



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 03:09 PM UTC

PDB ID : 9JK5 / pdb_00009jk5
EMDB ID : EMD-61544
Title : putative MgE1-ATP-H of TMEM94
Authors : Gong, D.S.
Deposited on : 2024-09-15
Resolution : 2.92 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

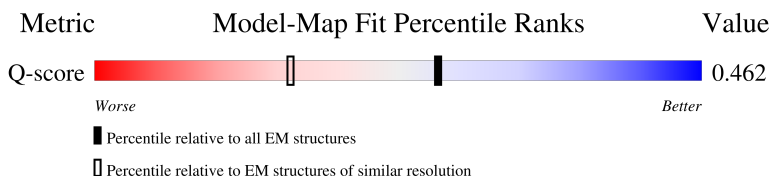
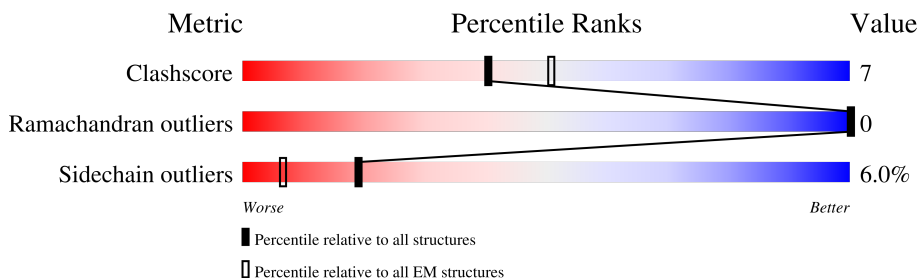
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.92 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13007 (2.42 - 3.42)

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 $\leq 5\%$. 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	1394	16% 59% 16% • 25%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8359 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 Endoplasmic reticulum magnesium-transporting P-type ATPase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1052	8279	5325	1421	1469	64	0	0

There are 38 discrepancies between the modelled and reference sequences:

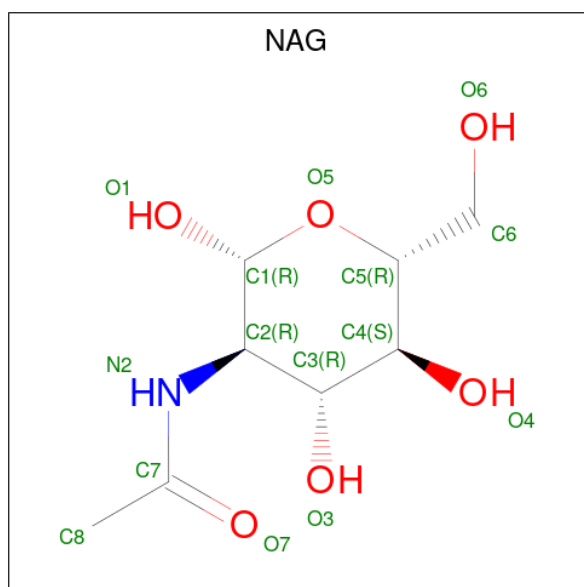
Chain	Residue	Modelled	Actual	Comment	Reference
A	1357	LEU	-	expression tag	UNP Q12767
A	1358	GLU	-	expression tag	UNP Q12767
A	1359	GLY	-	expression tag	UNP Q12767
A	1360	SER	-	expression tag	UNP Q12767
A	1361	ASP	-	expression tag	UNP Q12767
A	1362	GLU	-	expression tag	UNP Q12767
A	1363	VAL	-	expression tag	UNP Q12767
A	1364	ASP	-	expression tag	UNP Q12767
A	1365	ALA	-	expression tag	UNP Q12767
A	1366	GLY	-	expression tag	UNP Q12767
A	1367	SER	-	expression tag	UNP Q12767
A	1368	HIS	-	expression tag	UNP Q12767
A	1369	HIS	-	expression tag	UNP Q12767
A	1370	HIS	-	expression tag	UNP Q12767
A	1371	HIS	-	expression tag	UNP Q12767
A	1372	HIS	-	expression tag	UNP Q12767
A	1373	HIS	-	expression tag	UNP Q12767
A	1374	HIS	-	expression tag	UNP Q12767
A	1375	HIS	-	expression tag	UNP Q12767
A	1376	HIS	-	expression tag	UNP Q12767
A	1377	HIS	-	expression tag	UNP Q12767
A	1378	GLY	-	expression tag	UNP Q12767
A	1379	SER	-	expression tag	UNP Q12767
A	1380	VAL	-	expression tag	UNP Q12767
A	1381	GLU	-	expression tag	UNP Q12767
A	1382	ASP	-	expression tag	UNP Q12767
A	1383	TYR	-	expression tag	UNP Q12767

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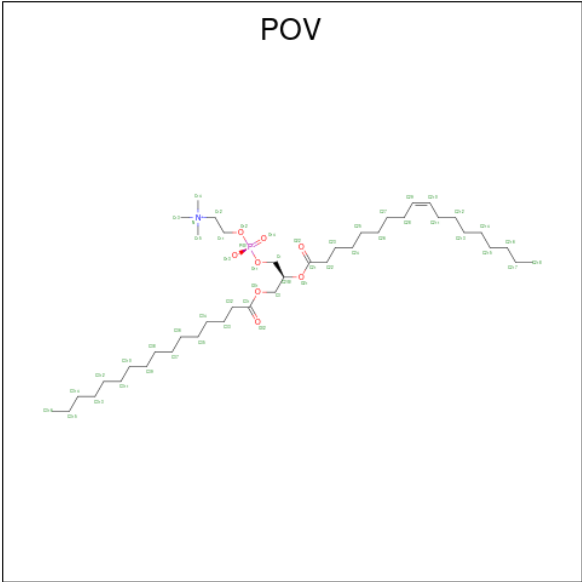
Chain	Residue	Modelled	Actual	Comment	Reference
A	1384	LYS	-	expression tag	UNP Q12767
A	1385	ASP	-	expression tag	UNP Q12767
A	1386	ASP	-	expression tag	UNP Q12767
A	1387	ASP	-	expression tag	UNP Q12767
A	1388	ASP	-	expression tag	UNP Q12767
A	1389	LYS	-	expression tag	UNP Q12767
A	1390	VAL	-	expression tag	UNP Q12767
A	1391	ILE	-	expression tag	UNP Q12767
A	1392	ALA	-	expression tag	UNP Q12767
A	1393	GLU	-	expression tag	UNP Q12767
A	1394	PRO	-	expression tag	UNP Q12767

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: $C_{42}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	

F851	F852	E859	L860	K863	K868	M869	G870	L871	W875	N876	S880	L881	T882	P883	ASN	GLY	ASP	MET	PRO	GLY	SER	ILE	PRO	PRO	SER	PRO	SER	HIS	ALA	GLY	SER	LEU	HIS	ASP	ASP	LEU	ASP	ASP	ALA	GLY	LEU	LEU	LEU	LEU	GLU	GLU			
GLU	GLY	HIS	SER	ASP	TYR	ALA	THR	ILE	SER	PHE	GLN	PRO	THR	ASP	SER	ASP	ILE	PRO	SER	PHE	LEU	GLU	ASP	ASN	ARG	ALA	LYS	L951	R959	P960	H961	L962	I965	D966	N967	L970	L971	V972	P973	T982	K988	Q991	N1005	S1015	L1021	S1027	ARG	CYS	TRP
I1137	S1138	H1145	S1146	M1149	S1150	M1151	A1152	L1170	L1173	S1181	L1184	I1185	S1193	R1199	S1213	L1230	K1234	S1248	L1258	W1259	R1260	L1267	W1268	W1269	T1272	V1273	V1281	V1282	Q1283	T1284	D1287	W1291	S1296	L1302	F1303	D1304	V1305	L1312											
L1319	V1322	T1323	N1324	Q1339	K1340	R1341	L1344	K1349	M1352	M1353	S1354	PRO	PHE	LEU	GLU	GLY	SER	ASP	GLU	VAL	ASP	ALA	GLY	SER	HIS	HIS	HIS	HIS	HIS	HIS	HIS	GLY	SER	VAL	GLU	ASP	TYR	LYS	ASP	ASP	ASP	ASP	LYS	VAL	ILE	ALA	GLU	PRO	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	318840	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.508	Depositor
Minimum map value	-1.600	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.043	Depositor
Recommended contour level	0.174	Depositor
Map size (Å)	298.8, 298.8, 298.8	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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: NAG, POV

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	0.14	0/8466	0.33	1/11504 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	213	PRO	CA-N-CD	-7.15	101.98	112.00

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	8279	0	8417	118	0
2	A	28	0	26	0	0
3	A	52	0	82	1	0
All	All	8359	0	8525	118	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 7.

