wwPDB EM Validation Summary Report

Nov 22, 2022 – 12:27 AM JST

PDB ID	:	7DTD
EMDB ID	:	EMD-30851
Title	:	Voltage-gated sodium channel Nav1.1 and beta4
Authors	:	Yan, N.; Pan, X.; Li, Z.; Huang, G.
Deposited on	:	2021-01-04
Resolution	:	3.30 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 ⓘ 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:

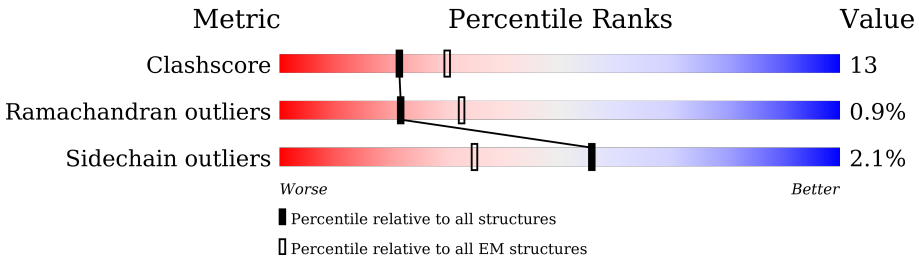
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

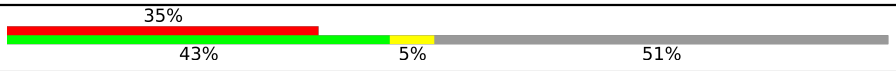
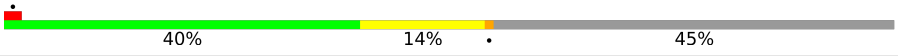
The reported resolution of this entry is 3.30 Å.

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	B	228	
2	A	2052	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10190 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 Sodium channel subunit beta-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	111	Total	C	N	O	S	5	0
			903	576	146	178	3		

- Molecule 2 is a protein called Sodium channel protein type 1 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	1138	Total	C	N	O	S	0	0
			9192	6097	1446	1574	75		

There are 43 discrepancies between the modelled and reference sequences:

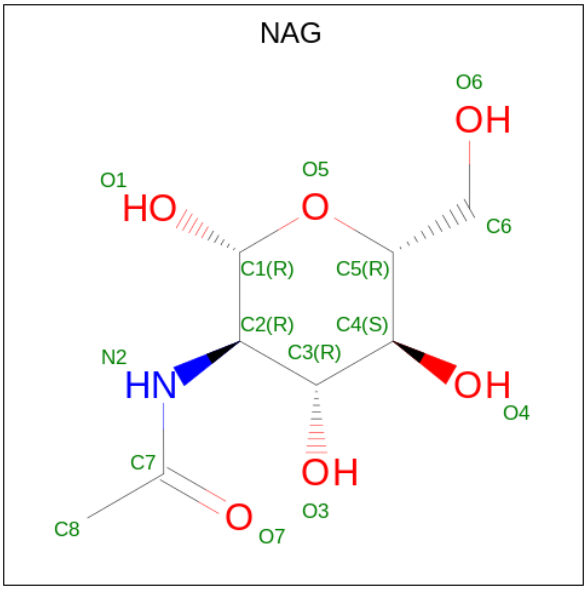
Chain	Residue	Modelled	Actual	Comment	Reference
A	-42	MET	-	initiating methionine	UNP P35498
A	-41	ALA	-	expression tag	UNP P35498
A	-40	SER	-	expression tag	UNP P35498
A	-39	TRP	-	expression tag	UNP P35498
A	-38	SER	-	expression tag	UNP P35498
A	-37	HIS	-	expression tag	UNP P35498
A	-36	PRO	-	expression tag	UNP P35498
A	-35	GLN	-	expression tag	UNP P35498
A	-34	PHE	-	expression tag	UNP P35498
A	-33	GLU	-	expression tag	UNP P35498
A	-32	LYS	-	expression tag	UNP P35498
A	-31	GLY	-	expression tag	UNP P35498
A	-30	GLY	-	expression tag	UNP P35498
A	-29	GLY	-	expression tag	UNP P35498
A	-28	ALA	-	expression tag	UNP P35498
A	-27	ARG	-	expression tag	UNP P35498
A	-26	GLY	-	expression tag	UNP P35498
A	-25	GLY	-	expression tag	UNP P35498
A	-24	SER	-	expression tag	UNP P35498
A	-23	GLY	-	expression tag	UNP P35498
A	-22	GLY	-	expression tag	UNP P35498

Continued on next page...

Continued from previous page...

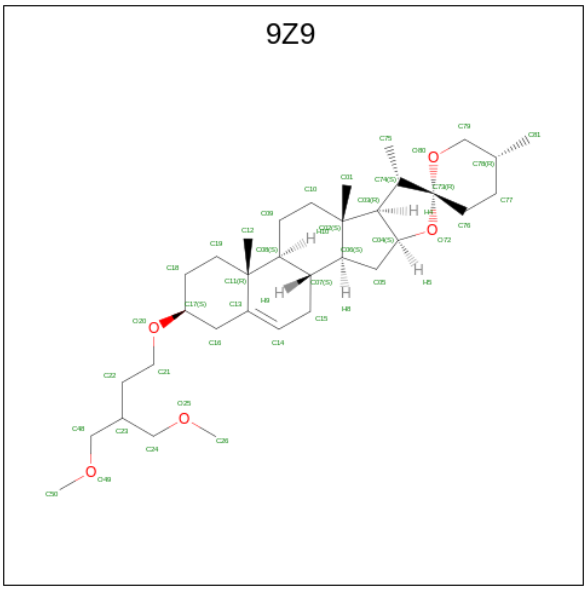
Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	GLY	-	expression tag	UNP P35498
A	-20	SER	-	expression tag	UNP P35498
A	-19	TRP	-	expression tag	UNP P35498
A	-18	SER	-	expression tag	UNP P35498
A	-17	HIS	-	expression tag	UNP P35498
A	-16	PRO	-	expression tag	UNP P35498
A	-15	GLN	-	expression tag	UNP P35498
A	-14	PHE	-	expression tag	UNP P35498
A	-13	GLU	-	expression tag	UNP P35498
A	-12	LYS	-	expression tag	UNP P35498
A	-11	GLY	-	expression tag	UNP P35498
A	-10	PHE	-	expression tag	UNP P35498
A	-9	ASP	-	expression tag	UNP P35498
A	-8	TYR	-	expression tag	UNP P35498
A	-7	LYS	-	expression tag	UNP P35498
A	-6	ASP	-	expression tag	UNP P35498
A	-5	ASP	-	expression tag	UNP P35498
A	-4	ASP	-	expression tag	UNP P35498
A	-3	ASP	-	expression tag	UNP P35498
A	-2	LYS	-	expression tag	UNP P35498
A	-1	GLY	-	expression tag	UNP P35498
A	0	THR	-	expression tag	UNP P35498

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			56	32	4	20	
3	A	1	Total	C	N	O	0
			56	32	4	20	
3	A	1	Total	C	N	O	0
			56	32	4	20	
3	A	1	Total	C	N	O	0
			56	32	4	20	

- Molecule 4 is (3beta,14beta,17beta,25R)-3-[4-methoxy-3-(methoxymethyl)butoxy]spirost-5-en (three-letter code: 9Z9) (formula: $C_{34}H_{56}O_5$).



