wwPDB EM Validation Summary Report (i)

Dec 20, 2022 – 02:20 PM JST

PDB ID	:	7XMG
EMDB ID	:	EMD-33296
Title	:	Cryo-EM structure of human NaV1.7/beta1/beta2-TCN-1752
Authors	:	Jiang, D.H.; Zhang, J.T.
Deposited on	:	2022-04-25
Resolution	:	3.09 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 (i)) were used in the production of this report:

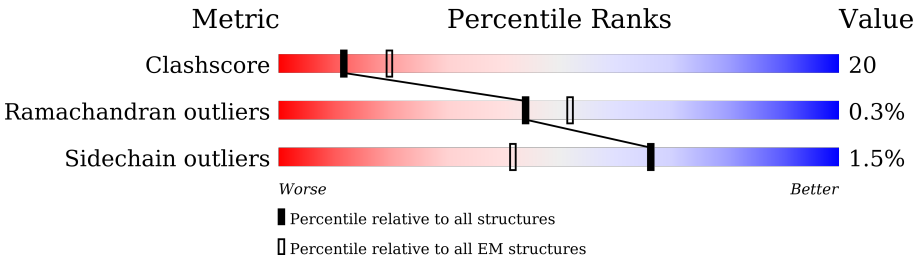
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.09 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	2250	32% 18% 49%
2	B	481	22% 13% 64%
3	F	215	53% 38% 17% 44%
4	D	2	50% 50%
4	E	2	50% 50%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 11692 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 Isoform 3 of Sodium channel protein type 9 subunit alpha,Green fluorescent protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1138	Total	C	N	O	S	0	0
			9175	6098	1434	1567	76		

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1161	ARG	TRP	engineered mutation	UNP Q15858
A	1989	ALA	-	linker	UNP Q15858
A	1990	ALA	-	linker	UNP Q15858
A	1991	ALA	-	linker	UNP Q15858
A	1992	LEU	-	linker	UNP Q15858
A	1993	GLU	-	linker	UNP Q15858
A	1994	VAL	-	linker	UNP Q15858
A	1995	LEU	-	linker	UNP Q15858
A	1996	PHE	-	linker	UNP Q15858
A	1997	GLN	-	linker	UNP Q15858
A	1998	GLY	-	linker	UNP Q15858
A	1999	PRO	-	linker	UNP Q15858
A	2000	SER	-	linker	UNP Q15858

- Molecule 2 is a protein called Sodium channel subunit beta-1,Green fluorescent protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	173	Total	C	N	O	S	0	0
			1416	902	232	272	10		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	219	ALA	-	linker	UNP Q07699
B	220	ALA	-	linker	UNP Q07699
B	221	ALA	-	linker	UNP Q07699

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Chain	Residue	Modelled	Actual	Comment	Reference
B	222	LEU	-	linker	UNP Q07699
B	223	GLU	-	linker	UNP Q07699
B	224	VAL	-	linker	UNP Q07699
B	225	LEU	-	linker	UNP Q07699
B	226	PHE	-	linker	UNP Q07699
B	227	GLN	-	linker	UNP Q07699
B	228	GLY	-	linker	UNP Q07699
B	229	PRO	-	linker	UNP Q07699
B	230	SER	-	linker	UNP Q07699

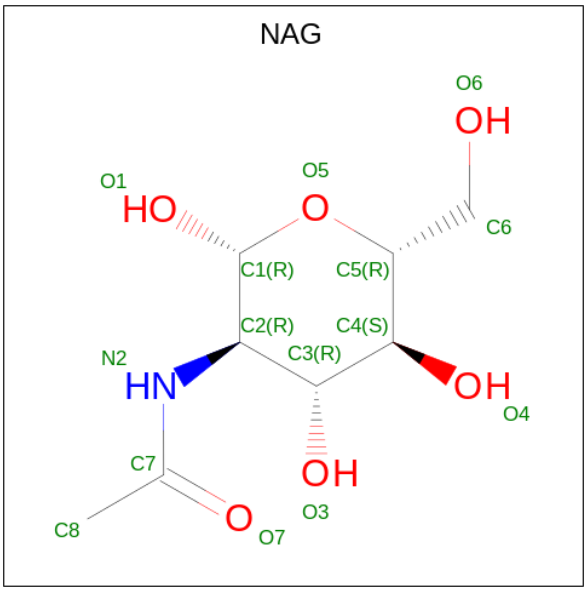
- Molecule 3 is a protein called Sodium channel subunit beta-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	120	Total	C	N	O	S	0	0
			938	582	166	180	10		

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

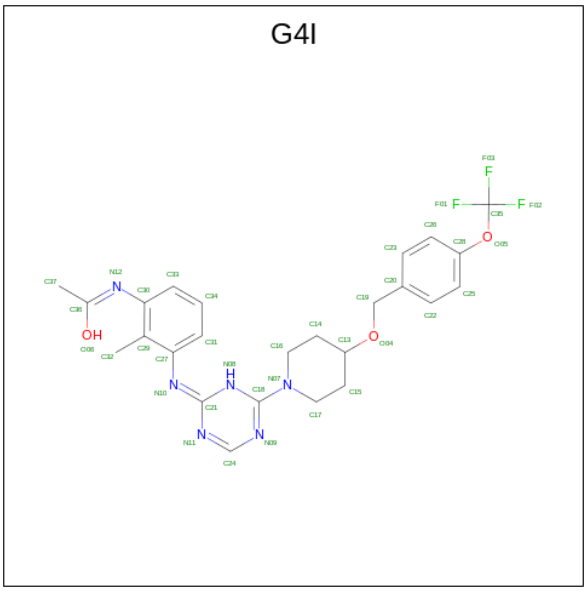
Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total C N O 14 8 1 5	0
5	B	1	Total C N O 56 32 4 20	0
5	B	1	Total C N O 56 32 4 20	0
5	B	1	Total C N O 56 32 4 20	0
5	B	1	Total C N O 56 32 4 20	0

- Molecule 6 is (1 {Z})- {N}-[2-methyl-3-[({E})-[6-[4-[[4-(trifluoromethyloxy)phenyl]methoxy]piperidin-1-yl]-1 {H}-1,3,5-triazin-2-ylidene]amino]phenyl]ethanimidic acid (three-letter code: G4I) (formula: $C_{25}H_{27}F_3N_6O_3$) (labeled as "Ligand of Interest" by depositor).



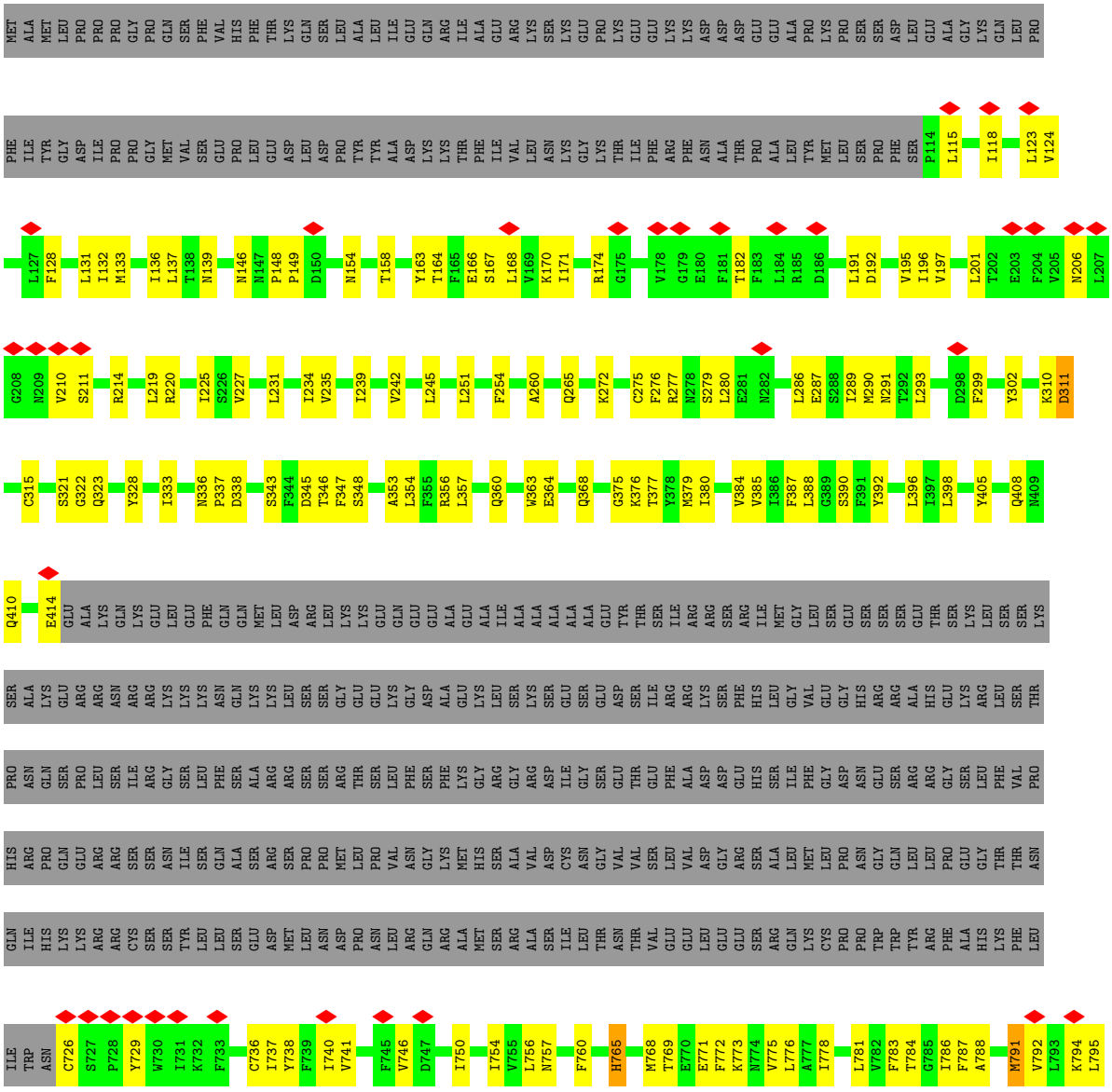
Mol	Chain	Residues	Atoms					AltConf
			Total	C	F	N	O	
6	A	1	37	25	3	6	3	0

