	0	17,19,21	0.91	1 (5%)
6	NAG	S	1	6,1	14,14,15	0.31	0	17,19,21	0.67	0
6	NAG	S	2	6	14,14,15	0.30	0	17,19,21	0.76	0
6	NAG	T	1	6,1	14,14,15	0.31	0	17,19,21	0.65	0
6	NAG	T	2	6	14,14,15	0.32	0	17,19,21	0.78	0
7	NAG	U	1	7,1	14,14,15	0.29	0	17,19,21	0.62	0
7	NAG	U	2	7	14,14,15	0.31	0	17,19,21	0.56	0
7	BMA	U	3	7	11,11,12	0.25	0	15,15,17	0.75	0
6	NAG	V	1	6,1	14,14,15	0.41	0	17,19,21	1.17	2 (11%)
6	NAG	V	2	6	14,14,15	0.27	0	17,19,21	0.80	0
6	NAG	W	1	6,1	14,14,15	0.28	0	17,19,21	0.71	0
6	NAG	W	2	6	14,14,15	0.29	0	17,19,21	0.67	0
8	NAG	X	1	8,1	14,14,15	0.56	0	17,19,21	0.96	1 (5%)
8	NAG	X	2	8	14,14,15	0.34	0	17,19,21	0.96	1 (5%)
8	BMA	X	3	8	11,11,12	0.26	0	15,15,17	0.95	1 (6%)
8	MAN	X	4	8	11,11,12	0.25	0	15,15,17	0.63	0
8	MAN	X	5	8	11,11,12	0.21	0	15,15,17	0.66	0
6	NAG	Y	1	6,1	14,14,15	0.73	1 (7%)	17,19,21	1.29	1 (5%)
6	NAG	Y	2	6	14,14,15	0.39	0	17,19,21	0.84	1 (5%)
8	NAG	Z	1	8,1	14,14,15	0.38	0	17,19,21	0.84	1 (5%)
8	NAG	Z	2	8	14,14,15	0.30	0	17,19,21	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	BMA	Z	3	8	11,11,12	0.20	0	15,15,17	0.69	0
8	MAN	Z	4	8	11,11,12	0.23	0	15,15,17	0.66	0
8	MAN	Z	5	8	11,11,12	0.20	0	15,15,17	0.66	0
6	NAG	a	1	6,1	14,14,15	0.32	0	17,19,21	0.68	0
6	NAG	a	2	6	14,14,15	0.36	0	17,19,21	0.70	0
6	NAG	b	1	6,1	14,14,15	0.31	0	17,19,21	1.10	2 (11%)
6	NAG	b	2	6	14,14,15	0.32	0	17,19,21	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
6	NAG	E	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	E	2	6	-	3/6/23/26	0/1/1/1
7	NAG	F	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	F	2	7	-	1/6/23/26	0/1/1/1
7	BMA	F	3	7	-	0/2/19/22	0/1/1/1
6	NAG	M	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	M	2	6	-	0/6/23/26	0/1/1/1
6	NAG	N	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	N	2	6	-	3/6/23/26	0/1/1/1
8	NAG	O	1	8,1	-	3/6/23/26	0/1/1/1
8	NAG	O	2	8	-	2/6/23/26	0/1/1/1
8	BMA	O	3	8	-	0/2/19/22	0/1/1/1
8	MAN	O	4	8	-	0/2/19/22	0/1/1/1
8	MAN	O	5	8	-	0/2/19/22	0/1/1/1
6	NAG	P	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	P	2	6	-	2/6/23/26	0/1/1/1
8	NAG	Q	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	Q	2	8	-	1/6/23/26	0/1/1/1
8	BMA	Q	3	8	-	0/2/19/22	0/1/1/1
8	MAN	Q	4	8	-	0/2/19/22	0/1/1/1
8	MAN	Q	5	8	-	0/2/19/22	0/1/1/1
6	NAG	R	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	R	2	6	-	1/6/23/26	0/1/1/1
6	NAG	S	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	S	2	6	-	0/6/23/26	0/1/1/1
6	NAG	T	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	T	2	6	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	U	1	7,1	-	1/6/23/26	0/1/1/1
7	NAG	U	2	7	-	0/6/23/26	0/1/1/1
7	BMA	U	3	7	-	0/2/19/22	0/1/1/1
6	NAG	V	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	V	2	6	-	1/6/23/26	0/1/1/1
6	NAG	W	1	6,1	-	4/6/23/26	0/1/1/1
6	NAG	W	2	6	-	2/6/23/26	0/1/1/1
8	NAG	X	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	X	2	8	-	0/6/23/26	0/1/1/1
8	BMA	X	3	8	-	2/2/19/22	0/1/1/1
8	MAN	X	4	8	-	0/2/19/22	0/1/1/1
8	MAN	X	5	8	-	0/2/19/22	0/1/1/1
6	NAG	Y	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	Y	2	6	-	0/6/23/26	0/1/1/1
8	NAG	Z	1	8,1	-	1/6/23/26	0/1/1/1
8	NAG	Z	2	8	-	0/6/23/26	0/1/1/1
8	BMA	Z	3	8	-	0/2/19/22	0/1/1/1
8	MAN	Z	4	8	-	0/2/19/22	0/1/1/1
8	MAN	Z	5	8	-	0/2/19/22	0/1/1/1
6	NAG	a	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	a	2	6	-	0/6/23/26	0/1/1/1
6	NAG	b	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	b	2	6	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Y	1	NAG	C1-C2	2.40	1.55	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	O	1	NAG	C1-O5-C5	4.38	118.12	112.19
6	Y	1	NAG	C1-O5-C5	3.71	117.21	112.19
7	F	1	NAG	O5-C5-C6	3.66	112.95	107.20
8	O	1	NAG	O5-C1-C2	-3.65	105.52	111.29
6	V	1	NAG	C1-O5-C5	-3.56	107.37	112.19
6	b	1	NAG	C1-O5-C5	3.46	116.88	112.19
6	N	2	NAG	C1-O5-C5	3.13	116.43	112.19
7	F	1	NAG	O5-C1-C2	-2.83	106.83	111.29
6	N	1	NAG	O5-C1-C2	-2.82	106.84	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	O	2	NAG	C1-O5-C5	2.68	115.82	112.19
8	Q	1	NAG	C1-C2-N2	-2.57	106.10	110.49
7	F	1	NAG	C2-N2-C7	-2.50	119.35	122.90
8	X	3	BMA	C1-C2-C3	2.42	112.64	109.67
8	X	1	NAG	O5-C1-C2	-2.42	107.47	111.29
6	b	1	NAG	O5-C1-C2	-2.32	107.63	111.29
6	Y	2	NAG	O5-C5-C6	2.28	110.78	107.20
8	Q	2	NAG	C1-O5-C5	2.20	115.17	112.19
6	R	2	NAG	C1-O5-C5	2.19	115.16	112.19
6	N	1	NAG	C3-C4-C5	2.19	114.14	110.24
7	F	1	NAG	C1-O5-C5	-2.18	109.23	112.19
6	E	1	NAG	C1-O5-C5	2.16	115.12	112.19
7	F	2	NAG	O5-C1-C2	-2.16	107.88	111.29
8	Z	1	NAG	C2-N2-C7	2.15	125.96	122.90
8	X	2	NAG	O5-C1-C2	-2.15	107.90	111.29
8	O	3	BMA	C1-O5-C5	2.13	115.07	112.19
6	E	2	NAG	C2-N2-C7	2.04	125.81	122.90
6	V	1	NAG	O5-C5-C6	2.04	110.41	107.20
7	F	3	BMA	C1-O5-C5	2.02	114.93	112.19
6	E	2	NAG	O5-C1-C2	-2.00	108.13	111.29

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	N	2	NAG	C8-C7-N2-C2
6	N	2	NAG	O7-C7-N2-C2
7	F	1	NAG	C8-C7-N2-C2
7	F	1	NAG	O7-C7-N2-C2
6	E	1	NAG	C8-C7-N2-C2
6	W	1	NAG	C1-C2-N2-C7
6	E	1	NAG	O7-C7-N2-C2
6	Y	1	NAG	C8-C7-N2-C2
6	Y	1	NAG	O7-C7-N2-C2
8	X	3	BMA	O5-C5-C6-O6
6	b	2	NAG	C8-C7-N2-C2
6	N	2	NAG	O5-C5-C6-O6
6	b	2	NAG	O7-C7-N2-C2
6	N	1	NAG	C1-C2-N2-C7
6	W	1	NAG	C8-C7-N2-C2
8	O	1	NAG	C8-C7-N2-C2
6	P	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	Q	2	NAG	O5-C5-C6-O6
6	E	2	NAG	O5-C5-C6-O6
6	V	2	NAG	O5-C5-C6-O6
6	b	1	NAG	O5-C5-C6-O6
7	U	1	NAG	O5-C5-C6-O6
6	W	1	NAG	O7-C7-N2-C2
8	O	1	NAG	O7-C7-N2-C2
8	X	3	BMA	C4-C5-C6-O6
6	P	2	NAG	C1-C2-N2-C7
6	E	2	NAG	C3-C2-N2-C7
6	R	2	NAG	C3-C2-N2-C7
6	W	1	NAG	C3-C2-N2-C7
6	W	2	NAG	C8-C7-N2-C2
8	O	2	NAG	C8-C7-N2-C2
7	F	2	NAG	C1-C2-N2-C7
6	E	2	NAG	C1-C2-N2-C7
8	O	2	NAG	O7-C7-N2-C2
6	N	1	NAG	C3-C2-N2-C7
8	Z	1	NAG	C3-C2-N2-C7
8	O	1	NAG	C4-C5-C6-O6
6	W	2	NAG	O7-C7-N2-C2
6	T	1	NAG	C8-C7-N2-C2

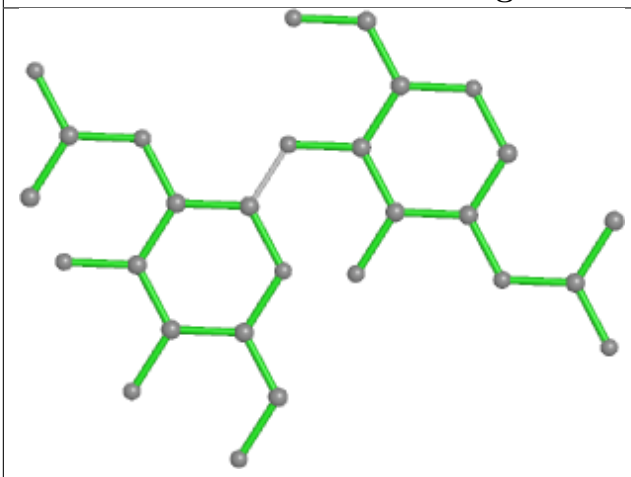
There are no ring outliers.

6 monomers are involved in 6 short contacts:

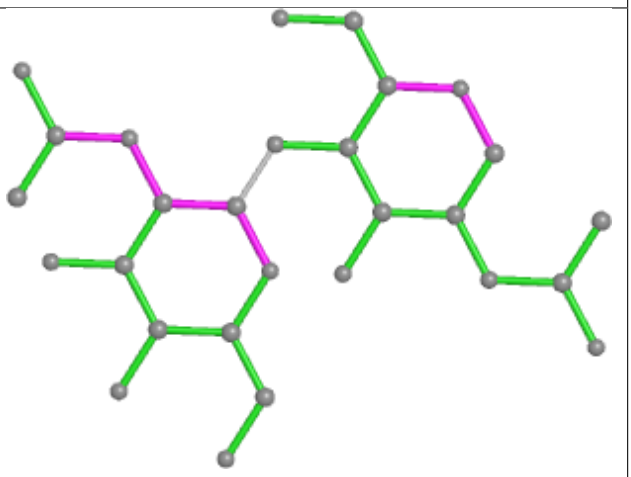
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	X	1	NAG	1	0
8	Q	1	NAG	2	0
7	U	1	NAG	1	0
6	V	1	NAG	1	0
6	Y	1	NAG	1	0
8	Q	2	NAG	1	0

