wwPDB EM Validation Summary Report

Nov 10, 2026 – 06:48 pm GMT

PDB ID	:	9T7E / pdb_00009t7e
EMDB ID	:	EMD-55634
Title	:	cryo-EM structure of Lipin1 TOS peptide bound to human mTOR complex 1
Authors	:	Craigie, L.M.; Maier, T.
Deposited on	:	2025-11-10
Resolution	:	3.20 Å(reported)
Based on initial model	:	9F44

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:

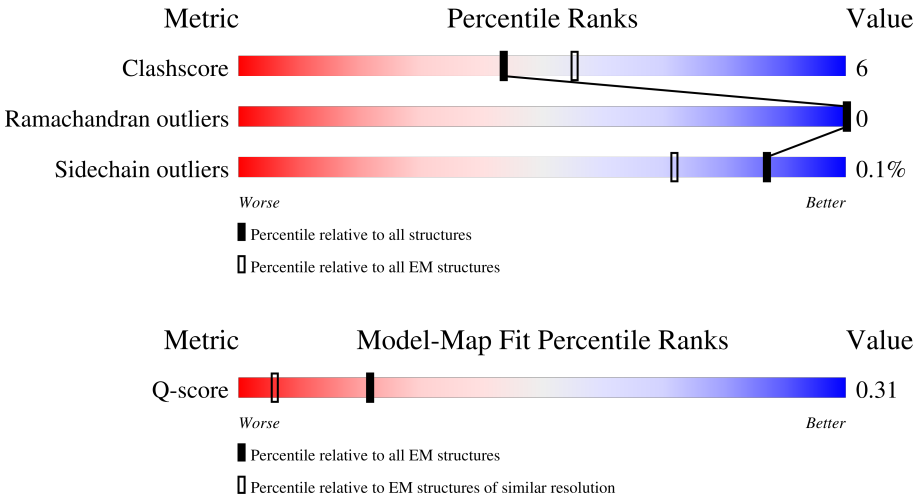
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.51

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 3.20 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.



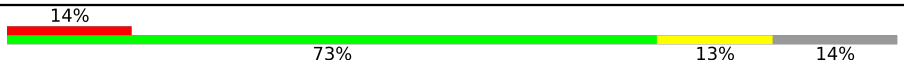
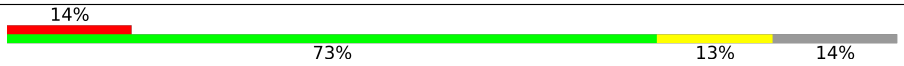
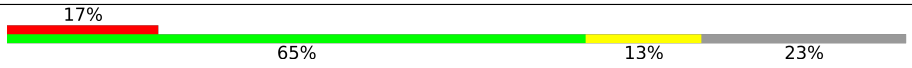
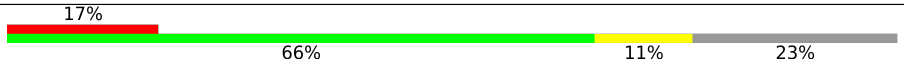
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	C	326	7% 85% 12% ·
1	D	326	7% 84% 13% ·
2	G	11	9% 82% 18%
2	H	11	9% 82% 18%

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Mol	Chain	Length	Quality of chain
3	A	2549	
3	B	2549	
4	E	1363	
4	F	1363	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 113518 atoms, of which 56678 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 Target of rapamycin complex subunit LST8.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	C	317	Total	C	H	N	O	S	0	0
			4797	1526	2341	436	476	18		
1	D	317	Total	C	H	N	O	S	0	0
			4797	1526	2341	436	476	18		

- Molecule 2 is a protein called Phosphatidate phosphatase LPIN1.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	G	9	Total	C	H	N	O	S	0	0
			140	48	64	9	17	2		
2	H	9	Total	C	H	N	O	S	0	0
			140	48	64	9	17	2		

- Molecule 3 is a protein called Serine/threonine-protein kinase mTOR.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	A	2192	Total	C	H	N	O	S	0	0
			35020	11158	17553	3060	3137	112		
3	B	2192	Total	C	H	N	O	S	0	0
			35020	11158	17553	3060	3137	112		

- Molecule 4 is a protein called Regulatory-associated protein of mTOR.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	E	1052	Total	C	H	N	O	S	0	0
			16760	5361	8375	1450	1518	56		
4	F	1052	Total	C	H	N	O	S	0	0
			16760	5361	8375	1450	1518	56		

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-27	HIS	-	expression tag	UNP Q8N122

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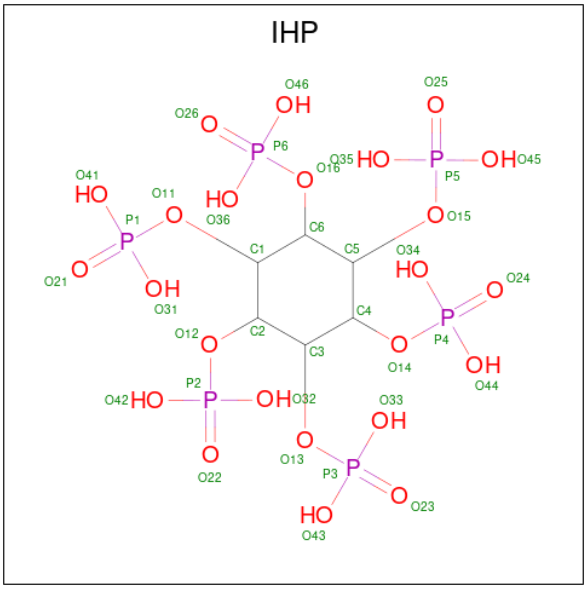
Chain	Residue	Modelled	Actual	Comment	Reference
E	-26	HIS	-	expression tag	UNP Q8N122
E	-25	HIS	-	expression tag	UNP Q8N122
E	-24	HIS	-	expression tag	UNP Q8N122
E	-23	HIS	-	expression tag	UNP Q8N122
E	-22	HIS	-	expression tag	UNP Q8N122
E	-21	HIS	-	expression tag	UNP Q8N122
E	-20	HIS	-	expression tag	UNP Q8N122
E	-19	HIS	-	expression tag	UNP Q8N122
E	-18	HIS	-	expression tag	UNP Q8N122
E	-17	GLU	-	expression tag	UNP Q8N122
E	-16	GLN	-	expression tag	UNP Q8N122
E	-15	LYS	-	expression tag	UNP Q8N122
E	-14	LEU	-	expression tag	UNP Q8N122
E	-13	ILE	-	expression tag	UNP Q8N122
E	-12	SER	-	expression tag	UNP Q8N122
E	-11	GLU	-	expression tag	UNP Q8N122
E	-10	GLU	-	expression tag	UNP Q8N122
E	-9	ASP	-	expression tag	UNP Q8N122
E	-8	LEU	-	expression tag	UNP Q8N122
E	-7	ASP	-	expression tag	UNP Q8N122
E	-6	TYR	-	expression tag	UNP Q8N122
E	-5	LYS	-	expression tag	UNP Q8N122
E	-4	ASP	-	expression tag	UNP Q8N122
E	-3	ASP	-	expression tag	UNP Q8N122
E	-2	ASP	-	expression tag	UNP Q8N122
E	-1	ASP	-	expression tag	UNP Q8N122
E	0	LYS	-	expression tag	UNP Q8N122
F	-27	HIS	-	expression tag	UNP Q8N122
F	-26	HIS	-	expression tag	UNP Q8N122
F	-25	HIS	-	expression tag	UNP Q8N122
F	-24	HIS	-	expression tag	UNP Q8N122
F	-23	HIS	-	expression tag	UNP Q8N122
F	-22	HIS	-	expression tag	UNP Q8N122
F	-21	HIS	-	expression tag	UNP Q8N122
F	-20	HIS	-	expression tag	UNP Q8N122
F	-19	HIS	-	expression tag	UNP Q8N122
F	-18	HIS	-	expression tag	UNP Q8N122
F	-17	GLU	-	expression tag	UNP Q8N122
F	-16	GLN	-	expression tag	UNP Q8N122
F	-15	LYS	-	expression tag	UNP Q8N122
F	-14	LEU	-	expression tag	UNP Q8N122
F	-13	ILE	-	expression tag	UNP Q8N122

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-12	SER	-	expression tag	UNP Q8N122
F	-11	GLU	-	expression tag	UNP Q8N122
F	-10	GLU	-	expression tag	UNP Q8N122
F	-9	ASP	-	expression tag	UNP Q8N122
F	-8	LEU	-	expression tag	UNP Q8N122
F	-7	ASP	-	expression tag	UNP Q8N122
F	-6	TYR	-	expression tag	UNP Q8N122
F	-5	LYS	-	expression tag	UNP Q8N122
F	-4	ASP	-	expression tag	UNP Q8N122
F	-3	ASP	-	expression tag	UNP Q8N122
F	-2	ASP	-	expression tag	UNP Q8N122
F	-1	ASP	-	expression tag	UNP Q8N122
F	0	LYS	-	expression tag	UNP Q8N122

- Molecule 5 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$).

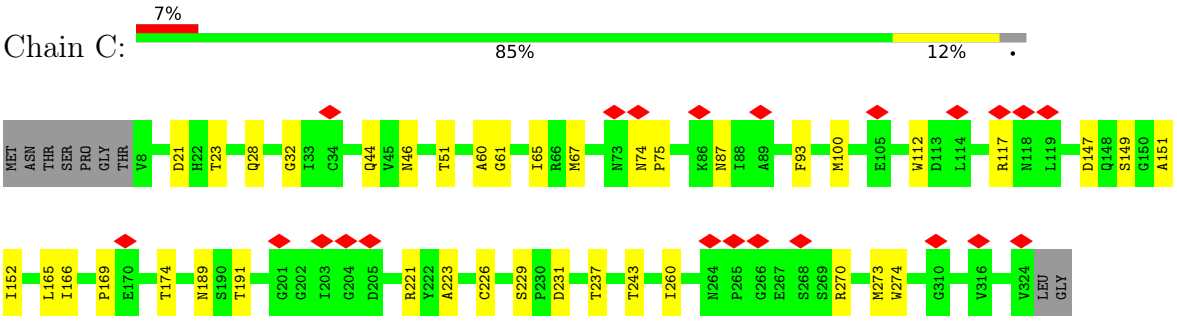


Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	H	O	P	0
			42	6	6	24	6	
5	B	1	Total	C	H	O	P	0
			42	6	6	24	6	

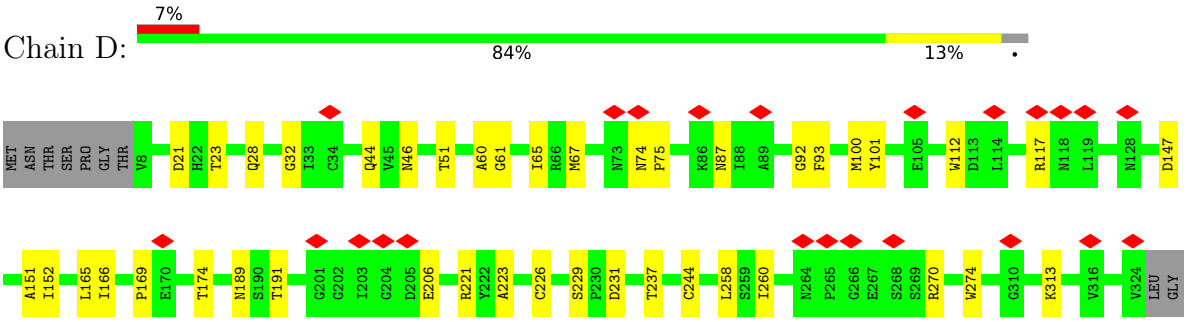
3 Residue-property plots (i)

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.