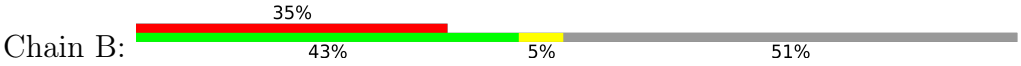
Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			39	34	5	

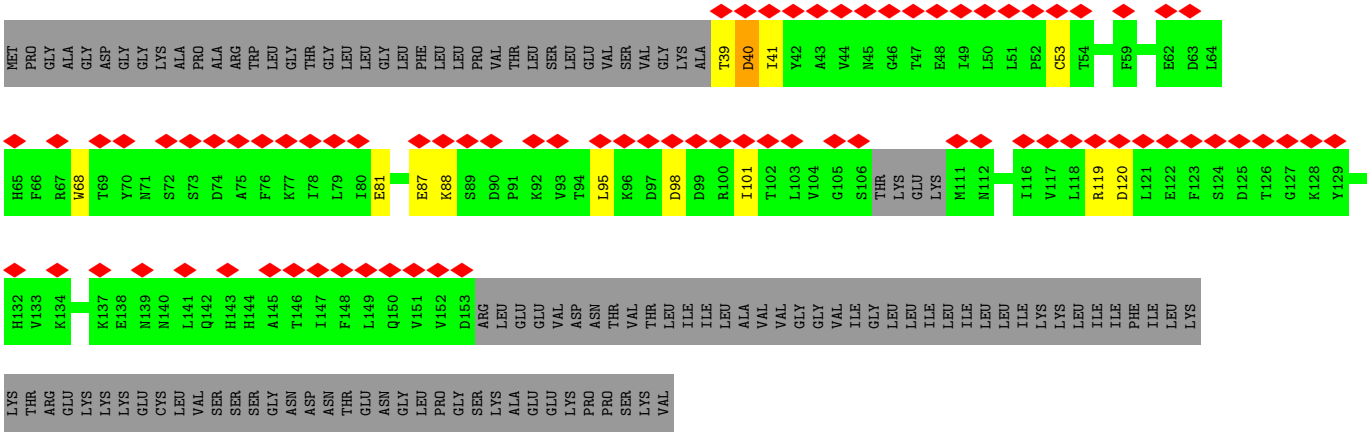
3 Residue-property plots (i)

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: Sodium channel subunit beta-4

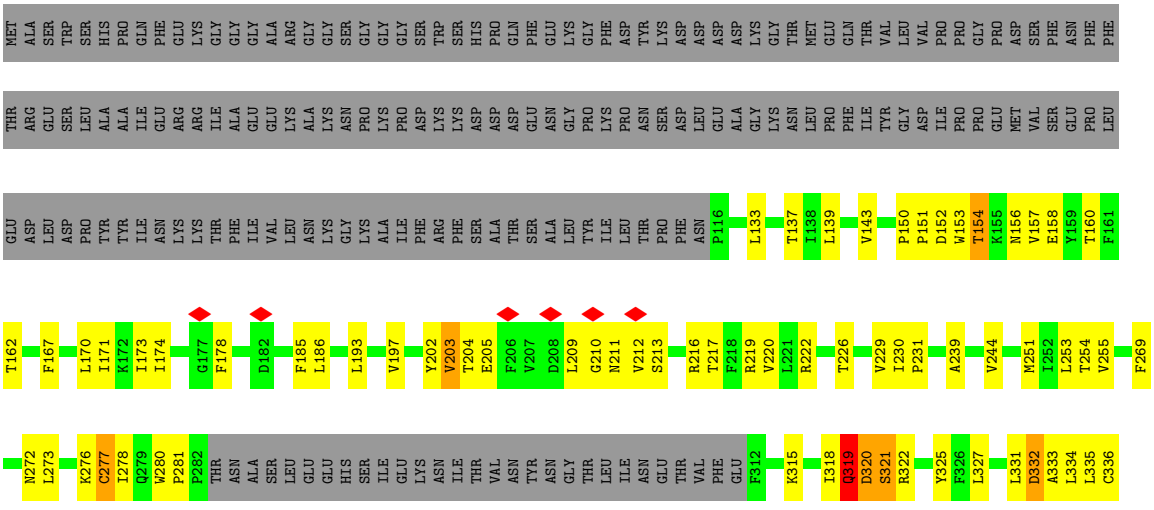
Chain B:

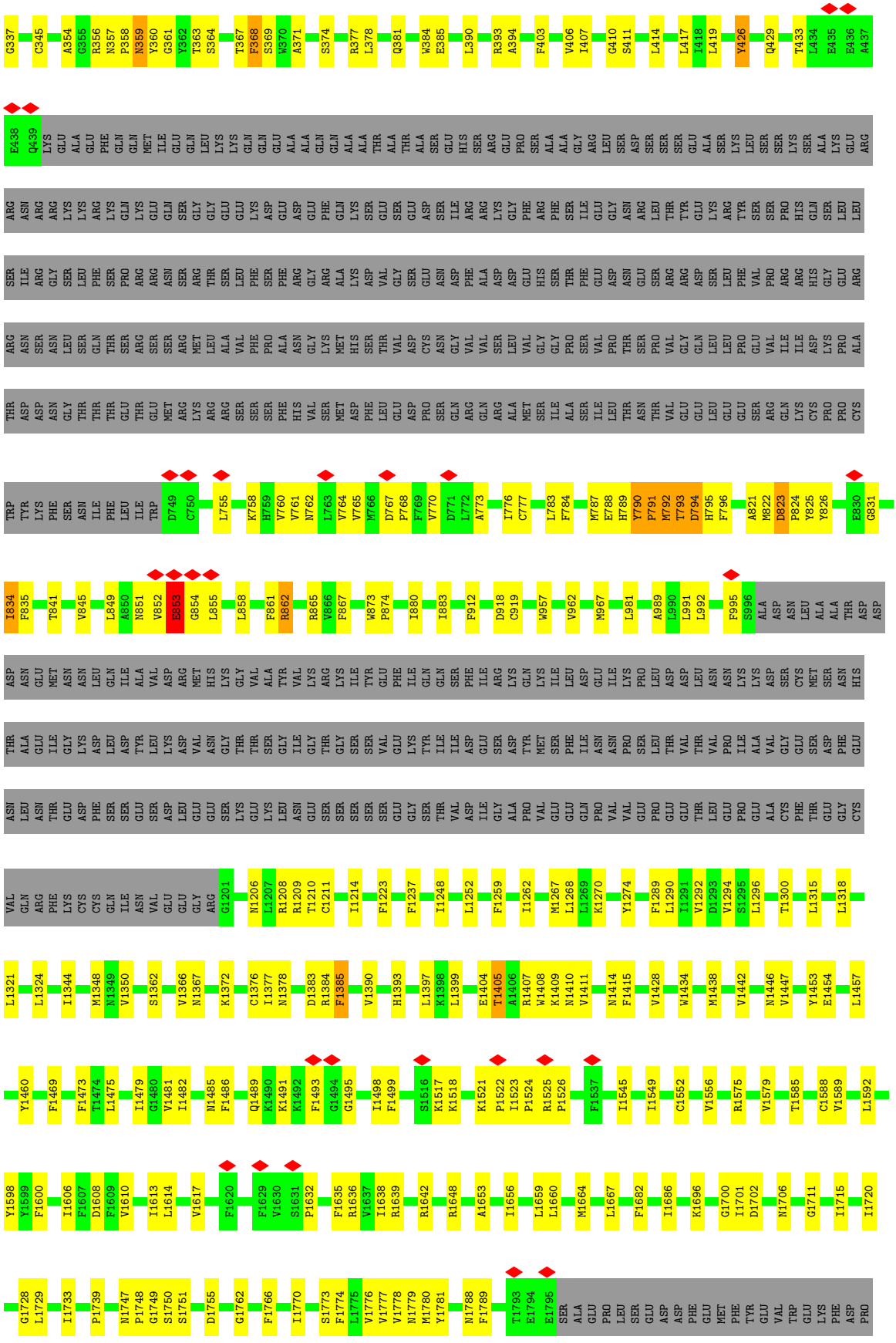


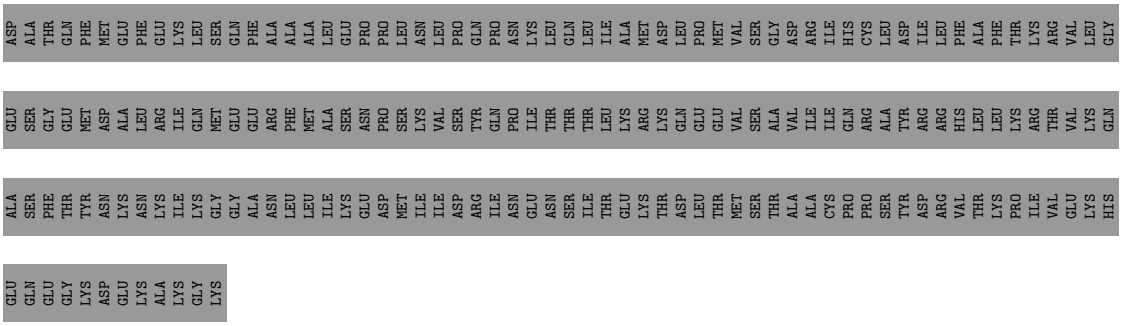


• Molecule 2: Sodium channel protein type 1 subunit alpha

Chain A:




G337 C345 A354 G355 R356 N357 P358 N359 Y360 G361 Y362 T363 S364 T367 F368 S369 W370 A371 S374 R377 L378 Q381 W384 E385 L390 R393 A394 F403 V406 I407 G410 S411 L414 L417 I418 L419 Y426 Q429 T433 L434 E435 E436 A437
E438 Q439 LYS GLU ALA GLU PHE GLN GLN MET ILE GLU GLN LEU LYS LYS GLN GLN GLU ALA ALA GLN GLN ALA ALA THR ALA THR ALA SER GLU HIS SER ARG GLU PRO SER ALA ALA GLY ARG LEU SER ASP SER SER GLU ALA SER LYS LEU SER SER SER LYS SER ALA LYS GLU ARG
ARG ASN ARG ARG LYS LYS ARG LYS GLN LYS GLU GLN SER GLY GLY GLU GLU LYS ASP GLU ASP GLU PHE GLN ALA LYS SER GLU SER GLU ASP SER ILE ARG ARG LYS GLY PHE ARG PHE SER ILE GLU GLY ASP GLU SER ARG LEU THR TYR GLU LYS ARG TYR SER SER PRO HIS GLN SER LEU LEU
SER ILE ARG GLY SER LEU PHE SER PRO ARG ARG ASN SER ARG THR SER LEU PHE SER PHE ARG GLY ALA LYS ASP GLU ASN ASP PHE ARG ASP GLU HIS SER THR PHE GLU ASP ASN GLU SER ARG ARG ASP SER LEU PHE VAL PRO ARG ARG HIS GLY GLU ARG
ARG ASN SER ASN LEU SER GLN THR SER ARG SER ARG MET LEU ALA VAL PHE PRO ALA ASN GLY LYS MET HIS SER THR VAL ASP CYS ASN GLY VAL VAL SER LEU VAL GLY GLY PRO SER VAL PRO THR SER PRO VAL GLY GLN LEU LEU LEU PRO GLU VAL PRO ARG ILE ILE ASP LYS PRO ALA
THR ASP ASP ASN GLY THR THR THR GLU THR GLU MET ARG LYS ARG ARG SER SER SER PHE HIS VAL SER MET ASP PHE LEU GLU ASP PRO SER GLN ARG GLN ARG ARG ALA MET SER ILE ALA SER ILE LEU LEU THR ASN THR VAL GLU GLU LEU LEU GLU GLU SER ARG GLN LYS CYS PRO PRO CYS
TRP TYR LYS PHE SER ASN ILE PHE LEU ILE TRP D749 C750 L755 K758 H759 V760 V761 N762 L763 V764 V765 W766 D767 P768 F769 V770 D771 L772 A773 I776 C777 L783 F784 M787 E788 H789 Y790 P791 M792 T793 D794 H795 F796 A821 M822 D823 P824 Y825 Y826 E830 G831
I834 F835 T841 V845 L849 A850 N851 V852 E853 G854 L855 L858 F861 R862 R865 V866 F867 W873 P874 I880 I883 F912 D918 C919 W957 V962 M967 L981 A989 L990 L991 L992 F995 S996 ALA ASP ASN LEU ALA ALA THR ASP ASP
ASP ASN GLU MET ASN ASN LEU GLN ILE ALA VAL ASP ARG MET HIS LYS GLY VAL ALA TYR VAL LYS ARG LYS ILE TYR GLU PHE ILE GLN GLN SER PHE ILE ARG LYS GLN LYS ILE LEU ASP GLU ILE LYS PRO LEU ASP ASP LEU ASN ASN LYS LYS ASP SER CYS MET SER ASN HIS
THR ALA GLU ILE GLY LYS ASP LEU ASP TYR LEU LEU LYS ASP VAL ASN GLY THR THR SER GLY ILE GLY THR GLY SER SER VAL GLU LYS TYR ILE ILE ASP GLU SER ASP TYR MET SER PHE ILE ASN ASN PRO SER LEU THR VAL THR VAL PRO ILE ALA VAL GLY GLU SER ASP PHE GLU
ASN LEU ASN THR GLU ASP PHE SER SER GLU SER LYS GLU LYS LEU ASN GLU SER SER SER SER GLU GLY SER THR SER VAL GLU ILE ASP PRO VAL GLU GLU GLN PRO VAL GLU PRO GLU THR LEU GLU GLU PRO GLU ALA CYS PHE THR GLU GLY CYS
VAL GLN ARG PHE LYS CYS CYS GLN ILE ASN VAL GLU GLU GLY ARG G1201 N1206 L1207 R1208 R1209 T1210 C1211 I1214 F1223 F1237 I1248 L1252 F1259 I1262 M1267 L1268 L1269 K1270 Y1274 F1289 L1290 I1291 V1292 D1293 V1294 S1295 L1296 T1300 L1315 L1318
L1321 L1324 I1344 M1348 N1349 V1350 S1362 V1366 N1367 K1372 C1376 I1377 N1378 D1383 R1384 F1385 V1390 H1393 L1397 K1398 L1399 E1404 T1405 A1406 R1407 W1408 K1409 N1410 V1411 N1414 F1415 V1428 W1434 M1438 V1442 N1446 V1447 Y1453 E1454 L1457
Y1460 F1469 F1473 T1474 L1475 I1479 G1480 V1481 I1482 N1485 F1486 Q1489 K1490 K1491 K1492 F1493 G1494 G1495 I1498 F1499 S1516 K1517 K1518 K1521 P1522 I1523 P1524 R1525 P1526 F1537 I1545 I1549 C1552 V1556 R1575 V1579 T1585 C1588 V1589 L1592
Y1598 Y1599 F1600 I1606 F1607 D1608 F1609 V1610 I1613 L1614 V1617 F1620 F1629 V1630 S1631 P1632 F1635 R1636 V1637 I1638 R1639 R1642 R1648 A1653 I1656 L1659 L1660 M1664 L1667 F1682 I1686 K1696 G1700 I1701 D1702 N1706 G1711 I1715 I1720
G1728 L1729 I1733 P1739 N1747 P1748 G1749 S1750 S1751 D1755 G1762 F1766 I1770 S1773 F1774 L1775 V1776 V1777 V1778 N1779 M1780 Y1781 N1788 F1789 T1793 E1794 E1795 SER ALA GLU PRO LEU SER GLU ASP ASP PHE GLU MET PHE TYR GLU VAL TRP GLU LYS PHE ASP PRO