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

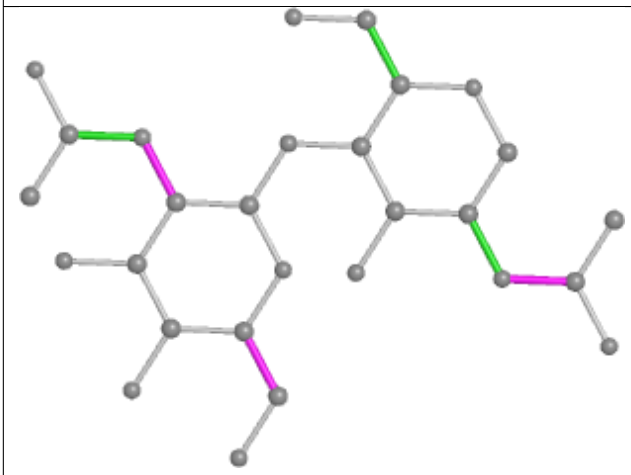
Oligosaccharide Chain E



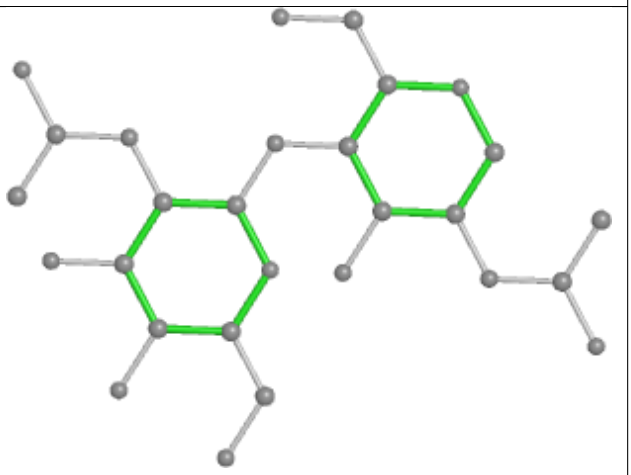
Bond lengths



Bond angles

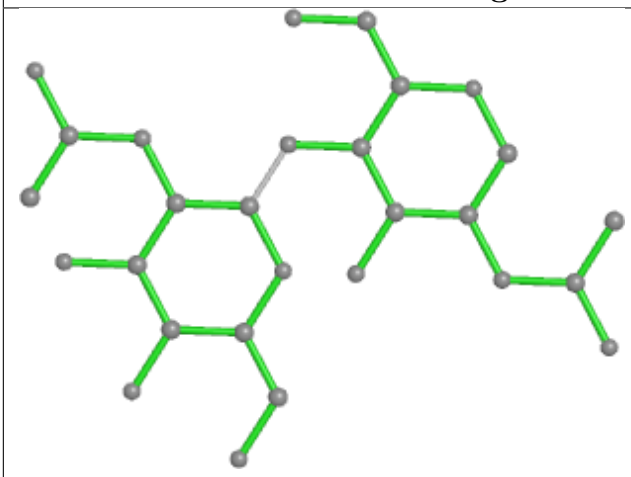


Torsions

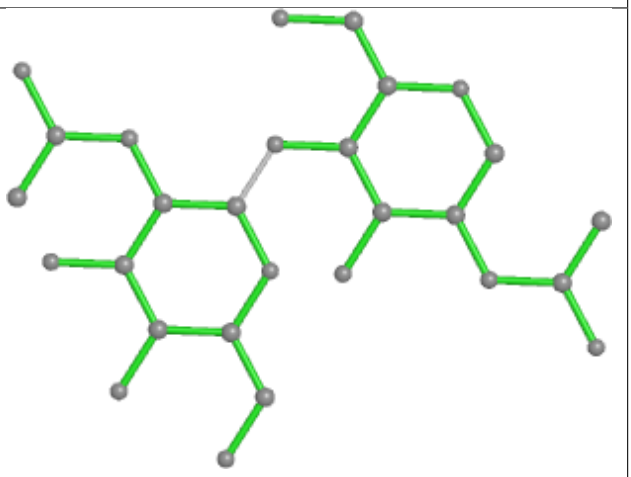


Rings

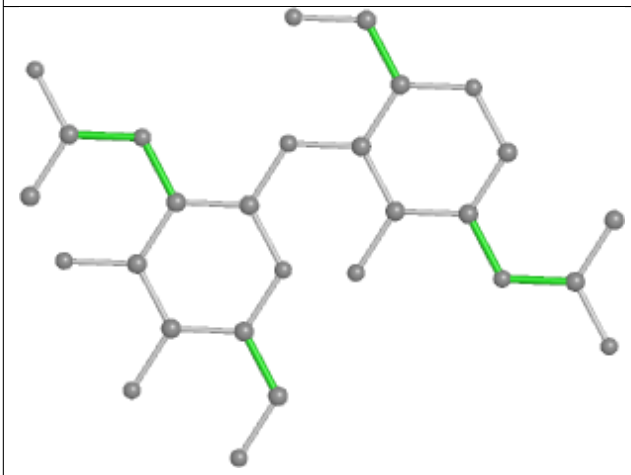
Oligosaccharide Chain M



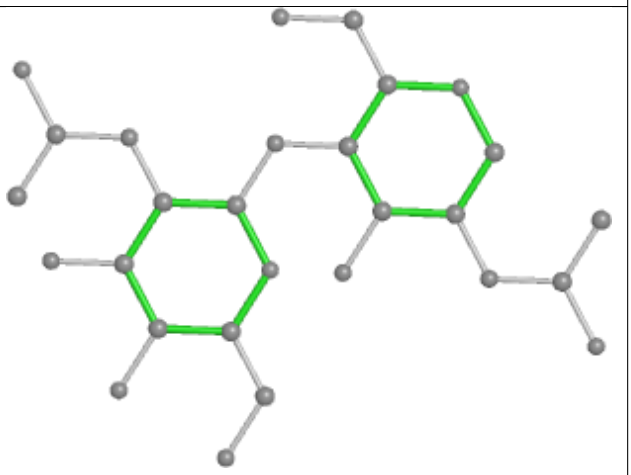
Bond lengths



Bond angles

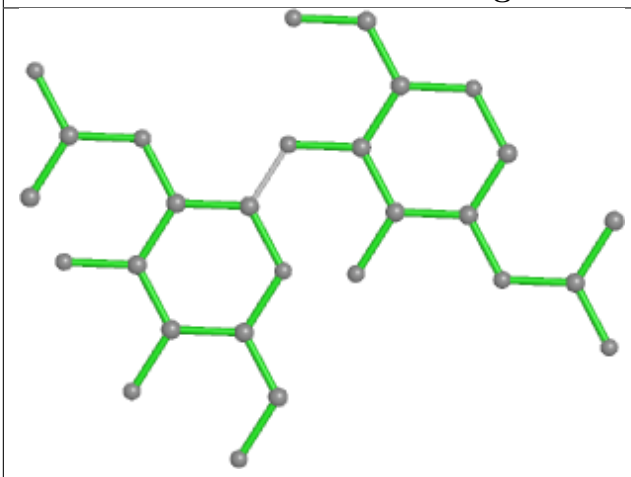


Torsions

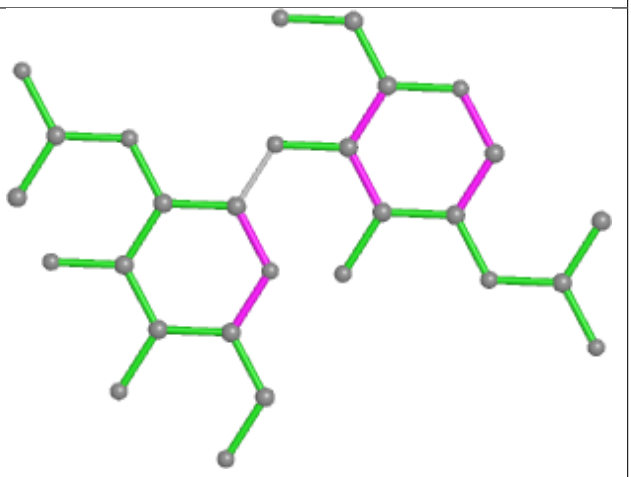


Rings

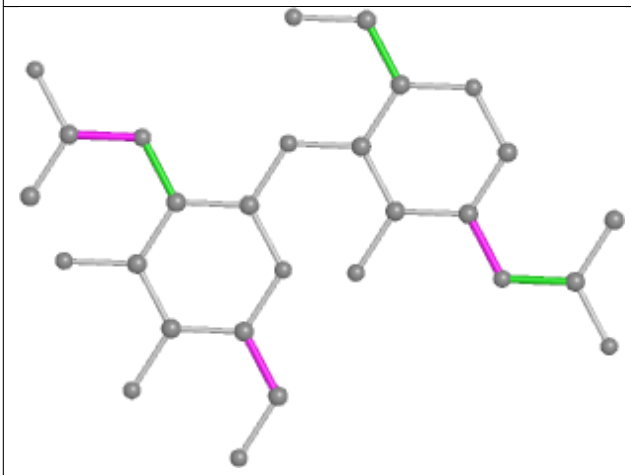
Oligosaccharide Chain N



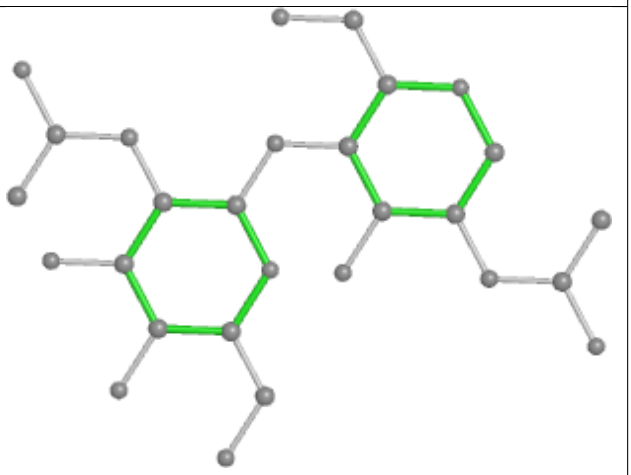
Bond lengths



Bond angles

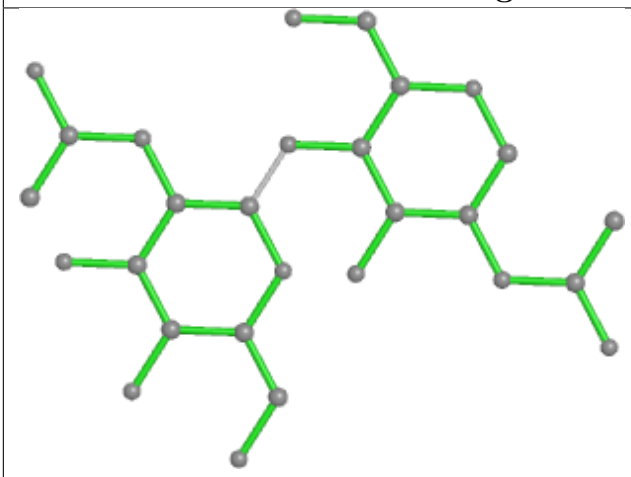


Torsions

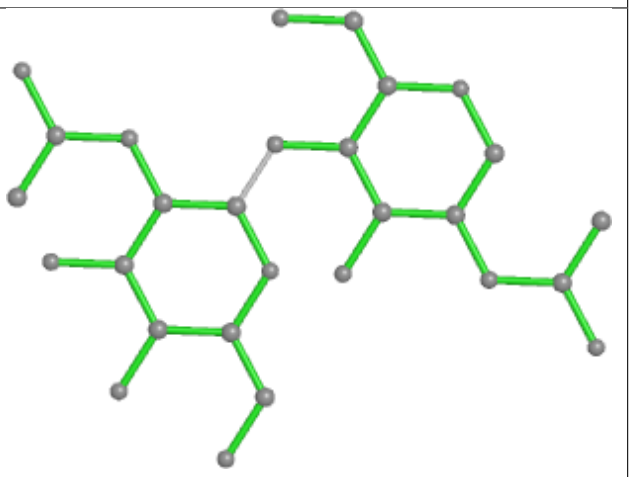


Rings

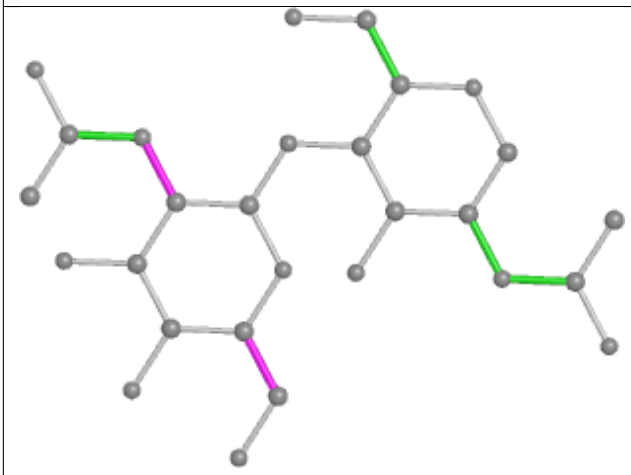
Oligosaccharide Chain P



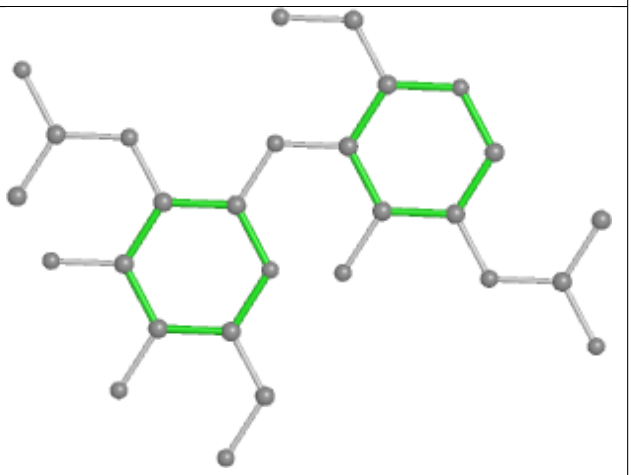
Bond lengths



Bond angles

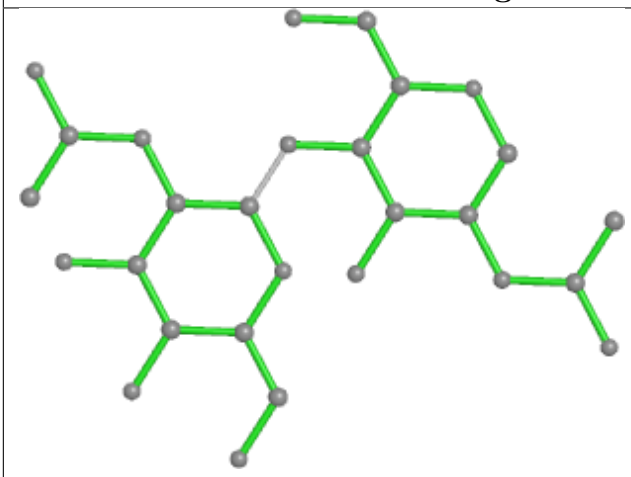


Torsions

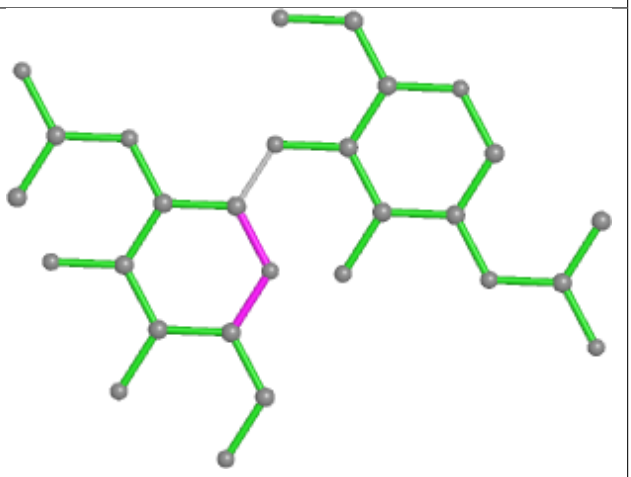


Rings

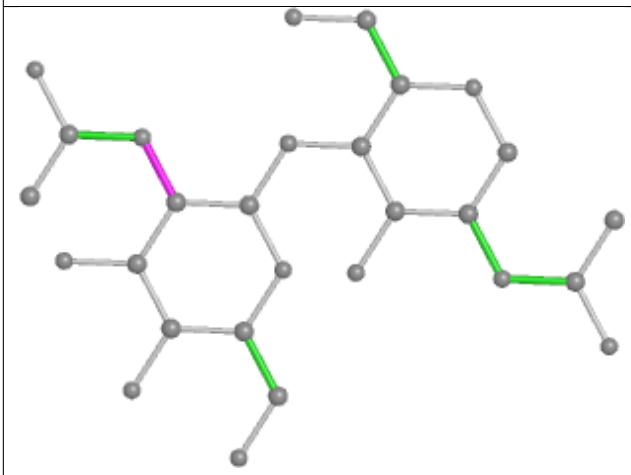
Oligosaccharide Chain R



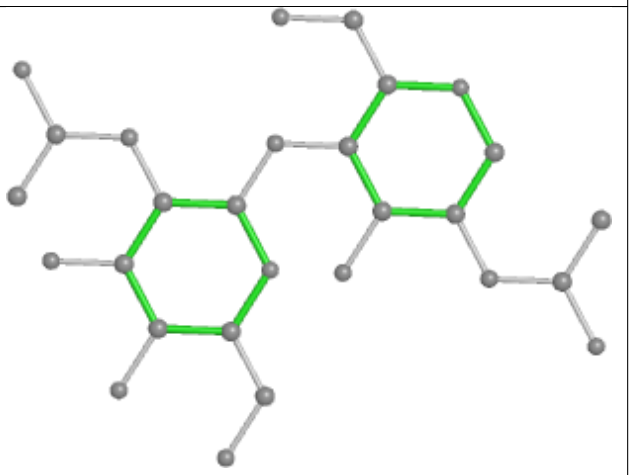
Bond lengths



Bond angles

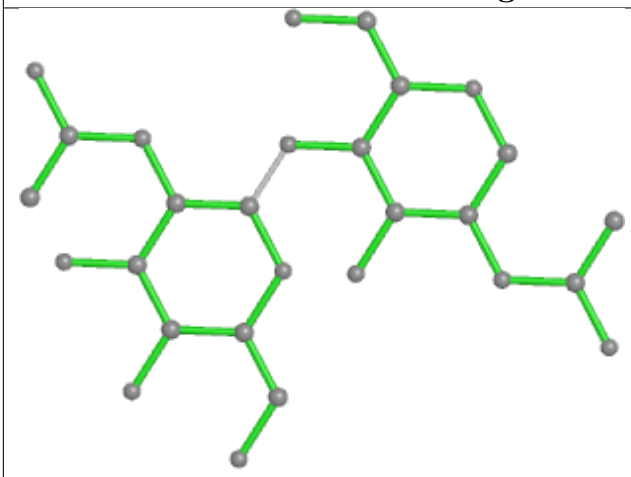


Torsions