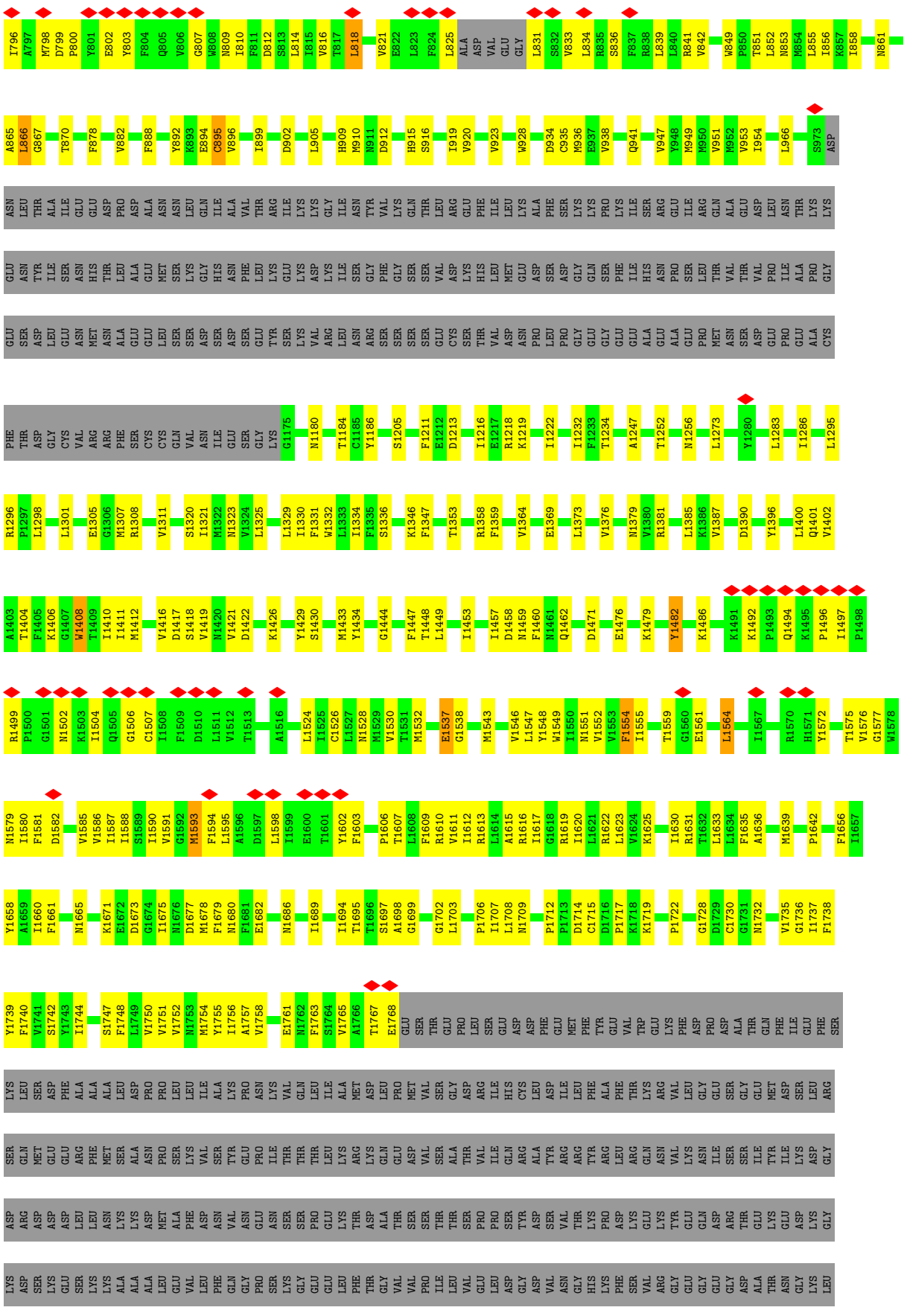
3 Residue-property plots (i)

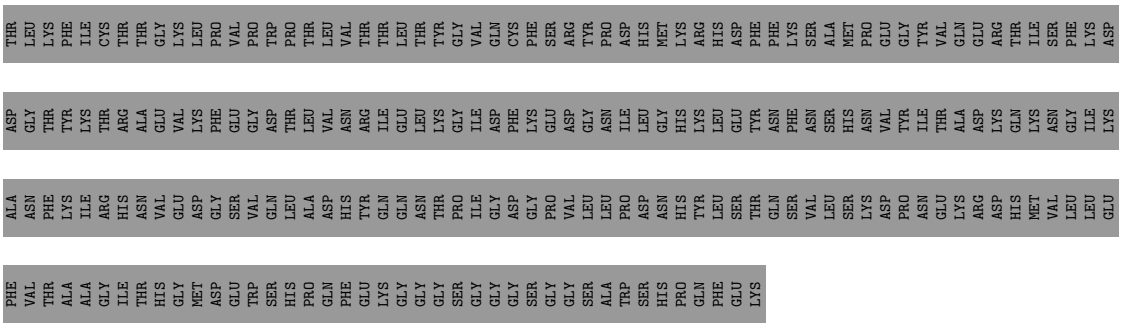
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Isoform 3 of Sodium channel protein type 9 subunit alpha,Green fluorescent protein

Chain A:

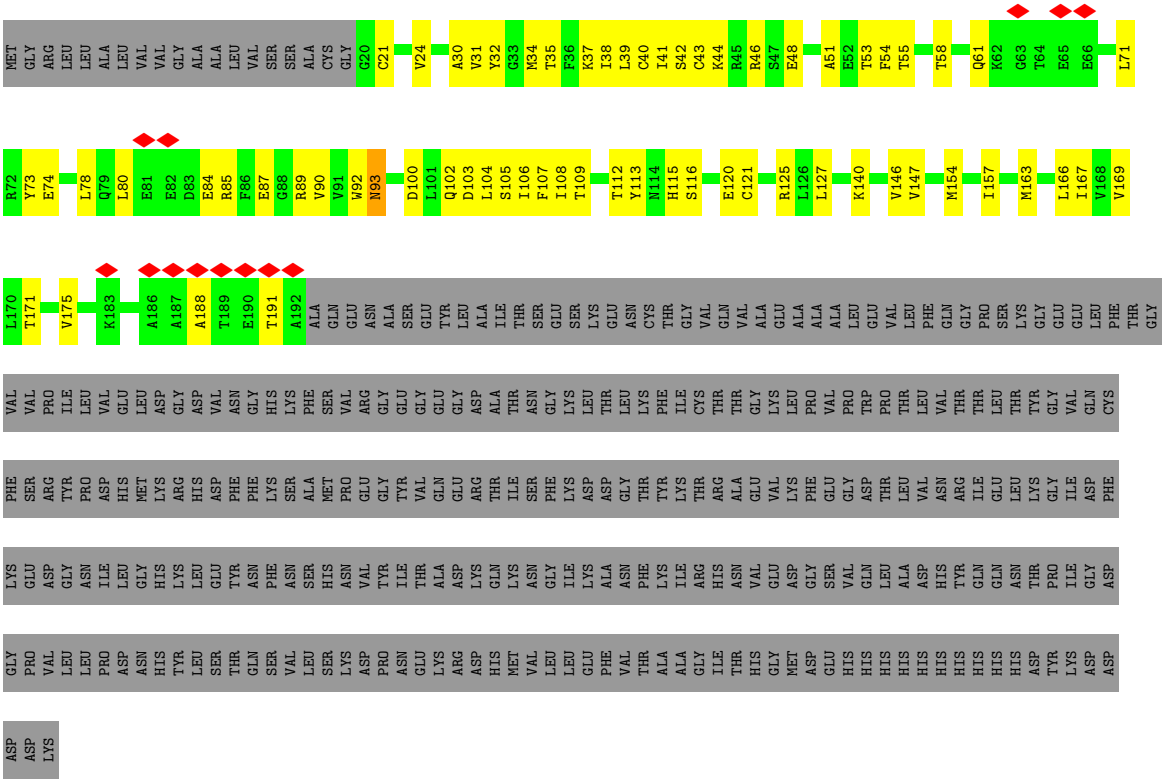



I796 A797 M798 D799 P800 Y801 E802 Y803 F804 Q805 V806 G807 W808 N809 I810 F811 D812 S813 L814 I815 V816 T817 L818 V821 E822 L823 F824 L825 ALA ASP VAL GLU GLY L831 S832 V833 L834 R835 S836 F837 R838 L839 L840 R841 V842 W849 P850 T851 L852 N853 M854 L855 I856 K857 I858 N861
A865 L866 G867 T870 F878 V882 F888 Y892 K893 E894 C895 V896 I899 D902 L905 H909 M910 N911 D912 H915 S916 I919 V920 V923 W928 D934 C935 M936 E937 V938 Q941 V947 Y948 M949 N950 V951 M952 V953 I954 L966 S973 ASP
ASN LEU THR ALA ILE GLU GLU ASP PRO ASP ALA ASN ASN LEU GLN ILE ALA VAL THR ARG ILE LYS GLY ILE ASN TYR VAL LYS GLN THR LEU ARG GLU PHE ILE LEU LYS ALA PHE SER LYS LYS PRO LYS ILE SER ARG GLU ILE ARG GLN ALA GLU ASP LEU ASN THR LYS LYS
GLU ASN TYR ILE SER ASN HIS THR LEU ALA GLU MET SER LYS GLY HIS ASN PHE LEU LYS GLU LYS ASP ILE SER GLY PHE GLY SER SER VAL ASP LYS HIS LEU MET GLU ASP SER ASP GLY GLN SER PHE ILE HIS ASN PRO SER LEU THR VAL THR VAL PRO ILE ALA PRO GLY
GLU SER ASP LEU GLU ASN MET ASN ALA GLU GLU LEU SER SER ASP SER ASP SER GLU TYR SER LYS VAL ARG LEU ASN ARG SER SER SER SER GLU CYS SER THR VAL ASP ASN PRO LEU PRO GLY GLU GLY GLU GLU ALA GLU ALA GLU PRO MET ASN SER ASP GLU PRO GLU ALA CYS
PHE THR ASP GLY CYS VAL ASN ILE GLU SER CYS CYS GLN VAL ASN ILE GLU SER GLY LYS G1175 N1180 T1184 C1185 Y1186 S1205 F1211 E1212 D1213 I1216 E1217 R1218 K1219 I1222 I1232 F1233 T1234 A1247 T1252 N1256 L1273 Y1280 L1283 I1286 L1295
R1296 P1297 L1298 L1301 E1305 G1306 M1307 R1308 V1311 S1320 I1321 M1322 N1323 Y1324 L1325 L1329 I1330 F1331 W1332 L1333 I1334 F1335 S1336 K1346 F1347 T1353 R1358 F1359 V1364 E1369 L1373 V1376 N1379 V1380 R1381 L1385 K1386 V1387 D1390 Y1396 L1400 Q1401 V1402
A1403 T1404 F1405 K1406 G1407 W1408 T1409 I1410 I1411 M1412 V1416 D1417 S1418 V1419 N1420 V1421 D1422 K1426 Y1429 S1430 M1433 Y1434 G1444 F1447 T1448 L1449 I1453 I1457 D1458 N1459 F1460 N1461 Q1462 D1471 E1476 K1479 Y1482 K1486 K1491 K1492 P1493 Q1494 K1495 P1496 I1497 P1498
R1499 P1500 G1501 N1502 K1503 I1504 Q1505 G1506 C1507 I1508 F1509 D1510 L1511 V1512 T1513 A1516 L1524 I1525 C1526 L1527 N1528 M1529 V1530 T1531 M1532 E1537 G1538 M1543 V1546 L1547 Y1548 W1549 I1550 N1551 V1552 V1553 F1554 I1555 T1559 G1560 E1561 L1564 I1567 R1570 H1571 Y1572 T1575 V1576 G1577 W1578
N1579 I1580 F1581 D1582 V1585 V1586 I1587 I1588 S1589 I1590 V1591 G1592 M1593 F1594 L1595 A1596 D1597 L1598 I1599 E1600 T1601 Y1602 F1603 P1606 T1607 L1608 F1609 R1610 V1611 I1612 R1613 L1614 A1615 R1616 I1617 G1618 R1619 I1620 L1621 R1622 L1623 V1624 K1625 I1630 R1631 T1632 L1633 L1634 F1635 A1636 M1639 P1642 F1656 I1657
Y1658 A1659 I1660 F1661 N1665 K1671 E1672 D1673 G1674 I1675 N1676 D1677 M1678 F1679 N1680 F1681 E1682 N1686 I1689 I1694 T1695 T1696 S1697 A1698 G1699 G1702 L1703 P1706 I1707 L1708 N1709 P1712 P1713 D1714 C1715 D1716 P1717 K1718 K1719 P1722 G1728 D1729 C1730 G1731 N1732 V1735 G1736 I1737 F1738
Y1739 F1740 V1741 S1742 Y1743 I1744 S1747 F1748 L1749 V1750 V1751 V1752 N1753 M1754 Y1755 I1756 A1757 V1758 E1761 N1762 F1763 S1764 V1765 A1766 T1767 E1768 GLU SER THR GLU PRO LEU SER GLU ASP ASP PHE GLU MET PHE TYR GLU VAL TRP GLU LYS PHE ASP PRO GLU ILE ILE GLU PHE SER
LYS LEU SER ASP PHE ALA ALA LEU ASP PRO PRO LEU LEU ILE ALA LYS PRO ASN LYS VAL GLN LEU ILE ALA MET ASP LEU PRO MET VAL SER GLY ASP ARG ILE HIS CYS LEU ASP ILE LEU PHE ALA PHE THR LYS ARG VAL LEU GLY GLU SER GLY GLU MET ASP SER LEU ARG
SER GLN MET GLU GLU ARG PHE MET SER ALA ASN PRO SER LYS VAL SER TYR GLU PRO ILE THR THR LEU LYS ARG LYS GLN GLU ASP VAL SER ALA THR VAL ILE GLN ARG ALA TYR ARG ARG TYR ARG LEU ARG GLN ASN VAL LYS ASN ILE SER SER ILE TYR ILE LYS ASP GLY
ASP ARG ASP ASP LEU LEU ASN LYS LYS ASP MET ALA PHE ASP ASN VAL ASN GLU LYS ASP SER SER PRO GLU LYS THR ASP ALA THR SER SER THR THR SER PRO PRO SER TYR ASP SER VAL THR LYS PRO ASP LYS GLU LYS TYR GLU GLN ASP ARG THR GLU LYS GLU ASP LYS GLY
LYS ASP SER LYS GLU SER LYS LYS ALA ALA LEU GLU VAL VAL LEU PHE GLN GLY PRO SER LYS GLY GLU GLU LEU PHE THR GLY VAL VAL PRO ILE LEU VAL GLU LEU ASP GLY ASP VAL ASN GLY HIS LYS PHE SER VAL ARG GLY GLU GLY GLU GLY ASP ALA THR ASN GLY LYS LEU



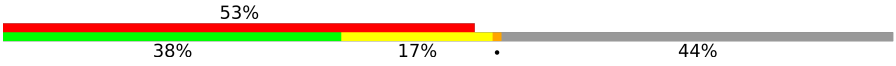
• Molecule 2: Sodium channel subunit beta-1,Green fluorescent protein

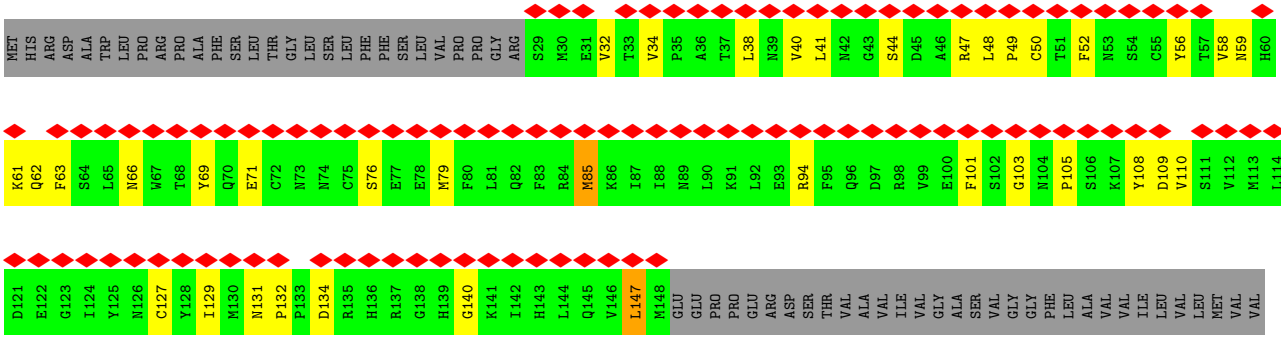
Chain B:

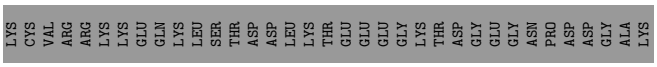


• Molecule 3: Sodium channel subunit beta-2

Chain F:







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

Chain D:

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

Chain E:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	158142	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 ($e^-/Å^2$)	60.0	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	4.571	Depositor
Minimum map value	-3.007	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.094	Depositor
Recommended contour level	0.376	Depositor
Map size (Å)	266.24, 266.24, 266.24	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: G4I, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.30	0/9400	0.49	3/12740 (0.0%)
2	B	0.28	0/1442	0.46	0/1949
3	F	0.51	1/957 (0.1%)	0.71	2/1298 (0.2%)
All	All	0.32	1/11799 (0.0%)	0.51	5/15987 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	127	CYS	CB-SG	11.06	2.01	1.82

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	127	CYS	CA-CB-SG	7.90	128.22	114.00
3	F	85	MET	CB-CA-C	-6.32	97.76	110.40
1	A	866	LEU	CA-CB-CG	-5.71	102.16	115.30
1	A	895	CYS	CA-CB-SG	5.49	123.88	114.00
1	A	1677	ASP	CB-CG-OD2	5.18	122.96	118.30

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	9175	0	9398	339	0
2	B	1416	0	1382	62	0
3	F	938	0	874	64	0
4	D	28	0	25	1	0
4	E	28	0	25	1	0
5	A	14	0	13	0	0
5	B	56	0	52	0	0
6	A	37	0	0	0	0
All	All	11692	0	11769	463	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 20.

