wwPDB EM Validation Summary Report (i)

Jul 27, 2025 – 11:24 PM EDT

PDB ID	:	9NWE / pdb_00009nwe
EMDB ID	:	EMD-49876
Title	:	E3 ligase UBR4-KCMF1-calmodulin complex
Authors	:	Yang, Z.; Rape, M.P.
Deposited on	:	2025-03-22
Resolution	:	3.20 Å(reported)

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

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

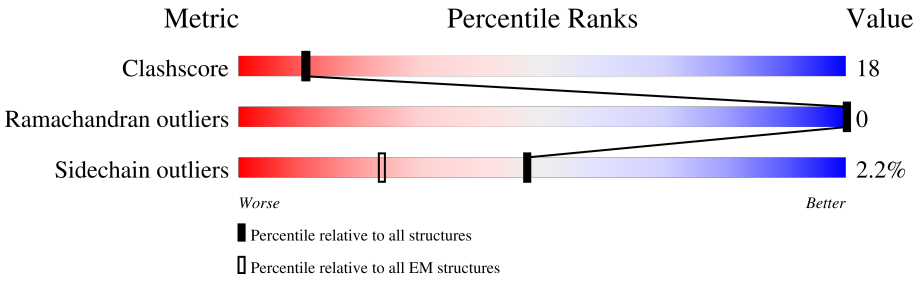
EMDB validation analysis	:	0.0.1.dev126
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.45.1

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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	5205	8% 23% 8% 68%
1	B	5205	8% 23% 9% 68%
2	C	149	17% 45% 46% 6%
2	D	149	15% 31% 55% 10%
3	E	381	7% 6% 88%
3	F	381	7% 88%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ZN	A	5203	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 29288 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called E3 ubiquitin-protein ligase UBR4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1660	Total	C	N	O	S	0	0
			13132	8325	2255	2465	87		
1	B	1660	Total	C	N	O	S	0	0
			13134	8325	2255	2467	87		

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP Q5T4S7
A	-20	ASP	-	expression tag	UNP Q5T4S7
A	-19	TYR	-	expression tag	UNP Q5T4S7
A	-18	LYS	-	expression tag	UNP Q5T4S7
A	-17	ASP	-	expression tag	UNP Q5T4S7
A	-16	HIS	-	expression tag	UNP Q5T4S7
A	-15	ASP	-	expression tag	UNP Q5T4S7
A	-14	GLY	-	expression tag	UNP Q5T4S7
A	-13	ASP	-	expression tag	UNP Q5T4S7
A	-12	TYR	-	expression tag	UNP Q5T4S7
A	-11	LYS	-	expression tag	UNP Q5T4S7
A	-10	ASP	-	expression tag	UNP Q5T4S7
A	-9	HIS	-	expression tag	UNP Q5T4S7
A	-8	ASP	-	expression tag	UNP Q5T4S7
A	-7	ILE	-	expression tag	UNP Q5T4S7
A	-6	ASP	-	expression tag	UNP Q5T4S7
A	-5	TYR	-	expression tag	UNP Q5T4S7
A	-4	LYS	-	expression tag	UNP Q5T4S7
A	-3	ASP	-	expression tag	UNP Q5T4S7
A	-2	ASP	-	expression tag	UNP Q5T4S7
A	-1	ASP	-	expression tag	UNP Q5T4S7
A	0	ASP	-	expression tag	UNP Q5T4S7
A	1	LYS	-	expression tag	UNP Q5T4S7
B	-21	MET	-	initiating methionine	UNP Q5T4S7
B	-20	ASP	-	expression tag	UNP Q5T4S7
B	-19	TYR	-	expression tag	UNP Q5T4S7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	LYS	-	expression tag	UNP Q5T4S7
B	-17	ASP	-	expression tag	UNP Q5T4S7
B	-16	HIS	-	expression tag	UNP Q5T4S7
B	-15	ASP	-	expression tag	UNP Q5T4S7
B	-14	GLY	-	expression tag	UNP Q5T4S7
B	-13	ASP	-	expression tag	UNP Q5T4S7
B	-12	TYR	-	expression tag	UNP Q5T4S7
B	-11	LYS	-	expression tag	UNP Q5T4S7
B	-10	ASP	-	expression tag	UNP Q5T4S7
B	-9	HIS	-	expression tag	UNP Q5T4S7
B	-8	ASP	-	expression tag	UNP Q5T4S7
B	-7	ILE	-	expression tag	UNP Q5T4S7
B	-6	ASP	-	expression tag	UNP Q5T4S7
B	-5	TYR	-	expression tag	UNP Q5T4S7
B	-4	LYS	-	expression tag	UNP Q5T4S7
B	-3	ASP	-	expression tag	UNP Q5T4S7
B	-2	ASP	-	expression tag	UNP Q5T4S7
B	-1	ASP	-	expression tag	UNP Q5T4S7
B	0	ASP	-	expression tag	UNP Q5T4S7
B	1	LYS	-	expression tag	UNP Q5T4S7

- Molecule 2 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	144	Total	C	N	O	S	0	0
			1134	696	182	247	9		
2	D	143	Total	C	N	O	S	0	0
			1127	692	181	245	9		

- Molecule 3 is a protein called E3 ubiquitin-protein ligase KCMF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	46	Total	C	N	O	S	0	0
			380	231	68	79	2		
3	F	45	Total	C	N	O	S	0	0
			371	226	67	76	2		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
4	A	3	Total	Zn	0
			3	3	

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Mol	Chain	Residues	Atoms	AltConf
4	B	3	Total Zn 3 3	0

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

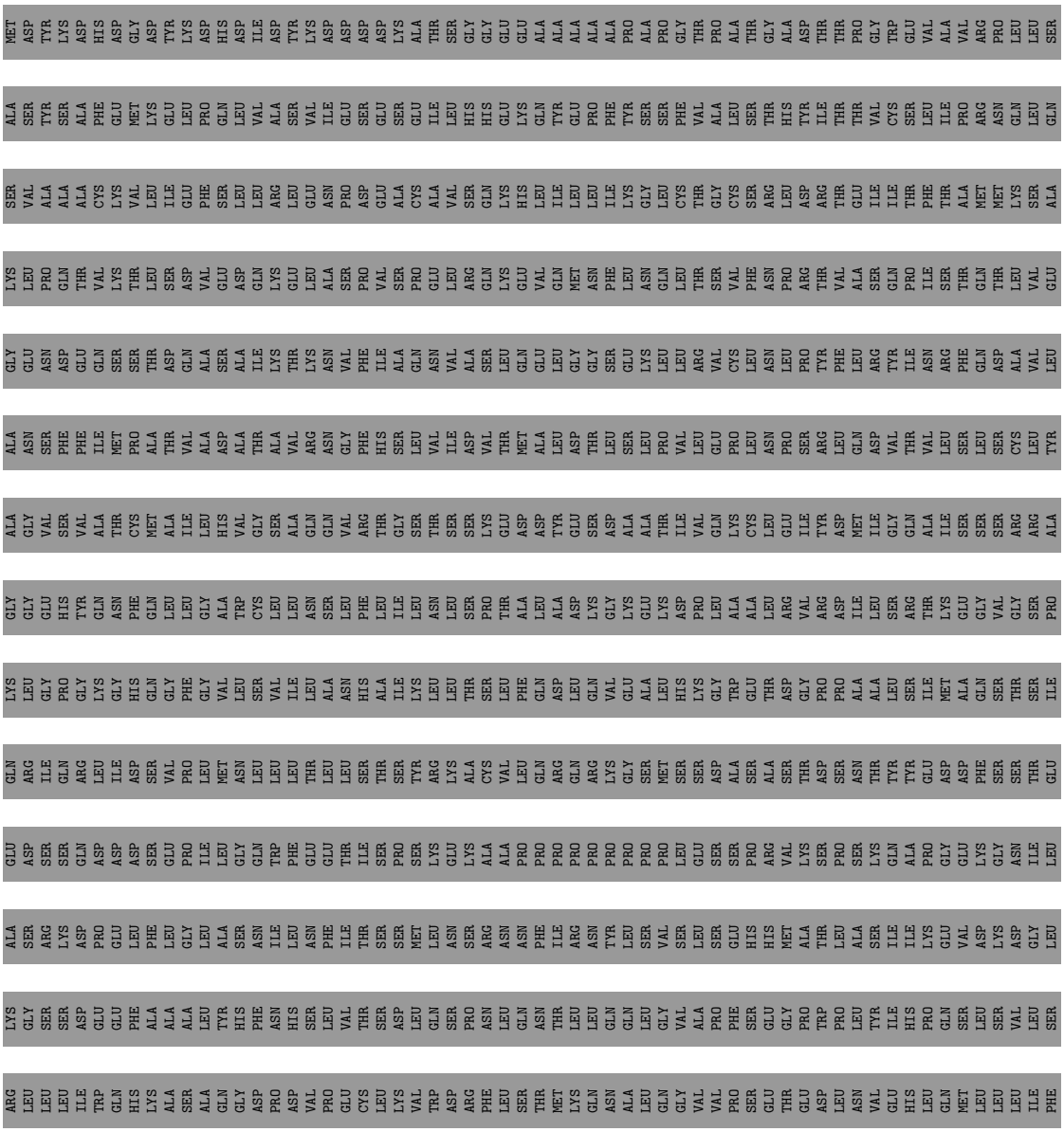
Mol	Chain	Residues	Atoms	AltConf
5	C	2	Total Ca 2 2	0
5	D	2	Total Ca 2 2	0