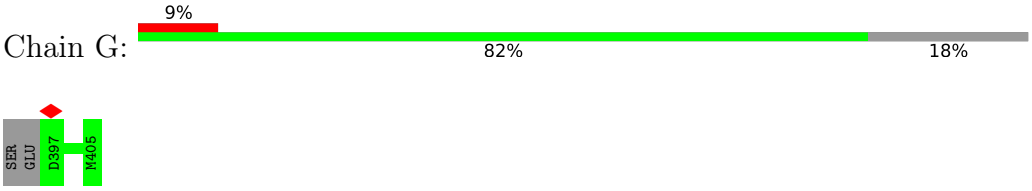
• Molecule 1: Target of rapamycin complex subunit LST8



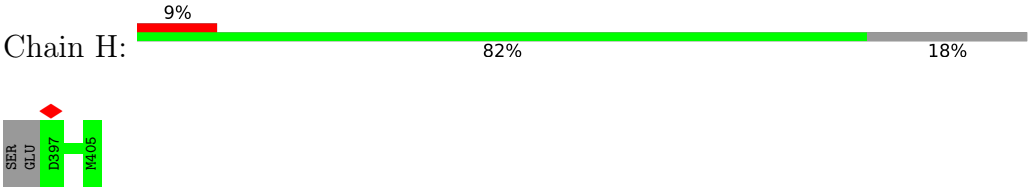
• Molecule 1: Target of rapamycin complex subunit LST8



• Molecule 2: Phosphatidate phosphatase LPIN1



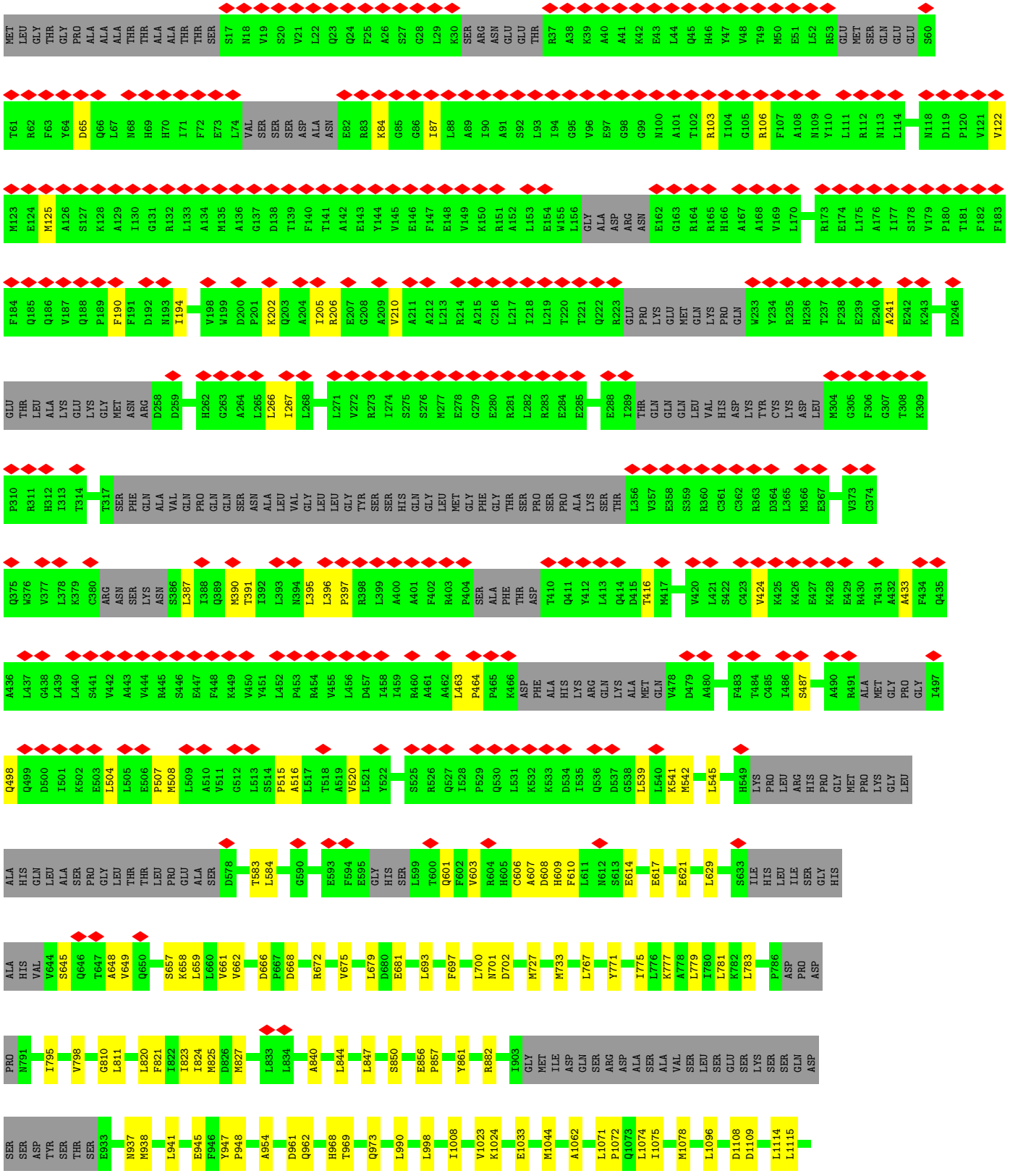
• Molecule 2: Phosphatidate phosphatase LPIN1

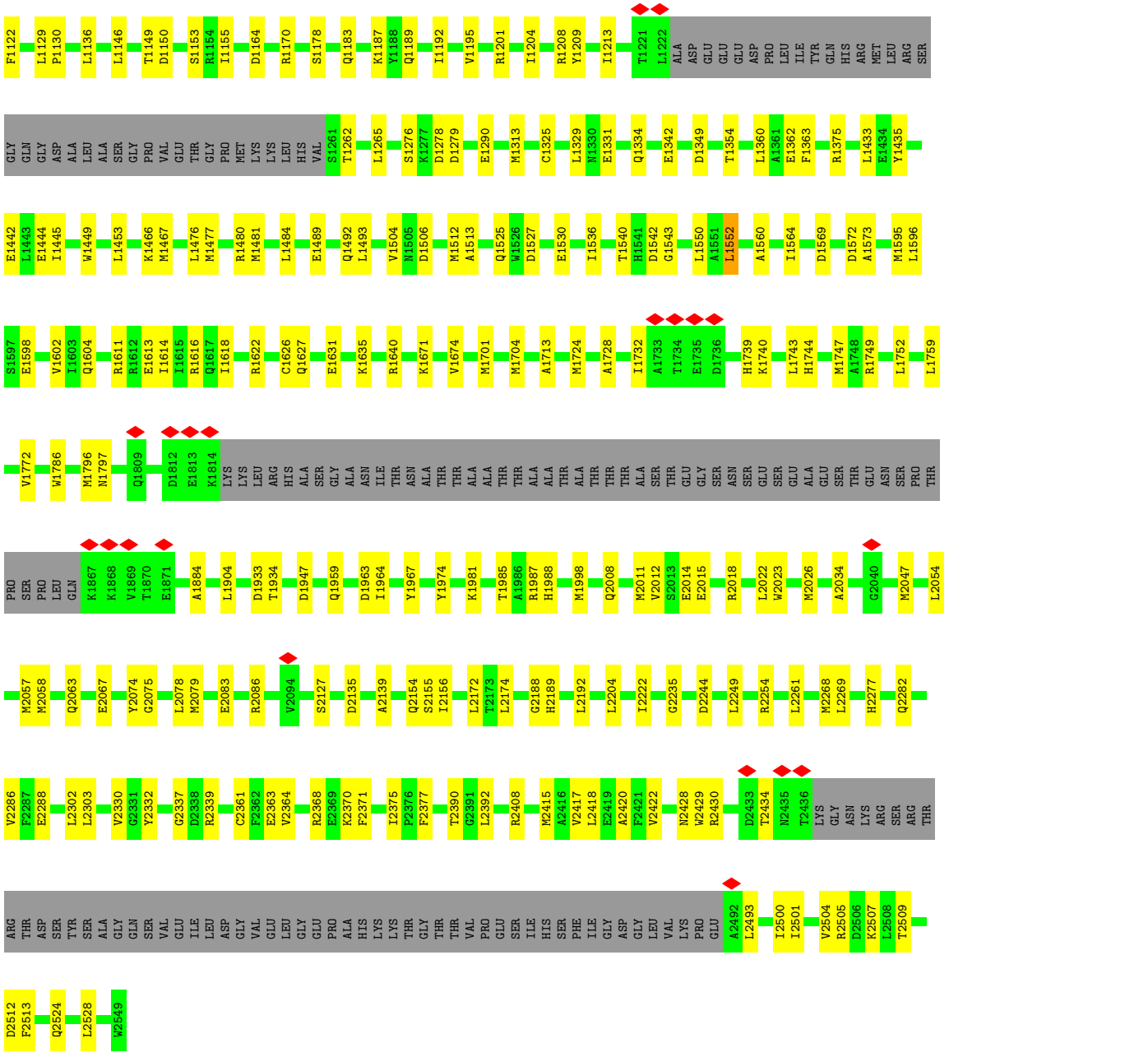


• Molecule 3: Serine/threonine-protein kinase mTOR

Chain A:



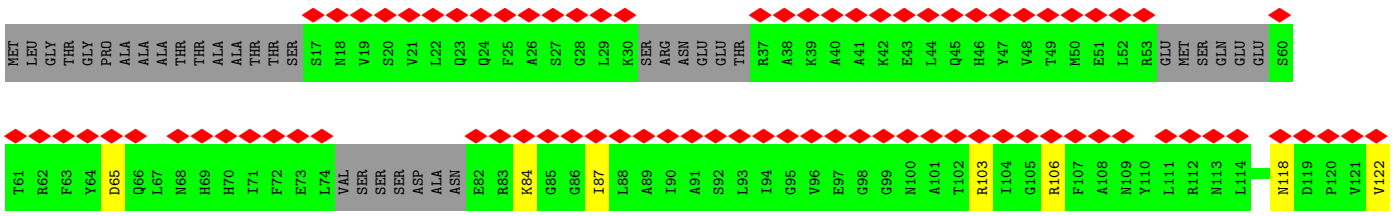




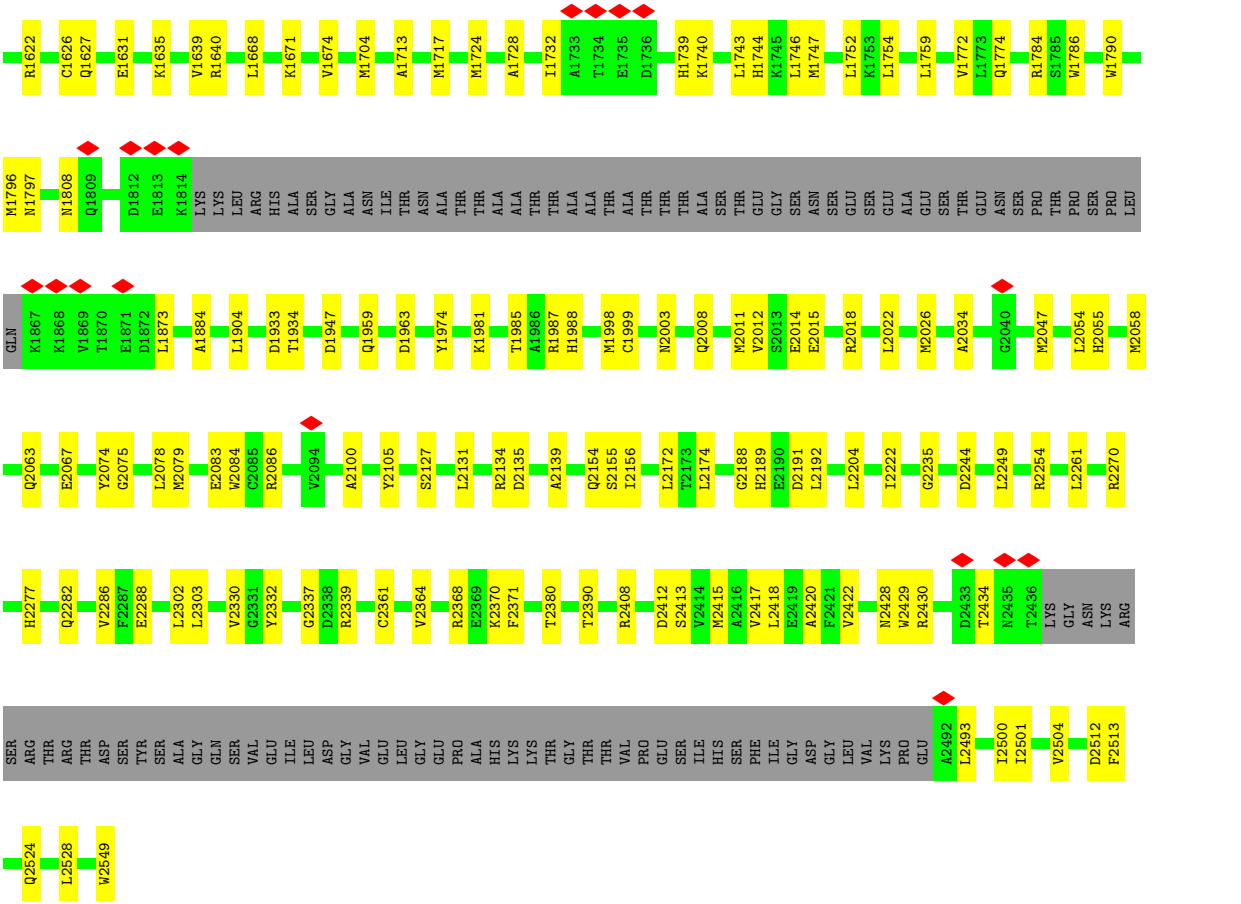
• Molecule 3: Serine/threonine-protein kinase mTOR