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

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	133127	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 ($e^-/Å^2$)	48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.162	Depositor
Minimum map value	-0.085	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.017	Depositor
Map size (Å)	219.58, 219.58, 219.58	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0979, 1.0979, 1.0979	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, 9Z9

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	B	0.36	0/935	0.57	0/1266
2	A	0.27	0/9421	0.44	0/12773
All	All	0.28	0/10356	0.45	0/14039

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	B	903	0	881	7	0
2	A	9192	0	9339	260	0
3	A	56	0	52	3	0
4	A	39	0	0	4	0
All	All	10190	0	10272	267	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 13.

The worst 5 of 267 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)
2:A:318:ILE:O	2:A:319:GLN:HG2	1.16	1.26
2:A:1376:CYS:SG	2:A:1408:TRP:CE3	2.45	1.09
2:A:419:LEU:HD23	4:A:2105:9Z9:C01	1.84	1.06
2:A:417:LEU:HD23	2:A:1788:ASN:HD21	1.18	1.05
2:A:1385:PHE:HZ	3:A:2103:NAG:H82	1.22	1.04

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	B	112/228 (49%)	110 (98%)	2 (2%)	0	100	100
2	A	1130/2052 (55%)	1025 (91%)	94 (8%)	11 (1%)	15	46
All	All	1242/2280 (54%)	1135 (91%)	96 (8%)	11 (1%)	21	48

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	368	PHE
2	A	791	PRO
2	A	359	ASN
2	A	794	ASP
2	A	319	GLN

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	B	106/200 (53%)	104 (98%)	2 (2%)	57	77
2	A	1013/1824 (56%)	992 (98%)	21 (2%)	53	75
All	All	1119/2024 (55%)	1096 (98%)	23 (2%)	56	75

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	793	THR
2	A	862	ARG
2	A	853	GLU
2	A	918	ASP
2	A	277	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	1496	GLN
2	A	1788	ASN
2	A	789	HIS
2	A	933	HIS
2	A	980	ASN

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)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

5 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	$\#\|Z\| > 2$
3	NAG	A	2103	2	14,14,15	0.50	0	17,19,21	0.63	1 (5%)
3	NAG	A	2102	2	14,14,15	0.17	0	17,19,21	0.38	0
3	NAG	A	2104	2	14,14,15	0.24	0	17,19,21	0.42	0
4	9Z9	A	2105	-	44,44,44	0.63	2 (4%)	66,68,68	1.03	4 (6%)
3	NAG	A	2101	2	14,14,15	0.28	0	17,19,21	0.59	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	2103	2	-	4/6/23/26	0/1/1/1
3	NAG	A	2102	2	-	2/6/23/26	0/1/1/1
3	NAG	A	2104	2	-	2/6/23/26	0/1/1/1
4	9Z9	A	2105	-	-	8/12/100/100	0/6/6/6
3	NAG	A	2101	2	-	3/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2105	9Z9	O80-C79	-2.04	1.40	1.43
4	A	2105	9Z9	O72-C04	-2.02	1.39	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	2105	9Z9	O80-C73-C76	4.59	115.04	110.77
4	A	2105	9Z9	C77-C78-C79	3.09	112.85	108.56
4	A	2105	9Z9	C79-O80-C73	2.38	118.23	113.72
3	A	2103	NAG	C1-O5-C5	2.17	115.14	112.19
4	A	2105	9Z9	O80-C73-O72	-2.02	104.14	109.78

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2105	9Z9	C22-C21-O20-C17
4	A	2105	9Z9	C48-C23-C24-O25
4	A	2105	9Z9	C24-C23-C48-O49
3	A	2103	NAG	O5-C5-C6-O6
3	A	2104	NAG	O5-C5-C6-O6

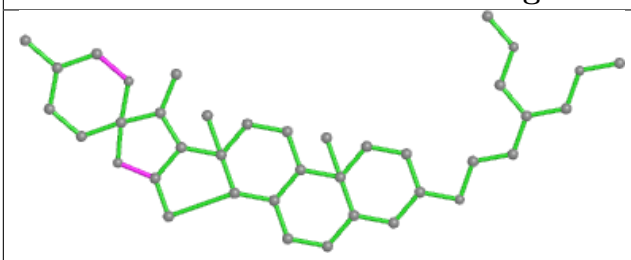
There are no ring outliers.