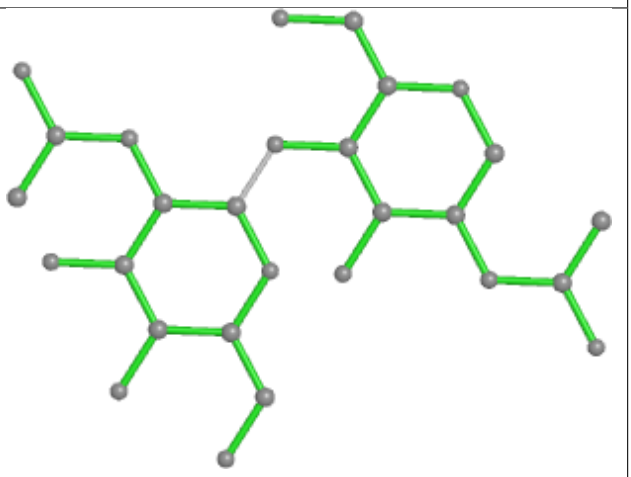


Rings

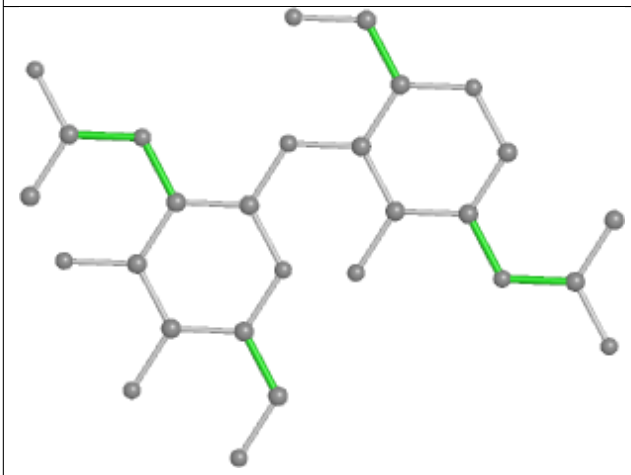
Oligosaccharide Chain S



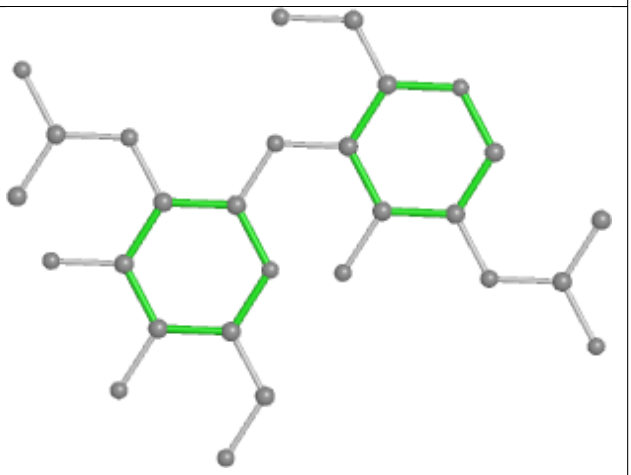
Bond lengths



Bond angles

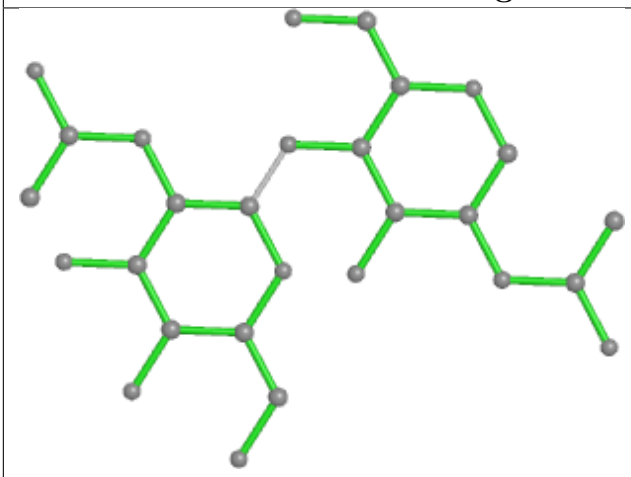


Torsions

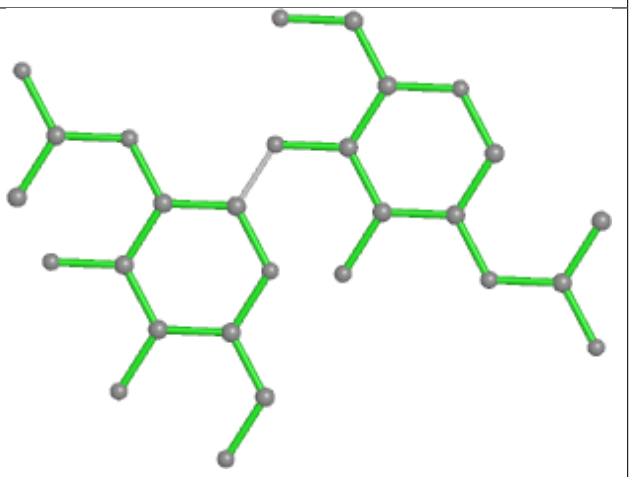


Rings

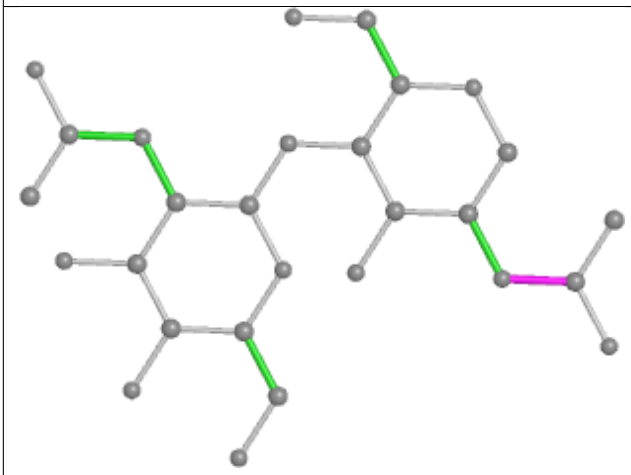
Oligosaccharide Chain T



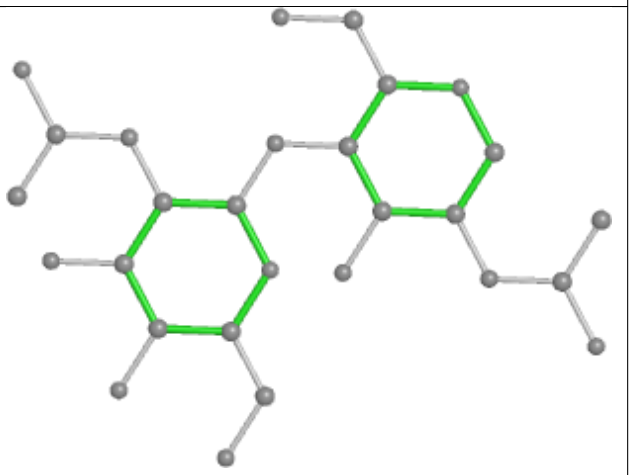
Bond lengths



Bond angles

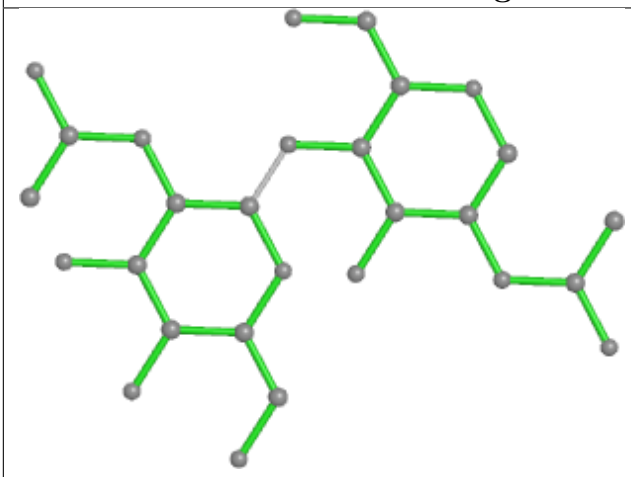


Torsions

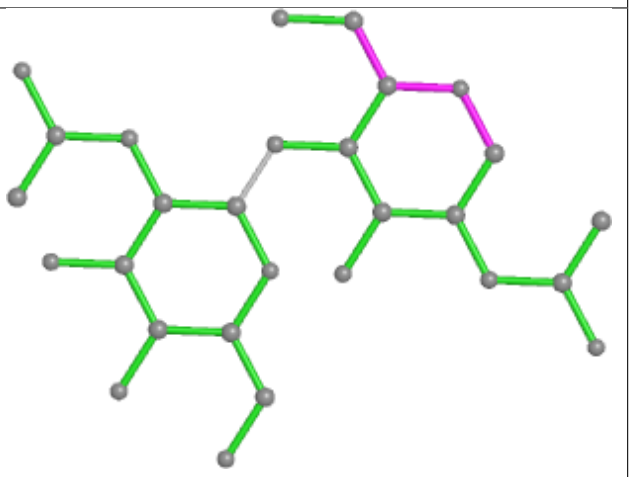


Rings

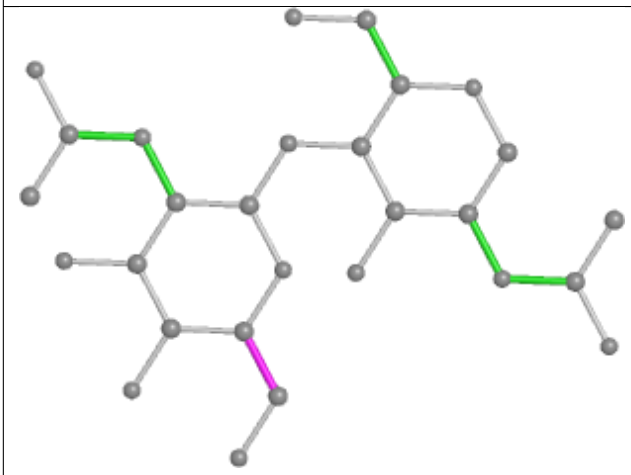
Oligosaccharide Chain V



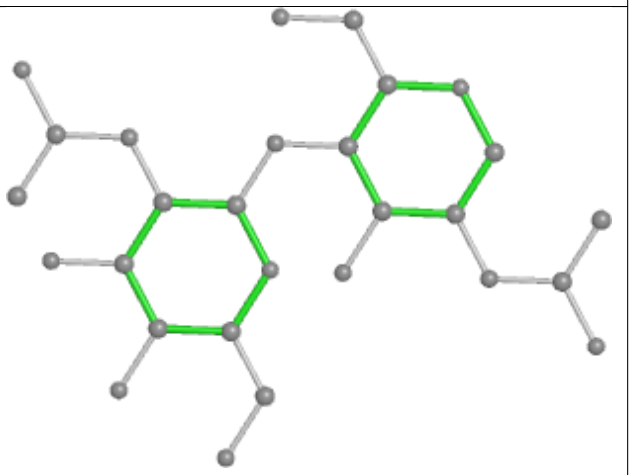
Bond lengths



Bond angles

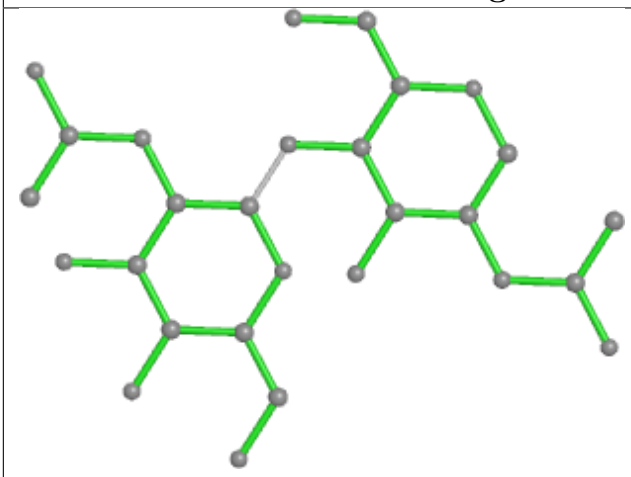


Torsions

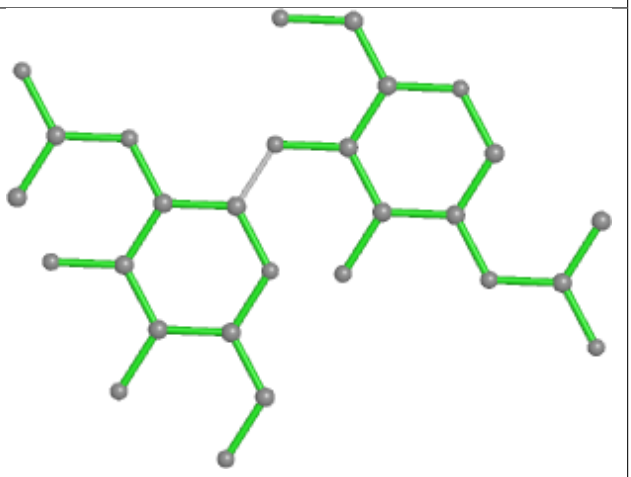


Rings

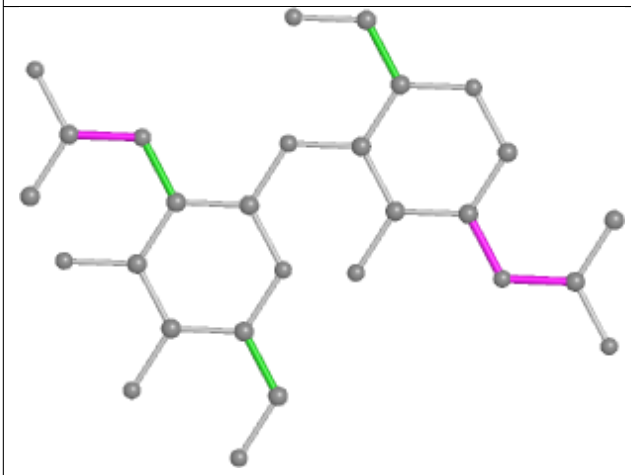
Oligosaccharide Chain W



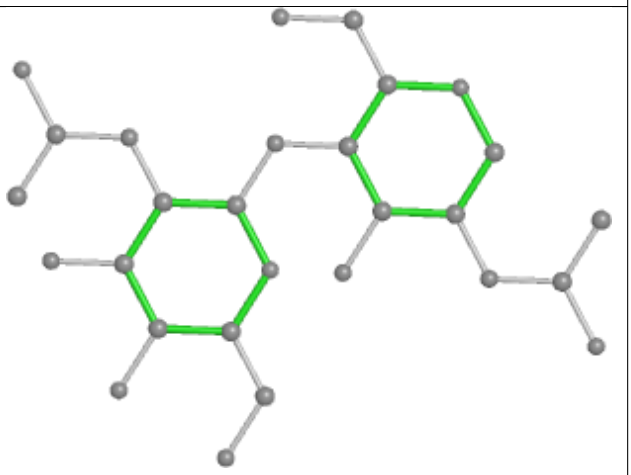
Bond lengths



Bond angles

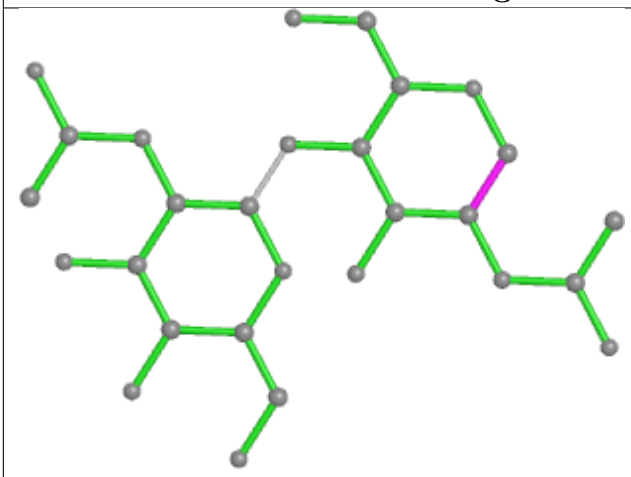


Torsions

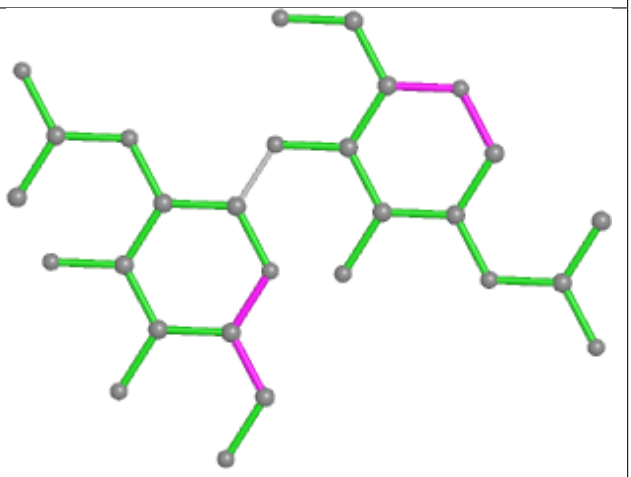


Rings

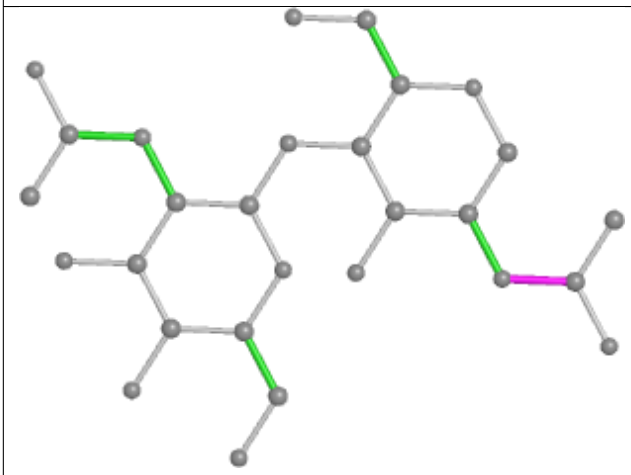
Oligosaccharide Chain Y



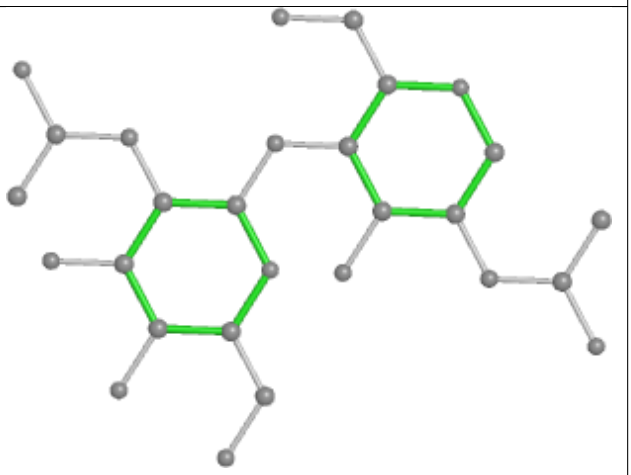
Bond lengths



Bond angles

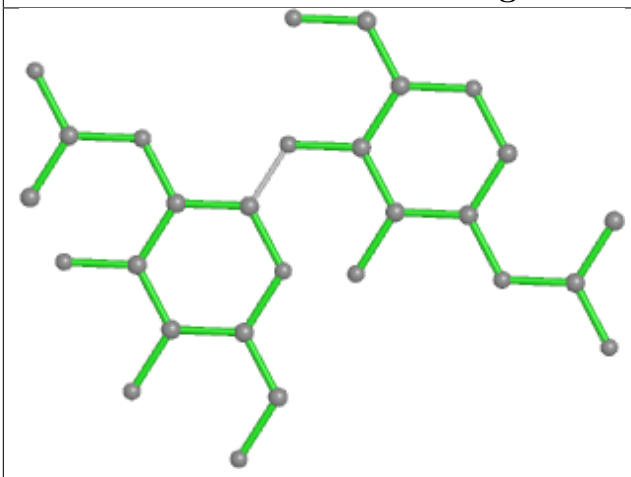


Torsions