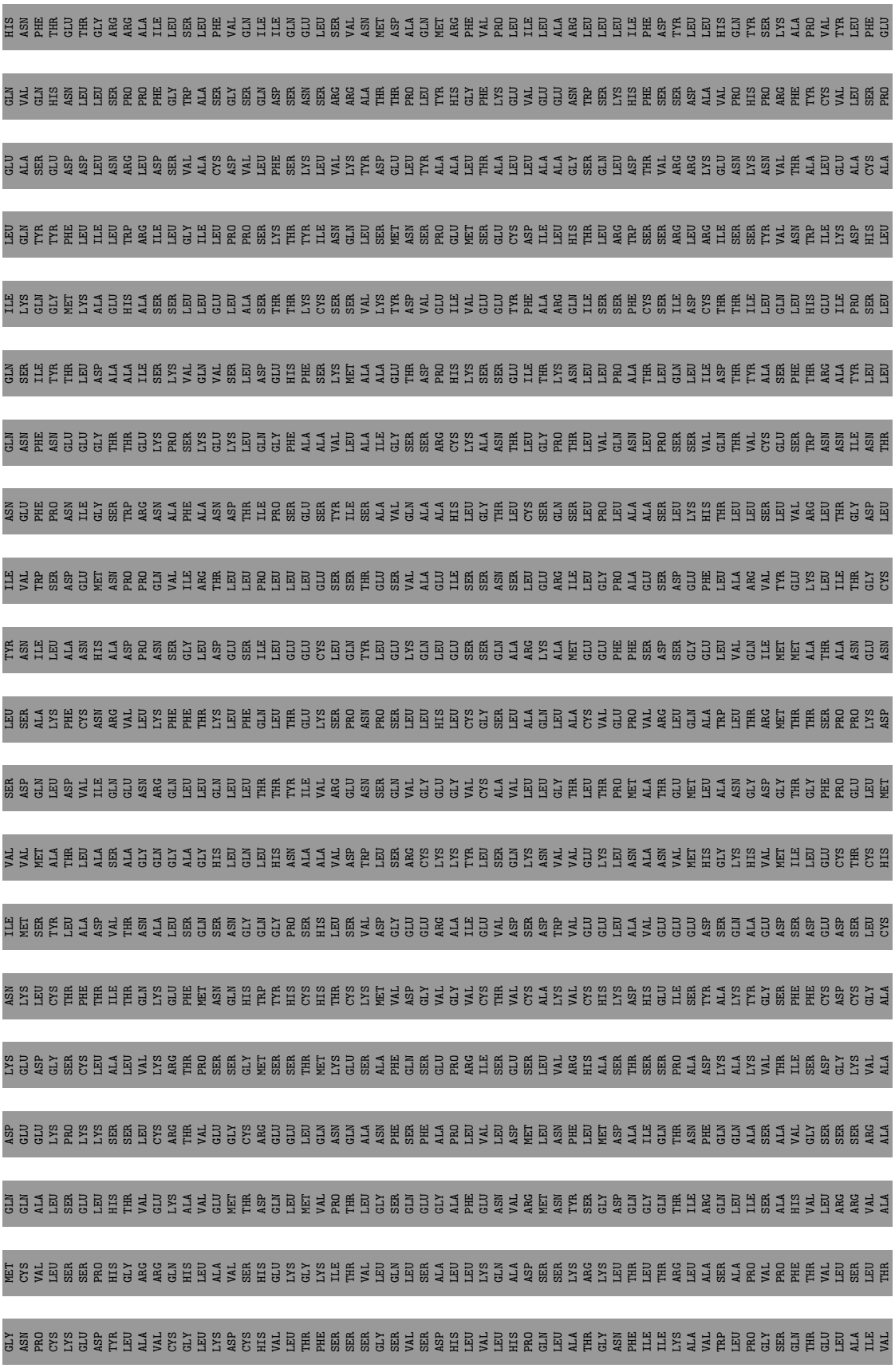
3 Residue-property plots (i)

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: E3 ubiquitin-protein ligase UBR4

Chain A:

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GLN VAL GLN HIS ASN LEU LEU SER PRO PRO PHE GLY TRP ALA SER GLY SER GLN ASP SER ASN SER ARG ARG ALA THR THR PRO LEU TYR HIS GLY PHE LYS GLU VAL GLU GLU ASN TRP SER LYS HIS PHE SER SER ASP ALA VAL THR PHE TYR CYS VAL LEU SER PRO
GLU ALA SER GLU ASP ASP LEU ASN ARG LEU ASP SER VAL ALA CYS ASP VAL LEU PHE SER LYS LEU VAL LYS TYR ASP GLU LEU TYR ALA ALA LEU THR PRO LEU TYR ALA GLU ALA ALA GLY SER GLN LEU ASP THR VAL ARG ARG LYS GLU ASN VAL THR ALA LEU GLU ASP ALA CYS ALA
LEU GLN TYR TYR PHE LEU ILE LEU TRP ARG ILE LEU GLY ILE LEU PRO PRO SER LYS THR TYR ILE ASN GLN LEU SER MET ASN SER PRO GLU MET SER GLU CYS ASP ILE LEU ARG TRP SER SER ARG LEU ARG ILE SER SER TYR VAL ASN TRP ILE LYS ASP HIS LEU
ILE LYS GLN GLY MET LYS ALA GLU HIS ALA ILE SER SER LEU LEU GLU LEU ALA SER THR THR LYS CYS SER SER VAL LYS TYR ASP VAL GLU ILE VAL GLU GLU TYR PHE ALA ARG GLN ILE SER SER PHE CYS SER ILE ASP CYS THR THR ILE LEU GLN LEU HIS GLU ILE LEU PRO SER LEU
GLN SER ILE TYR THR LEU ASP ALA ALA ILE SER LYS LEU GLN VAL SER LEU ASP GLU HIS PHE SER LYS MET ALA ALA GLU THR ASP PRO HIS LYS LYS VAL GLN ILE THR LYS ASN LEU LEU PRO ALA THR LEU GLN LEU ILE ASP THR TYR ALA SER PHE THR ARG ALA TYR LEU LEU
GLN ASN PHE ASN GLU GLU GLY THR THR GLU LYS LEU ALA ILE GLY SER SER ARG CYS SER ALA ASN LEU PRO SER SER VAL GLN THR THR VAL CYS SER GLU SER TRP ASN ASN LEU ILE ASN THR
ASN GLU PHE PRO ASN ILE GLY SER TRP ARG ASN ALA PHE ALA ASP THR ILE PRO SER GLU SER TYR ILE SER ALA ALA VAL GLN ALA ALA HIS LEU LEU GLY SER THR LEU CYS SER GLN SER LEU PRO LEU ALA ALA SER LEU LYS HIS THR LEU LEU SER LEU VAL LEU ARG LEU THR GLY ASP LEU
ILE VAL TRP SER ASP GLU MET ASN PRO PRO GLN VAL ILE ARG THR LEU LEU LEU GLU SER SER THR GLU SER VAL ALA GLU ILE SER SER ASN SER LEU CYS SER GLN SER LEU PRO LEU ALA ALA GLU SER ASP GLU PHE LEU ALA ARG VAL TYR GLU LYS LEU ILE THR GLY CYS
TYR ASN ILE LEU ALA ASN HIS ALA ASP PRO ASN SER GLY LEU GLN ILE GLU SER GLU ALA ASP SER LEU GLU ALA ARG LYS ALA MET GLU GLU PHE PHE SER ASP SER GLY GLU LEU VAL GLN ILE MET MET ALA THR ALA ASN GLU ASN
LEU SER ALA LYS PHE CYS ASN ARG VAL LEU LYS PHE PHE PHE THR LYS LEU PHE GLN LEU THR GLU LYS SER PRO ASN PRO SER LEU LEU HIS LEU CYS GLY SER LEU LEU ALA ALA GLN LEU LEU ALA CYS VAL GLU PRO VAL ARG LEU GLN ALA TRP LEU LEU THR ARG MET THR THR SER PRO PRO LYS ASP
SER ASP GLN LEU ASP VAL ILE GLN GLU ASN ARG GLN LEU LEU LEU GLU LEU GLN LEU LEU THR THR TYR ILE VAL ARG GLU ASN SER GLN VAL GLY GLU GLY VAL CYS ALA VAL LEU LEU GLY THR LEU THR PRO MET ALA THR GLU MET LEU ALA GLY PHE PRO GLU LEU MET