Chain B:





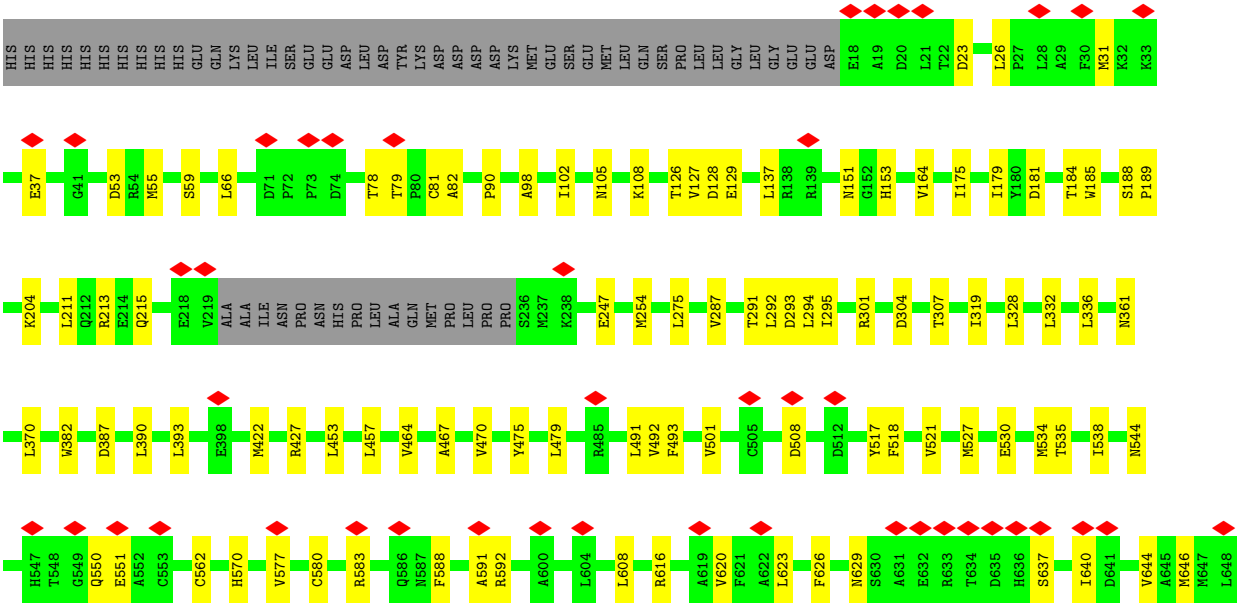

M123 E124 M125 A126 S127 K128 A129 I130 G131 R132 L133 A134 M135 A136 G137 D138 T139 F140 T141 A142 E143 Y144 V145 E146 F147 E148 V149 K150 R151 A152 L153 E154 W155 L156 GLY ALA ASP ARG ASN E162 G163 R164 R165 H166 A167 A168 V169 L170 R173 E174 L175 A176 I177 S178 V179 P180 T181 F182 F183
F184 Q185 Q186 V187 Q188 P189 F190 F191 D192 N193 I194 V198 W199 D200 P201 K202 Q203 A204 I205 R206 E207 G208 A209 V210 A211 A212 L213 R214 A215 C216 L217 I218 L219 T220 T221 Q222 R223 GLU PRO LYS GLU MET GLN LYS PRO GLN W233 Y234 R235 H236 T237 F238 E239 E240 A241 E242 K243 D246
GLU THR LEU ALA LYS GLU LYS GLY MET ASN ARG D258 D259 H262 G263 A264 L265 L266 I267 L268 L271 V272 R273 I274 S275 S276 M277 E278 G279 E280 R281 L282 R283 E284 E285 E288 I289 THR GLN GLN GLN LEU VAL HIS ASP LYS TYR CYS LYS ASP LEU M304 G305 F306 G307 T308 K309
P310 R311 H312 I313 T314 T317 SER PHE GLN ALA VAL GLN PRO GLN GLN GLN SER ASN ALA LEU VAL GLY LEU LEU GLY TYR SER SER HIS GLN GLY LEU MET GLY PHE GLY THR SER PRO SER PRO ALA LYS SER THR L356 V357 E358 S359 R360 C361 C362 R363 D364 L365 M366 E367 V373 C374
Q375 W376 V377 L378 K379 C380 ARG ASN SER LYS ASN S386 L387 I388 Q389 M390 T391 I392 L393 N394 L395 L396 P397 R398 L399 A400 A401 A402 R403 P404 SER ALA PHE THR ASP T410 Q411 Y412 L413 Q414 D415 T416 M417 V420 L421 S422 C423 V424 K425 K426 E427 K428 E429 R430 T431 A432 A433 F434 Q435
A436 L437 G438 L439 L440 S441 V442 A443 V444 R445 S446 E447 F448 K449 V450 Y451 L452 P453 R454 V455 L456 D457 I458 I459 R460 A461 A462 L463 P464 P465 K466 ASP PHE ALA HIS LYS ARG GLN LYS ALA MET GLN V478 D479 A480 F483 T484 C485 I486 S487 M488 L489 A490 R491 ALA MET GLY PRO GLY
I497 Q498 Q499 D500 I501 K502 E503 L504 L505 E506 P507 M508 L509 A510 V511 G512 L513 S514 P515 T518 A519 V520 L521 Y522 S525 R526 Q527 I528 P529 Q530 L531 K532 K533 D534 I535 Q536 D537 G538 L539 L540 K541 M542 L545 H549 LYS PRO LEU ARG HIS PRO GLY MET PRO LYS GLY LEU
ALA HIS GLN LEU ALA SER PRO GLY LEU THR THR LEU PRO GLU ALA SER D578 T583 L584 G590 E593 F594 E595 GLY HIS SER L599 T600 Q601 F602 V603 R604 H605 C606 A607 D608 H609 F610 L611 N612 S613 E614 E617 E621 L629 S633 ILE HIS LEU ILE SER GLY HIS
ALA HIS VAL V644 S645 Q646 T647 A648 V649 Q650 S657 K658 L659 L660 V661 V662 R672 V675 L679 D680 E681 L693 F697 L700 N701 D702 I712 M727 K732 M733 V761 L767 I768 Y771 I775 L776 K777 A778 L779 I780 L781 K782 L783 P786 ASP
PRO ASP PRO N791 V798 G810 L811 L820 F821 I822 I823 I824 L833 L834 A840 L844 L847 S850 E856 P857 R882 I903 GLY MET ILE ASP GLN SER ARG ASP ALA SER ALA VAL SER LEU SER GLU SER LYS SER SER GLN ASP SER SER ASP TYR SER
THR SER E933 N937 M938 L941 E945 F946 Y947 P948 R960 D961 Q962 H968 T969 Q973 T976 L990 L998 I1008 L1019 V1023 K1024 S1025 H1026 E1033 M1044 A1062 L1071 P1072 I1100 D1108 D1109 L1114 L1115 F1122 L1129 P1130
L1136 L1146 T1149 S1153 R1154 I1155 D1164 R1170 S1178 Q1183 K1187 Y1188 Q1189 I1192 V1195 R1201 I1204 R1208 Y1209 I1213 Y1220 T1221 L1222 ALA ASP GLU GLU GLU ASP PRO LEU ILE TYR GLN HIS ARG MET LEU ARG SER GLY GLN GLY ASP ALA
LEU ALA SER GLY PRO VAL GLU THR GLY PRO MET LYS LYS LEU HIS VAL S1261 T1262 L1265 D1278 D1279 E1290 C1325 L1329 N1330 E1331 D1332 Q1333 Q1334 E1342 D1349 T1354 L1360 F1363 R1375 L1433 E1434 Y1435 E1442 L1443 E1444 I1445 W1449 L1453
K1466 L1476 M1477 R1480 L1484 E1489 Q1492 V1504 N1505 D1506 M1512 A1513 Q1525 W1526 D1527 E1530 I1536 T1540 H1541 D1542 G1543 L1550 A1551 L1552 A1560 I1564 D1569 D1572 A1573 M1595 L1596 S1597 E1598 V1602 I1603 Q1604 R1611 R1612 E1613 R1616

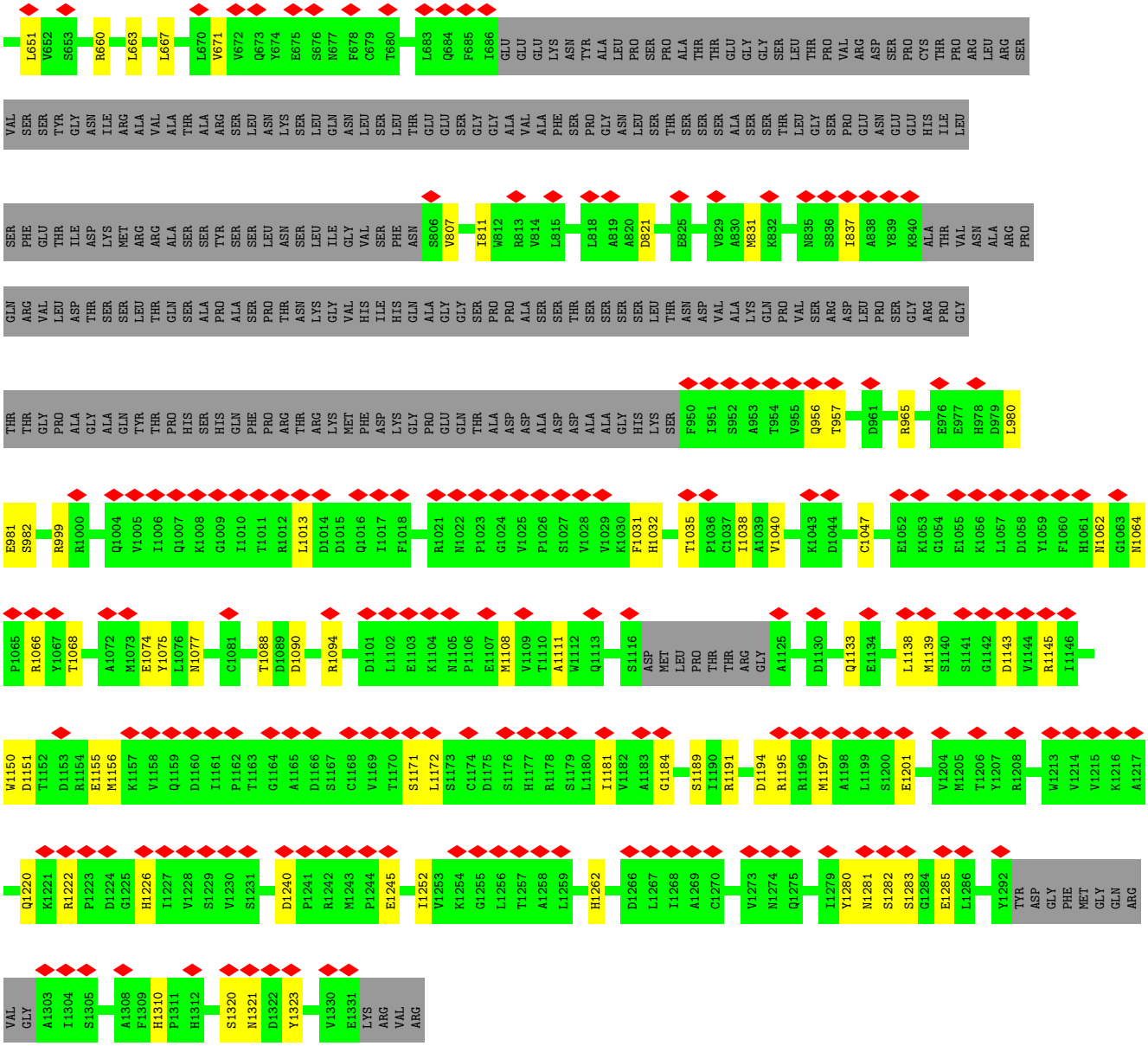


• Molecule 4: Regulatory-associated protein of mTOR

Chain E:



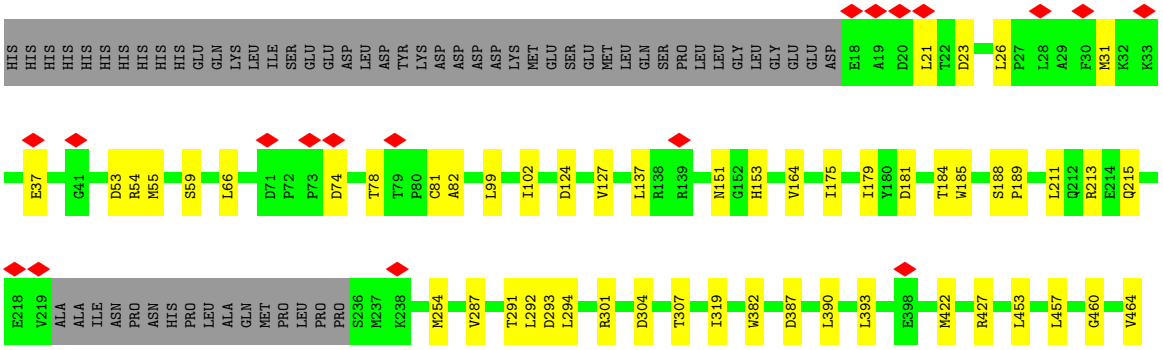


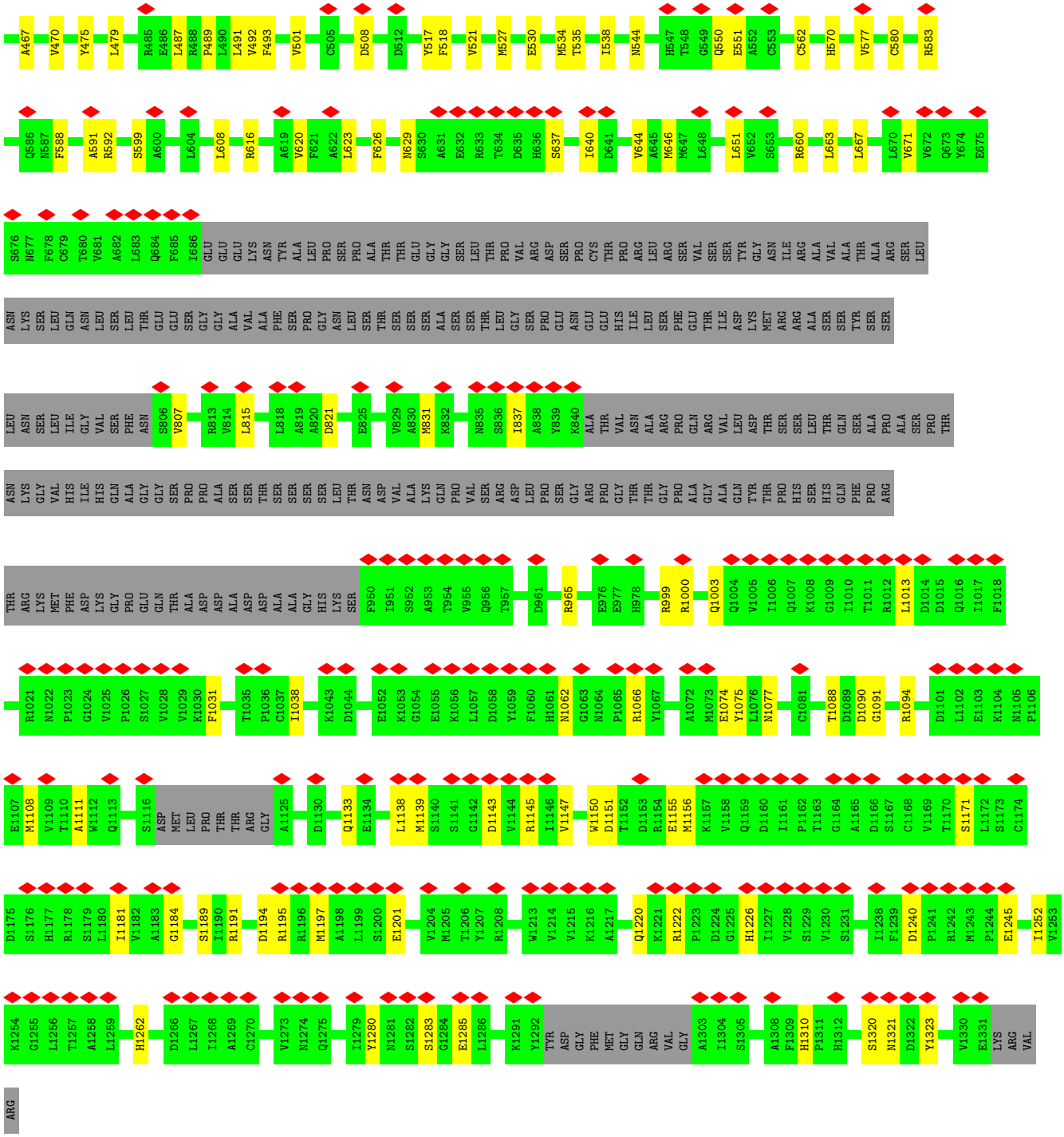


• Molecule 4: Regulatory-associated protein of mTOR

Chain F:






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Q586 N587 F588 A591 R592 S599 A600 L604 L608 R616 A619 V620 F621 A622 L623 F626 W629 S630 A631 E632 R633 T634 D635 H636 S637 I640 D641 V644 A645 M646 M647 L648 L651 V652 S653 R660 L663 L667 L670 V671 V672 Q673 Y674 E675
S676 N677 F678 C679 T680 V681 A682 L683 Q684 F685 I686 GLU GLU GLU LYS ASN TYR ALA LEU PRO SER PRO ALA THR THR GLU GLY GLY SER LEU THR PRO VAL ARG ASP SER PRO CYS THR PRO ARG LEU ARG SER VAL SER SER TYR GLY ASN ILE ARG ALA VAL ALA THR ALA ARG SER LEU
ASN LYS SER LEU GLN ASN LEU SER LEU THR GLU GLU SER GLY GLY ALA VAL ALA PHE SER PRO GLY ASN LEU SER THR SER SER ALA SER SER THR LEU GLY SER PRO GLU ASN GLU GLU HIS ILE LEU SER PHE GLU THR ILE ASP LYS MET ARG ARG ALA SER SER TYR SER SER
LEU ASN SER LEU ILE GLY VAL SER PHE ASN S806 V807 R813 V814 L815 L818 A819 A820 D821 E825 V829 A830 M831 K832 N835 S836 I837 A838 Y839 K840 ALA THR VAL ASN ALA ARG PRO GLN ARG VAL LEU ASP THR SER SER LEU THR GLN SER ALA PRO ALA SER PRO THR
ASN LYS GLY VAL HIS ILE HIS GLN ALA GLY GLY SER PRO PRO ALA SER SER THR SER SER SER SER LEU THR ASN ASP VAL ALA LYS GLN PRO VAL SER ARG ASP LEU PRO SER GLY ARG PRO GLY THR THR GLY PRO ALA ALA GLY ALA GLN TYR THR PRO HIS SER HIS GLN PHE PRO ARG
THR ARG LYS MET PHE ASP LYS GLY PRO GLU GLN THR ALA ASP ASP ALA ASP ASP ALA ALA GLY HIS LYS SER F950 I951 S952 A953 T954 V955 Q956 T957 D961 R965 E976 E977 H978 R999 R1000 Q1003 Q1004 V1005 I1006 Q1007 K1008 G1009 I1010 T1011 R1012 L1013 D1014 D1015 Q1016 I1017 F1018
R1021 N1022 P1023 G1024 V1025 P1026 S1027 V1028 V1029 K1030 F1031 T1035 P1036 C1037 I1038 K1043 D1044 E1052 K1053 G1054 E1055 K1056 L1057 D1058 Y1059 F1060 H1061 N1062 G1063 N1064 P1065 R1066 Y1067 A1072 M1073 E1074 Y1075 L1076 N1077 C1081 T1088 D1089 D1090 G1091 R1094 D1101 L1102 E1103 K1104 N1105 P1106
E1107 M1108 V1109 T1110 A1111 W1112 Q1113 S1116 ASP MET LEU PRO THR THR ARG GLY A1125 D1130 Q1133 E1134 L1138 M1139 S1140 S1141 G1142 D1143 V1144 R1145 I1146 V1147 W1150 D1151 T1152 D1153 R1154 E1155 M1156 K1157 V1158 Q1159 D1160 I1161 P1162 T1163 G1164 A1165 D1166 S1167 C1168 V1169 T1170 S1171 L1172 S1173 C1174
D1175 S1176 H1177 R1178 S1179 L1180 I1181 V1182 A1183 G1184 S1189 T1190 R1191 D1194 R1195 R1196 M1197 A1198 L1199 S1200 E1201 V1204 M1205 T1206 Y1207 R1208 W1213 V1214 V1215 K1216 A1217 Q1220 K1221 R1222 P1223 D1224 G1225 H1226 I1227 V1228 S1229 V1230 S1231 I1238 F1239 D1240 P1241 R1242 M1243 P1244 E1245 I1252 V1253
K1254 G1255 L1256 T1257 A1258 L1259 H1262 D1266 L1267 I1268 A1269 C1270 V1273 N1274 Q1275 I1279 Y1280 N1281 S1282 S1283 G1284 E1285 L1286 K1291 Y1292 TYR ASP GLY PHE MET GLY GLN ARG VAL GLY A1303 I1304 S1305 A1308 F1309 H1310 P1311 H1312 S1320 N1321 D1322 Y1323 V1330 E1331 LYS ARG VAL
ARG

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	425626	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.566	Depositor
Minimum map value	-0.296	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	467.2, 467.2, 467.2	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.97333336, 0.97333336, 0.97333336	Depositor

5 Model quality

5.1 Standard geometry

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

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	C	0.07	0/2514	0.23	0/3426
1	D	0.07	0/2514	0.23	0/3426
2	G	0.11	0/77	0.30	0/102
2	H	0.09	0/77	0.23	0/102
3	A	0.10	0/17814	0.25	0/24116
3	B	0.10	0/17814	0.25	0/24116
4	E	0.09	0/8585	0.23	0/11680
4	F	0.09	0/8585	0.24	0/11680
All	All	0.10	0/57980	0.24	0/78648

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	C	2456	2341	2341	23	0
1	D	2456	2341	2341	26	0
2	G	76	64	64	0	0
2	H	76	64	64	0	0
3	A	17467	17553	17553	231	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	17467	17553	17553	234	0
4	E	8385	8375	8375	120	0
4	F	8385	8375	8375	110	0
5	A	36	6	6	0	0
5	B	36	6	6	0	0
All	All	56840	56678	56678	735	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 6.