All (118) 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:207:GLU:N	1:A:207:GLU:OE2	2.23	0.70
1:A:267:THR:O	1:A:271:ASN:ND2	2.23	0.69
1:A:830:GLN:OE1	1:A:831:TYR:N	2.28	0.67
1:A:318:GLN:N	1:A:318:GLN:OE1	2.28	0.67
1:A:313:THR:O	1:A:317:LEU:HB2	1.95	0.66
1:A:1151:MET:HE3	1:A:1339:GLN:HB3	1.78	0.64
1:A:832:GLN:OE1	1:A:868:LYS:NZ	2.30	0.64
1:A:192:PRO:HG2	1:A:607:ASP:HB3	1.79	0.64
1:A:1133:PRO:O	1:A:1137:ILE:HG12	1.99	0.63
1:A:710:LEU:O	1:A:730:ARG:NH1	2.33	0.61
1:A:161:PRO:O	1:A:1005:ASN:ND2	2.35	0.60
1:A:154:ASP:O	1:A:176:ASN:ND2	2.34	0.59
1:A:1083:ARG:NH1	1:A:1149:MET:SD	2.73	0.58
1:A:625:HIS:O	1:A:745:TYR:OH	2.20	0.58
1:A:1128:SER:O	1:A:1133:PRO:HD2	2.02	0.58
1:A:200:LEU:HB3	1:A:243:PHE:HB3	1.85	0.58
1:A:430:GLU:OE2	1:A:868:LYS:NZ	2.35	0.58
1:A:589:VAL:HG13	1:A:593:LEU:HD12	1.85	0.57
1:A:377:GLU:OE1	1:A:377:GLU:N	2.38	0.57
1:A:327:PRO:HG3	3:A:1403:POV:H21G	1.87	0.56
1:A:146:GLN:O	1:A:146:GLN:NE2	2.39	0.56
1:A:177:LEU:HD22	1:A:178:PRO:HD2	1.88	0.56
1:A:742:LEU:HB3	1:A:860:LEU:HD21	1.86	0.56
1:A:1283:GLN:NE2	1:A:1287:ASP:OD2	2.39	0.55
1:A:428:SER:HB3	1:A:832:GLN:HE21	1.72	0.55
1:A:1135:LEU:O	1:A:1138:SER:OG	2.21	0.55
1:A:348:GLN:OE1	1:A:1077:ARG:NH1	2.39	0.54
1:A:427:PRO:HD3	1:A:831:TYR:CE1	2.43	0.54
1:A:297:ALA:O	1:A:301:ILE:HG23	2.07	0.54
1:A:433:LEU:O	1:A:826:MET:N	2.40	0.53
1:A:113:ILE:HD11	1:A:331:PRO:HB3	1.90	0.53
1:A:430:GLU:HG3	1:A:832:GLN:HE22	1.73	0.53
1:A:876:ASN:ND2	1:A:1353:ASN:O	2.42	0.53
1:A:967:ASN:HB2	1:A:970:LEU:HD12	1.89	0.53
1:A:324:PRO:HG2	1:A:1104:VAL:HG22	1.92	0.53
1:A:418:LYS:HG2	1:A:419:GLN:N	2.24	0.52
1:A:1234:LYS:HD2	1:A:1284:THR:HG23	1.92	0.52
1:A:1319:LEU:O	1:A:1323:THR:HG23	2.07	0.52
1:A:280:MET:HE3	1:A:1097:LEU:HD11	1.92	0.52
1:A:1021:LEU:HD23	1:A:1067:PHE:HB2	1.91	0.52
1:A:653:LEU:HB3	1:A:687:SER:HB2	1.92	0.52
1:A:1181:SER:O	1:A:1185:ILE:HG13	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1341:ARG:HH11	1:A:1341:ARG:HG2	1.75	0.51
1:A:851:PHE:HD2	1:A:871:LEU:HD21	1.76	0.51
1:A:1352:MET:O	1:A:1352:MET:HG2	2.10	0.51
1:A:1134:LEU:HD23	1:A:1137:ILE:HD11	1.93	0.51
1:A:762:LEU:HD11	1:A:785:PRO:HD2	1.92	0.50
1:A:55:PHE:CE2	1:A:56:LEU:HG	2.47	0.50
1:A:267:THR:HG21	1:A:405:HIS:HB3	1.93	0.50
1:A:46:THR:O	1:A:50:VAL:HG23	2.11	0.49
1:A:875:TRP:CE3	1:A:876:ASN:HB3	2.48	0.48
1:A:1113:VAL:HG23	1:A:1115:LEU:HG	1.94	0.48
1:A:216:LEU:HD21	1:A:614:LEU:HD13	1.96	0.47
1:A:703:HIS:CE1	1:A:749:PHE:HD1	2.33	0.47
1:A:157:MET:HE3	1:A:157:MET:HB2	1.77	0.47
1:A:432:VAL:HG22	1:A:827:VAL:HG22	1.95	0.47
1:A:716:PHE:HB3	1:A:725:LEU:HD13	1.96	0.47
1:A:1268:TRP:O	1:A:1272:THR:HG23	2.15	0.47
1:A:141:ASP:OD1	1:A:141:ASP:N	2.45	0.47
1:A:427:PRO:HD3	1:A:831:TYR:HE1	1.80	0.47
1:A:1248:SER:OG	1:A:1269:TRP:NE1	2.44	0.46
1:A:613:ALA:O	1:A:617:SER:OG	2.32	0.46
1:A:859:GLU:O	1:A:863:LYS:HG2	2.15	0.46
1:A:1099:CYS:O	1:A:1102:THR:HG22	2.16	0.45
1:A:737:TYR:HB2	1:A:826:MET:HE1	1.98	0.45
1:A:743:SER:O	1:A:830:GLN:NE2	2.49	0.45
1:A:196:SER:OG	1:A:212:GLU:O	2.35	0.45
1:A:700:MET:HB3	1:A:754:MET:HE2	1.98	0.45
1:A:333:LEU:HD11	1:A:1133:PRO:HB3	1.97	0.45
1:A:961:HIS:ND1	1:A:965:ILE:HD12	2.32	0.45
1:A:848:CYS:HB3	1:A:1152:ALA:HB2	1.99	0.45
1:A:55:PHE:CD2	1:A:55:PHE:C	2.95	0.44
1:A:417:ASP:HB3	1:A:421:ILE:HG13	2.00	0.44
1:A:556:LEU:HD23	1:A:556:LEU:HA	1.84	0.44
1:A:310:TRP:CE2	1:A:311:GLN:HG2	2.52	0.44
1:A:595:ASP:O	1:A:599:THR:OG1	2.28	0.44
1:A:871:LEU:HD22	1:A:973:PRO:HB2	1.98	0.44
1:A:25:VAL:O	1:A:29:GLN:HG3	2.18	0.44
1:A:988:LYS:HE3	1:A:988:LYS:HB2	1.62	0.43
1:A:842:ASP:HA	1:A:845:VAL:HG12	2.00	0.43
1:A:39:ARG:HA	1:A:42:LYS:HG2	2.00	0.43
1:A:217:PHE:HE2	1:A:241:ARG:HG3	1.84	0.43
1:A:876:ASN:CG	1:A:876:ASN:O	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1118:LEU:HD23	1:A:1119:LEU:HG	2.00	0.43
1:A:655:LEU:O	1:A:685:MET:N	2.48	0.43
1:A:1260:ARG:HD3	1:A:1260:ARG:HA	1.64	0.43
1:A:91:SER:HB3	1:A:1291:TRP:HB3	2.00	0.43
1:A:991:GLN:NE2	1:A:1015:SER:HA	2.34	0.43
1:A:588:ASN:OD1	1:A:701:LEU:HB3	2.18	0.42
1:A:1193:SER:OG	1:A:1304:ASP:O	2.37	0.42
1:A:700:MET:HE2	1:A:700:MET:HB2	1.92	0.42
1:A:951:LEU:HD23	1:A:951:LEU:HA	1.87	0.42
1:A:432:VAL:HG12	1:A:434:PHE:HD1	1.84	0.42
1:A:657:ARG:HB2	1:A:769:LEU:HB2	2.02	0.42
1:A:691:LYS:HA	1:A:698:GLU:HA	2.01	0.42
1:A:962:LEU:HD23	1:A:967:ASN:HA	2.01	0.42
1:A:280:MET:CE	1:A:1097:LEU:HD11	2.49	0.42
1:A:967:ASN:O	1:A:971:LEU:HD13	2.20	0.42
1:A:762:LEU:HD22	1:A:767:ILE:HD11	2.02	0.42
1:A:869:MET:HE2	1:A:871:LEU:HD11	2.01	0.42
1:A:48:LYS:HD3	1:A:48:LYS:HA	1.81	0.41
1:A:67:TRP:CG	1:A:68:PRO:HD3	2.55	0.41
1:A:346:LEU:O	1:A:349:MET:HG3	2.20	0.41
1:A:613:ALA:HB2	1:A:682:LEU:HD22	2.01	0.41
1:A:251:ILE:HD13	1:A:251:ILE:HA	1.86	0.41
1:A:1269:TRP:O	1:A:1273:VAL:HG23	2.20	0.41
1:A:752:LYS:HB2	1:A:821:GLN:HA	2.01	0.41
1:A:147:TRP:CE3	1:A:1051:PRO:HG3	2.56	0.41
1:A:119:LEU:HD23	1:A:119:LEU:HA	1.85	0.41
1:A:1199:ARG:HH11	1:A:1199:ARG:HB3	1.86	0.41
1:A:125:GLU:O	1:A:129:ARG:HG3	2.21	0.41
1:A:691:LYS:HB2	1:A:698:GLU:HG2	2.03	0.41
1:A:1073:ILE:HD12	1:A:1073:ILE:HA	1.88	0.41
1:A:35:GLU:O	1:A:39:ARG:HG3	2.21	0.40
1:A:1151:MET:HE3	1:A:1339:GLN:OE1	2.21	0.40
1:A:598:VAL:O	1:A:602:LEU:HD23	2.22	0.40
1:A:436:SER:N	1:A:552:HIS:O	2.47	0.40
1:A:1173:LEU:HD23	1:A:1173:LEU:HA	1.91	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1034/1394 (74%)	992 (96%)	42 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	941/1242 (76%)	885 (94%)	56 (6%)	17	45

