wwPDB EM Validation Summary Report

Nov 10, 2026 – 06:47 pm GMT

PDB ID	:	9T77 / pdb_00009t77
EMDB ID	:	EMD-55628
Title	:	cryo-EM structure of human LARP1 bound to human mTOR complex 1
Authors	:	Craigie, L.M.; Maier, T.
Deposited on	:	2025-11-10
Resolution	:	3.28 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:

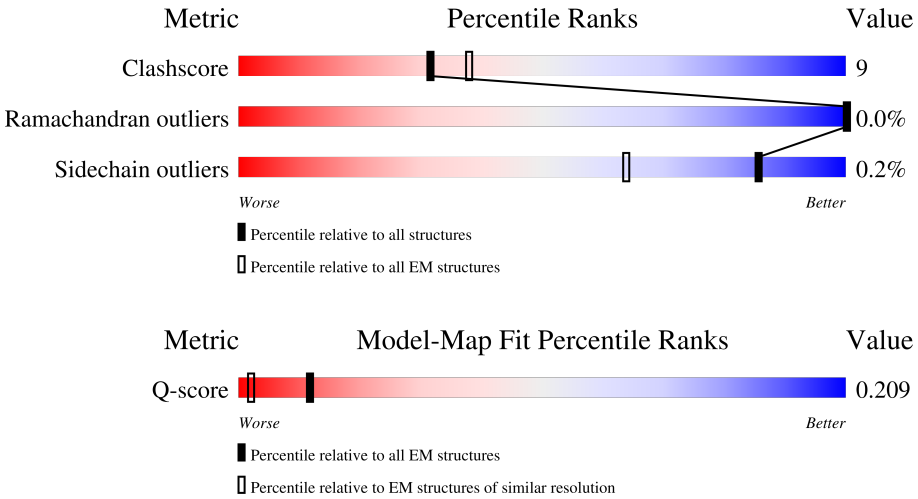
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

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

The reported resolution of this entry is 3.28 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.



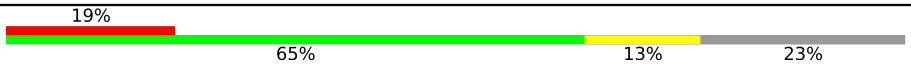
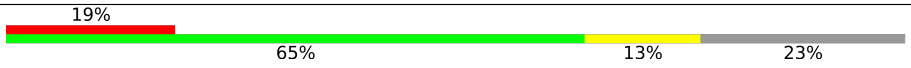
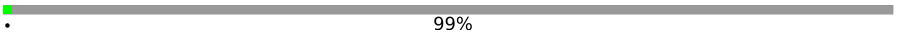
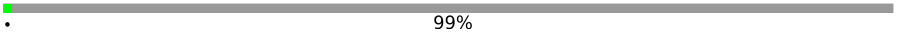
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14492 (2.78 - 3.78)

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	A	2549	68% 17% 14%
1	B	2549	68% 18% 14%
2	C	326	5% 87% 10%
2	D	326	5% 90% 8%

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Mol	Chain	Length	Quality of chain
3	E	1363	
3	F	1363	
4	G	1096	
4	H	1096	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 113464 atoms, of which 56648 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	2192	Total	C	H	N	O	S	0	0
			35020	11158	17553	3060	3137	112		
1	B	2192	Total	C	H	N	O	S	0	0
			35020	11158	17553	3060	3137	112		

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

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

- Molecule 3 is a protein called Regulatory-associated protein of mTOR.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	E	1052	Total	C	H	N	O	S	0	0
			16760	5361	8375	1450	1518	56		
3	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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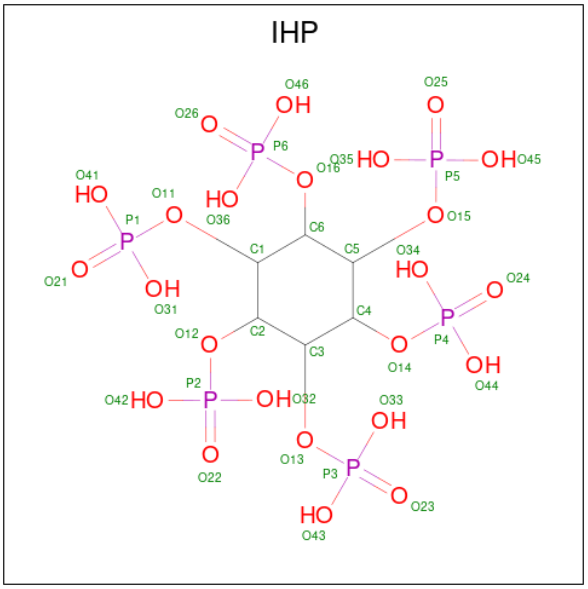
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Chain	Residue	Modelled	Actual	Comment	Reference
F	-4	ASP	-	expression tag	UNP Q8N122
F	-3	ASP	-	expression tag	UNP Q8N122
F	-2	ASP	-	expression tag	UNP Q8N122
F	-1	ASP	-	expression tag	UNP Q8N122
F	0	LYS	-	expression tag	UNP Q8N122

- Molecule 4 is a protein called La-related protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	7	Total	C	H	N	O	0	0
			113	42	49	7	15		
4	H	7	Total	C	H	N	O	0	0
			113	42	49	7	15		

- 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	

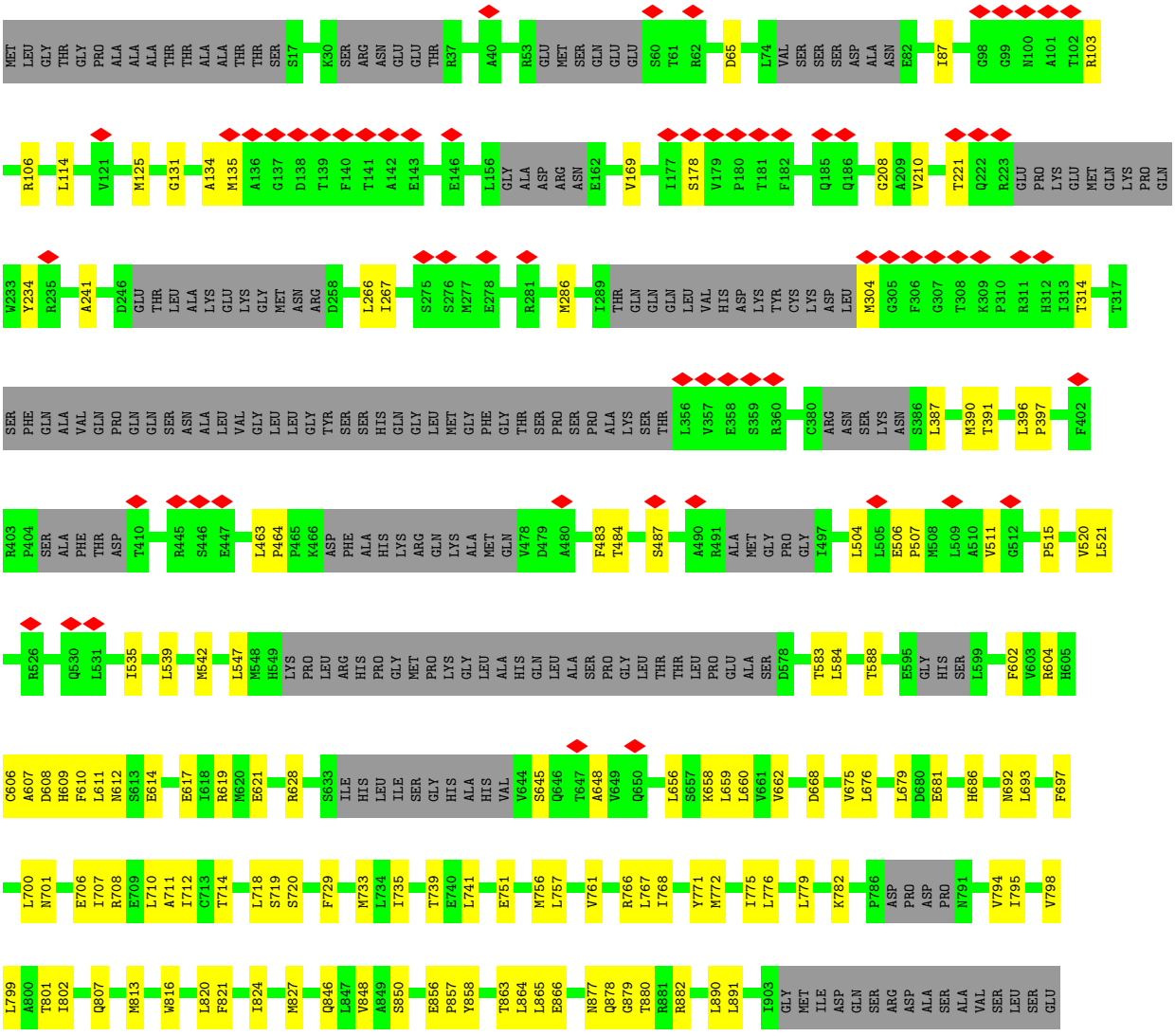
3 Residue-property plots (i)

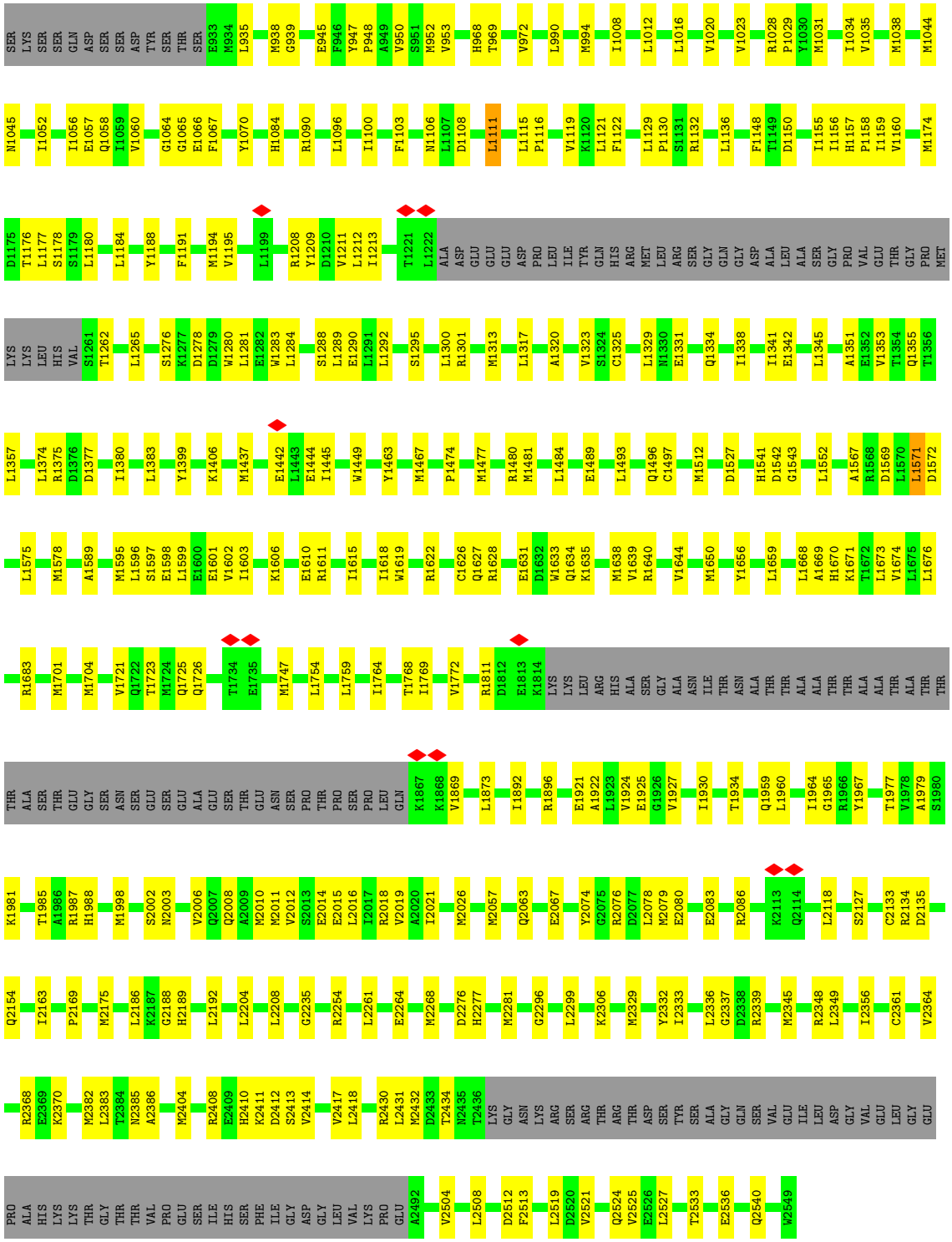
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Serine/threonine-protein kinase mTOR