The worst 5 of 735 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)
4:F:304:ASP:OD1	4:F:307:THR:OG1	1.93	0.86
4:E:620:VAL:HG11	4:E:663:LEU:HD23	1.58	0.86
4:F:620:VAL:HG11	4:F:663:LEU:HD23	1.59	0.85
3:B:1146:LEU:O	3:B:1183:GLN:NE2	2.13	0.81
3:A:1146:LEU:O	3:A:1183:GLN:NE2	2.14	0.80

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	C	315/326 (97%)	304 (96%)	11 (4%)	0	100	100
1	D	315/326 (97%)	304 (96%)	11 (4%)	0	100	100
2	G	7/11 (64%)	6 (86%)	1 (14%)	0	100	100
2	H	7/11 (64%)	7 (100%)	0	0	100	100
3	A	2150/2549 (84%)	2099 (98%)	51 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	B	2150/2549 (84%)	2095 (97%)	55 (3%)	0	100	100
4	E	1040/1363 (76%)	1005 (97%)	35 (3%)	0	100	100
4	F	1040/1363 (76%)	1007 (97%)	33 (3%)	0	100	100
All	All	7024/8498 (83%)	6827 (97%)	197 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	C	269/276 (98%)	268 (100%)	1 (0%)	84	86
1	D	269/276 (98%)	268 (100%)	1 (0%)	84	86
2	G	9/11 (82%)	9 (100%)	0	100	100
2	H	9/11 (82%)	9 (100%)	0	100	100
3	A	1876/2220 (84%)	1873 (100%)	3 (0%)	87	89
3	B	1876/2220 (84%)	1876 (100%)	0	100	100
4	E	928/1191 (78%)	926 (100%)	2 (0%)	87	89
4	F	928/1191 (78%)	926 (100%)	2 (0%)	87	89
All	All	6164/7396 (83%)	6155 (100%)	9 (0%)	87	91

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	F	551	GLU
4	F	1323	TYR
3	A	1552	LEU
3	A	2392	LEU
4	E	551	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
3	B	1157	HIS
3	B	2154	GLN
3	B	1915	HIS
4	E	242	GLN
3	A	1157	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	IHP	A	2601	-	36,36,36	0.77	1 (2%)	54,60,60	0.36	0
5	IHP	B	2601	-	36,36,36	0.77	1 (2%)	54,60,60	0.36	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	IHP	A	2601	-	-	4/30/54/54	0/1/1/1
5	IHP	B	2601	-	-	4/30/54/54	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	2601	IHP	P3-O13	2.98	1.64	1.59
5	A	2601	IHP	P3-O13	2.98	1.64	1.59

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

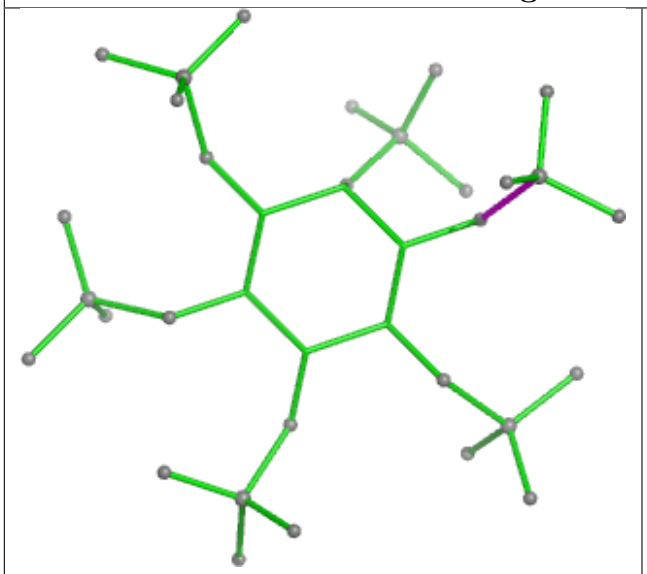
Mol	Chain	Res	Type	Atoms
5	A	2601	IHP	C2-O12-P2-O22
5	B	2601	IHP	C2-O12-P2-O22
5	A	2601	IHP	C1-O11-P1-O31
5	A	2601	IHP	C2-O12-P2-O32
5	A	2601	IHP	C4-O14-P4-O34

There are no ring outliers.

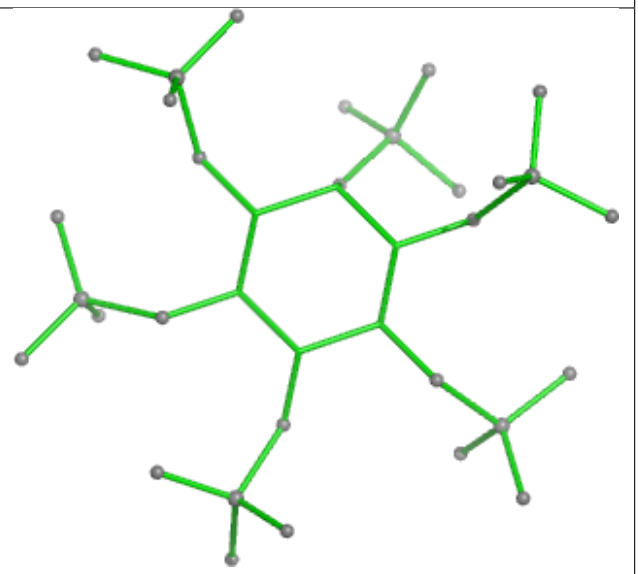
No monomer is involved in short contacts.

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

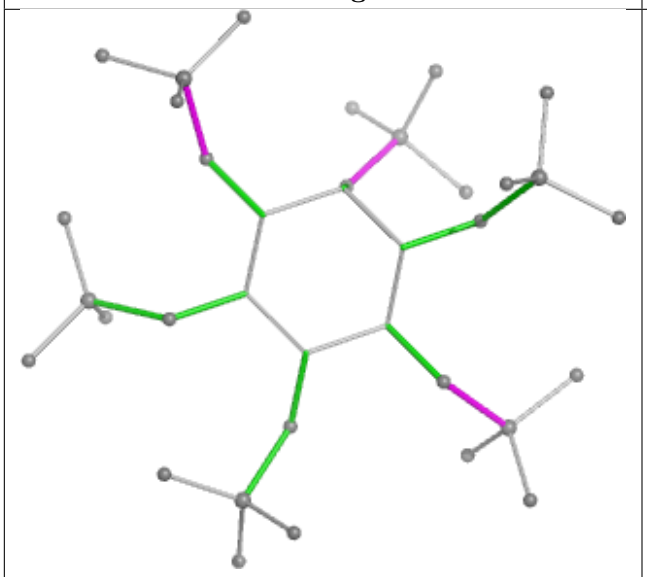
Ligand IHP A 2601



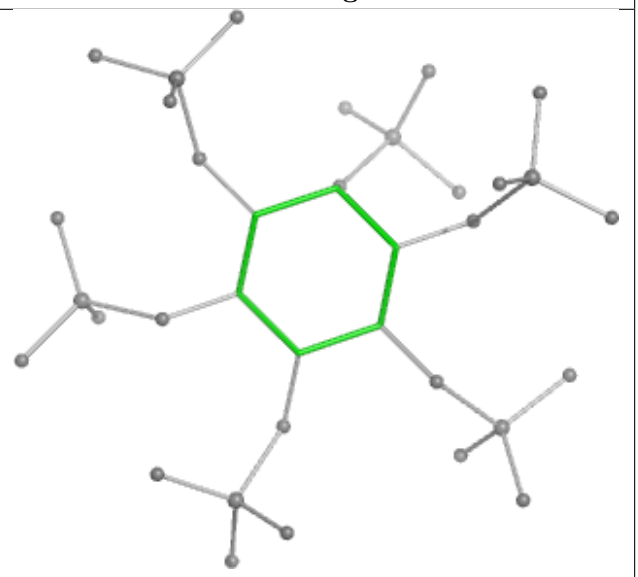
Bond lengths



Bond angles

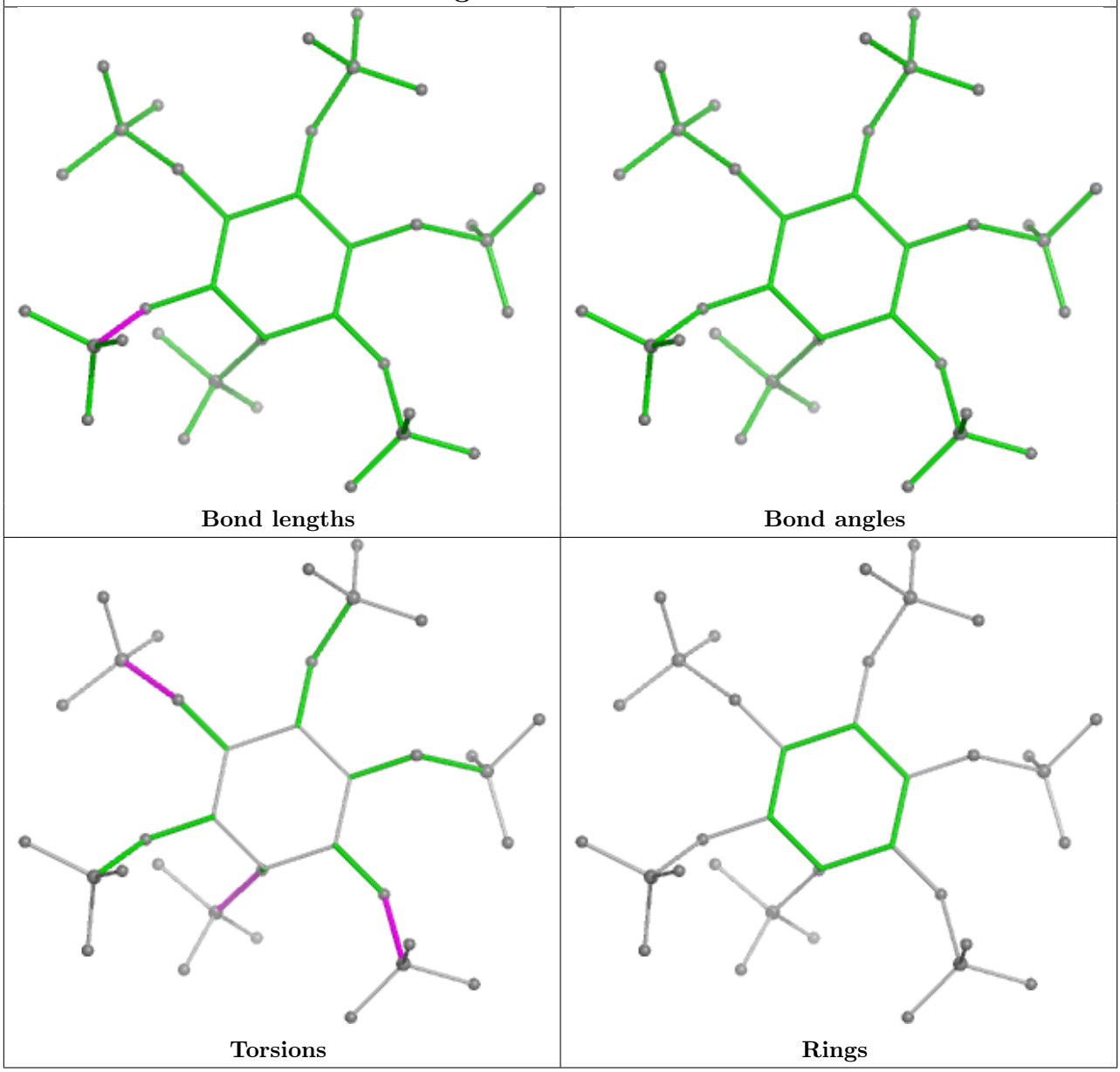


Torsions



Rings

Ligand IHP B 2601



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.