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	SER
1	A	24	SER
1	A	78	LEU
1	A	79	LEU
1	A	94	VAL
1	A	119	LEU
1	A	139	LEU
1	A	141	ASP
1	A	164	SER
1	A	166	HIS
1	A	177	LEU
1	A	179	VAL
1	A	188	ILE

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Mol	Chain	Res	Type
1	A	200	LEU
1	A	206	ASP
1	A	216	LEU
1	A	242	LEU
1	A	245	VAL
1	A	318	GLN
1	A	323	LEU
1	A	417	ASP
1	A	423	SER
1	A	428	SER
1	A	551	TYR
1	A	582	LEU
1	A	852	VAL
1	A	880	SER
1	A	881	LEU
1	A	959	ARG
1	A	972	VAL
1	A	982	THR
1	A	1057	GLN
1	A	1070	GLU
1	A	1072	THR
1	A	1092	CYS
1	A	1112	LEU
1	A	1122	THR
1	A	1145	HIS
1	A	1146	SER
1	A	1151	MET
1	A	1170	LEU
1	A	1184	LEU
1	A	1199	ARG
1	A	1213	SER
1	A	1230	LEU
1	A	1248	SER
1	A	1258	LEU
1	A	1267	LEU
1	A	1281	VAL
1	A	1296	SER
1	A	1302	LEU
1	A	1305	VAL
1	A	1312	LEU
1	A	1322	VAL
1	A	1324	ASN

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Mol	Chain	Res	Type
1	A	1344	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	277	GLN
1	A	419	GLN
1	A	426	ASN
1	A	611	ASN
1	A	1057	GLN
1	A	1227	ASN
1	A	1345	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	POV	A	1403	-	51,51,51	0.50	0	57,59,59	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	1401	1	14,14,15	0.91	1 (7%)	17,19,21	1.34	1 (5%)
2	NAG	A	1402	1	14,14,15	0.23	0	17,19,21	0.49	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	POV	A	1403	-	-	22/55/55/55	-
2	NAG	A	1401	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1402	1	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1401	NAG	O5-C1	3.30	1.49	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1401	NAG	C1-O5-C5	5.25	119.23	112.19

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1403	POV	C22-C21-O21-C2
3	A	1403	POV	O22-C21-O21-C2
2	A	1401	NAG	O5-C5-C6-O6
2	A	1401	NAG	C4-C5-C6-O6
2	A	1402	NAG	C8-C7-N2-C2
2	A	1402	NAG	O7-C7-N2-C2
3	A	1403	POV	C35-C36-C37-C38
3	A	1403	POV	C310-C311-C312-C313
3	A	1403	POV	C1-C2-C3-O31
3	A	1403	POV	C312-C313-C314-C315
3	A	1403	POV	C25-C26-C27-C28
3	A	1403	POV	C39-C310-C311-C312
3	A	1403	POV	O11-C1-C2-C3

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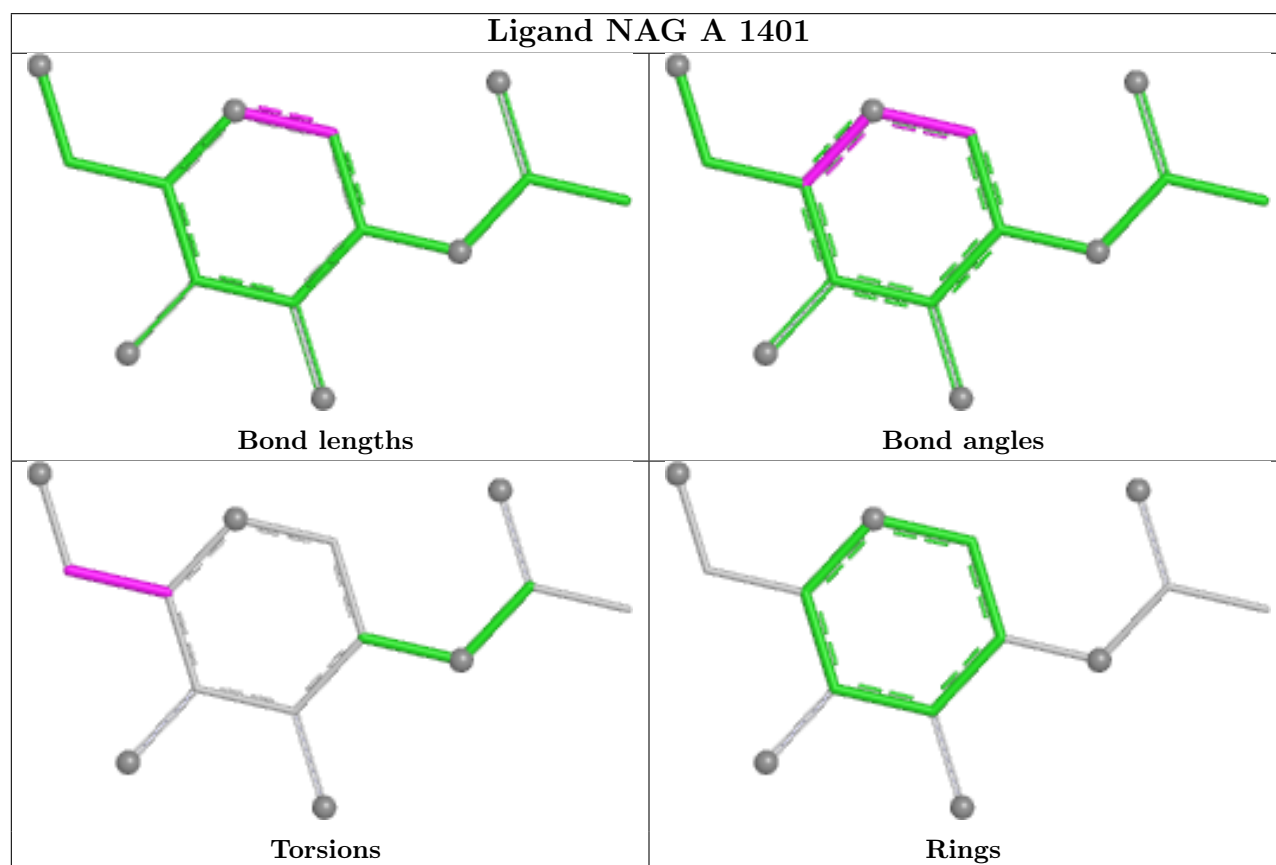
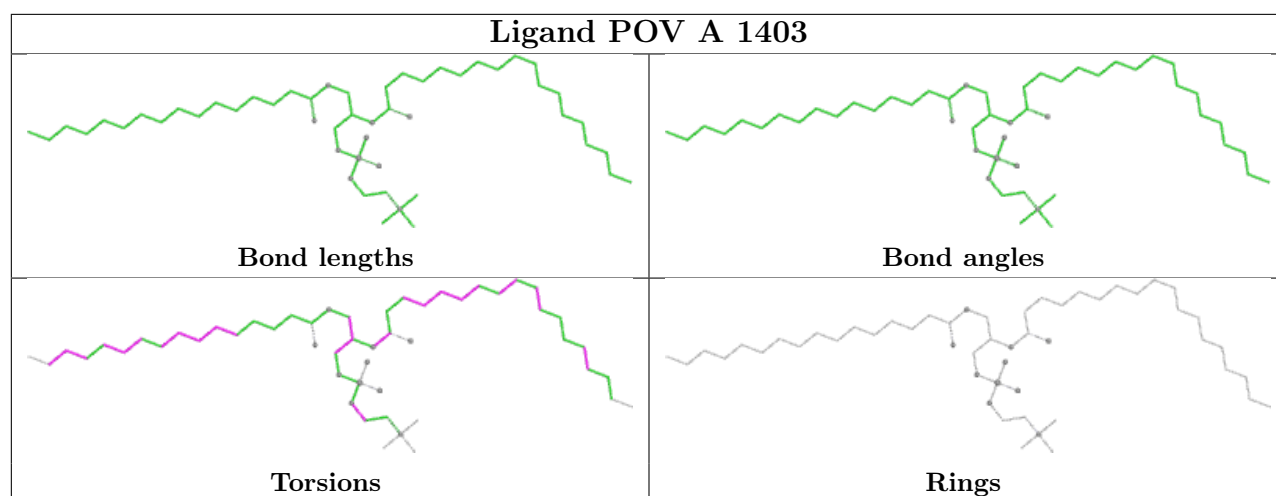
Mol	Chain	Res	Type	Atoms
3	A	1403	POV	C34-C35-C36-C37
3	A	1403	POV	O11-C1-C2-O21
3	A	1403	POV	C12-C11-O12-P
3	A	1403	POV	O21-C2-C3-O31
3	A	1403	POV	C23-C24-C25-C26
3	A	1403	POV	C213-C214-C215-C216
2	A	1402	NAG	C4-C5-C6-O6
3	A	1403	POV	C37-C38-C39-C310
3	A	1403	POV	C24-C25-C26-C27
3	A	1403	POV	C313-C314-C315-C316
3	A	1403	POV	C22-C23-C24-C25
3	A	1403	POV	C27-C28-C29-C210
3	A	1403	POV	C29-C210-C211-C212
3	A	1403	POV	C36-C37-C38-C39

