



## wwPDB EM Validation Summary Report ⓘ

Apr 16, 2026 – 04:38 pm BST

PDB ID : 9TPW / pdb\_00009tpw  
EMDB ID : EMD-56117  
Title : cryo-ET structure of mTOR complex 2 on a PIP2-containing membrane  
Authors : Hay, I.M.; Ahsan, B.; Williams, R.L.  
Deposited on : 2025-12-18  
Resolution : 6.40 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](mailto: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:

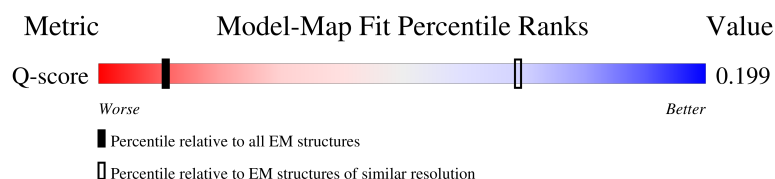
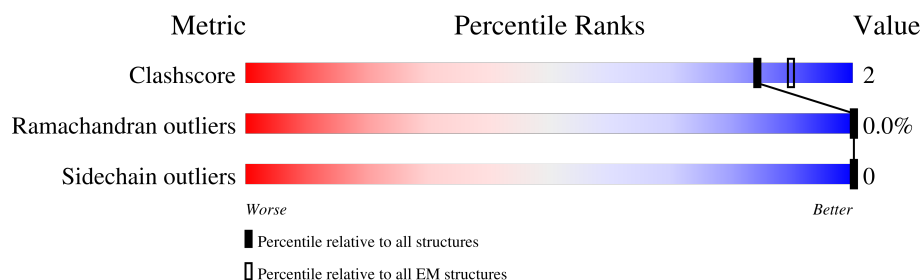
EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 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 6.40 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	544 ( 5.90 - 6.90 )

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  $\geq 3$ , 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	2590	<div> <div>35%</div> <div>82%</div> <div>6%</div> <div>13%</div> </div>
1	B	2590	<div> <div>36%</div> <div>81%</div> <div>6%</div> <div>13%</div> </div>
2	C	326	<div> <div>66%</div> <div>88%</div> <div>8%</div> <div>.</div> </div>
2	D	326	<div> <div>67%</div> <div>89%</div> <div>8%</div> <div>.</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	E	1734	<div><div>24%</div><div>60%</div><div>5%</div><div>35%</div></div>
3	F	1734	<div><div>22%</div><div>60%</div><div>•</div><div>35%</div></div>
4	G	522	<div><div>17%</div><div>22%</div><div>•</div><div>77%</div></div>
4	H	522	<div><div>17%</div><div>22%</div><div>•</div><div>77%</div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 61288 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 Serine/threonine-protein kinase mTOR.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2265	Total	C	N	O	S	0	0
			18242	11626	3206	3284	126		
1	B	2263	Total	C	N	O	S	0	0
			18230	11619	3204	3282	125		

There are 82 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-40	MET	-	initiating methionine	UNP P42345
A	-39	ALA	-	expression tag	UNP P42345
A	-38	SER	-	expression tag	UNP P42345
A	-37	TRP	-	expression tag	UNP P42345
A	-36	SER	-	expression tag	UNP P42345
A	-35	HIS	-	expression tag	UNP P42345
A	-34	PRO	-	expression tag	UNP P42345
A	-33	GLN	-	expression tag	UNP P42345
A	-32	PHE	-	expression tag	UNP P42345
A	-31	GLU	-	expression tag	UNP P42345
A	-30	LYS	-	expression tag	UNP P42345
A	-29	GLY	-	expression tag	UNP P42345
A	-28	GLY	-	expression tag	UNP P42345
A	-27	GLY	-	expression tag	UNP P42345
A	-26	ALA	-	expression tag	UNP P42345
A	-25	ARG	-	expression tag	UNP P42345
A	-24	GLY	-	expression tag	UNP P42345
A	-23	GLY	-	expression tag	UNP P42345
A	-22	SER	-	expression tag	UNP P42345
A	-21	GLY	-	expression tag	UNP P42345
A	-20	GLY	-	expression tag	UNP P42345
A	-19	GLY	-	expression tag	UNP P42345
A	-18	SER	-	expression tag	UNP P42345
A	-17	TRP	-	expression tag	UNP P42345
A	-16	SER	-	expression tag	UNP P42345
A	-15	HIS	-	expression tag	UNP P42345

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	PRO	-	expression tag	UNP P42345
A	-13	GLN	-	expression tag	UNP P42345
A	-12	PHE	-	expression tag	UNP P42345
A	-11	GLU	-	expression tag	UNP P42345
A	-10	LYS	-	expression tag	UNP P42345
A	-9	GLY	-	expression tag	UNP P42345
A	-8	GLU	-	expression tag	UNP P42345
A	-7	ASN	-	expression tag	UNP P42345
A	-6	LEU	-	expression tag	UNP P42345
A	-5	TYR	-	expression tag	UNP P42345
A	-4	PHE	-	expression tag	UNP P42345
A	-3	GLN	-	expression tag	UNP P42345
A	-2	GLY	-	expression tag	UNP P42345
A	-1	GLY	-	expression tag	UNP P42345
A	0	THR	-	expression tag	UNP P42345
B	-40	MET	-	initiating methionine	UNP P42345
B	-39	ALA	-	expression tag	UNP P42345
B	-38	SER	-	expression tag	UNP P42345
B	-37	TRP	-	expression tag	UNP P42345
B	-36	SER	-	expression tag	UNP P42345
B	-35	HIS	-	expression tag	UNP P42345
B	-34	PRO	-	expression tag	UNP P42345
B	-33	GLN	-	expression tag	UNP P42345
B	-32	PHE	-	expression tag	UNP P42345
B	-31	GLU	-	expression tag	UNP P42345
B	-30	LYS	-	expression tag	UNP P42345
B	-29	GLY	-	expression tag	UNP P42345
B	-28	GLY	-	expression tag	UNP P42345
B	-27	GLY	-	expression tag	UNP P42345
B	-26	ALA	-	expression tag	UNP P42345
B	-25	ARG	-	expression tag	UNP P42345
B	-24	GLY	-	expression tag	UNP P42345
B	-23	GLY	-	expression tag	UNP P42345
B	-22	SER	-	expression tag	UNP P42345
B	-21	GLY	-	expression tag	UNP P42345
B	-20	GLY	-	expression tag	UNP P42345
B	-19	GLY	-	expression tag	UNP P42345
B	-18	SER	-	expression tag	UNP P42345
B	-17	TRP	-	expression tag	UNP P42345
B	-16	SER	-	expression tag	UNP P42345
B	-15	HIS	-	expression tag	UNP P42345
B	-14	PRO	-	expression tag	UNP P42345

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	GLN	-	expression tag	UNP P42345
B	-12	PHE	-	expression tag	UNP P42345
B	-11	GLU	-	expression tag	UNP P42345
B	-10	LYS	-	expression tag	UNP P42345
B	-9	GLY	-	expression tag	UNP P42345
B	-8	GLU	-	expression tag	UNP P42345
B	-7	ASN	-	expression tag	UNP P42345
B	-6	LEU	-	expression tag	UNP P42345
B	-5	TYR	-	expression tag	UNP P42345
B	-4	PHE	-	expression tag	UNP P42345
B	-3	GLN	-	expression tag	UNP P42345
B	-2	GLY	-	expression tag	UNP P42345
B	-1	GLY	-	expression tag	UNP P42345
B	0	THR	-	expression tag	UNP P42345

- Molecule 2 is a protein called Target of rapamycin complex subunit LST8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	315	Total	C	N	O	S	0	0
			2443	1518	434	473	18		
2	D	315	Total	C	N	O	S	0	0
			2443	1518	434	473	18		

- Molecule 3 is a protein called Rapamycin-insensitive companion of mTOR.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	1119	Total	C	N	O	S	0	0
			8990	5732	1584	1625	49		
3	F	1119	Total	C	N	O	S	0	0
			8990	5732	1584	1625	49		

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-25	MET	-	initiating methionine	UNP Q6R327
E	-24	ALA	-	expression tag	UNP Q6R327
E	-23	ASP	-	expression tag	UNP Q6R327
E	-22	TYR	-	expression tag	UNP Q6R327
E	-21	LYS	-	expression tag	UNP Q6R327
E	-20	ASP	-	expression tag	UNP Q6R327
E	-19	HIS	-	expression tag	UNP Q6R327
E	-18	ASP	-	expression tag	UNP Q6R327

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
E	-17	GLY	-	expression tag	UNP Q6R327
E	-16	ASP	-	expression tag	UNP Q6R327
E	-15	TYR	-	expression tag	UNP Q6R327
E	-14	LYS	-	expression tag	UNP Q6R327
E	-13	ASP	-	expression tag	UNP Q6R327
E	-12	HIS	-	expression tag	UNP Q6R327
E	-11	ASP	-	expression tag	UNP Q6R327
E	-10	ILE	-	expression tag	UNP Q6R327
E	-9	ASP	-	expression tag	UNP Q6R327
E	-8	TYR	-	expression tag	UNP Q6R327
E	-7	LYS	-	expression tag	UNP Q6R327
E	-6	ASP	-	expression tag	UNP Q6R327
E	-5	ASP	-	expression tag	UNP Q6R327
E	-4	ASP	-	expression tag	UNP Q6R327
E	-3	ASP	-	expression tag	UNP Q6R327
E	-2	LYS	-	expression tag	UNP Q6R327
E	-1	GLY	-	expression tag	UNP Q6R327
E	0	THR	-	expression tag	UNP Q6R327
F	-25	MET	-	initiating methionine	UNP Q6R327
F	-24	ALA	-	expression tag	UNP Q6R327
F	-23	ASP	-	expression tag	UNP Q6R327
F	-22	TYR	-	expression tag	UNP Q6R327
F	-21	LYS	-	expression tag	UNP Q6R327
F	-20	ASP	-	expression tag	UNP Q6R327
F	-19	HIS	-	expression tag	UNP Q6R327
F	-18	ASP	-	expression tag	UNP Q6R327
F	-17	GLY	-	expression tag	UNP Q6R327
F	-16	ASP	-	expression tag	UNP Q6R327
F	-15	TYR	-	expression tag	UNP Q6R327
F	-14	LYS	-	expression tag	UNP Q6R327
F	-13	ASP	-	expression tag	UNP Q6R327
F	-12	HIS	-	expression tag	UNP Q6R327
F	-11	ASP	-	expression tag	UNP Q6R327
F	-10	ILE	-	expression tag	UNP Q6R327
F	-9	ASP	-	expression tag	UNP Q6R327
F	-8	TYR	-	expression tag	UNP Q6R327
F	-7	LYS	-	expression tag	UNP Q6R327
F	-6	ASP	-	expression tag	UNP Q6R327
F	-5	ASP	-	expression tag	UNP Q6R327
F	-4	ASP	-	expression tag	UNP Q6R327
F	-3	ASP	-	expression tag	UNP Q6R327
F	-2	LYS	-	expression tag	UNP Q6R327