2 monomers are involved in 7 short contacts:

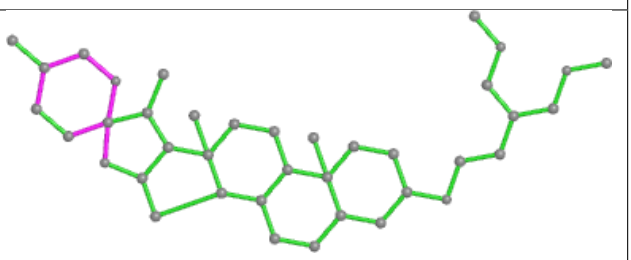
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2103	NAG	3	0
4	A	2105	9Z9	4	0

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.

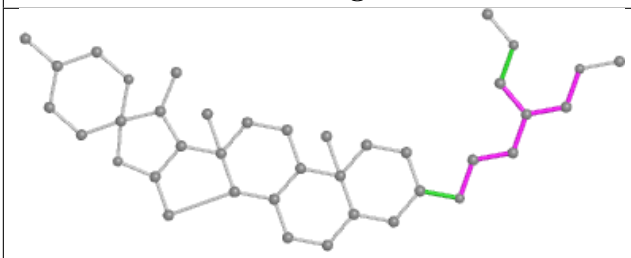
Ligand 9Z9 A 2105



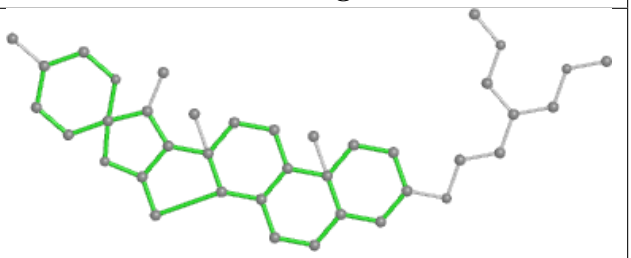
Bond lengths



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.

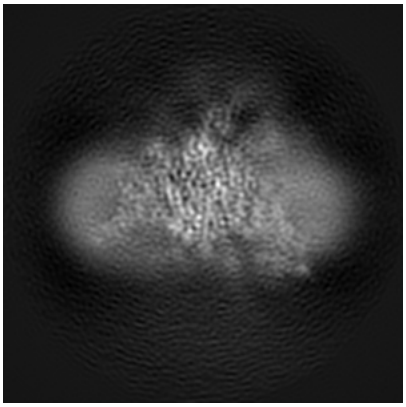
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-30851. 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.

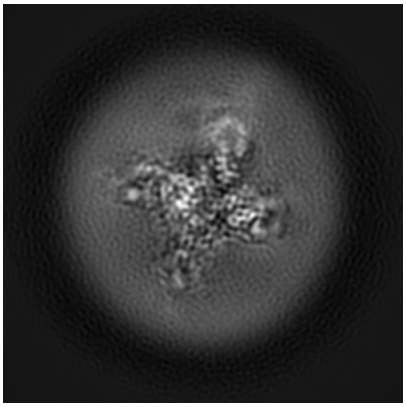
6.1 Orthogonal projections

6.1.1 Primary map



X

Y

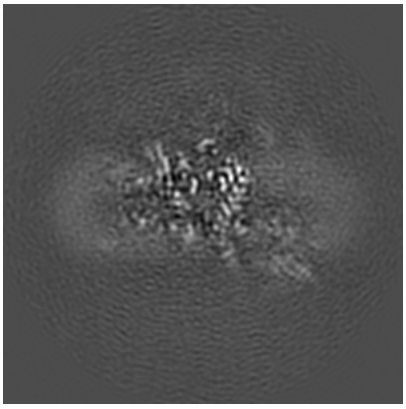


Z

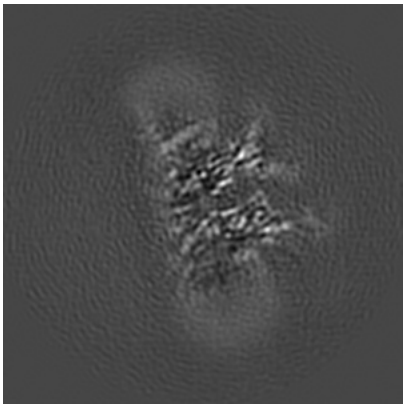
The images above show the map projected in three orthogonal directions.

6.2 Central slices

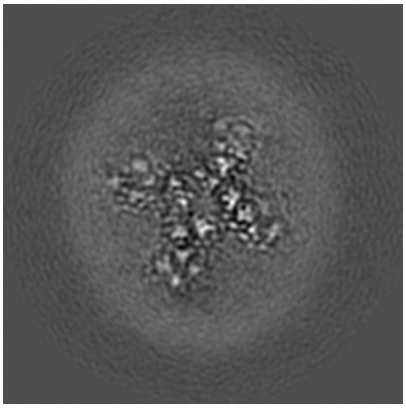
6.2.1 Primary map



X Index: 100



Y Index: 100

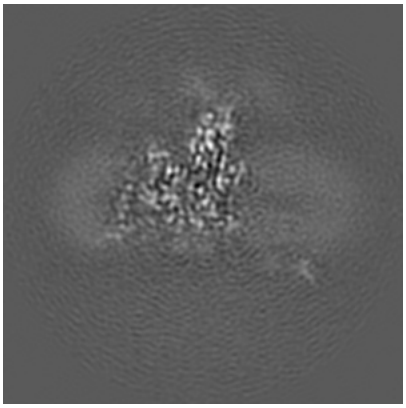


Z Index: 100

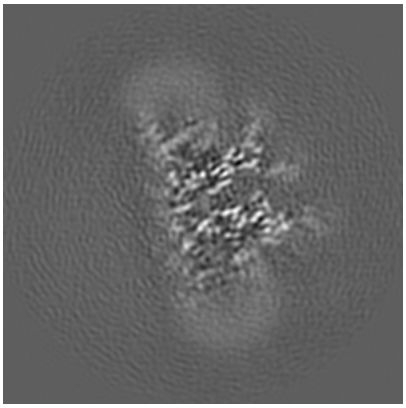
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

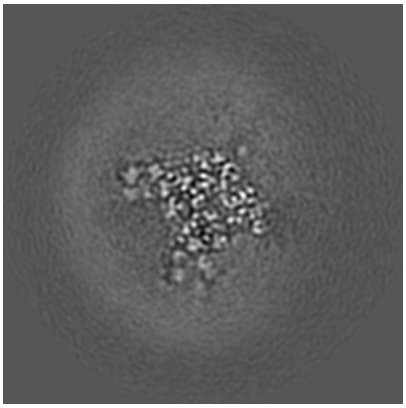
6.3.1 Primary map



X Index: 90



Y Index: 101



Z Index: 112

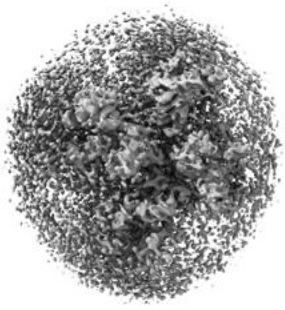
The images above show the largest variance slices of the map in three orthogonal directions.