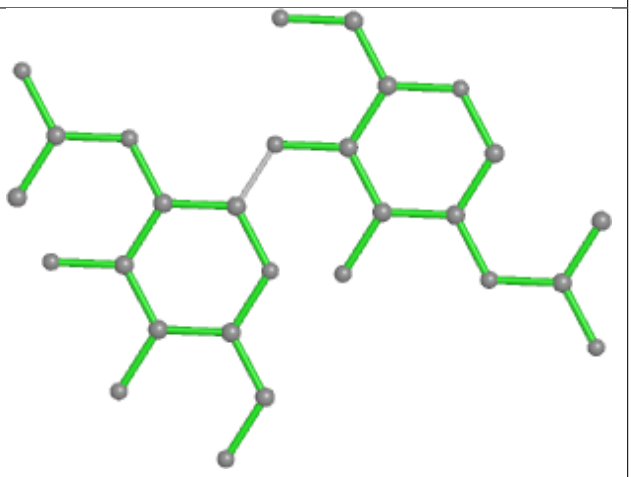


Rings

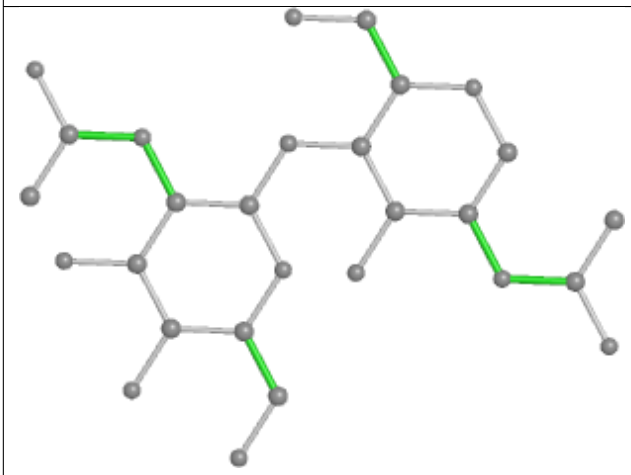
Oligosaccharide Chain a



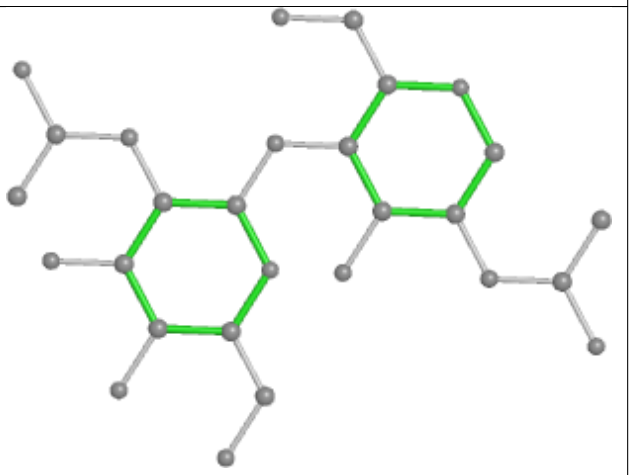
Bond lengths



Bond angles

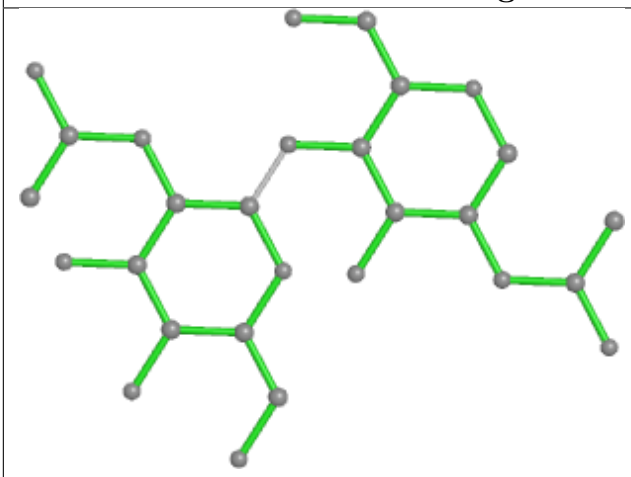


Torsions

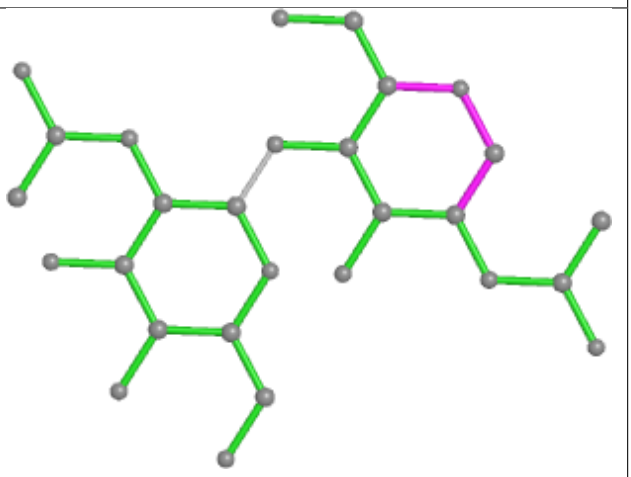


Rings

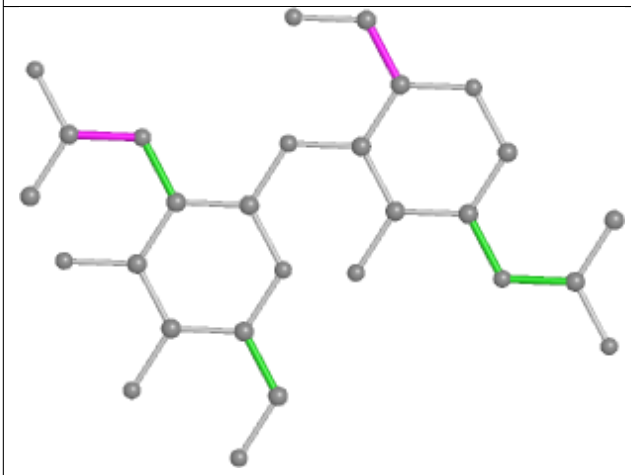
Oligosaccharide Chain b



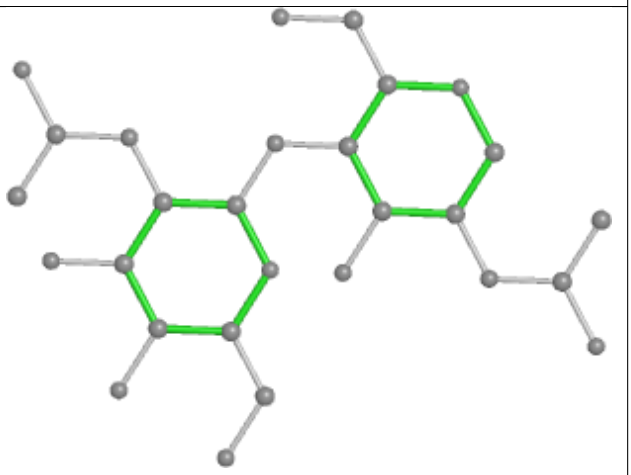
Bond lengths



Bond angles

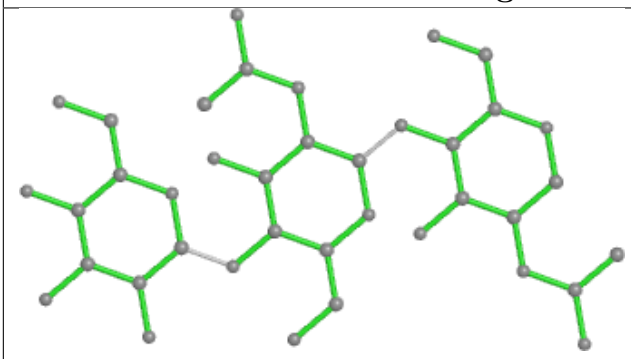


Torsions

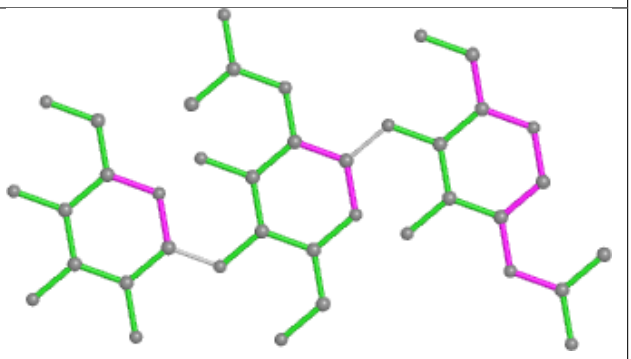


Rings

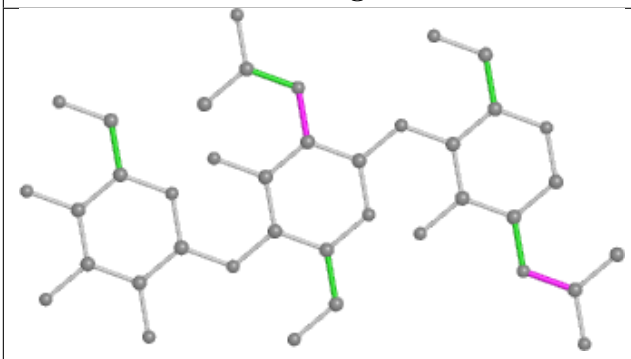
Oligosaccharide Chain F



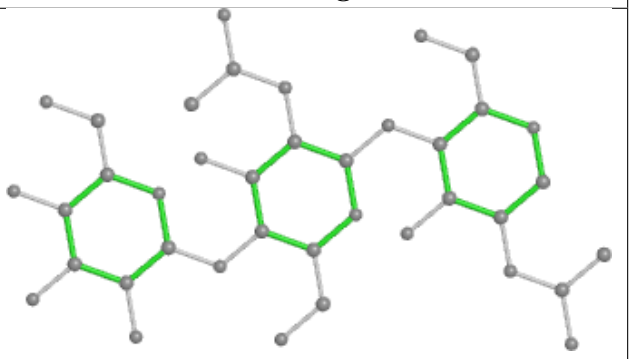
Bond lengths



Bond angles

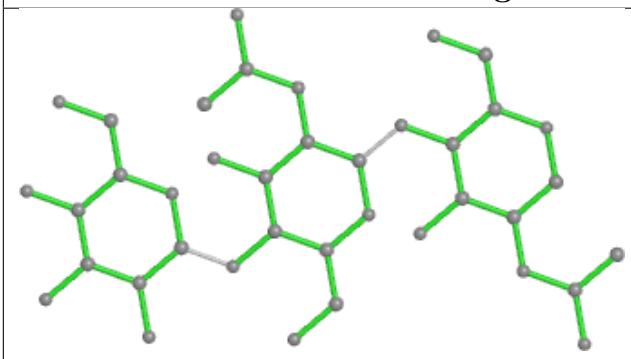


Torsions

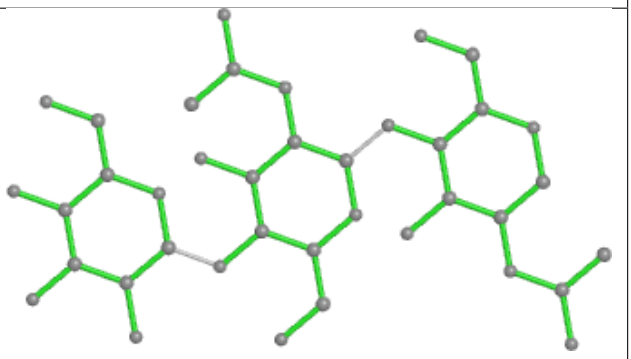


Rings

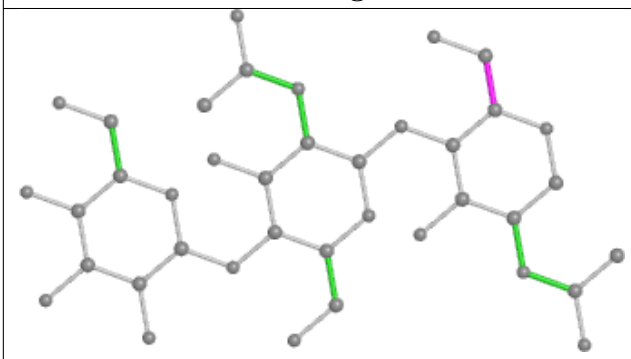
Oligosaccharide Chain U



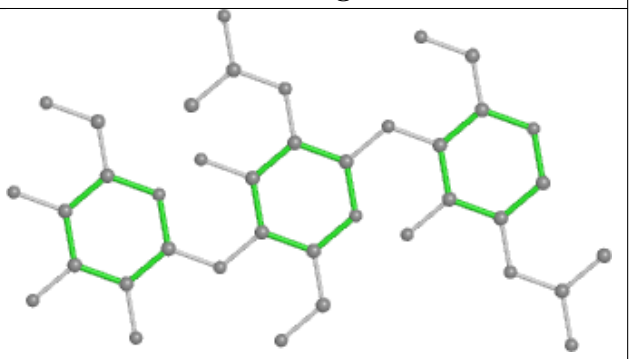
Bond lengths



Bond angles

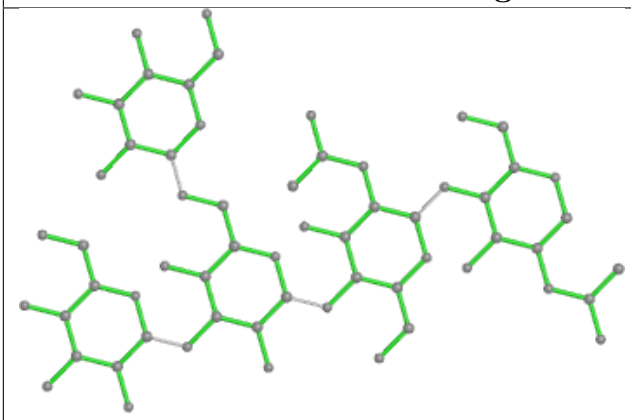


Torsions

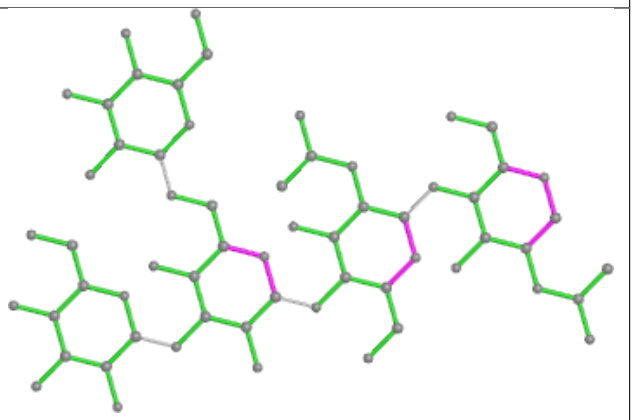


Rings

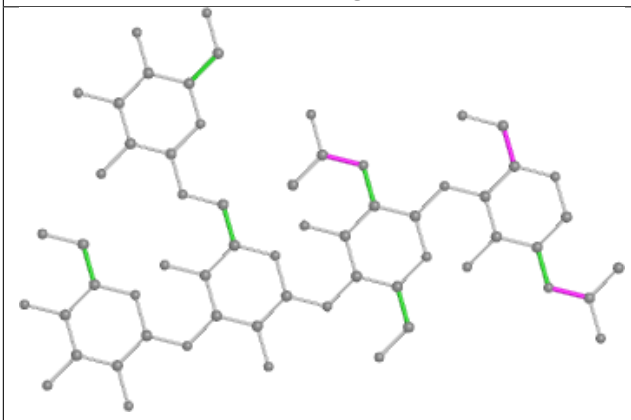
Oligosaccharide Chain O



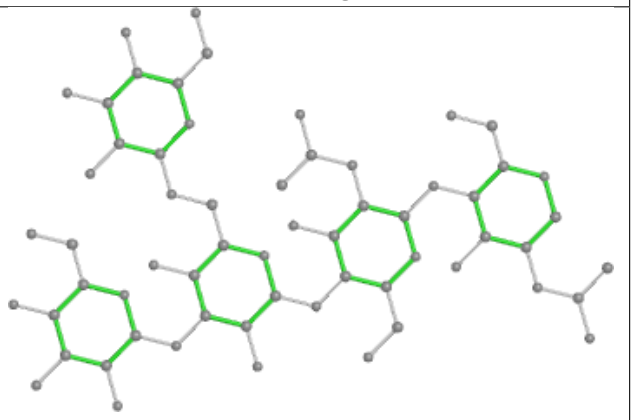
Bond lengths



Bond angles

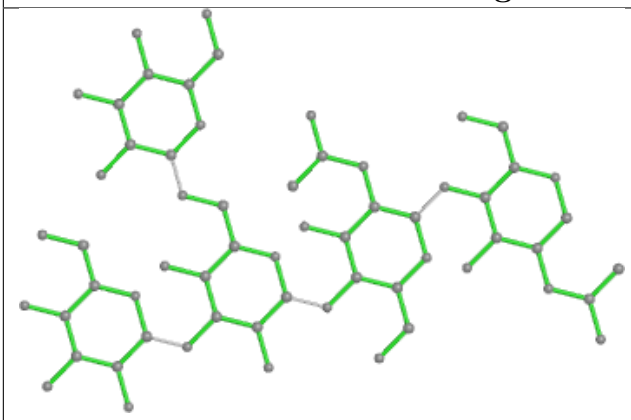


Torsions

