wwPDB EM Validation Summary Report

Nov 10, 2026 – 06:48 pm GMT

PDB ID	:	9T79 / pdb_00009t79
EMDB ID	:	EMD-55630
Title	:	cryo-EM structure of human Lipin1 bound to human mTOR complex 1
Authors	:	Craigie, L.M.; Maier, T.
Deposited on	:	2025-11-10
Resolution	:	3.33 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

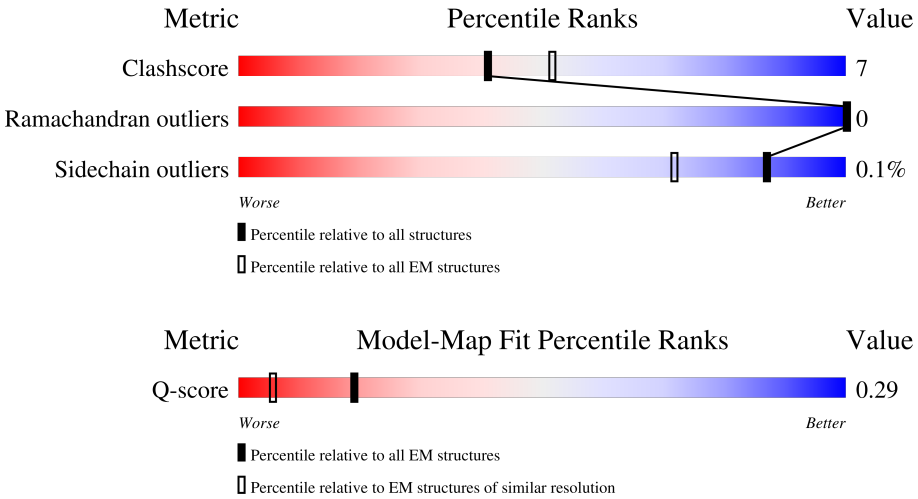
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

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

The reported resolution of this entry is 3.33 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	14484 (2.83 - 3.83)

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	8% 84% 13% .
1	D	326	8% 86% 11% .
2	G	890	. 99%
2	H	890	. 99%

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Mol	Chain	Length	Quality of chain
3	A	2549	11% 72% 14% 14%
3	B	2549	11% 72% 14% 14%
4	E	1363	12% 64% 13% 23%
4	F	1363	12% 64% 13% 23%

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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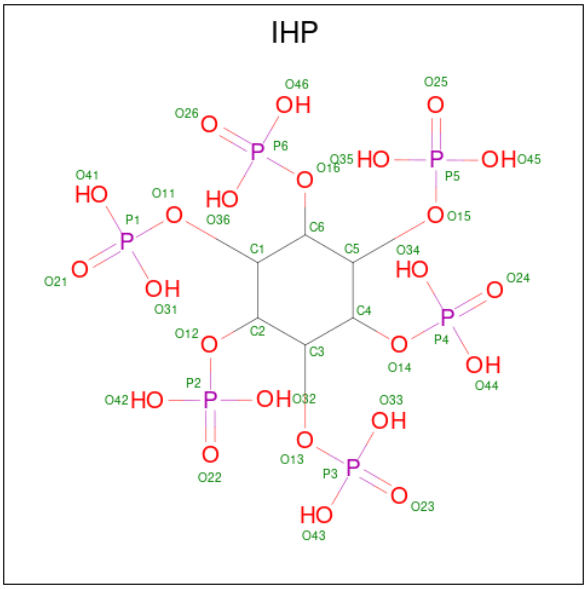
Chain	Residue	Modelled	Actual	Comment	Reference
E	-26	HIS	-	expression tag	UNP Q8N122
E	-25	HIS	-	expression tag	UNP Q8N122
E	-24	HIS	-	expression tag	UNP Q8N122
E	-23	HIS	-	expression tag	UNP Q8N122
E	-22	HIS	-	expression tag	UNP Q8N122
E	-21	HIS	-	expression tag	UNP Q8N122
E	-20	HIS	-	expression tag	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: $C_6H_{18}O_{24}P_6$).



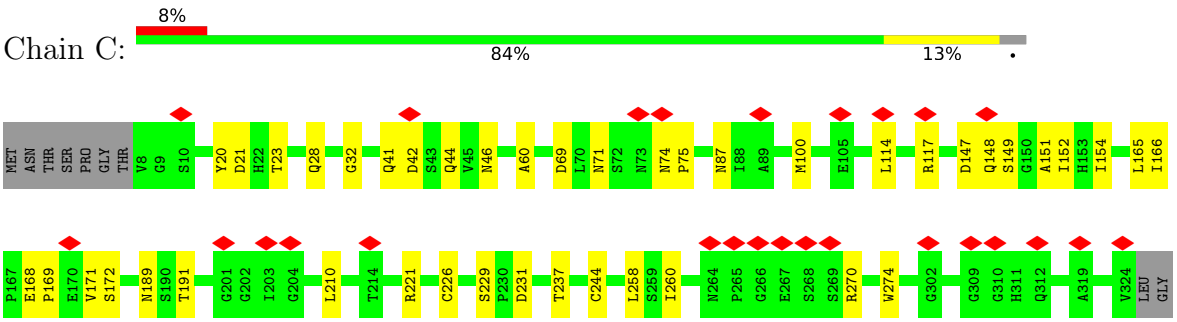
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	H	O	P	0
			42	6	6	24	6	
5	B	1	Total	C	H	O	P	0
			42	6	6	24	6	

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.

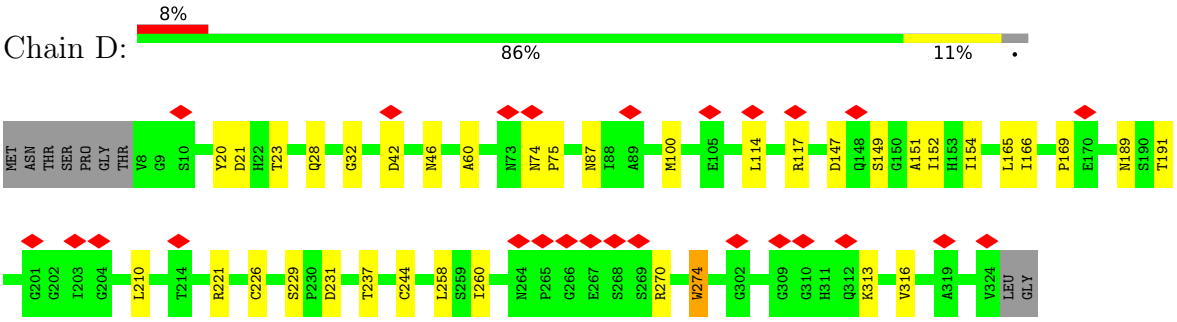
• Molecule 1: Target of rapamycin complex subunit LST8

Chain C:



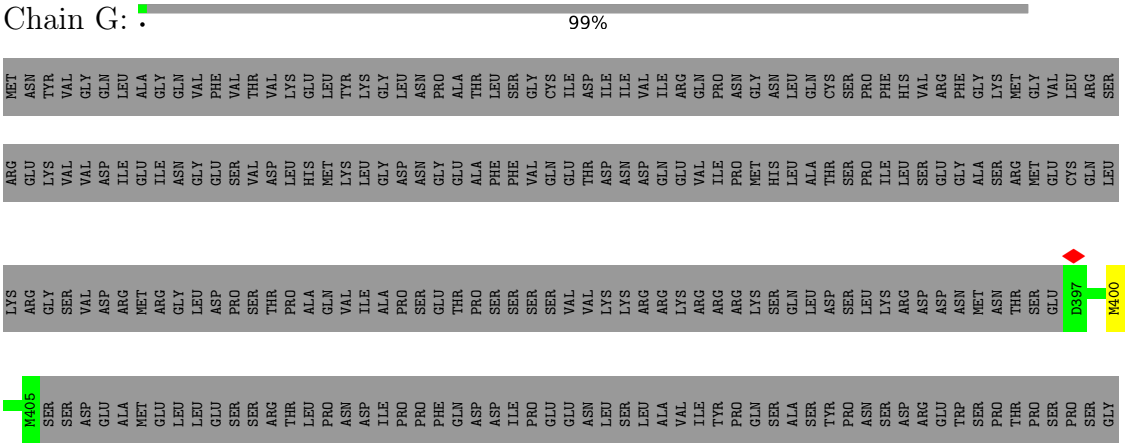
• Molecule 1: Target of rapamycin complex subunit LST8

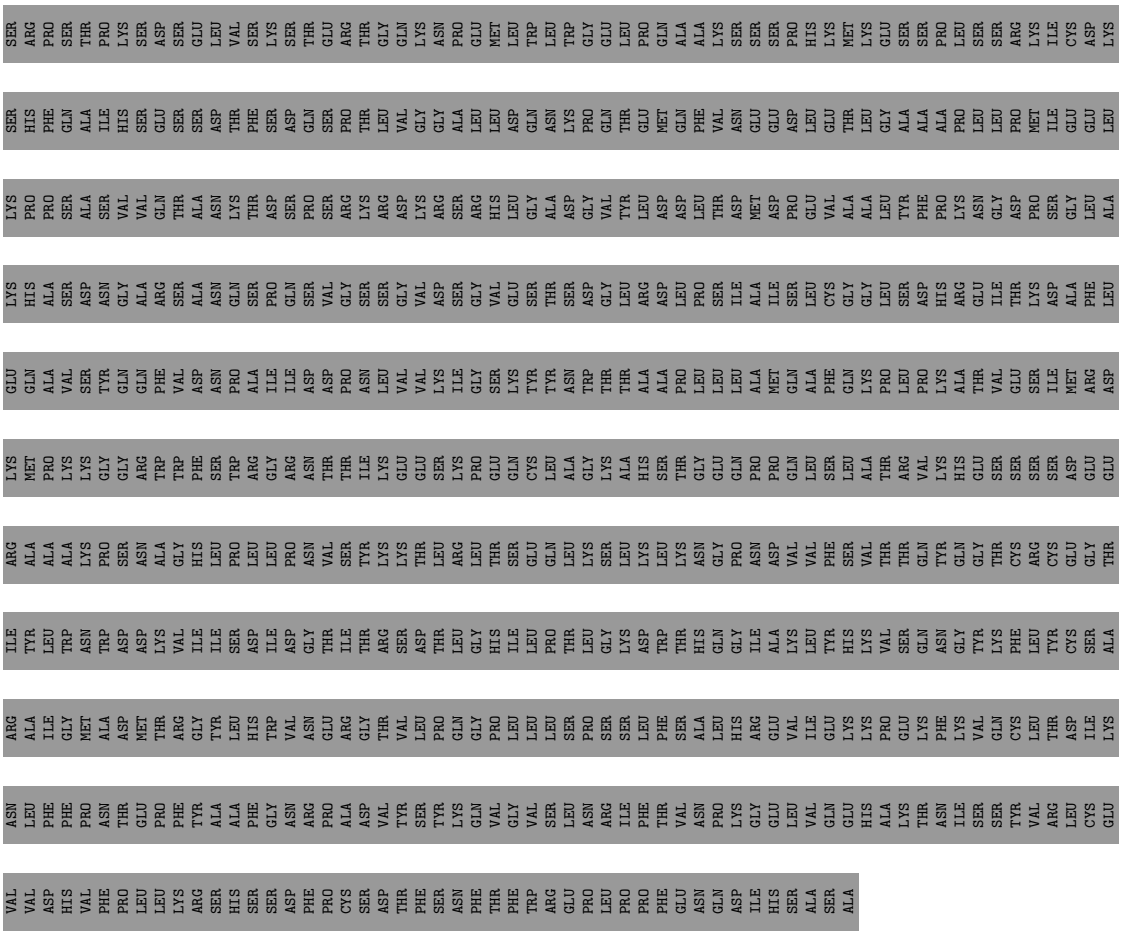
Chain D:



• Molecule 2: Phosphatidate phosphatase LPIN1

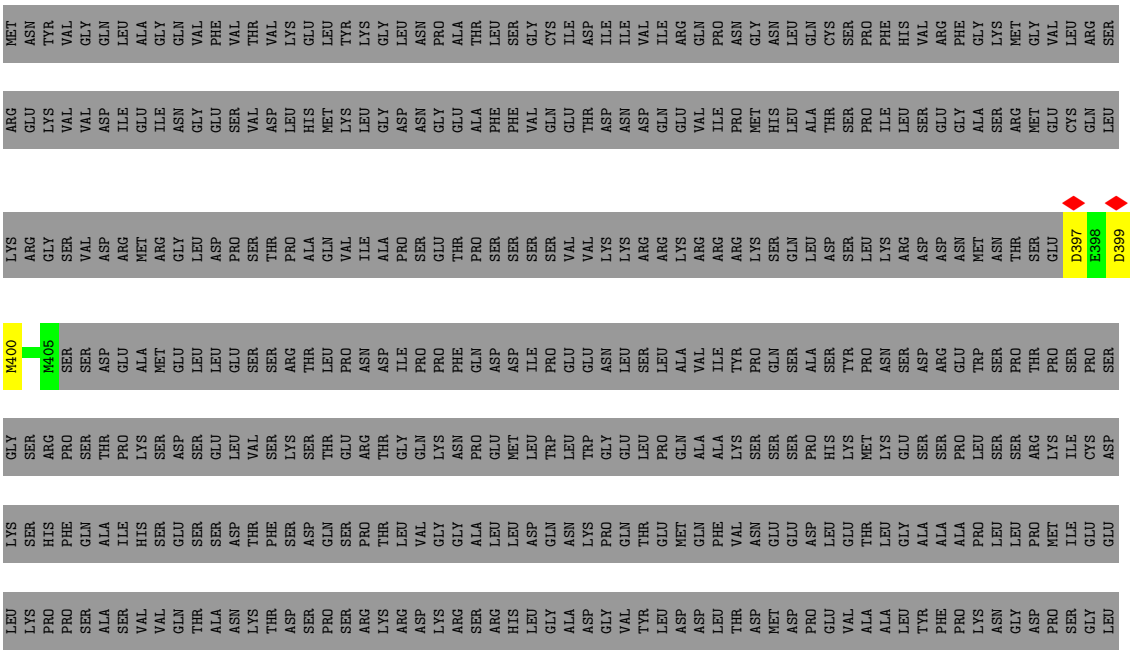
Chain G:

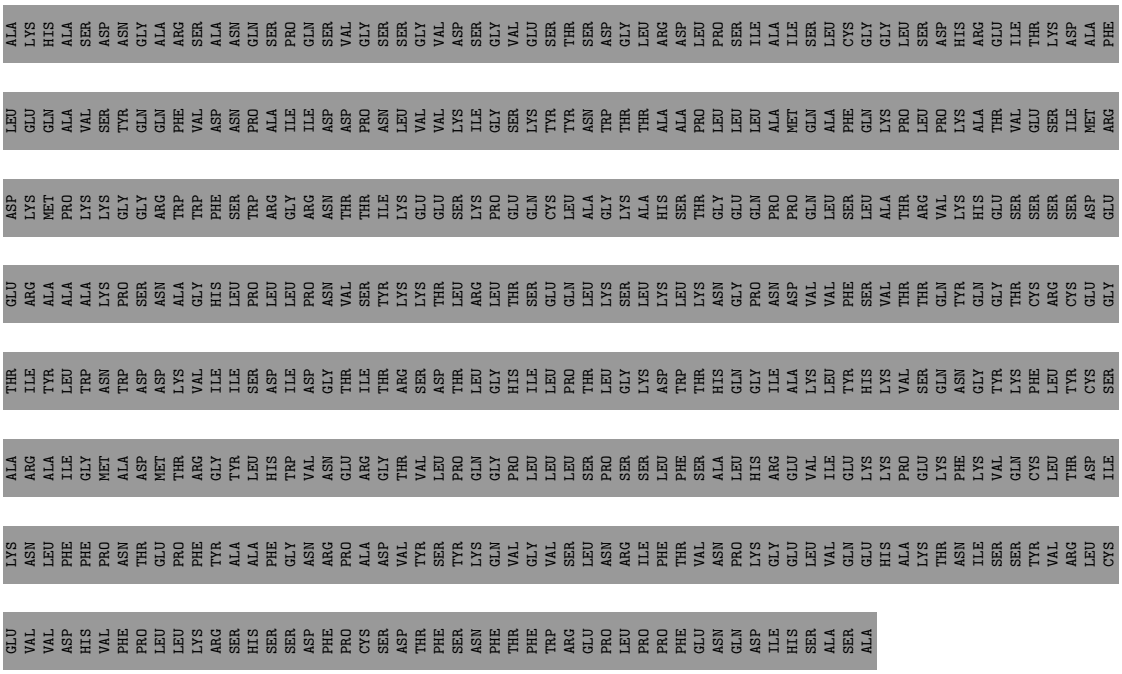




• Molecule 2: Phosphatidate phosphatase LPIN1

Chain H: 99%

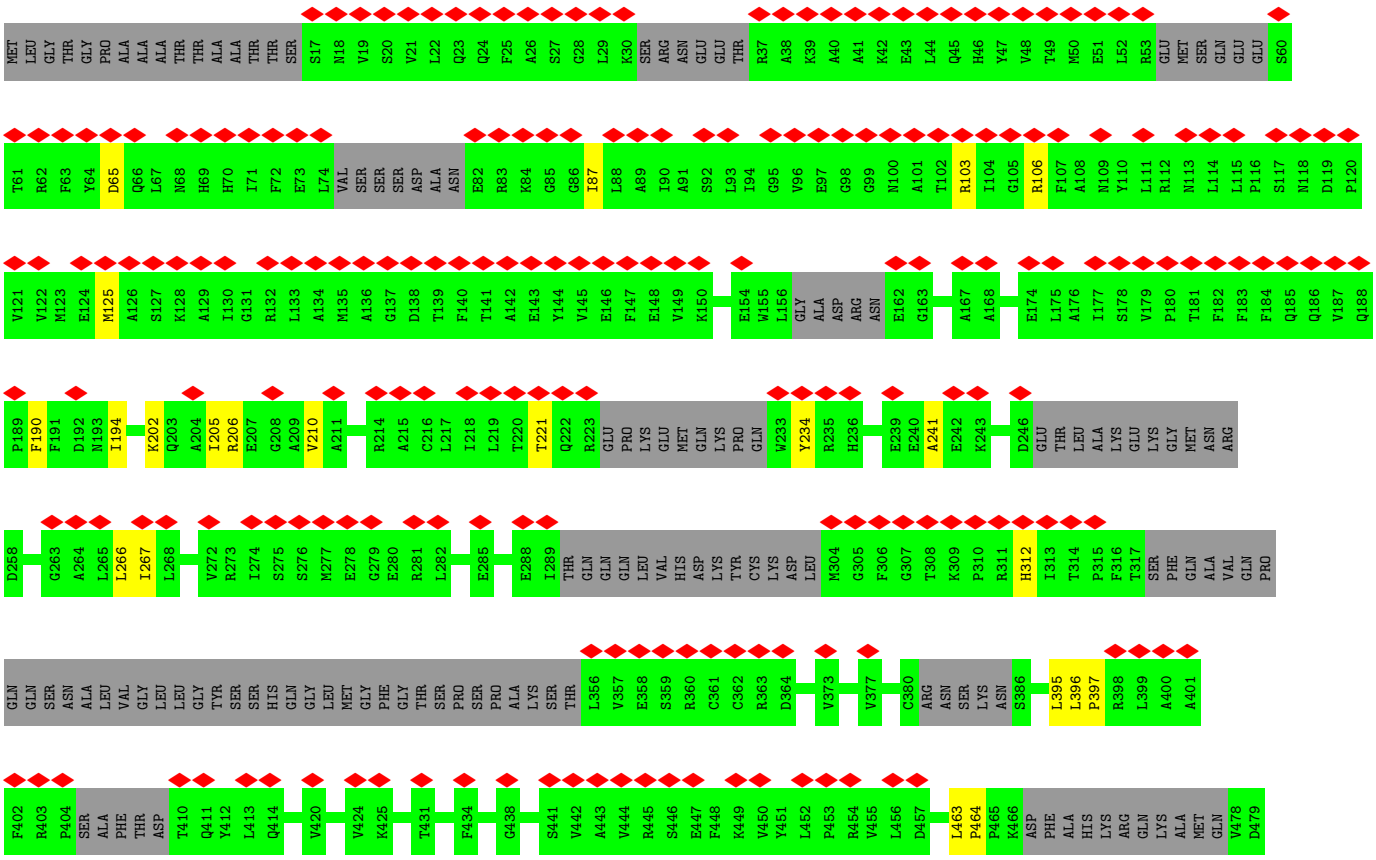


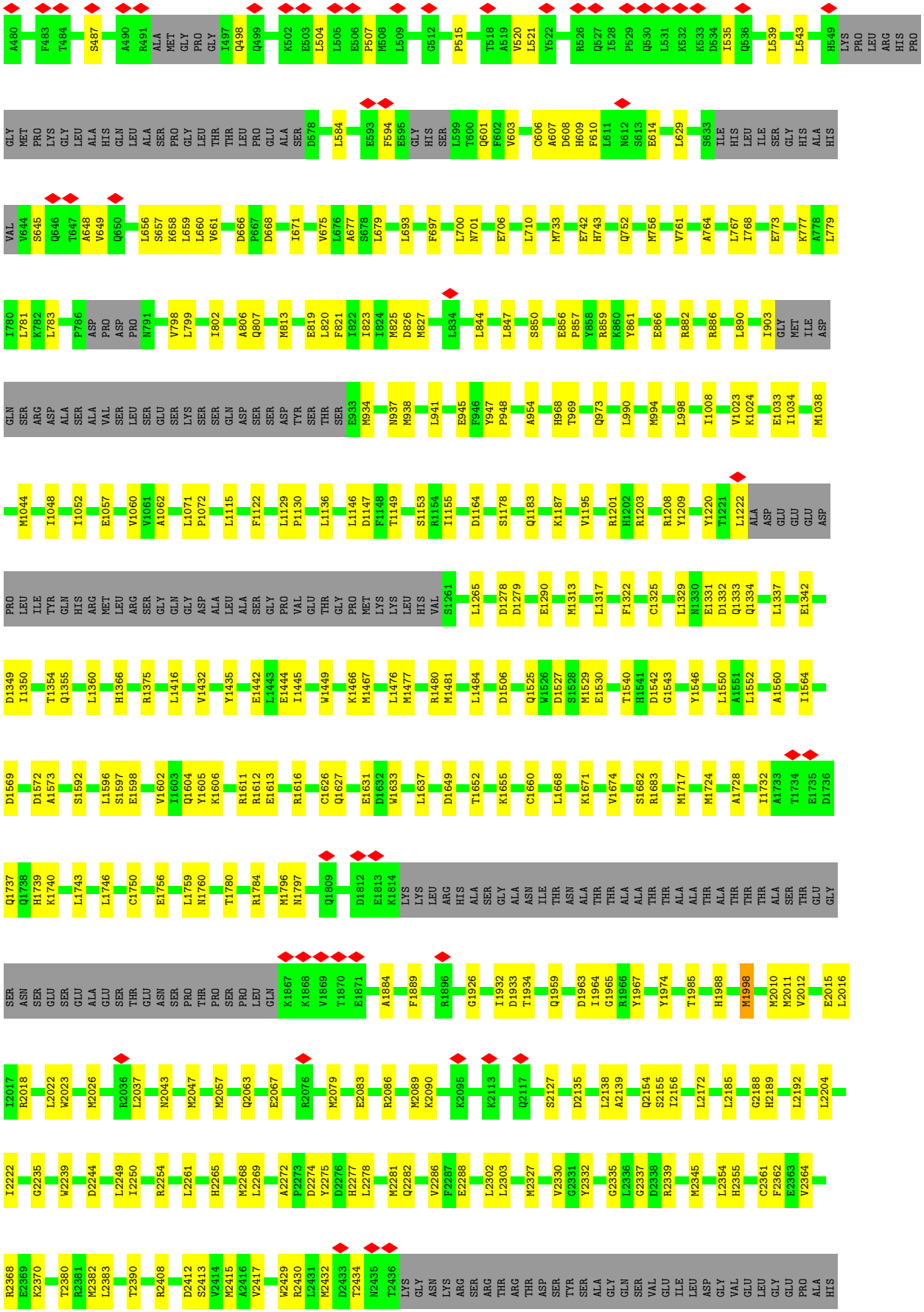


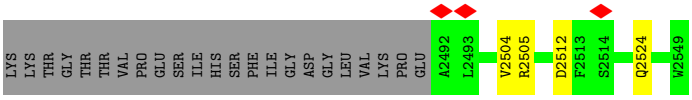
• Molecule 3: Serine/threonine-protein kinase mTOR

