wwPDB EM Validation Summary Report (i)

Nov 20, 2022 – 02:41 PM EST

PDB ID	:	7MIX
EMDB ID	:	EMD-23867
Title	:	Human N-type voltage-gated calcium channel Cav2.2 in the presence of ziconotide at 3.0 Angstrom resolution
Authors	:	Yan, N.; Gao, S.; Yao, X.
Deposited on	:	2021-04-18
Resolution	:	3.00 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

The following versions of software and data (see references (1)) were used in the production of this report:

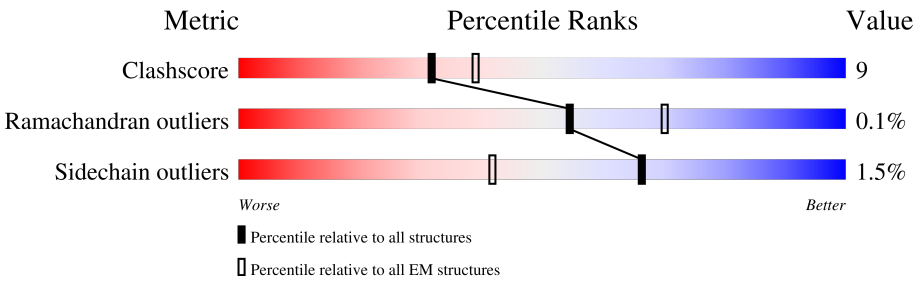
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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	2339	10%; 45%; 11%; •; 43%
2	B	25	80%; 16%; •
3	D	1103	7%; 68%; 18%; 14%
4	C	484	44%; 50%; 17%; 33%
5	G	3	33%; 33%; 33%; 33%
6	J	2	100%; 100%
6	P	2	50%; 100%
6	S	2	50%; 50%; 50%

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Mol	Chain	Length	Quality of chain
7	L	4	25% 25% 25% 50%

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 21652 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 Voltage-dependent N-type calcium channel subunit alpha-1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1326	10740	7049	1746	1868	77	1	0

- Molecule 2 is a protein called Omega-conotoxin MVIIA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	25	176	102	35	32	7	0	0

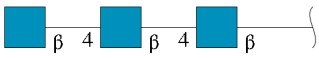
- Molecule 3 is a protein called Voltage-dependent calcium channel subunit alpha-2/delta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	948	7570	4803	1269	1467	31	0	0

- Molecule 4 is a protein called Voltage-dependent L-type calcium channel subunit beta-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	324	2575	1619	467	479	10	0	0

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	G	3	42	24	3	15	0	0

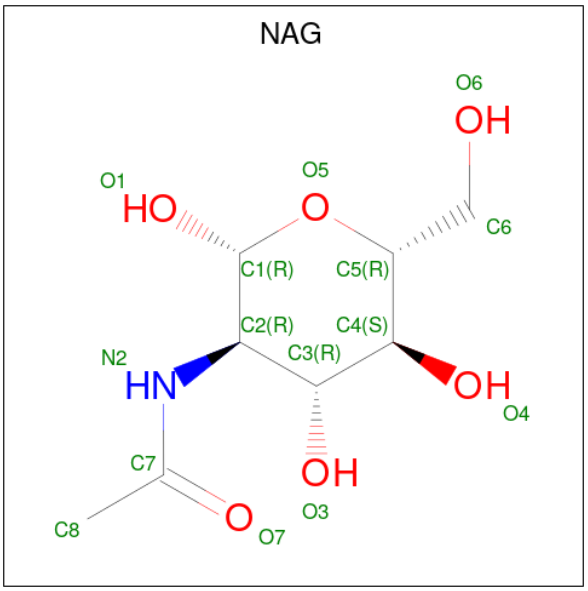
- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	L	4	56	32	4	20	0	0

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

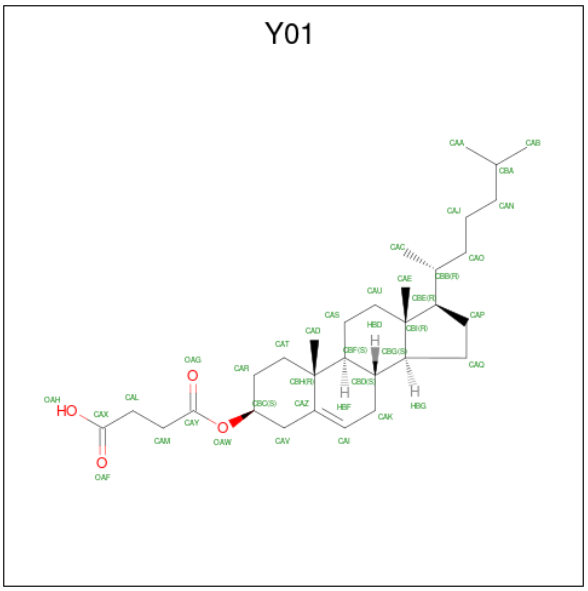


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
8	A	1	14	8	1	5	0
			Total	C	N	O	
8	D	1	28	16	2	10	0
			Total	C	N	O	
8	D	1	28	16	2	10	0

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

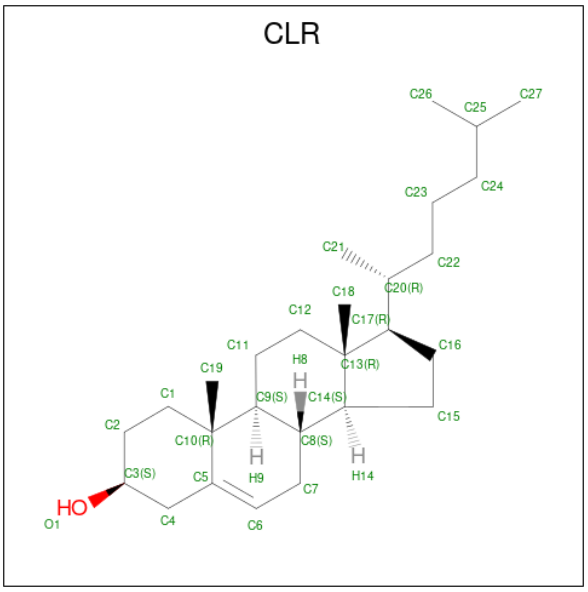
Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
9	A	1	1	1	0
			Total	Ca	
9	D	1	1	1	0

- Molecule 10 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: $C_{31}H_{50}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
10	A	1	70	62	8	0
			Total	C	O	
10	A	1	70	62	8	0

- Molecule 11 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
11	A	1	140	135	5	0

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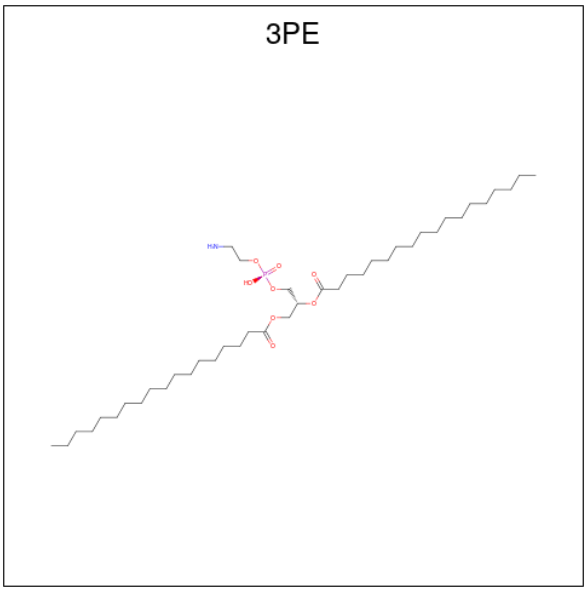
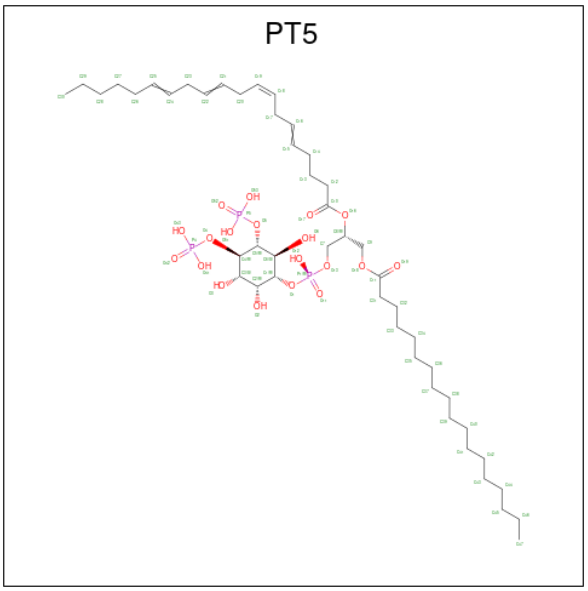
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
11	A	1	140	135	5	0
			Total	C	O	
11	A	1	140	135	5	0
			Total	C	O	
11	A	1	140	135	5	0
			Total	C	O	
11	A	1	140	135	5	0

- Molecule 12 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
12	A	1	91	71	2	16	2	0
			Total	C	N	O	P	
12	A	1	91	71	2	16	2	0

- Molecule 13 is [(2R)-1-octadecanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonooxy-cyclohexyl]oxy-phospho ryl]oxy-propan-2-yl] (8Z)-icosa-5,8,11,14-tetraenoate (three-letter code: PT5) (formula: $C_{47}H_{85}O_{19}P_3$) (labeled as "Ligand of Interest" by depositor).



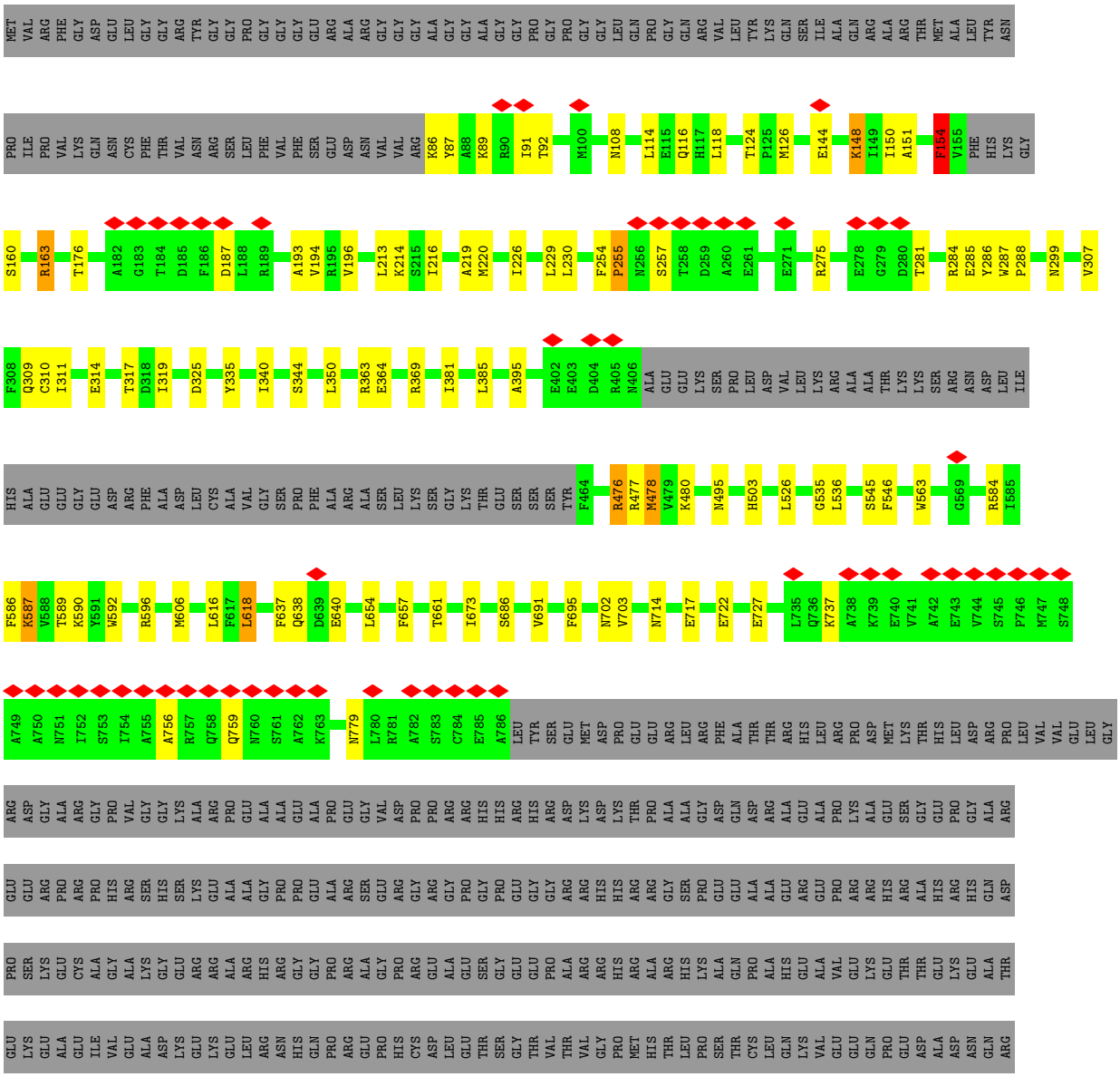
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
13	A	1	64	42	19	3	0