Chain A:

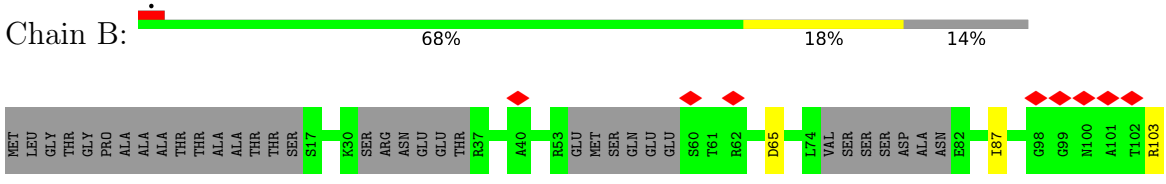


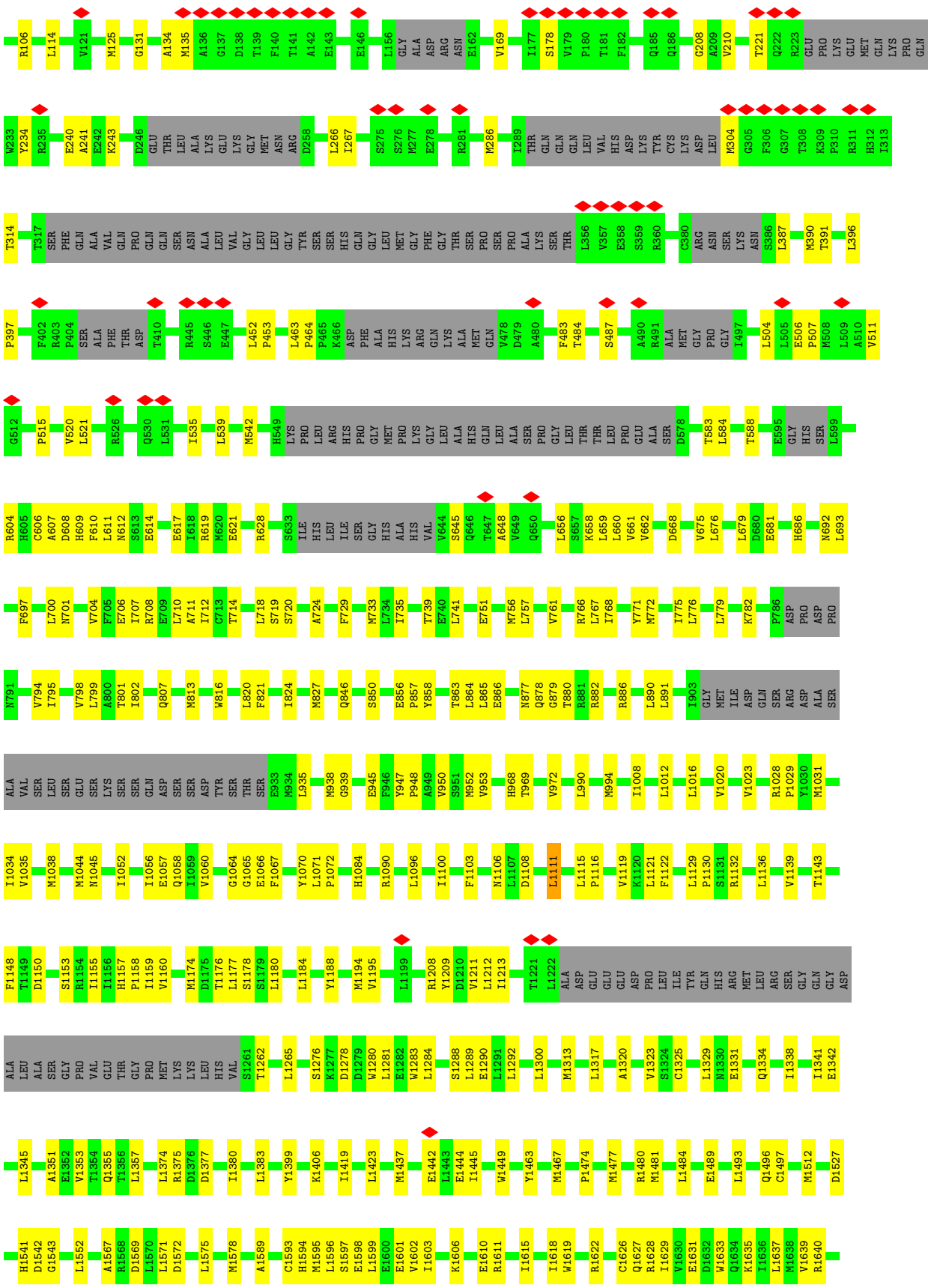


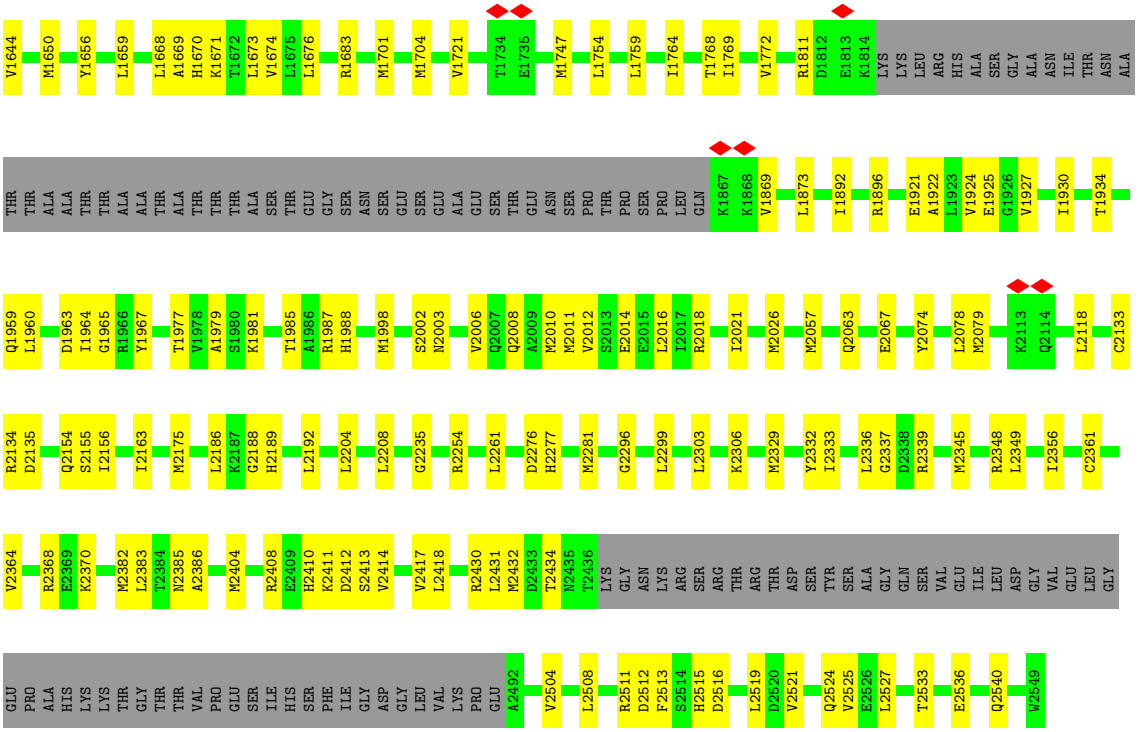


• Molecule 1: Serine/threonine-protein kinase mTOR

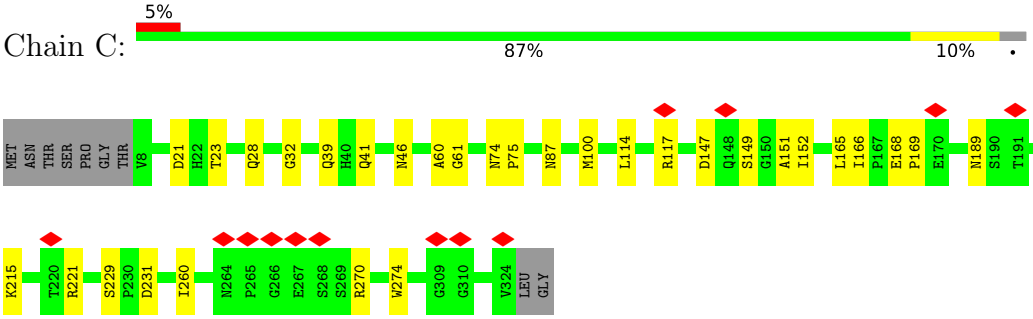
Chain B:



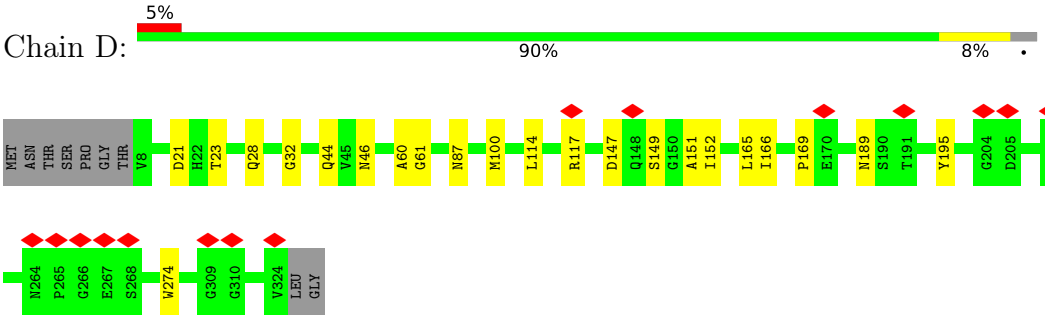




• Molecule 2: Target of rapamycin complex subunit LST8

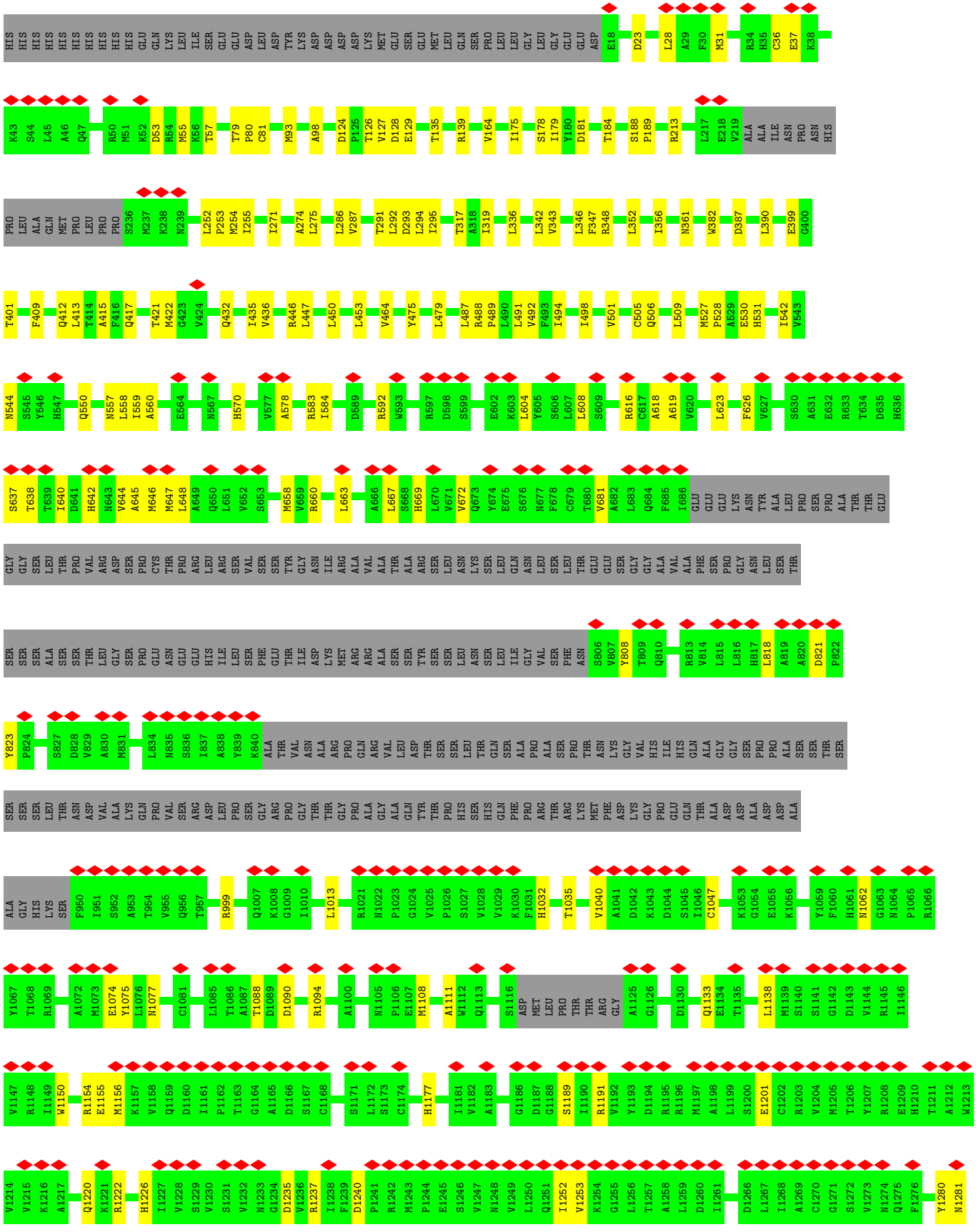


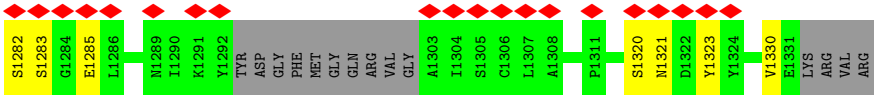
• Molecule 2: Target of rapamycin complex subunit LST8



• Molecule 3: Regulatory-associated protein of mTOR



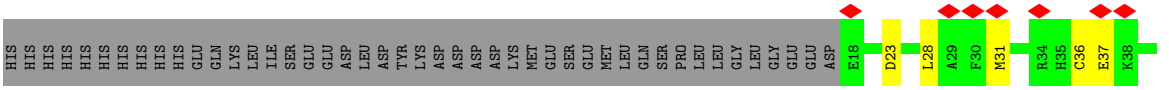

HIS HIS HIS HIS HIS HIS HIS HIS GLU GLN LYS LEU ILE SER GLU GLU ASP LEU ASP TYR LYS ASP ASP ASP LYS MET GLU SER GLU MET LEU GLN SER PRO LEU LEU GLY LEU GLY GLU GLU ASP
E18 D23 L28 A29 F30 M31 R34 H35 C36 E37 K38
K43 S44 L45 A46 Q47 R50 M51 K52 D53 R54 M55 K56 T57 T79 P80 C81 M93 A98 D124 P125 T126 V127 D128 E129 T135 R139 V164 I175 S178 I179 Y180 D181 T184 S188 P189 R213 L217 E218 V219 ALA ALA ILE ASN PRO ASN HIS
PRO LEU ALA GLN MET PRO LEU PRO PRO S236 M237 K238 N239 L252 P253 M254 I255 I271 A274 L275 L286 V287 T291 L292 D293 L294 I295 T317 A318 I319 L336 L342 V343 L346 F347 R348 L352 I356 N361 W382 D387 L390 E399 G400
T401 F409 Q412 L413 T414 A415 F416 Q417 T421 M422 G423 V424 Q432 I435 V436 R446 L447 L450 L453 V464 Y475 L479 L487 R488 P489 L490 L491 V492 F493 I494 I498 V501 C505 Q506 L509 M527 P528 A529 E530 H531 I542 V543
N544 S545 Y546 H547 Q550 N557 L558 I559 A560 E564 N567 H570 V577 A578 R583 I584 D589 R592 W593 R597 D598 S599 E602 K603 L604 Y605 S606 L607 L608 S609 R616 C617 A618 A619 V620 L623 F626 V627 S630 A631 E632 R633 T634 D635 H636
S637 T638 T639 I640 D641 H642 M643 V644 A645 M646 M647 L648 A649 Q650 L651 V652 S653 M658 V659 R660 L663 A666 L667 S668 H669 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 ALA THR ALA ARG SER LEU 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 SER ALA SER SER THR LEU GLY SER PRO PRO GLU ASN GLU 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 Y808 T809 Q810 R813 V814 L815 L816 H817 L818 A819 A820 D821 P822
Y823 P824 S827 D828 V829 A830 M831 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 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 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 ALA ASP ASP ALA
ALA GLY HIS LYS SER F950 I951 S952 A953 T954 V955 Q956 T957 R999 Q1007 K1008 G1009 I1010 L1013 R1021 N1022 P1023 G1024 V1025 P1026 S1027 V1028 V1029 K1030 F1031 H1032 T1035 V1040 A1041 D1042 K1043 D1044 S1045 I1046 C1047 K1053 G1054 E1055 K1056 Y1059 F1060 H1061 N1062 G1063 N1064 P1065 R1066
Y1067 T1068 R1069 A1072 M1073 E1074 Y1075 L1076 N1077 C1081 L1085 T1086 A1087 T1088 D1089 D1090 R1094 A1100 N1105 P1106 E1107 M1108 A1111 W1112 Q1113 S1116 ASP MET LEU PRO THR THR ARG GLY A1125 G1126 D1130 Q1133 E1134 T1135 L1138 M1139 S1140 S1141 G1142 D1143 V1144 R1145 I1146
V1147 R1148 I1149 W1150 R1154 E1155 M1156 K1157 V1158 Q1159 D1160 I1161 P1162 T1163 G1164 A1165 D1166 S1167 C1168 S1171 L1172 S1173 C1174 H1177 I1181 V1182 A1183 G1186 D1187 G1188 S1189 I1190 R1191 V1192 Y1193 D1194 R1195 R1196 M1197 A1198 L1199 S1200 E1201 C1202 R1203 V1204 M1205 T1206 Y1207 R1208 E1209 H1210 T1211 A1212 W1213
V1214 V1215 K1216 A1217 Q1220 K1221 R1222 H1226 I1227 V1228 S1229 V1230 S1231 V1232 N1233 G1234 D1235 V1236 R1237 I1238 F1239 D1240 P1241 R1242 M1243 P1244 E1245 S1246 V1247 N1248 V1249 L1250 Q1251 I1252 V1253 K1254 G1255 L1256 T1257 A1258 L1259 D1260 I1261 D1266 L1267 I1268 A1269 C1270 G1271 S1272 V1273 N1274 Q1275 F1276 Y1280 N1281

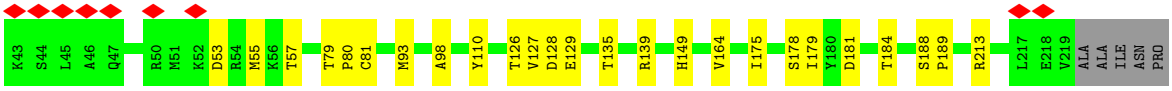


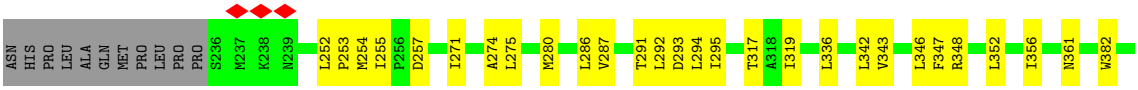
• Molecule 3: Regulatory-associated protein of mTOR

Chain F:

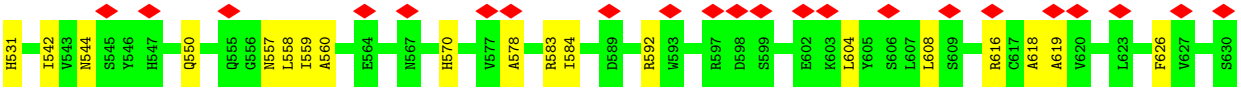


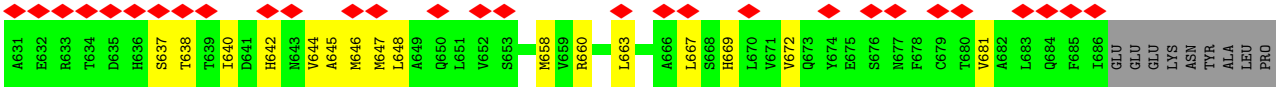






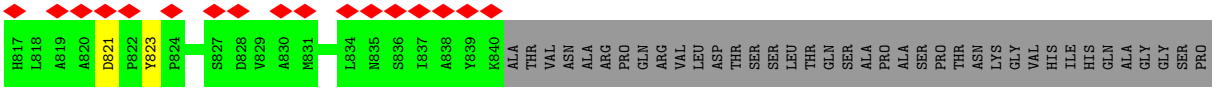


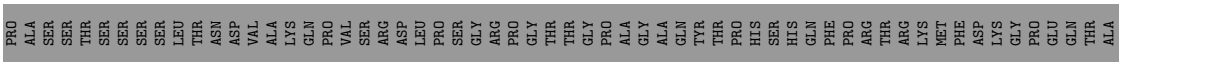


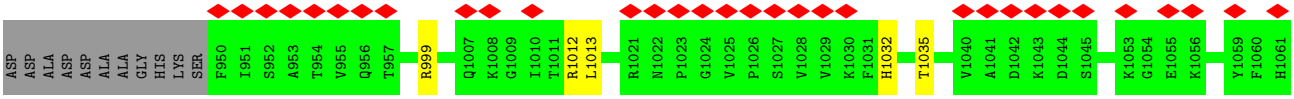


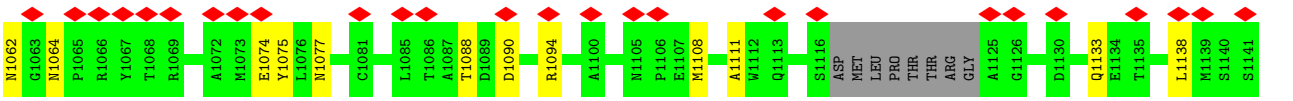


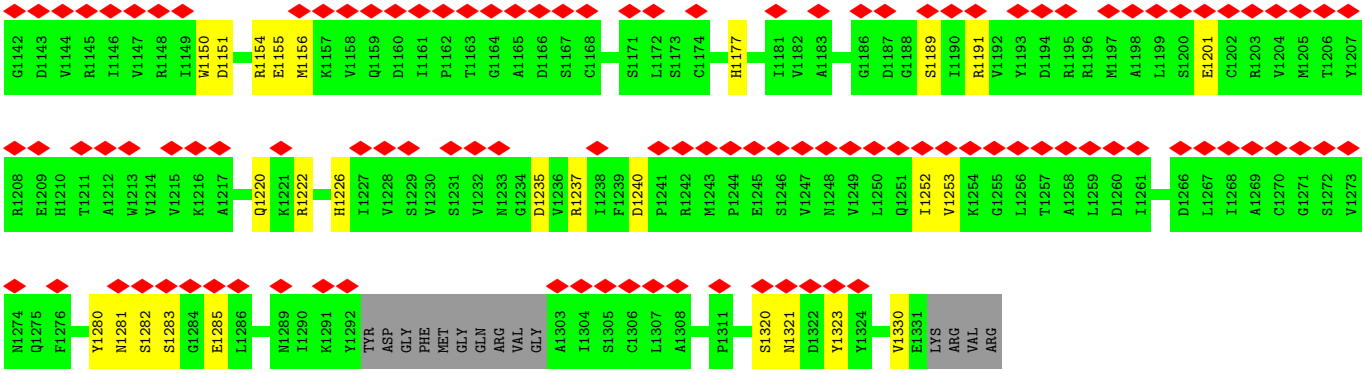






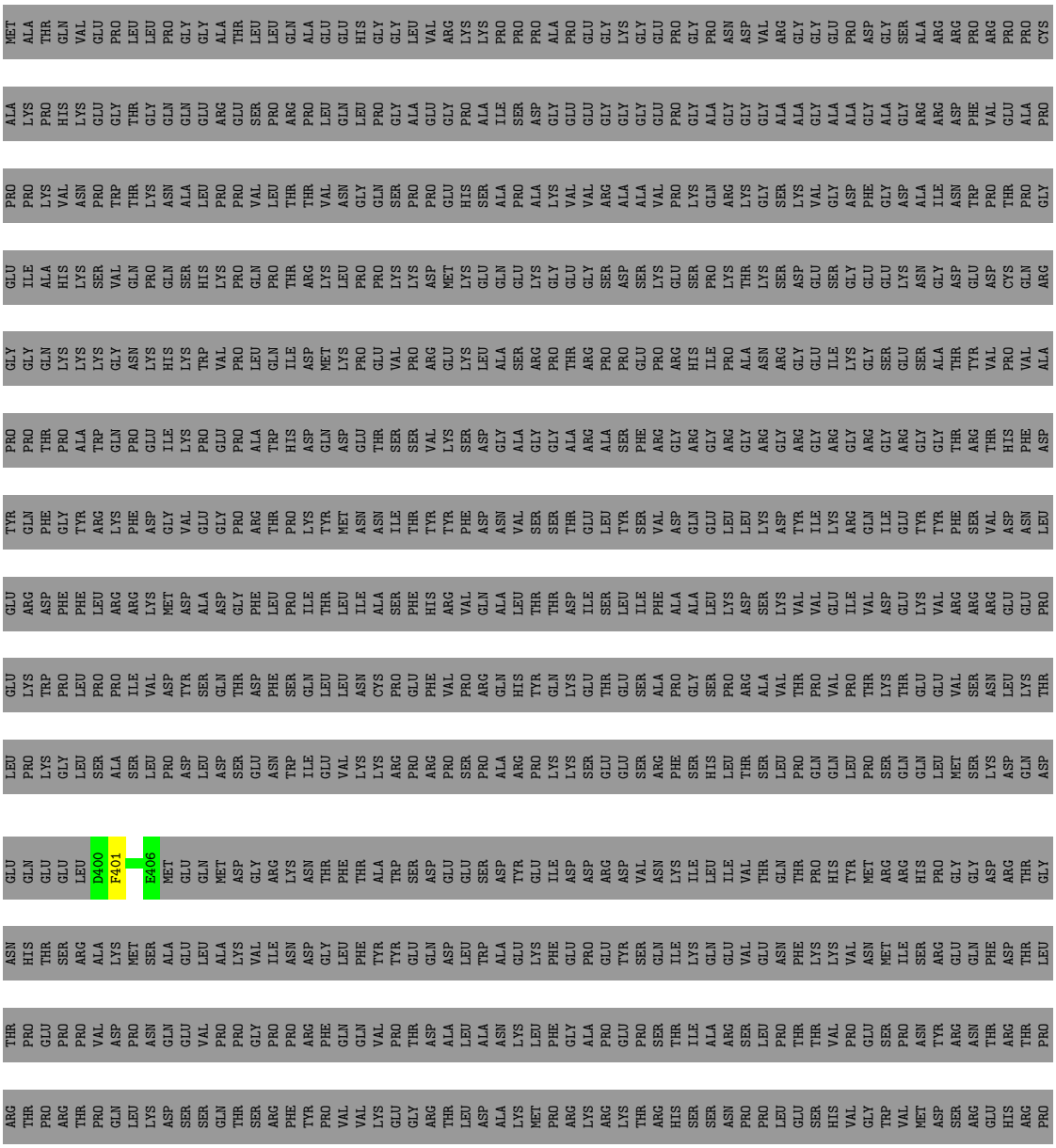


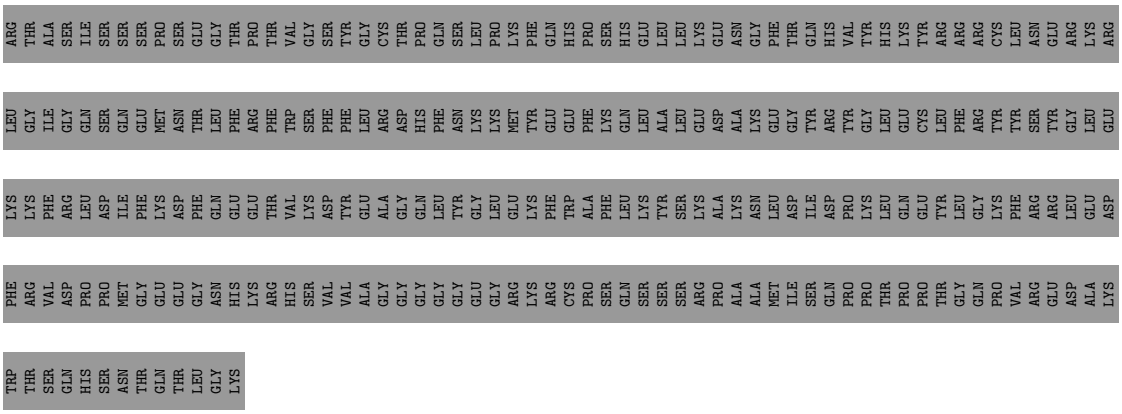




• Molecule 4: La-related protein 1

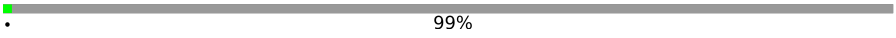
Chain G: 99%

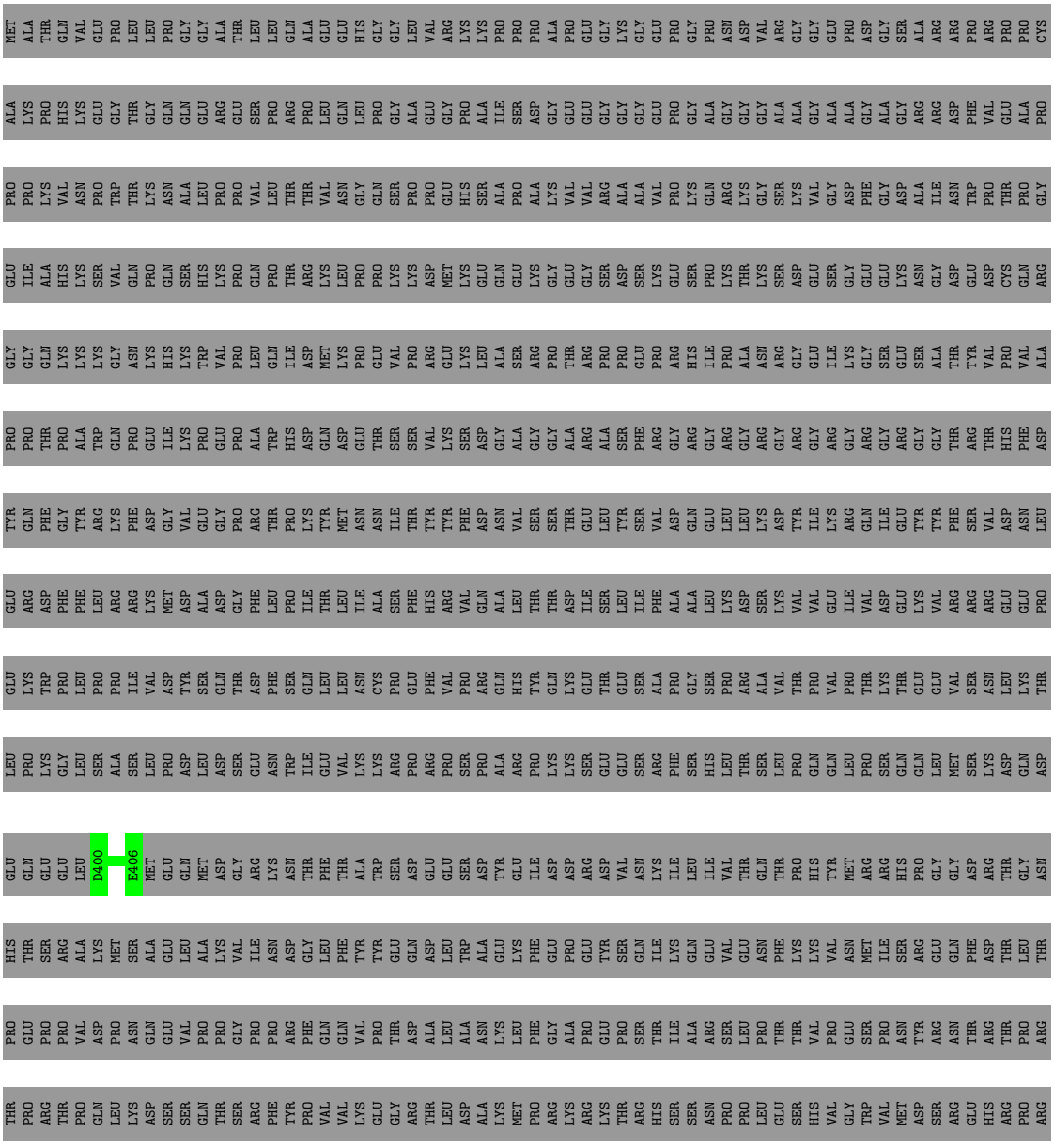


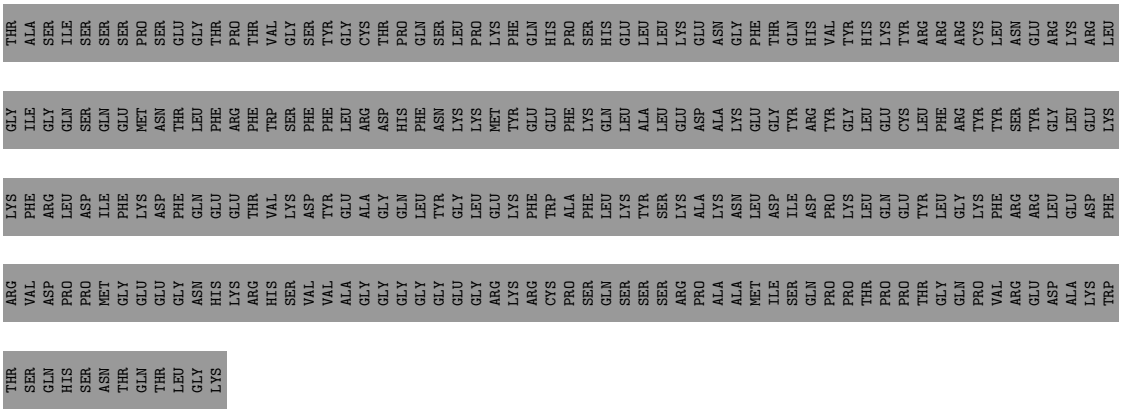


• Molecule 4: La-related protein 1

Chain H:






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

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	597046	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	0.438	Depositor
Minimum map value	-0.203	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.045	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	A	0.12	0/17814	0.30	0/24116
1	B	0.12	0/17814	0.29	0/24116
2	C	0.09	0/2514	0.27	0/3426
2	D	0.10	0/2514	0.27	0/3426
3	E	0.11	0/8585	0.27	0/11680
3	F	0.11	0/8585	0.27	0/11680
4	G	0.08	0/65	0.28	0/86
4	H	0.11	0/65	0.30	0/86
All	All	0.12	0/57956	0.28	0/78616

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	A	17467	17553	17553	357	0
1	B	17467	17553	17553	362	0
2	C	2456	2341	2341	17	0
2	D	2456	2341	2341	14	0
3	E	8385	8375	8375	121	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	8385	8375	8375	122	0
4	G	64	49	48	1	0
4	H	64	49	48	0	0
5	A	36	6	6	0	0
5	B	36	6	6	0	0
All	All	56816	56648	56646	981	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 9.