Chain A:





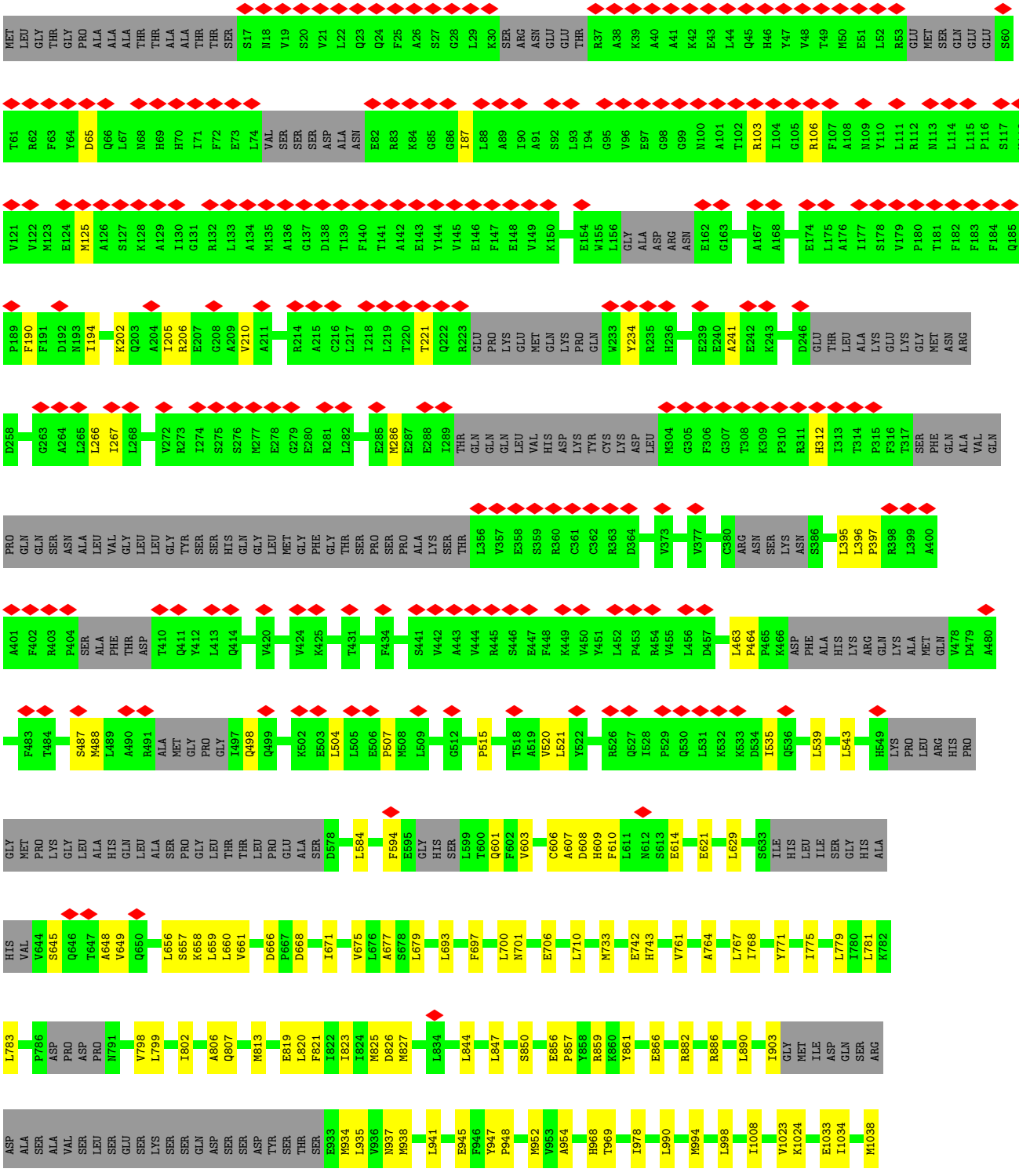


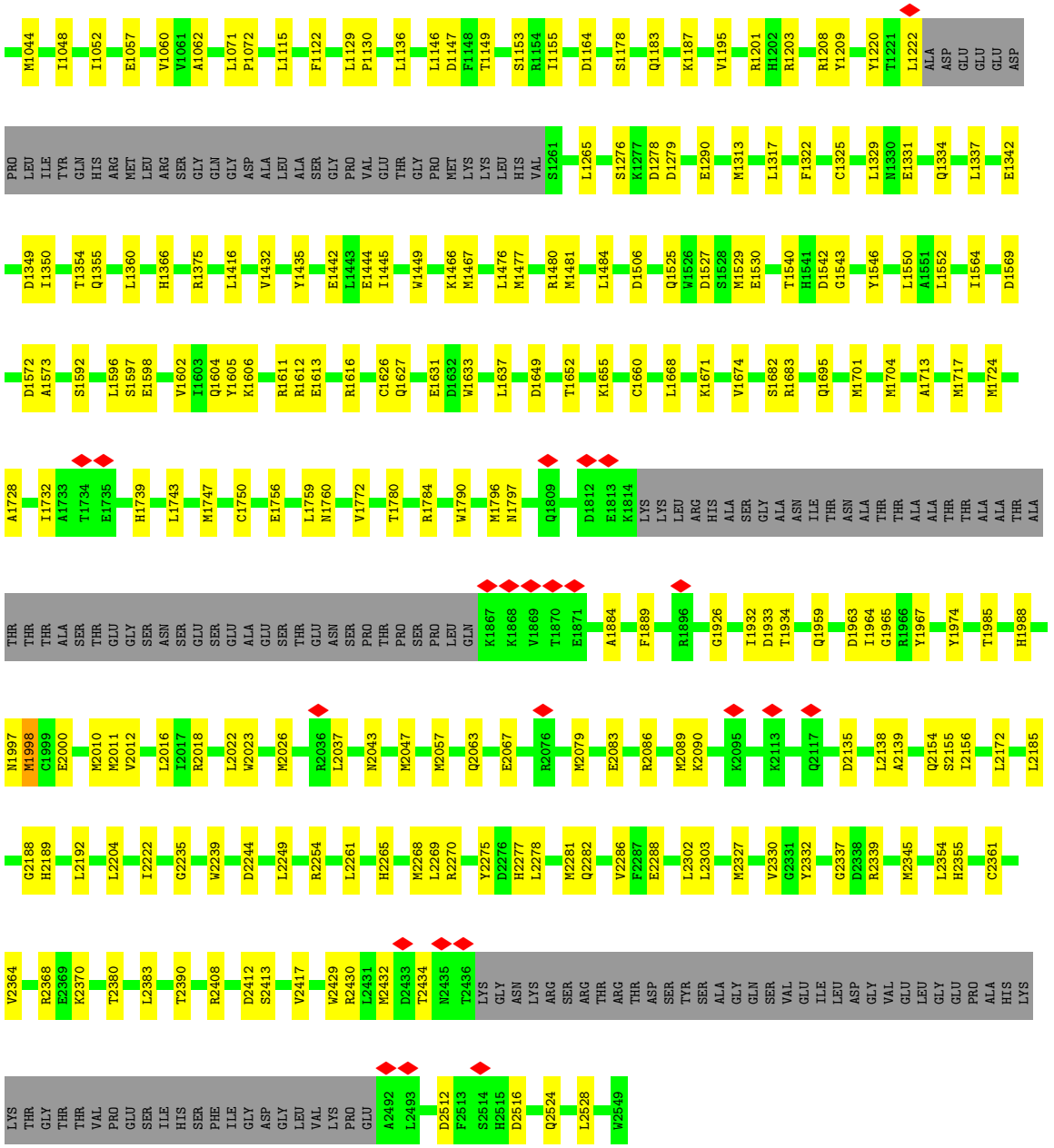


• Molecule 3: Serine/threonine-protein kinase mTOR

Chain B:



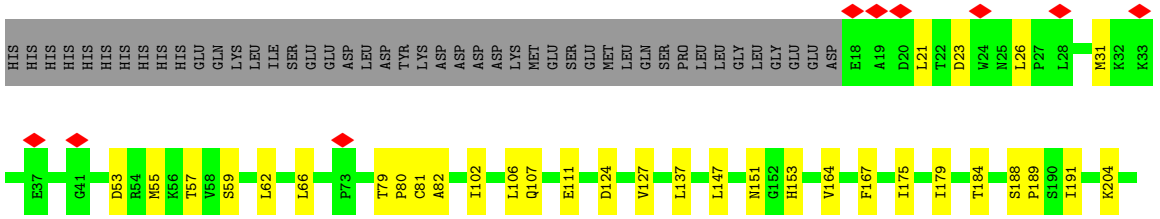


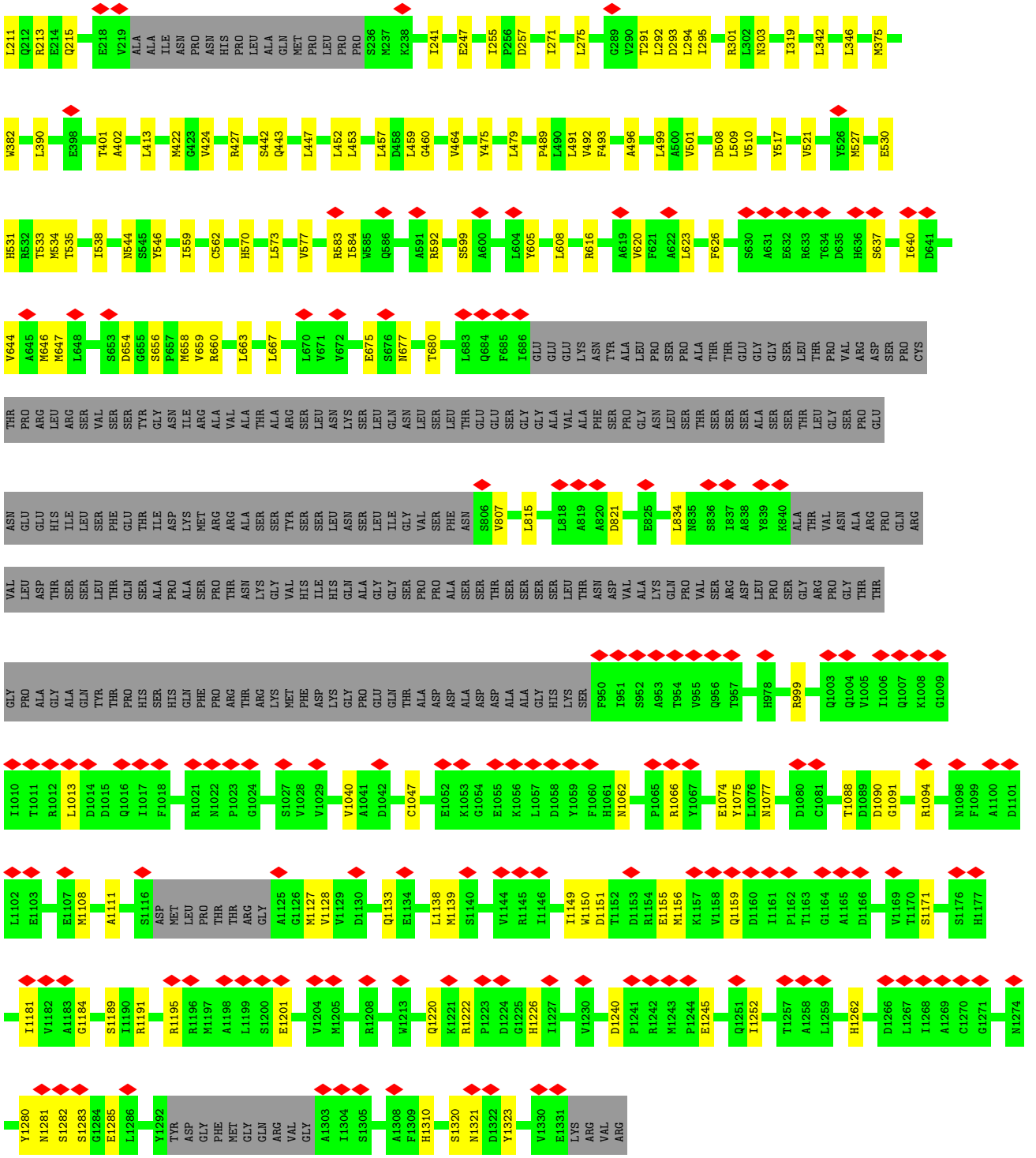


• Molecule 4: Regulatory-associated protein of mTOR

Chain E:



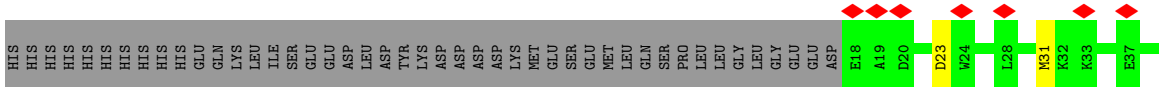


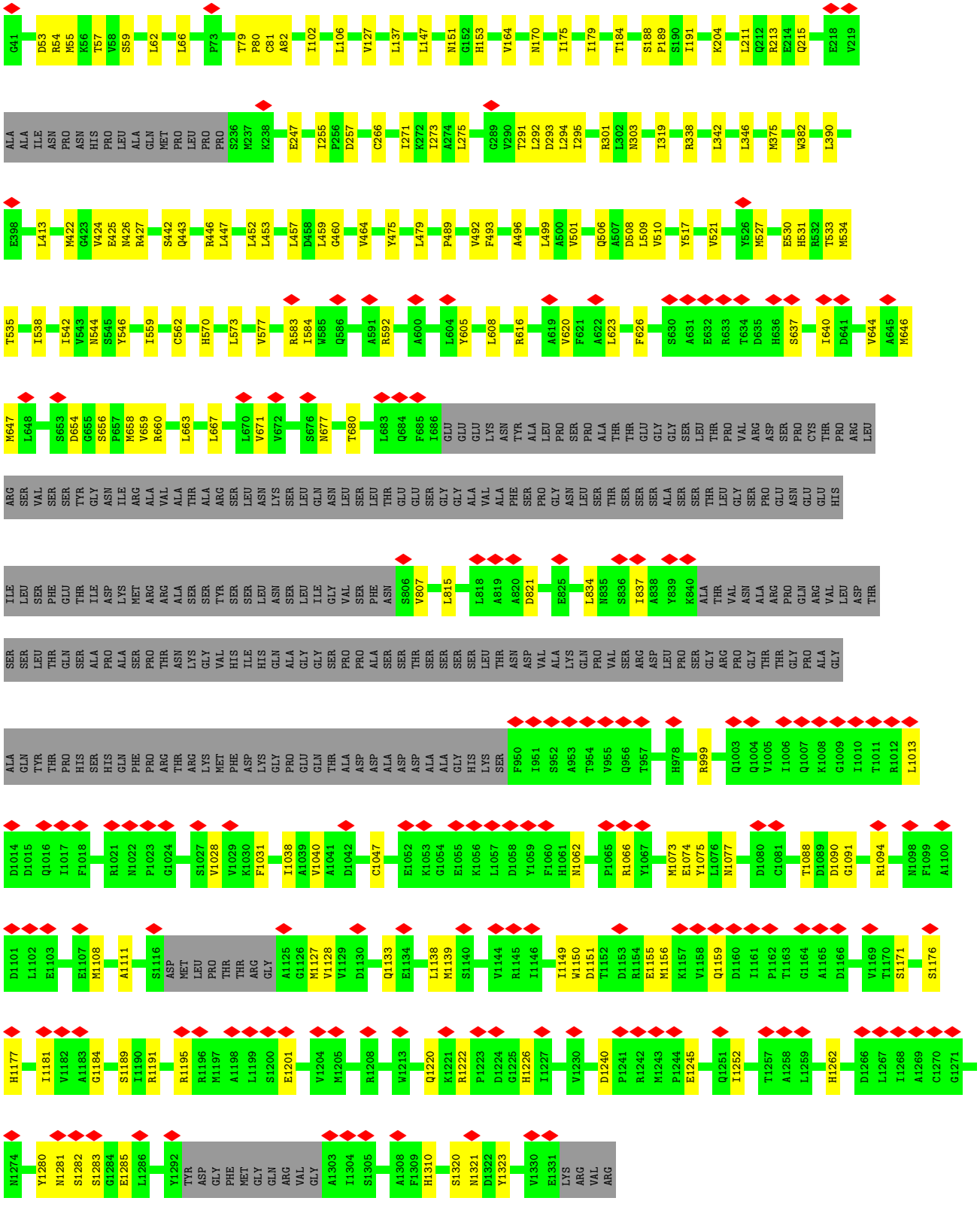


• Molecule 4: Regulatory-associated protein of mTOR

Chain F:






G41 D53 R54 M55 K56 T57 V58 S59 L62 L66 P73 T79 P80 C81 A82 I102 L106 V127 L137 L147 N151 G152 H153 V164 N170 I175 I179 T184 S188 P189 S190 I191 K204 L211 Q212 R213 E214 Q215 E218 V219
ALA ALA ILE ASN PRO ASN HIS PRO LEU ALA GLN MET PRO LEU PRO PRO S236 M237 K238 E247 I255 P256 D257 C266 I271 K272 I273 A274 L275 G289 V290 T291 L292 D293 L294 I295 R301 L302 N303 I319 R338 L342 L346 M375 W382 L390
E398 L413 M422 G423 V424 E425 N426 R427 S442 Q443 R446 L447 L452 L453 L457 D458 L459 G460 V464 Y475 L479 P489 V492 F493 A496 L499 A500 V501 Q506 A507 D508 L509 V510 Y517 V521 Y526 M527 E530 H531 R532 T533 M534
T535 I538 I542 V543 N544 S545 Y546 I559 C562 H570 L573 V577 R583 I584 W585 Q586 A591 R592 A600 L604 Y605 L608 R616 A619 V620 F621 A622 L623 F626 S630 A631 E632 R633 T634 D635 H636 S637 I640 D641 V644 A645 M646
M647 L648 S653 D654 G655 S656 P657 M658 V659 R660 L663 L667 L670 V671 V672 S676 N677 T680 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 L815 L818 A819 A820 D821 E825 L834 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 PRO THR ASN LYS GLY VAL HIS ILE HIS GLN ALA GLY GLY SER PRO PRO ALA SER SER THR 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 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 ASP ALA ALA GLY HIS LYS SER F950 I951 S952 A953 T954 V955 Q956 T957 H978 R999 Q1003 Q1004 V1005 I1006 Q1007 K1008 G1009 I1010 T1011 R1012 L1013
D1014 D1015 Q1016 I1017 F1018 R1021 N1022 P1023 G1024 S1027 V1028 V1029 K1030 F1031 I1038 A1039 V1040 A1041 D1042 C1047 E1052 K1053 G1054 E1055 K1056 L1057 D1058 Y1059 F1060 H1061 N1062 P1065 R1066 Y1067 M1073 E1074 Y1075 L1076 N1077 D1080 C1081 T1088 D1089 D1090 G1091 R1094 N1098 F1099 A1100
D1101 L1102 E1103 E1107 M1108 A1111 S1116 ASP MET LEU PRO THR THR ARG GLY A1125 G1126 M1127 V1128 V1129 D1130 Q1133 E1134 L1138 M1139 S1140 V1144 R1145 I1146 I1149 W1150 D1151 T1152 D1153 R1154 E1155 M1156 K1157 V1158 Q1159 D1160 I1161 P1162 T1163 G1164 A1165 D1166 V1169 T1170 S1171 S1176
H1177 I1181 V1182 A1183 G1184 S1189 I1190 R1191 R1195 R1196 M1197 A1198 L1199 S1200 E1201 V1204 M1205 R1208 W1213 Q1220 K1221 R1222 P1223 D1224 G1225 H1226 I1227 V1230 D1240 P1241 R1242 M1243 P1244 E1245 Q1251 I1252 T1257 A1258 L1259 H1262 D1266 L1267 I1268 A1269 C1270 G1271
N1274 Y1280 N1281 S1282 S1283 G1284 E1285 L1286 Y1292 TYR ASP GLY PHE MET GLY GLN ARG VAL GLY A1303 I1304 S1305 A1308 F1309 H1310 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, C2	Depositor
Number of particles used	211482	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	0.419	Depositor
Minimum map value	-0.251	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.05	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	0.09	0/2514	0.25	0/3426
1	D	0.09	0/2514	0.25	0/3426
2	G	0.17	0/77	0.34	0/102
2	H	0.16	0/77	0.29	0/102
3	A	0.12	0/17814	0.26	0/24116
3	B	0.12	0/17814	0.26	0/24116
4	E	0.11	0/8585	0.25	0/11680
4	F	0.11	0/8585	0.25	0/11680
All	All	0.11	0/57980	0.25	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	28	0
1	D	2456	2341	2341	22	0
2	G	76	64	64	1	0
2	H	76	64	64	3	0
3	A	17467	17553	17553	246	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	17467	17553	17553	247	0
4	E	8385	8375	8375	124	0
4	F	8385	8375	8375	126	0
5	A	36	6	6	1	0
5	B	36	6	6	1	0
All	All	56840	56678	56678	779	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.

The worst 5 of 779 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:620:VAL:HG11	4:F:663:LEU:HD23	1.48	0.95
4:E:620:VAL:HG11	4:E:663:LEU:HD23	1.55	0.87
3:A:1416:LEU:HD21	3:A:1432:VAL:HG21	1.58	0.86
3:B:1044:MET:HE3	3:B:1044:MET:O	1.76	0.84
3:A:1044:MET:HE3	3:A:1044:MET:O	1.77	0.83

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%)	305 (97%)	10 (3%)	0	100	100
1	D	315/326 (97%)	307 (98%)	8 (2%)	0	100	100
2	G	7/890 (1%)	5 (71%)	2 (29%)	0	100	100
2	H	7/890 (1%)	7 (100%)	0	0	100	100
3	A	2150/2549 (84%)	2095 (97%)	55 (3%)	0	100	100

Continued on next page...