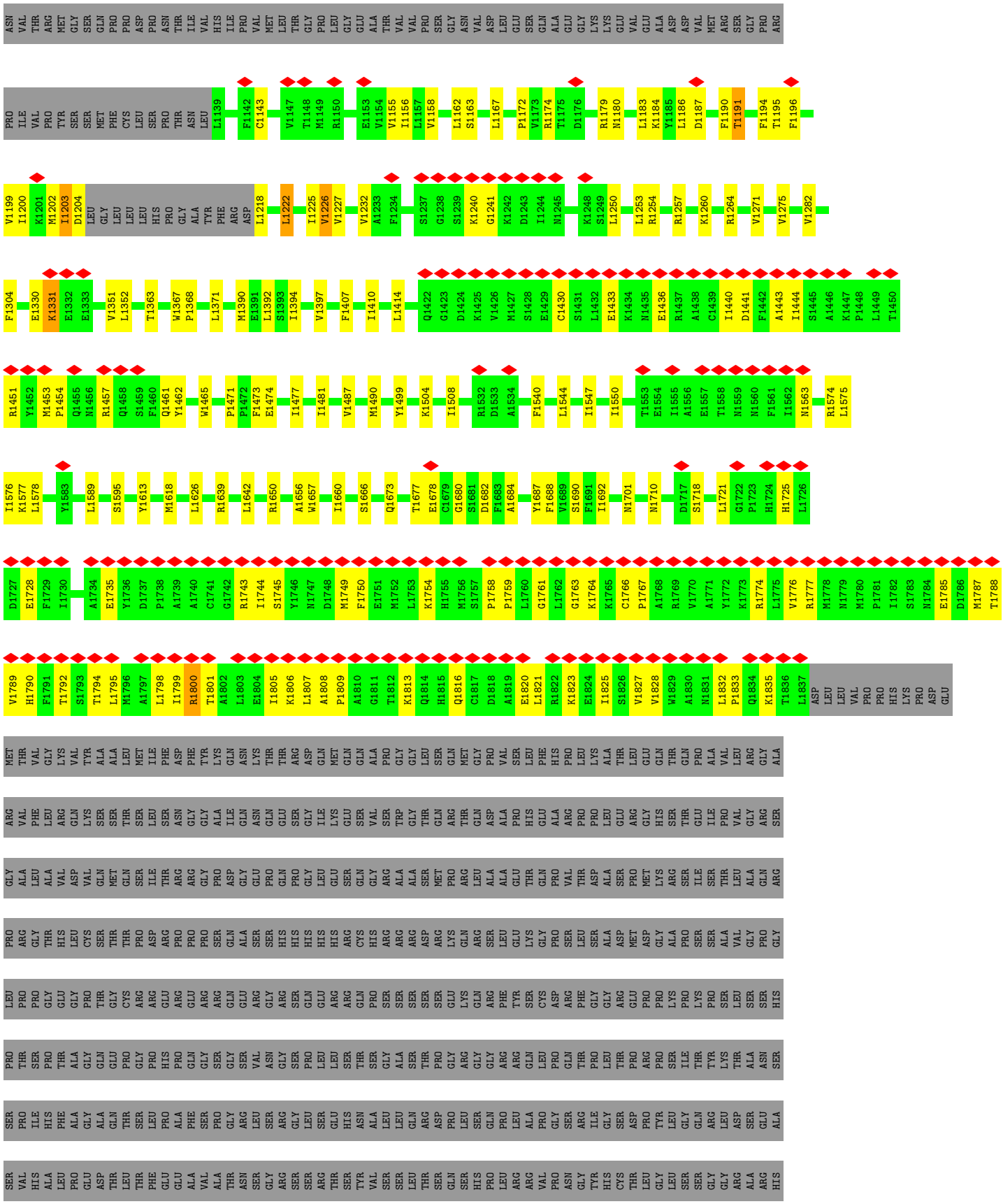
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Voltage-dependent N-type calcium channel subunit alpha-1B

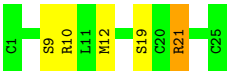
Chain A: 10% 45% 11% 43%




ASN VAL THR ARG MET GLY SER GLN PRO PRO ASP PRO ASN THR ILE VAL HIS ILE PRO VAL MET LEU THR GLY PRO LEU GLY GLU ALA THR VAL VAL PRO SER GLY ASN VAL ASP LEU GLU SER GLN ALA GLU GLY LYS LYS GLU VAL GLU ALA ASP ASP VAL MET ARG SER GLY PRO ARG
PRO ILE VAL PRO TYR SER SER MET PHE CYS LEU SER PRO THR ASN LEU L1139 F1142 C1143 V1147 T1148 M1149 R1150 E1153 V1154 V1155 I1156 L1157 V1158 L1162 S1163 L1167 P1172 V1173 R1174 T1175 D1176 R1179 N1180 L1183 K1184 Y1185 L1186 D1187 F1190 T1191 F1194 T1195 F1196
V1199 I1200 K1201 M1202 I1203 D1204 LEU GLY LEU LEU LEU HIS PRO GLY ALA TYR PHE ARG ASP L1218 L1222 I1225 V1226 V1227 V1232 A1233 F1234 S1237 G1238 S1239 K1240 G1241 K1242 D1243 I1244 N1245 K1248 S1249 L1250 L1253 R1254 R1257 K1260 R1264 V1271 V1275 V1282
F1304 E1330 K1331 E1332 E1333 V1351 L1352 T1363 W1367 P1368 L1371 M1390 E1391 L1392 S1393 I1394 V1397 F1407 I1410 L1414 Q1422 G1423 D1424 K1425 V1426 M1427 S1428 E1429 C1430 S1431 L1432 E1433 K1434 N1435 E1436 R1437 A1438 C1439 I1440 D1441 F1442 A1443 I1444 S1445 A1446 K1447 P1448 L1449 T1450
R1451 Y1452 M1453 P1454 Q1455 N1456 R1457 Q1458 S1459 F1460 Q1461 Y1462 W1465 P1471 P1472 F1473 E1474 I1477 I1481 V1487 M1490 Y1499 K1504 I1508 R1532 D1533 A1534 F1540 L1544 I1547 I1550 T1553 E1554 I1555 A1556 E1557 T1558 N1559 N1560 F1561 I1562 N1563 R1574 L1575
I1576 K1577 L1578 Y1583 L1589 S1595 Y1613 M1618 L1626 R1639 L1642 R1650 A1656 W1657 I1660 S1666 Q1673 T1677 E1678 C1679 G1680 S1681 D1682 F1683 A1684 Y1687 F1688 V1689 S1690 F1691 I1692 N1701 N1710 D1717 S1718 L1721 G1722 P1723 H1724 H1725 L1726
D1727 E1728 F1729 I1730 A1734 E1735 Y1736 D1737 P1738 A1739 A1740 C1741 G1742 R1743 I1744 S1745 Y1746 N1747 D1748 M1749 F1750 E1751 M1752 L1753 K1754 H1755 M1756 S1757 P1758 P1759 L1760 G1761 L1762 G1763 K1764 K1765 C1766 P1767 A1768 R1769 V1770 A1771 Y1772 K1773 R1774 L1775 V1776 R1777 M1778 N1779 M1780 P1781 I1782 S1783 N1784 E1785 D1786 M1787 T1788
V1789 H1790 F1791 T1792 S1793 T1794 L1795 M1796 A1797 L1798 I1799 R1800 T1801 A1802 L1803 E1804 I1805 K1806 L1807 A1808 P1809 A1810 G1811 T1812 K1813 Q1814 H1815 Q1816 C1817 D1818 A1819 E1820 L1821 R1822 K1823 E1824 I1825 S1826 V1827 V1828 W1829 A1830 N1831 L1832 P1833 Q1834 K1835 T1836 L1837 ASP LEU LEU VAL PRO PRO HIS LYS PRO ASP GLU
MET THR VAL GLY LYS VAL TYR ALA ALA LEU MET ILE PHE ASP PHE TYR LYS GLN ASN LYS THR THR ARG ASP GLN MET GLN GLN ALA PRO GLY GLY LEU SER GLN MET GLY PRO VAL SER LEU PHE HIS PRO LEU LYS ALA THR LEU GLU GLN THR GLN PRO ALA VAL LEU ARG GLY ALA
ARG VAL PHE LEU ARG GLN LYS SER SER THR SER SER LEU SER ASN GLY GLY ALA ILE GLN ASN GLN GLU SER GLY ILE LYS GLU SER VAL SER TRP GLY THR GLN ARG THR GLN ASP ALA PRO HIS GLU ALA ARG PRO PRO LEU GLU ARG GLY HIS SER THR GLN ILE PRO VAL GLY ARG SER
GLY ALA LEU ALA VAL ASP VAL GLN MET GLN SER ILE THR ARG ARG GLY PRO ASP GLY ARG GLU PRO GLN PRO GLY LEU GLU SER GLN GLY ARG ALA ALA SER MET PRO ARG LEU ALA ALA GLU THR GLN PRO ARG ALA VAL THR ASP ALA SER PRO MET LYS ARG SER ILE SER THR GLN ARG
PRO ARG GLY THR HIS LEU CYS SER THR THR PRO ASP ARG PRO PRO SER GLN ALA SER SER HIS HIS HIS HIS HIS ARG CYS HIS ARG ARG ARG ASP ARG LYS GLN ARG SER LEU GLU LYS GLY PRO SER LEU SER ALA ASP MET ASP GLY ALA PRO SER SER ALA VAL GLY PRO GLY
LEU PRO PRO GLY GLU GLY PRO THR GLY CYS ARG ARG GLU ARG GLU ARG GLN GLU ARG GLY GLN GLU ARG ARG ARG GLN PRO SER SER SER SER GLU LYS GLN ARG PHE TYR SER CYS ASP ARG PHE GLY ARG GLU PRO PRO LYS PRO LYS PRO SER LEU SER HIS
PRO THR SER PRO THR ALA GLY GLN GLU PRO GLY PRO HIS PRO GLN GLY SER VAL ASN GLY SER PRO LEU LEU SER THR SER GLY ALA SER THR PRO GLY ARG GLY GLN THR PRO LEU THR PRO ARG PRO SER ILE THR TYR LYS THR ALA ASN SER
SER PRO ILE HIS PHE ALA GLY ALA GLN THR SER LEU PRO ALA PHE SER PRO GLY ARG LEU SER ARG GLY LEU SER GLU HIS ASN ALA LEU LEU SER LEU ARG ASP PRO LEU SER GLN PRO LEU ALA PRO GLY SER ARG ILE GLY SER ASP PRO TYR LEU GLY GLN ARG LEU ASP SER GLU ALA
SER VAL HIS ALA LEU PRO GLU ASP THR LEU THR PHE GLU GLU ALA VAL ALA THR ASN SER GLY ARG SER SER ARG THR SER TYR VAL SER SER LEU THR SER GLN SER HIS PRO LEU ARG ARG VAL PRO ASN GLY TYR HIS CYS THR LEU GLY LEU LEU SER SER GLY GLY ARG LEU ALA ARG HIS

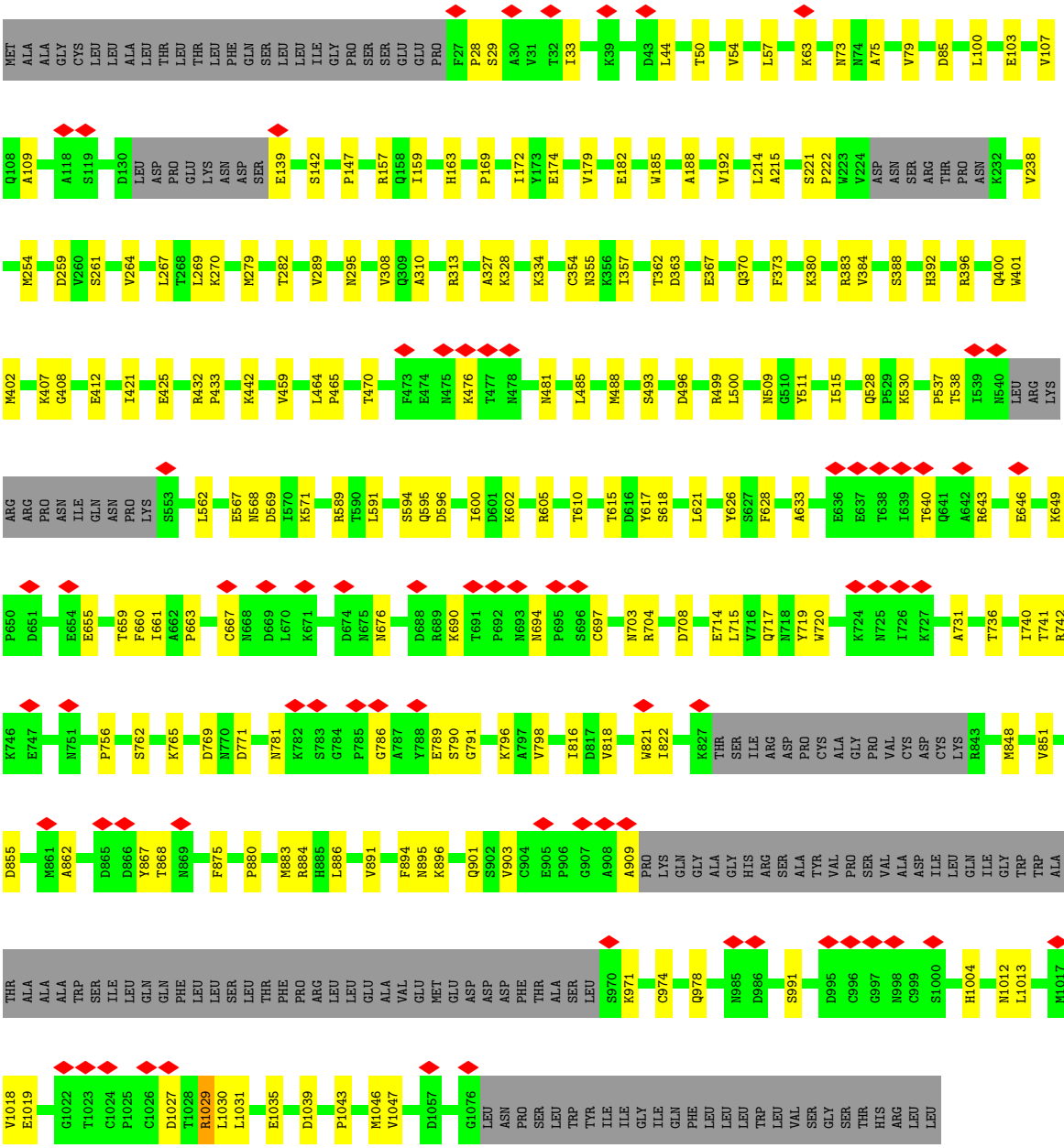
- Molecule 2: Omega-conotoxin MVIIA

Chain B:



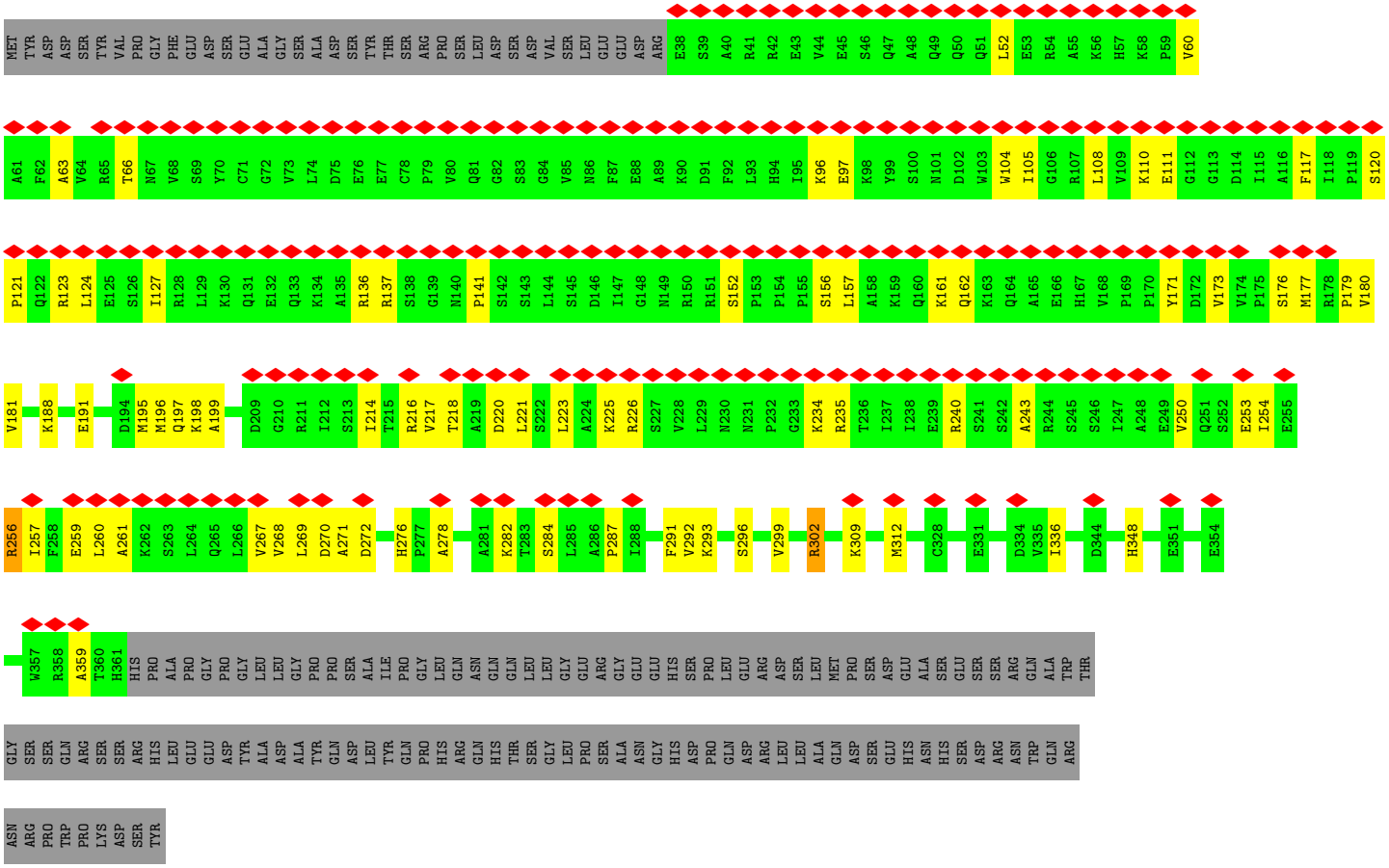
- Molecule 3: Voltage-dependent calcium channel subunit alpha-2/delta-1

Chain D:



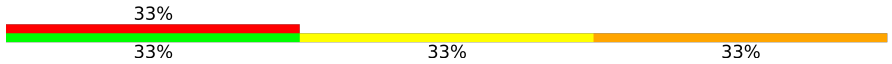
• Molecule 4: Voltage-dependent L-type calcium channel subunit beta-3

Chain C:



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

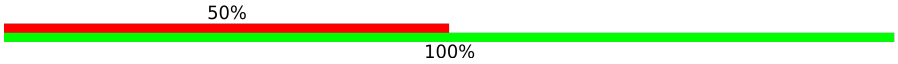
Chain G:



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

Chain J:

• 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 S:

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

Chain L:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	170839	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.200	Depositor
Minimum map value	-0.128	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	311.91998, 311.91998, 311.91998	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.114, 1.114, 1.114	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, NAG, PT5, 3PE, CLR, Y01

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	0.27	0/11002	0.48	2/14897 (0.0%)
2	B	0.26	0/176	0.50	0/228
3	D	0.25	0/7728	0.49	0/10477
4	C	0.25	0/2624	0.51	0/3544
All	All	0.26	0/21530	0.48	2/29146 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	596[A]	ARG	CA-C-O	5.86	132.40	120.10
1	A	596[B]	ARG	CA-C-O	5.86	132.40	120.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10740	0	10851	212	0
2	B	176	0	176	5	0
3	D	7570	0	7369	118	0
4	C	2575	0	2619	54	0
5	G	42	0	37	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	J	28	0	25	0	0
6	P	28	0	25	0	0
6	S	28	0	25	1	0
7	L	56	0	49	4	0
8	A	14	0	13	0	0
8	D	28	0	26	1	0
9	A	1	0	0	0	0
9	D	1	0	0	0	0
10	A	70	0	98	16	0
11	A	140	0	230	11	0
12	A	91	0	139	5	0
13	A	64	0	67	12	0
All	All	21652	0	21749	410	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 9.

The worst 5 of 410 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:1187:ASP:O	1:A:1191:THR:HG22	1.67	0.94
1:A:1195:THR:HG22	1:A:1227:VAL:HG13	1.48	0.94
1:A:254:PHE:HB3	1:A:284:ARG:NH2	1.83	0.92
1:A:160:SER:HA	1:A:163:ARG:HG3	1.52	0.90
1:A:476:ARG:HH11	1:A:476:ARG:HB3	1.35	0.89

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	1317/2339 (56%)	1237 (94%)	77 (6%)	3 (0%)	47	82
2	B	23/25 (92%)	23 (100%)	0	0	100	100
3	D	936/1103 (85%)	895 (96%)	41 (4%)	0	100	100
4	C	322/484 (66%)	307 (95%)	15 (5%)	0	100	100
All	All	2598/3951 (66%)	2462 (95%)	133 (5%)	3 (0%)	54	85

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	154	PHE
1	A	286	TYR
1	A	255	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1165/1991 (58%)	1139 (98%)	26 (2%)	52	81
2	B	20/20 (100%)	19 (95%)	1 (5%)	24	60
3	D	837/971 (86%)	835 (100%)	2 (0%)	93	98
4	C	287/426 (67%)	282 (98%)	5 (2%)	60	85
All	All	2309/3408 (68%)	2275 (98%)	34 (2%)	66	87

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	1029	ARG
4	C	198	LYS
4	C	296	SER
1	A	606	MET
1	A	590	LYS

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

Mol	Chain	Res	Type
1	A	702	ASN
1	A	1673	GLN
1	A	1725	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

13 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	$\#\|Z\| > 2$
5	NAG	G	1	3,5	14,14,15	0.53	0	17,19,21	0.56	0
5	NAG	G	2	5	14,14,15	0.45	0	17,19,21	1.27	1 (5%)
5	NAG	G	3	5	14,14,15	0.35	0	17,19,21	0.37	0
6	NAG	J	1	3,6	14,14,15	0.34	0	17,19,21	0.50	0
6	NAG	J	2	6	14,14,15	0.49	0	17,19,21	0.77	0
7	NAG	L	1	3,7	14,14,15	0.26	0	17,19,21	0.44	0
7	NAG	L	2	7	14,14,15	0.26	0	17,19,21	0.40	0
7	NAG	L	3	7	14,14,15	0.98	1 (7%)	17,19,21	1.66	2 (11%)
7	NAG	L	4	7	14,14,15	0.52	0	17,19,21	1.26	1 (5%)
6	NAG	P	1	3,6	14,14,15	0.26	0	17,19,21	0.47	0
6	NAG	P	2	6	14,14,15	0.44	0	17,19,21	0.54	0
6	NAG	S	1	3,6	14,14,15	0.88	1 (7%)	17,19,21	1.25	1 (5%)
6	NAG	S	2	6	14,14,15	0.21	0	17,19,21	0.45	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	G	1	3,5	-	2/6/23/26	0/1/1/1
5	NAG	G	2	5	-	5/6/23/26	0/1/1/1
5	NAG	G	3	5	-	4/6/23/26	0/1/1/1
6	NAG	J	1	3,6	-	3/6/23/26	0/1/1/1
6	NAG	J	2	6	-	3/6/23/26	0/1/1/1
7	NAG	L	1	3,7	-	2/6/23/26	0/1/1/1
7	NAG	L	2	7	-	2/6/23/26	0/1/1/1
7	NAG	L	3	7	-	5/6/23/26	0/1/1/1
7	NAG	L	4	7	-	5/6/23/26	0/1/1/1
6	NAG	P	1	3,6	-	2/6/23/26	0/1/1/1
6	NAG	P	2	6	-	2/6/23/26	0/1/1/1
6	NAG	S	1	3,6	-	3/6/23/26	0/1/1/1
6	NAG	S	2	6	-	4/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	3	NAG	O5-C1	3.16	1.48	1.43
6	S	1	NAG	O5-C1	2.57	1.47	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	S	1	NAG	C1-O5-C5	4.81	118.71	112.19
7	L	3	NAG	C1-O5-C5	4.60	118.42	112.19
7	L	3	NAG	C2-N2-C7	4.34	129.09	122.90
7	L	4	NAG	C2-N2-C7	4.29	129.02	122.90
5	G	2	NAG	C2-N2-C7	4.26	128.97	122.90

There are no chirality outliers.

5 of 42 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	2	NAG	O5-C5-C6-O6
7	L	3	NAG	C4-C5-C6-O6
6	P	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	P	2	NAG	O5-C5-C6-O6
7	L	3	NAG	O5-C5-C6-O6

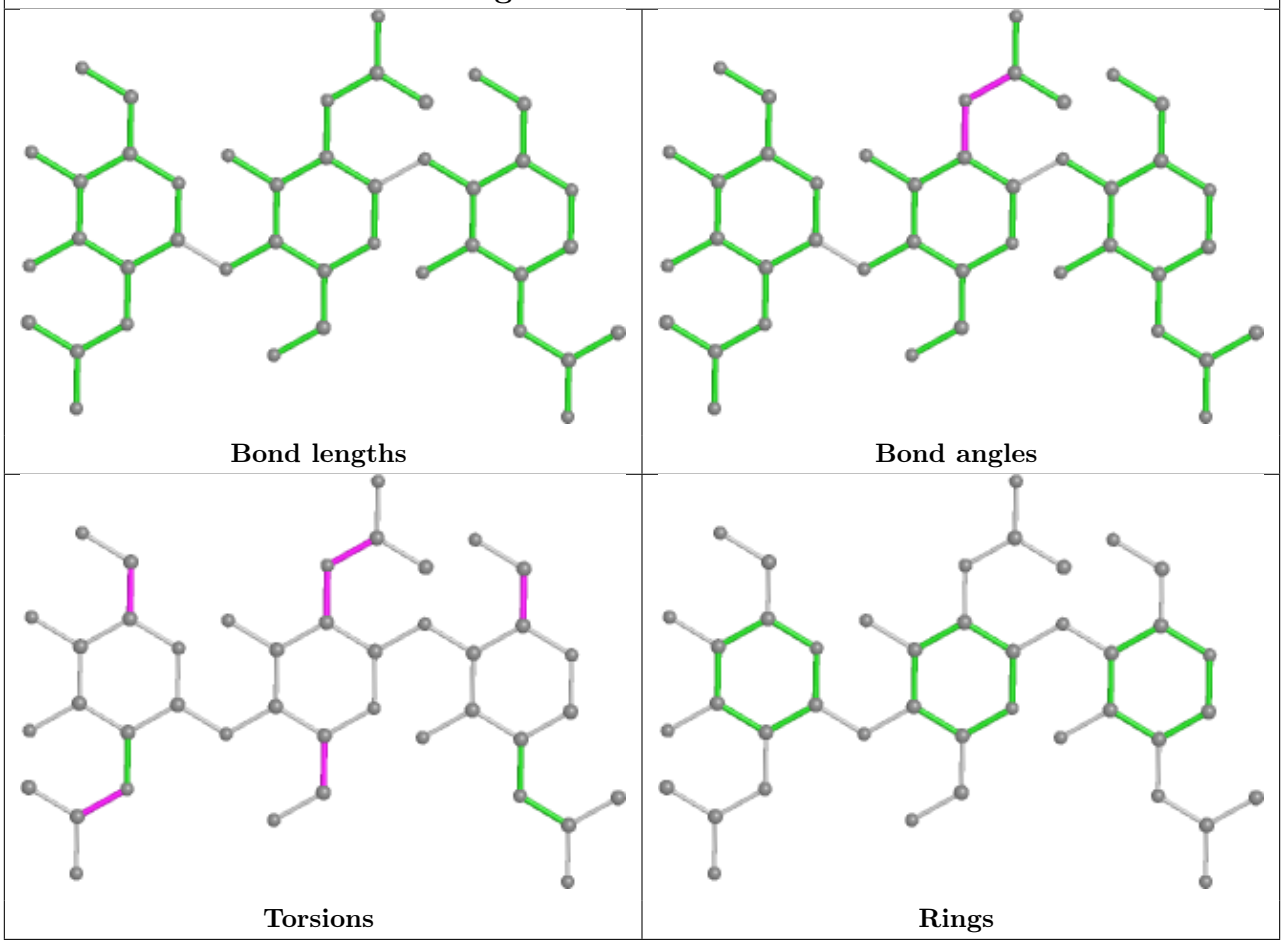
There are no ring outliers.