The worst 5 of 981 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:712:ILE:HG21	1:B:756:MET:HE1	1.42	1.01
1:A:712:ILE:HG21	1:A:756:MET:HE1	1.41	1.00
3:E:421:THR:OG1	3:E:422:MET:SD	2.21	0.98
3:F:421:THR:OG1	3:F:422:MET:SD	2.21	0.97
1:A:2521:VAL:O	1:A:2525:VAL:HG23	1.78	0.84

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	A	2150/2549 (84%)	2102 (98%)	48 (2%)	0	100	100
1	B	2150/2549 (84%)	2102 (98%)	48 (2%)	0	100	100
2	C	315/326 (97%)	302 (96%)	13 (4%)	0	100	100
2	D	315/326 (97%)	301 (96%)	14 (4%)	0	100	100
3	E	1040/1363 (76%)	1017 (98%)	22 (2%)	1 (0%)	48	76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	F	1040/1363 (76%)	1016 (98%)	23 (2%)	1 (0%)	48 76
4	G	5/1096 (0%)	5 (100%)	0	0	100 100
4	H	5/1096 (0%)	5 (100%)	0	0	100 100
All	All	7020/10668 (66%)	6850 (98%)	168 (2%)	2 (0%)	100 100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	81	CYS
3	F	81	CYS

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	A	1876/2220 (84%)	1874 (100%)	2 (0%)	88 91
1	B	1876/2220 (84%)	1875 (100%)	1 (0%)	88 91
2	C	269/276 (98%)	267 (99%)	2 (1%)	76 80
2	D	269/276 (98%)	267 (99%)	2 (1%)	76 80
3	E	928/1191 (78%)	927 (100%)	1 (0%)	88 91
3	F	928/1191 (78%)	926 (100%)	2 (0%)	87 88
4	G	7/948 (1%)	7 (100%)	0	100 100
4	H	7/948 (1%)	7 (100%)	0	100 100
All	All	6160/9270 (66%)	6150 (100%)	10 (0%)	85 88

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	1323	TYR
3	F	390	LEU
3	F	1323	TYR
2	C	221	ARG

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Mol	Chain	Res	Type
2	C	274	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	2154	GLN
3	E	67	ASN
1	B	2277	HIS
2	C	189	ASN
3	E	555	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	0.74	1 (2%)	54,60,60	0.34	0
5	IHP	A	2601	-	36,36,36	0.74	1 (2%)	54,60,60	0.34	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	-	-	3/30/54/54	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	2.84	1.64	1.59
5	A	2601	IHP	P3-O13	2.84	1.64	1.59

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

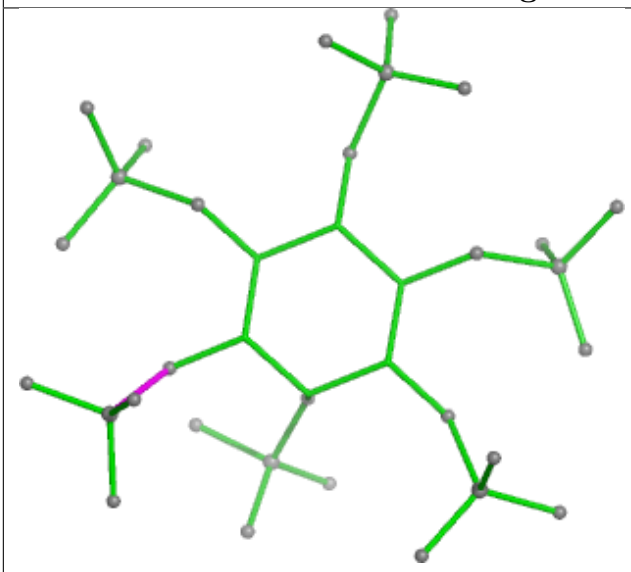
Mol	Chain	Res	Type	Atoms
5	A	2601	IHP	C2-O12-P2-O22
5	B	2601	IHP	C2-O12-P2-O22
5	A	2601	IHP	C3-O13-P3-O23
5	B	2601	IHP	C3-O13-P3-O23
5	A	2601	IHP	C3-O13-P3-O33

There are no ring outliers.

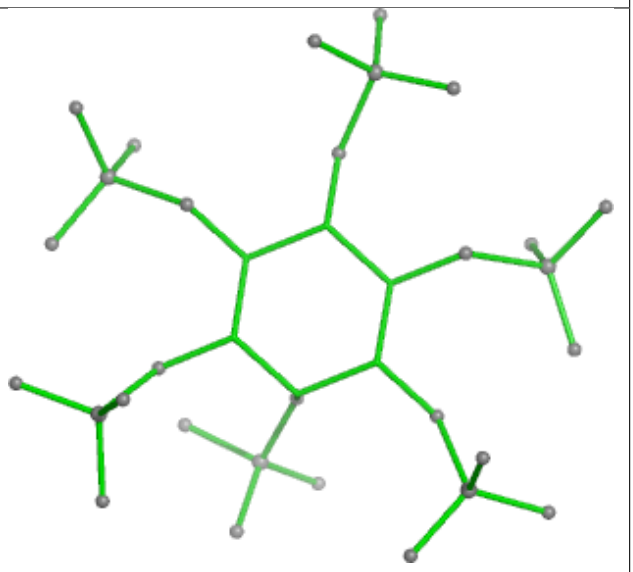
No monomer is involved in short contacts.

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.

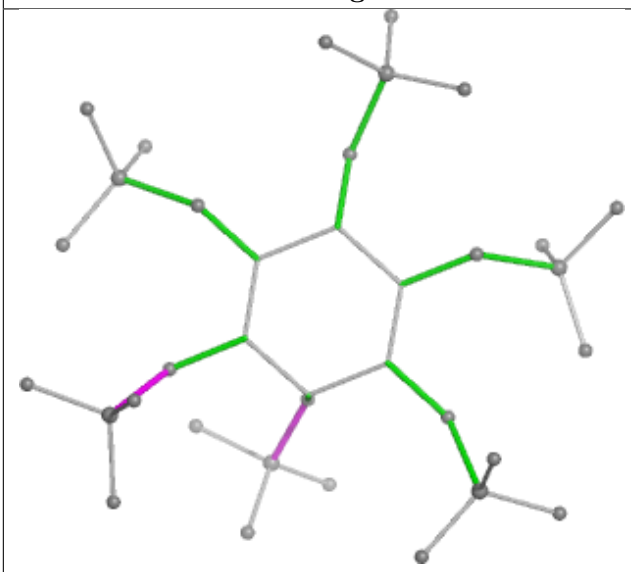
Ligand IHP B 2601



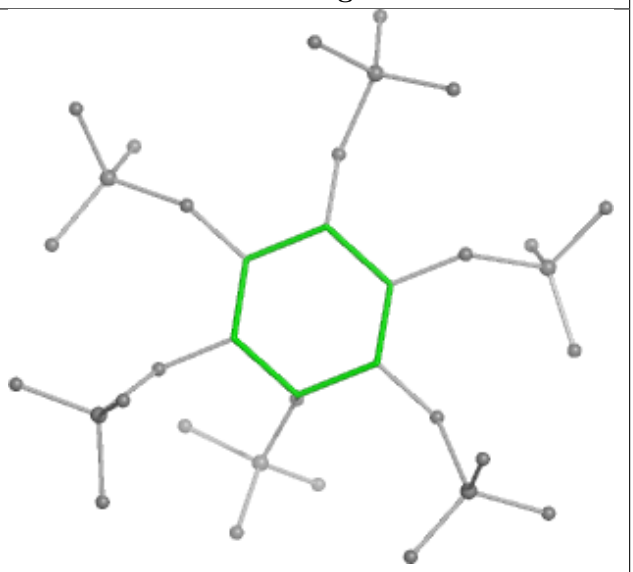
Bond lengths



Bond angles

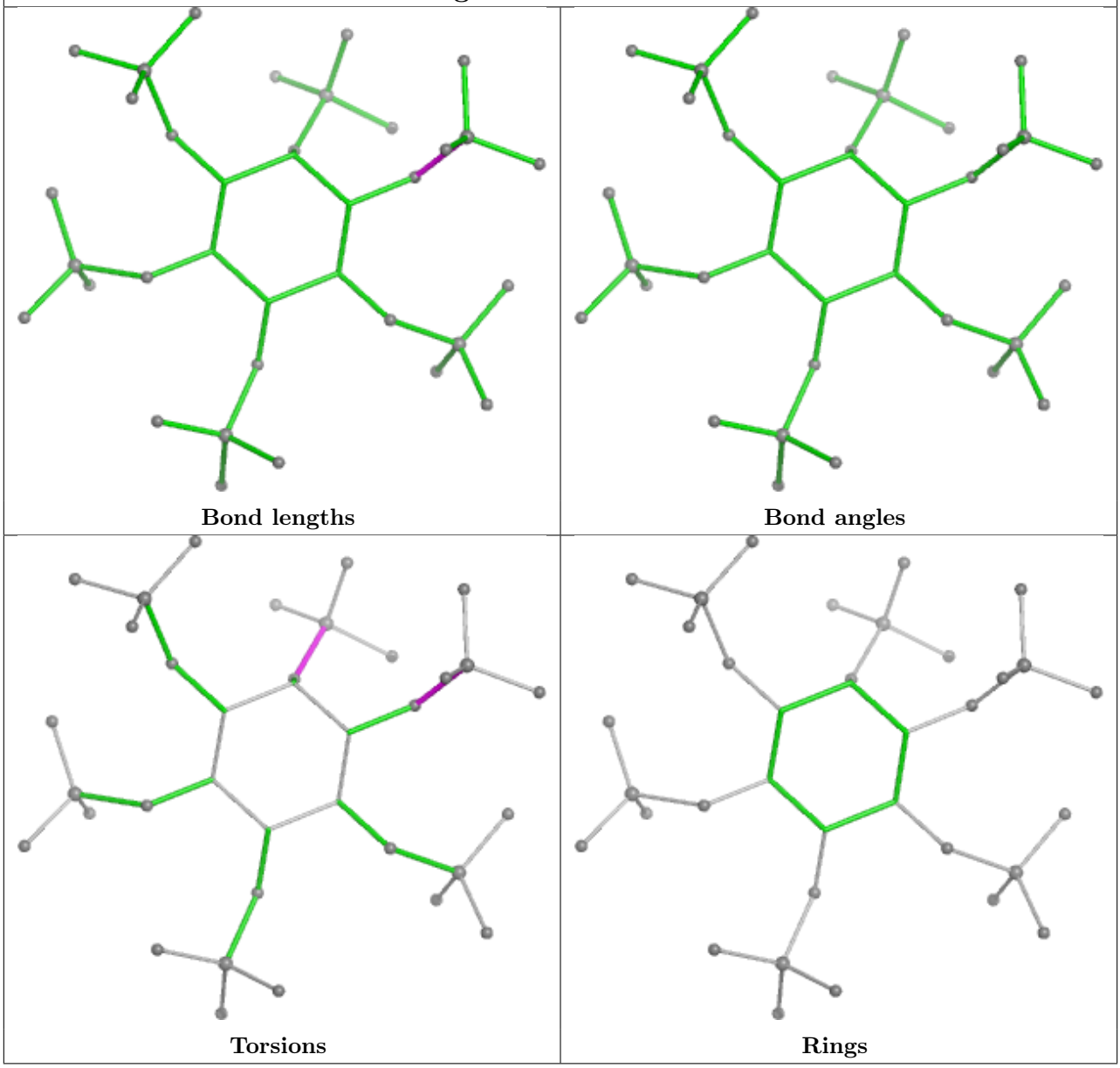


Torsions



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.

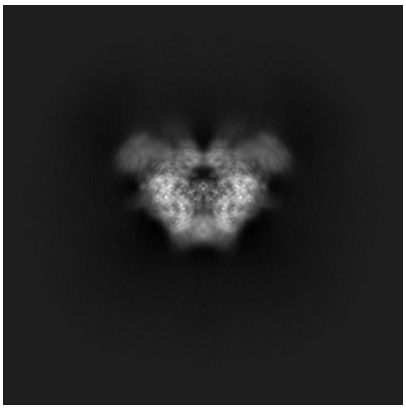
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-55628. These allow visual inspection of the internal detail of the map and identification of artifacts.