The worst 5 of 463 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:866:LEU:CD1	1:A:966:LEU:HD11	1.56	1.34
1:A:1496:PRO:O	1:A:1497:ILE:HG13	1.29	1.32
3:F:34:VAL:HG13	3:F:50:CYS:SG	1.86	1.16
1:A:139:ASN:HD21	1:A:220:ARG:HD3	1.01	1.10
3:F:34:VAL:CG1	3:F:50:CYS:SG	2.39	1.10

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	1130/2250 (50%)	1046 (93%)	83 (7%)	1 (0%)	51 83
2	B	171/481 (36%)	157 (92%)	14 (8%)	0	100 100
3	F	118/215 (55%)	108 (92%)	7 (6%)	3 (2%)	5 27
All	All	1419/2946 (48%)	1311 (92%)	104 (7%)	4 (0%)	44 73

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	56	TYR
3	F	76	SER
3	F	147	LEU
1	A	800	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	1017/1998 (51%)	999 (98%)	18 (2%)	59 82
2	B	157/419 (38%)	156 (99%)	1 (1%)	86 94
3	F	105/193 (54%)	105 (100%)	0	100 100
All	All	1279/2610 (49%)	1260 (98%)	19 (2%)	66 85

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1564	LEU
1	A	1603	PHE
2	B	93	ASN
1	A	1602	TYR
1	A	1390	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1680	ASN
3	F	59	ASN
3	F	118	GLN
3	F	66	ASN
2	B	115	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)

4 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	$\#\|Z\| > 2$
4	NAG	D	1	4,1	14,14,15	0.31	0	17,19,21	0.45	0
4	NAG	D	2	4	14,14,15	0.25	0	17,19,21	0.46	0
4	NAG	E	1	4,1	14,14,15	0.53	0	17,19,21	1.37	1 (5%)
4	NAG	E	2	4	14,14,15	0.79	1 (7%)	17,19,21	1.02	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	NAG	E	1	4,1	-	5/6/23/26	0/1/1/1
4	NAG	E	2	4	-	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)
4	E	2	NAG	O5-C1	2.59	1.47	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	1	NAG	C2-N2-C7	4.27	128.99	122.90
4	E	2	NAG	C1-O5-C5	3.95	117.54	112.19

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	1	NAG	C4-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
4	E	1	NAG	C8-C7-N2-C2
4	E	1	NAG	O7-C7-N2-C2
4	E	2	NAG	C4-C5-C6-O6

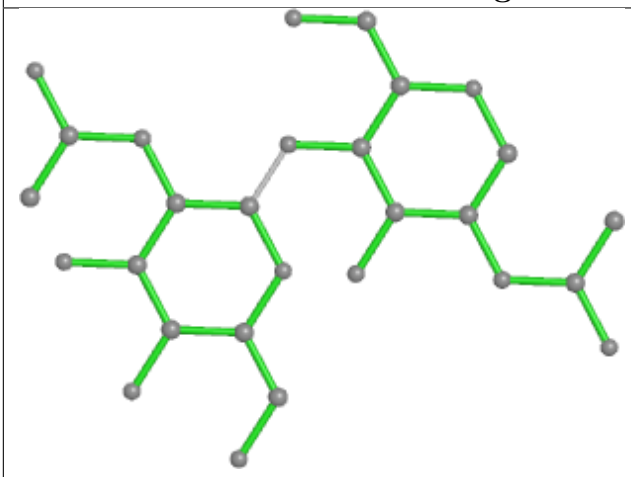
There are no ring outliers.

2 monomers are involved in 2 short contacts:

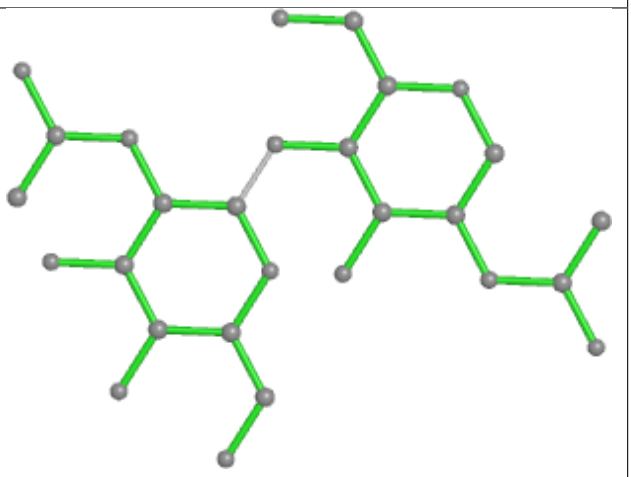
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	NAG	1	0
4	E	1	NAG	1	0

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

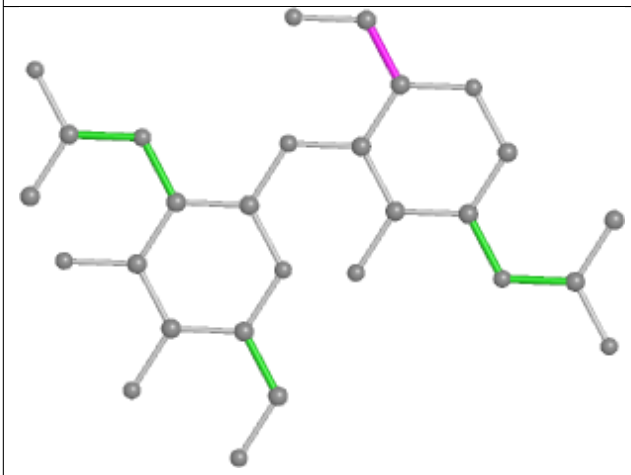
Oligosaccharide Chain D



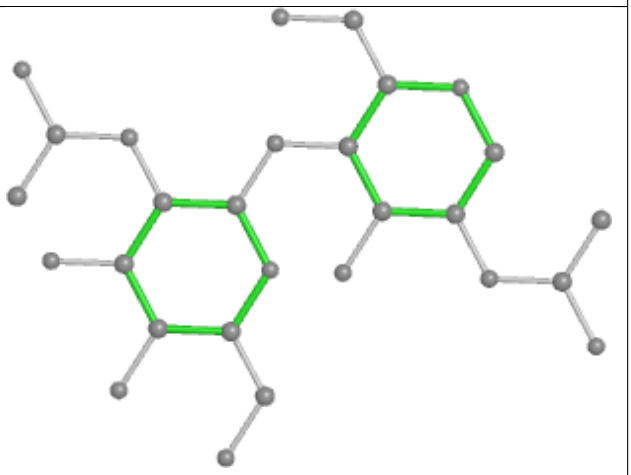
Bond lengths



Bond angles

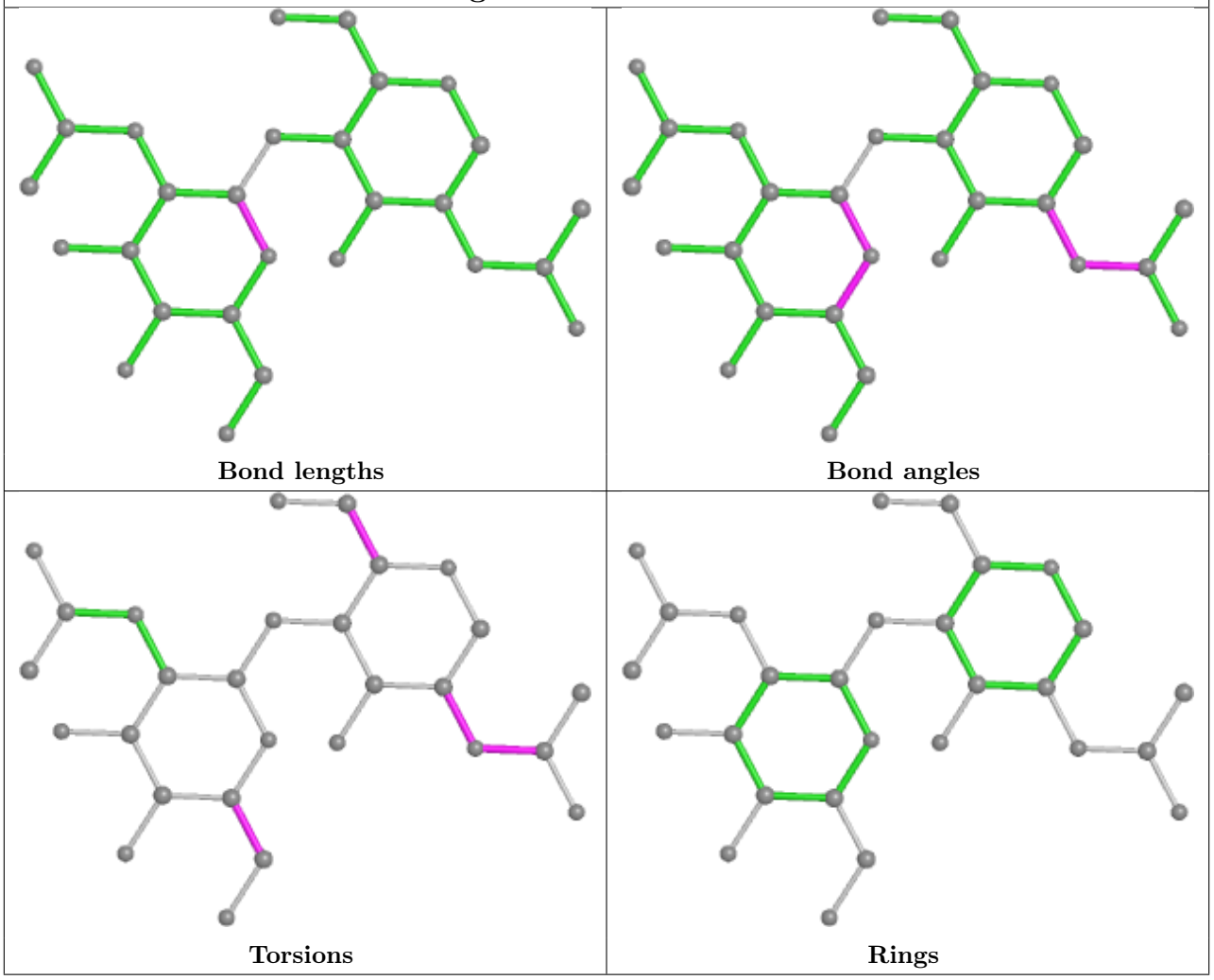


Torsions



Rings

Oligosaccharide Chain E



5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	B	504	2	14,14,15	0.22	0	17,19,21	0.36	0
5	NAG	A	2301	1	14,14,15	0.38	0	17,19,21	0.54	0
5	NAG	B	502	2	14,14,15	0.23	0	17,19,21	0.43	0
5	NAG	B	501	2	14,14,15	0.44	0	17,19,21	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	G4I	A	2302	-	40,40,40	2.18	7 (17%)	49,56,56	1.42	7 (14%)
5	NAG	B	503	2	14,14,15	0.19	0	17,19,21	0.38	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	B	504	2	-	2/6/23/26	0/1/1/1
5	NAG	A	2301	1	-	2/6/23/26	0/1/1/1
5	NAG	B	502	2	-	1/6/23/26	0/1/1/1
5	NAG	B	501	2	-	2/6/23/26	0/1/1/1
6	G4I	A	2302	-	-	3/19/32/32	0/4/4/4
5	NAG	B	503	2	-	1/6/23/26	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2302	G4I	C21-N10	10.28	1.47	1.29
6	A	2302	G4I	C36-N12	3.78	1.44	1.29
6	A	2302	G4I	C18-N07	3.62	1.47	1.34
6	A	2302	G4I	C21-N08	-3.60	1.33	1.38
6	A	2302	G4I	O06-C36	-3.41	1.18	1.29

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	2302	G4I	N10-C21-N11	-4.79	120.41	126.47
6	A	2302	G4I	N09-C24-N11	-4.68	119.96	128.82
6	A	2302	G4I	C29-C30-N12	3.09	120.95	118.14
6	A	2302	G4I	C18-N08-C21	-2.63	119.93	123.75
6	A	2302	G4I	C16-N07-C17	2.57	117.57	112.62

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	2302	G4I	N11-C21-N10-C27
5	A	2301	NAG	O5-C5-C6-O6

Continued on next page...