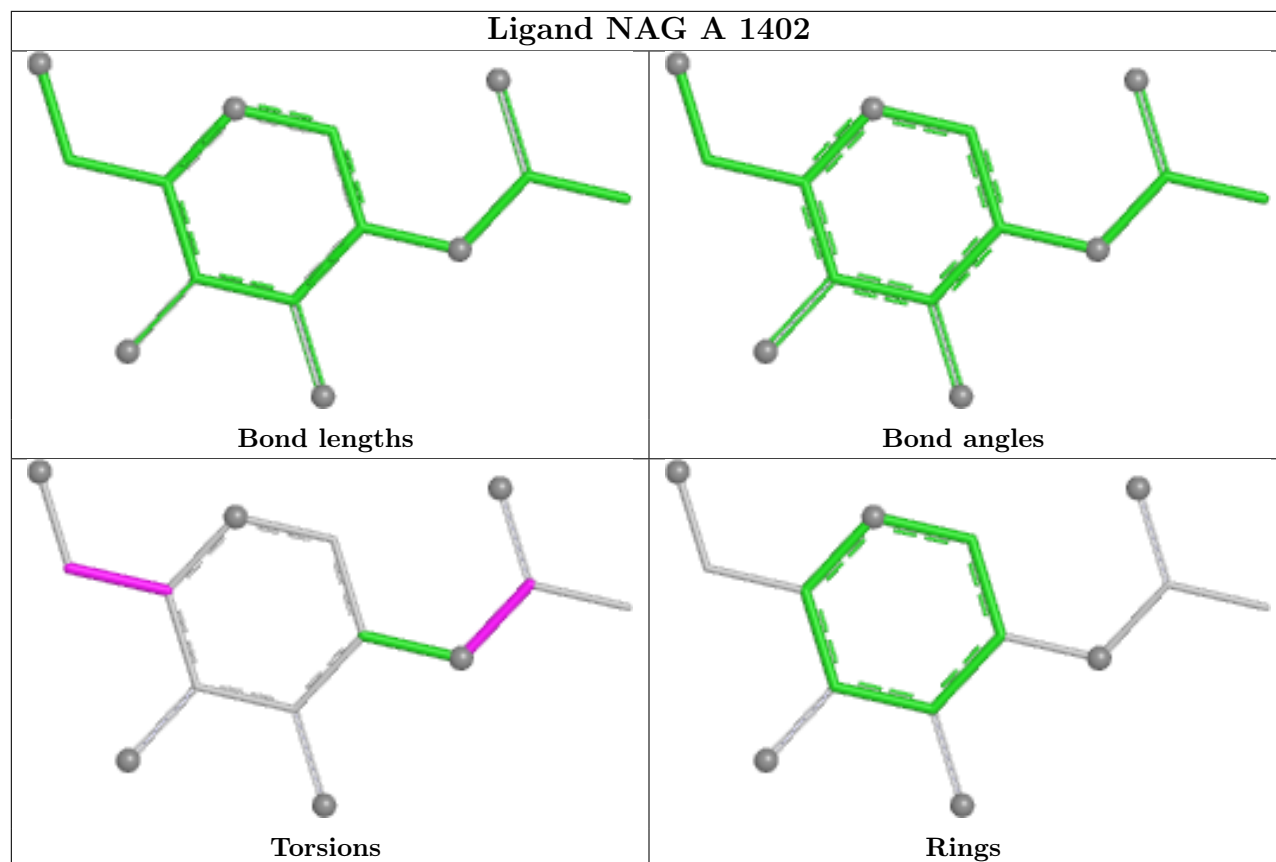
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1403	POV	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 than 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.

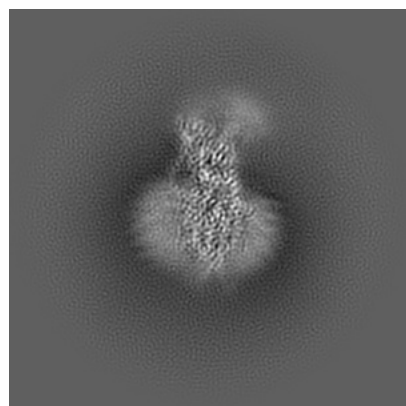
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61544. These allow visual inspection of the internal detail of the map and identification of artifacts.

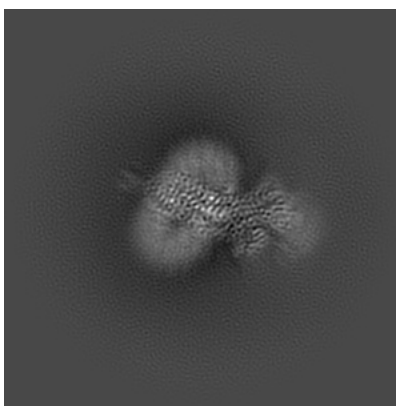
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

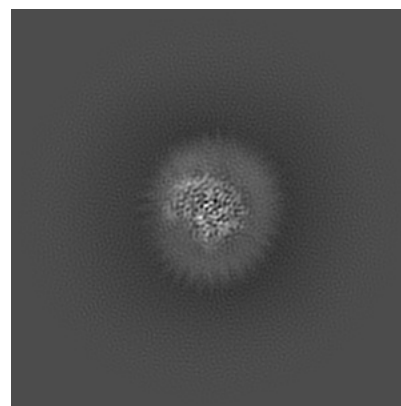
6.1.1 Primary map



X

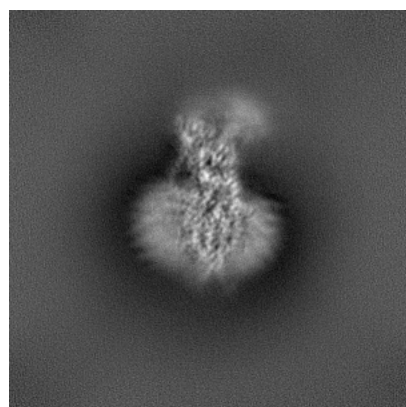


Y

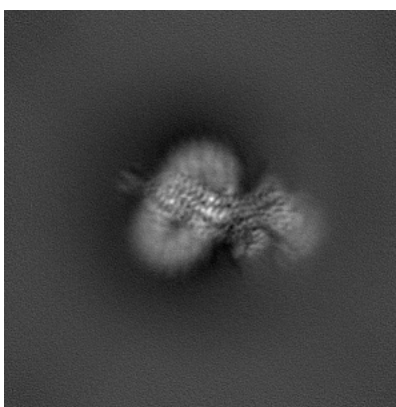


Z

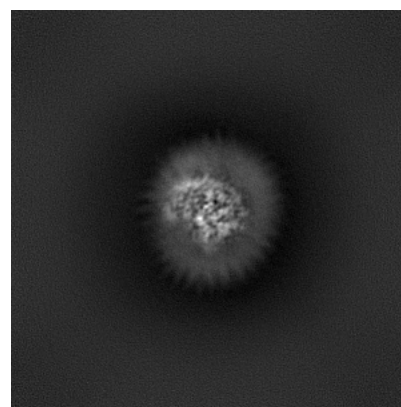
6.1.2 Raw map



X



Y

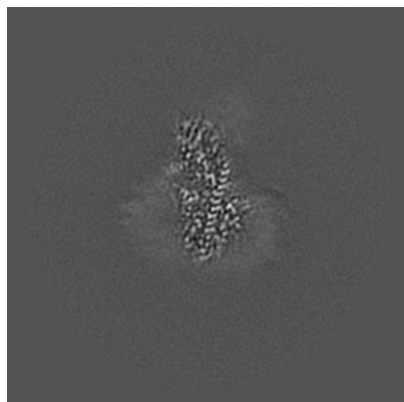


Z

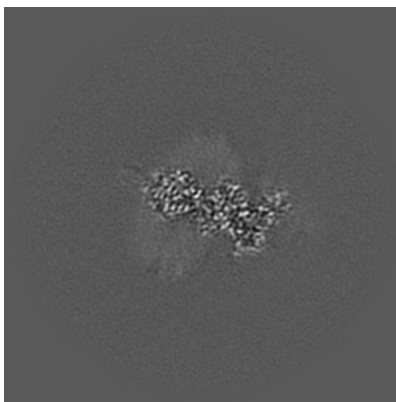
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