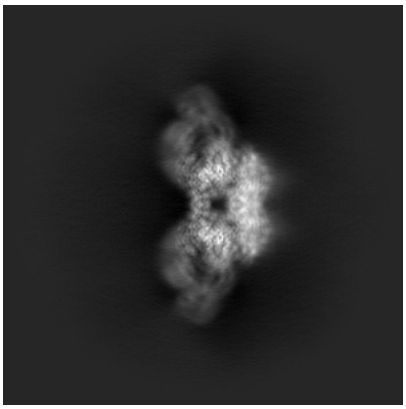
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

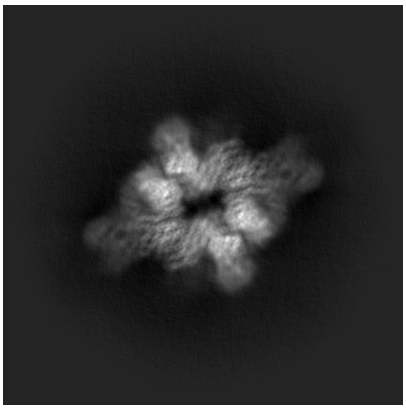
6.1.1 Primary map



X

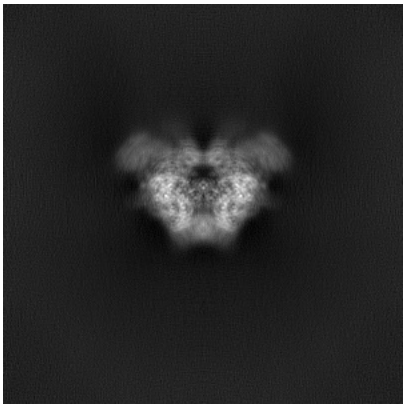


Y

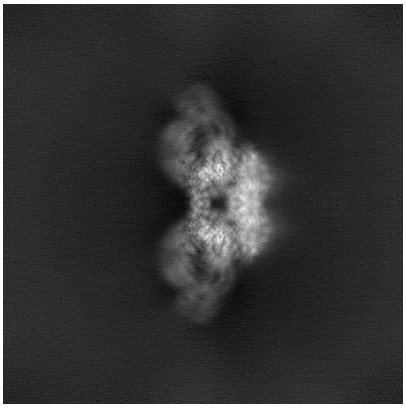


Z

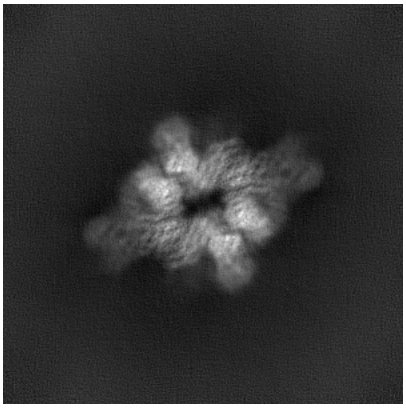
6.1.2 Raw map



X



Y

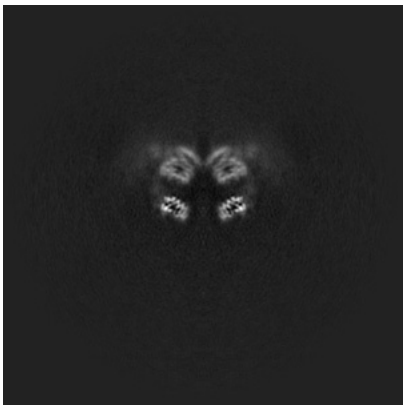


Z

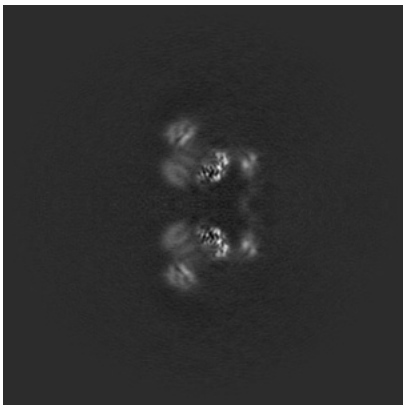
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

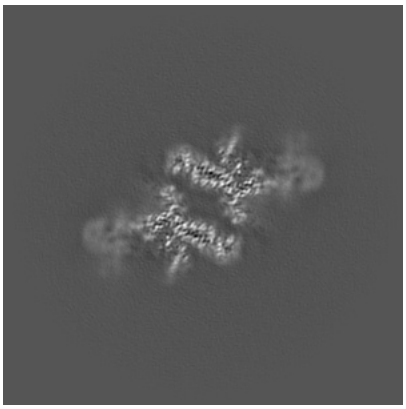
6.2.1 Primary map



X Index: 240



Y Index: 240

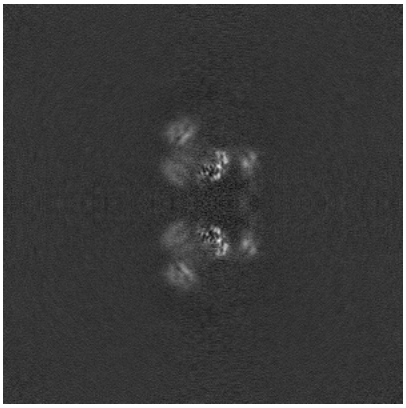


Z Index: 240

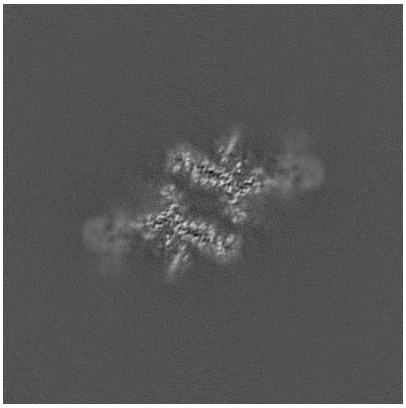
6.2.2 Raw map



X Index: 240



Y Index: 240

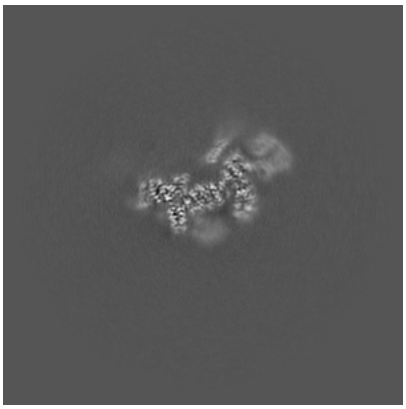


Z Index: 240

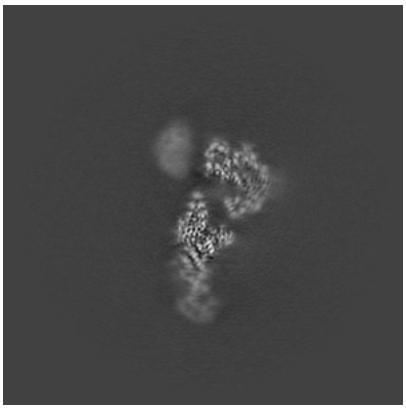
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

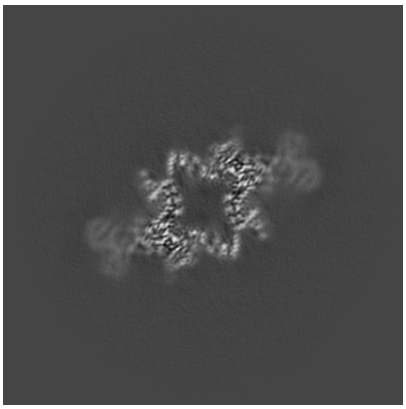
6.3.1 Primary map



X Index: 205

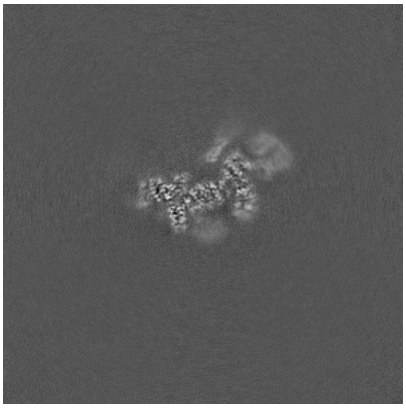


Y Index: 215

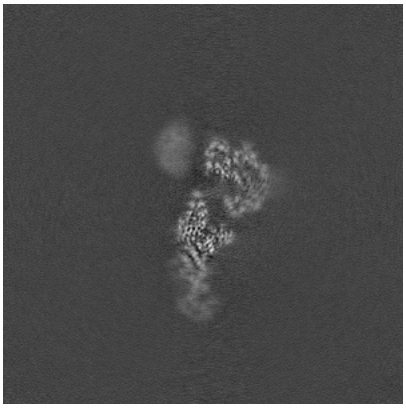


Z Index: 248

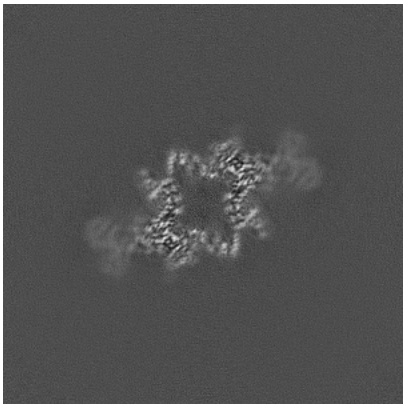
6.3.2 Raw map



X Index: 205



Y Index: 215

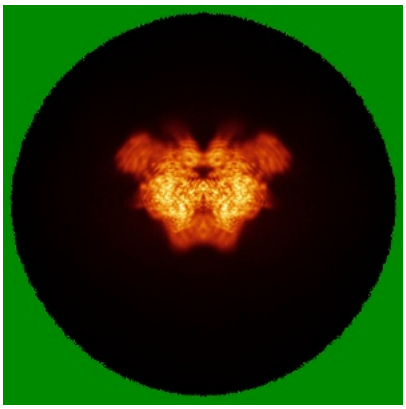


Z Index: 248

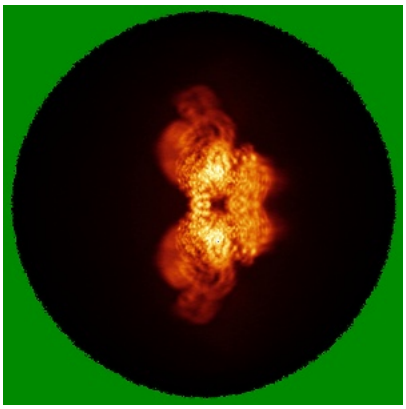
The images above show the largest variance slices of the map in three orthogonal directions.

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

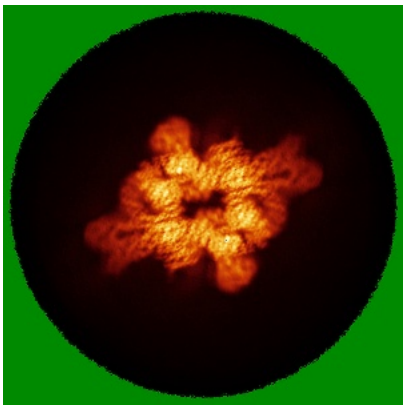
6.4.1 Primary map



X

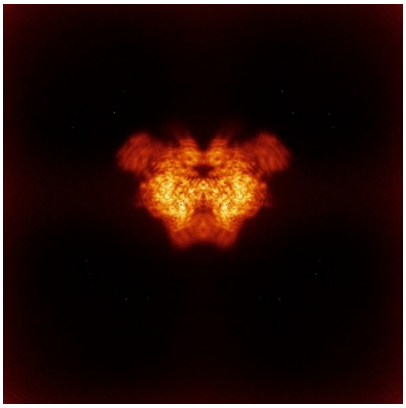


Y

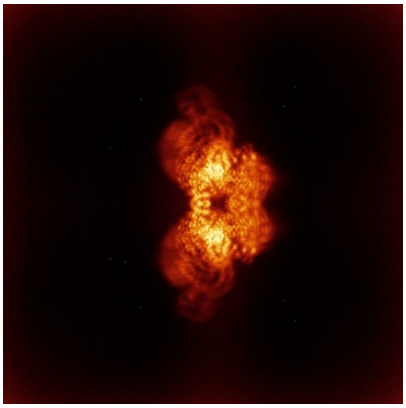


Z

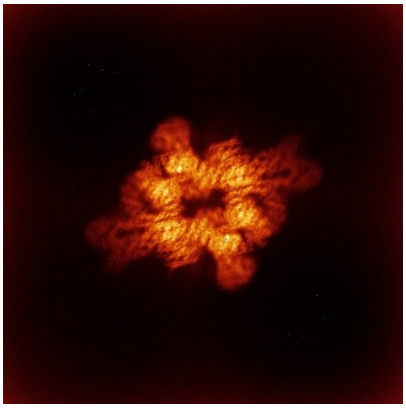
6.4.2 Raw map



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 0.045. 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.