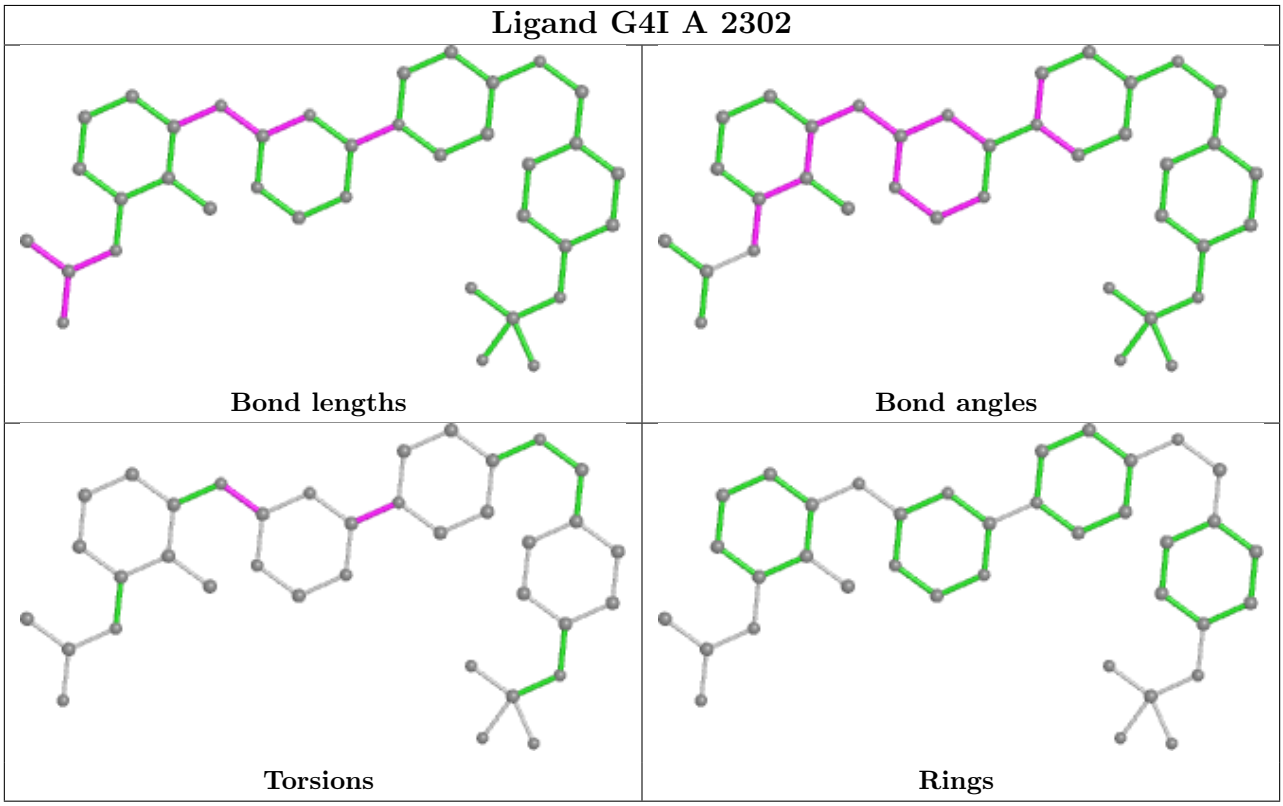
Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	2301	NAG	C4-C5-C6-O6
5	B	504	NAG	O5-C5-C6-O6
5	B	501	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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



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.

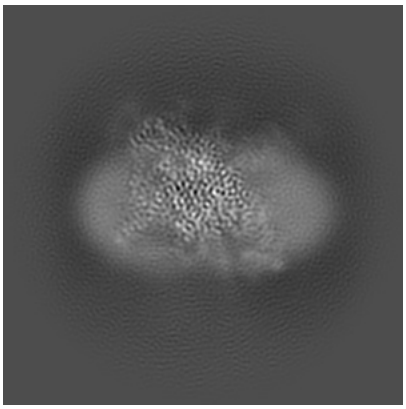
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-33296. These allow visual inspection of the internal detail of the map and identification of artifacts.

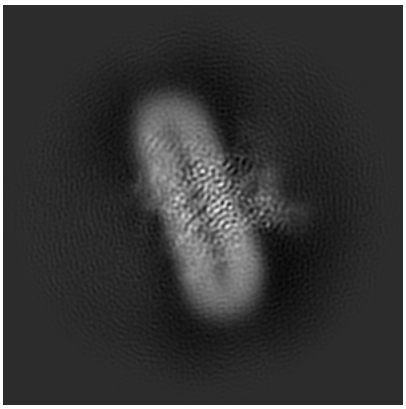
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

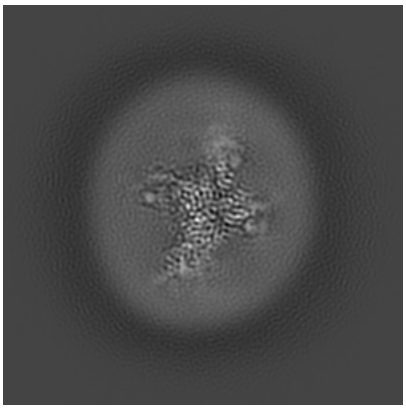
6.1.1 Primary map



X

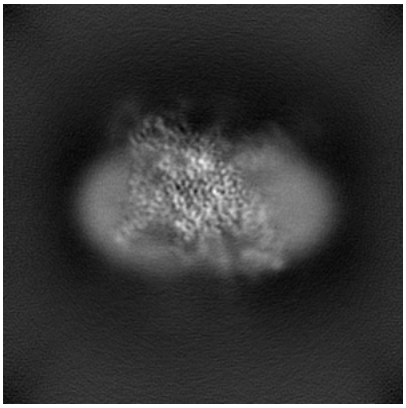


Y

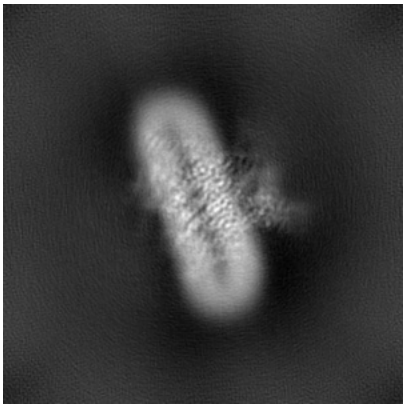


Z

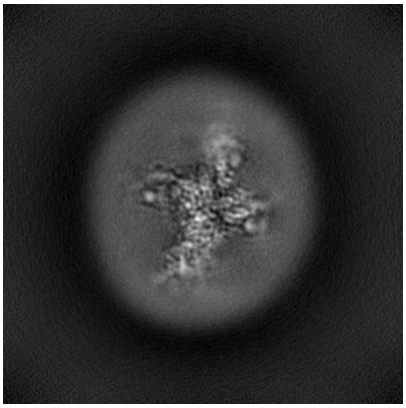
6.1.2 Raw map



X



Y

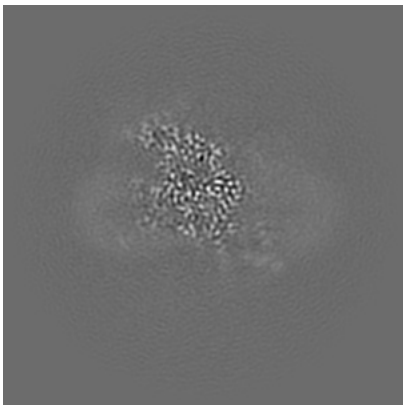


Z

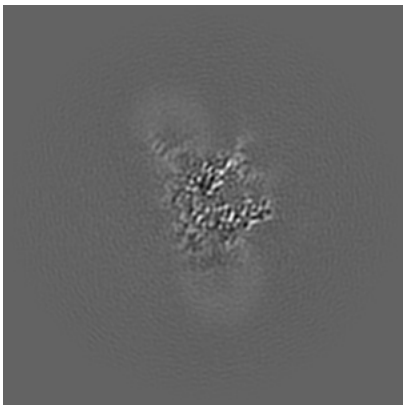
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