VAL VAL MET ALA THR LEU ALA GLY GLN GLY ALA GLY HIS LEU GLN LEU HIS ASN ALA ALA VAL ASP TRP LEU SER ARG CYS LYS LYS TYR LEU SER ALA ASP GLY GLU ASN SER GLN VAL GLY GLU GLY VAL CYS ALA VAL GLN VAL VAL GLU LYS LEU ASN ALA VAL MET HIS GLY LYS HIS VAL MET ILE LEU GLU GLU ASP SER CYS HIS
ILE MET SER TYR LEU ALA ASP VAL THR ASN ALA LEU SER GLN SER HIS LEU SER VAL ASP GLY GLU GLY ARG ALA ILE GLU VAL ASP SER ASP TRP VAL GLU GLU LEU ALA VAL GLU GLU GLU ASP SER GLN ALA LYS ASP GLU ASP SER CYS
ASN LYS LEU CYS THR PHE THR ILE THR GLN GLU PHE MET ASN GLN HIS TRP TYR HIS CYS HIS THR CYS LYS MET VAL ASP GLY VAL GLY VAL CYS THR VAL CYS HIS LYS ASP HIS GLU ILE SER TYR ALA LYS TYR GLY SER PHE CYS ASP CYS GLY ALA
LYS GLU ASP GLY SER CYS LEU VAL LYS ARG THR PRO SER SER GLY MET SER SER THR MET LYS GLU SER ALA PHE GLN SER GLU PRO ARG ILE SER GLU SER LEU VAL ARG HIS ALA SER THR SER SER PRO ALA ASP LYS ALA LYS VAL THR ILE SER ASP GLY LYS VAL ALA
ASP GLU GLU LYS PRO LYS LYS SER LEU CYS ARG GLU GLU LEU GLN ASN GLN ALA ASN PHE SER PHE ALA PRO LEU VAL LEU ASP MET LEU ASN PHE LEU MET ASP ALA ILE GLN THR ASN PHE GLN GLN ALA LYS ALA SER VAL ALA ASP SER SER SER ARG ALA
GLN GLN ALA LEU SER GLU LEU HIS THR VAL GLU LYS ALA PHE GLU ASN VAL ARG MET ASN TYR SER GLY ASP GLN GLY GLN THR ILE ARG GLN LEU LEU ILE SER ALA HIS VAL LEU ARG ARG VAL ALA
MET CYS VAL LEU SER SER PRO HIS GLY ARG ARG GLN HIS LEU LEU LYS GLN ALA ASP SER SER LYS ARG LYS LEU THR LEU THR ARG LEU ALA SER ALA PRO VAL PRO PHE THR VAL LEU SER LEU THR
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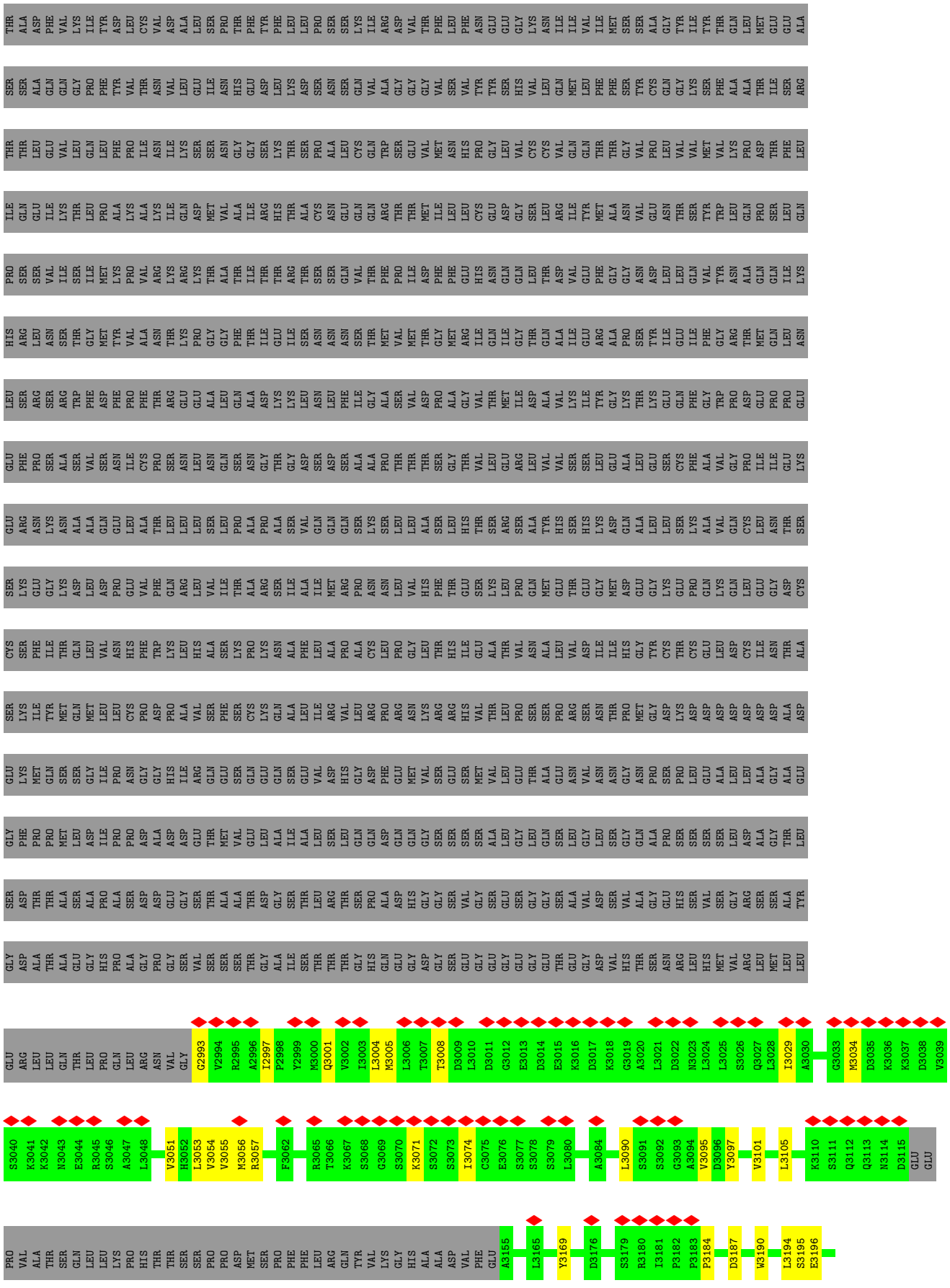
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SER SER ALA GLN GLN GLY PRO PHE TYR VAL THR ASN VAL LEU GLU ILE ASN HIS GLU ASP LEU LYS SER ASP SER ASN SER GLN VAL ALA GLY GLY GLY VAL SER VAL TYR TYR SER HIS VAL LEU GLN MET LEU PHE PHE SER TYR CYS GLN GLY LYS SER PHE ALA ALA THR ILE SER ARG
THR THR LEU GLU VAL LEU GLN LEU PHE PRO ILE ASN ILE LYS SER SER ASN GLY GLY SER LYS THR SER PRO ALA LEU CYS GLN TRP SER GLU VAL MET ASN HIS PRO GLY LEU VAL CYS CYS VAL GLN GLN THR THR GLY VAL PRO LEU VAL VAL MET VAL LYS PRO ASP THR PHE LEU
ILE GLN GLU ILE LYS THR LEU PRO ALA LYS ALA LYS ILE GLN ASP MET VAL ALA ILE ARG HIS THR ALA CYS ASN GLU GLN GLN ARG THR THR MET ILE LEU LEU CYS GLU ASP GLY SER LEU ARG ILE TYR MET ALA ASN VAL GLU ASN THR SER TYR TRP LEU GLN LEU SER GLN
PRO SER SER VAL ILE SER ILE MET LYS PRO VAL ARG LYS ARG LYS THR ALA ALA THR ILE THR THR ARG THR SER SER GLN VAL THR PHE PRO PRO ILE ASP PHE PHE GLU HIS ASN GLN GLN LEU THR ASP VAL GLU PHE GLY GLY ASN ASP LEU LEU GLN VAL THR LYS ILE LEU
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LEU SER ARG SER ARG TRP PHE ASP PHE PRO PHE THR ARG GLU GLU ALA ALA LEU GLN ALA ASP LYS LYS LEU ASN LEU PHE ILE GLY ALA ALA SER VAL ASP PRO ALA GLY VAL THR MET ILE ASP ALA ALA VAL LYS ILE TYR GLY LYS THR LYS GLU ALA LEU GLU GLY TRP PRO ASP GLU PRO PRO GLU