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	B	2150/2549 (84%)	2097 (98%)	53 (2%)	0	100	100
4	E	1040/1363 (76%)	1010 (97%)	30 (3%)	0	100	100
4	F	1040/1363 (76%)	1007 (97%)	33 (3%)	0	100	100
All	All	7024/10256 (68%)	6833 (97%)	191 (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	83
1	D	269/276 (98%)	268 (100%)	1 (0%)	84	83
2	G	9/785 (1%)	9 (100%)	0	100	100
2	H	9/785 (1%)	9 (100%)	0	100	100
3	A	1876/2220 (84%)	1875 (100%)	1 (0%)	88	89
3	B	1876/2220 (84%)	1875 (100%)	1 (0%)	88	89
4	E	928/1191 (78%)	926 (100%)	2 (0%)	87	87
4	F	928/1191 (78%)	927 (100%)	1 (0%)	88	89
All	All	6164/8944 (69%)	6157 (100%)	7 (0%)	87	89

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	1998	MET
4	E	675	GLU
4	F	1323	TYR
4	E	1323	TYR
3	A	1998	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
3	B	2117	GLN
4	E	1310	HIS
3	B	2154	GLN
4	E	392	GLN
4	F	392	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)

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	B	2601	-	36,36,36	0.76	1 (2%)	54,60,60	0.37	0
5	IHP	A	2601	-	36,36,36	0.76	1 (2%)	54,60,60	0.37	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	B	2601	-	-	2/30/54/54	0/1/1/1
5	IHP	A	2601	-	-	3/30/54/54	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	2.97	1.64	1.59
5	A	2601	IHP	P3-O13	2.96	1.64	1.59

There are no bond angle outliers.

There are no chirality outliers.

All (5) 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	B	2601	IHP	C2-O12-P2-O32
5	A	2601	IHP	C2-C1-O11-P1
5	A	2601	IHP	C2-O12-P2-O32

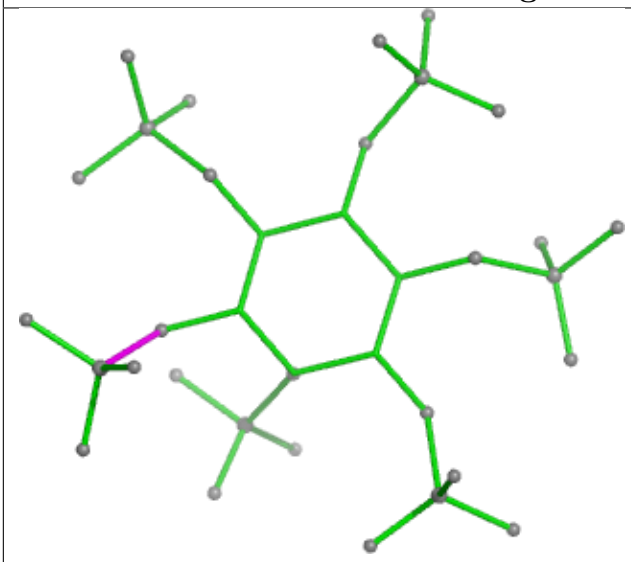
There are no ring outliers.

2 monomers are involved in 2 short contacts:

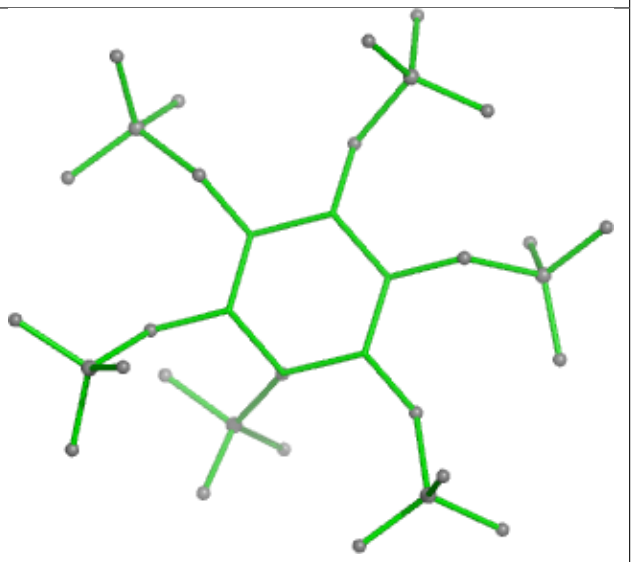
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	2601	IHP	1	0
5	A	2601	IHP	1	0

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 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.

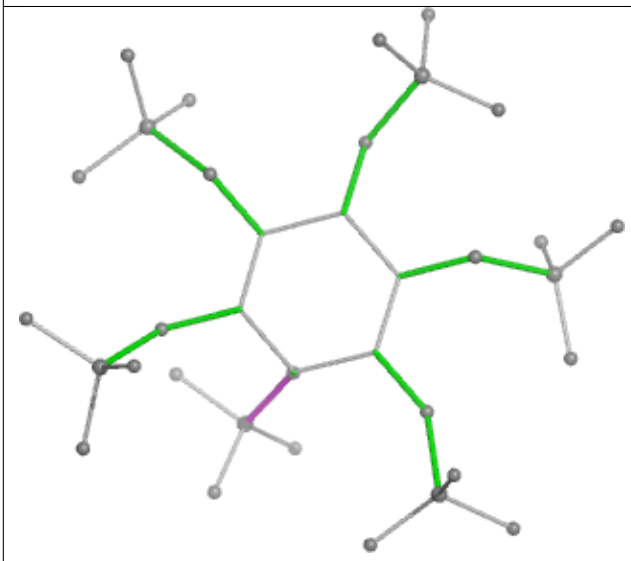
Ligand IHP B 2601



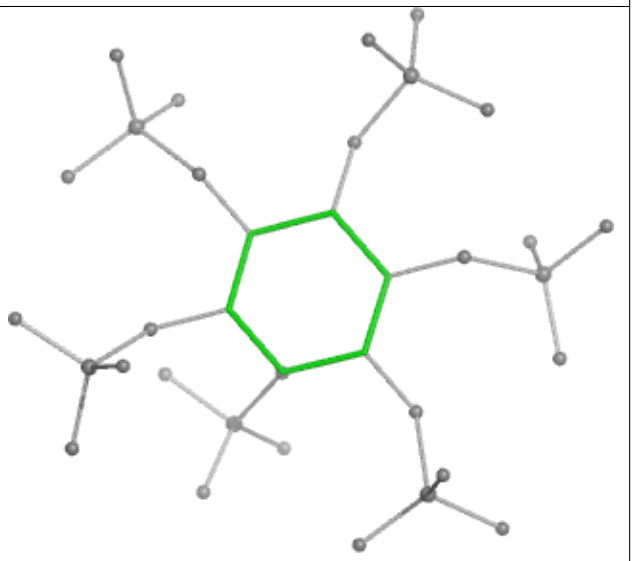
Bond lengths



Bond angles

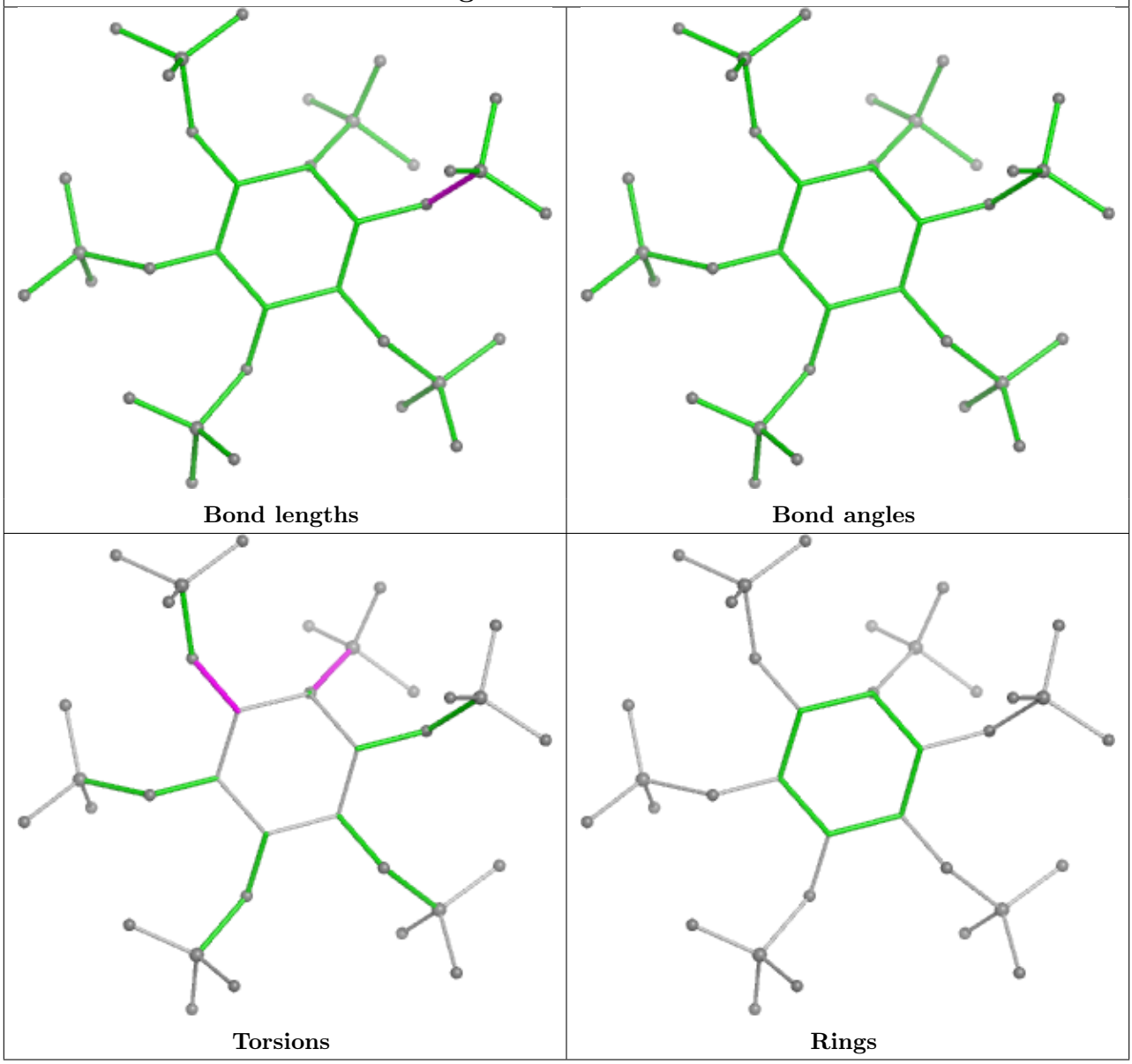


Torsions



Rings

Ligand IHP A 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.

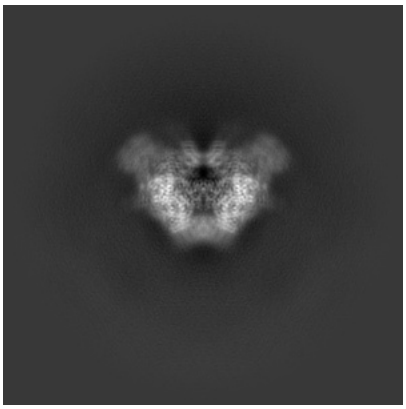
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-55630. These allow visual inspection of the internal detail of the map and identification of artifacts.