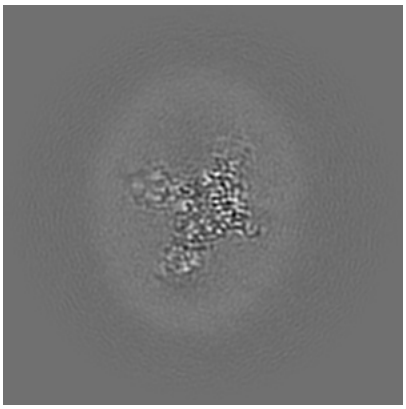
6.2.1 Primary map



X Index: 128

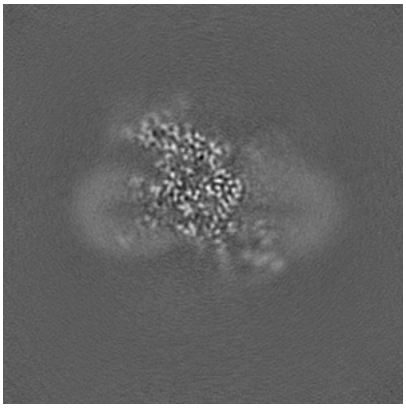


Y Index: 128

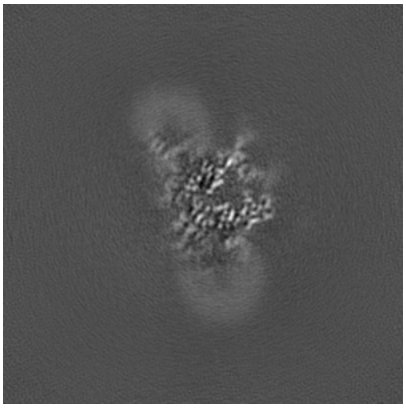


Z Index: 128

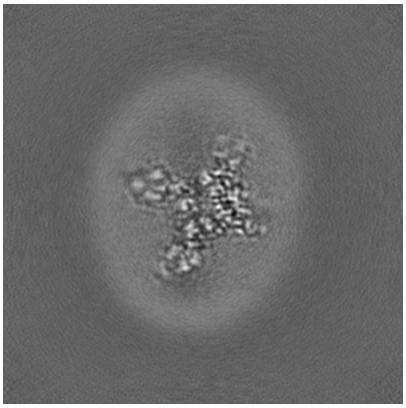
6.2.2 Raw map



X Index: 128



Y Index: 128

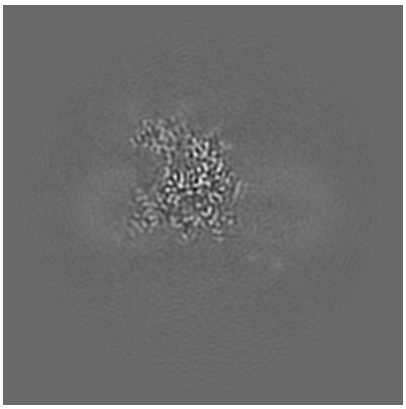


Z Index: 128

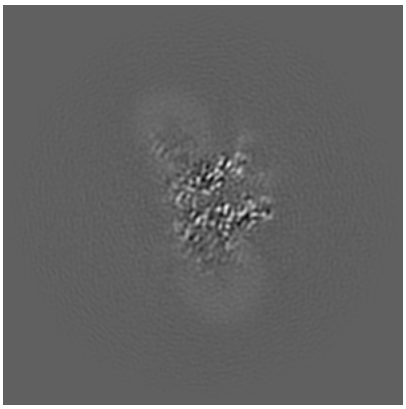
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

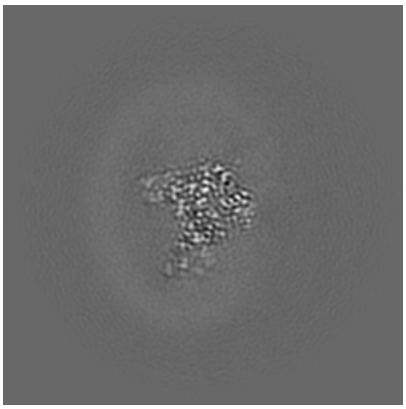
6.3.1 Primary map



X Index: 122

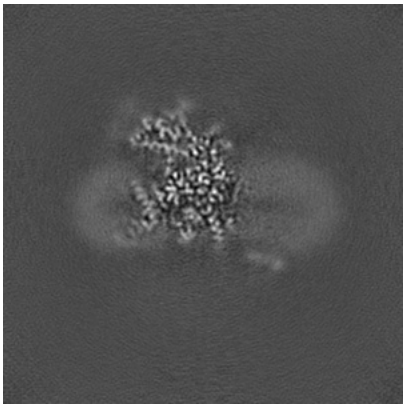


Y Index: 129

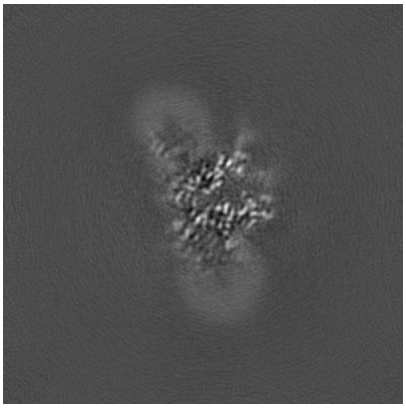


Z Index: 138

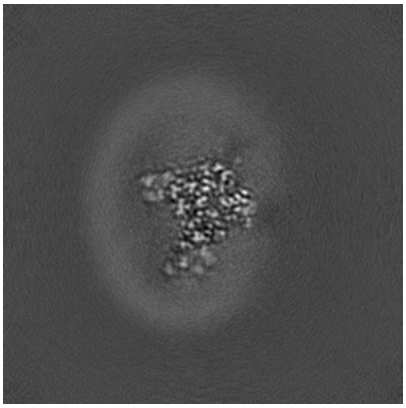
6.3.2 Raw map



X Index: 123



Y Index: 129



Z Index: 138

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 0.376. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

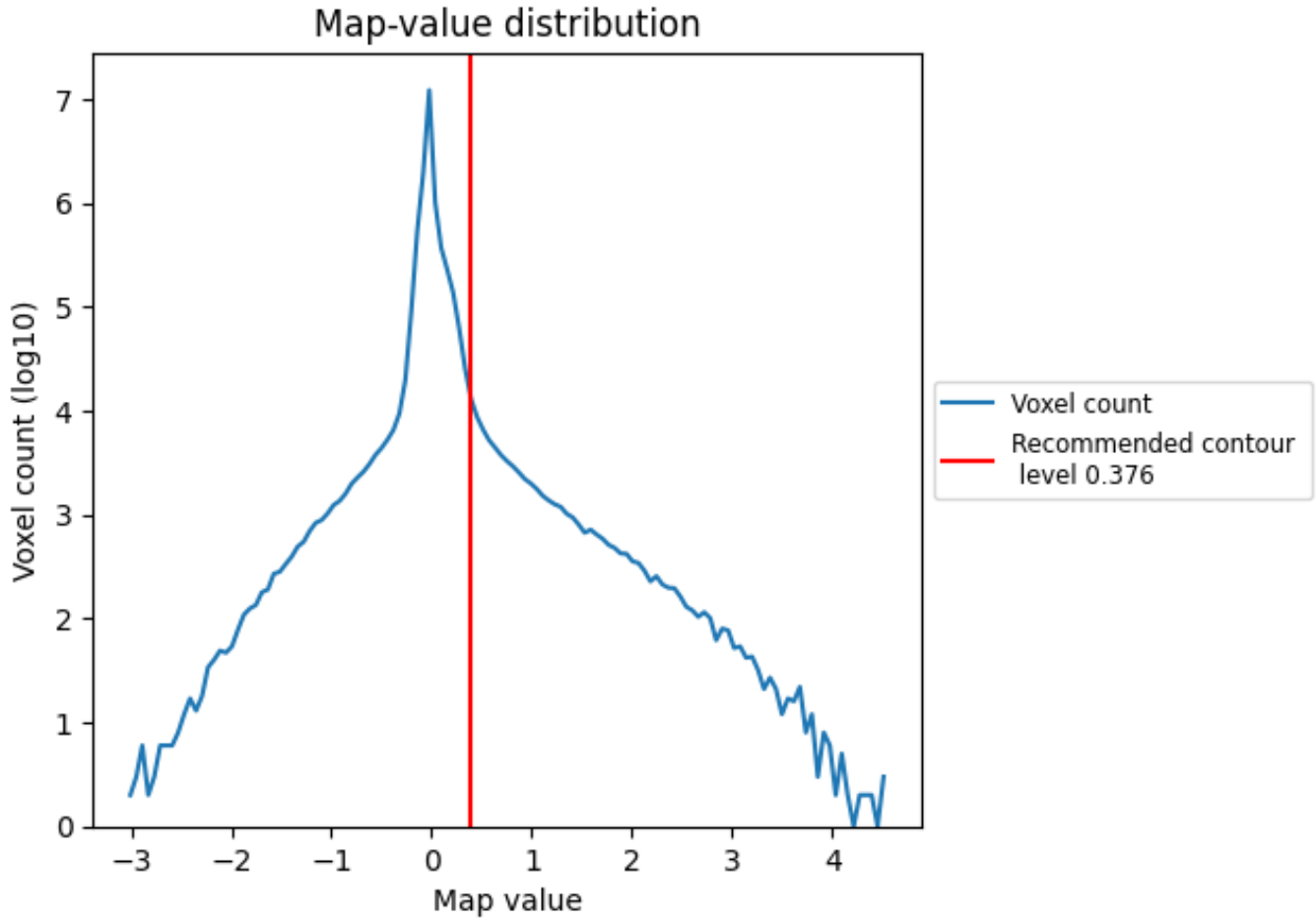
6.5 Mask visualisation (i)