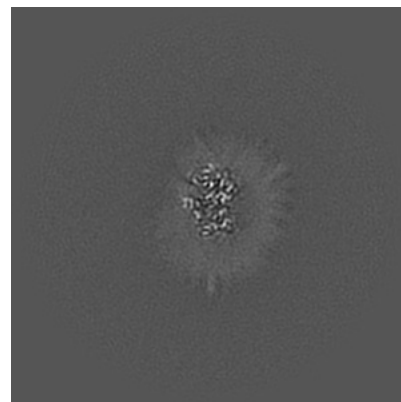
6.2.1 Primary map



X Index: 180

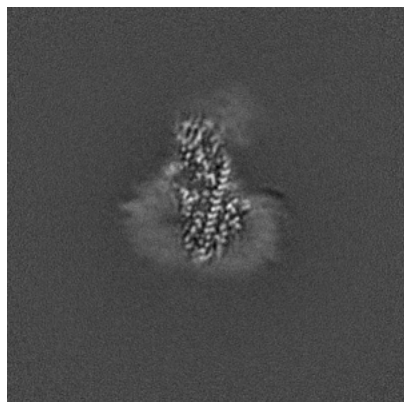


Y Index: 180

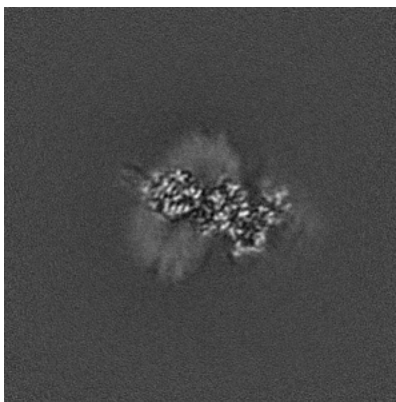


Z Index: 180

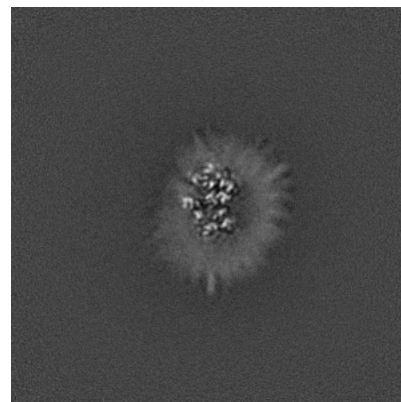
6.2.2 Raw map



X Index: 180



Y Index: 180

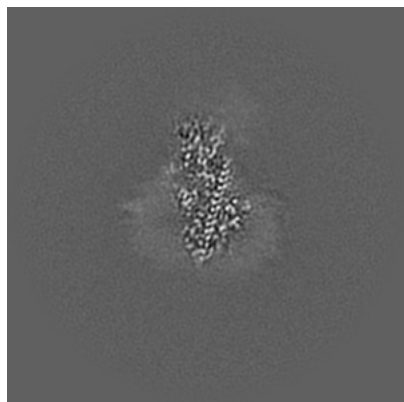


Z Index: 180

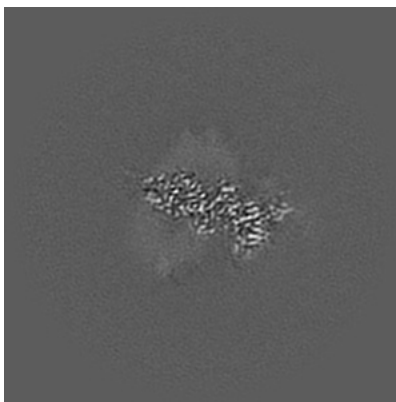
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