GLU PHE PRO SER ALA SER VAL SER ASN ILE CYS PRO SER ASN GLN SER ASN GLY THR GLY ASP SER ASP SER ALA ALA PRO THR THR THR SER GLY THR VAL LEU GLU THR VAL VAL SER SER LEU GLU ALA LEU GLU SER CYS PHE ALA ALA VAL GLY PRO ILE ILE GLU LYS
GLU ARG ASN LYS ASN ALA ALA GLN GLU LEU ALA THR LEU LEU LEU SER LEU LEU SER VAL GLN GLN GLN SER LYS SER LEU LEU ALA SER LEU HIS THR SER ARG SER ALA TYR HIS SER HIS LYS ASP GLN ALA LEU LEU SER LYS ALA VAL GLN CYS LEU ASN THR SER
SER LYS GLU GLY LYS ASP LEU ASP PRO GLU VAL PHE GLN ARG ARG LEU LEU VAL ILE THR ALA ARG SER ILE ALA ILE MET ARG PRO ASN ASN LEU VAL HIS PHE THR GLU SER LYS LEU PRO GLN MET GLU THR GLU GLY MET ASP GLU GLY LYS GLU PRO GLN LYS GLN LEU GLU GLY ASP CYS
CYS SER PHE ILE THR GLN LEU VAL ASN HIS PHE TRP LYS LEU HIS ALA SER LYS PRO LYS ASN ALA PHE LEU ALA PRO ALA CYS LEU PRO GLY LEU THR HIS ILE GLU SER ALA THR VAL ASN ALA LEU VAL ASP ILE ILE HIS GLY TYR CYS THR CYS GLU LEU ASP CYS ILE ASN THR ALA
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GLY PHE PRO MET LEU ASP ILE PRO PRO ASP ALA ASP ASP GLU LEU ALA LEU SER LEU GLN GLN GLN GLY SER SER SER ALA LEU GLY LEU GLN SER LEU GLY LEU SER SER GLY GLN ALA PRO SER SER SER SER LEU ASP ASP ALA GLY THR LEU
SER ASP THR ALA SER ASP ASP GLU GLY SER THR ALA ALA LEU ARG THR SER PRO ALA ASP HIS GLY GLY GLY SER VAL GLY GLY SER GLU GLY SER ALA GLY GLU GLY VAL ALA GLY GLU HIS SER VAL SER GLY ASP SER VAL HIS ALA GLY GLU HIS SER VAL ASP ALA ALA TYR
GLY ASP ALA THR ALA GLU GLY HIS PRO GLY SER VAL SER SER SER THR GLY HIS GLN GLU GLY ASP GLY SER GLU GLY GLU GLY GLU GLY GLU GLY GLU THR GLU GLY ASP VAL HIS THR SER ASN ARG LEU MET LEU LEU LEU
GLU ARG LEU LEU GLN THR LEU GLN LEU ARG ASN VAL GLY
S3040 K3041 K3042 N3043 E3044 R3045 S3046 A3047 L3048 V3051 H3052 L3053 V3054 V3055 M3056 R3057 F3062 R3065 T3066 K3067 S3068 G3069 S3070 K3071 S3072 S3073 I3074 C3075 E3076 S3077 S3078 S3079 L3080 A3084 L3090 S3091 S3092 G3093 A3094 V3095 D3096 Y3097 V3101 L3105 K3110 S3111 Q3112 Q3113 N3114 D3115 GLU GLU
G2993 V2994 R2995 A2996 I2997 P2998 Y2999 M3000 Q3001 V3002 I3003 L3004 M3005 L3006 T3007 T3008 D3009 L3010 D3011 G3012 E3013 D3014 E3015 K3016 D3017 K3018 G3019 A3020 L3021 D3022 N3023 L3024 L3025 S3026 Q3027 L3028 I3029 A3030 G3033 M3034 D3035 K3036 K3037 D3038 V3039
PRO VAL ALA THR SER GLN LEU LEU LYS PRO HIS THR THR SER SER PRO PRO ASP MET SER PRO PHE PHE LEU ARG GLN TYR VAL LYS GLY HIS ALA ALA ASP VAL PHE GLU
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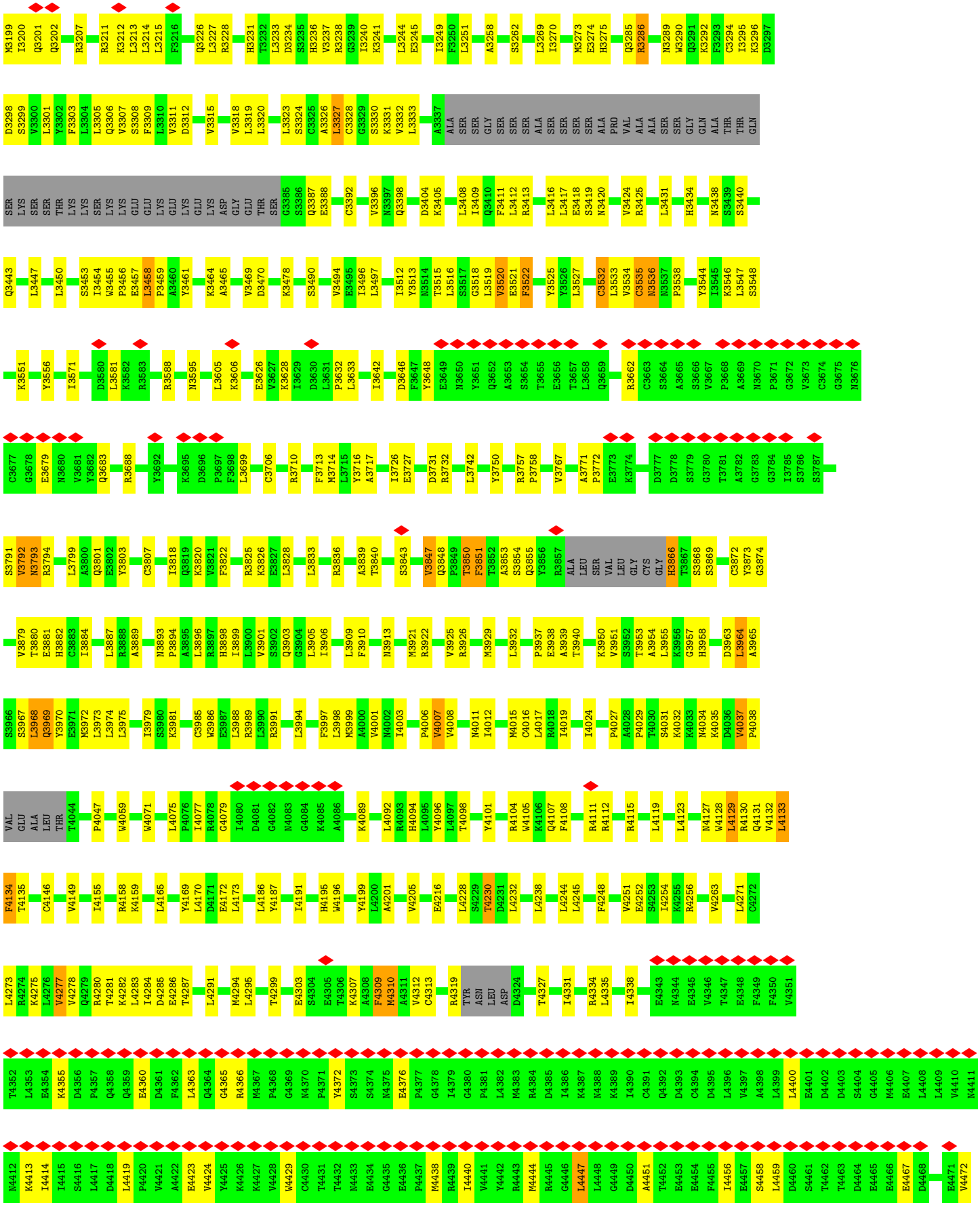
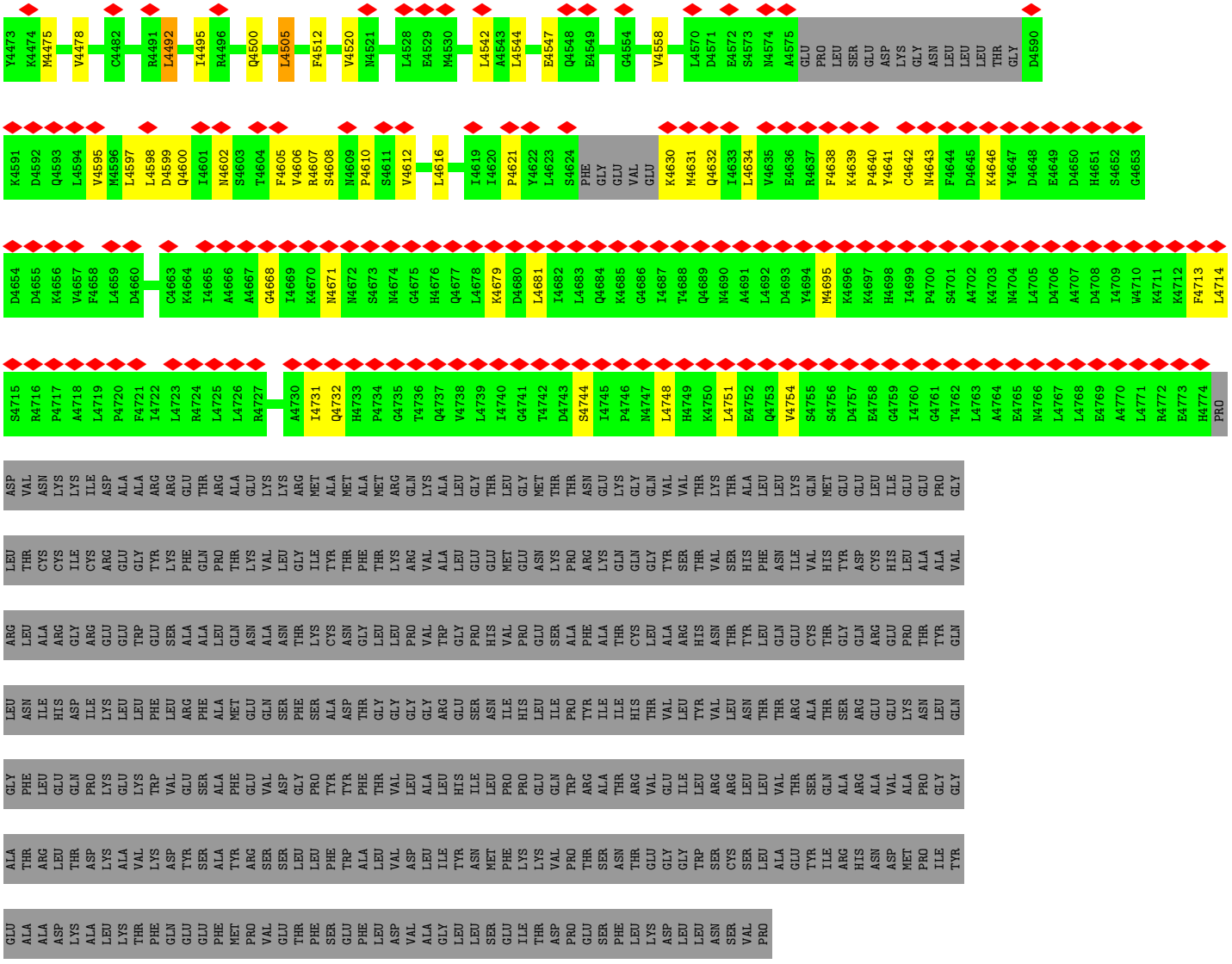
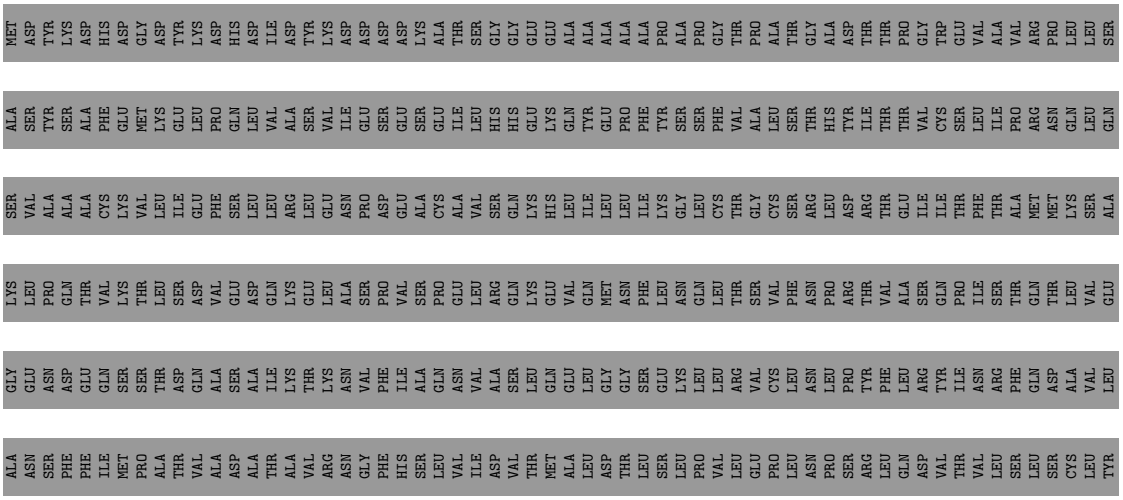
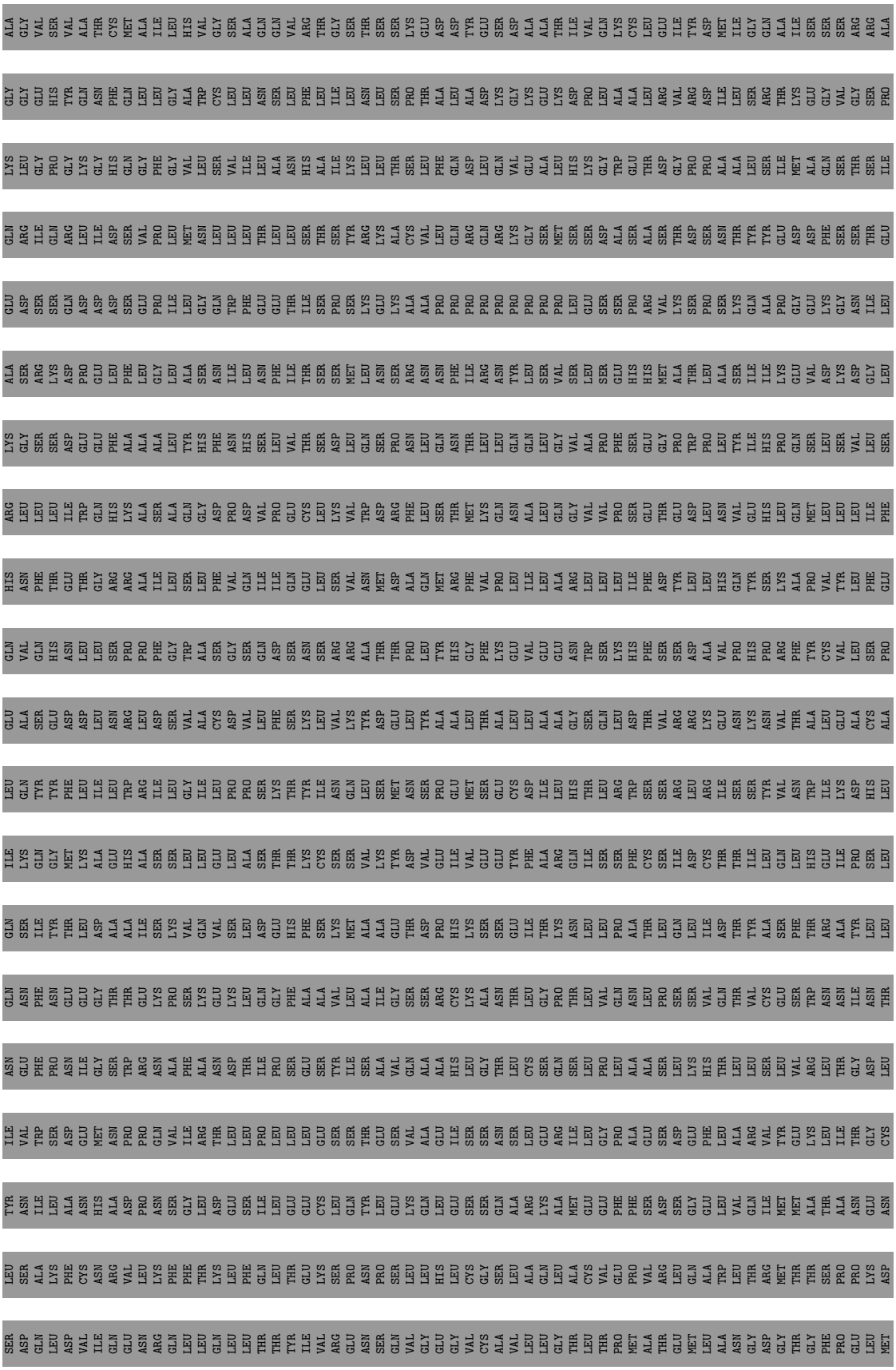