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
F	-1	GLY	-	expression tag	UNP Q6R327
F	0	THR	-	expression tag	UNP Q6R327

- Molecule 4 is a protein called Target of rapamycin complex 2 subunit MAPKAP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	120	Total	C	N	O	S	0	0
			974	603	182	185	4		
4	H	120	Total	C	N	O	S	0	0
			974	603	182	185	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	1	ACE	-	acetylation	UNP Q9BPZ7
H	1	ACE	-	acetylation	UNP Q9BPZ7

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

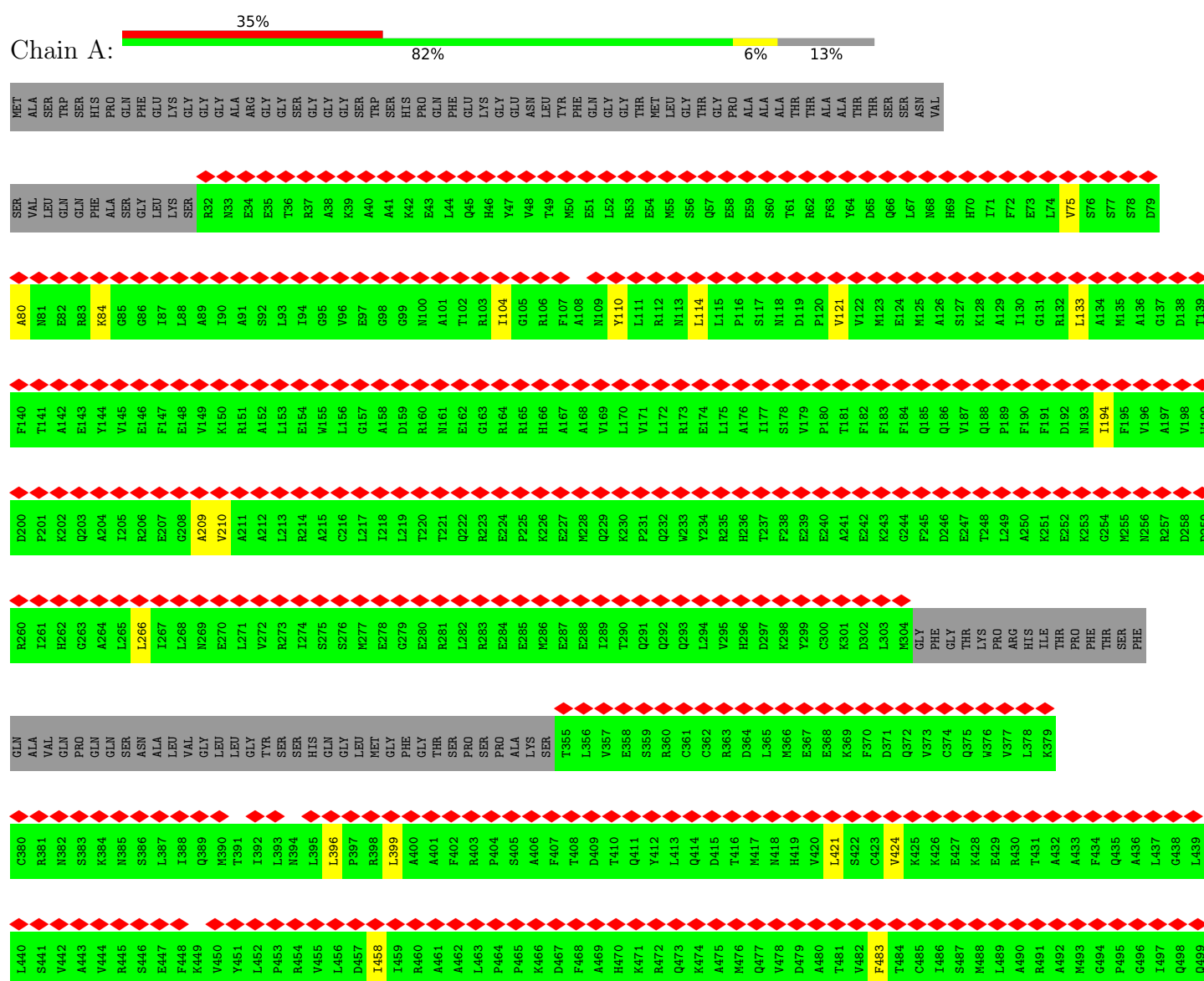
Mol	Chain	Residues	Atoms		AltConf
5	E	1	Total	Zn	0
			1	1	
5	F	1	Total	Zn	0
			1	1	



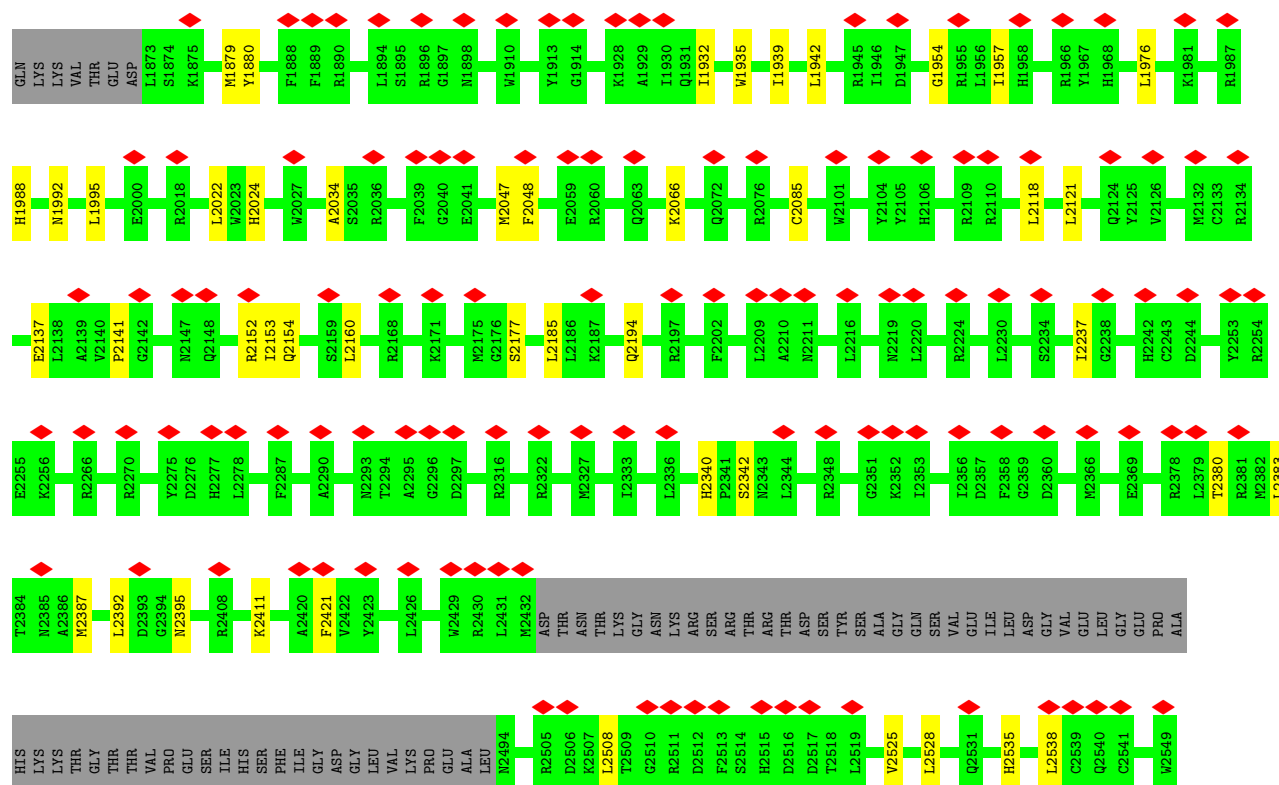
### 3 Residue-property plots

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.

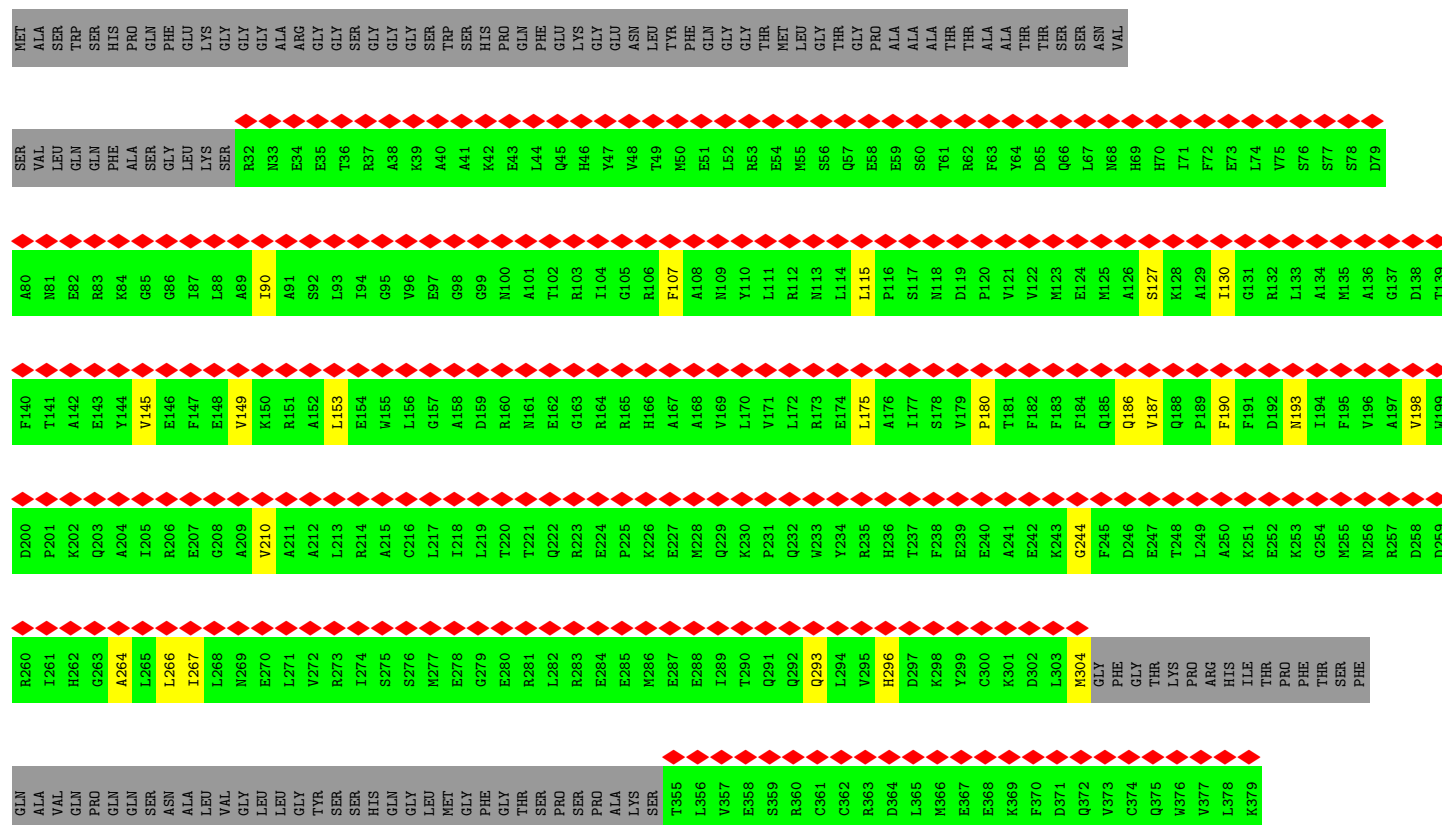
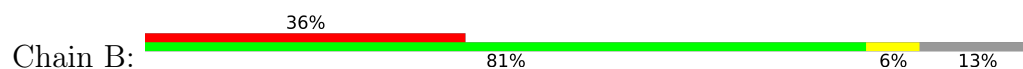
- Molecule 1: Serine/threonine-protein kinase mTOR