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

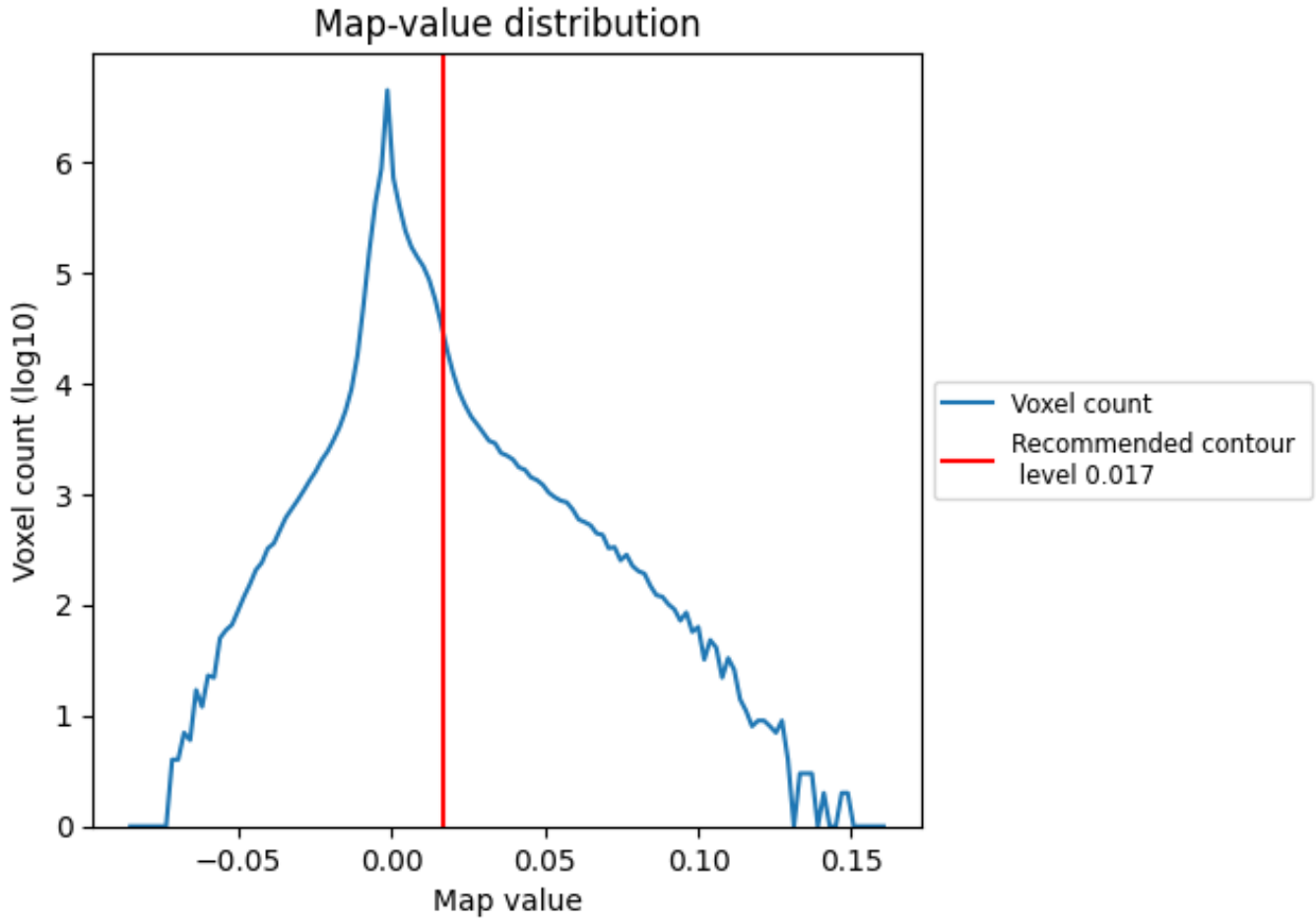
6.5 Mask visualisation (i)

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

7 Map analysis

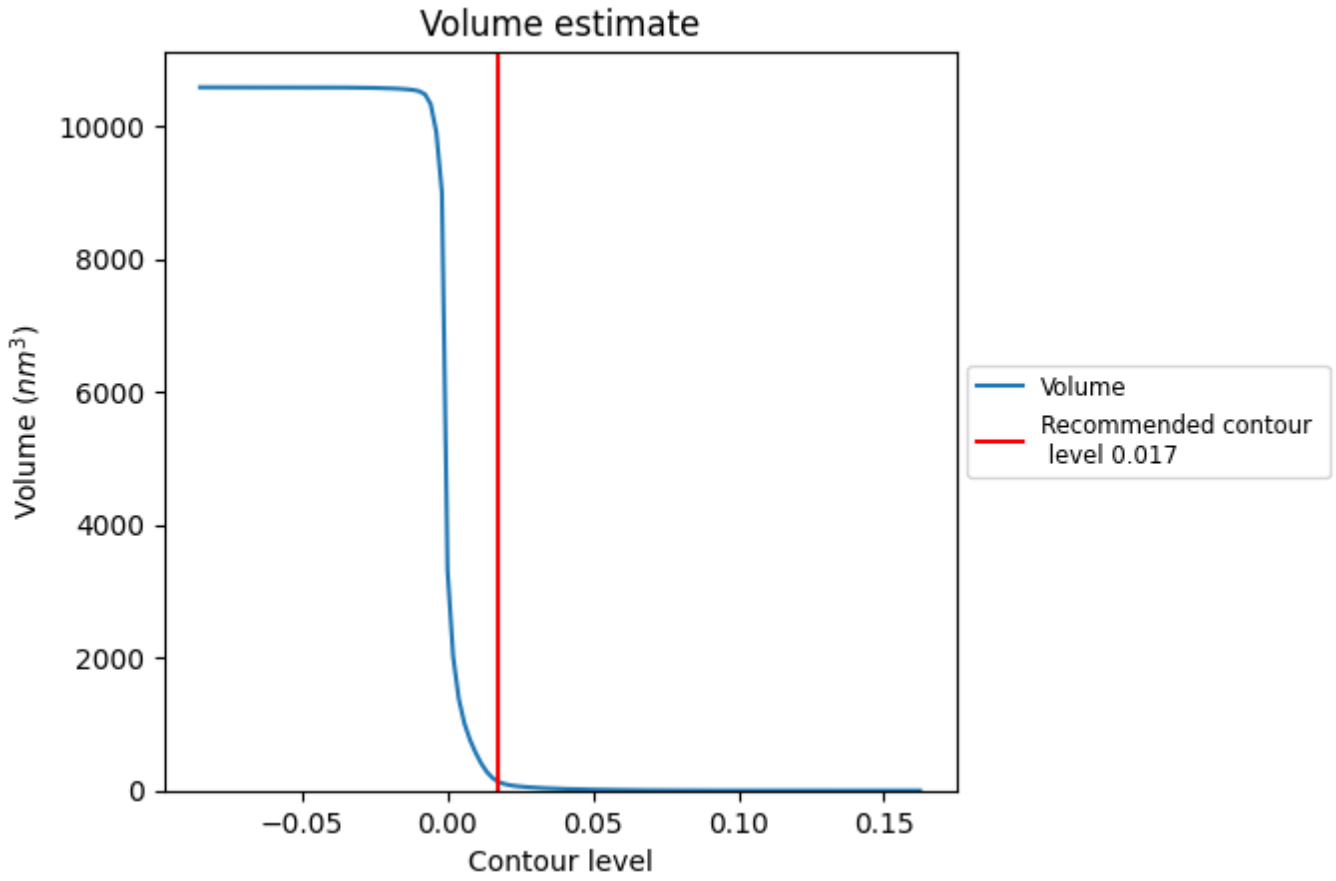
This section contains the results of statistical analysis of the map.