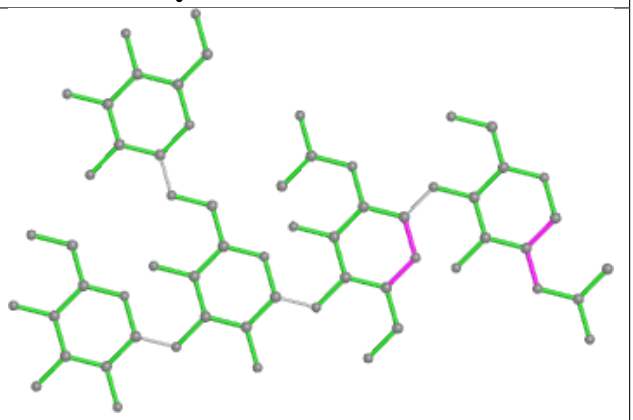


Rings

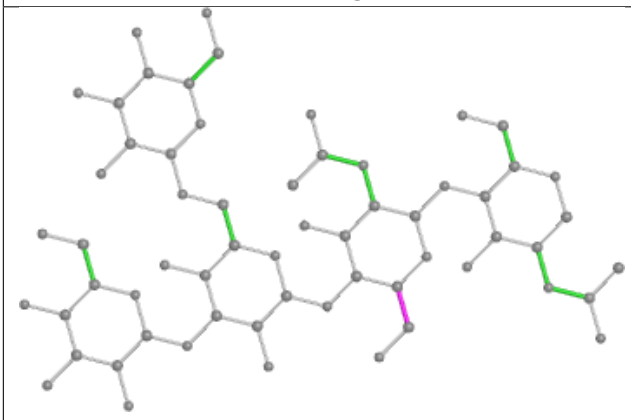
Oligosaccharide Chain Q



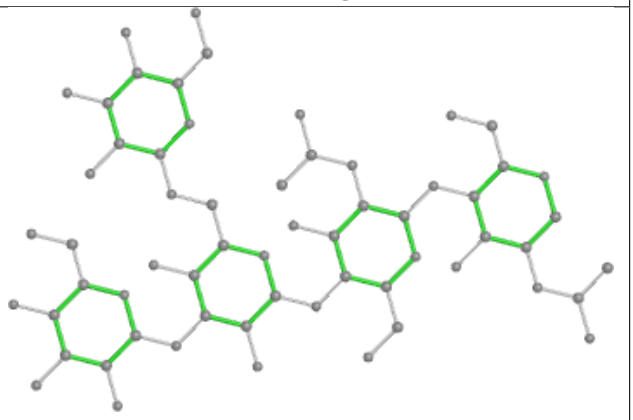
Bond lengths



Bond angles

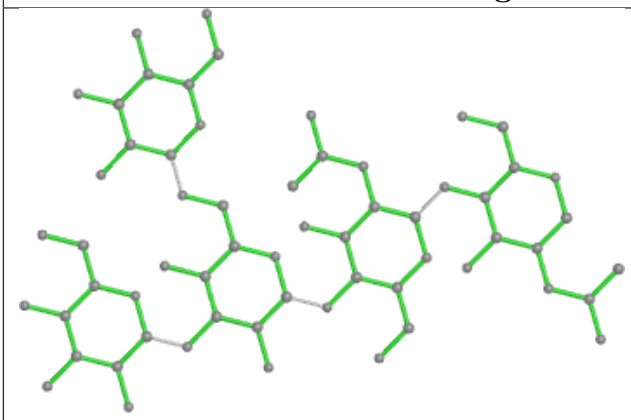


Torsions

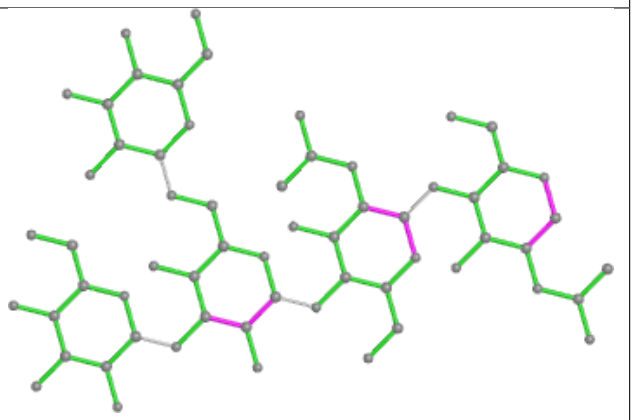


Rings

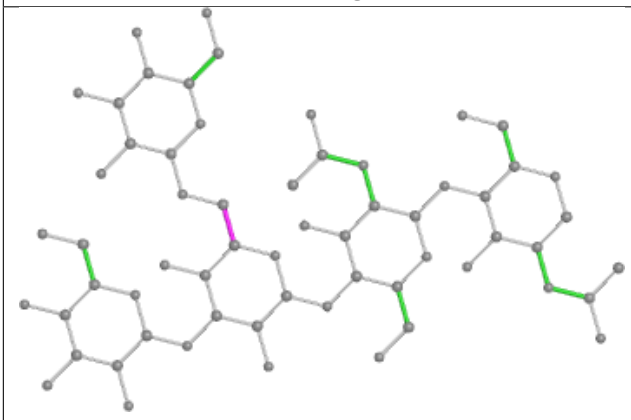
Oligosaccharide Chain X



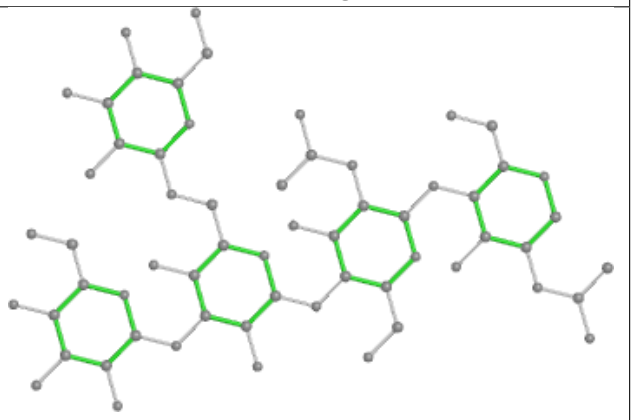
Bond lengths



Bond angles

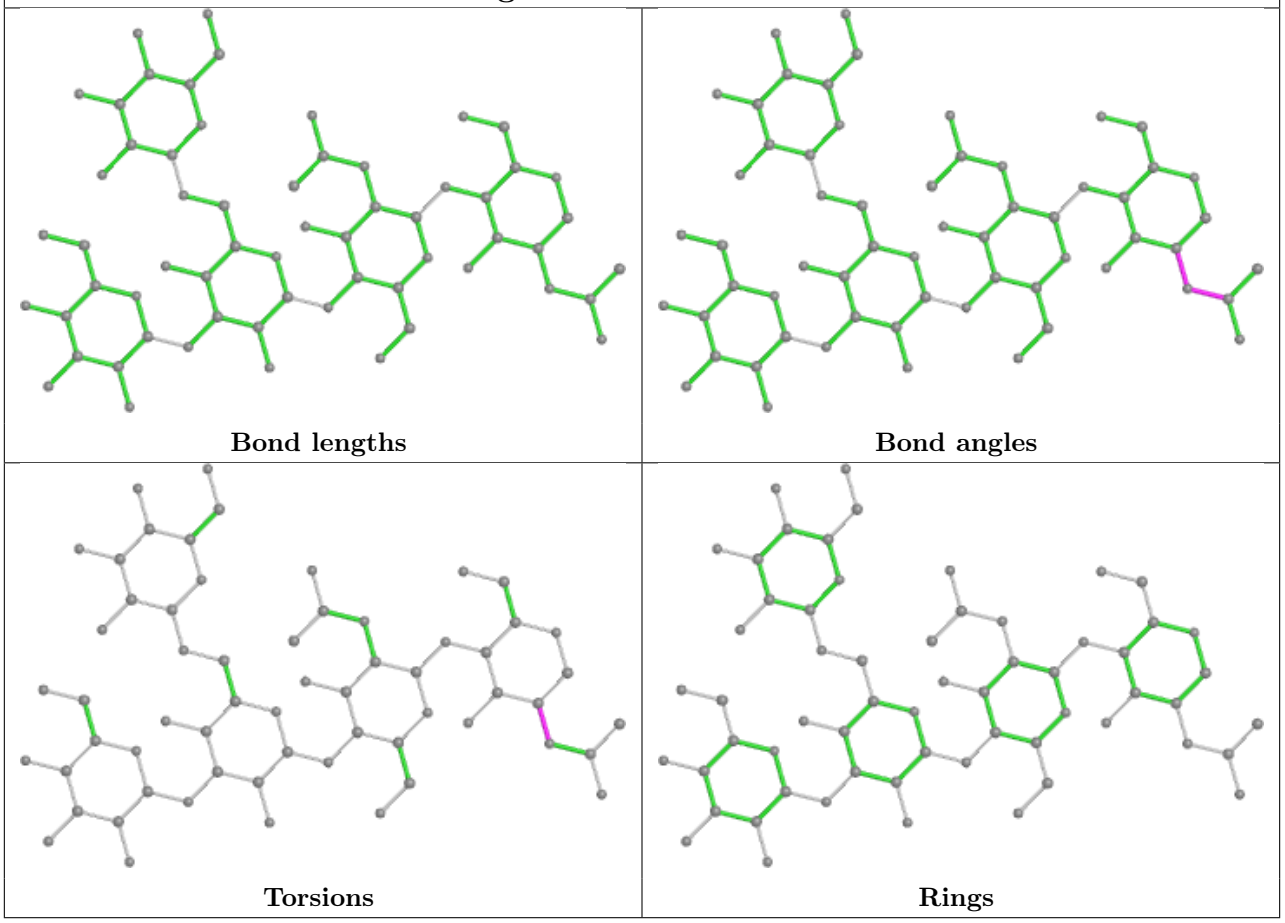


Torsions



Rings

Oligosaccharide Chain Z



5.6 Ligand geometry (i)

Of 22 ligands modelled in this entry, 12 are monoatomic - leaving 10 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	$\#\|Z\| > 2$
9	NAG	A	4702	1	14,14,15	0.33	0	17,19,21	0.91	1 (5%)
9	NAG	A	4703	1	14,14,15	0.36	0	17,19,21	1.05	1 (5%)
9	NAG	A	4701	1	14,14,15	0.40	0	17,19,21	2.23	3 (17%)
9	NAG	A	4704	1	14,14,15	0.38	0	17,19,21	0.85	0
10	A2G	B	4705	1	14,14,15	0.39	0	17,19,21	0.42	0
9	NAG	B	4704	1	14,14,15	0.50	0	17,19,21	2.14	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	NAG	B	4703	1	14,14,15	0.29	0	17,19,21	0.80	1 (5%)
10	A2G	A	4705	1	14,14,15	0.39	0	17,19,21	0.71	0
9	NAG	B	4701	1	14,14,15	0.34	0	17,19,21	0.75	1 (5%)
9	NAG	B	4702	1	14,14,15	0.53	0	17,19,21	1.94	3 (17%)