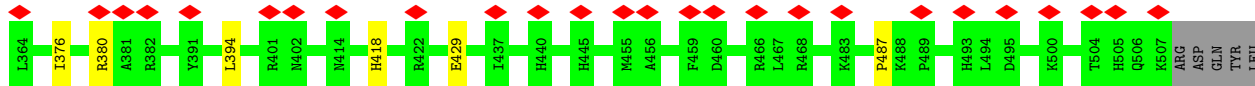


• Molecule 1: Serine/threonine-protein kinase mTOR

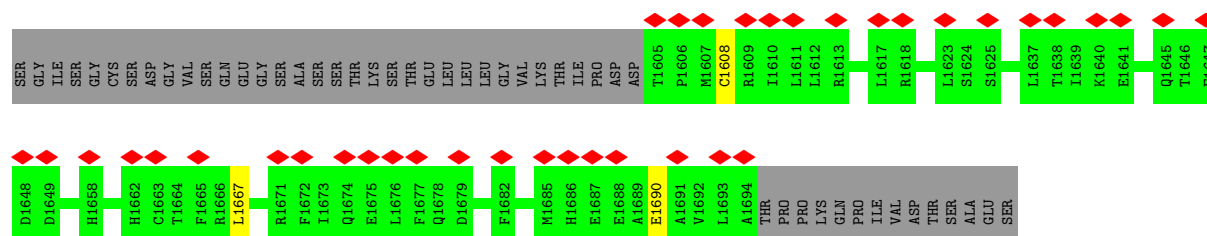


D1472	D1473	M1477	E1485	A1486	L1487	M1490	H1494	K1500	V1504	M1505	A1513	R1514	T1533	C1534	M1535	I1536	F1537	R1538	D1539	G1543	A1544	F1545	P1408	N1421	K1422	E1427	M1437	F1440	G1441	E1442	L1443	E1444	I1445	E1451	K1452	V1456	Y1463	D1464	M1467	D1468	T1469	N1470	K1471																	
Q1348	D1349	I1350	A1351	Q1355	E1365	H1366	K1369	L1374	R1375	D1376	D1377	N1378	G1379	I1380	R1386	K1389	C1390	R1391	A1392	Y1399	K1406	G1407	P1408	N1421	K1422	E1427	M1437	F1440	G1441	E1442	L1443	E1444	I1445	E1451	K1452	V1456	Y1463	D1464	M1467	D1468	T1469	N1470	K1471																	
D1150	R1154	H1157	V1160	R1161	T1162	L1163	D1164	Q1165	E1168	L1169	R1170	G1185	Y1188	M1196	K1197	V1198	L1199	V1200	R1201	H1202	R1203	T1204	H1205	Q1206	R1207	R1208	K1218	G1219	L1222	A1223	D1224	E1225	E1226	E1227	Y1232	Q1233	H1234	R1235	M1236	L1237	R1238	SER	GLY	GLN	GLY	ASP	ALA	LEU	ALA											
SER	GLY	PRO	VAL	GLU	THR	GLY	PRO	GLY	PRO	MET	LYS	LEU	HIS	V1260	S1261	T1262	I1263	M1264	Q1265	K1267	A1268	W1269	G1270	A1271	A1272	R1273	R1274	V1275	S1276	K1277	D1278	D1279	W1280	R1286	E1290	L1291	L1292	K1293	D1294	S1295	S1296	R1301	M1311	D1316	A1321	E1328	L1329	M1330	E1331	D1332	S1347									
F1041	V1042	V1043	M1044	H1045	T1048	Q1049	A1062	L1063	G1064	F1067	R1080	V1081	F1082	M1083	H1084	D1085	M1086	G1089	R1090	I1091	I1094	Q1101	L1102	M1106	L1107	D1108	D1109	Y1110	L1114	V1119	K1120	L1121	F1122	D1123	A1124	P1125	E1126	A1127	P1128	R1132	T1138	E1144	D1147	F1148	T1149															
ASP	SER	SER	LEU	LEU	ALA	R836	T843	Q846	Q852	Y853	Y854	Y858	R859	P862	T863	L864	L869	L872	K873	T874	E875	Q876	R881	R882	E883	R886	Q892	A893	L894	I903	GLY	MET	I1003	ASP	GLN	SER	ARG	ASP	ALA	SER	ALA	VAL	SER	LEU	SER	GLU	SER	LYS												
F729	L741	E742	H743	S744	G745	I746	G747	R748	I749	R755	M756	L757	GLY	H759	L760	S762	M763	R766	L776	L779	L780	L781	K782	L783	K784	ASP	PRO	ASP	PRO	ASP	PRO	N791	V794	I795	L799	T802	L805	L811	R814	T823	R824	M825	D826	N827	LEU	GLN														
R628	L629	T631	PRO	SER	I1E	HIS	LEU	SER	SER	GLY	HIS	ALA	HIS	VAL	VAL	SER	GLN	ALA	V652	L656	L659	T664	T665	P669	D670	I671	A677	S678	L679	R682	H686	L687	A688	L693	L696	L700	R708	I712	M721	N722																				
G560	L561	A562	H563	Q564	L565	A566	S567	P568	G569	L570	T571	L572	L573	P574	E575	A576	S577	D578	V579	S580	S581	I582	T583	L584	A585	L586	L587	T588	L589	G590	S591	F592	E593	F594	E595	G596	H597	S598	L599	T600	Q601	F602	V603	R604	H605	D608	H609	F610	L611	N612	S613	E614	R619	M620	E621	R624				
D500	I501	K502	E503	L504	L505	E506	P507	M508	L509	A510	V511	G512	L513	S514	P515	A516	L517	T518	A519	V520	L521	Y522	D523	L524	S525	R526	Q527	I528	P529	Q530	L531	K532	K533	D534	I535	Q536	D537	G538	L539	L540	Q541	M542	L543	F483	S544	L545	V546	L547	M548	H549	K550	P551	L552	R553	H554	P555	G556	M557	P558	K559
C380	R381	N382	S383	K384	N385	S386	L387	I388	Q389	M390	T391	I392	L393	N394	L395	L396	P397	R398	L399	A400	A401	F402	R403	P404	S405	A406	F407	T408	D409	T410	Q411	Y412	L413	Q414	D415	T416	M417	N418	H419	V420	L421	S422	C423	V424	K425	K426	E427	K428	E429	R430	T431	A432	F434	Q435	A436	G438	L439			
L440	S441	V442	A443	V444	R445	S446	E447	F448	K449	V450	Y451	L452	P453	R454	V455	L456	D457	I458	I459	A460	A461	A462	L463	P464	P465	K466	D467	F468	A469	H470	K471	Q472	Q473	K474	A475	M476	Q477	V478	D479	A480	T481	V482	F483	T484	C485	I486	S487	M488	L489	A490	R491	A492	M493	G494	P495	G496	I497	Q498	Q499	