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.

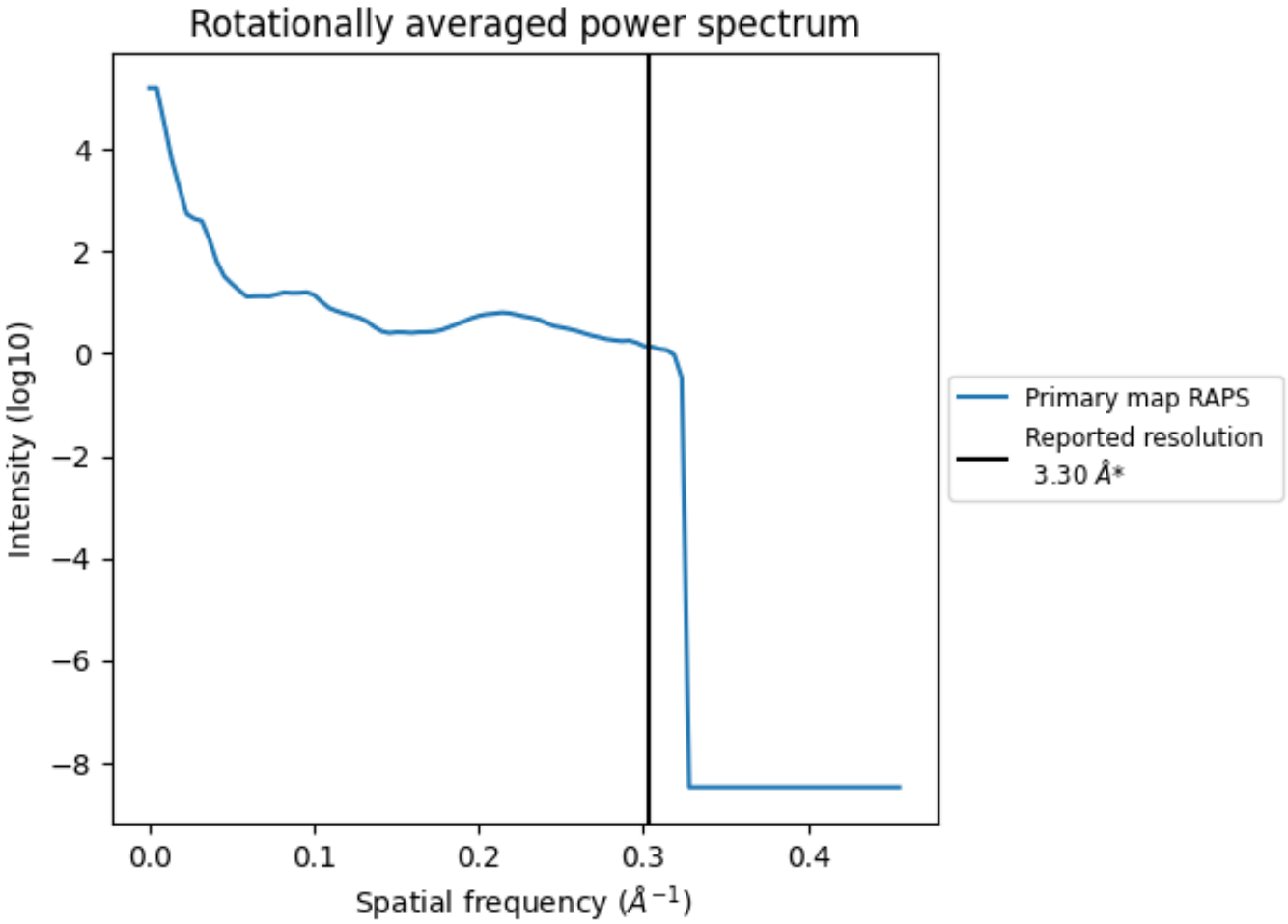
7.2 Volume estimate (i)



The volume at the recommended contour level is 143 nm^3; this corresponds to an approximate mass of 129 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}

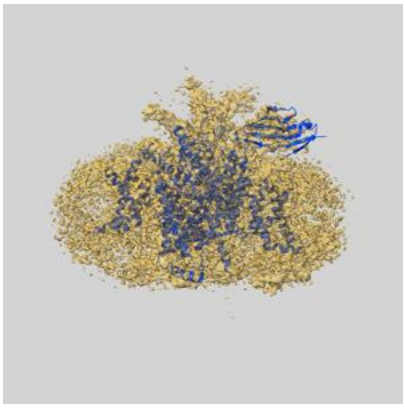
8 Fourier-Shell correlation

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

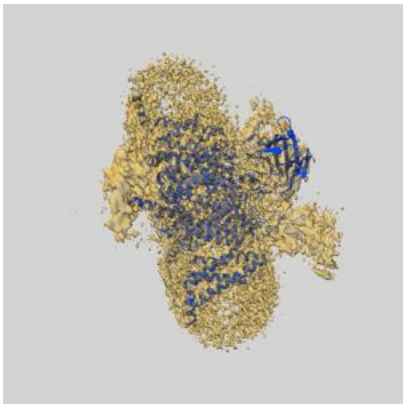
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-30851 and PDB model 7DTD. Per-residue inclusion information can be found in section 3 on page 6.