6 monomers are involved in 8 short contacts:

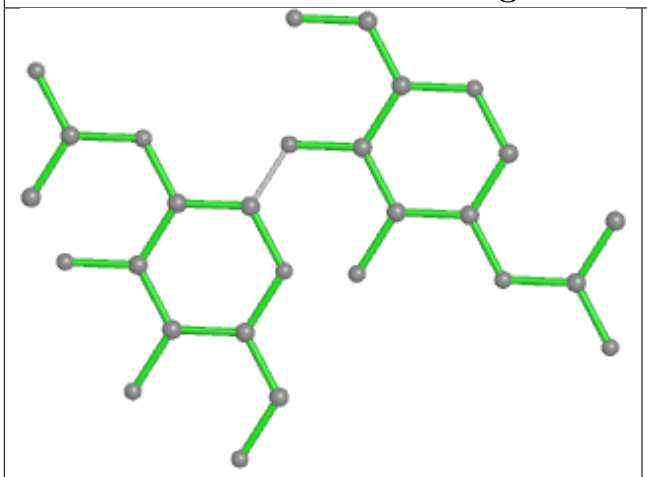
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	2	NAG	2	0
7	L	4	NAG	1	0
7	L	1	NAG	2	0
5	G	1	NAG	2	0
7	L	3	NAG	1	0
6	S	1	NAG	1	0

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

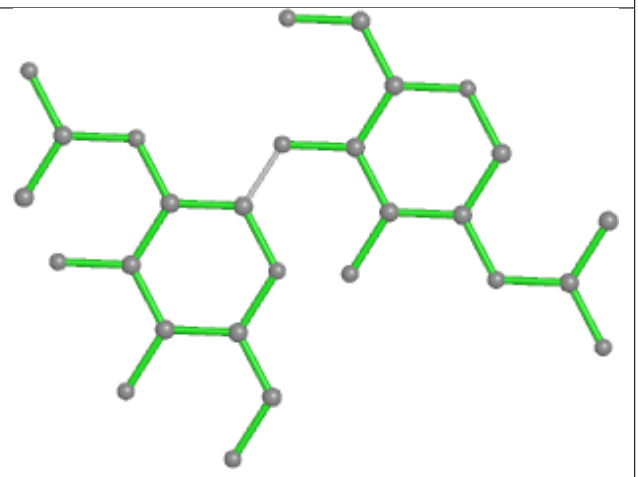
Oligosaccharide Chain G



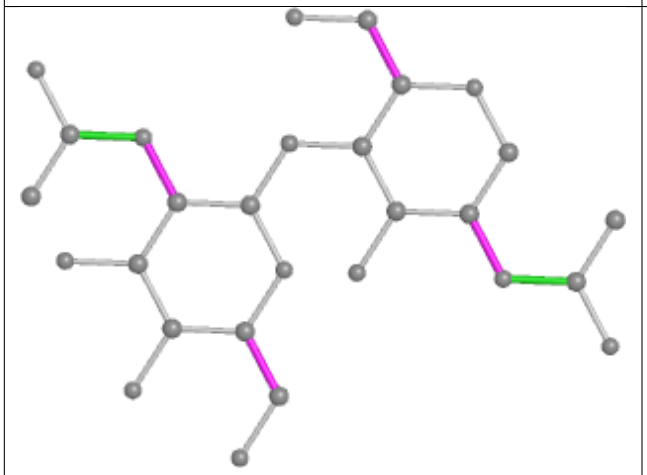
Oligosaccharide Chain J



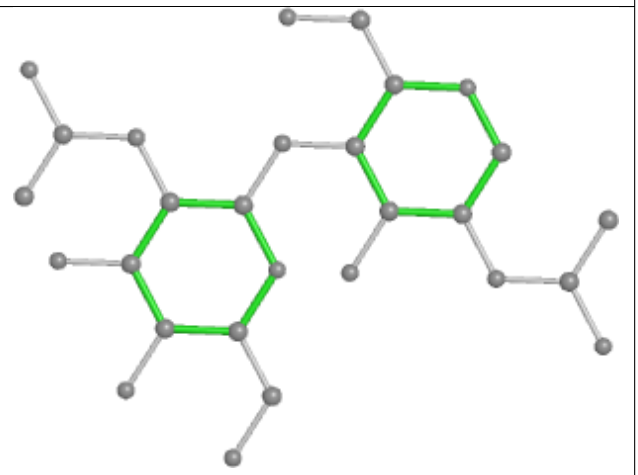
Bond lengths



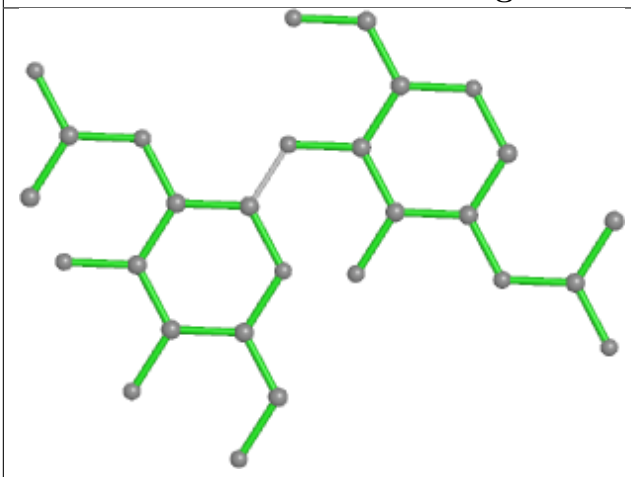
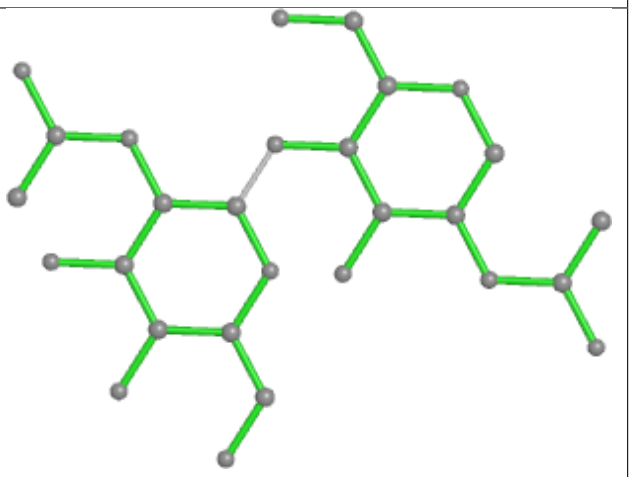
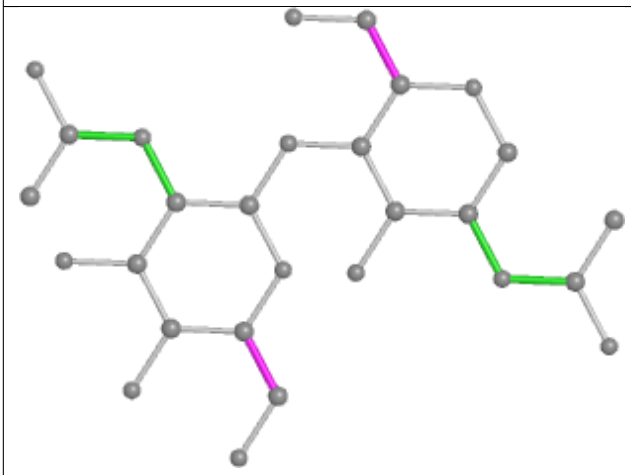
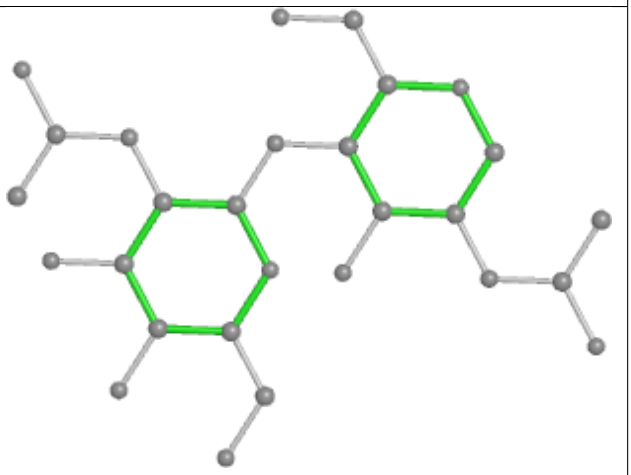
Bond angles

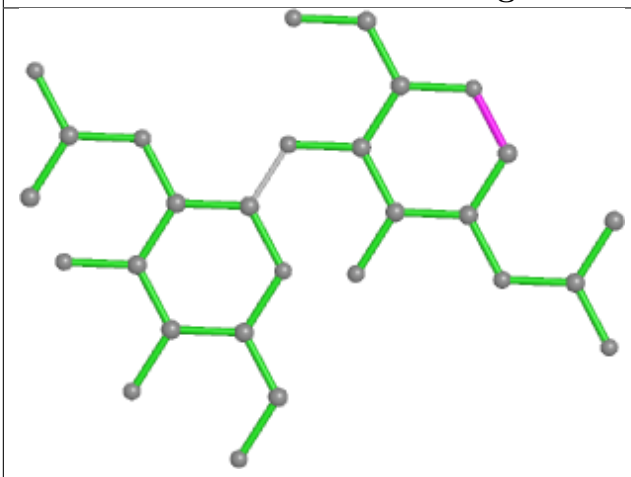
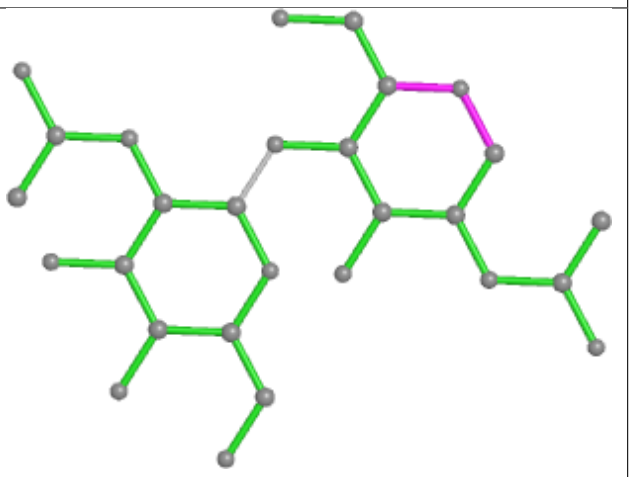
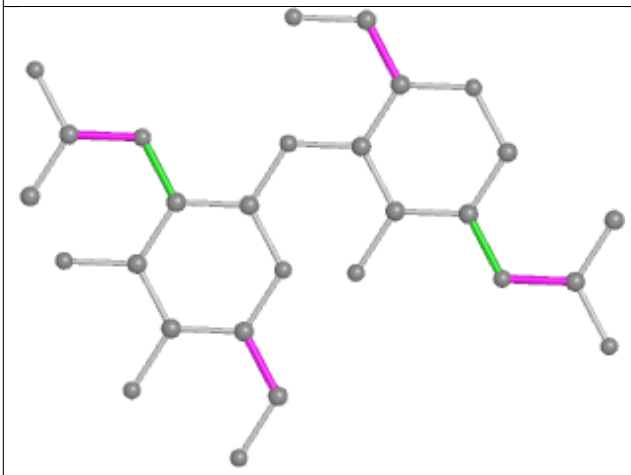
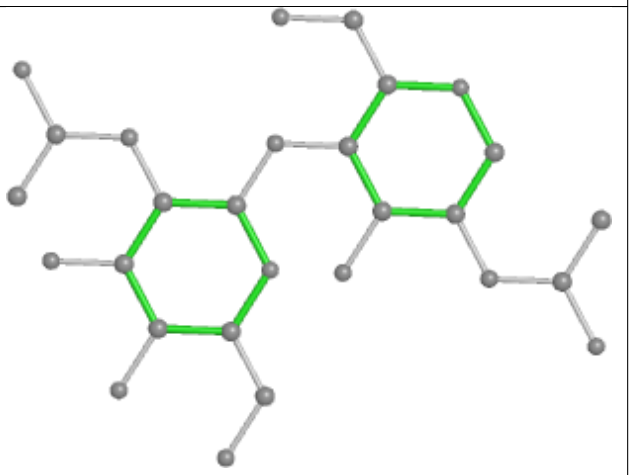