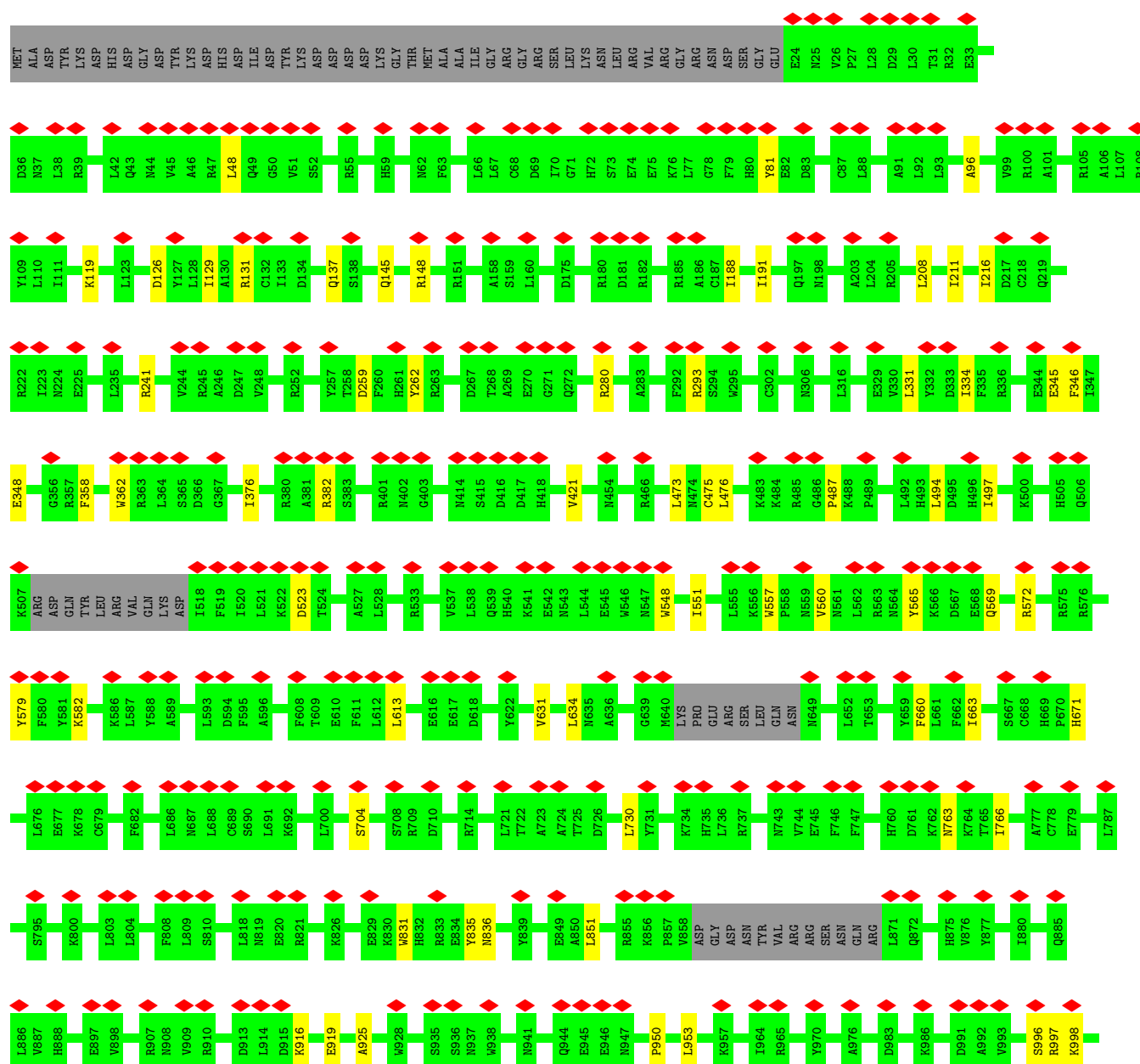




T1510	G1511	L1512	Q1513	E1514	H1515	T1516	D1517	D1518	C1520	L1521	Y1522	C1523	C1525	I1526	E1527	I1528	G1530	F1531	Q1532	M1535	L1537	S1538	A1539	I1540	C1541	SER	HIS	SER	ASP	PHE	GLN	ASP	ILE	PRO	PRO	ILE																																																																																																																																																																																																																																																																																																																																																																																																																																					
K586	L587	Y588	A589	P590	L591	D592	L593	D594	F595	A596	F598	L599	S600	Y601	F602	L603	D604	Q605	K606	S607	L608	Y609	F610	L611	D612	S613	H614	C615	G616	H617	L618	Y619	F620	L621	D622	Q623	K624	S625	L626	Y627	F628	L629	D630	Q631	K632	S633	H634	C635	G636	H637	L638	Y639	F640	L641	D642	Q643	K644	S645	H646	C647	G648	H649	L650	Y651	F652	L653	D654	Q655	K656	S657	H658	C659	G660	H661	L662	Y663	F664	L665	D666	Q667	K668	S669	H670	C671	G672	H673	L674	Y675	F676	L677	D678	Q679	K680	S681	H682	C683	G684	H685	L686	Y687	F688	L689	D690	Q691	K692	S693	H694	C695	G696	H697	L698	Y699	F700	L701	D702	Q703	K704	S705	H706	C707	G708	H709	L710	Y711	F712	L713	D714	Q715	K716	S717	H718	C719	G720	H721	L722	Y723	F724	L725	D726	Q727	K728	S729	H730	C731	G732	H733	L734	Y735	F736	L737	D738	Q739	K740	S741	H742	C743	G744	H745	L746	Y747	F748	L749	D750	Q751	K752	S753	H754	C755	G756	H757	L758	Y759	F760	L761	D762	Q763	K764	S765	H766	C767	G768	H769	L770	Y771	F772	L773	D774	Q775	K776	S777	H778	C779	G780	H781	L782	Y783	F784	L785	D786	Q787	K788	S789	H790	C791	G792	H793	L794	Y795	F796	L797	D798	Q799	K800	S801	H802	C803	G804	H805	L806	Y807	F808	L809	D810	Q811	K812	S813	H814	C815	G816	H817	L818	Y819	F820	L821	D822	Q823	K824	S825	H826	C827	G828	H829	L830	Y831	F832	L833	D834	Q835	K836	S837	H838	C839	G840	H841	L842	Y843	F844	L845	D846	Q847	K848	S849	H850	C851	G852	H853	L854	Y855	F856	L857	D858	Q859	K860	S861	H862	C863	G864	H865	L866	Y867	F868	L869	D870	Q871	K872	S873	H874	C875	G876	H877	L878	Y879	F880	L881	D882	Q883	K884	S885	H886	C887	G888	H889	L890	Y891	F892	L893	D894	Q895	K896	S897	H898	C899	G900	H901	L902	Y903	F904	L905	D906	Q907	K908	S909	H910	C911	G912	H913	L914	Y915	F916	L917	D918	Q919	K920	S921	H922	C923	G924	H925	L926	Y927	F928	L929	D930	Q931	K932	S933	H934	C935	G936	H937	L938	Y939	F940	L941	D942	Q943	K944	S945	H946	C947	G948	H949	L950	Y951	F952	L953	D954	Q955	K956	S957	H958	C959	G960	H961	L962	Y963	F964	L965	D966	Q967	K968	S969	H970	C971	G972	H973	L974	Y975	F976	L977	D978	Q979	K980	S981	H982	C983	G984	H985	L986	Y987	F988	L989	D990	Q991	K992	S993	H994	C995	G996	H997	L998	Y999	F1000	L1001	D1002	Q1003	K1004	S1005	H1006	C1007	G1008	H1009	L1010	Y1011	F1012	L1013	D1014	Q1015	K1016	S1017	H1018	C1019	G1020	H1021	L1022	Y1023	F1024	L1025	D1026	Q1027	K1028	S1029	H1030	C1031	G1032	H1033	L1034	Y1035	F1036	L1037	D1038	Q1039	K1040	S1041	H1042	C1043	G1044



• Molecule 3: Rapamycin-insensitive companion of mTOR









## 4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	38469	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	140	Depositor
Minimum defocus (nm)	3000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	81000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.030	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	532.92804, 532.92804, 532.92804	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.514, 1.514, 1.514	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	0.35	0/18617	0.79	0/25184
1	B	0.35	0/18604	0.81	0/25166
2	C	0.35	0/2501	0.78	0/3408
2	D	0.34	0/2501	0.79	0/3408
3	E	0.34	0/9154	0.77	0/12384
3	F	0.34	0/9154	0.79	0/12384
4	G	0.32	0/984	0.81	0/1318
4	H	0.31	0/984	0.83	0/1318
All	All	0.34	0/62499	0.80	0/84570

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1132	ARG	Sidechain
1	B	1132	ARG	Sidechain

## 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	18242	0	18471	80	0
1	B	18230	0	18458	84	0
2	C	2443	0	2327	15	0
2	D	2443	0	2327	15	0
3	E	8990	0	9187	43	0
3	F	8990	0	9187	44	0
4	G	974	0	993	4	0
4	H	974	0	993	4	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
All	All	61288	0	61943	282	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 2.

The worst 5 of 282 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:B:153:LEU:HD22	1:B:193:ASN:HB2	1.78	0.66
2:D:50:VAL:HG21	2:D:321:ASN:HB2	1.80	0.64
1:A:722:ASN:HD21	3:F:1001:TRP:HB3	1.63	0.62
1:A:2022:LEU:HD13	1:A:2066:LYS:HE2	1.82	0.60
3:E:1541:CYS:HA	3:E:1608:CYS:HB2	1.83	0.60

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	2245/2590 (87%)	2185 (97%)	59 (3%)	1 (0%)	100	100
1	B	2241/2590 (86%)	2184 (98%)	56 (2%)	1 (0%)	100	100
2	C	313/326 (96%)	301 (96%)	12 (4%)	0	100	100
2	D	313/326 (96%)	302 (96%)	11 (4%)	0	100	100
3	E	1103/1734 (64%)	1079 (98%)	24 (2%)	0	100	100
3	F	1103/1734 (64%)	1076 (98%)	27 (2%)	0	100	100
4	G	116/522 (22%)	111 (96%)	5 (4%)	0	100	100
4	H	116/522 (22%)	107 (92%)	9 (8%)	0	100	100
All	All	7550/10344 (73%)	7345 (97%)	203 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	180	PRO
1	A	569	GLY

### 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	1991/2248 (89%)	1991 (100%)	0	100	100
1	B	1990/2248 (88%)	1990 (100%)	0	100	100
2	C	267/276 (97%)	267 (100%)	0	100	100
2	D	267/276 (97%)	267 (100%)	0	100	100
3	E	1005/1562 (64%)	1005 (100%)	0	100	100
3	F	1005/1562 (64%)	1005 (100%)	0	100	100
4	G	111/470 (24%)	111 (100%)	0	100	100
4	H	111/470 (24%)	111 (100%)	0	100	100
All	All	6747/9112 (74%)	6747 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 97 such sidechains are listed below:

Mol	Chain	Res	Type
3	E	178	GLN
3	E	1632	HIS
3	E	242	GLN
3	E	694	GLN
3	F	242	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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.



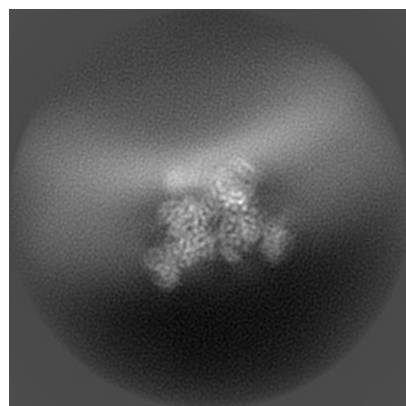
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-56117. These allow visual inspection of the internal detail of the map and identification of artifacts.