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
9	NAG	A	4702	1	-	2/6/23/26	0/1/1/1
9	NAG	A	4703	1	-	5/6/23/26	0/1/1/1
9	NAG	A	4701	1	-	3/6/23/26	0/1/1/1
9	NAG	A	4704	1	-	4/6/23/26	0/1/1/1
10	A2G	B	4705	1	-	1/6/23/26	0/1/1/1
9	NAG	B	4704	1	-	5/6/23/26	0/1/1/1
9	NAG	B	4703	1	-	3/6/23/26	0/1/1/1
10	A2G	A	4705	1	-	1/6/23/26	0/1/1/1
9	NAG	B	4701	1	-	2/6/23/26	0/1/1/1
9	NAG	B	4702	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	4701	NAG	C1-O5-C5	7.91	122.91	112.19
9	B	4702	NAG	C1-O5-C5	6.32	120.76	112.19
9	B	4704	NAG	C1-O5-C5	-6.25	103.72	112.19
9	B	4704	NAG	O5-C5-C6	5.52	115.86	107.20
9	A	4701	NAG	C4-C3-C2	-3.35	106.11	111.02
9	B	4702	NAG	C6-C5-C4	-3.26	105.36	113.00
9	A	4702	NAG	C1-O5-C5	2.99	116.24	112.19
9	B	4702	NAG	C4-C3-C2	-2.63	107.16	111.02
9	A	4703	NAG	C3-C4-C5	2.40	114.51	110.24
9	B	4701	NAG	C1-O5-C5	2.24	115.23	112.19
9	B	4703	NAG	C1-O5-C5	2.16	115.12	112.19
9	A	4701	NAG	C6-C5-C4	-2.12	108.03	113.00

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	4703	NAG	C3-C2-N2-C7
9	A	4704	NAG	C3-C2-N2-C7
9	A	4704	NAG	C8-C7-N2-C2
9	A	4704	NAG	O7-C7-N2-C2
9	B	4704	NAG	C3-C2-N2-C7
9	B	4704	NAG	C8-C7-N2-C2
9	B	4704	NAG	O7-C7-N2-C2
9	A	4703	NAG	C8-C7-N2-C2
9	A	4703	NAG	O7-C7-N2-C2
9	A	4703	NAG	O5-C5-C6-O6
9	B	4704	NAG	O5-C5-C6-O6
9	B	4703	NAG	C8-C7-N2-C2
9	A	4703	NAG	C4-C5-C6-O6
9	B	4703	NAG	O7-C7-N2-C2
9	B	4704	NAG	C4-C5-C6-O6
10	A	4705	A2G	O5-C5-C6-O6
9	A	4704	NAG	O5-C5-C6-O6
9	B	4703	NAG	C3-C2-N2-C7
10	B	4705	A2G	C1-C2-N2-C7
9	A	4701	NAG	O5-C5-C6-O6
9	A	4701	NAG	C8-C7-N2-C2
9	B	4701	NAG	C8-C7-N2-C2
9	A	4702	NAG	C4-C5-C6-O6
9	A	4701	NAG	O7-C7-N2-C2
9	A	4702	NAG	O5-C5-C6-O6
9	B	4701	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	4701	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.

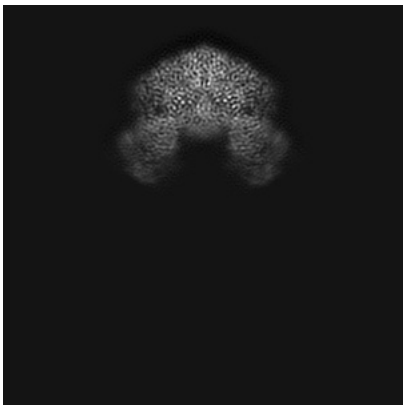
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-36692. These allow visual inspection of the internal detail of the map and identification of artifacts.

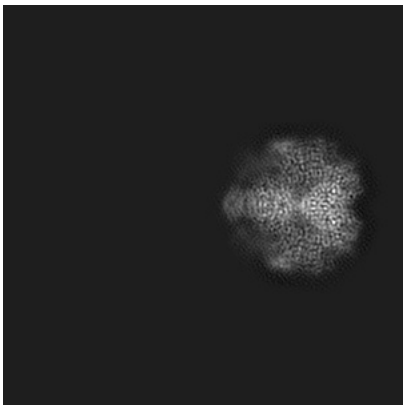
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

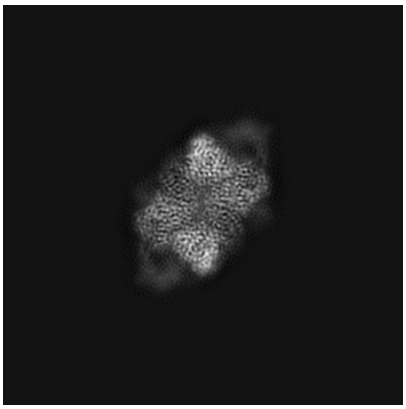
6.1.1 Primary map



X

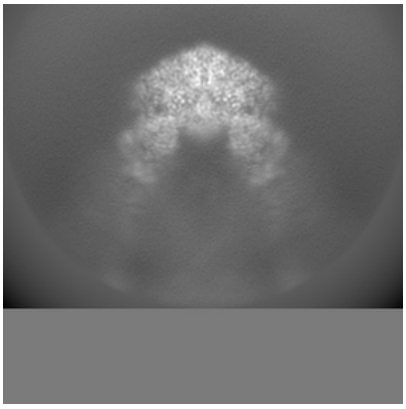


Y

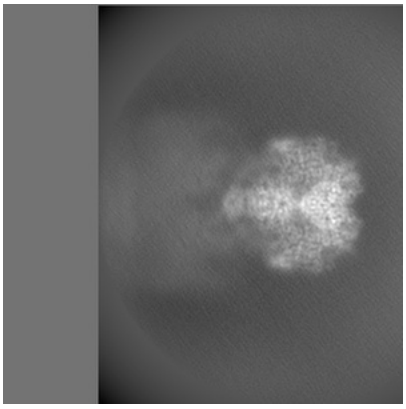


Z

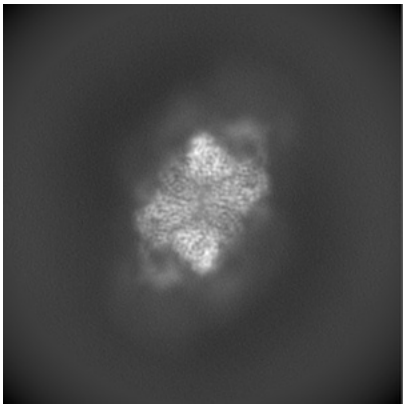
6.1.2 Raw map



X



Y

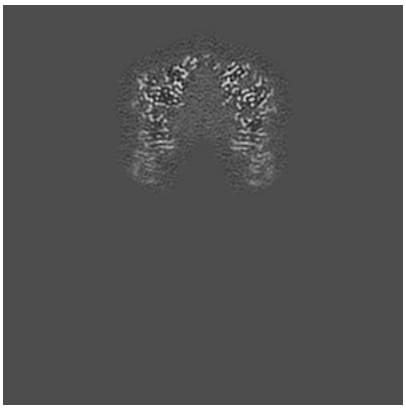


Z

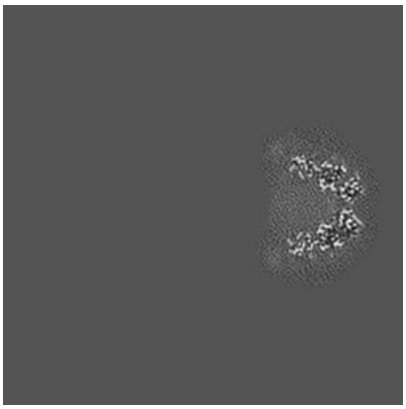
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

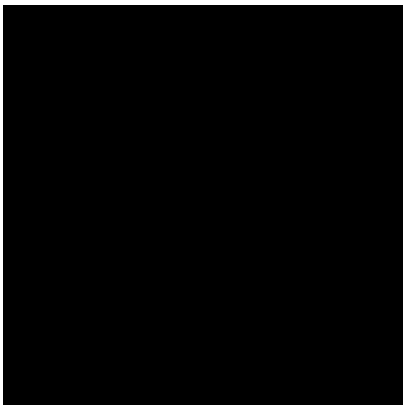
6.2.1 Primary map



X Index: 130

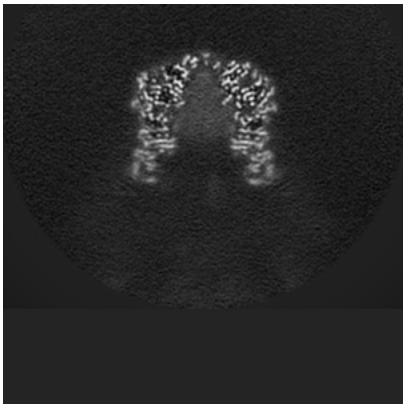


Y Index: 130

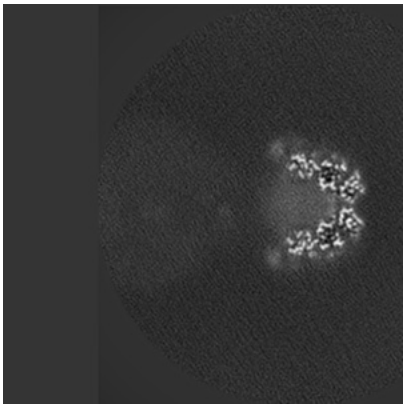


Z Index: 130

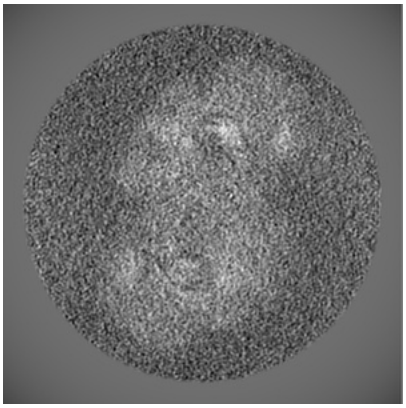
6.2.2 Raw map



X Index: 130



Y Index: 130



Z Index: 130

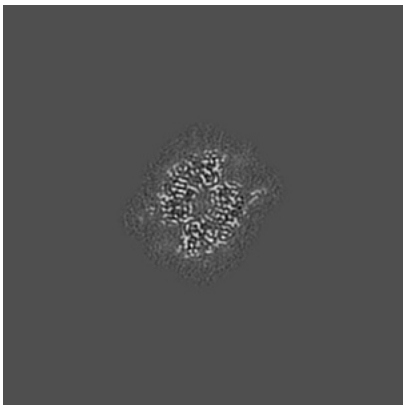
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

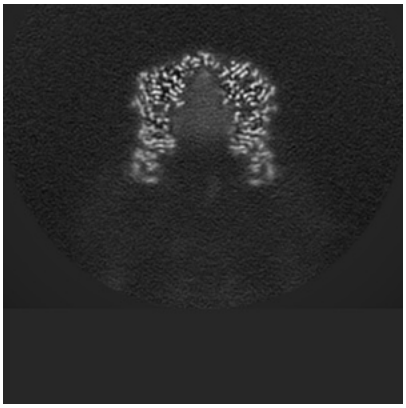
X Index: 131

Y Index: 134

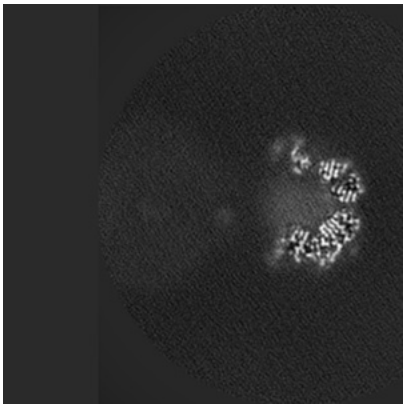


Z Index: 215

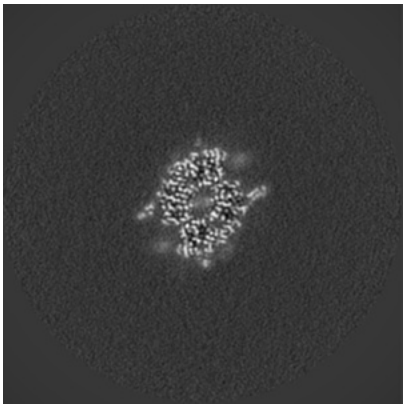
6.3.2 Raw map



X Index: 131



Y Index: 127

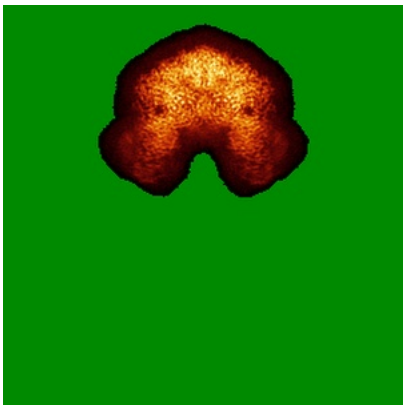


Z Index: 214

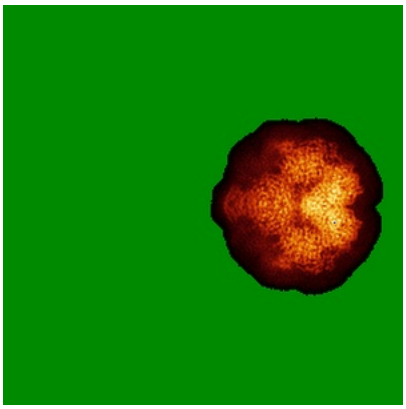
The images above show the largest variance slices of the map in three orthogonal directions.