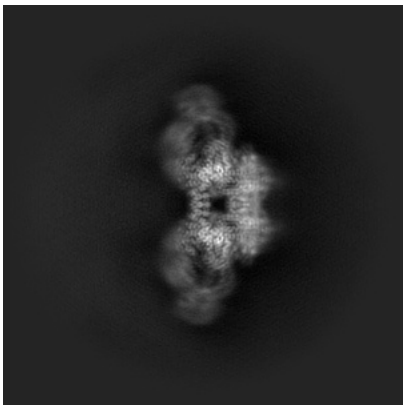
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

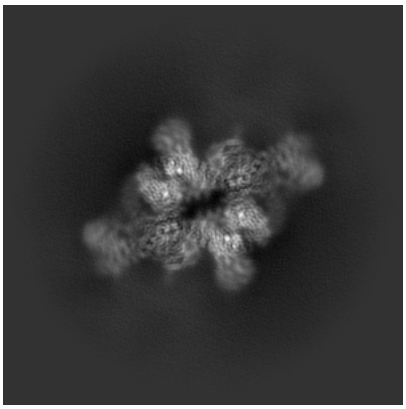
6.1.1 Primary map



X

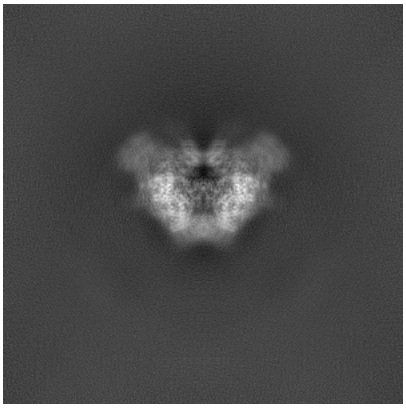


Y

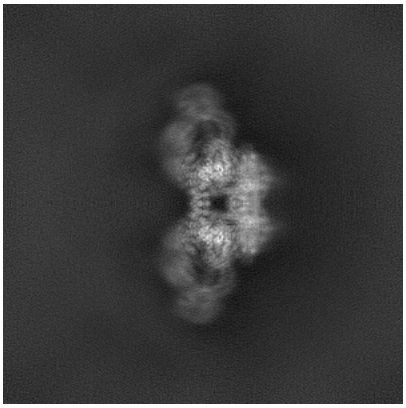


Z

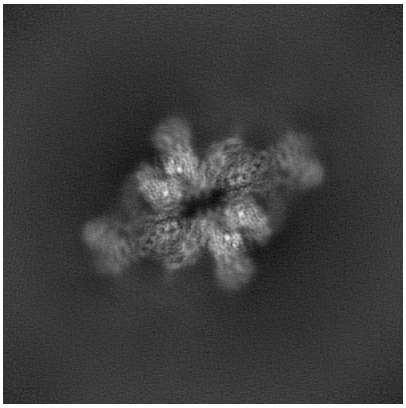
6.1.2 Raw map



X



Y

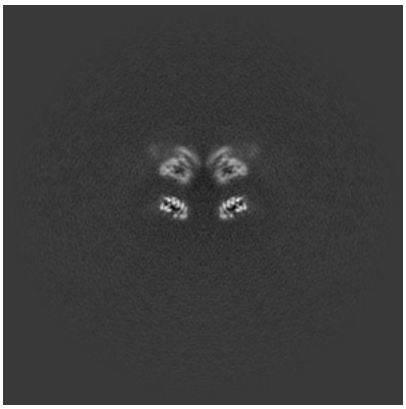


Z

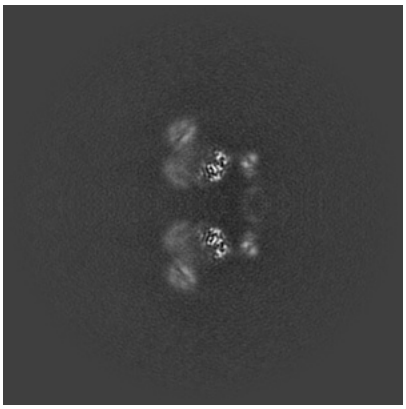
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

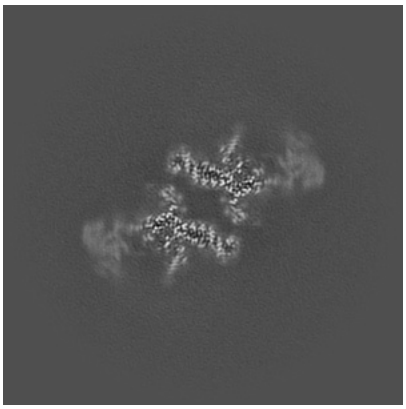
6.2.1 Primary map



X Index: 240



Y Index: 240

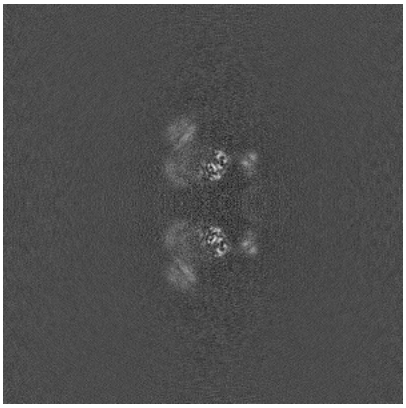


Z Index: 240

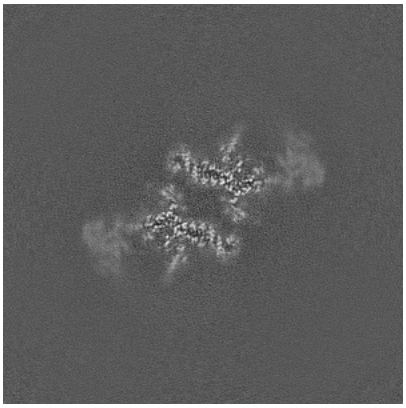
6.2.2 Raw map



X Index: 240



Y Index: 240



Z Index: 240

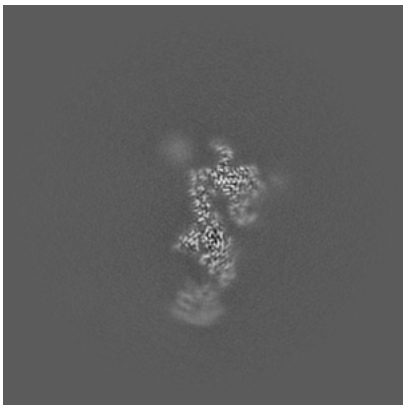
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

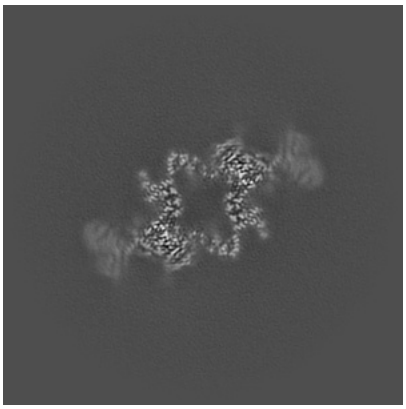
6.3.1 Primary map



X Index: 196



Y Index: 199

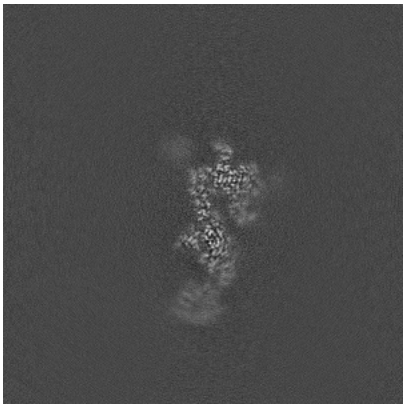


Z Index: 249

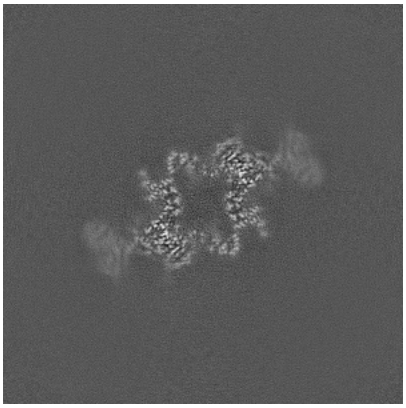
6.3.2 Raw map



X Index: 283



Y Index: 198

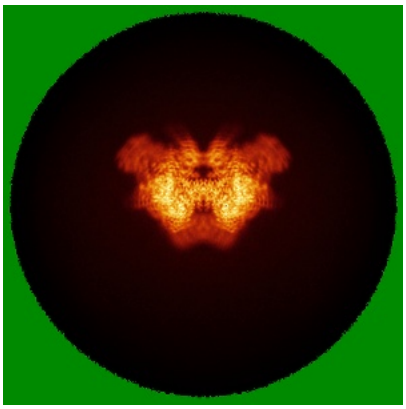


Z Index: 249

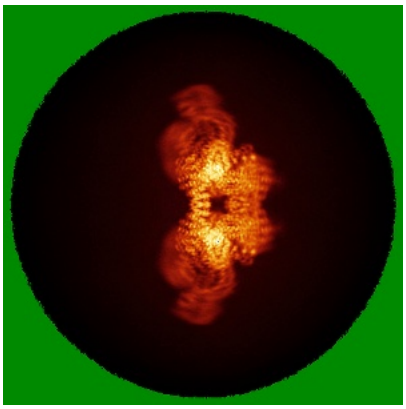
The images above show the largest variance slices of the map in three orthogonal directions.

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

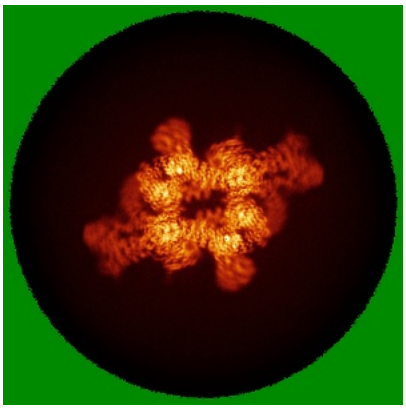
6.4.1 Primary map



X

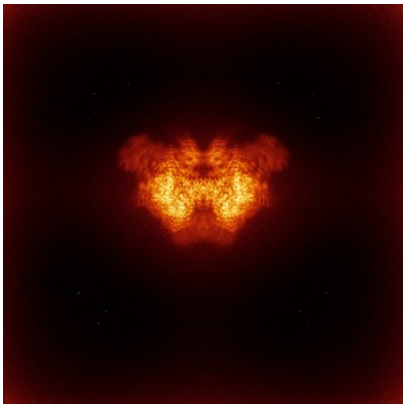


Y

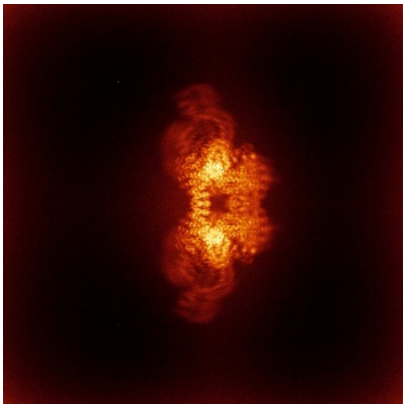


Z

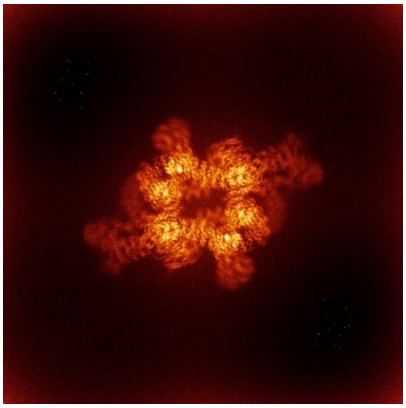
6.4.2 Raw map



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 0.05. 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.