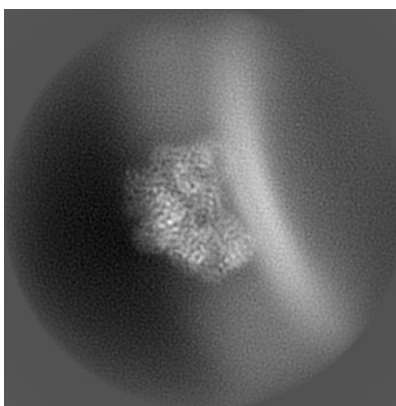
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

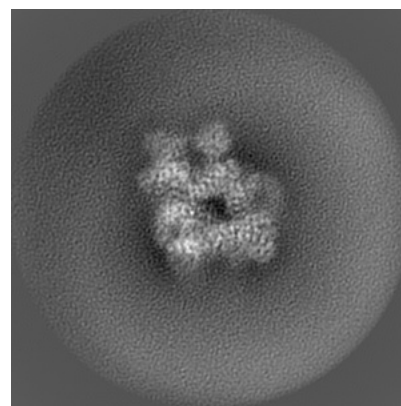
#### 6.1.1 Primary map



X

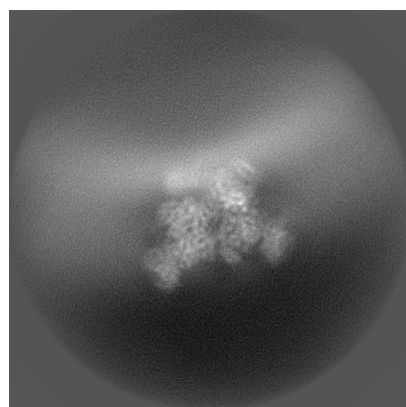


Y

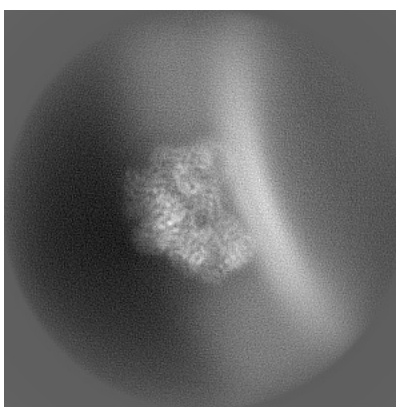


Z

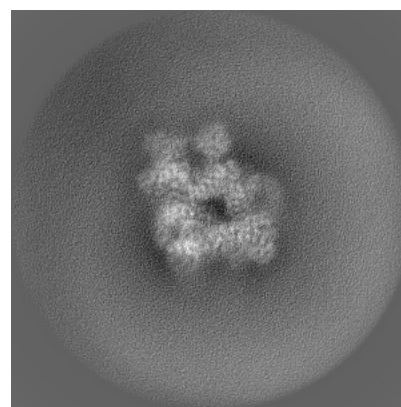
#### 6.1.2 Raw map



X



Y

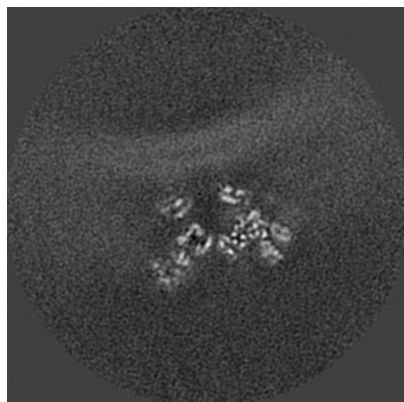


Z

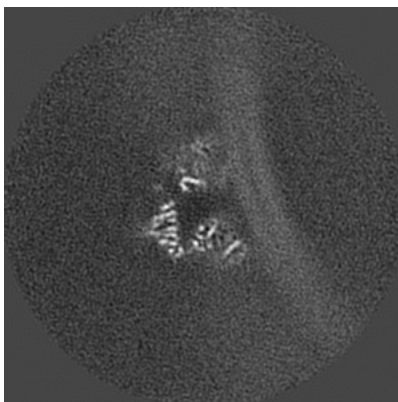
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

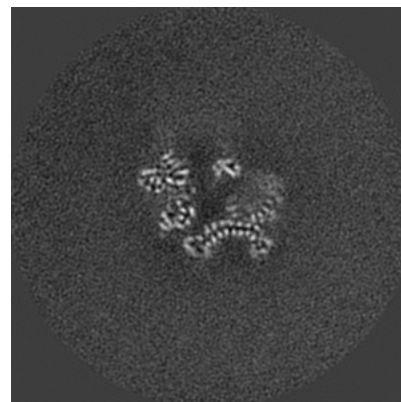
### 6.2.1 Primary map



X Index: 176

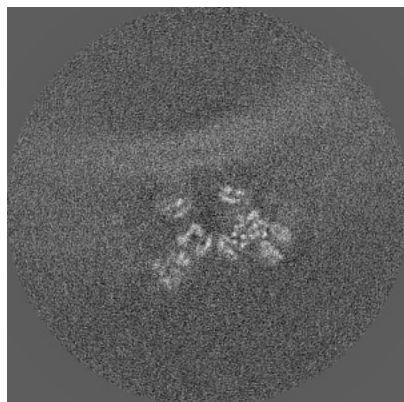


Y Index: 176

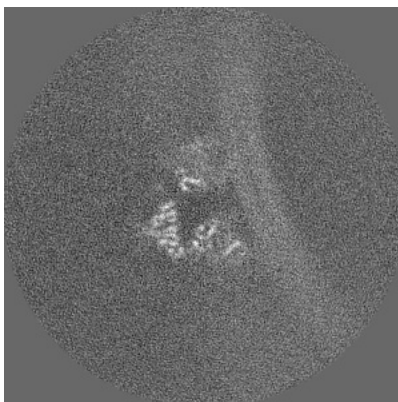


Z Index: 176

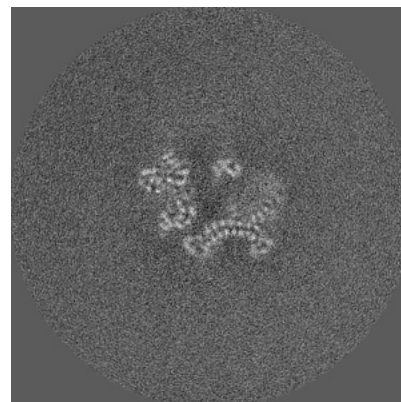
### 6.2.2 Raw map



X Index: 176



Y Index: 176

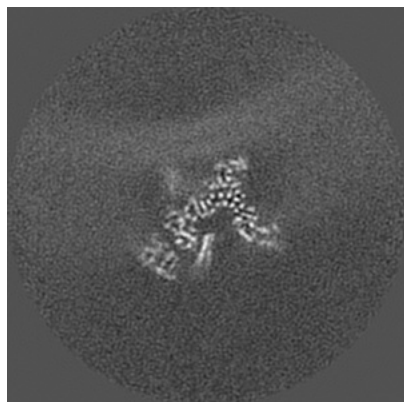


Z Index: 176

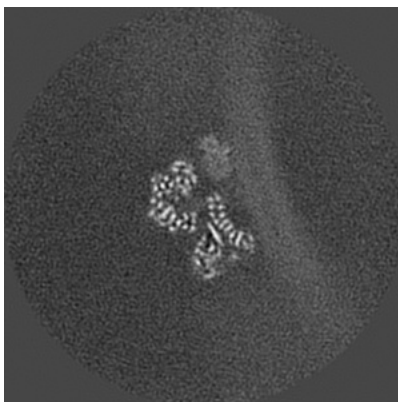
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