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

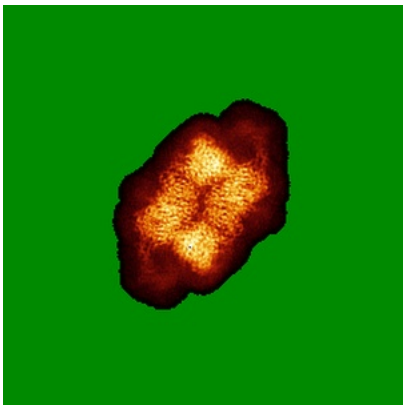
6.4.1 Primary map



X

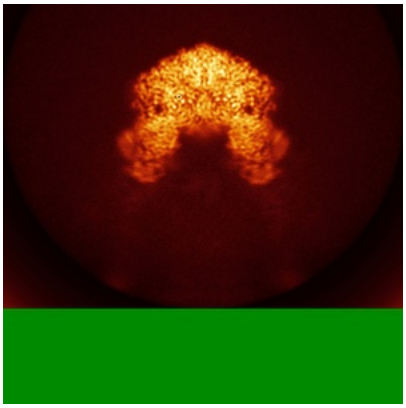


Y

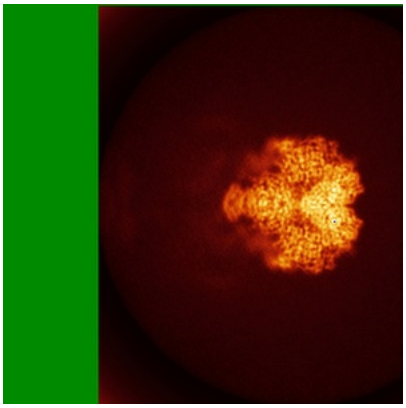


Z

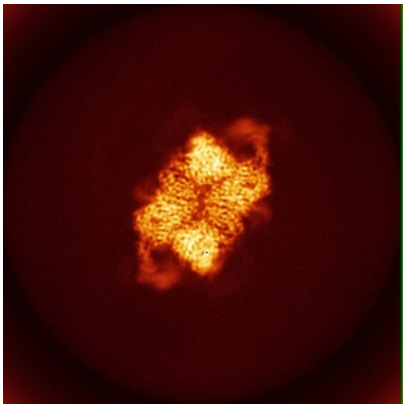
6.4.2 Raw map



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.

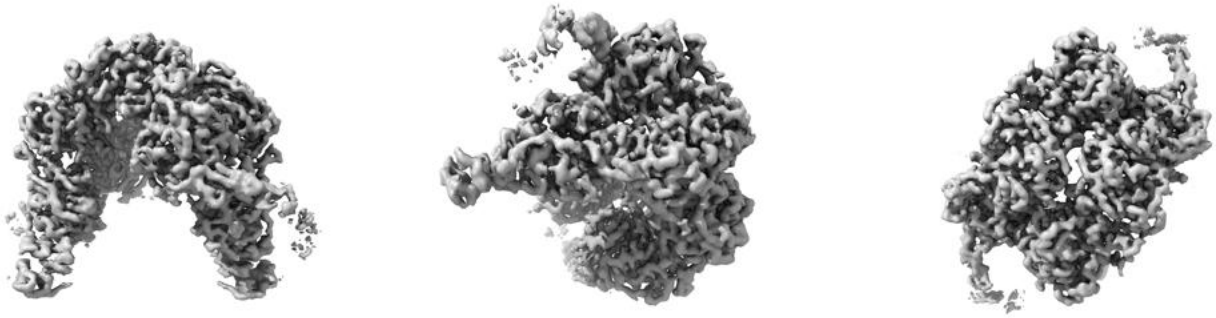
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0434. 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.

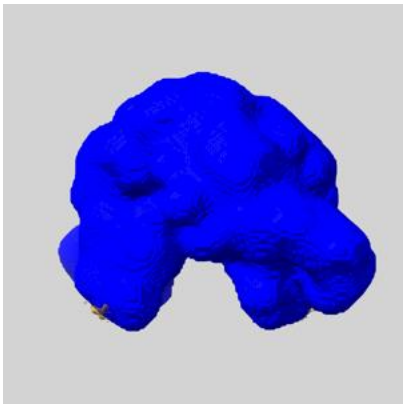
6.6 Mask visualisation (i)

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

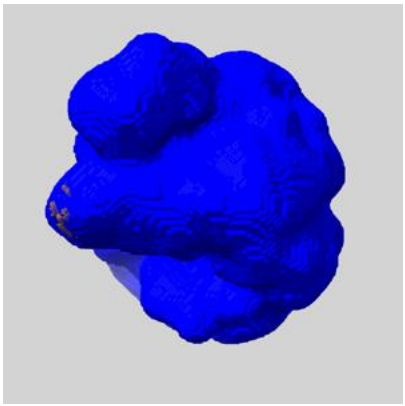
A mask typically either:

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

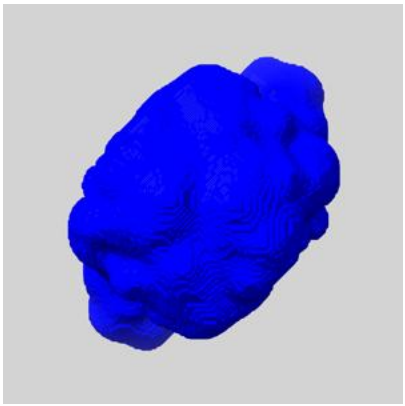
6.6.1 emd_36692_msk_1.map (i)



X



Y

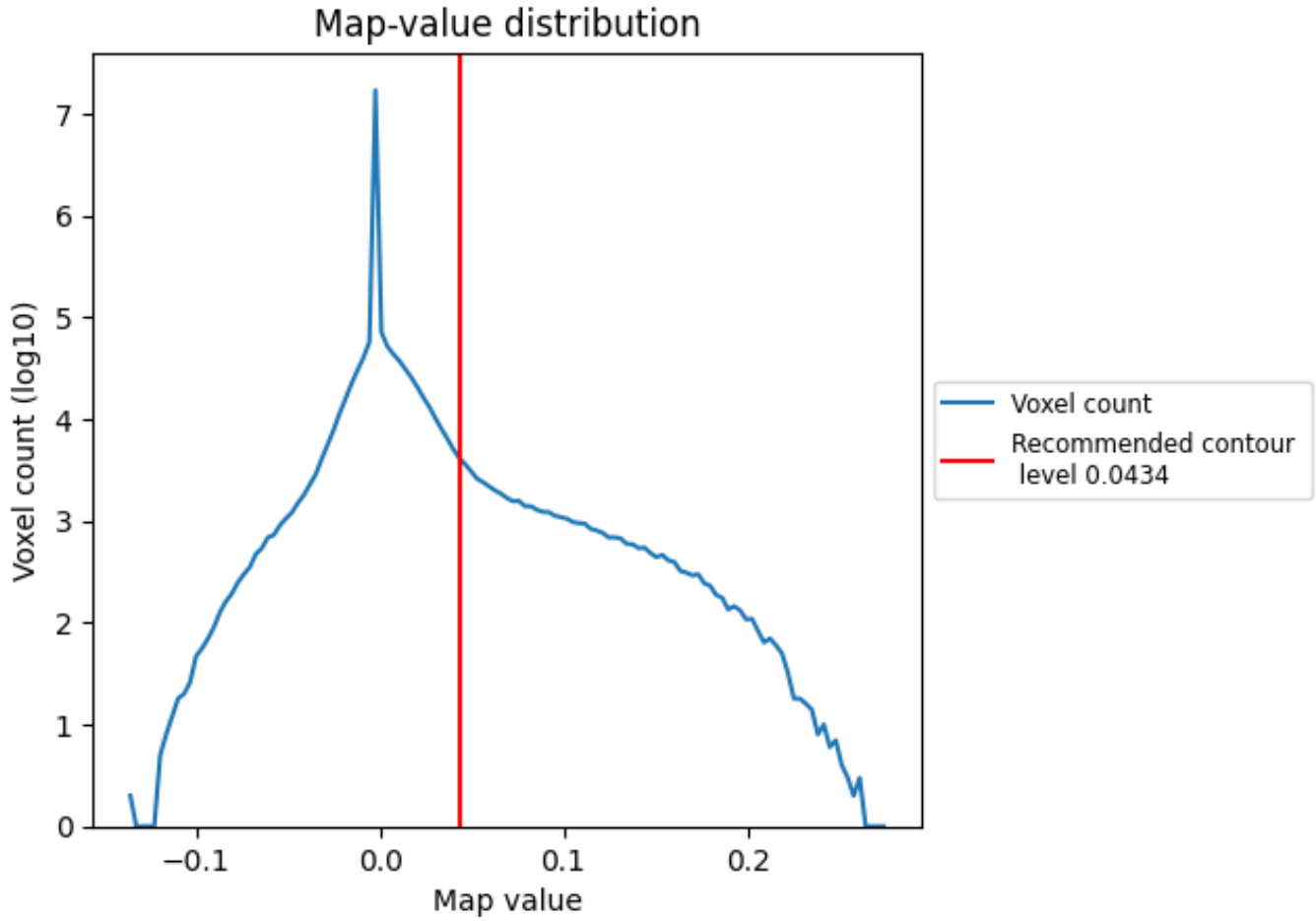


Z

7 Map analysis

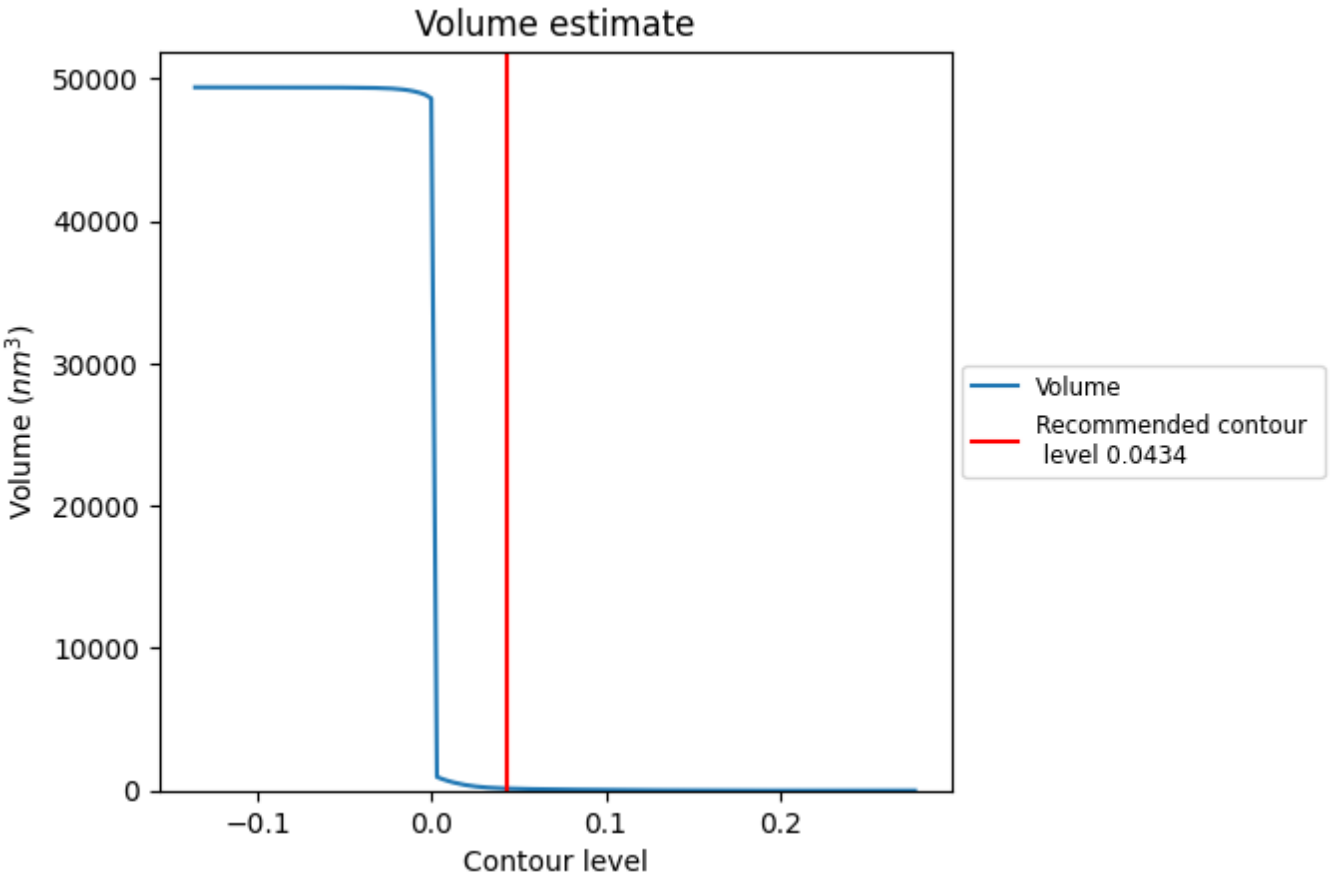
This section contains the results of statistical analysis of the map.

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.