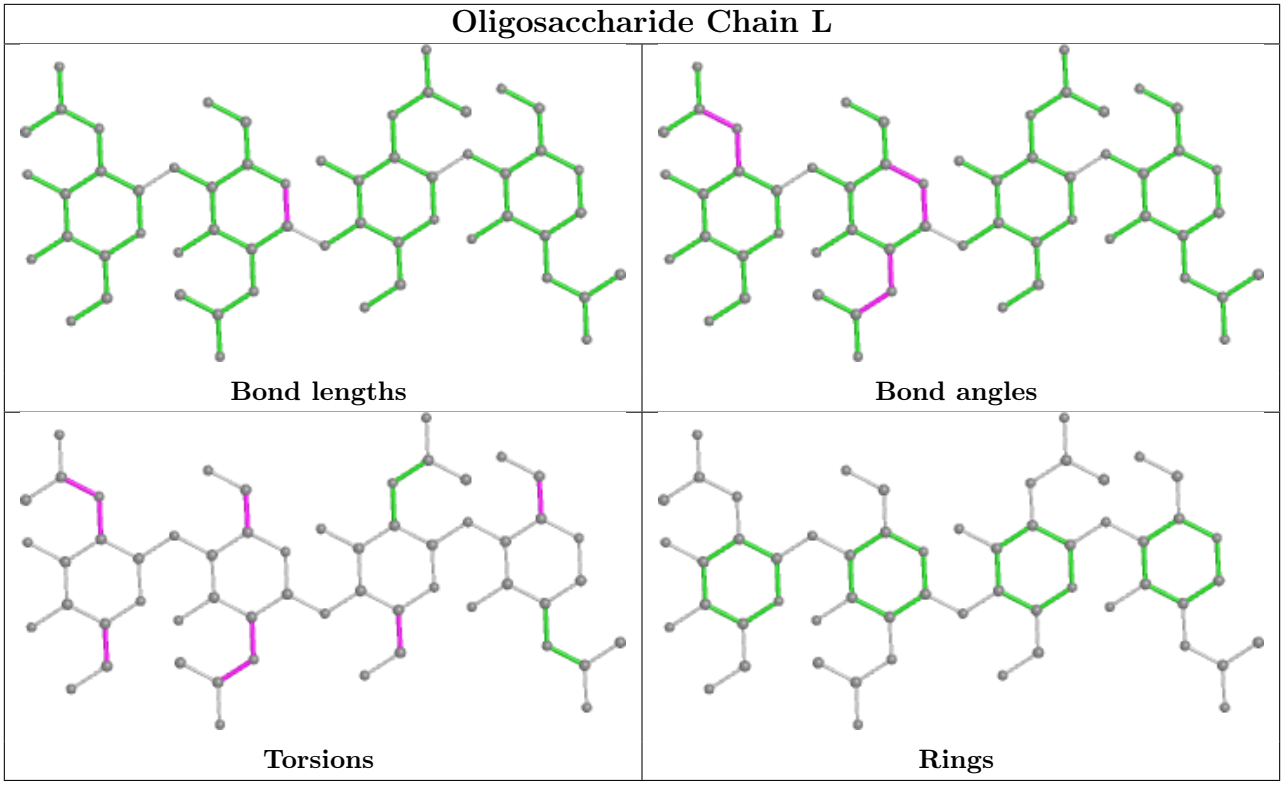
Torsions



Rings

Oligosaccharide Chain P	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain S	
 Bond lengths	 Bond angles
 Torsions	 Rings



5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 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	$\#\|Z\| > 2$
11	CLR	A	2404	-	31,31,31	1.08	2 (6%)	48,48,48	1.30	6 (12%)
11	CLR	A	2409	-	31,31,31	1.07	1 (3%)	48,48,48	1.28	7 (14%)
8	NAG	A	2401	1	14,14,15	0.33	0	17,19,21	0.47	0
11	CLR	A	2407	-	31,31,31	1.06	1 (3%)	48,48,48	1.33	7 (14%)
11	CLR	A	2408	-	31,31,31	1.04	2 (6%)	48,48,48	1.36	7 (14%)
13	PT5	A	2412	-	64,64,69	0.85	2 (3%)	78,82,87	1.01	3 (3%)
10	Y01	A	2406	-	38,38,38	2.71	11 (28%)	57,57,57	4.40	33 (57%)
11	CLR	A	2405	-	31,31,31	1.04	2 (6%)	48,48,48	1.37	9 (18%)
8	NAG	D	1202	3	14,14,15	0.87	1 (7%)	17,19,21	0.88	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	Y01	A	2403	-	38,38,38	2.43	11 (28%)	57,57,57	4.36	33 (57%)
12	3PE	A	2411	-	50,50,50	0.51	0	53,55,55	0.54	1 (1%)
12	3PE	A	2410	-	39,39,50	0.57	0	42,44,55	0.56	1 (2%)
8	NAG	D	1201	3	14,14,15	0.36	0	17,19,21	0.46	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
11	CLR	A	2404	-	-	7/10/68/68	0/4/4/4
11	CLR	A	2409	-	-	8/10/68/68	0/4/4/4
8	NAG	A	2401	1	-	2/6/23/26	0/1/1/1
11	CLR	A	2407	-	-	7/10/68/68	0/4/4/4
11	CLR	A	2408	-	-	6/10/68/68	0/4/4/4
13	PT5	A	2412	-	-	25/61/85/90	0/1/1/1
10	Y01	A	2406	-	-	13/19/77/77	0/4/4/4
11	CLR	A	2405	-	-	2/10/68/68	0/4/4/4
8	NAG	D	1202	3	-	2/6/23/26	0/1/1/1
10	Y01	A	2403	-	-	8/19/77/77	0/4/4/4
12	3PE	A	2411	-	-	25/54/54/54	-
12	3PE	A	2410	-	-	9/43/43/54	-
8	NAG	D	1201	3	-	1/6/23/26	0/1/1/1

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	2406	Y01	CAK-CBD	10.83	1.71	1.53
10	A	2403	Y01	CAK-CBD	8.36	1.67	1.53
10	A	2406	Y01	CBD-CBG	-6.36	1.41	1.53
10	A	2403	Y01	CBD-CBG	-6.09	1.42	1.53
10	A	2403	Y01	CAI-CAZ	4.33	1.42	1.33

The worst 5 of 108 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	2406	Y01	CAD-CBH-CAT	11.66	127.85	109.43
10	A	2403	Y01	CAD-CBH-CAT	11.29	127.26	109.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	2403	Y01	CAK-CBD-CBG	-9.58	97.02	110.91
10	A	2403	Y01	CAD-CBH-CAZ	-9.49	92.99	108.34
10	A	2406	Y01	CAD-CBH-CAZ	-9.03	93.72	108.34

There are no chirality outliers.

5 of 115 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	2403	Y01	OAG-CAY-OAW-CBC
10	A	2403	Y01	CAX-CAL-CAM-CAY
10	A	2406	Y01	OAG-CAY-OAW-CBC
10	A	2406	Y01	CAM-CAY-OAW-CBC
12	A	2410	3PE	C1-O11-P-O12

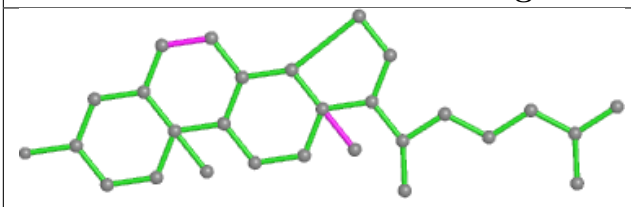
There are no ring outliers.

10 monomers are involved in 45 short contacts:

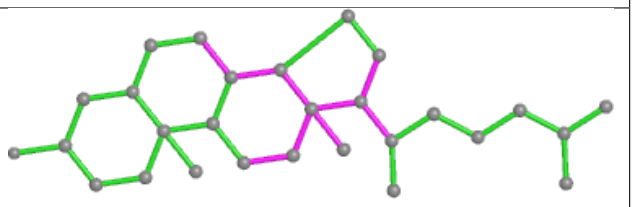
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	2404	CLR	3	0
11	A	2409	CLR	2	0
11	A	2408	CLR	4	0
13	A	2412	PT5	12	0
10	A	2406	Y01	5	0
11	A	2405	CLR	2	0
8	D	1202	NAG	1	0
10	A	2403	Y01	11	0
12	A	2411	3PE	4	0
12	A	2410	3PE	1	0