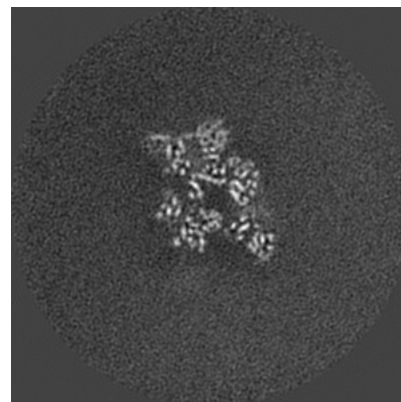
### 6.3.1 Primary map



X Index: 151

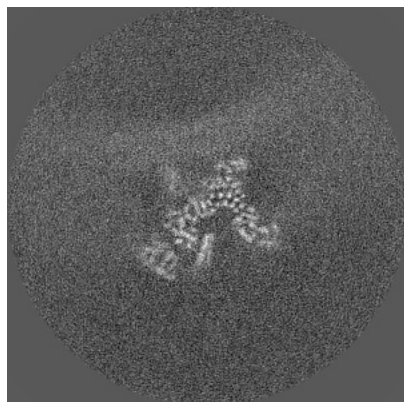


Y Index: 195

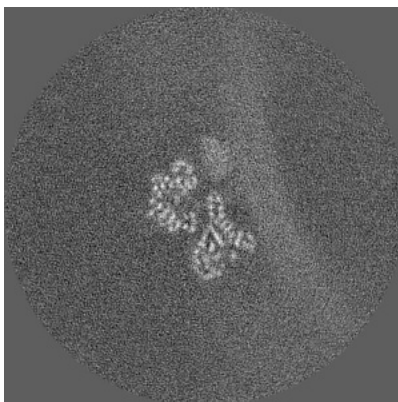


Z Index: 153

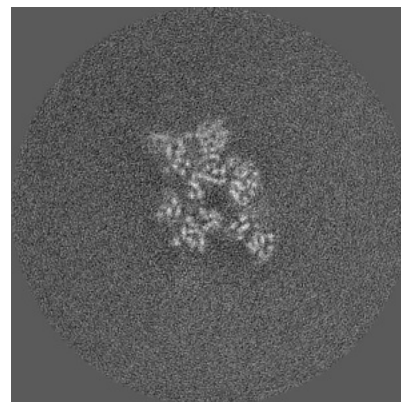
### 6.3.2 Raw map



X Index: 151



Y Index: 196



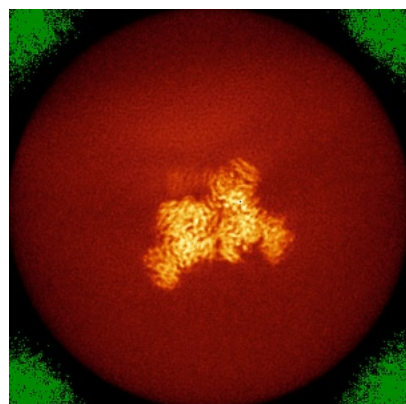
Z Index: 153

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

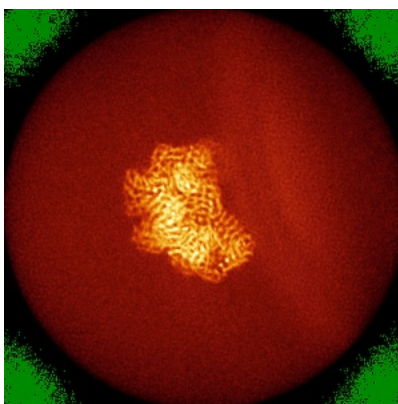


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

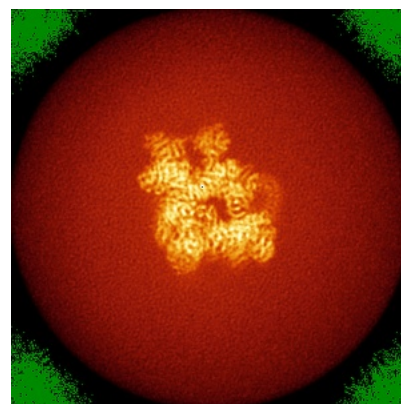
### 6.4.1 Primary map



X

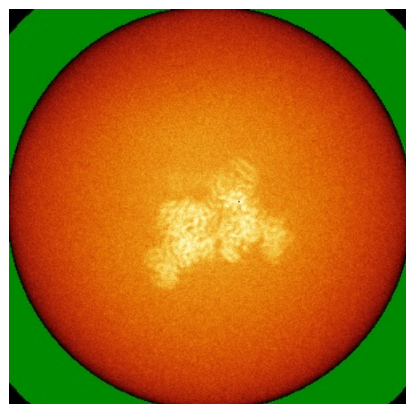


Y

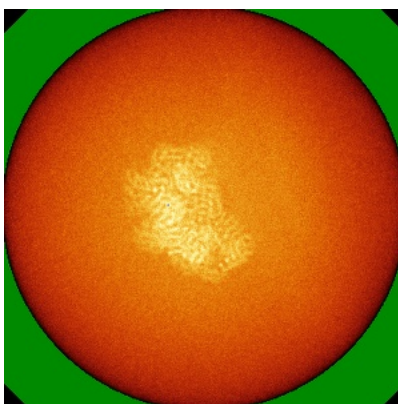


Z

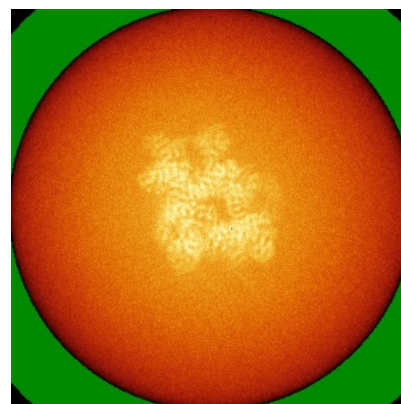
### 6.4.2 Raw map



X



Y



Z

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

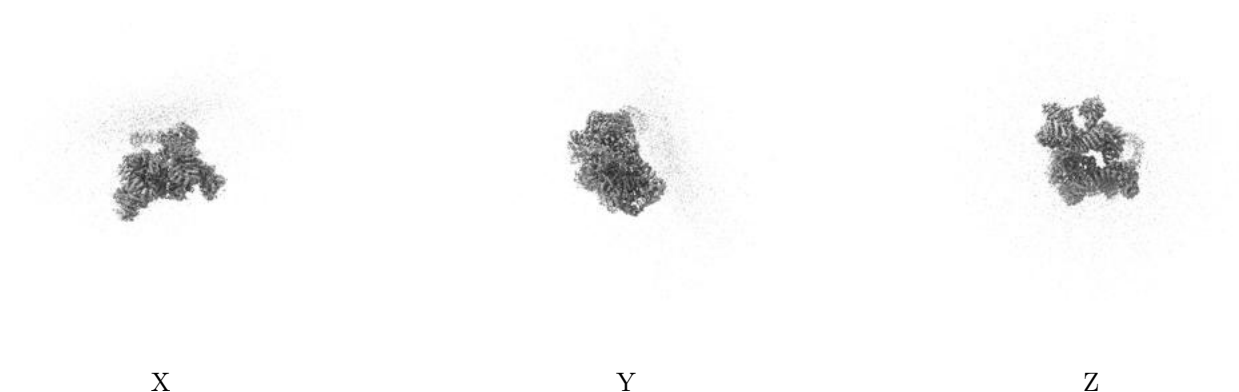
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

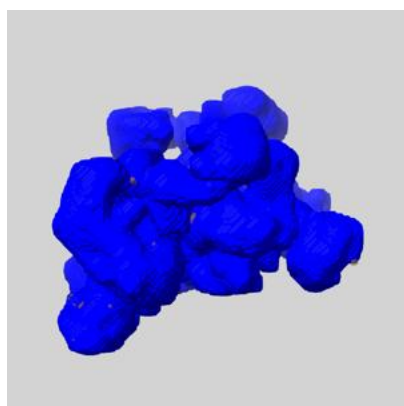
## 6.6 Mask visualisation [i](#)

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

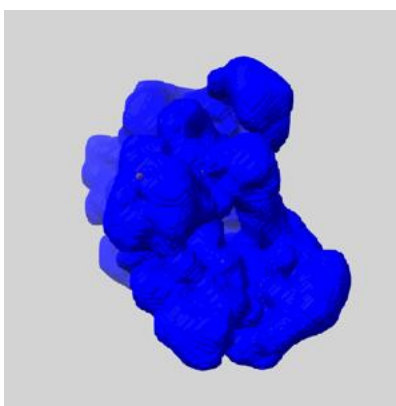
A mask typically either:

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

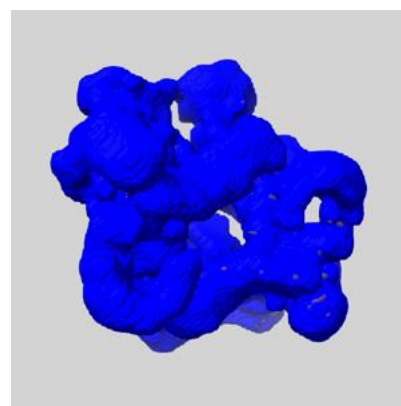
### 6.6.1 emd\_56117\_msk\_1.map [i](#)