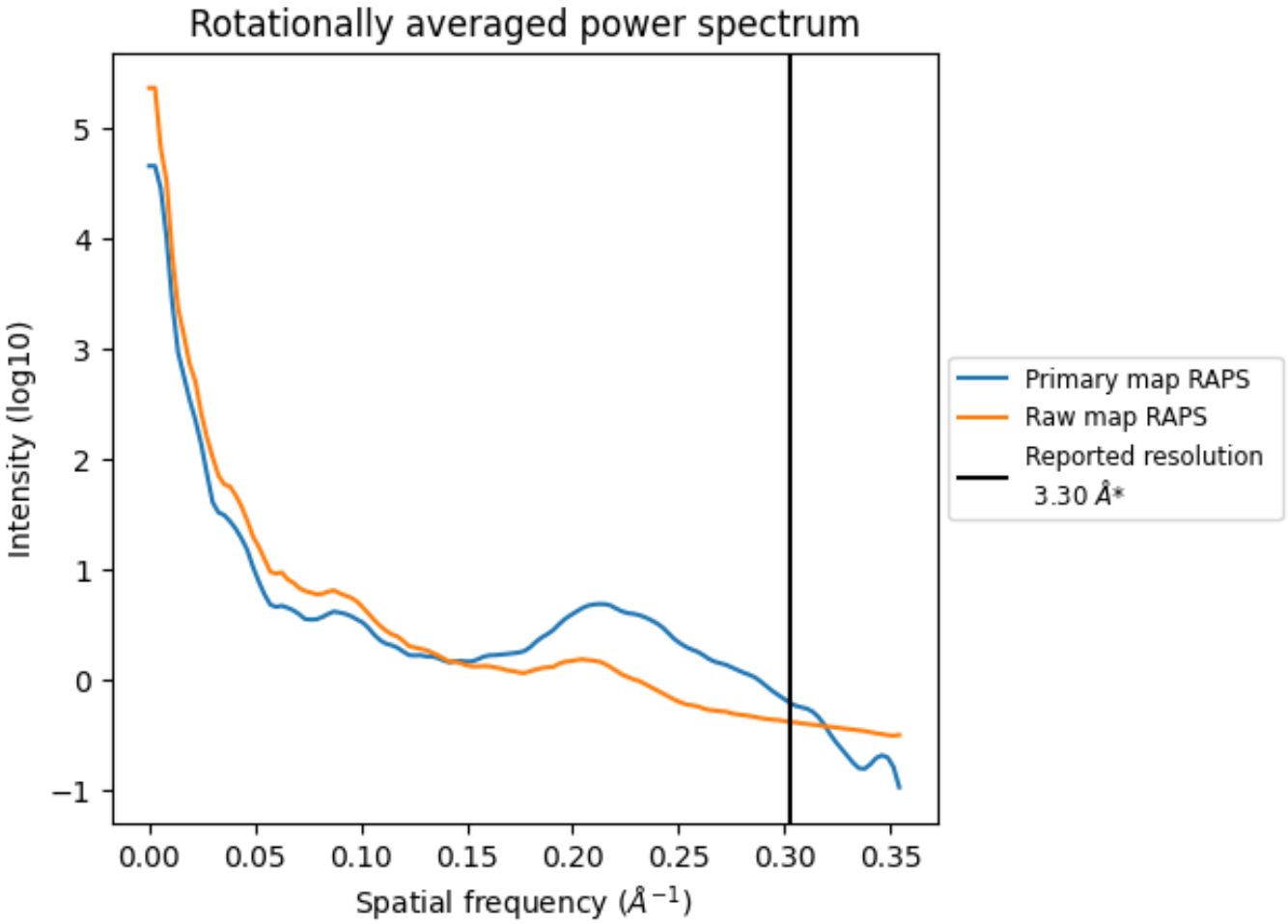
7.2 Volume estimate



The volume at the recommended contour level is 144 nm^3; this corresponds to an approximate mass of 130 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)

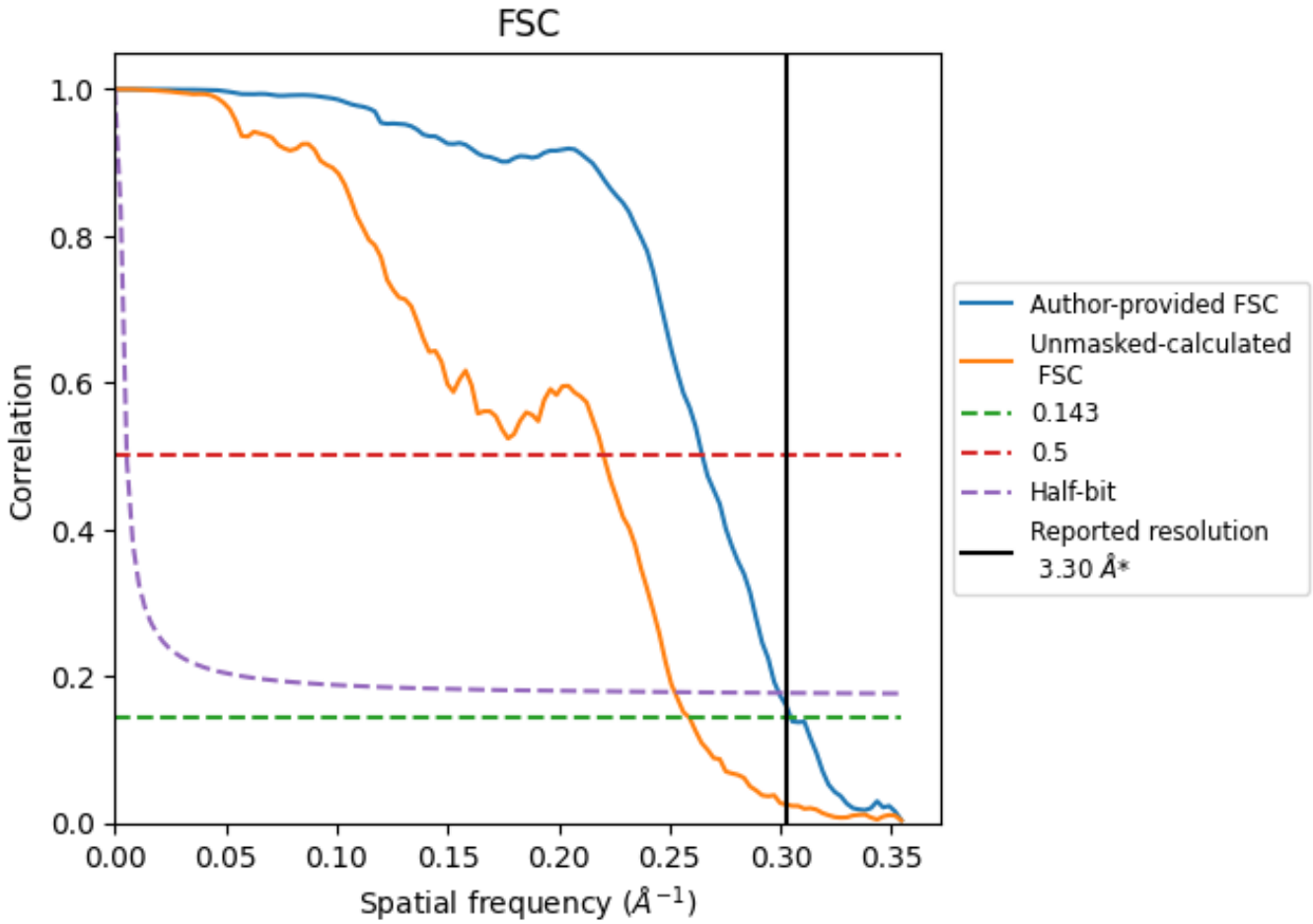


*Reported resolution corresponds to spatial frequency of 0.303 $Å^{-1}$

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 0.303 Å^{-1}

8.2 Resolution estimates (i)

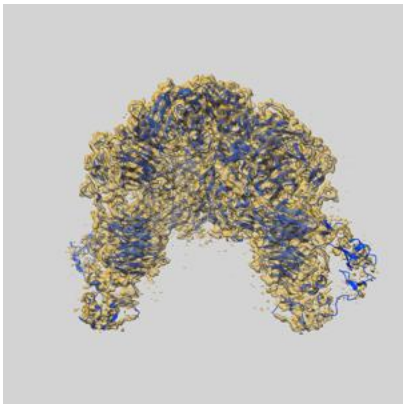
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.28	3.78	3.34
Unmasked-calculated*	3.86	4.54	3.96

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.86 differs from the reported value 3.3 by more than 10 %

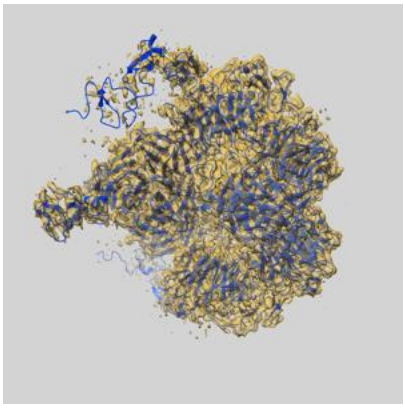
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-36692 and PDB model 8JX8. Per-residue inclusion information can be found in section 3 on page 9.

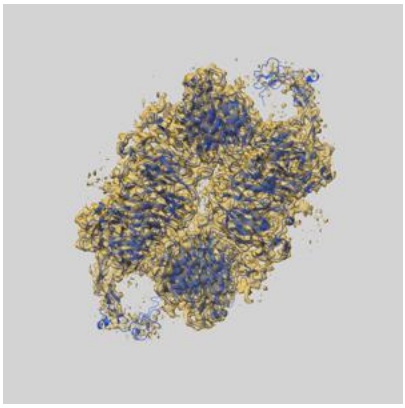
9.1 Map-model overlay



X



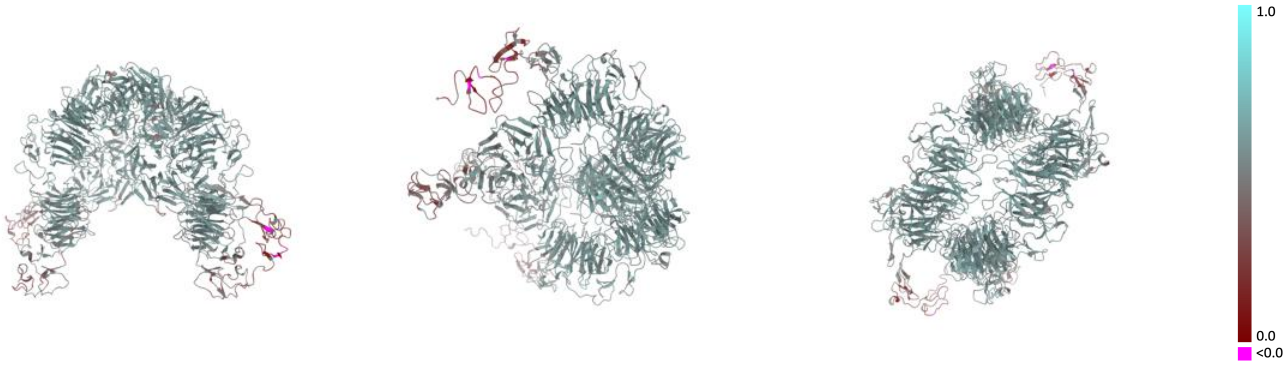
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0434 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

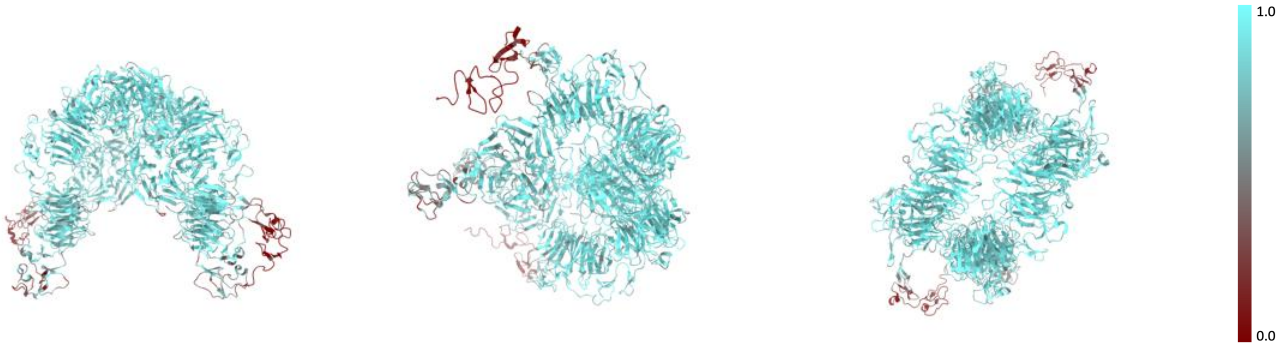
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

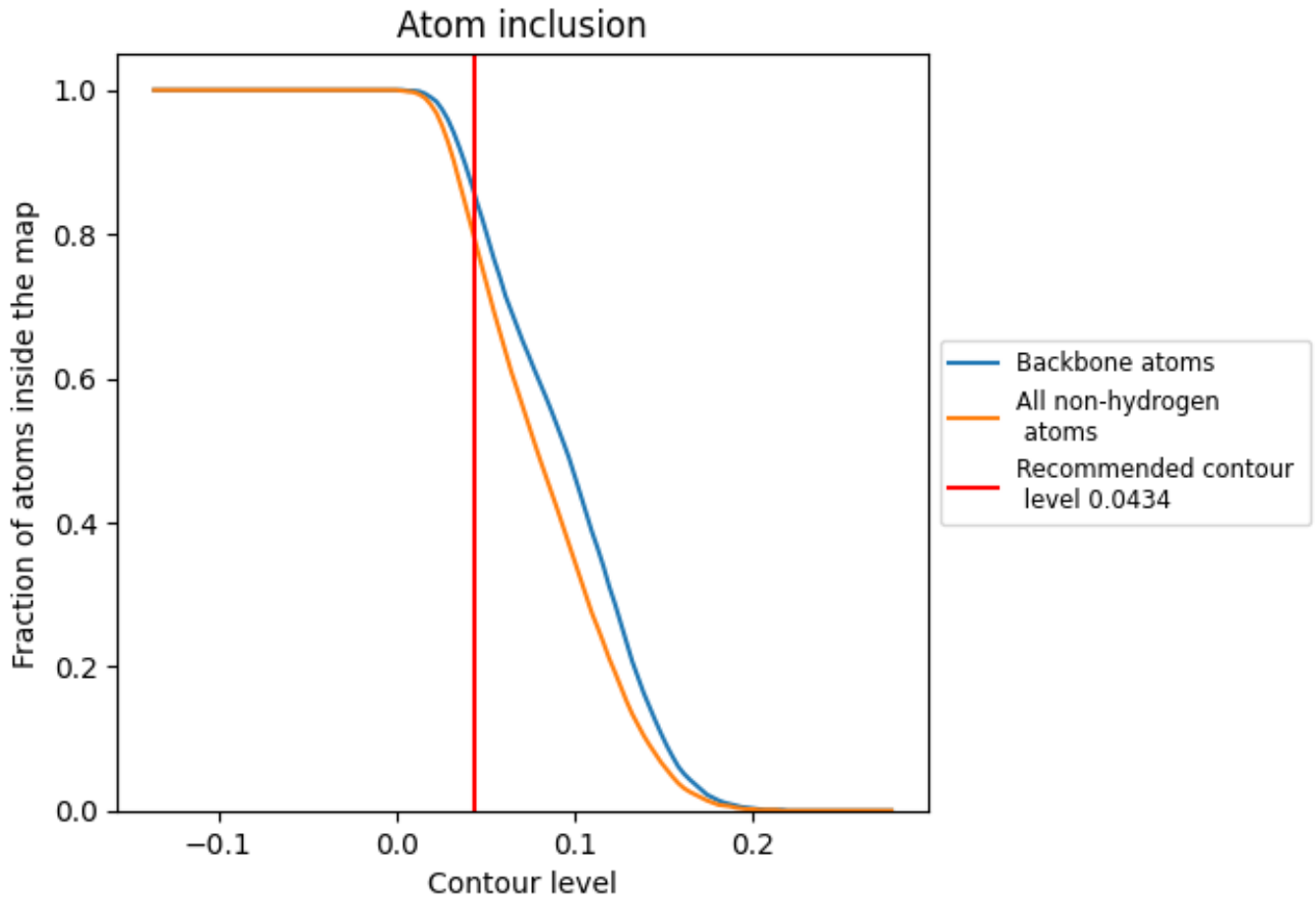
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0434).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 80% 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 (0.0434) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7970	0.5380
A	0.8060	0.5410
B	0.8070	0.5410
C	0.9090	0.5370
D	0.6250	0.4240
E	0.2860	0.3370
F	0.4100	0.3670
G	0.7270	0.5130
H	0.5000	0.4870
I	0.8180	0.5400
J	0.6880	0.4810
K	0.7270	0.4210
L	0.5710	0.4560
M	0.5000	0.4690
N	0.3570	0.3910
O	0.4750	0.4530
P	0.4290	0.4410
Q	0.7210	0.5280
R	0.4290	0.4540
S	0.5360	0.4510
T	0.4290	0.4100
U	0.5900	0.4420
V	0.5360	0.4680
W	0.2140	0.3240
X	0.3110	0.4030
Y	0.5000	0.5350
Z	0.7540	0.5460
a	0.3210	0.3710
b	0.5000	0.4690