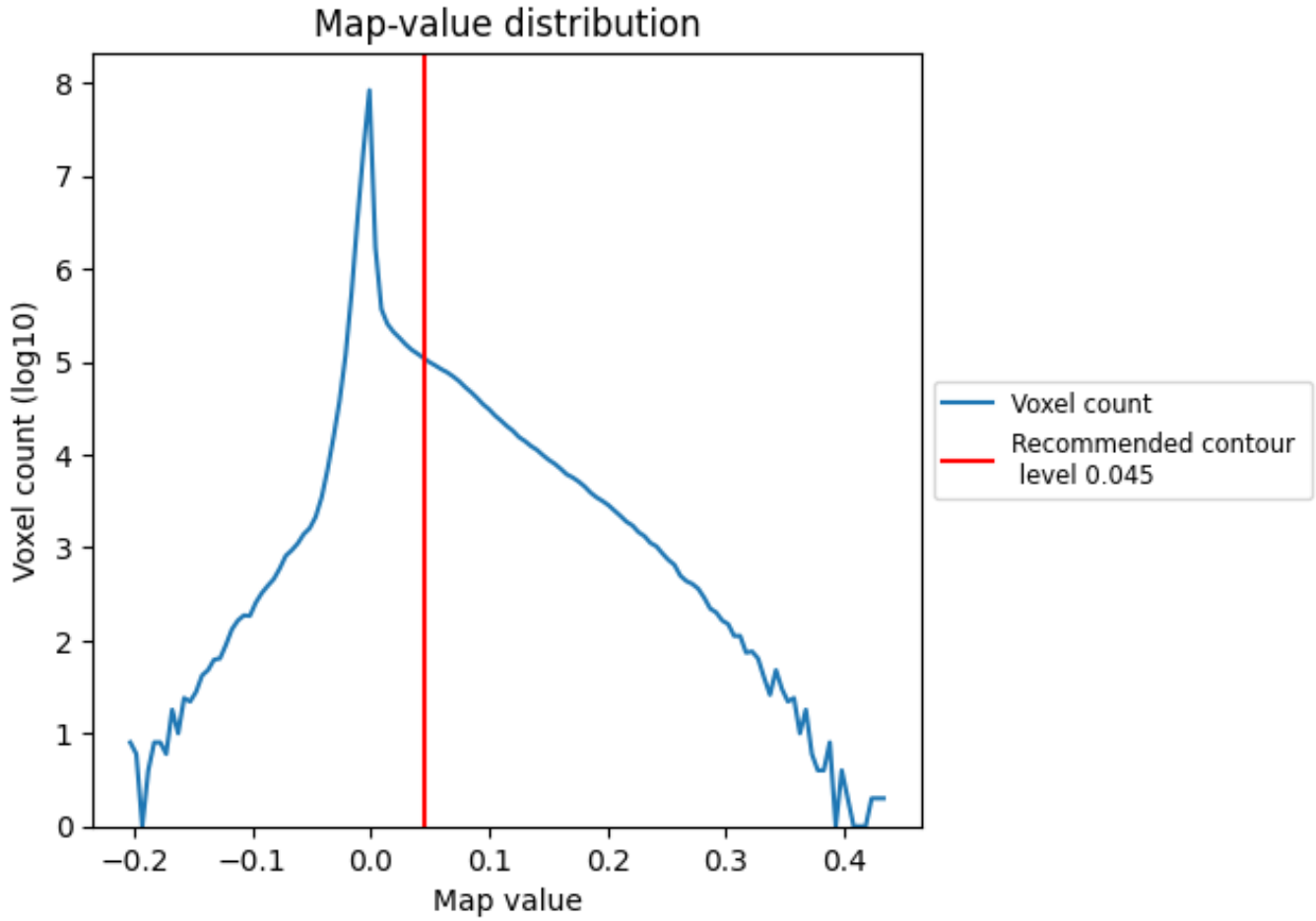
6.6 Mask visualisation (i)

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

7 Map analysis

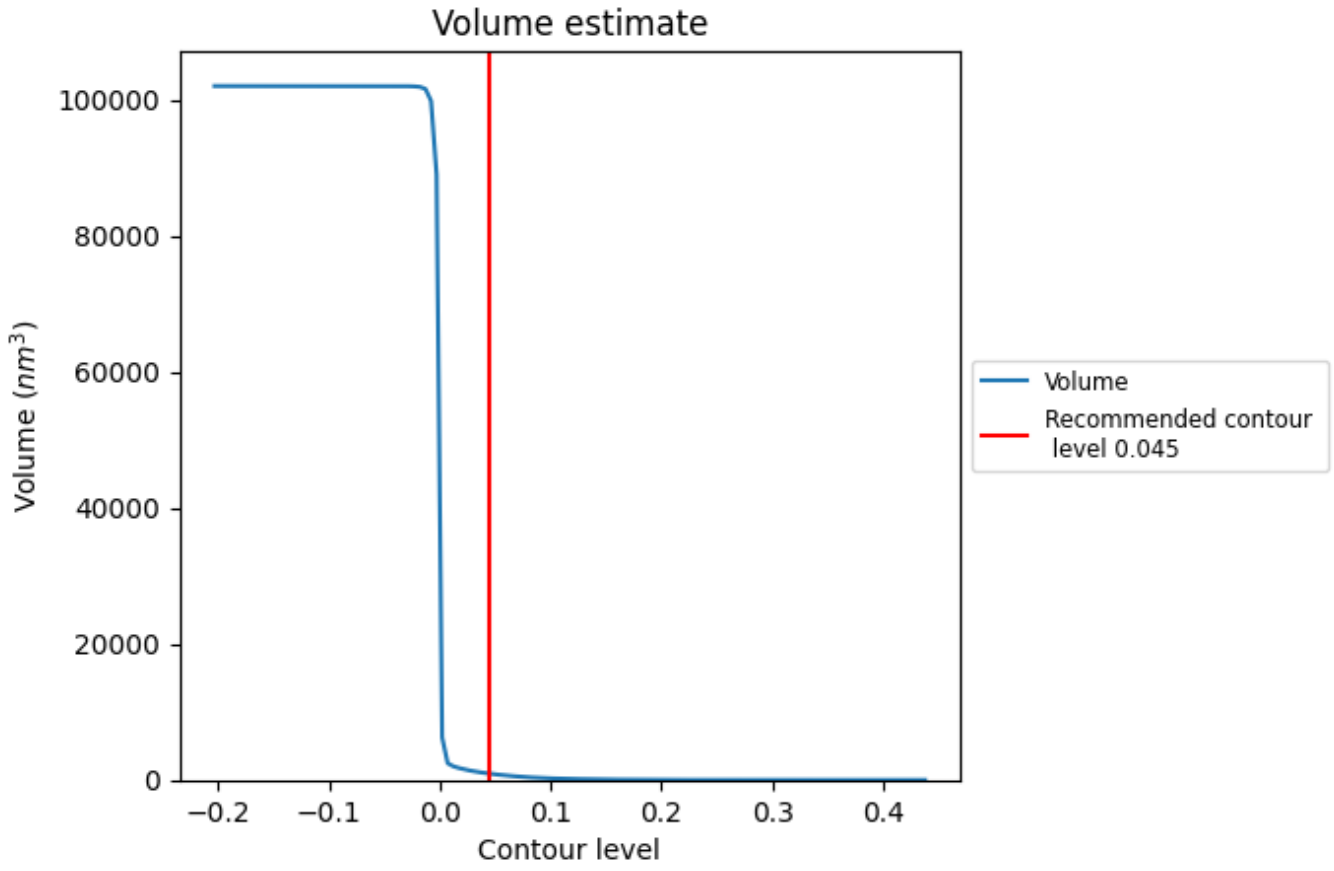
This section contains the results of statistical analysis of the map.

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.

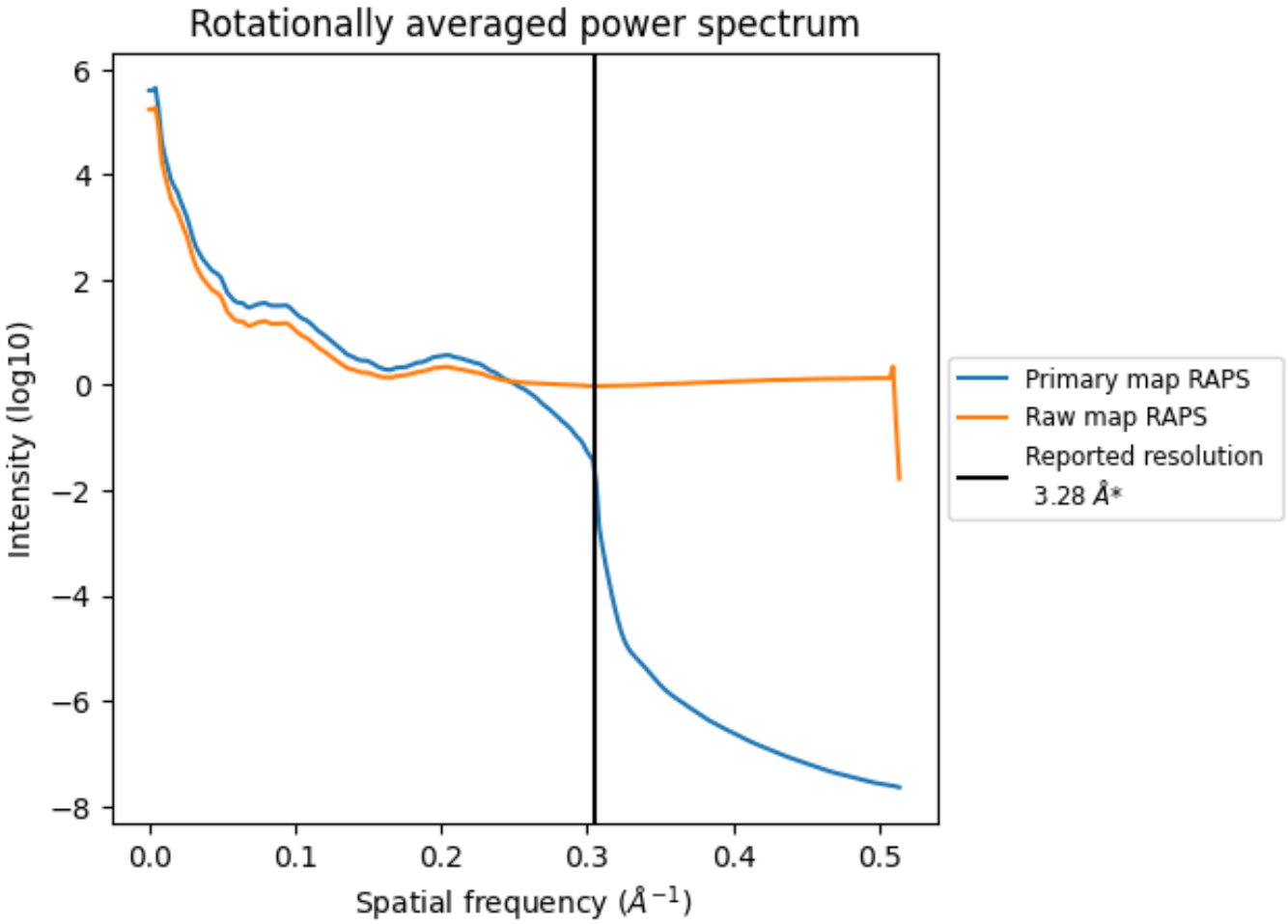
7.2 Volume estimate



The volume at the recommended contour level is 931 nm^3; this corresponds to an approximate mass of 841 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)