X



Y

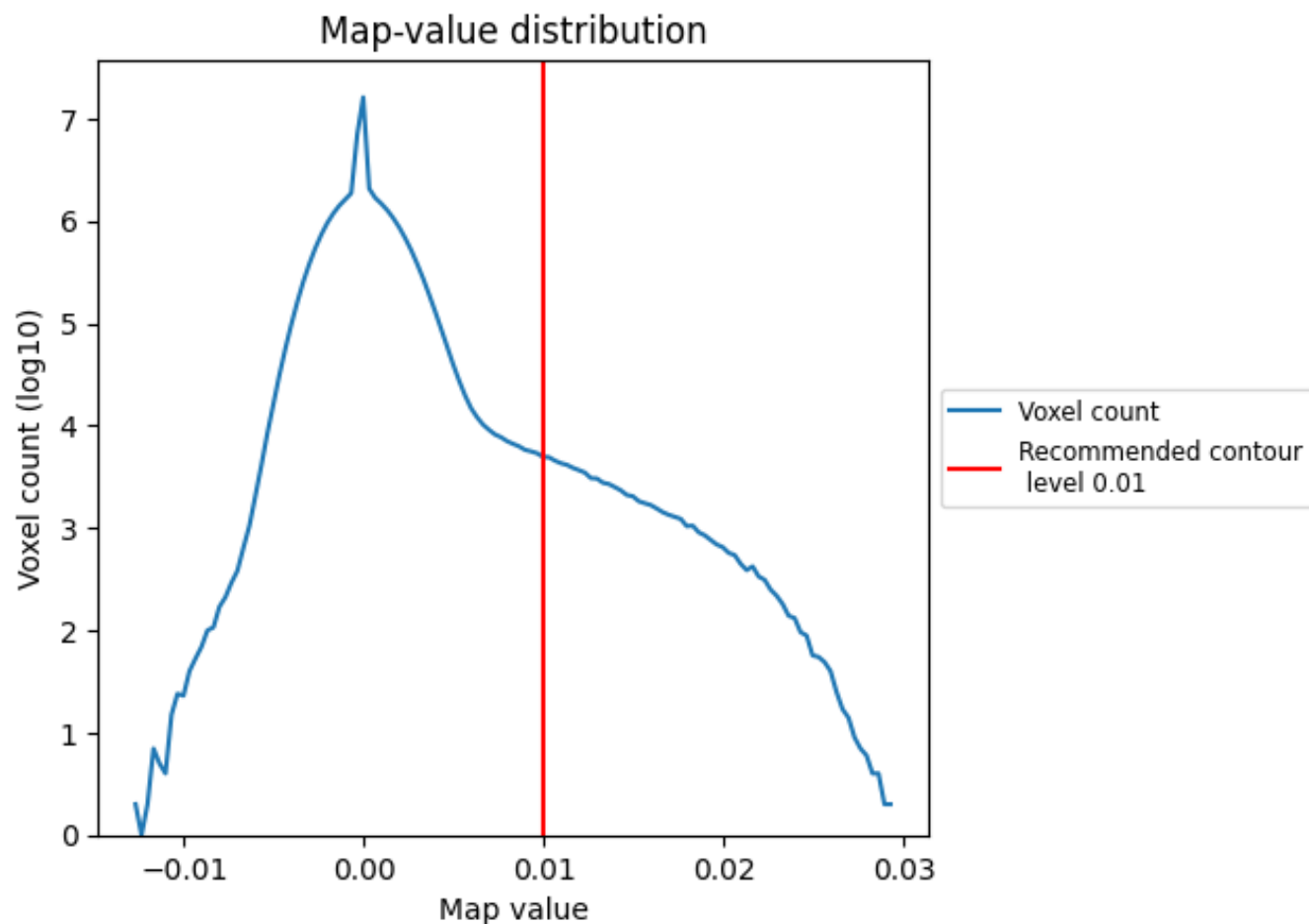


Z

## 7 Map analysis [i](#)

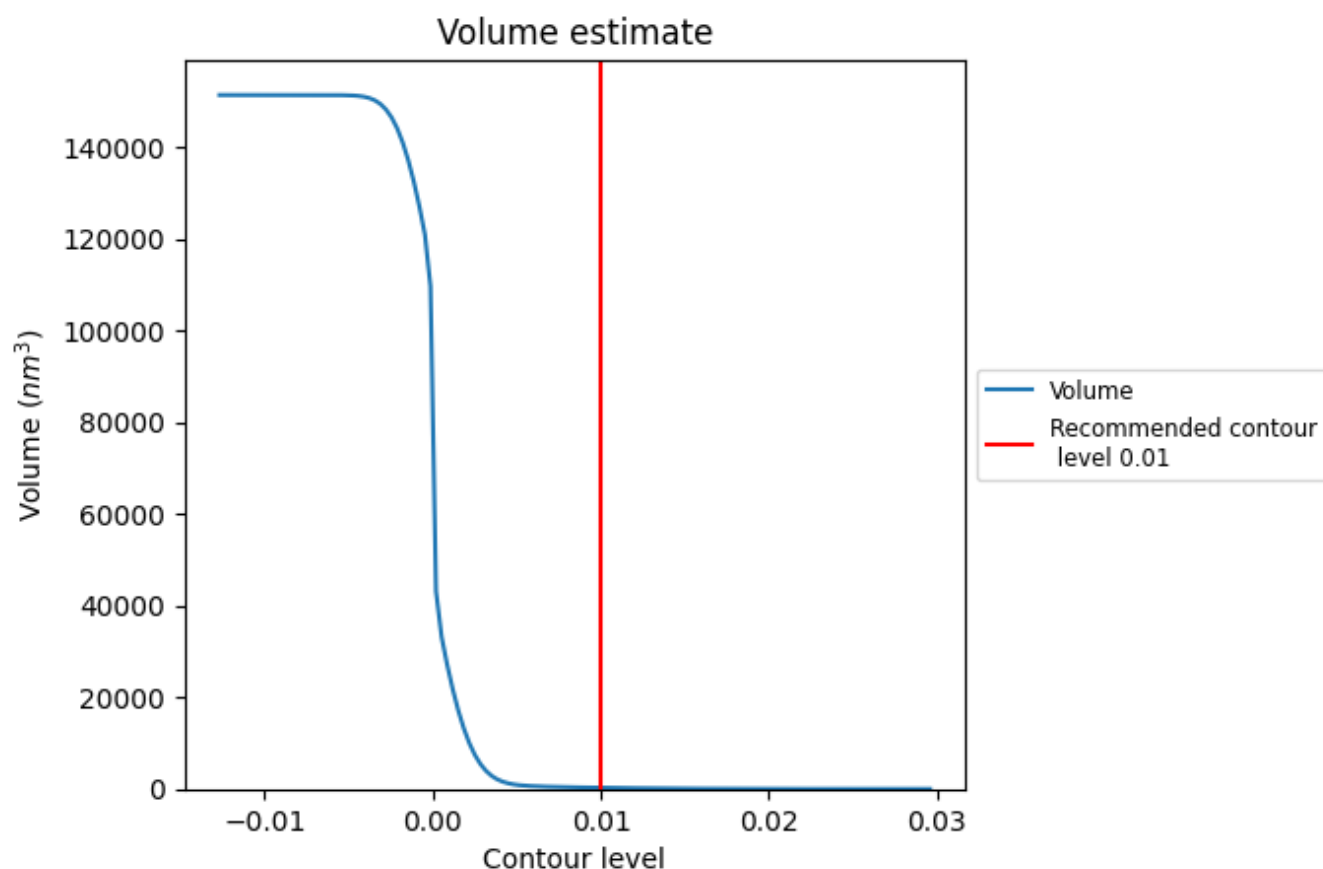
This section contains the results of statistical analysis of the map.

### 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](#)

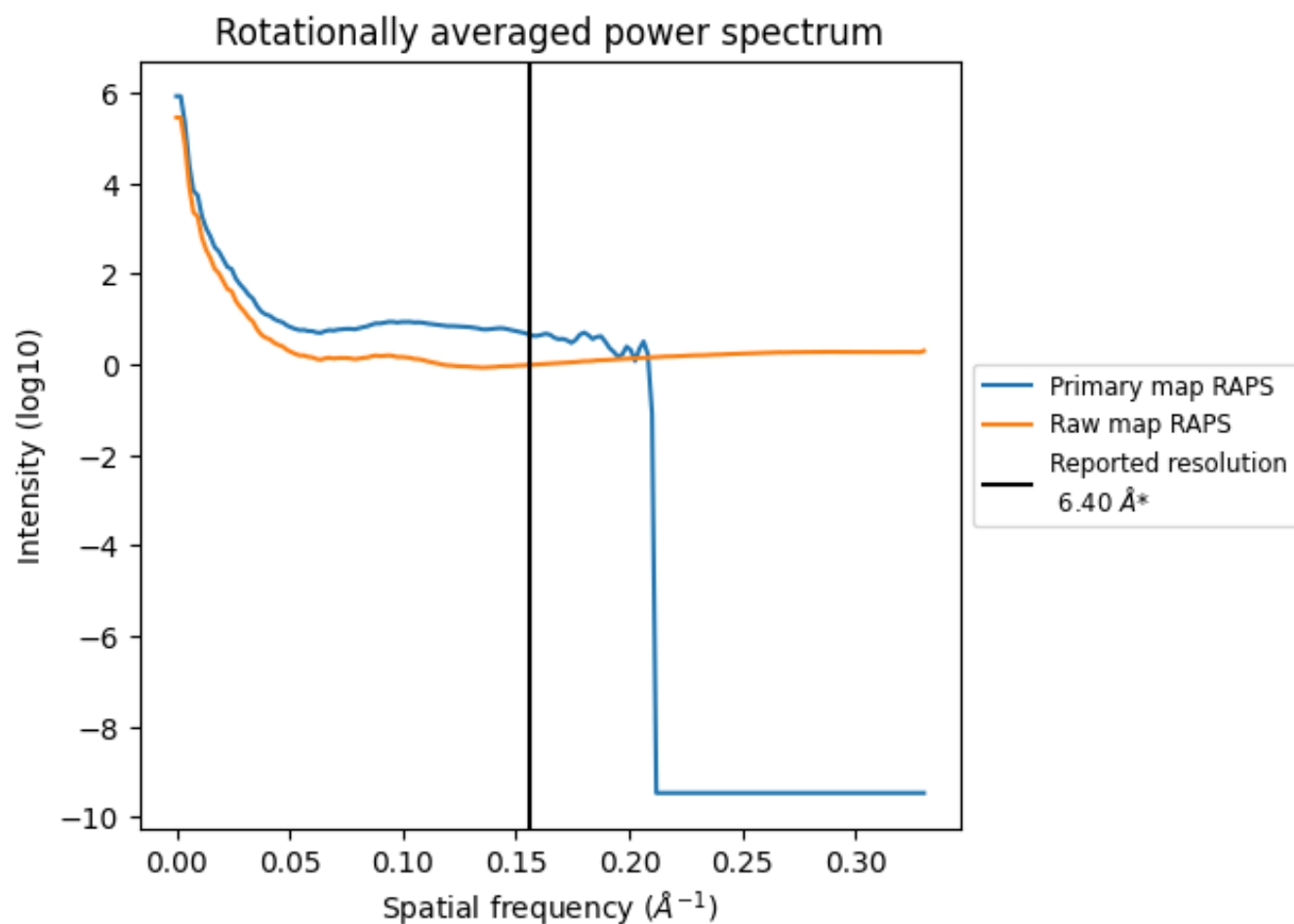


The volume at the recommended contour level is 265  $\text{nm}^3$ ; this corresponds to an approximate mass of 239 kDa.

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 ⓘ

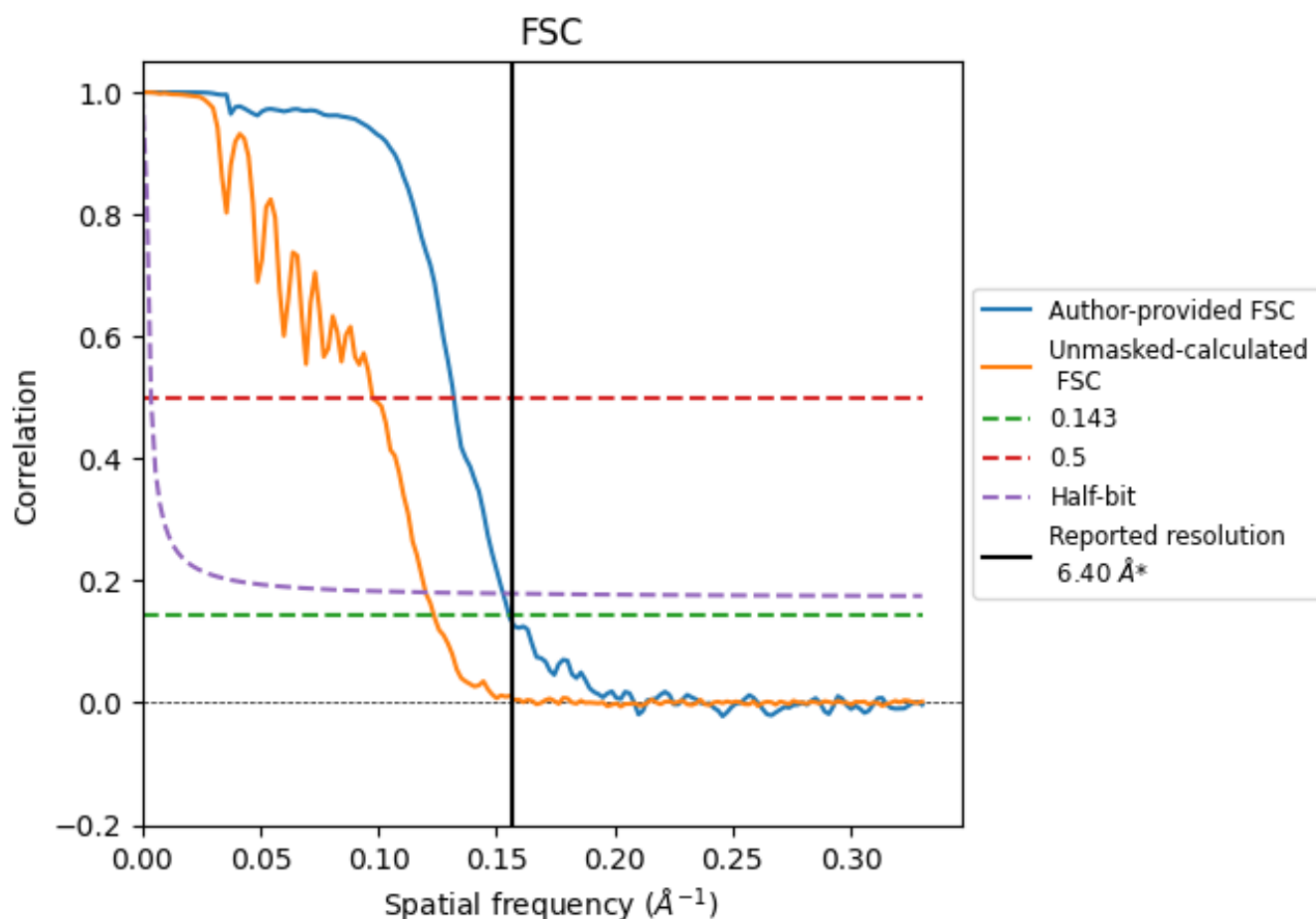


\*Reported resolution corresponds to spatial frequency of  $0.156 \text{ \AA}^{-1}$