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

7 Map analysis

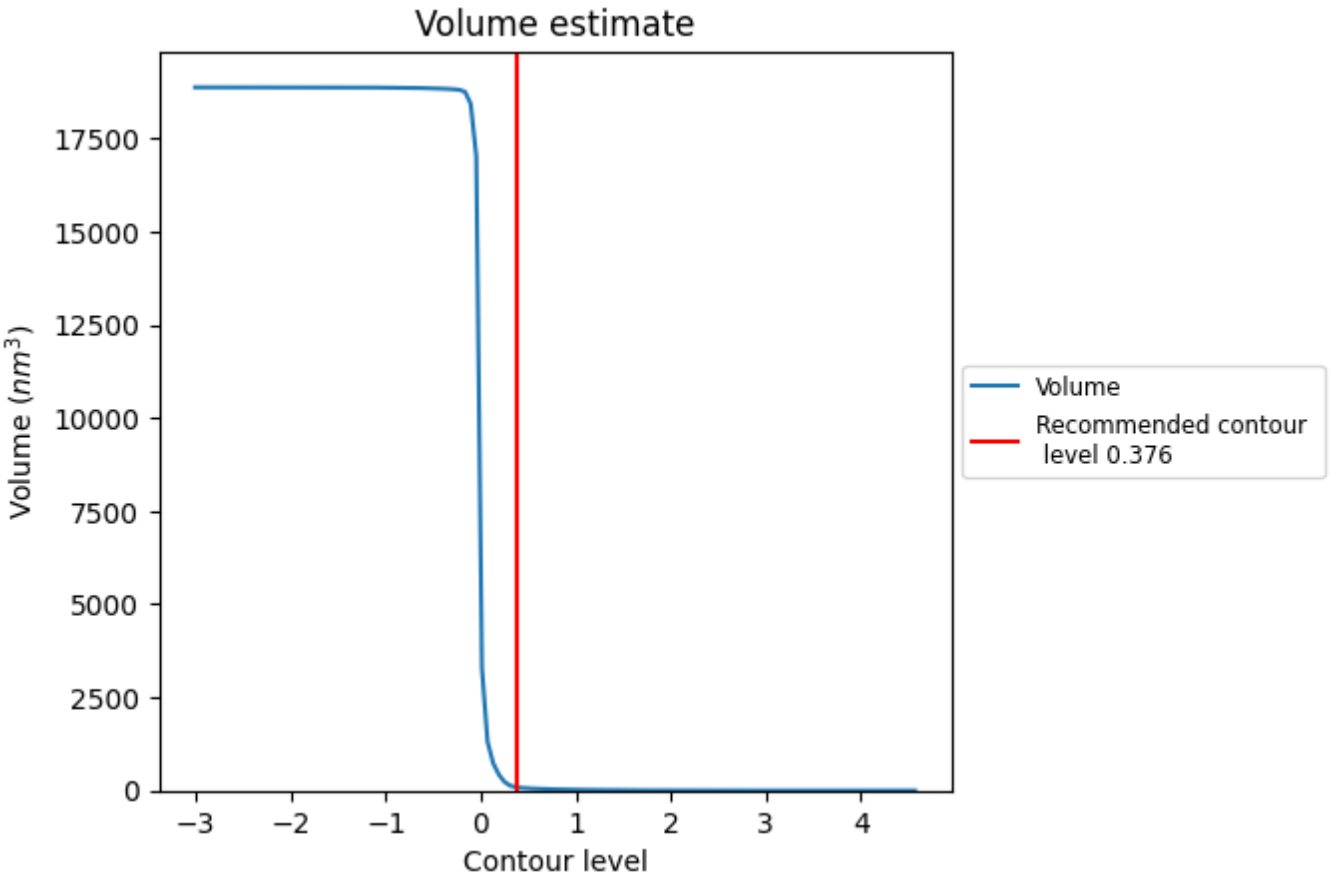
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

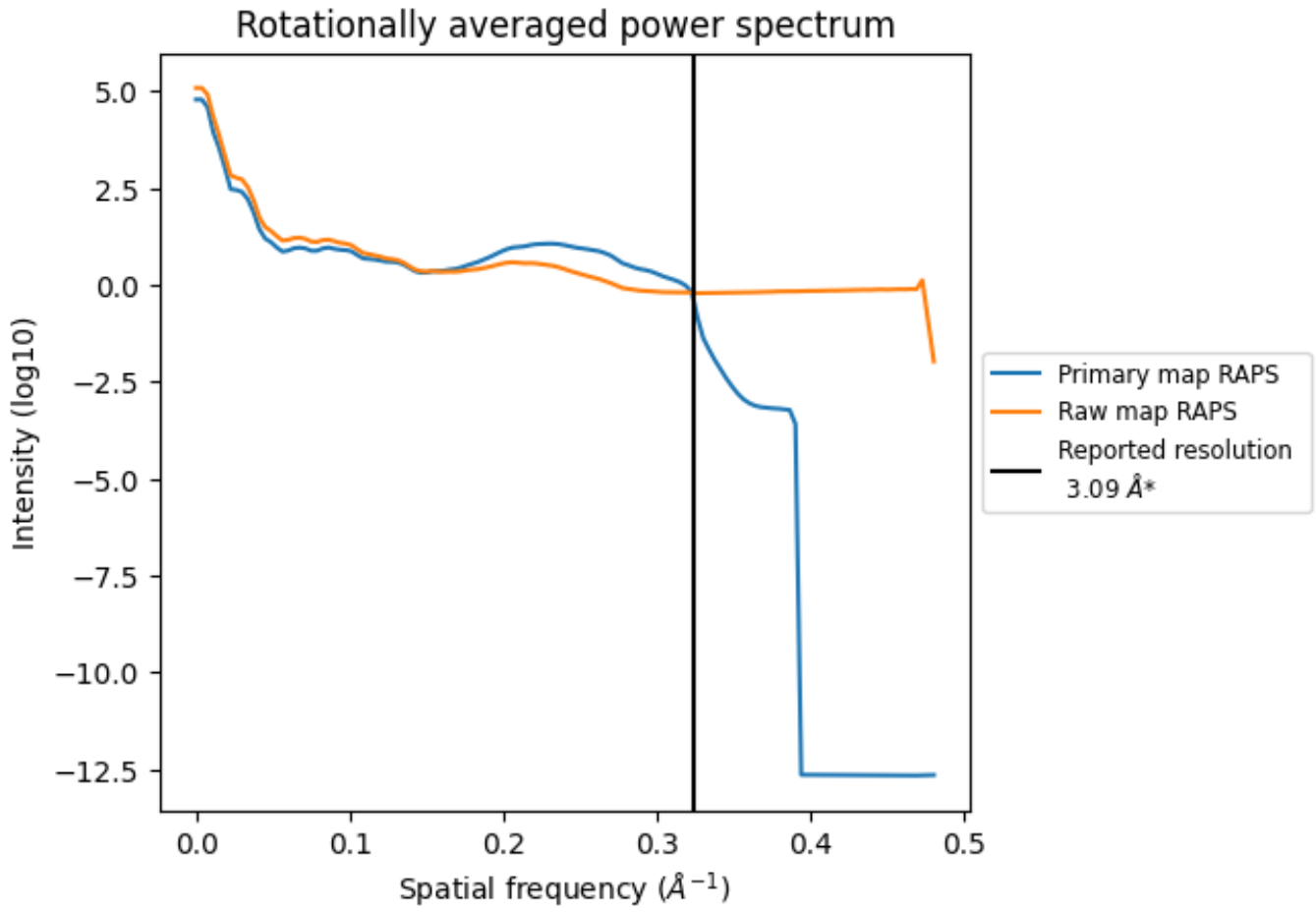
7.2 Volume estimate (i)



The volume at the recommended contour level is 89 nm^3; this corresponds to an approximate mass of 80 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)

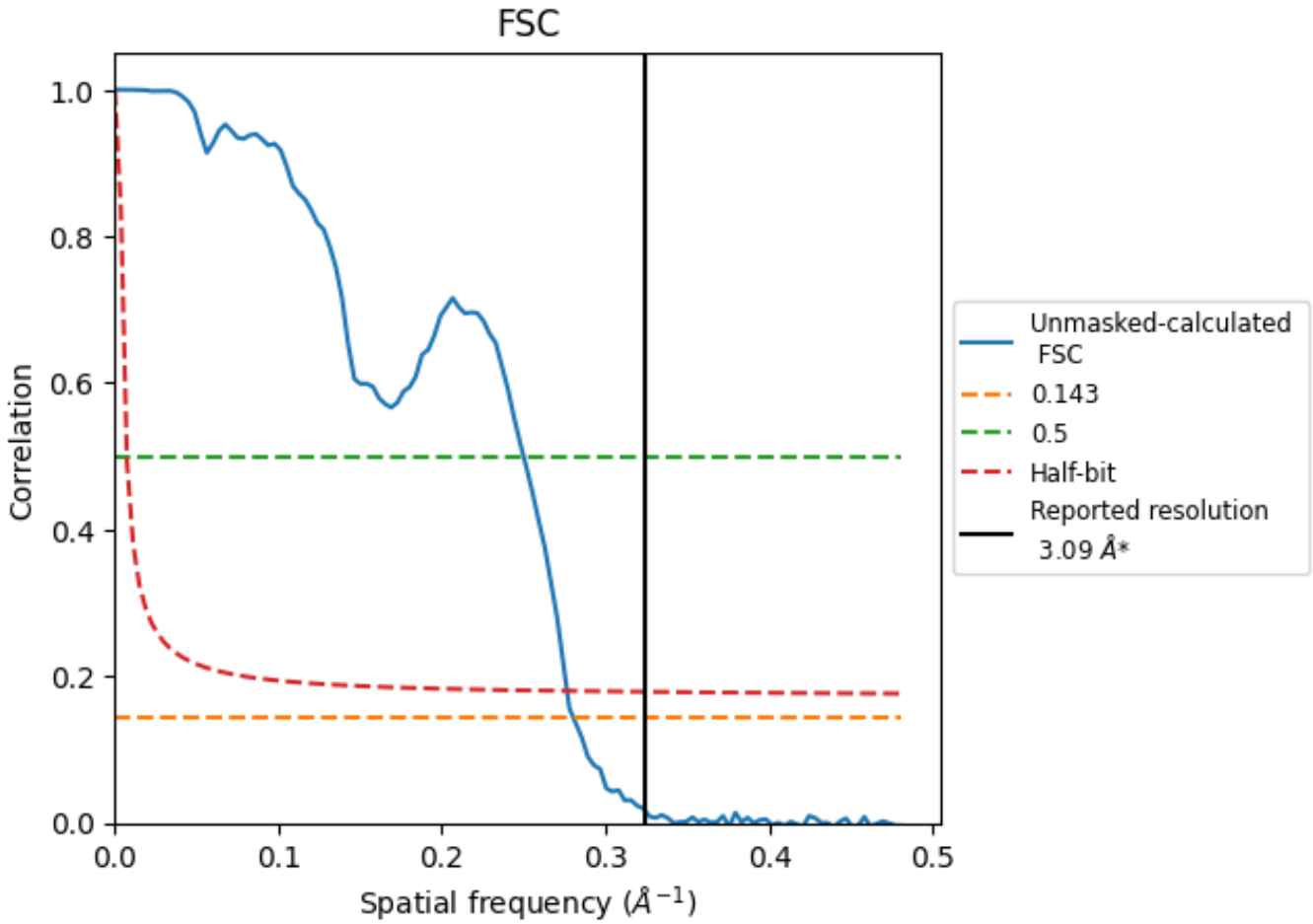


*Reported resolution corresponds to spatial frequency of 0.324 $Å^{-1}$

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 0.324 Å^{-1}

8.2 Resolution estimates (i)

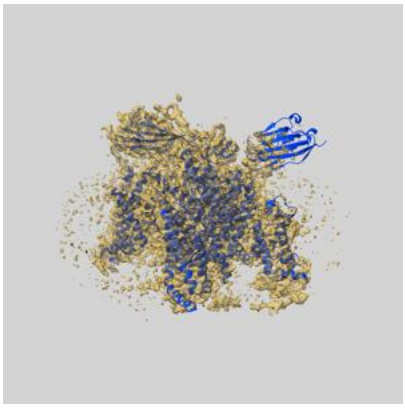
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.09	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.57	4.00	3.62