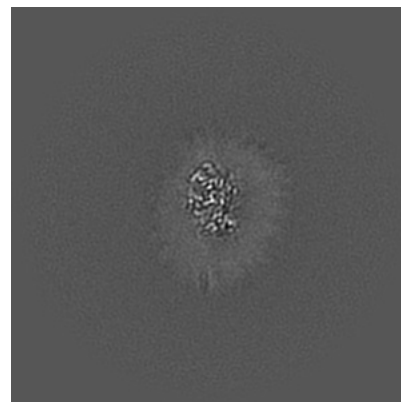
6.3.1 Primary map



X Index: 179

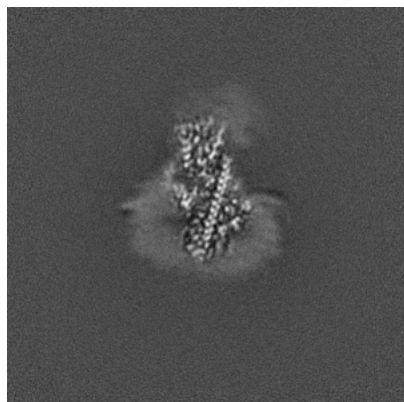


Y Index: 184

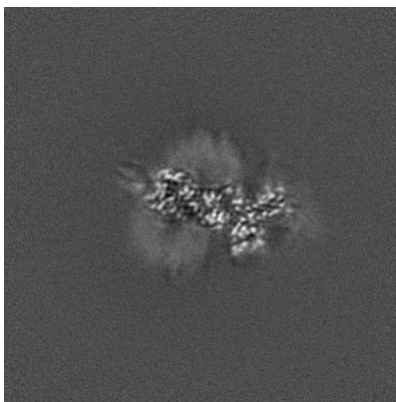


Z Index: 178

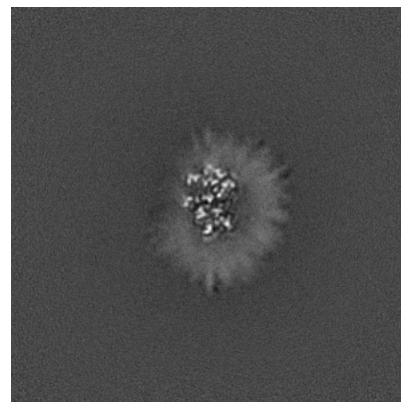
6.3.2 Raw map



X Index: 178



Y Index: 176

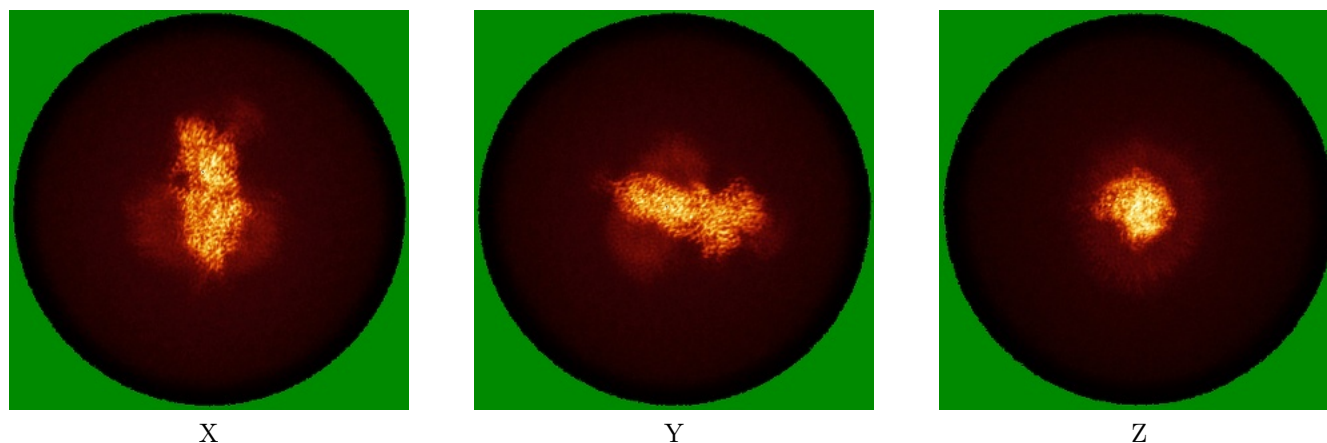


Z Index: 183

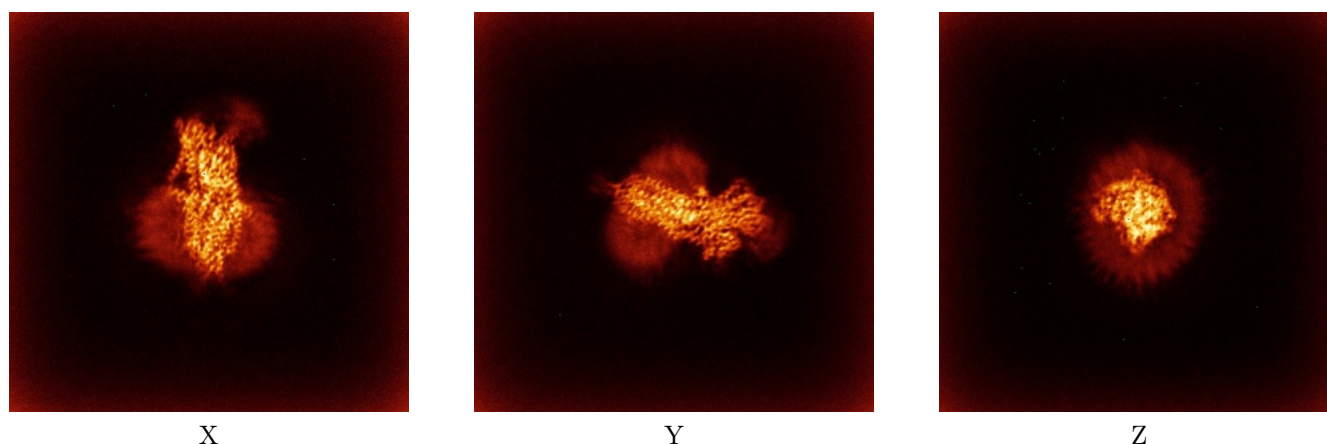
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

6.4.1 Primary map



6.4.2 Raw map



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

6.5 Orthogonal surface views [i](#)

This section was not generated.

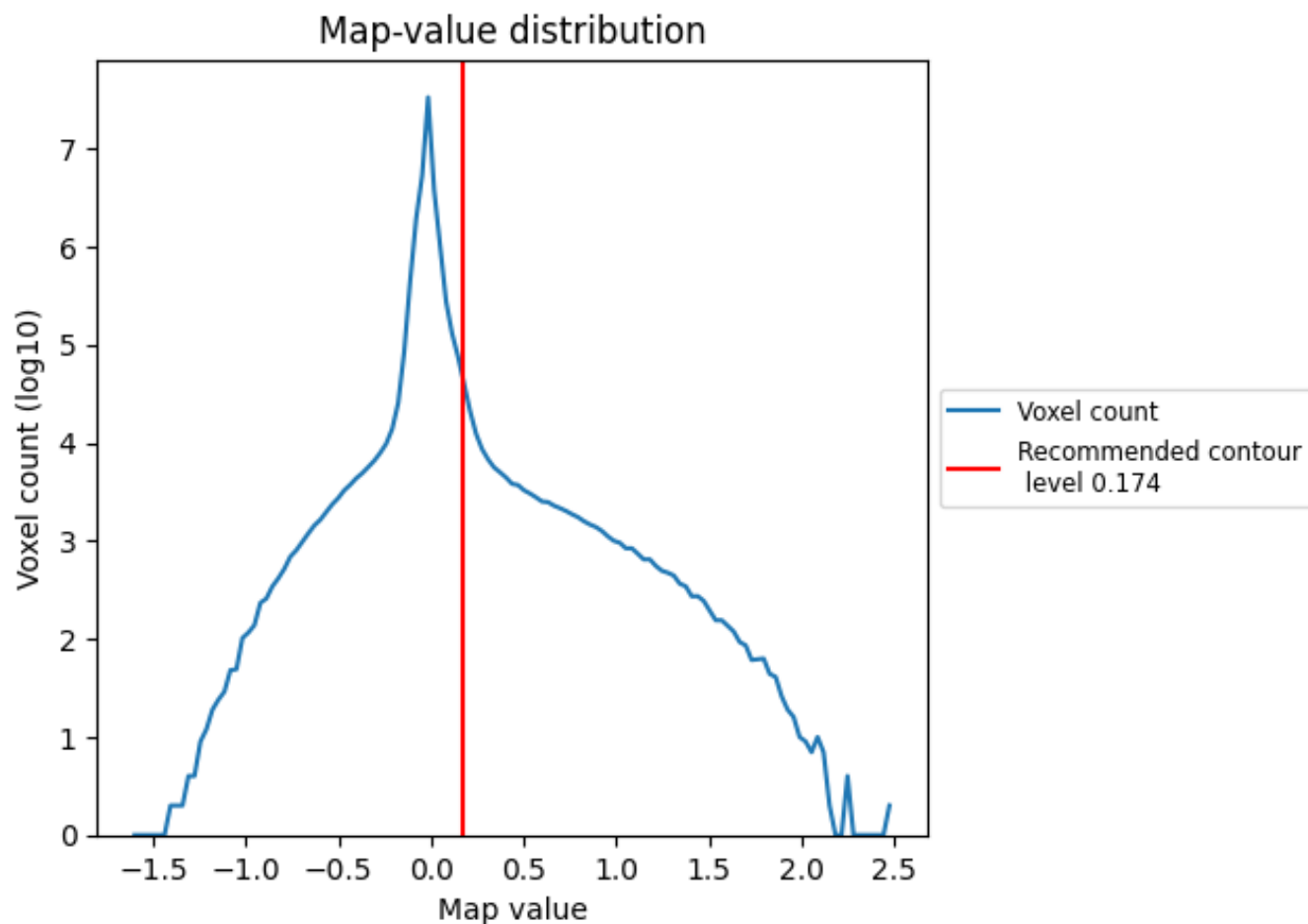
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

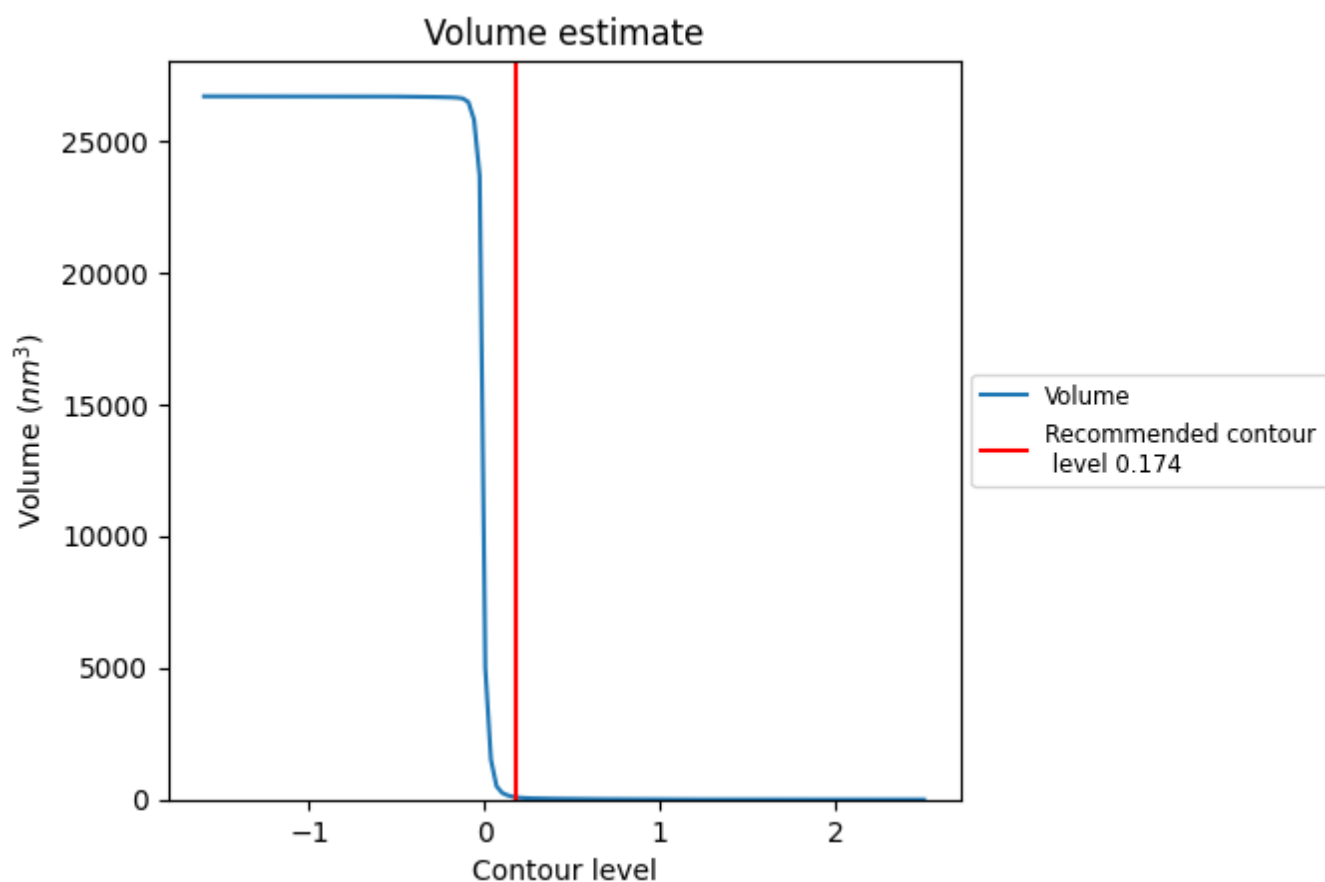
This section contains the results of statistical analysis of the map.