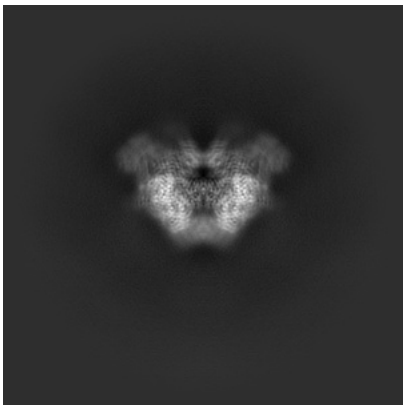
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-55634. These allow visual inspection of the internal detail of the map and identification of artifacts.

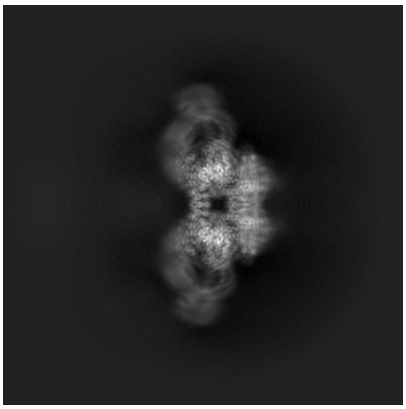
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

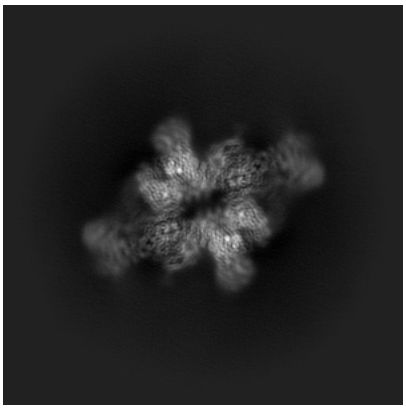
6.1.1 Primary map



X

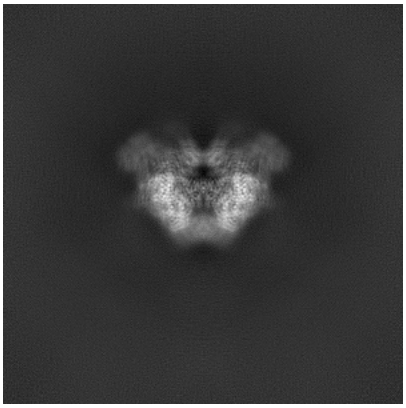


Y

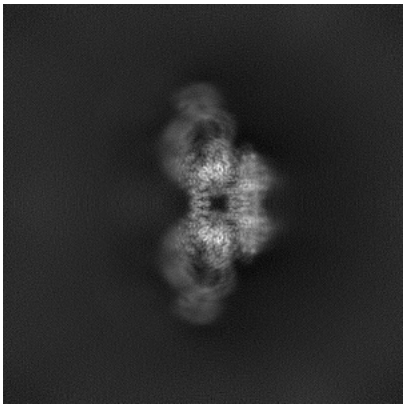


Z

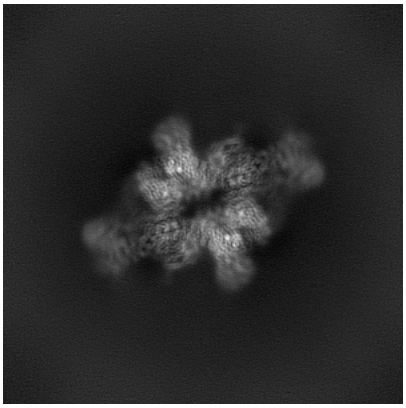
6.1.2 Raw map



X



Y



Z

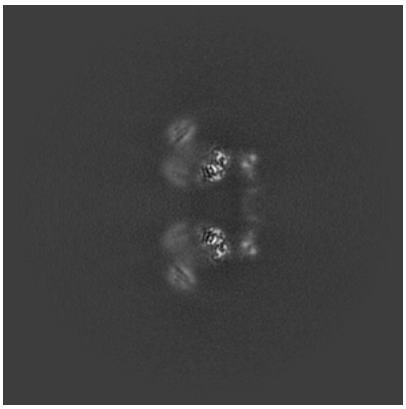
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

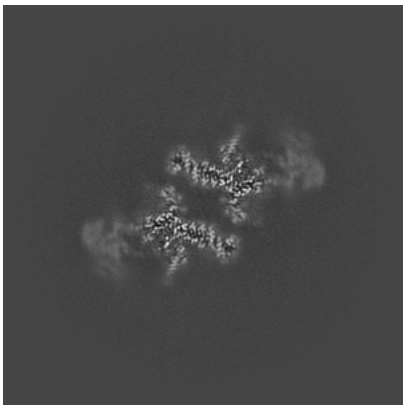
6.2.1 Primary map



X Index: 240



Y Index: 240

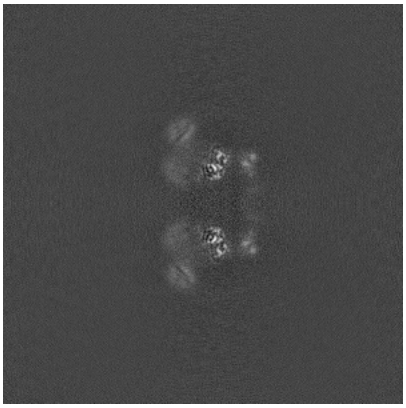


Z Index: 240

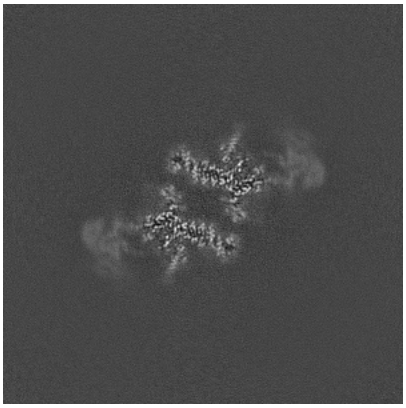
6.2.2 Raw map



X Index: 240



Y Index: 240

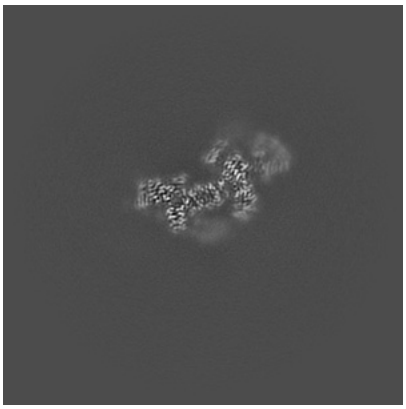


Z Index: 240

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

6.3 Largest variance slices (i)

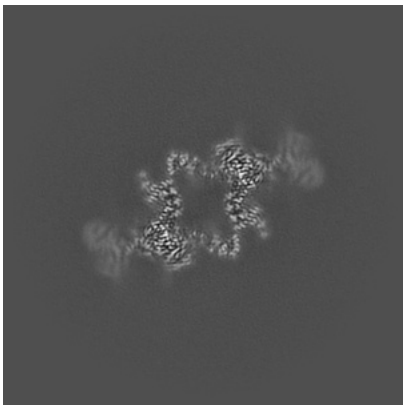
6.3.1 Primary map



X Index: 204

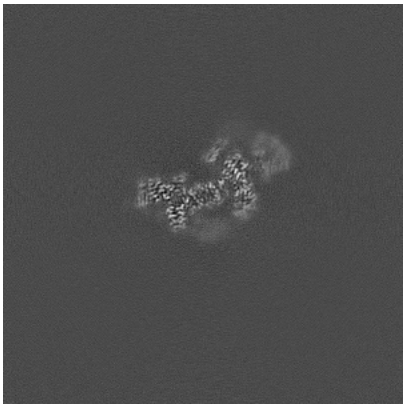


Y Index: 282

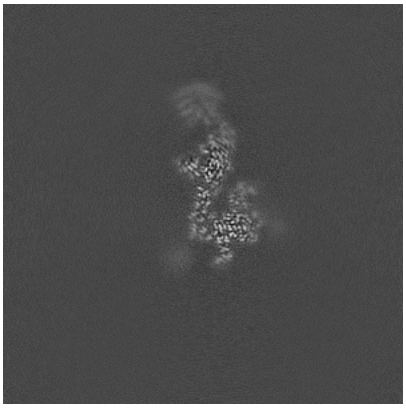


Z Index: 249

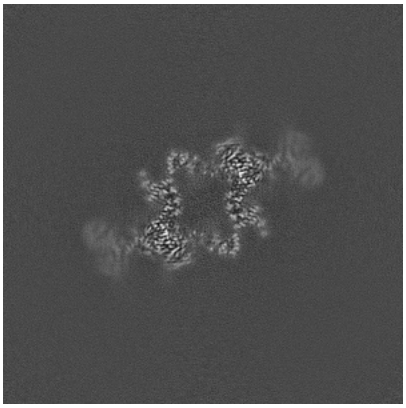
6.3.2 Raw map



X Index: 204



Y Index: 282



Z Index: 249

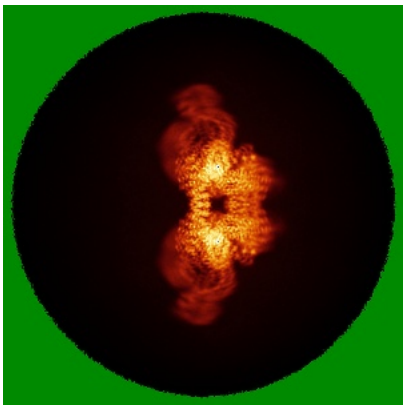
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

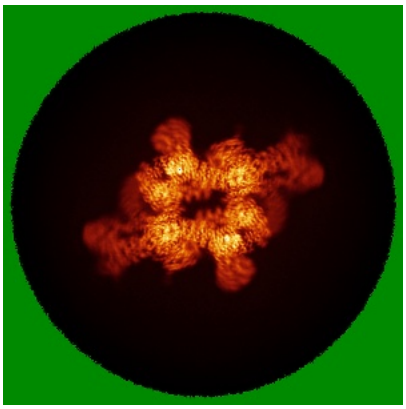
6.4.1 Primary map



X

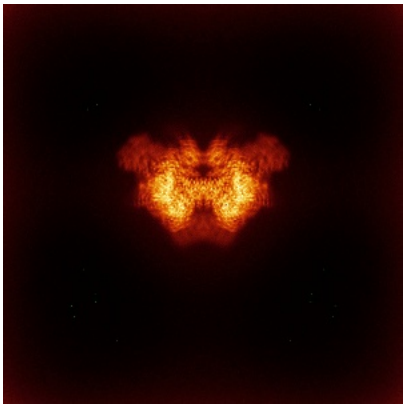


Y

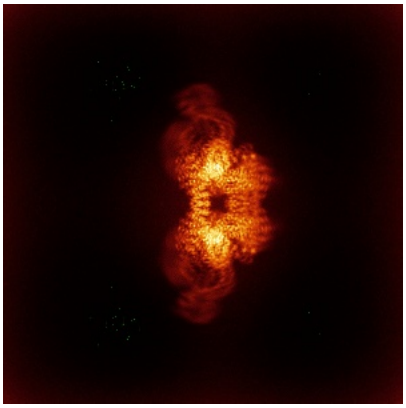


Z

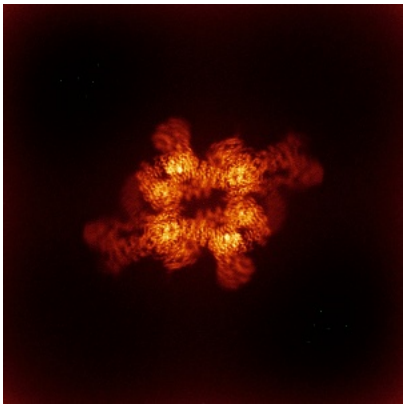
6.4.2 Raw map



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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. 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