*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 3.57 differs from the reported value 3.09 by more than 10 %

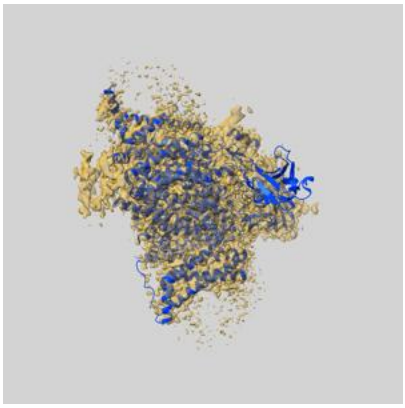
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-33296 and PDB model 7XMG. Per-residue inclusion information can be found in section 3 on page 7.

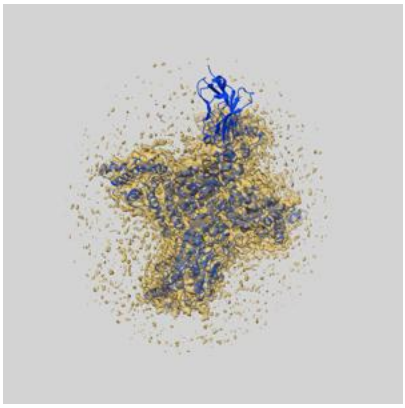
9.1 Map-model overlay



X



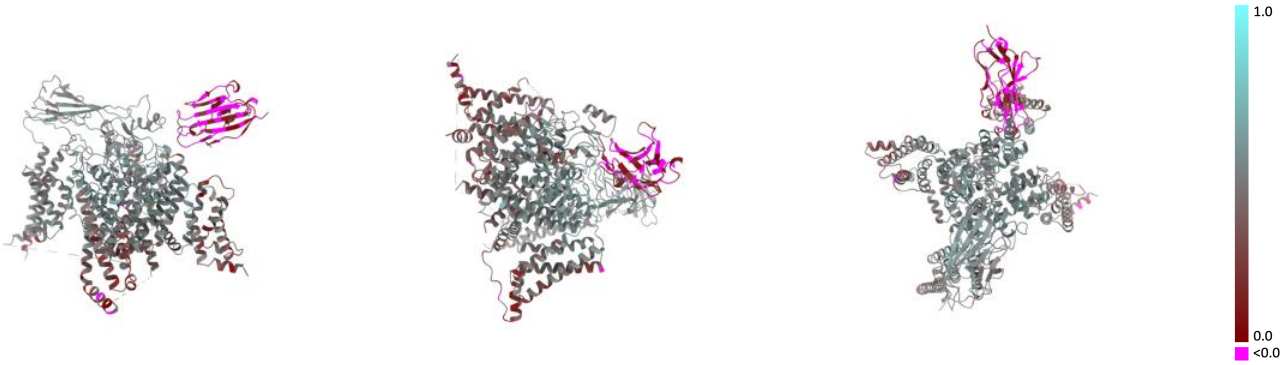
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.376 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.

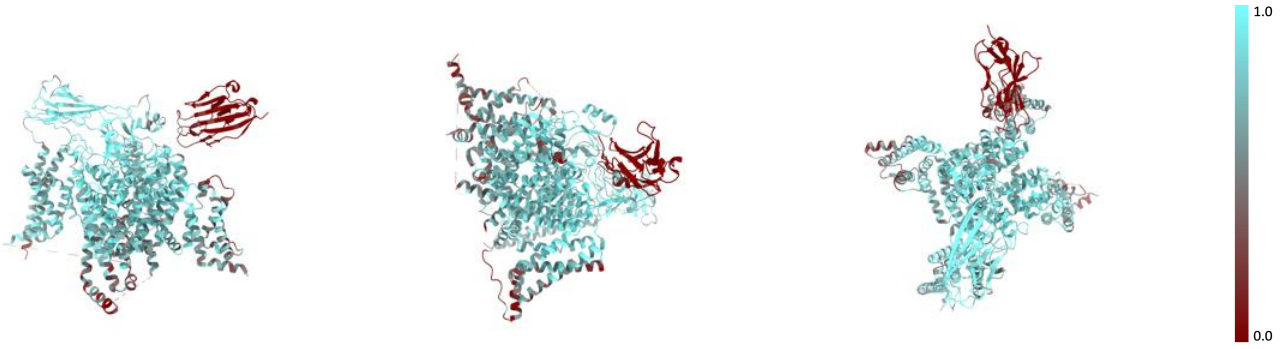
9.2 Q-score mapped to coordinate model (i)



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.

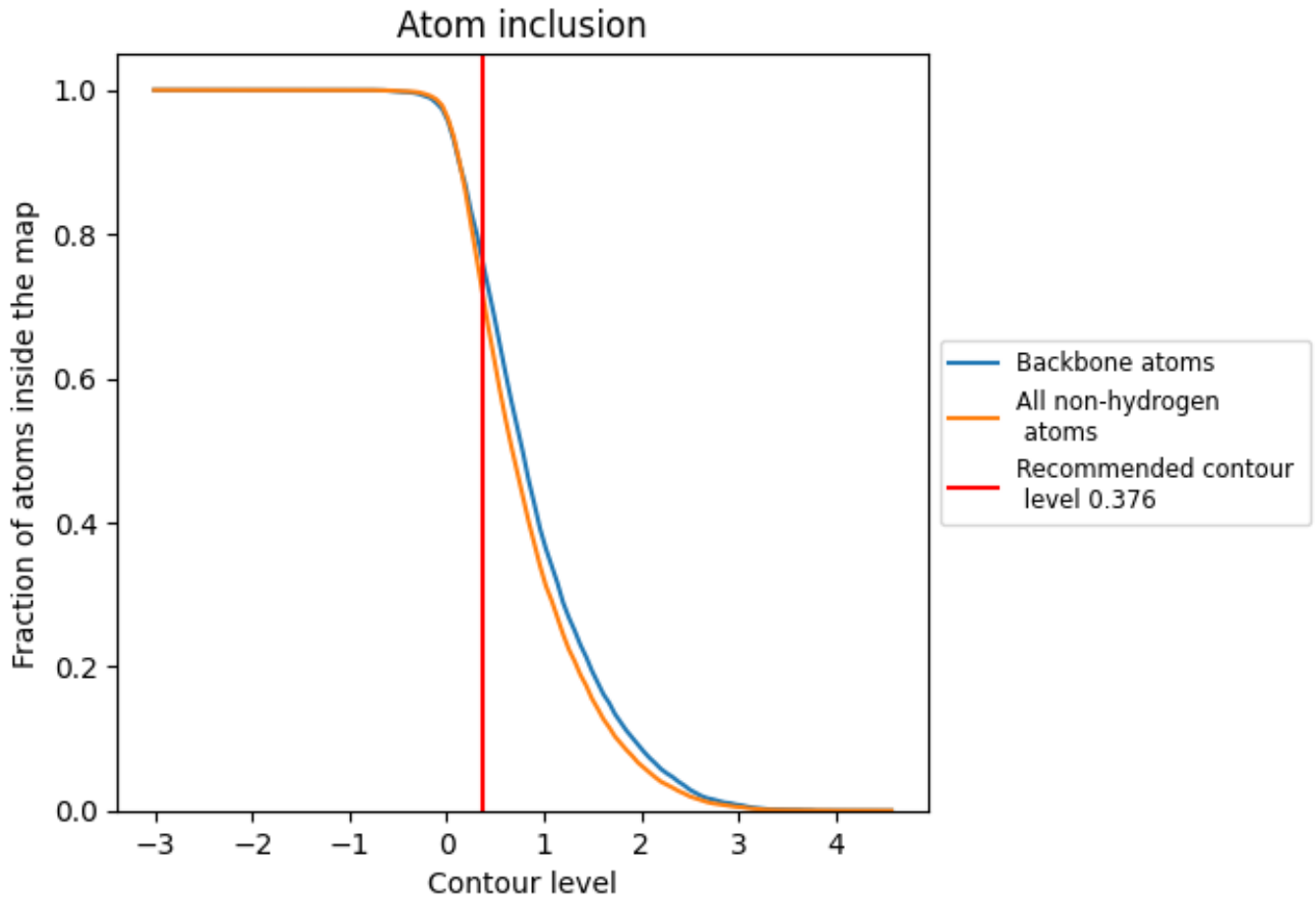
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.376).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 71% 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 (0.376) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7116	0.4360
A	0.7671	0.4700
B	0.7829	0.4800
D	0.7143	0.4230
E	0.6429	0.3950
F	0.0574	0.0350