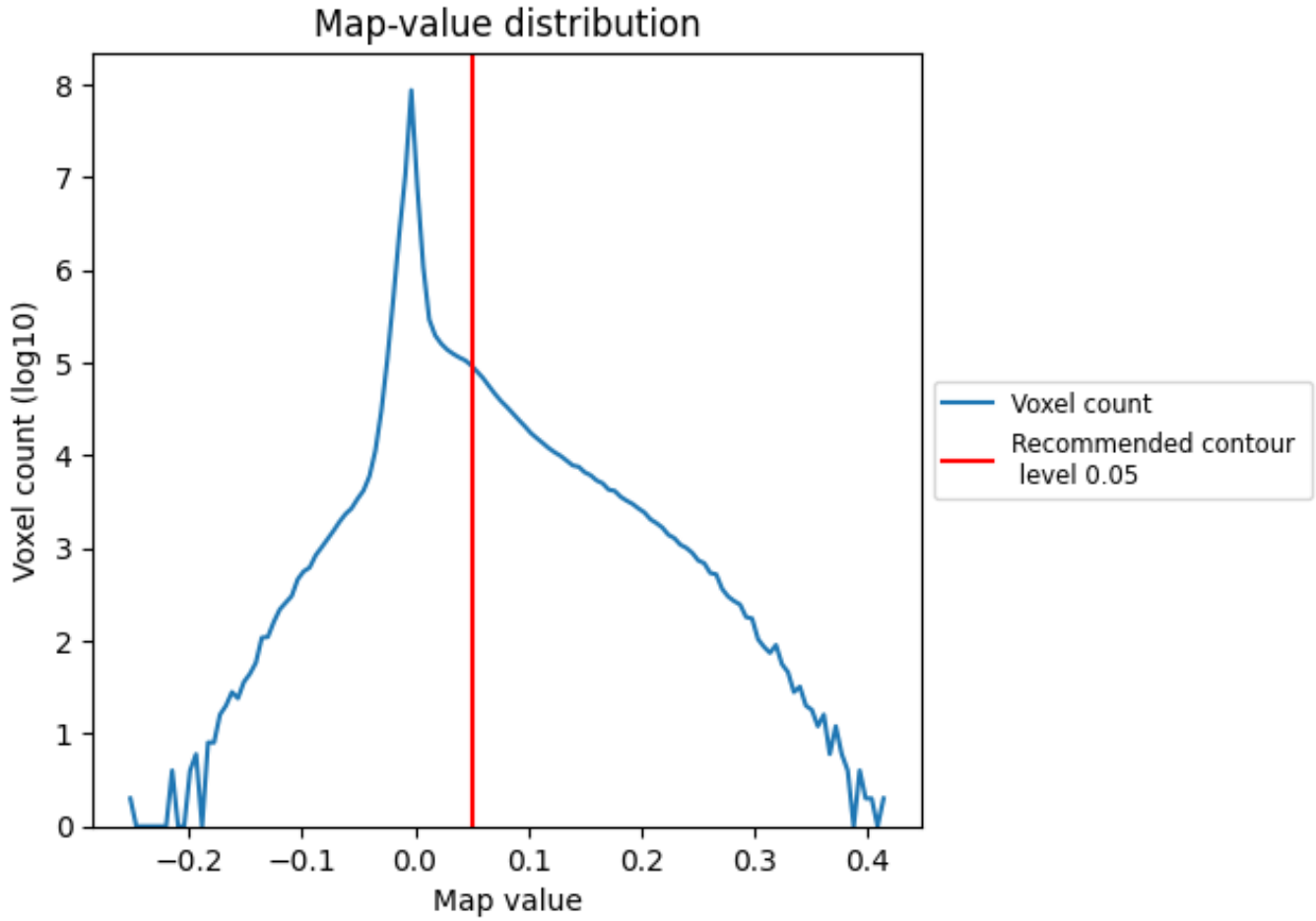
6.6 Mask visualisation (i)

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

7 Map analysis

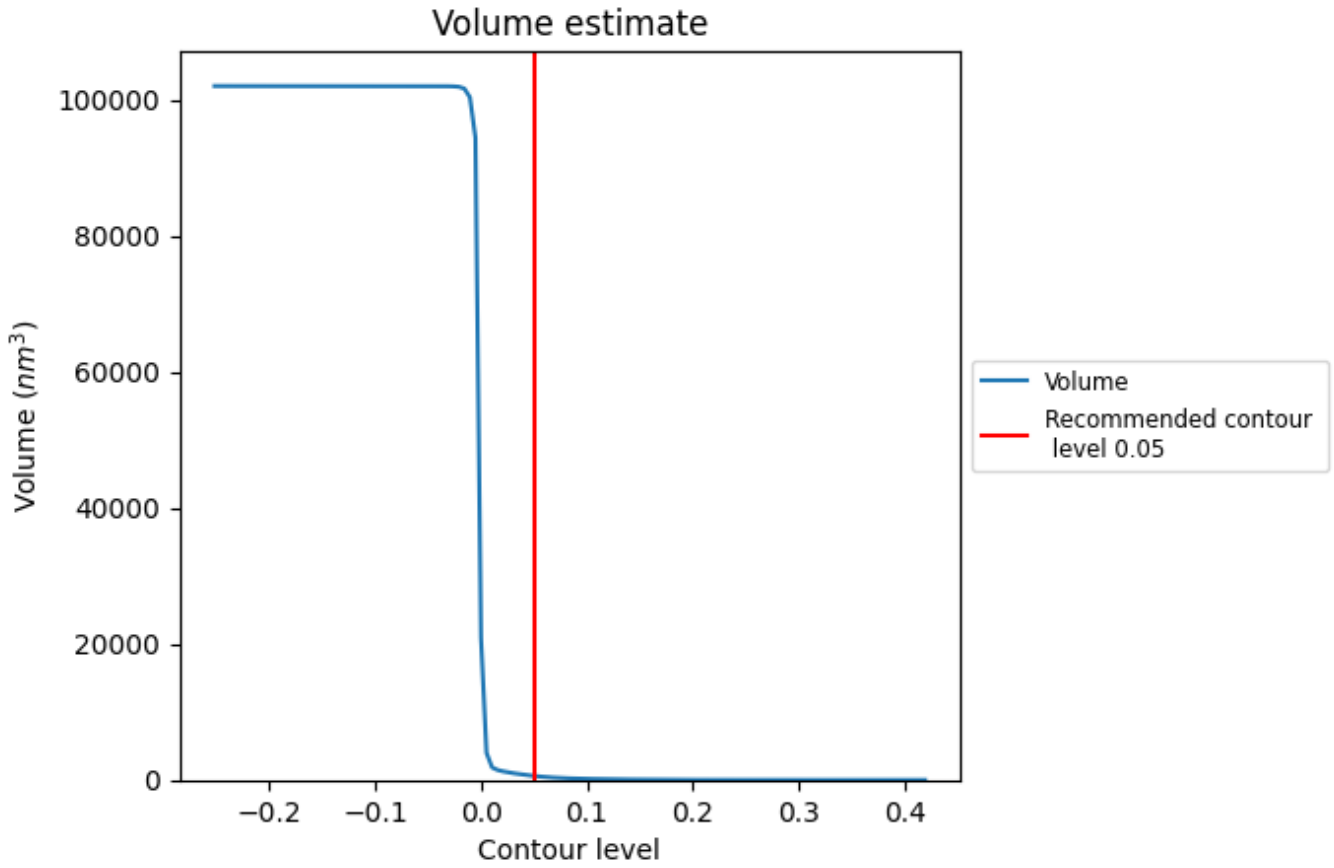
This section contains the results of statistical analysis of the map.

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.

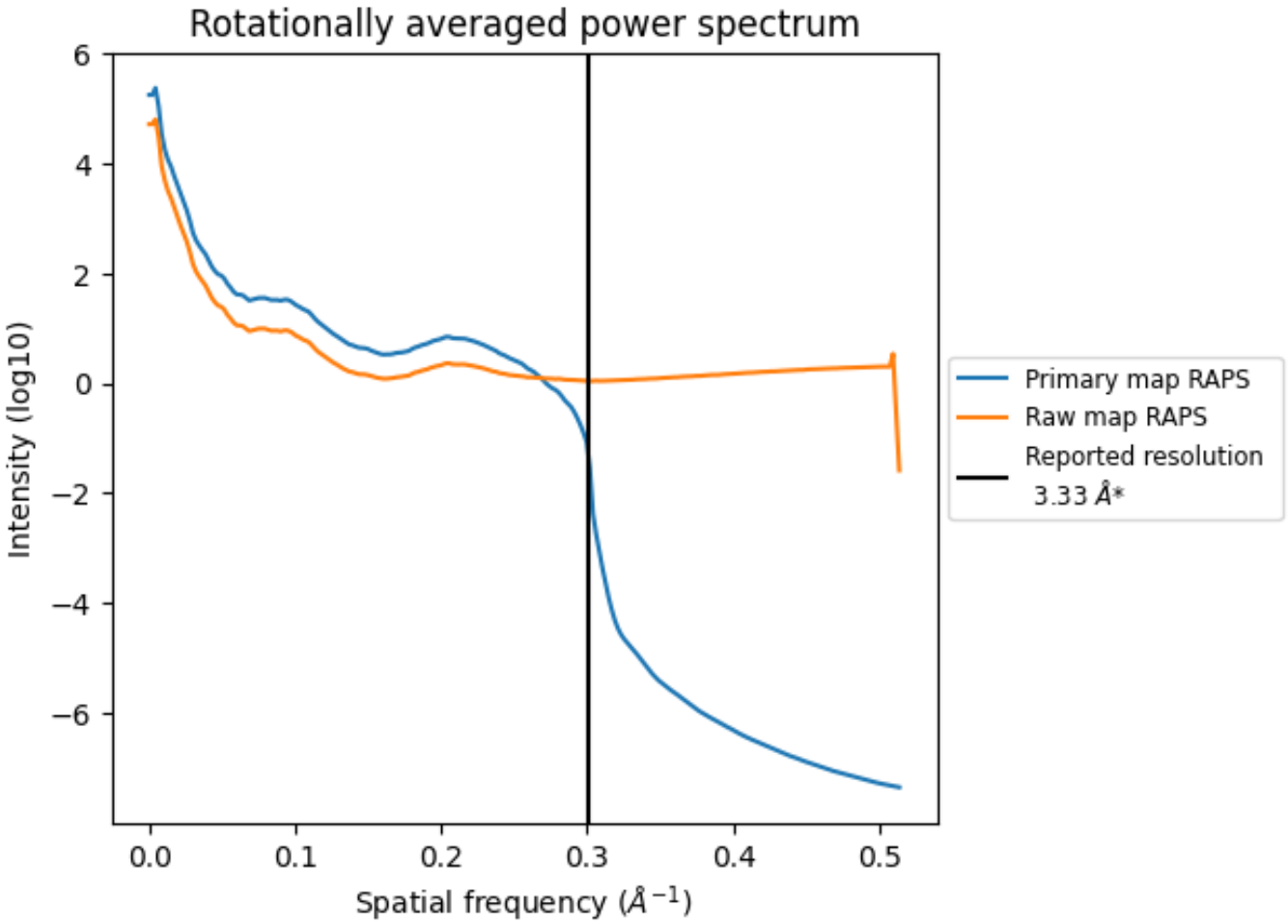
7.2 Volume estimate (i)



The volume at the recommended contour level is 594 nm^3; this corresponds to an approximate mass of 537 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)