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.

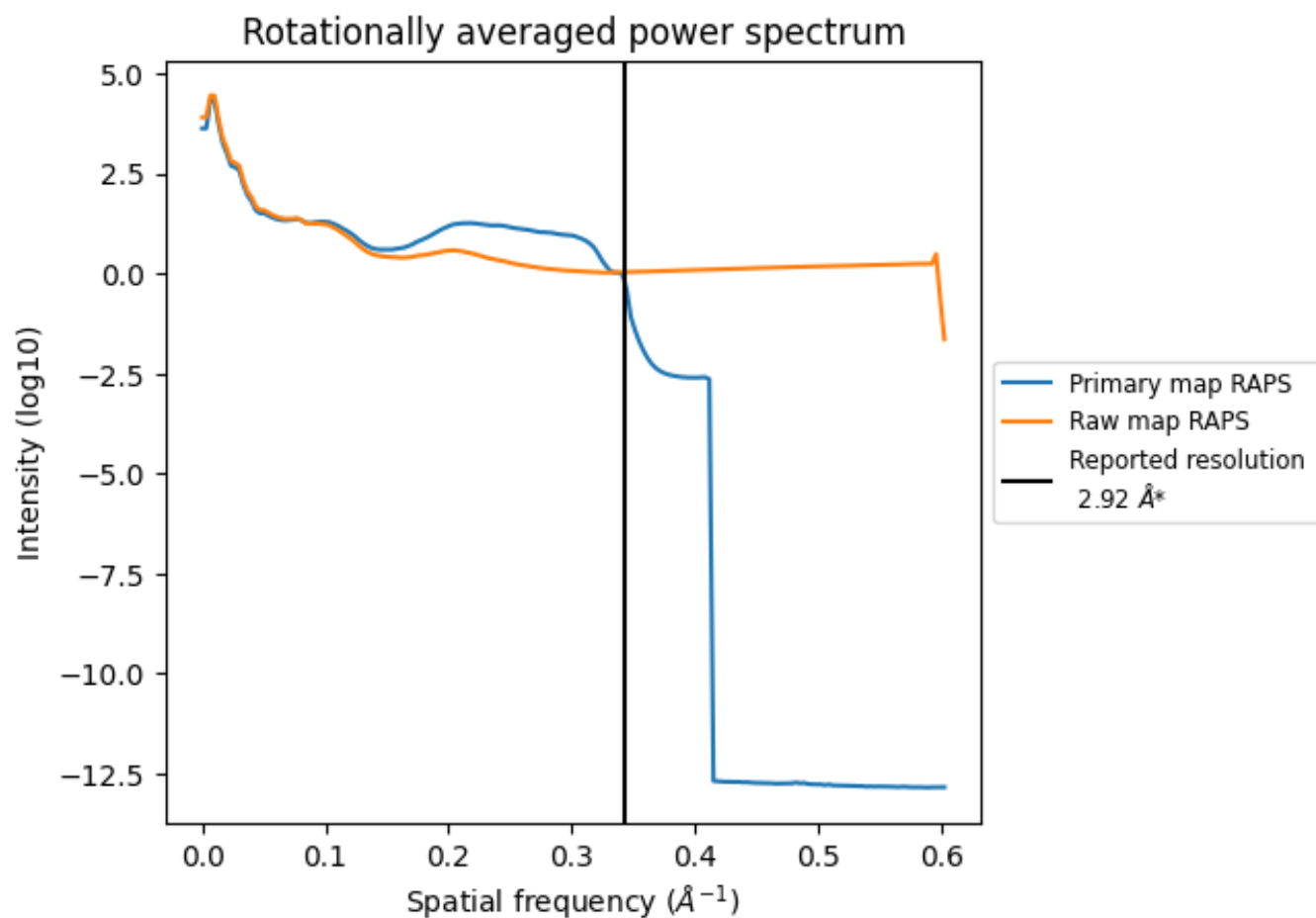
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 95 nm³; this corresponds to an approximate mass of 85 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 ⓘ

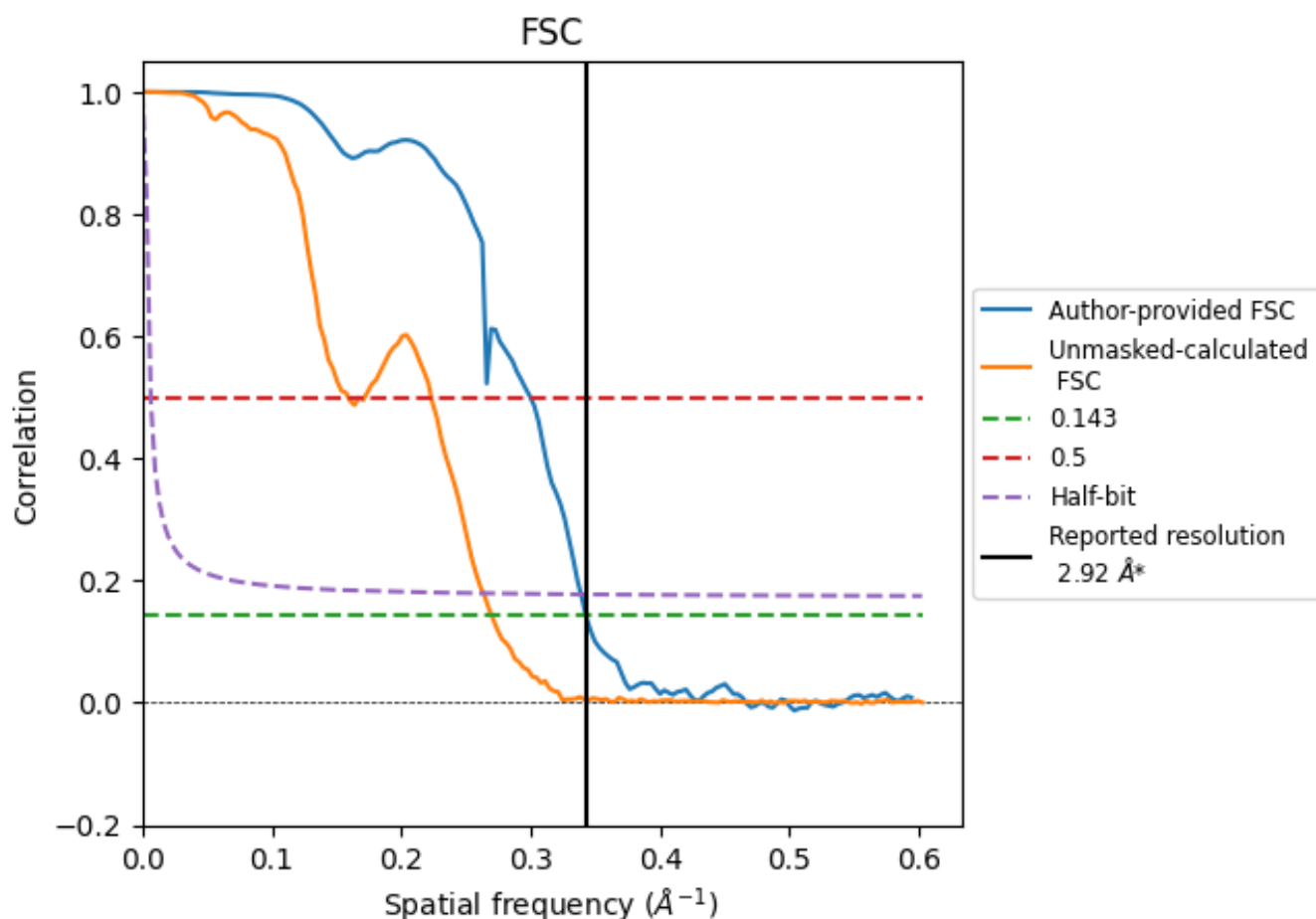


*Reported resolution corresponds to spatial frequency of 0.342 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.342 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