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

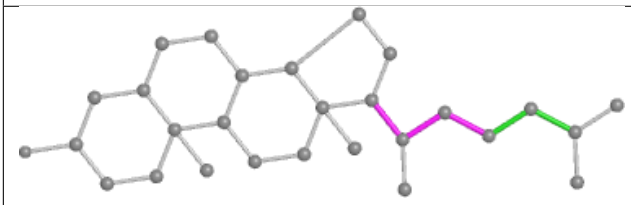
Ligand CLR A 2404



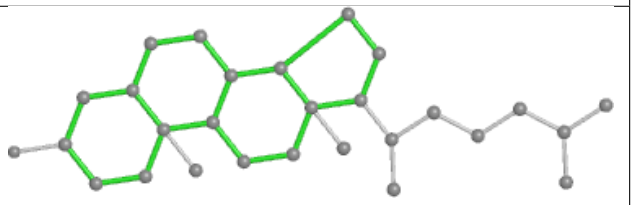
Bond lengths



Bond angles

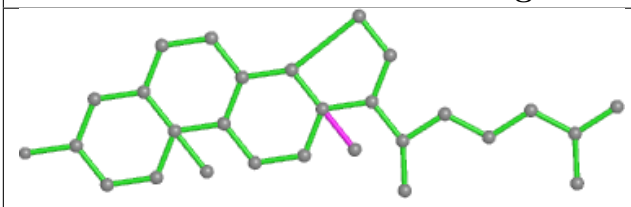


Torsions

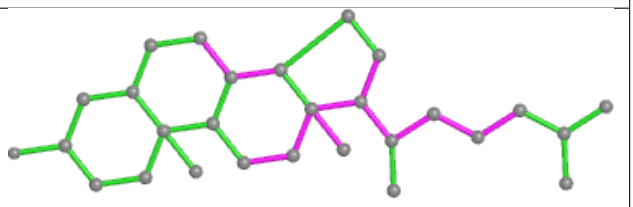


Rings

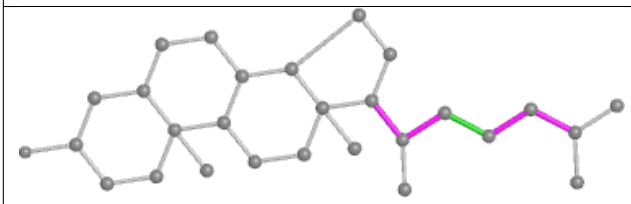
Ligand CLR A 2409



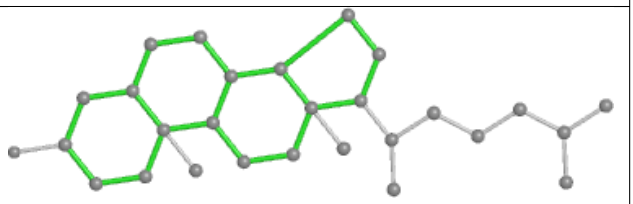
Bond lengths



Bond angles

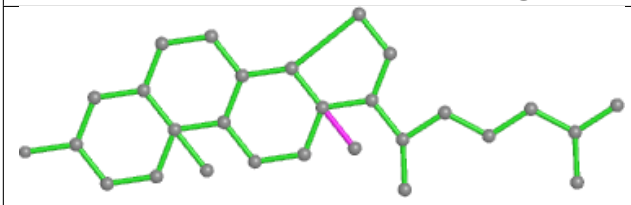


Torsions

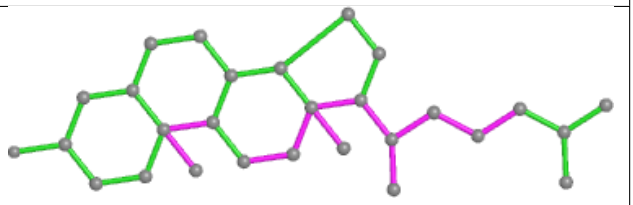


Rings

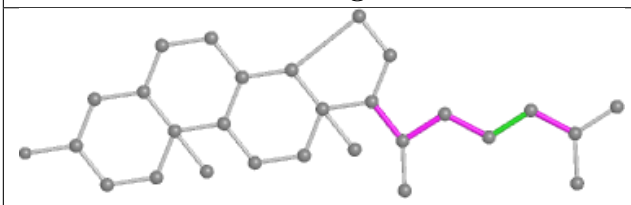
Ligand CLR A 2407



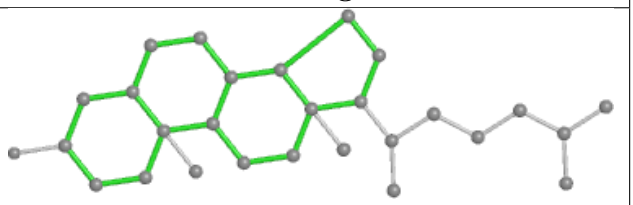
Bond lengths



Bond angles

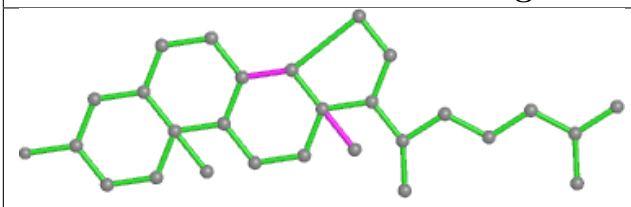


Torsions

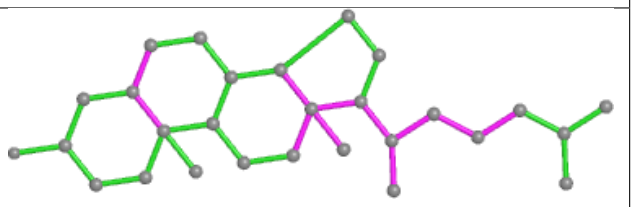


Rings

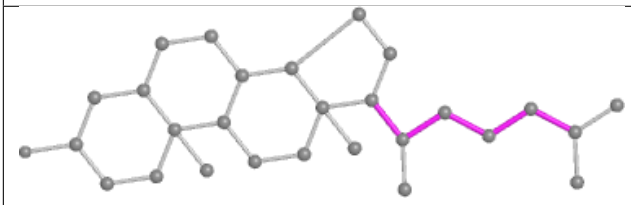
Ligand CLR A 2408



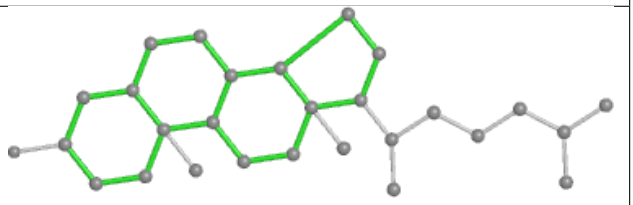
Bond lengths



Bond angles

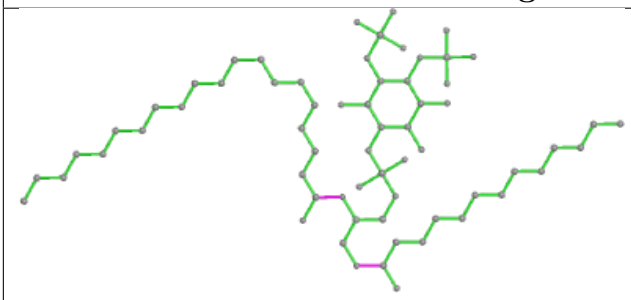


Torsions

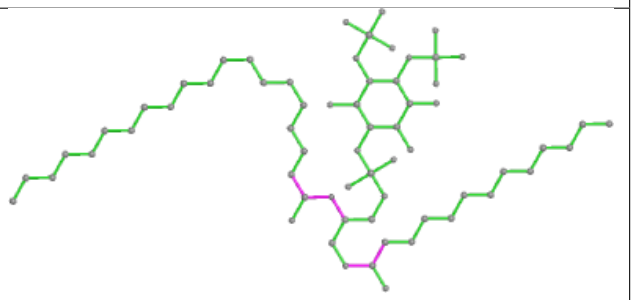


Rings

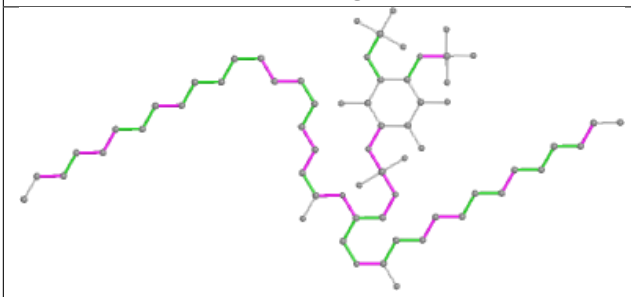
Ligand PT5 A 2412



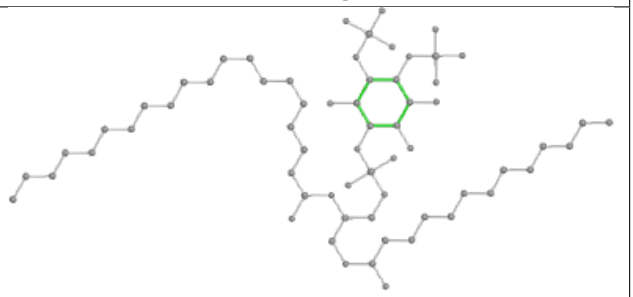
Bond lengths



Bond angles

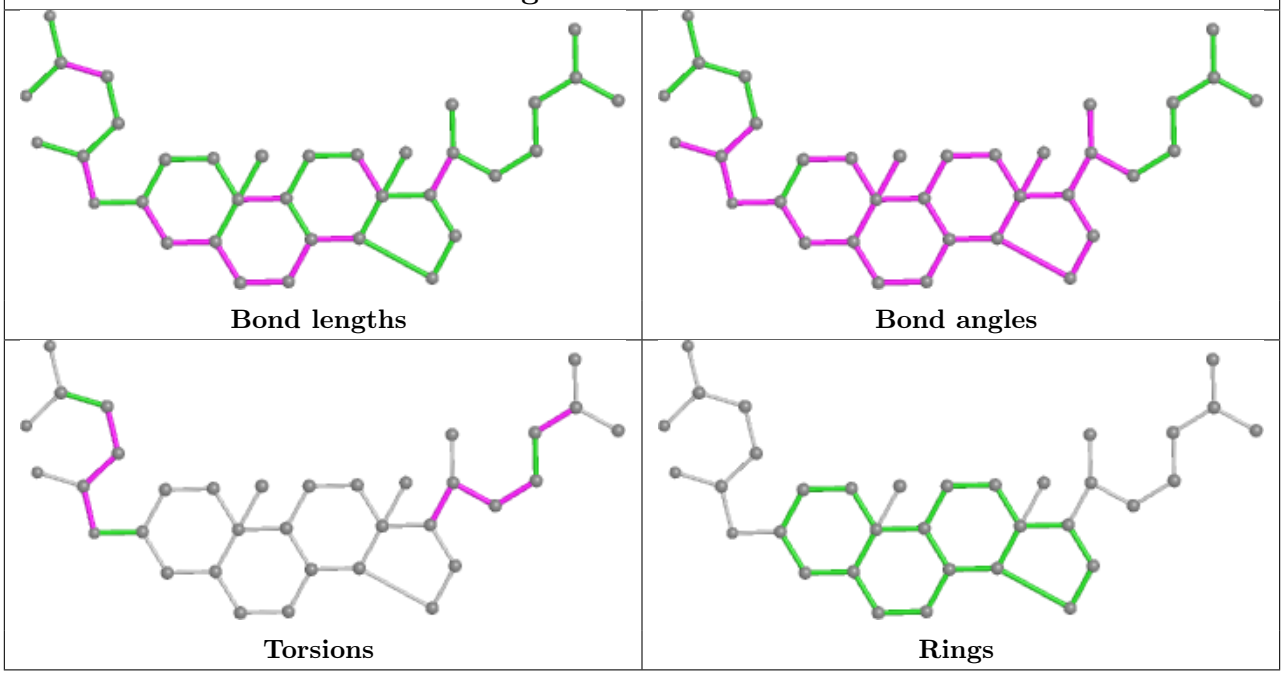


Torsions

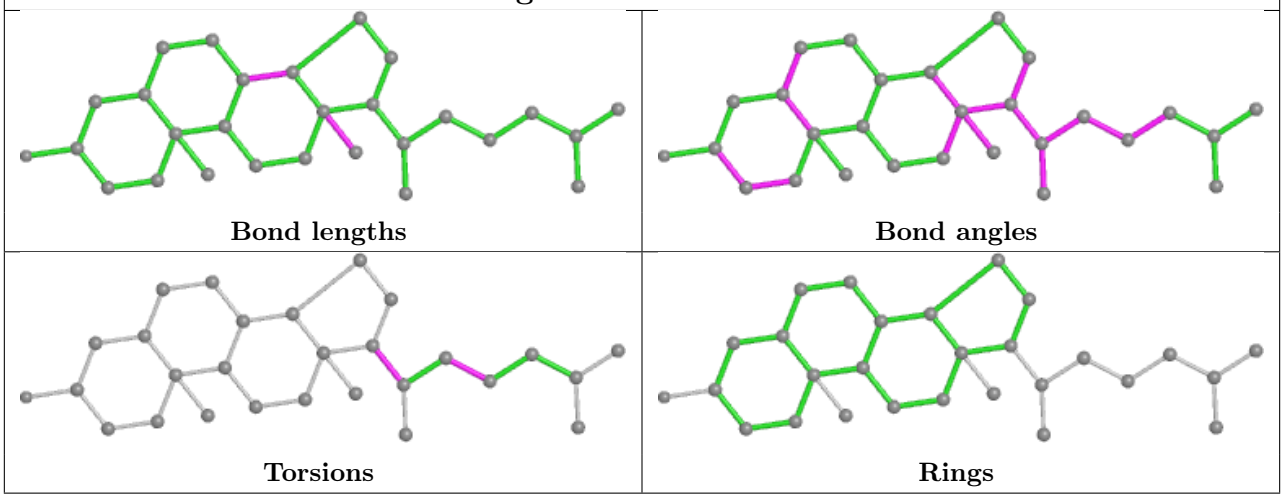


Rings

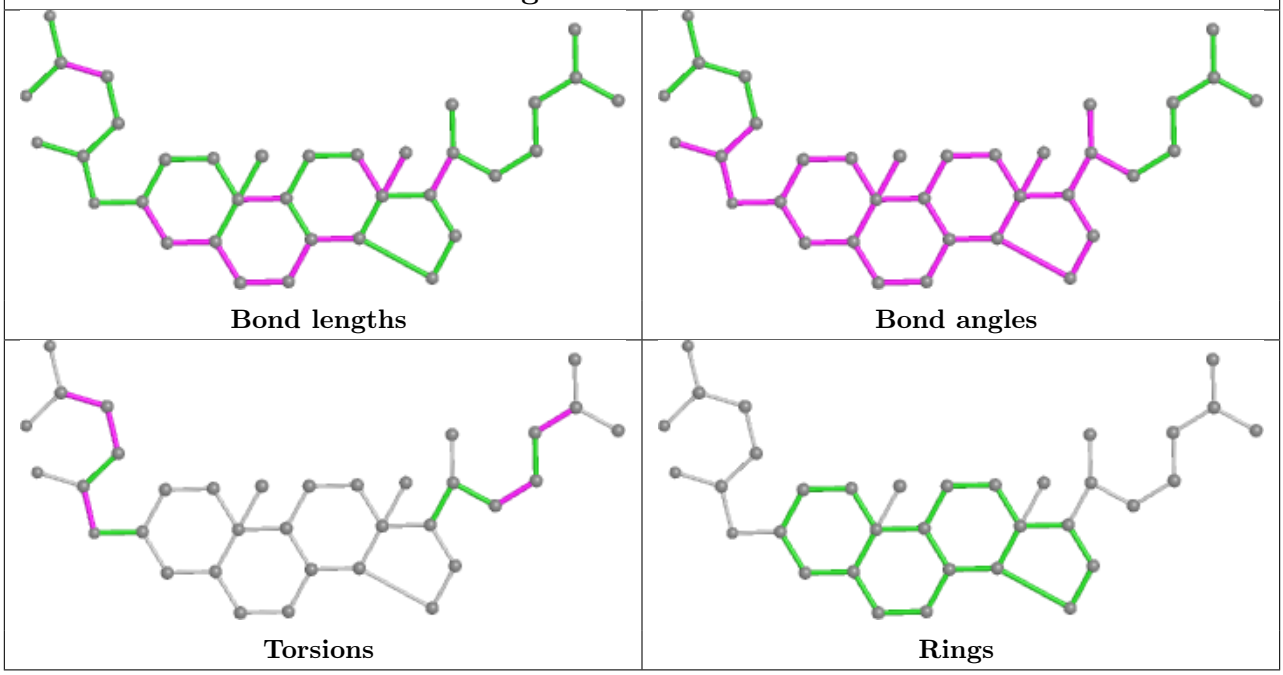
Ligand Y01 A 2406



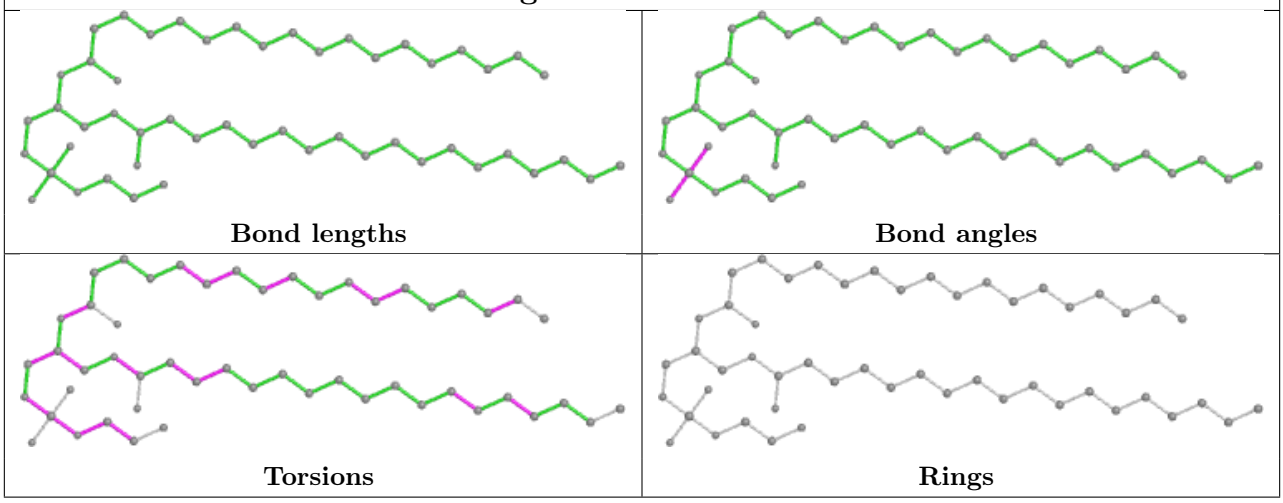
Ligand CLR A 2405

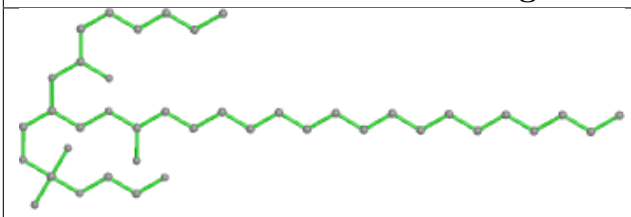
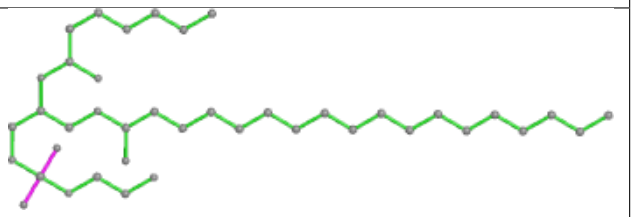
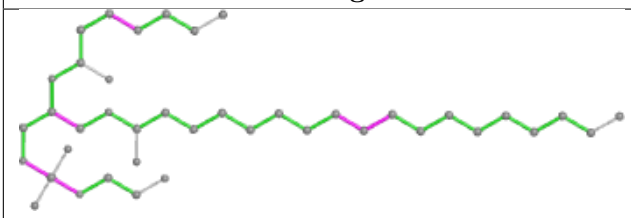
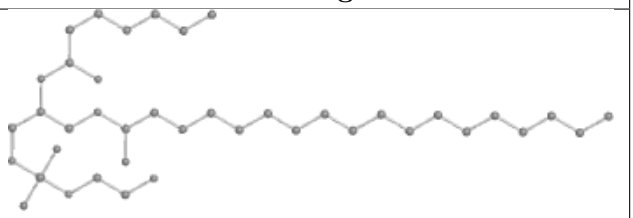