X Y Z

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

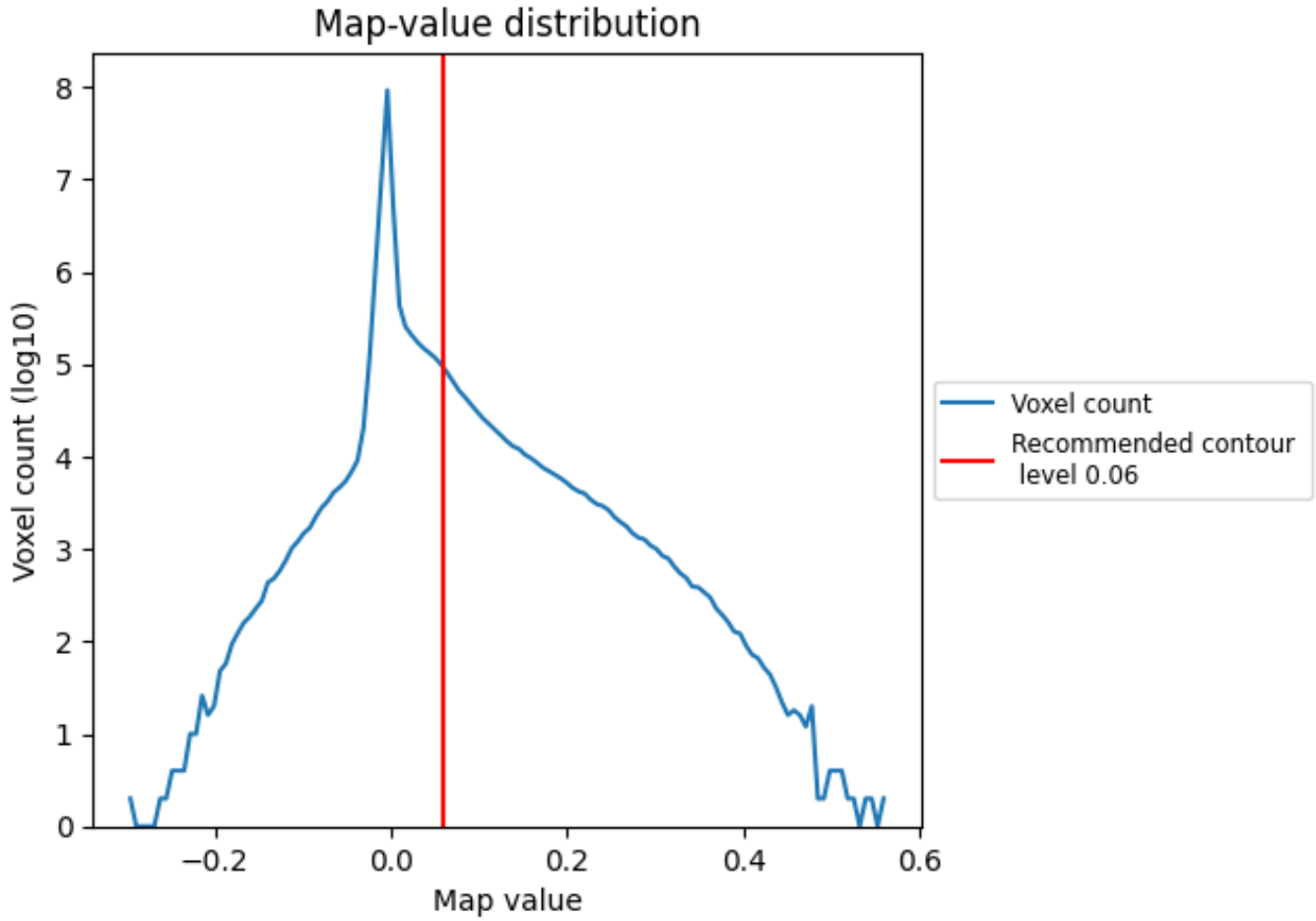
6.6 Mask visualisation (i)

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

7 Map analysis

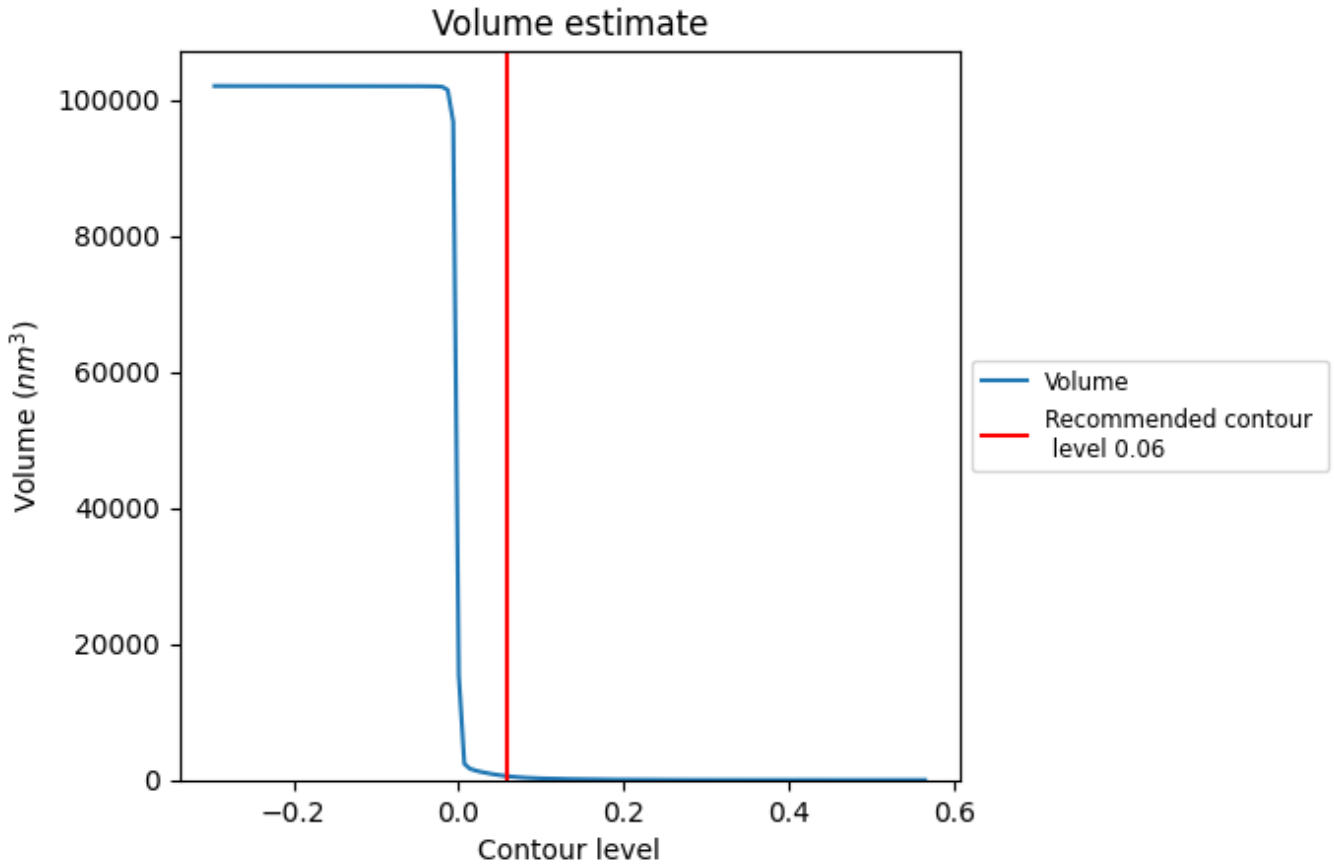
This section contains the results of statistical analysis of the map.

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.

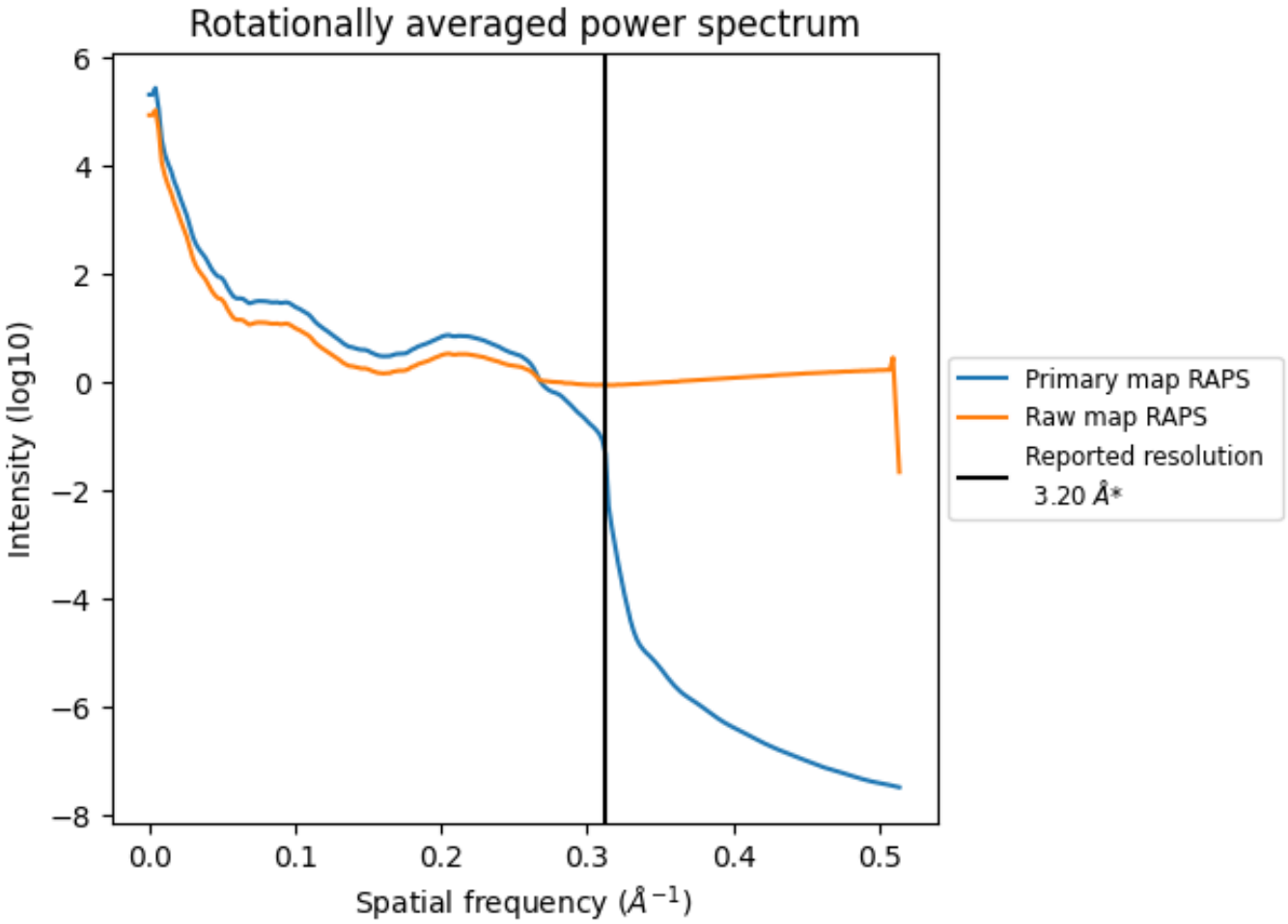
7.2 Volume estimate (i)



The volume at the recommended contour level is 545 nm^3; this corresponds to an approximate mass of 492 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)