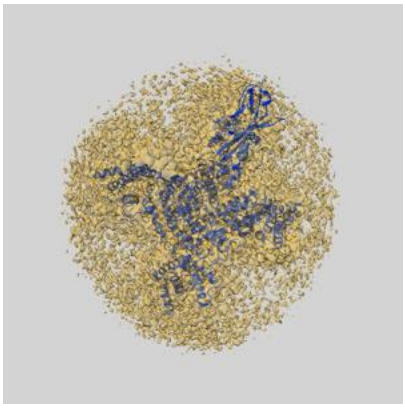
9.1 Map-model overlay



X



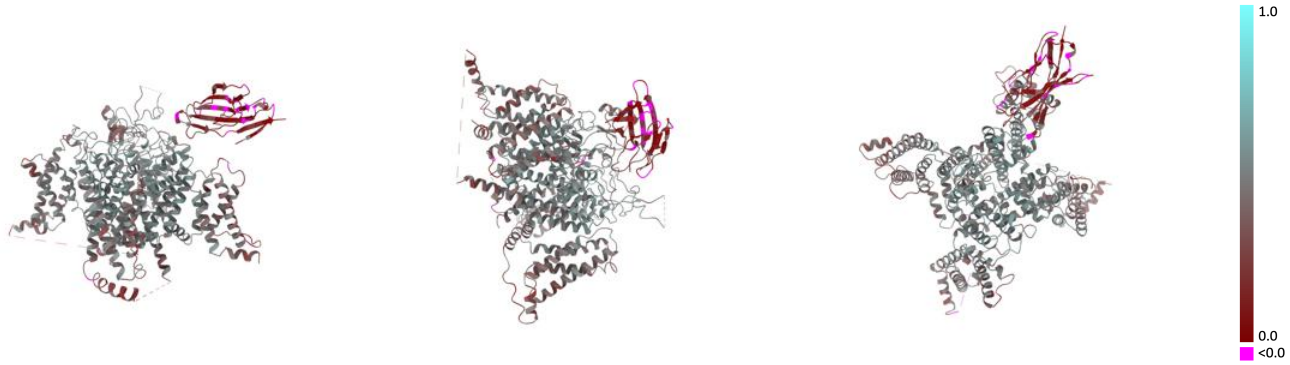
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.017 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.

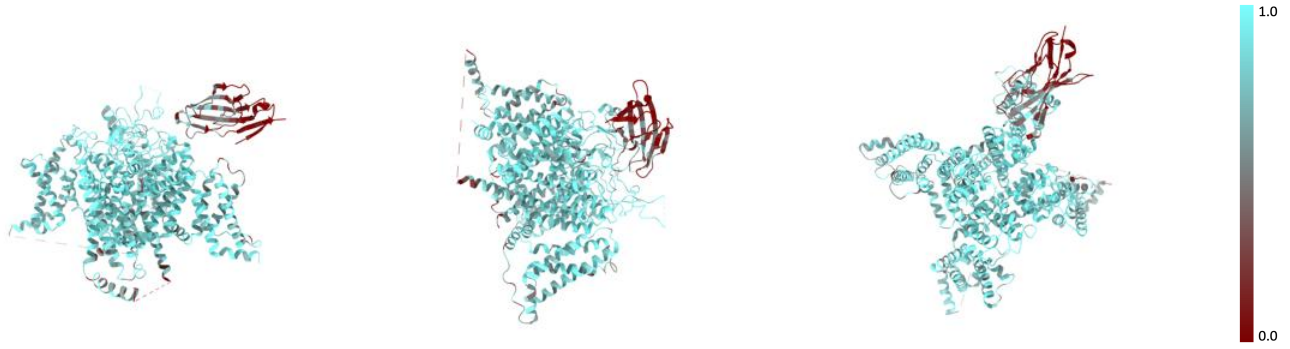
9.2 Q-score mapped to coordinate model (i)



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.

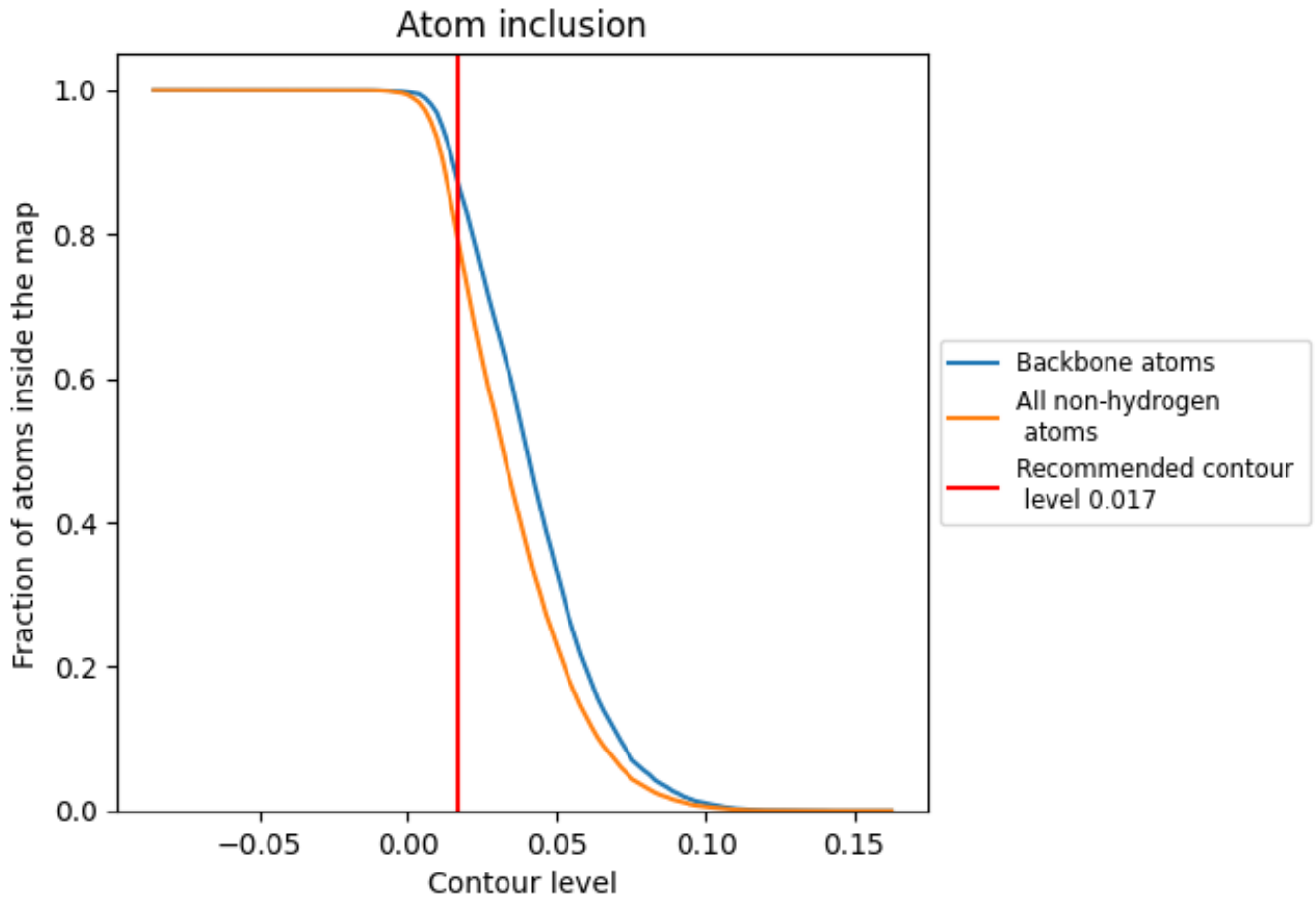
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.017).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 79% 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 (0.017) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7903	0.4280
A	0.8410	0.4560
B	0.2583	0.1370