Ligand Y01 A 2403



Ligand 3PE A 2411



Ligand 3PE A 2410	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

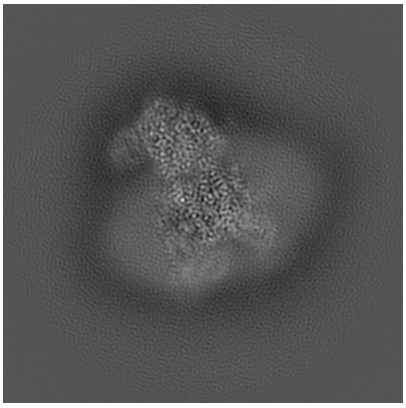
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-23867. These allow visual inspection of the internal detail of the map and identification of artifacts.

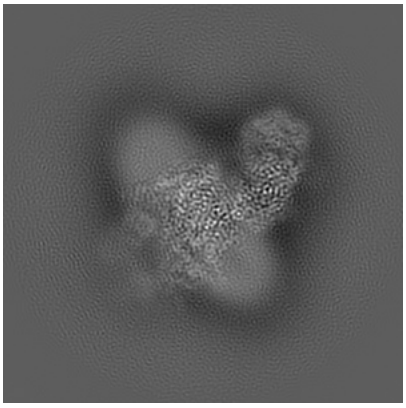
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

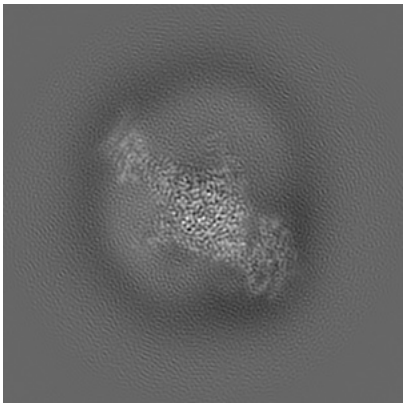
6.1.1 Primary map



X



Y

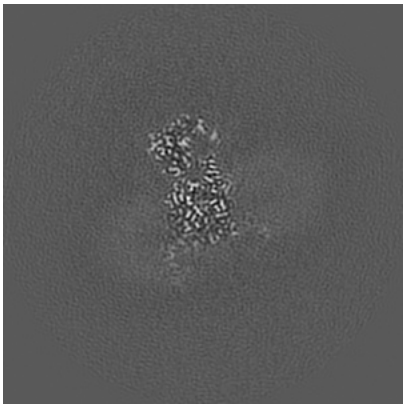


Z

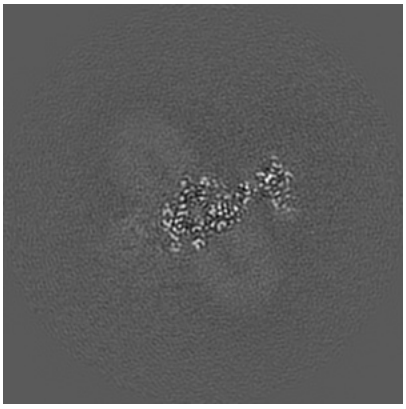
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

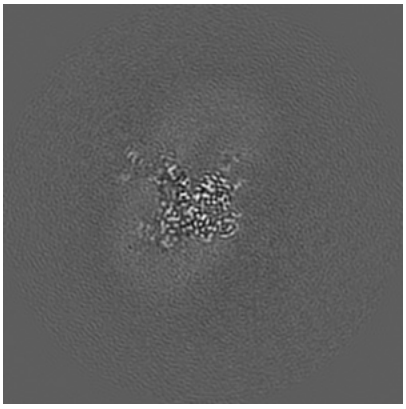
6.2.1 Primary map



X Index: 140



Y Index: 140

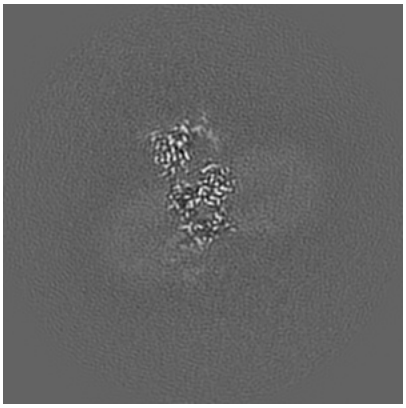


Z Index: 140

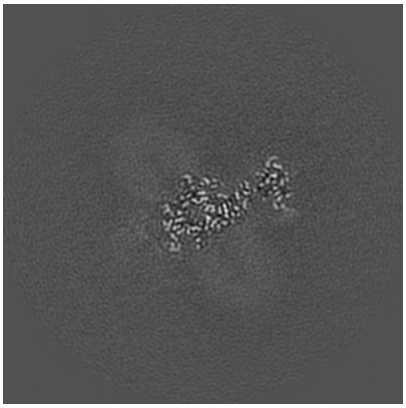
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

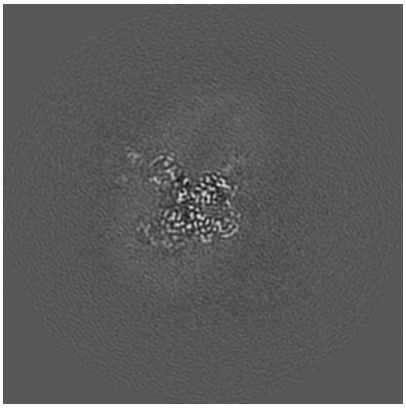
6.3.1 Primary map



X Index: 136



Y Index: 141



Z Index: 141

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

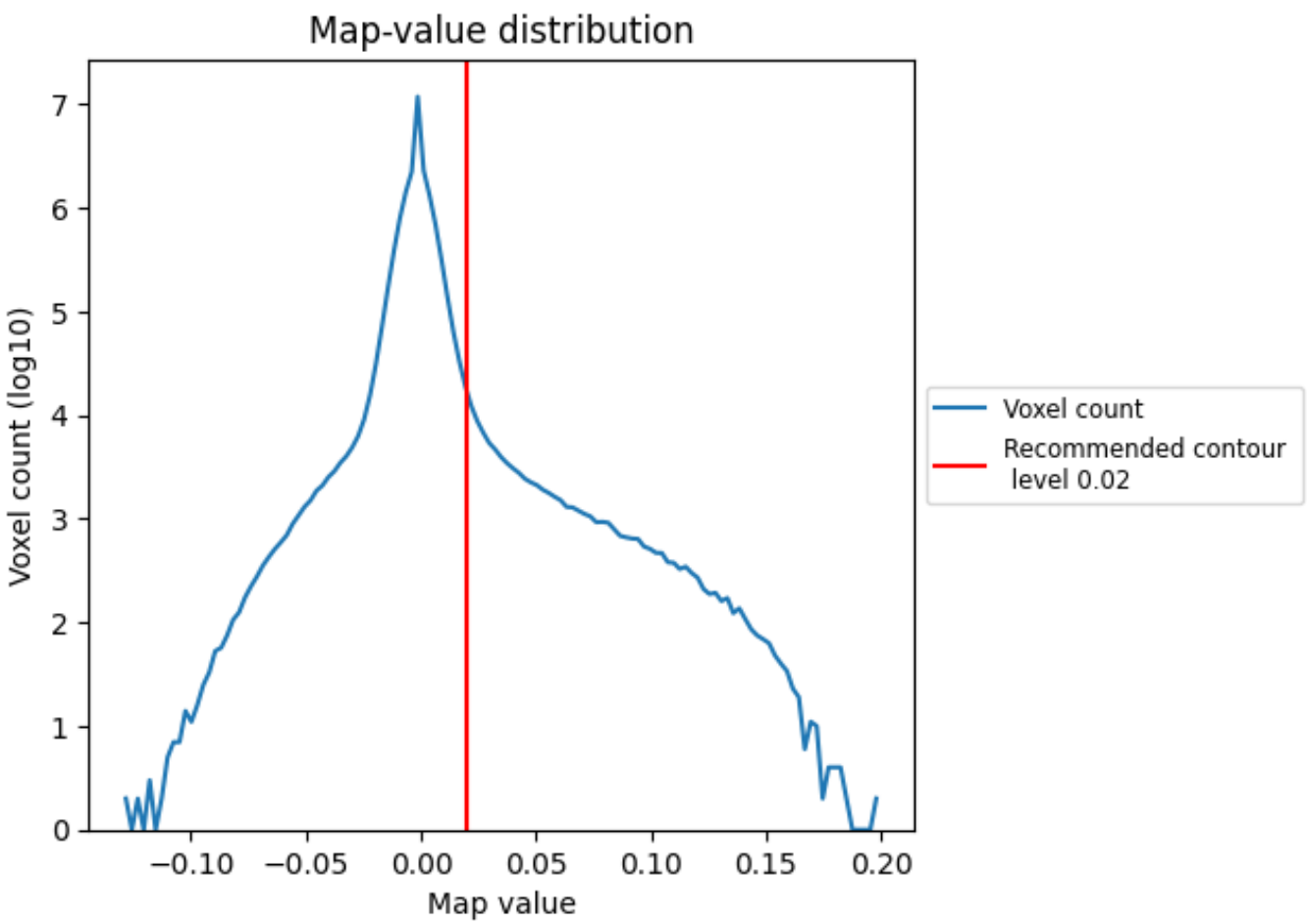
6.5 Mask visualisation (i)

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

7 Map analysis (i)

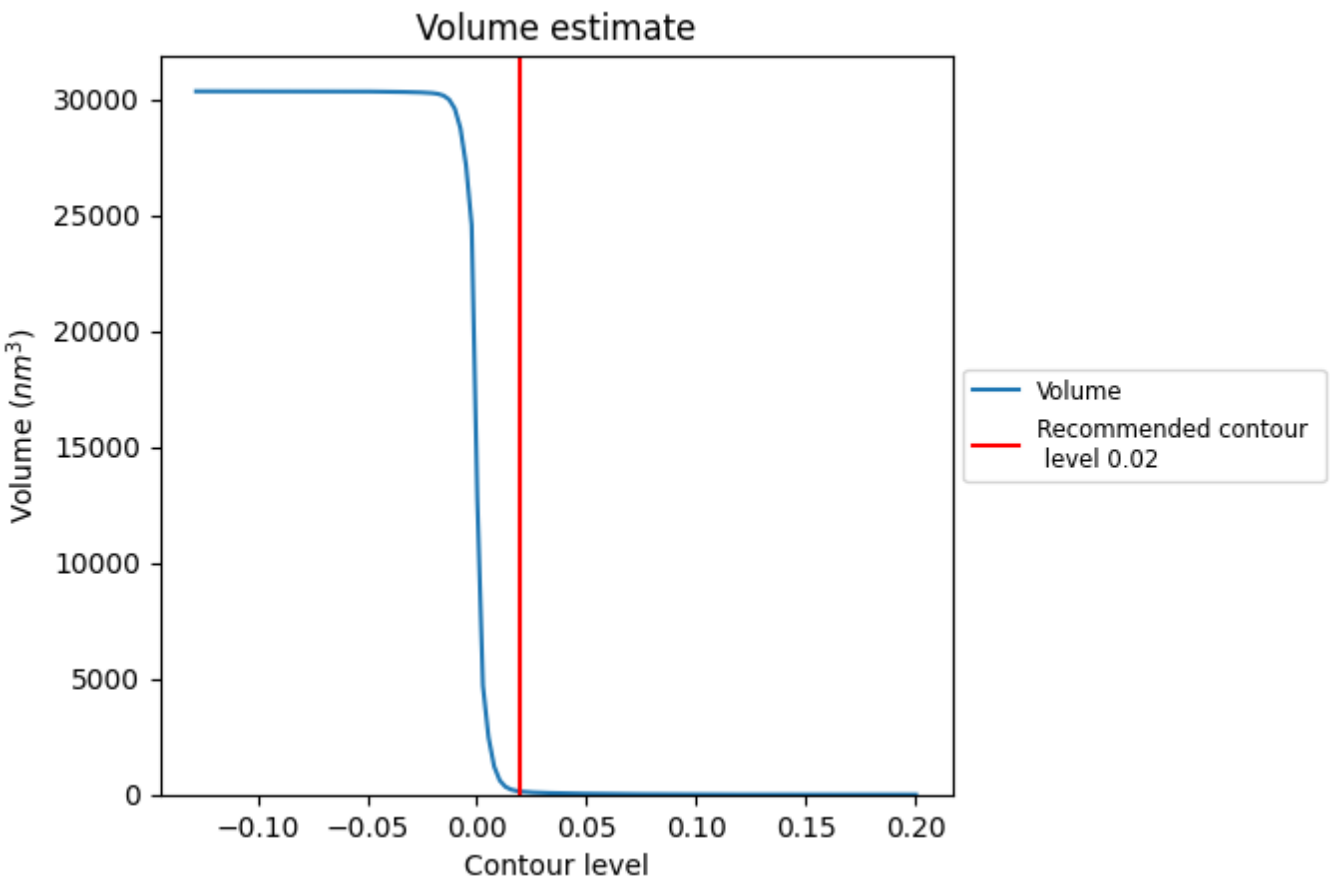
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