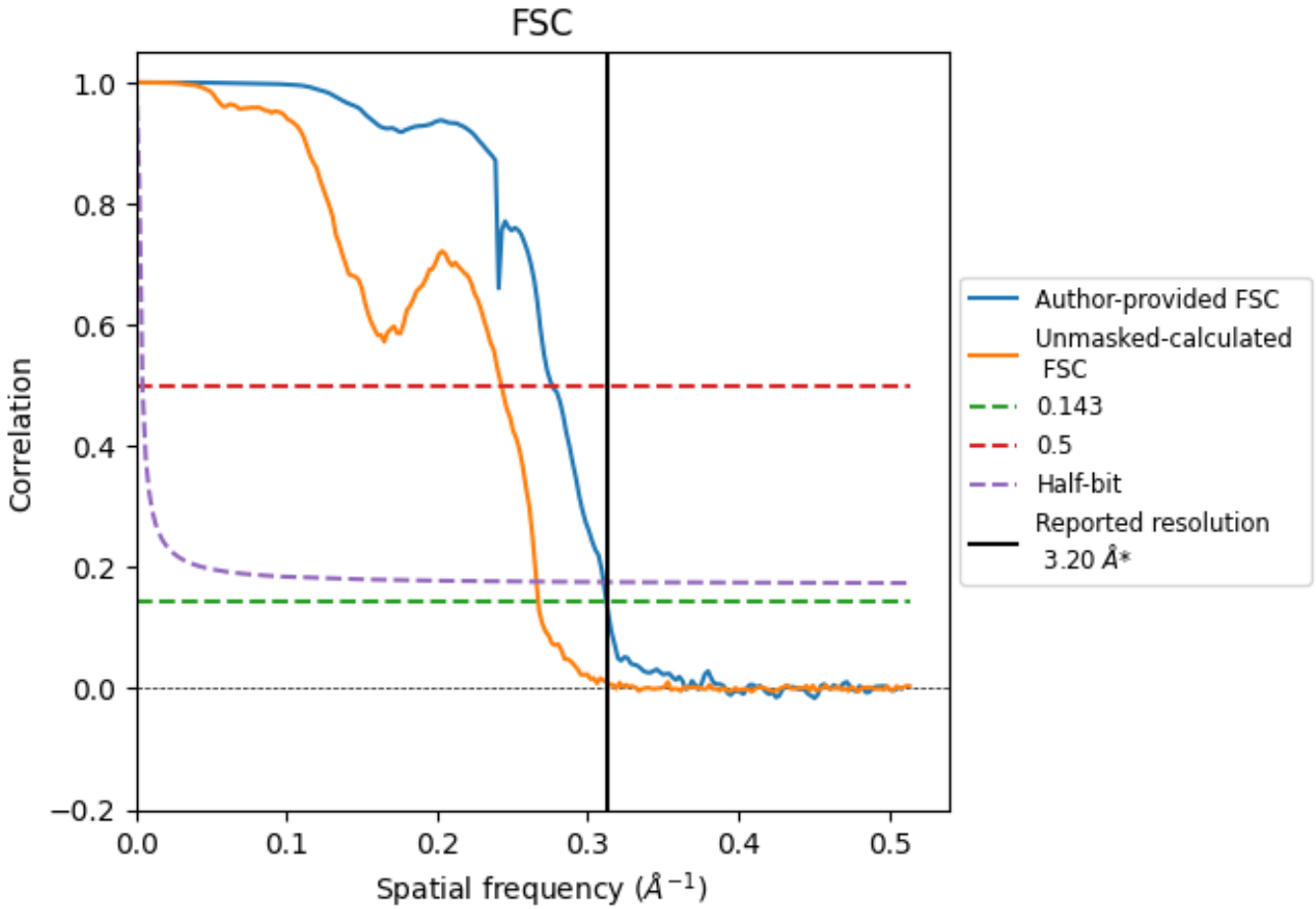


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8.2 Resolution estimates (i)

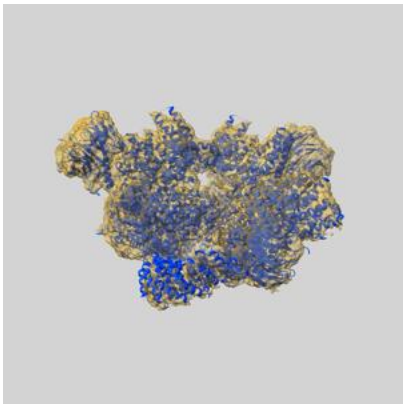
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.20	3.62	3.22
Unmasked-calculated*	3.75	4.12	3.76

*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 3.75 differs from the reported value 3.2 by more than 10 %

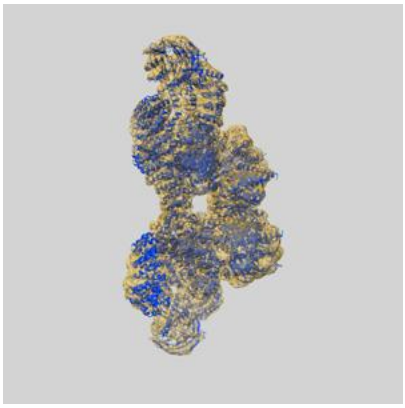
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-55634 and PDB model 9T7E. Per-residue inclusion information can be found in section 3 on page 7.

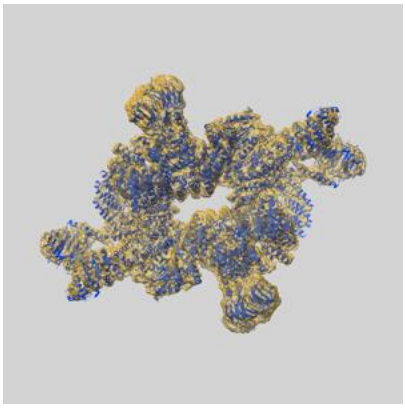
9.1 Map-model overlay



X



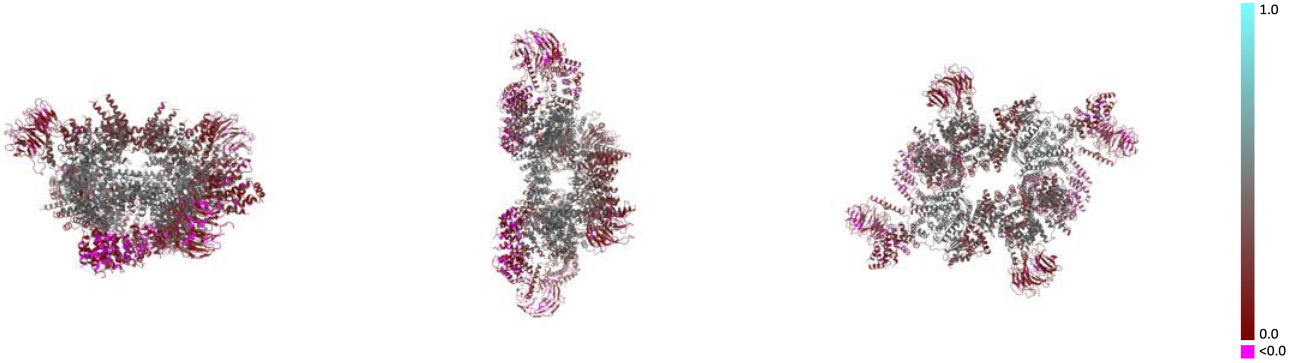
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06 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.

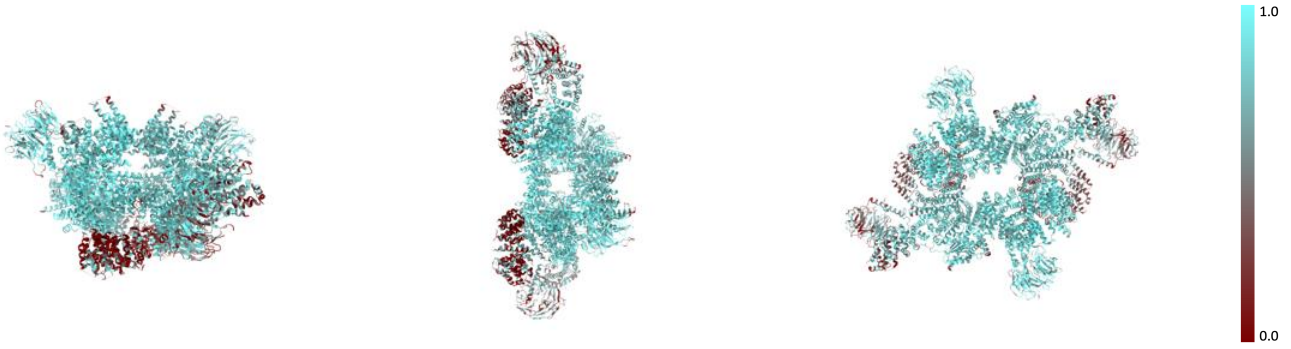
9.2 Q-score mapped to coordinate model



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.

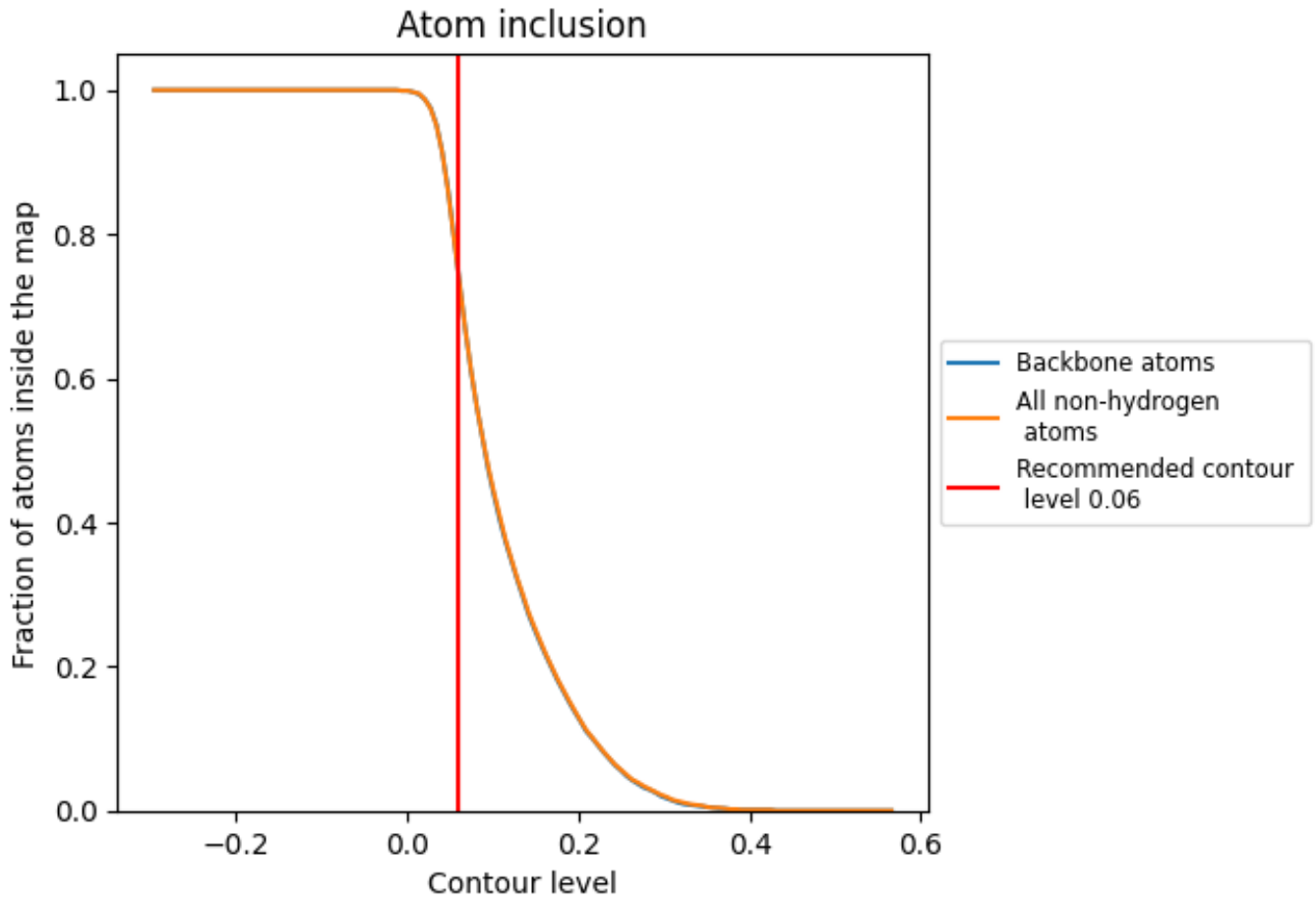
9.3 Atom inclusion mapped to coordinate model



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 (0.06).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 74% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7420	0.3100
A	0.7810	0.3460
B	0.7810	0.3450
C	0.7890	0.1730
D	0.7890	0.1720
E	0.6660	0.2750
F	0.6670	0.2720
G	0.7630	0.4760
H	0.8030	0.4620