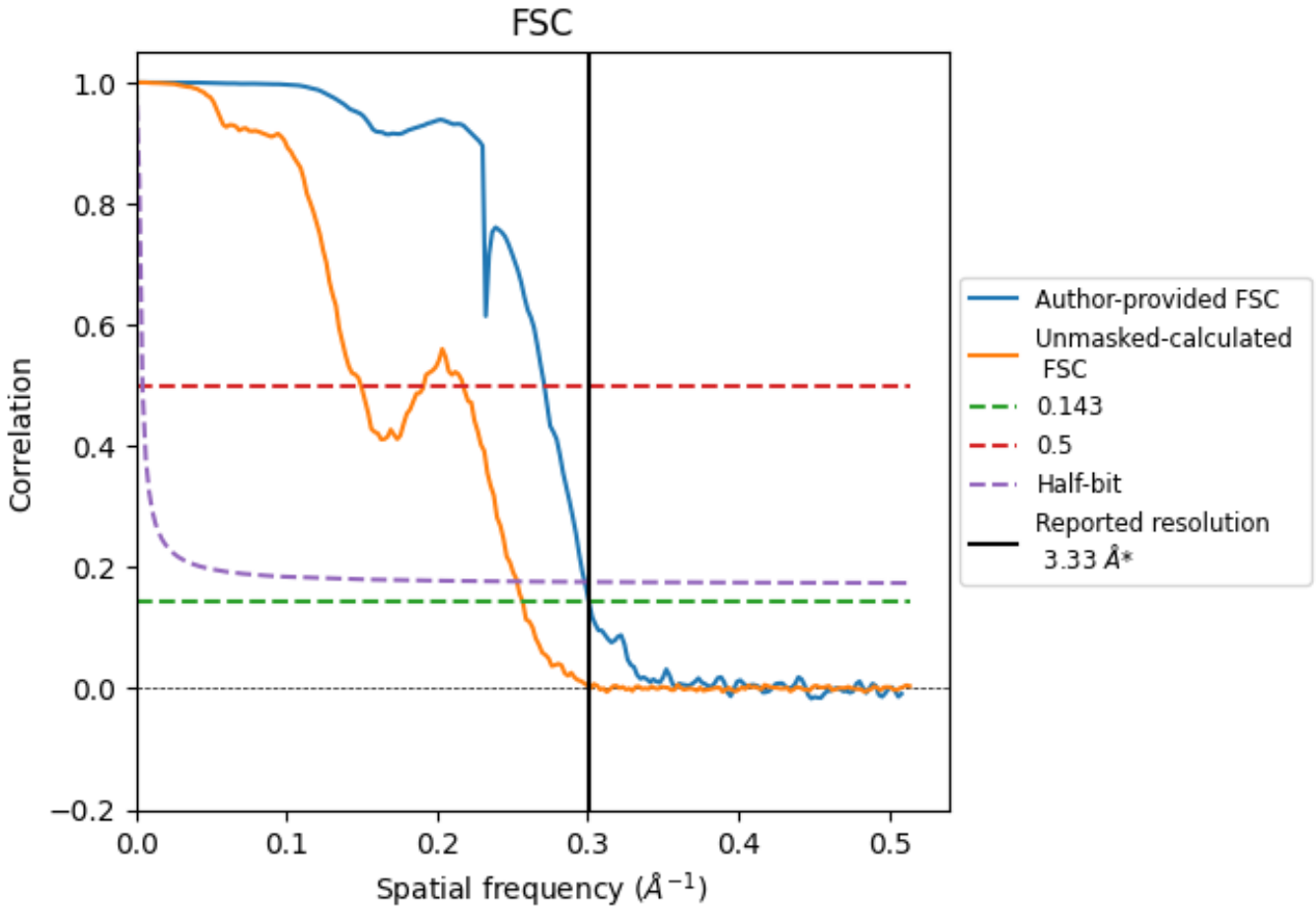


*Reported resolution corresponds to spatial frequency of 0.300 Å^{-1}

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 0.300 Å^{-1}

8.2 Resolution estimates (i)

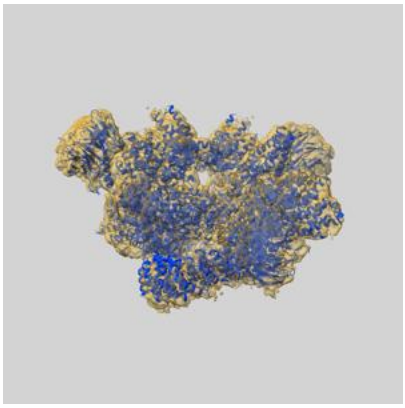
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.33	-	-
Author-provided FSC curve	3.33	3.69	3.36
Unmasked-calculated*	3.89	6.70	3.95

*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 3.89 differs from the reported value 3.33 by more than 10 %

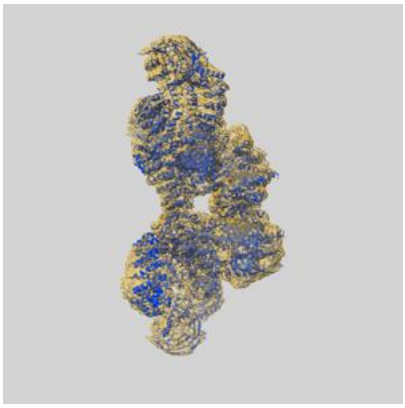
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-55630 and PDB model 9T79. Per-residue inclusion information can be found in section 3 on page 7.

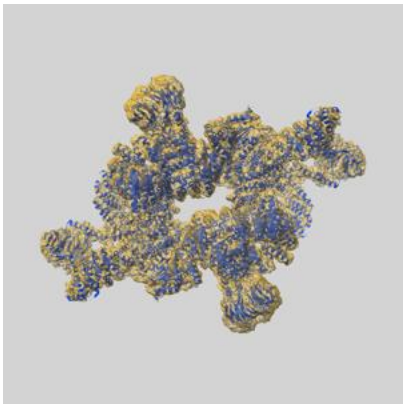
9.1 Map-model overlay



X



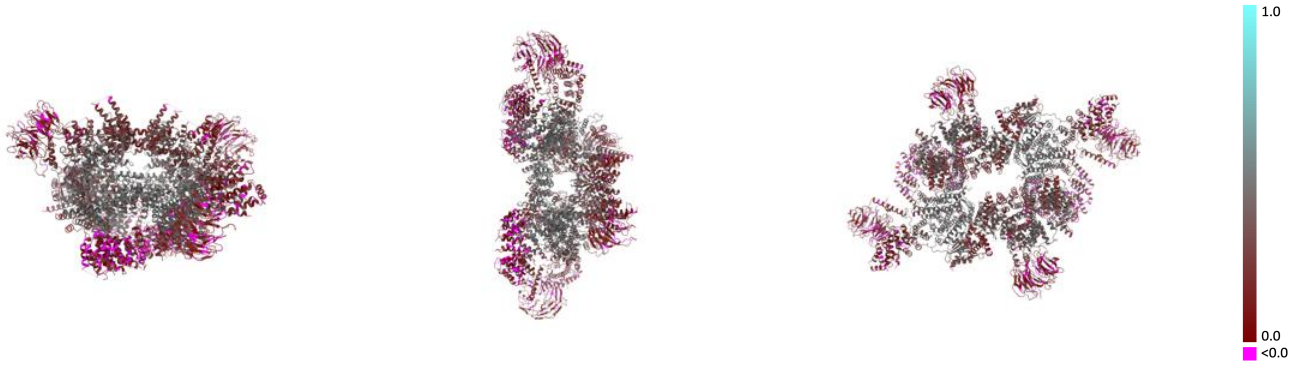
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 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.

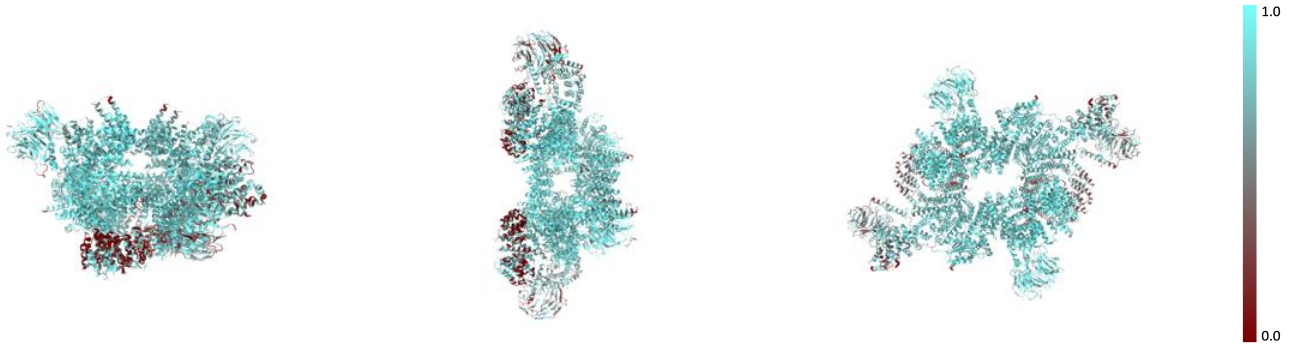
9.2 Q-score mapped to coordinate model



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.

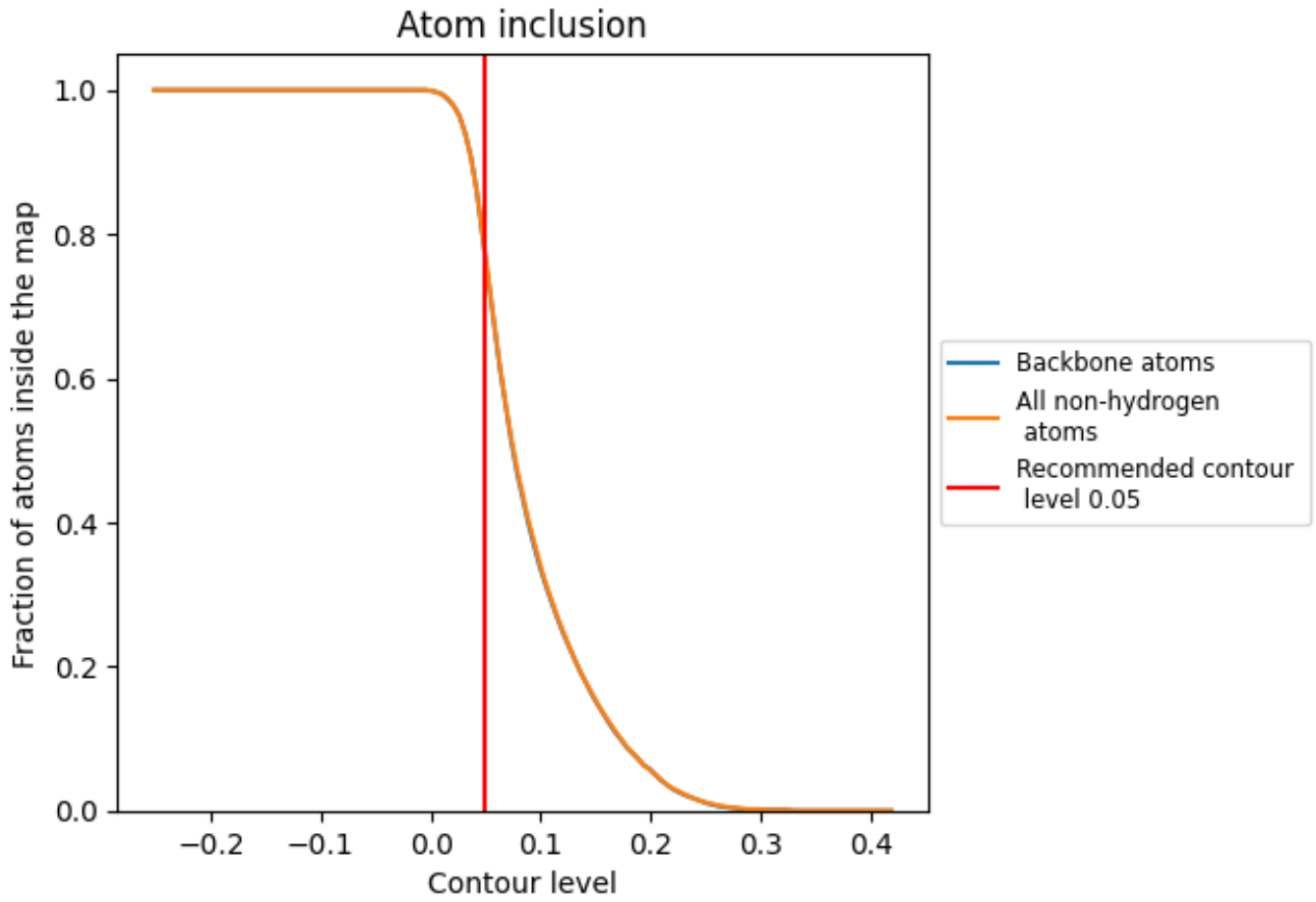
9.3 Atom inclusion mapped to coordinate model



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 (0.05).

9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 77% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7680	0.2900
A	0.8010	0.3230
B	0.8020	0.3230
C	0.7960	0.1420
D	0.7960	0.1420
E	0.7130	0.2650
F	0.7130	0.2610
G	0.7240	0.4400
H	0.6710	0.4570