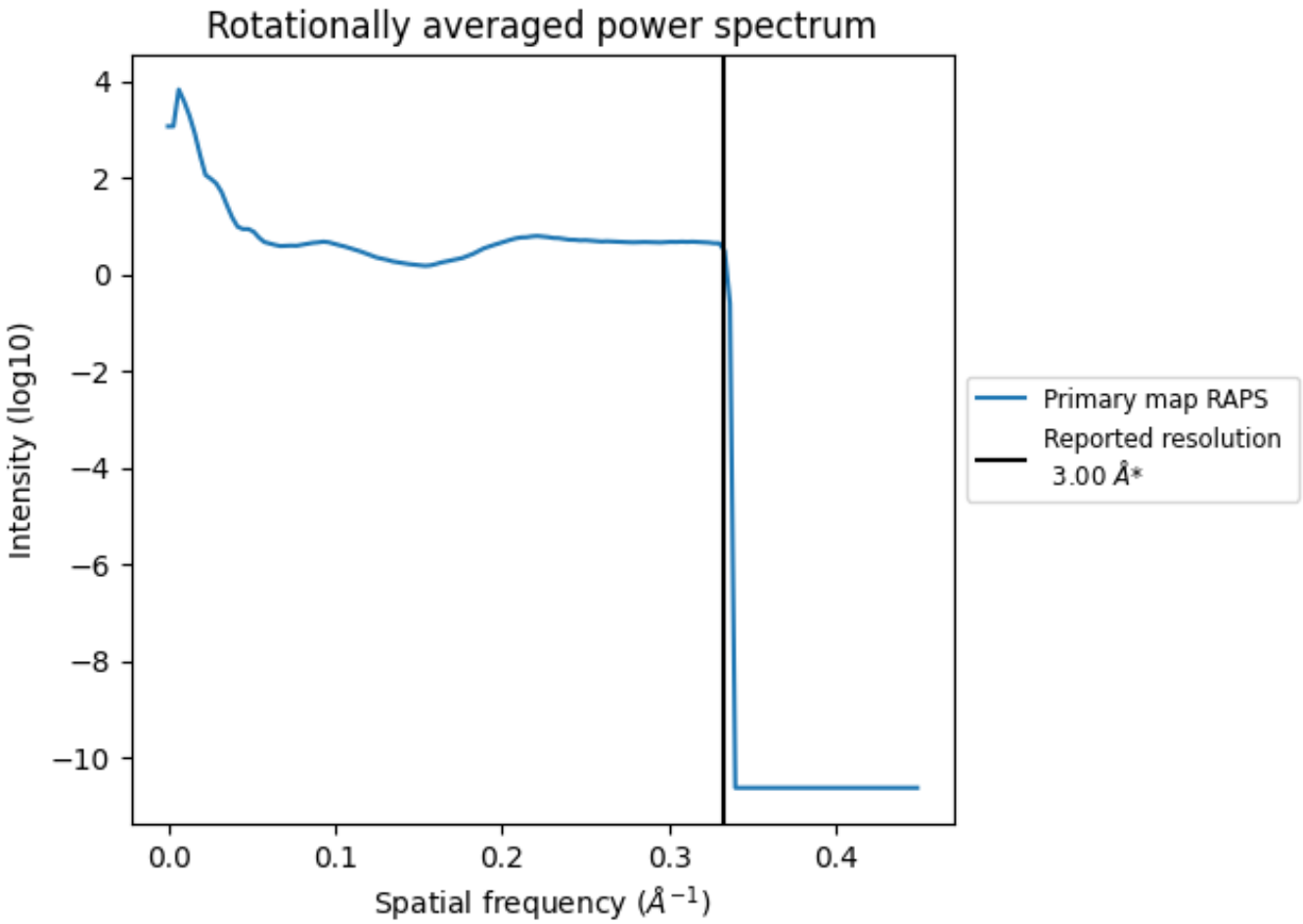
7.2 Volume estimate (i)



The volume at the recommended contour level is 135 nm^3; this corresponds to an approximate mass of 122 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 0.333 Å^{-1}

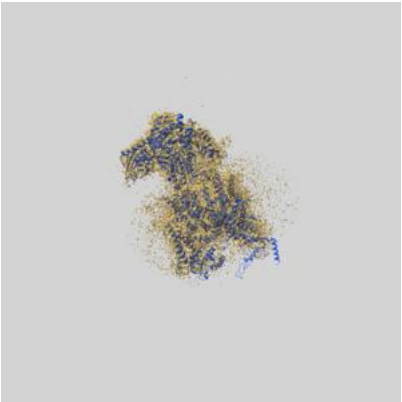
8 Fourier-Shell correlation (i)

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

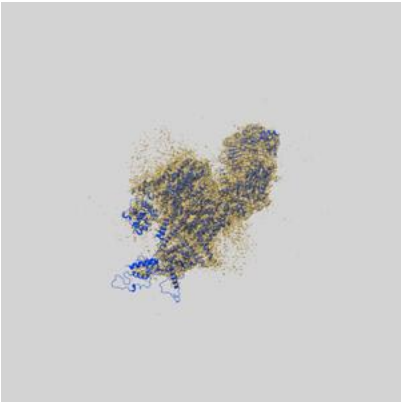
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-23867 and PDB model 7MIX. Per-residue inclusion information can be found in section 3 on page 10.

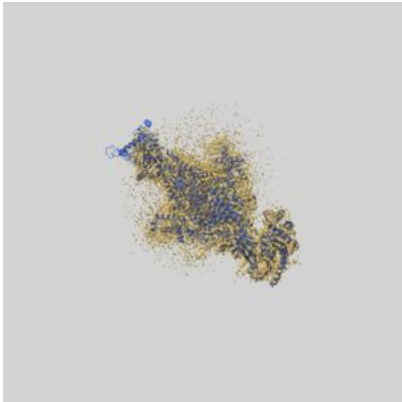
9.1 Map-model overlay (i)



X



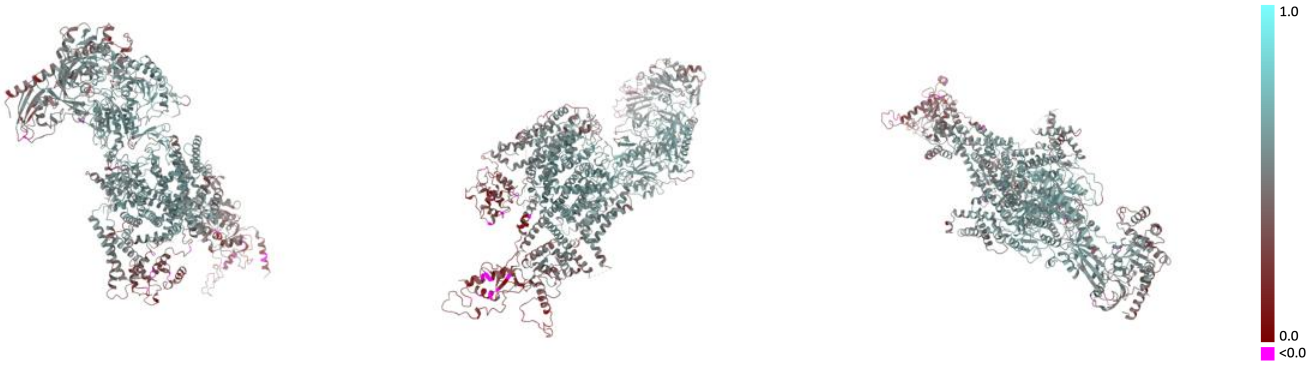
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

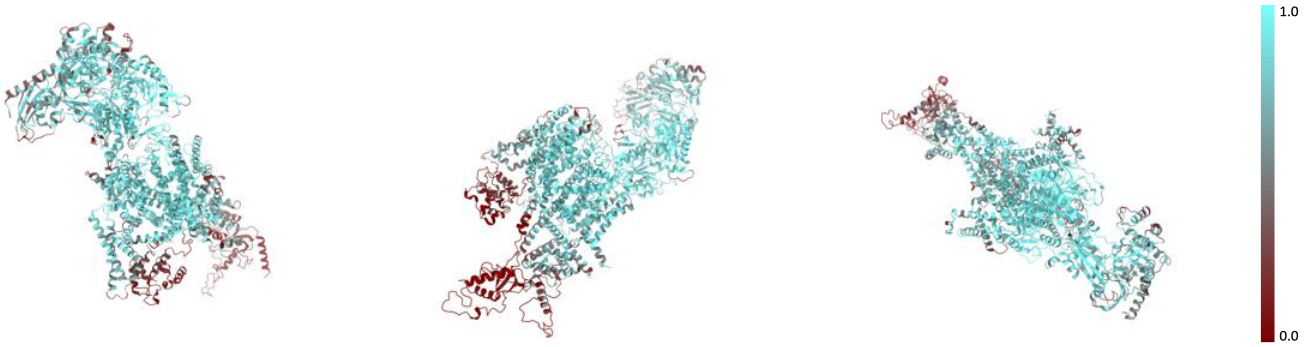
9.2 Q-score mapped to coordinate model (i)



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.

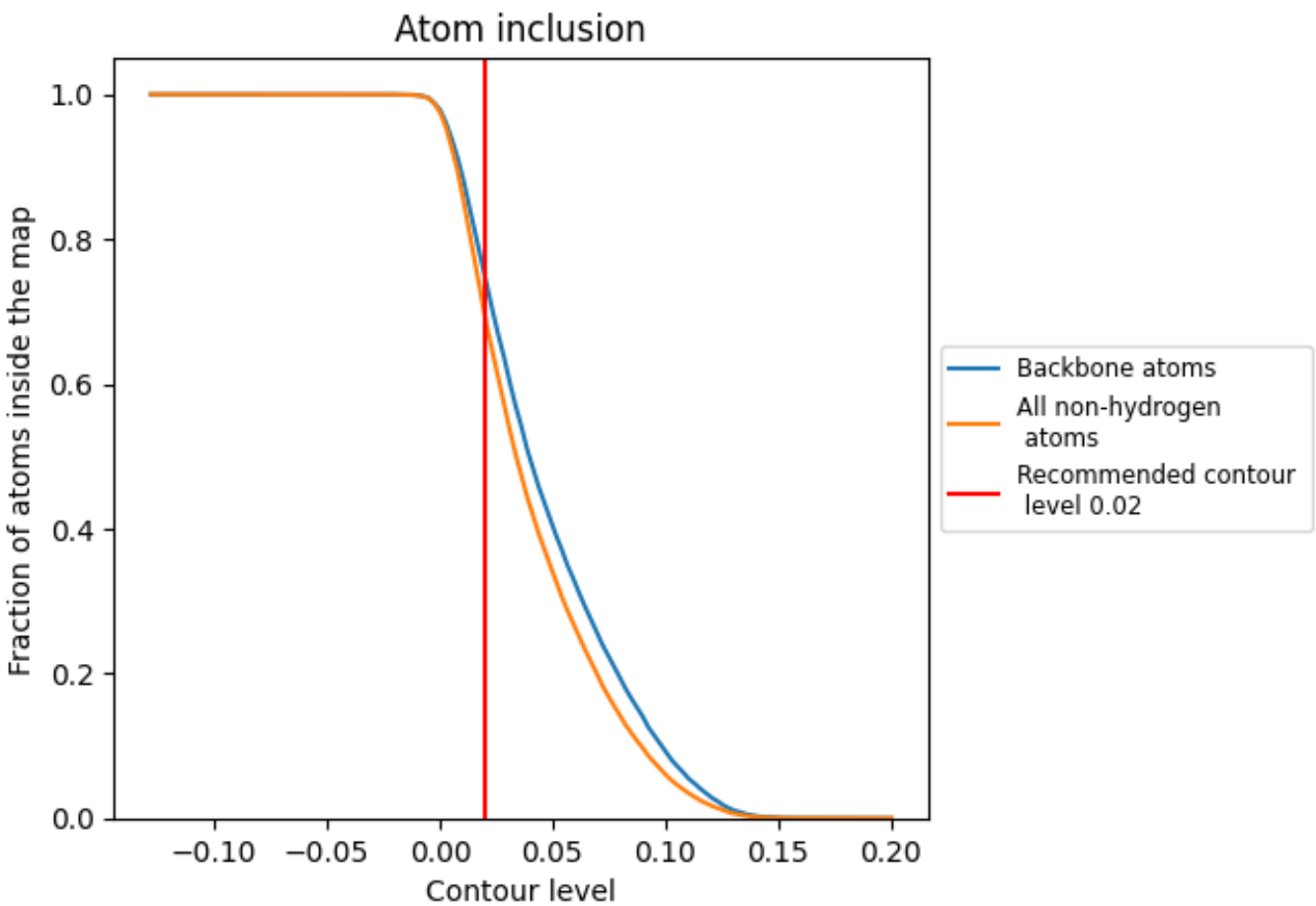
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6946	0.4960
A	0.7230	0.5090
B	0.9181	0.6050
C	0.2908	0.3270
D	0.7885	0.5320
G	0.5000	0.3530
J	0.2857	0.3440
L	0.7143	0.4910
P	0.4286	0.3640
S	0.4643	0.3820