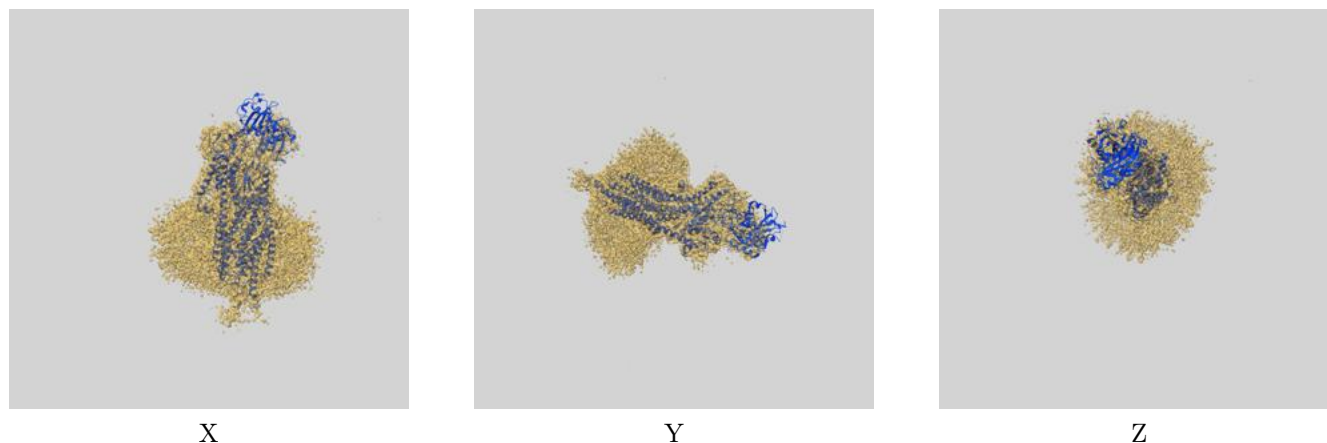
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.92	-	-
Author-provided FSC curve	2.92	3.33	2.95
Unmasked-calculated*	3.71	6.28	3.80

*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 3.71 differs from the reported value 2.92 by more than 10 %

9 Map-model fit [i](#)

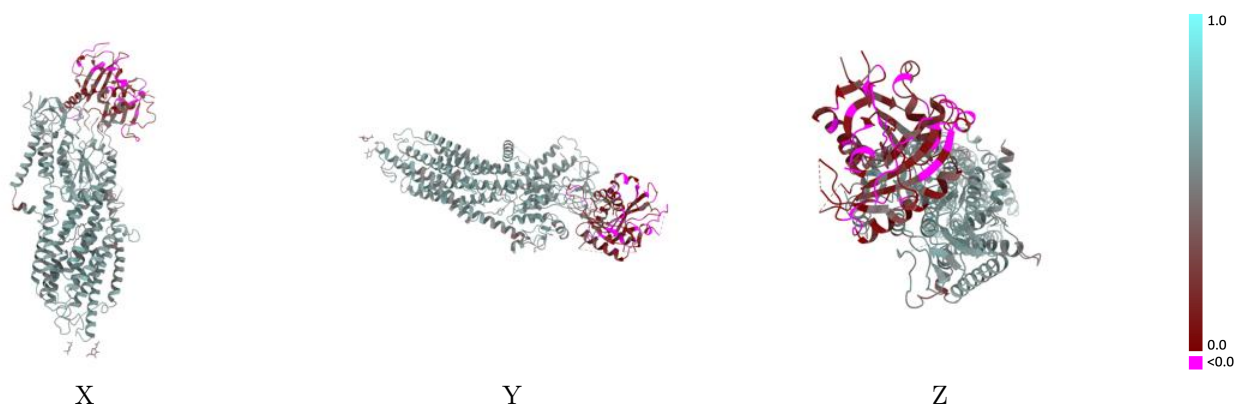
This section contains information regarding the fit between EMDB map EMD-61544 and PDB model 9JK5. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



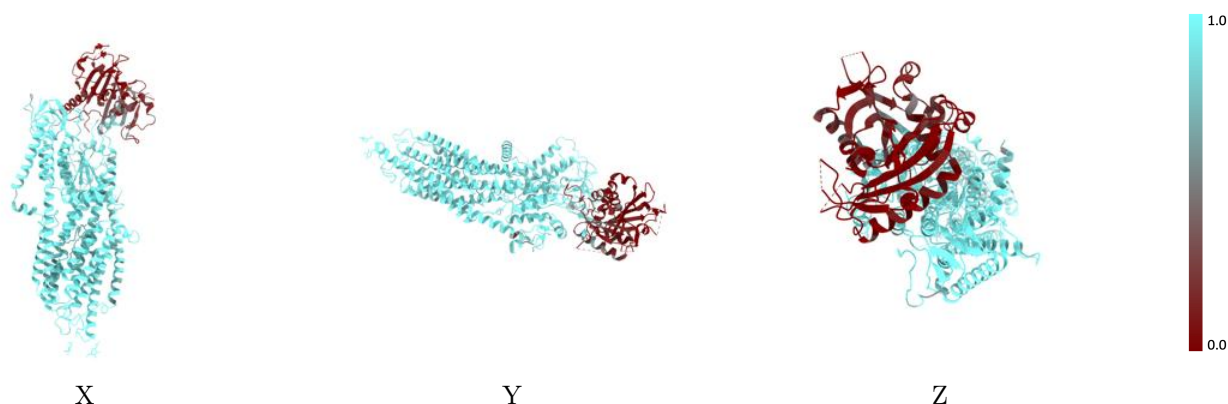
The images above show the 3D surface view of the map at the recommended contour level 0.174 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



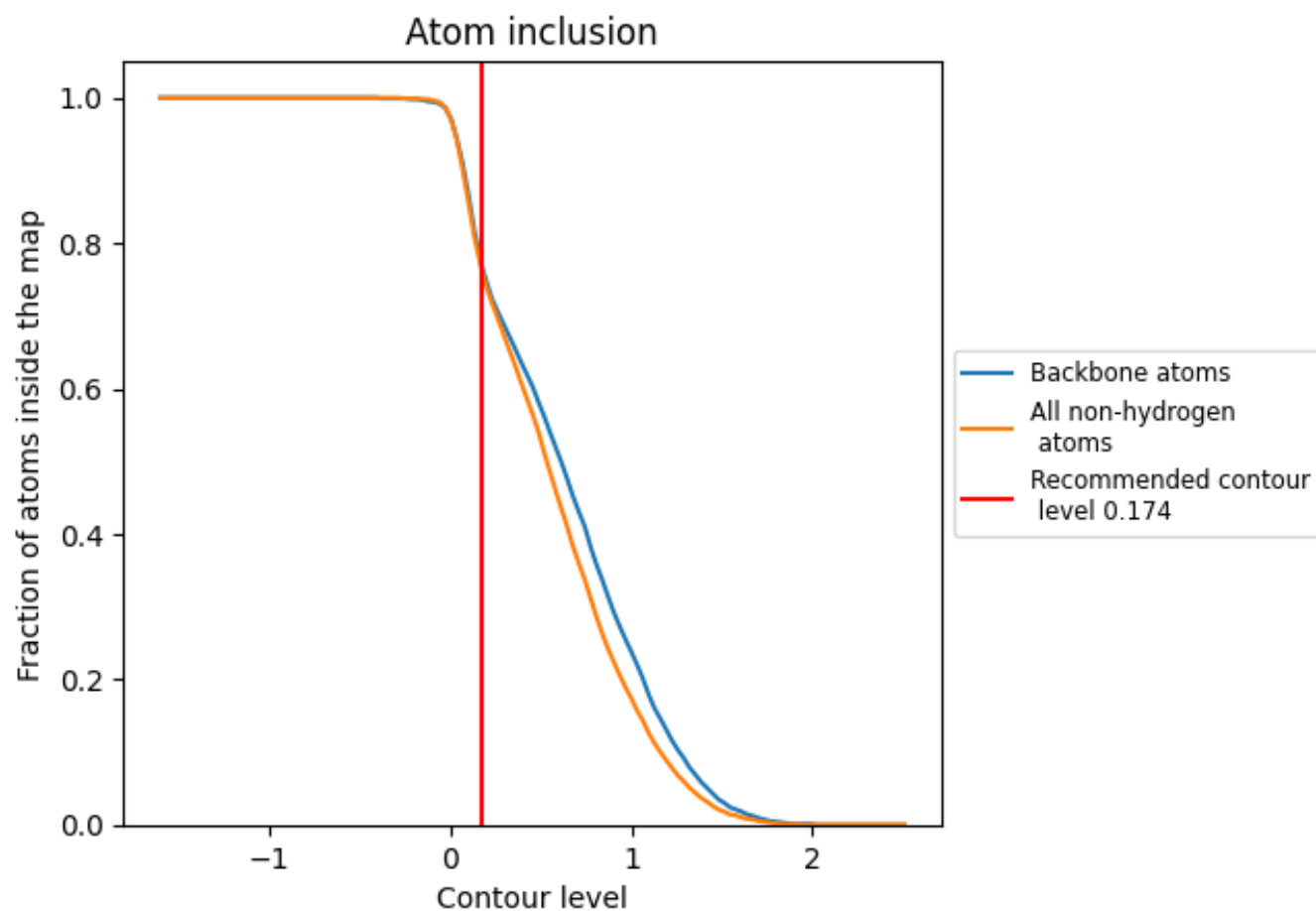
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.174).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 76% 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 (0.174) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7630	0.4620
A	0.7630	0.4620