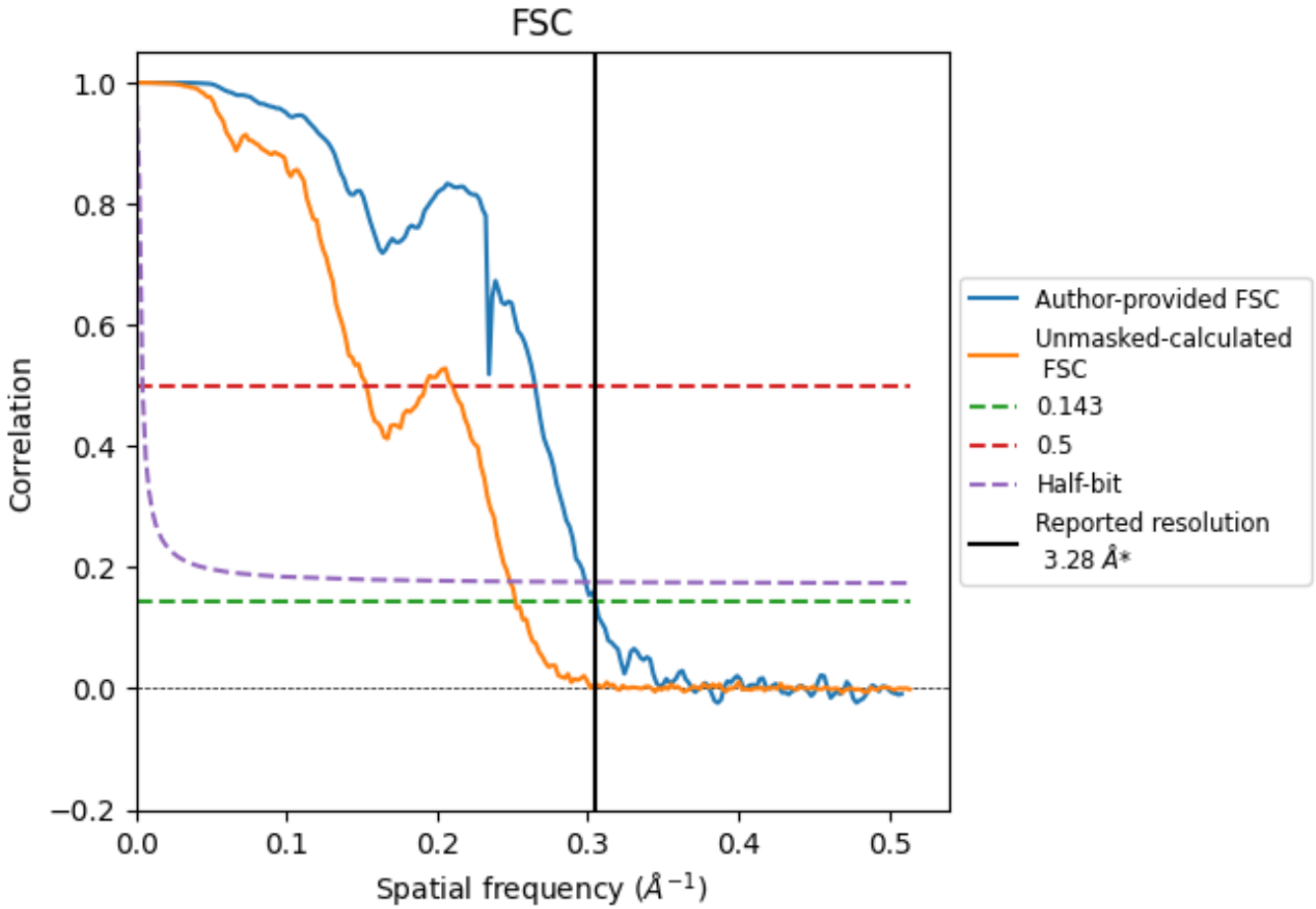


*Reported resolution corresponds to spatial frequency of 0.305 Å^{-1}

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 0.305 Å^{-1}

8.2 Resolution estimates (i)

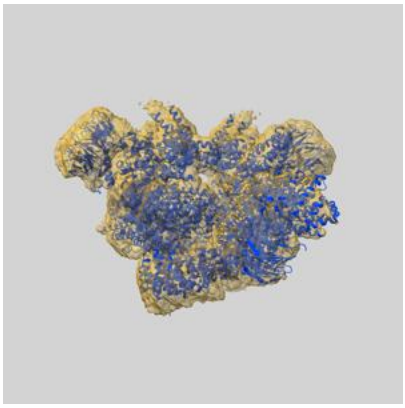
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.28	-	-
Author-provided FSC curve	3.28	3.78	3.35
Unmasked-calculated*	3.97	6.55	4.03

*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 3.97 differs from the reported value 3.28 by more than 10 %

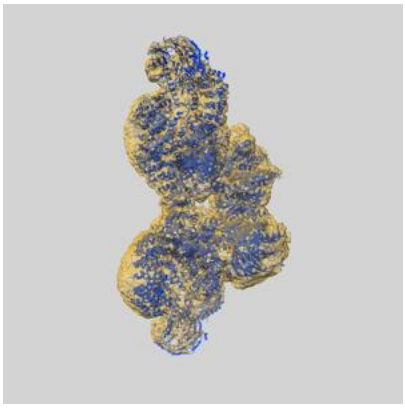
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-55628 and PDB model 9T77. Per-residue inclusion information can be found in section 3 on page 7.

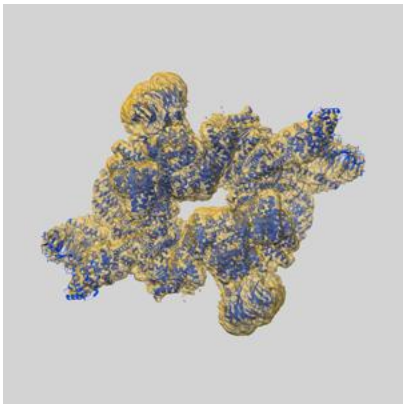
9.1 Map-model overlay



X



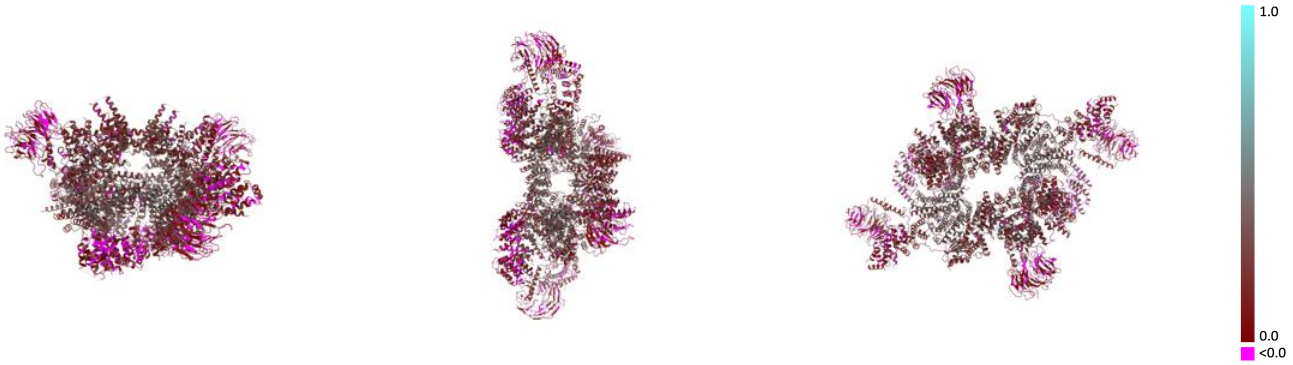
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

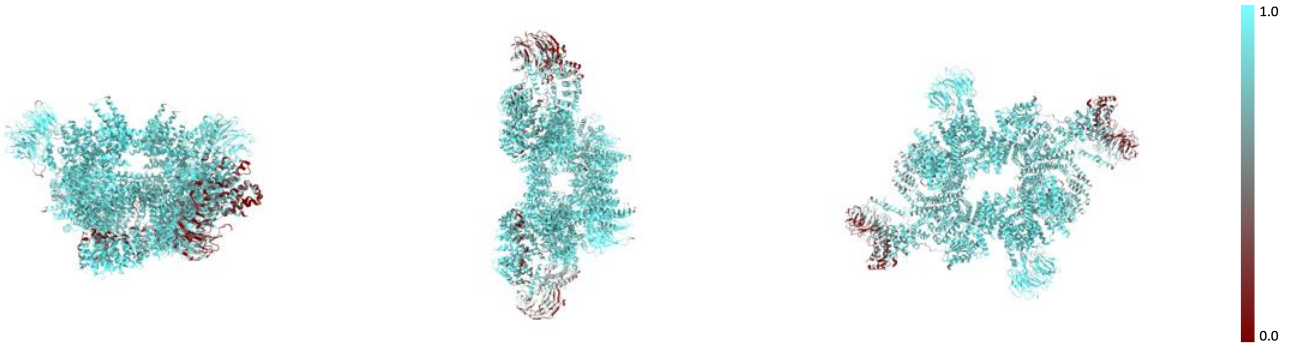
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

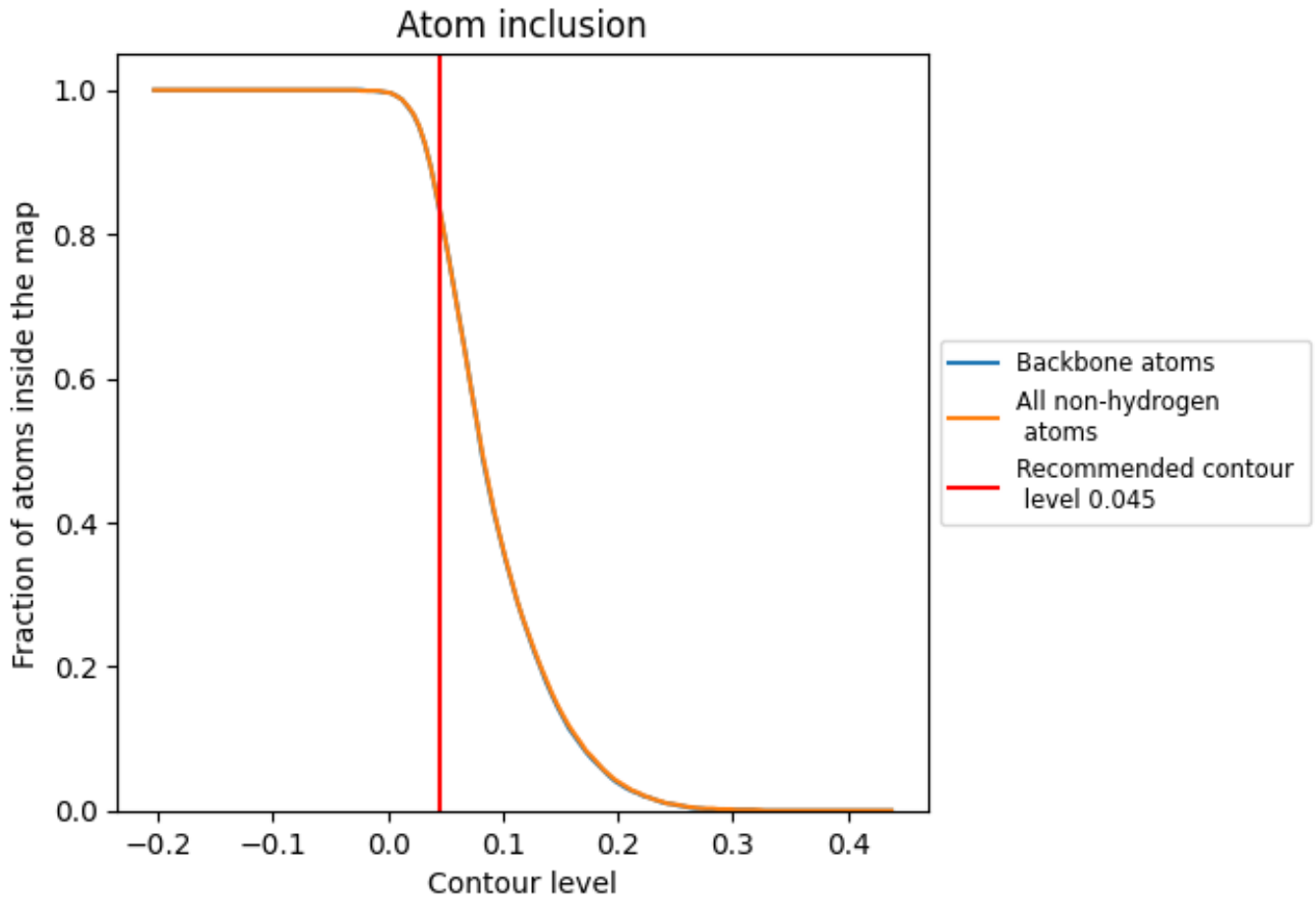
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.045).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8360	0.2090
A	0.9060	0.2320
B	0.9060	0.2320
C	0.9140	0.0770
D	0.9130	0.0750
E	0.6830	0.1980
F	0.6830	0.2010
G	0.8440	0.2260
H	0.8120	0.2370