## 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  $0.156 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

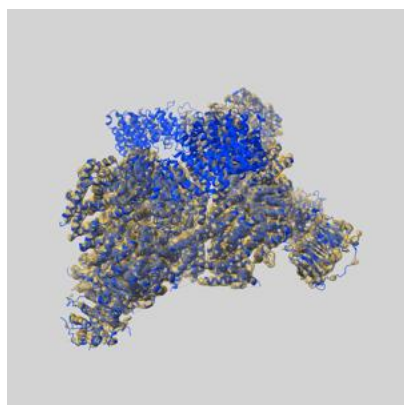
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.40	-	-
Author-provided FSC curve	6.44	7.58	6.54
Unmasked-calculated*	8.09	10.26	8.33

\*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 8.09 differs from the reported value 6.4 by more than 10 %

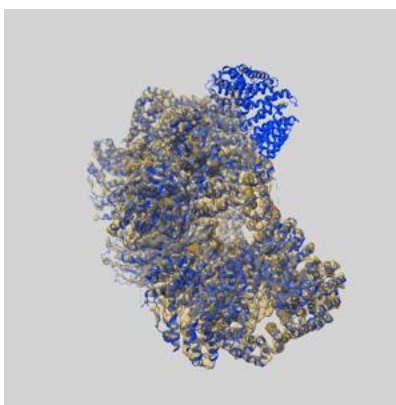
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-56117 and PDB model 9TPW. Per-residue inclusion information can be found in section [3](#) on page [9](#).

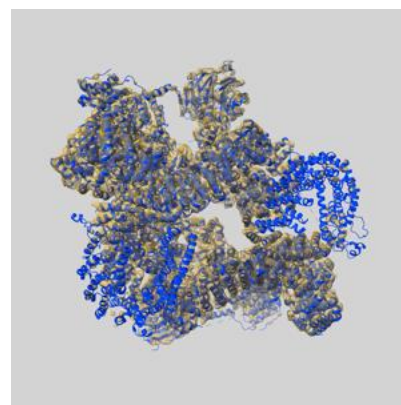
### 9.1 Map-model overlay [i](#)



X



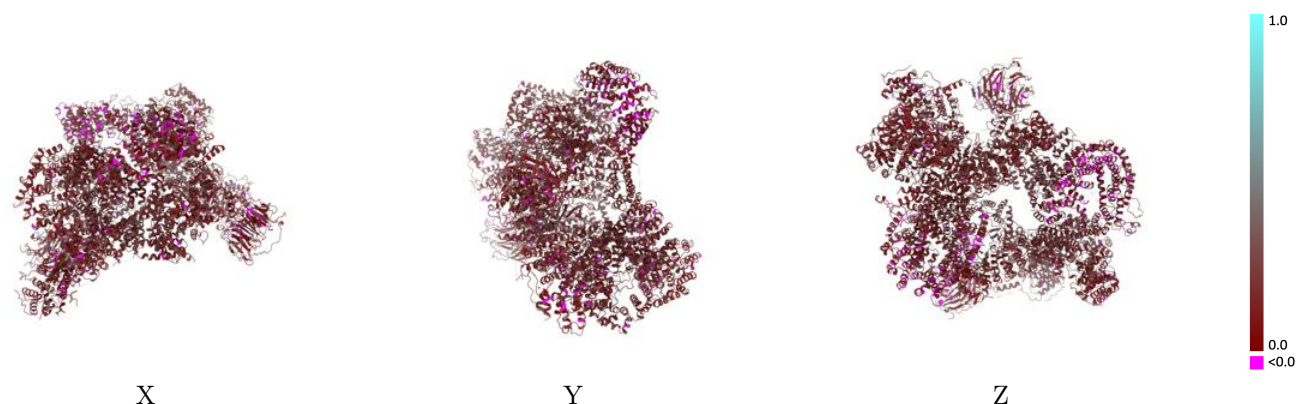
Y



Z

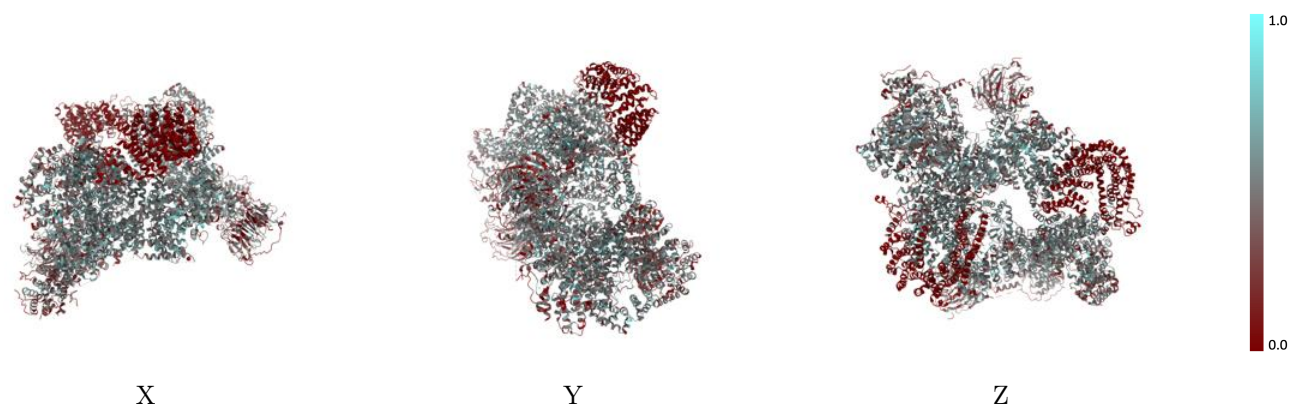
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



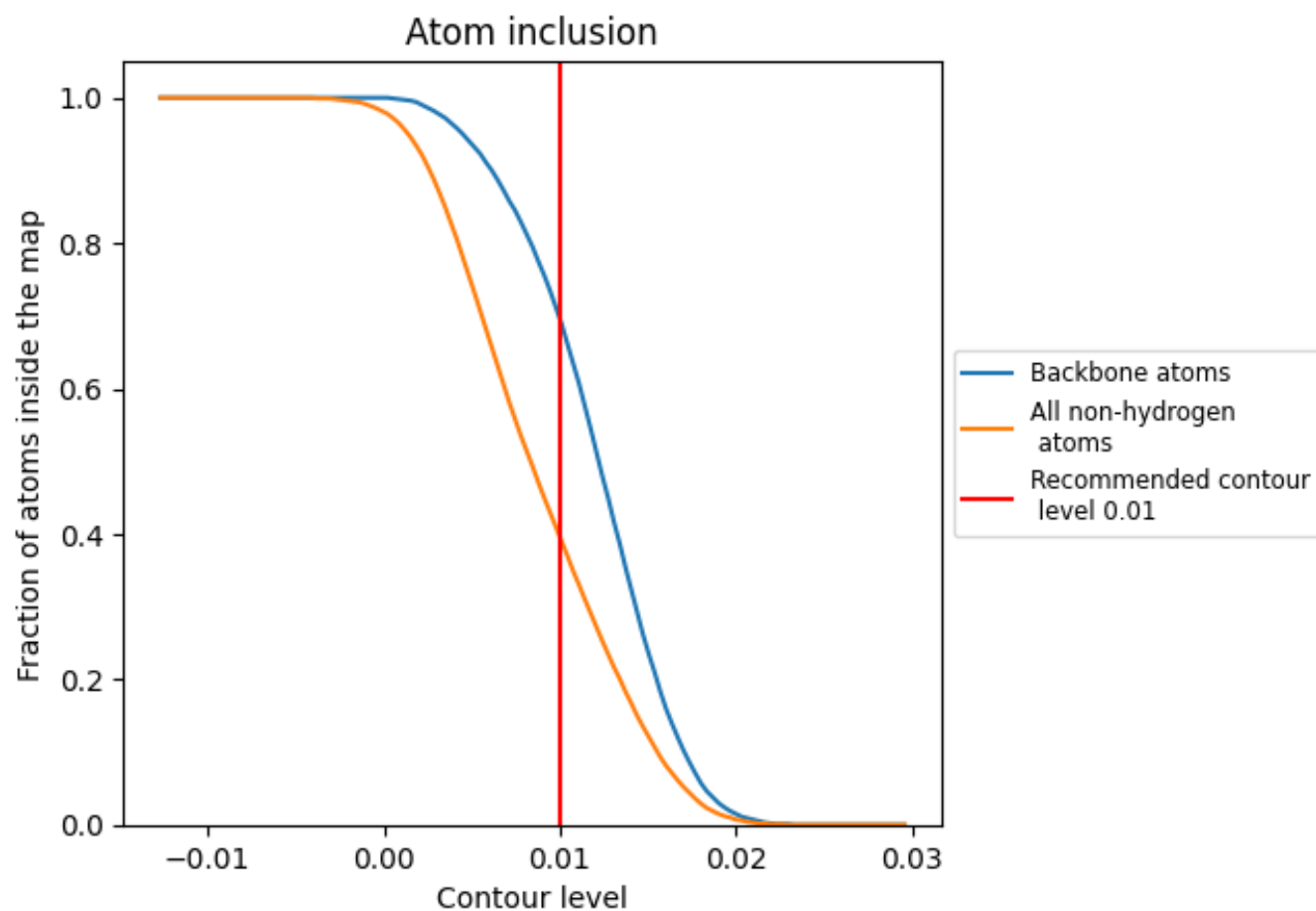
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 40% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.3960	<div></div> 0.1990
A	<div></div> 0.3940	<div></div> 0.1930
B	<div></div> 0.3900	<div></div> 0.1950
C	<div></div> 0.3030	<div></div> 0.1990
D	<div></div> 0.3120	<div></div> 0.1920
E	<div></div> 0.4350	<div></div> 0.2030
F	<div></div> 0.4540	<div></div> 0.2060
G	<div></div> 0.2340	<div></div> 0.2260
H	<div></div> 0.2560	<div></div> 0.2380

1.0

0.0

<0.0