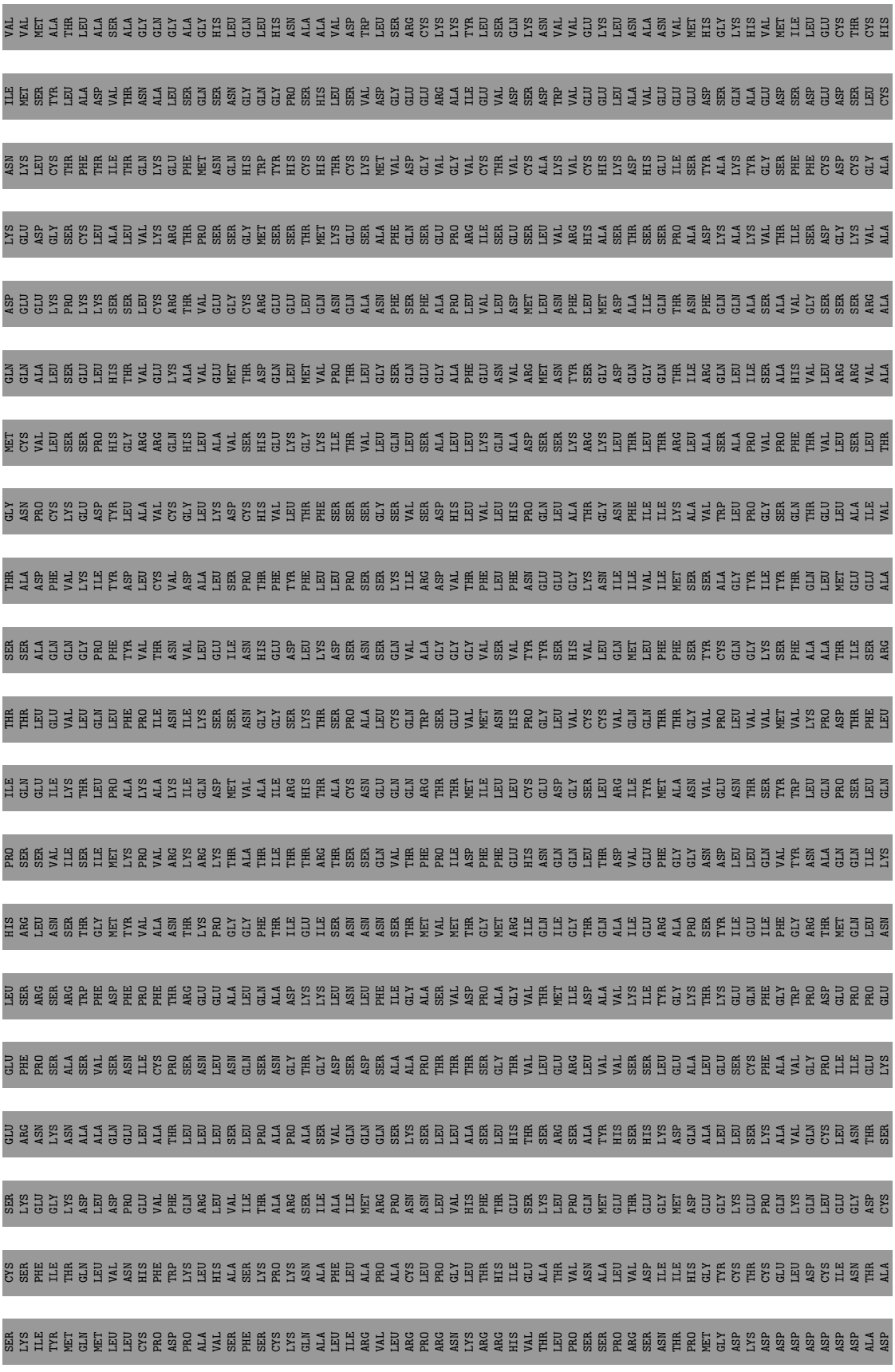


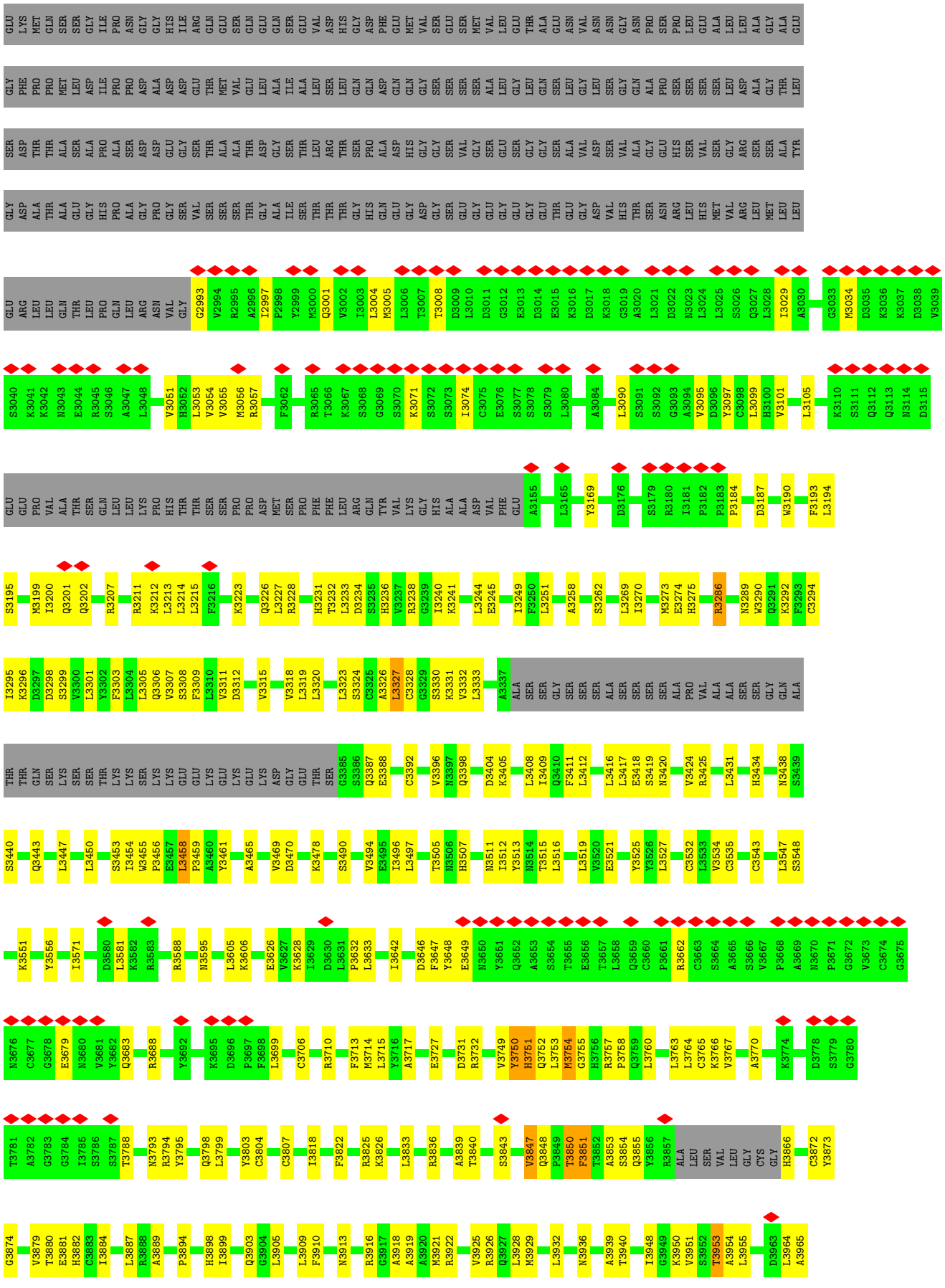
• Molecule 1: E3 ubiquitin-protein ligase UBR4

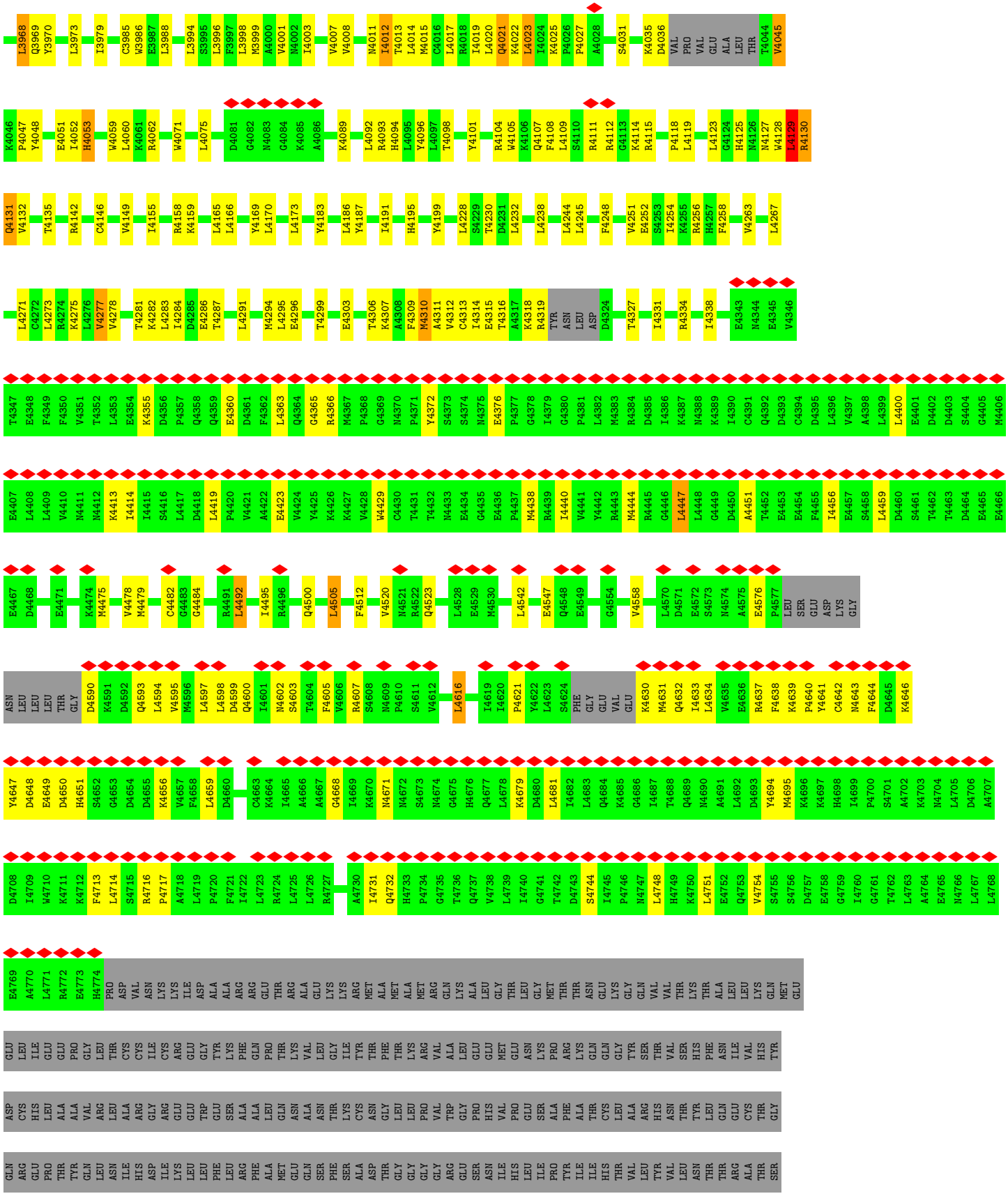
Chain B:







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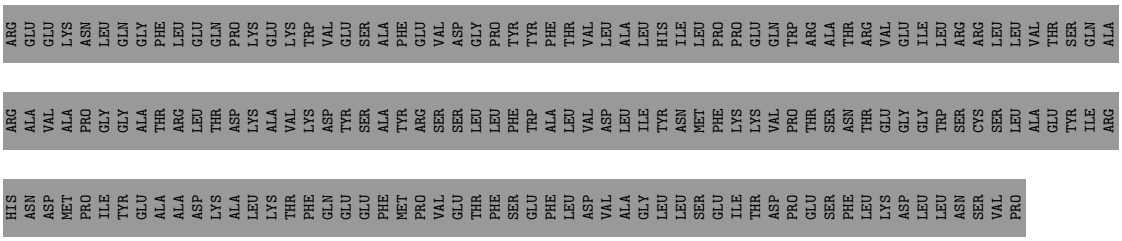
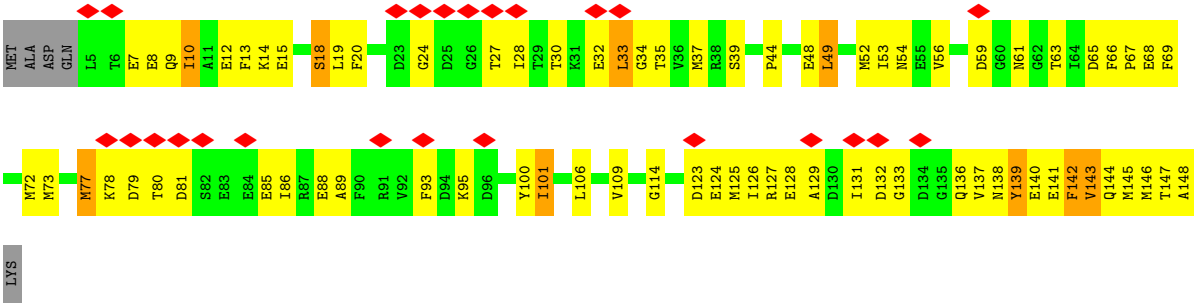
K4046 P4047 Y4048 E4051 I4052 H4053 W4059 L4060 K4061 R4062 W4071 L4075 D4081 G4082 N4083 G4084 K4085 A4086 K4089 L4092 R4093 H4094 L4095 Y4096 I4097 T4098 Y4101 R4104 W4105 Q4107 F4108 L4109 S4110 R4111 R4112 G4113 K4114 R4115 P4118 L4119 L4123 G4124 H4125 N4126 N4127 W4128 L4129 R4130
Q4131 V4132 T4135 R4142 C4146 V4149 I4155 R4158 K4159 L4165 L4166 Y4169 L4170 L4173 Y4183 L4186 Y4187 I4191 H4195 Y4199 L4228 S4229 T4230 D4231 L4232 L4238 L4244 L4245 F4248 V4251 E4252 S4253 I4254 K4255 R4256 H4257 F4258 V4263 L4267
L4271 C4272 L4273 R4274 K4275 L4276 V4277 V4278 T4281 K4282 L4283 I4284 D4285 E4286 T4287 L4291 M4294 L4295 E4296 T4299 E4303 T4306 K4307 A4308 F4309 M4310 A4311 V4312 C4313 I4314 E4315 T4316 A4317 K4318 R4319 TYR ASN LEU ASP D4324 T4327 I4331 R4334 I4338 E4343 N4344 E4345 V4346
T4347 E4348 F4349 F4350 V4351 T4352 L4353 E4354 K4355 D4356 P4357 Q4358 Q4359 E4360 D4361 F4362 L4363 Q4364 G4365 R4366 M4367 P4368 G4369 N4370 P4371 Y4372 S4373 S4374 N4375 E4376 P4377 G4378 I4379 G4380 P4381 L4382 M4383 R4384 D4385 I4386 K4387 N4388 K4389 I4390 C4391 Q4392 D4393 C4394 D4395 L4396 V4397 A4398 L4399 L4400 E4401 D4402 D4403 S4404 G4405 M4406
E4407 L4408 L4409 V4410 N4411 N4412 K4413 I4414 I4415 S4416 L4417 D4418 L4419 P4420 V4421 A4422 E4423 V4424 Y4425 K4426 K4427 V4428 W4429 C4430 T4431 T4432 N4433 E4434 G4435 E4436 P4437 M4438 R4439 I4440 V4441 Y4442 R4443 M4444 R4445 G4446 L4447 L4448 G4449 D4450 A4451 T4452 E4453 E4454 F4455 I4456 E4457 S4458 L4459 D4460 S4461 T4462 T4463 D4464 E4465 E4466
E4467 D4468 E4471 K4474 M4475 V4478 M4479 C4482 G4483 G4484 R4491 L4492 I4495 R4496 Q4500 L4505 F4512 V4520 N4521 R4522 Q4523 L4528 E4529 M4530 L4542 E4547 Q4548 E4549 G4554 V4558 L4570 D4571 E4572 S4573 N4574 A4575 E4576 P4577 LEU SER GLU ASP LYS GLY
ASN LEU LEU LEU THR GLY D4590 K4591 D4592 Q4593 L4594 V4595 M4596 L4597 L4598 D4599 Q4600 I4601 N4602 S4603 T4604 F4605 V4606 R4607 S4608 N4609 P4610 S4611 V4612 L4616 I4619 I4620 P4621 Y4622 L4623 S4624 PHE GLY GLU VAL GLU K4630 M4631 Q4632 I4633 L4634 V4635 E4636 R4637 F4638 K4639 P4640 Y4641 C4642 N4643 F4644 D4645 K4646
Y4647 D4648 E4649 D4650 H4651 S4652 G4653 D4654 D4655 K4656 V4657 F4658 L4659 D4660 C4663 K4664 I4665 A4666 A4667 G4668 I4669 K4670 N4671 N4672 S4673 N4674 G4675 H4676 Q4677 L4678 K4679 D4680 L4681 I4682 L4683 Q4684 K4685 G4686 I4687 T4688 Q4689 M4690 A4691 L4692 D4693 Y4694 M4695 K4696 K4697 H4698 I4699 P4700 S4701 A4702 K4703 N4704 L4705 D4706 A4707
D4708 I4709 W4710 K4711 K4712 F4713 L4714 S4715 R4716 P4717 A4718 L4719 P4720 F4721 I4722 L4723 R4724 I4725 L4726 R4727 A4730 I4731 Q4732 H4733 P4734 G4735 T4736 Q4737 V4738 L4739 I4740 G4741 T4742 D4743 S4744 I4745 P4746 N4747 L4748 H4749 K4750 L4751 E4752 Q4753 V4754 S4755 S4756 D4757 E4758 G4759 I4760 G4761 T4762 L4763 A4764 E4765 N4766 L4767 L4768
E4769 A4770 L4771 R4772 E4773 H4774 PRO ASP VAL ASN LYS LYS ILE ASP ALA ALA ARG ARG GLU THR ARG ALA GLU LYS LYS ARG MET ALA MET THR ALA MET ARG GLN LYS ALA LEU GLY THR LEU GLY MET THR THR ASN GLU LYS GLY GLN VAL VAL THR LYS THR ALA LEU LEU LEU LYS GLN MET GLU
GLU LEU ILE GLU GLU PRO GLY LEU THR CYS CYS ILE CYS ARG GLU GLY TYR LYS PHE GLN PRO THR LYS VAL LEU GLY ILE TYR THR PHE THR LYS ARG VAL ALA LEU GLU GLU MET GLU ASN LYS PRO ARG LYS GLN GLN GLY GLY TYR SER THR VAL SER HIS PHE ASN ILE VAL HIS TYR
ASP CYS HIS LEU ALA ALA VAL ARG LEU ALA ARG GLY ARG GLU GLU TRP GLU SER ALA ALA LEU GLN ASN ASN ALA ASN THR LYS CYS ASN GLY LEU LEU LEU PRO VAL TRP GLY PRO HIS VAL PRO GLU SER ALA PHE ALA THR CYS LEU ALA ARG HIS ASN THR TYR LEU GLN GLU CYS THR GLY
GLN ARG GLU PRO THR TYR GLN LEU ASN ILE HIS ASP ILE LYS LEU LEU PHE LEU ARG PHE ALA MET GLU GLN SER PHE SER ALA ASP THR GLY GLY GLY GLY ARG GLU SER ASN ILE HIS LEU LEU ILE PRO TYR ILE ILE HIS THR VAL LEU TYR VAL LEU ASN THR THR ARG ALA THR SER



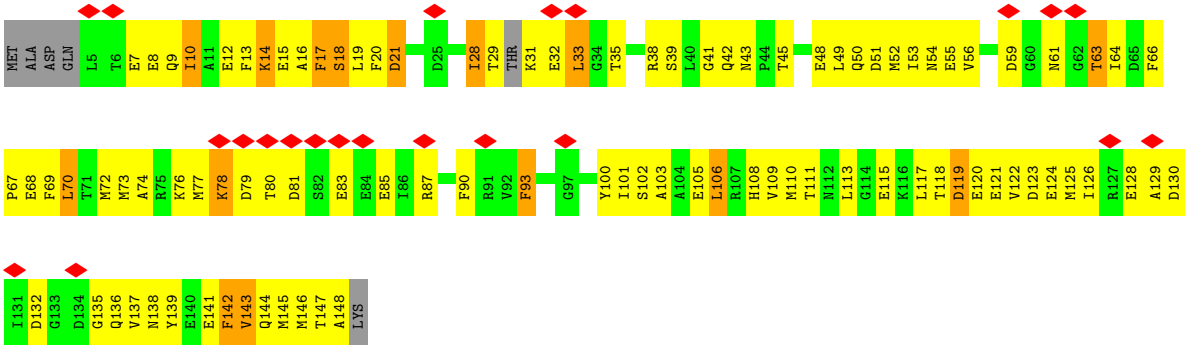
• Molecule 2: Calmodulin-1

Chain C:



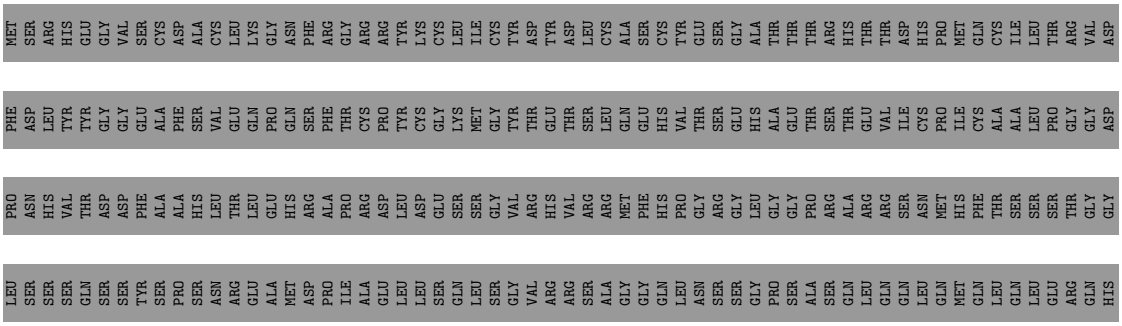
• Molecule 2: Calmodulin-1

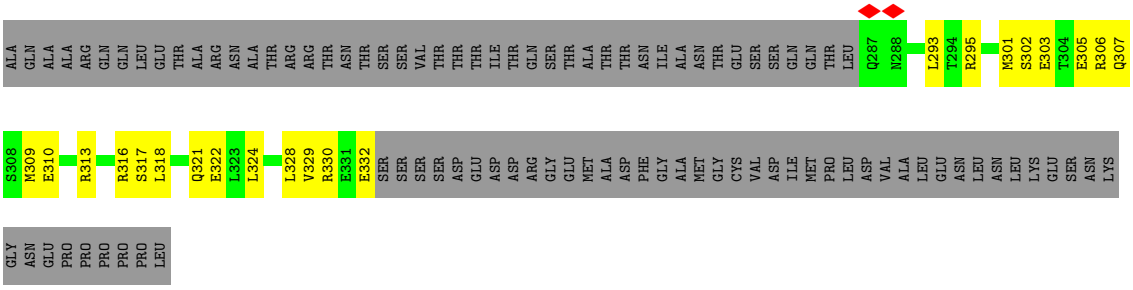
Chain D:



• Molecule 3: E3 ubiquitin-protein ligase KCMF1

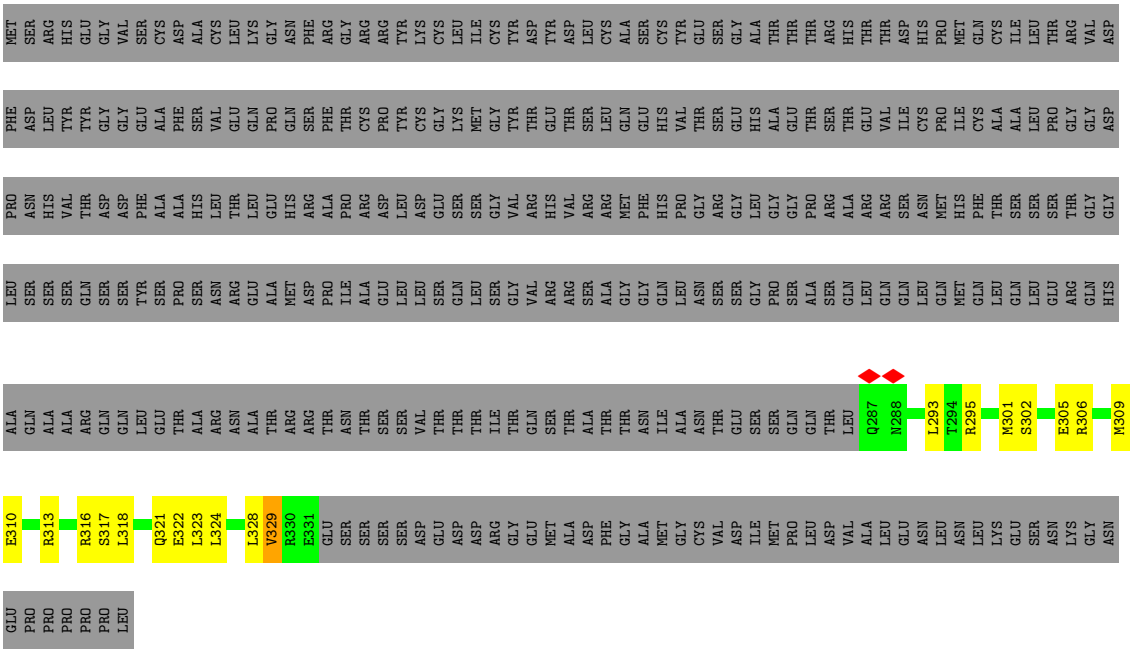
Chain E:





• Molecule 3: E3 ubiquitin-protein ligase KCMF1

Chain F: 7% 88%



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	87263	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40.0	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.493	Depositor
Minimum map value	-0.698	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.146	Depositor
Map size (Å)	419.19998, 419.19998, 419.19998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.048, 1.048, 1.048	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.61	1/13355 (0.0%)	0.90	24/18055 (0.1%)
1	B	0.64	6/13357 (0.0%)	0.91	24/18057 (0.1%)
2	C	1.06	2/1146 (0.2%)	1.31	5/1539 (0.3%)
2	D	1.14	2/1138 (0.2%)	1.34	8/1526 (0.5%)
3	E	0.36	0/382	0.68	0/511
3	F	0.35	0/373	0.77	1/499 (0.2%)
All	All	0.66	11/29751 (0.0%)	0.94	62/40187 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	4013	THR	C-O	-6.08	1.17	1.24
1	B	4023	LEU	C-O	-6.06	1.17	1.24
1	A	3968	LEU	C-O	-5.96	1.16	1.24
2	D	14	LYS	CA-C	-5.91	1.45	1.52
2	C	14	LYS	CA-C	-5.89	1.45	1.52

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	3792	VAL	CA-C-N	-17.13	96.38	120.71
1	A	3792	VAL	C-N-CA	-17.13	96.38	120.71
1	A	3792	VAL	O-C-N	13.47	136.41	122.54
1	A	3969	GLN	CB-CA-C	-12.40	91.86	110.96
2	C	86	ILE	N-CA-C	-11.11	97.20	111.09

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3286	ARG	Sidechain
1	A	4319	ARG	Sidechain
1	B	4112	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	13132	0	13358	477	0
1	B	13134	0	13352	460	0
2	C	1134	0	1063	91	0
2	D	1127	0	1055	112	0
3	E	380	0	376	30	0
3	F	371	0	370	17	0
4	A	3	0	0	3	0
4	B	3	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
All	All	29288	0	29574	1056	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 18.

The worst 5 of 1056 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4032:LYS:CE	3:E:307:GLN:HG3	1.25	1.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4307:LYS:CG	1:A:4475:MET:HE1	1.45	1.44
1:A:4307:LYS:HG3	1:A:4475:MET:CE	1.47	1.42
1:A:4032:LYS:CE	3:E:307:GLN:CG	2.11	1.28
1:B:4098:THR:OG1	2:D:113:LEU:HD21	1.18	1.26

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	1644/5205 (32%)	1590 (97%)	54 (3%)	0	100	100
1	B	1644/5205 (32%)	1599 (97%)	45 (3%)	0	100	100
2	C	142/149 (95%)	131 (92%)	11 (8%)	0	100	100
2	D	139/149 (93%)	127 (91%)	12 (9%)	0	100	100
3	E	44/381 (12%)	44 (100%)	0	0	100	100
3	F	43/381 (11%)	43 (100%)	0	0	100	100
All	All	3656/11470 (32%)	3534 (97%)	122 (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	A	1471/4542 (32%)	1439 (98%)	32 (2%)	47	73
1	B	1471/4542 (32%)	1443 (98%)	28 (2%)	52	76
2	C	123/127 (97%)	118 (96%)	5 (4%)	26	59
2	D	122/127 (96%)	114 (93%)	8 (7%)	14	45
3	E	45/330 (14%)	45 (100%)	0	100	100
3	F	44/330 (13%)	44 (100%)	0	100	100
All	All	3276/9998 (33%)	3203 (98%)	73 (2%)	47	73

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	4542	LEU
2	D	78	LYS
1	B	4649	GLU
2	D	21	ASP
1	A	4400	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	4002	ASN
1	B	4651	HIS
1	B	4011	ASN
1	B	4500	GLN
2	C	43	ASN

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

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

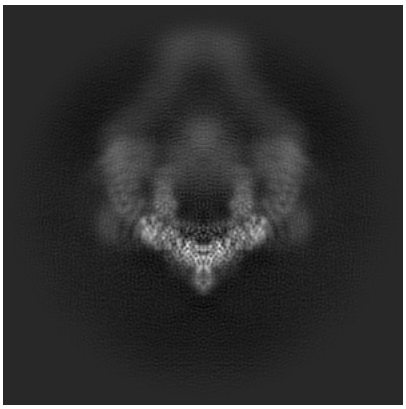
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-49876. 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



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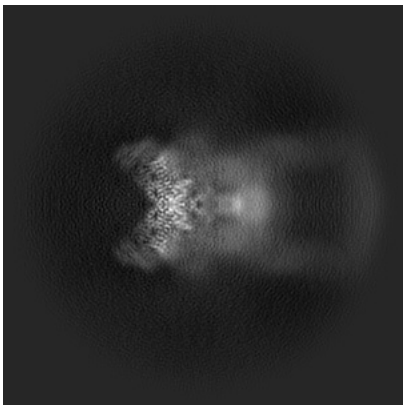

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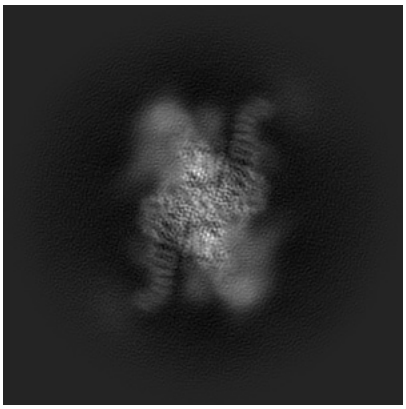
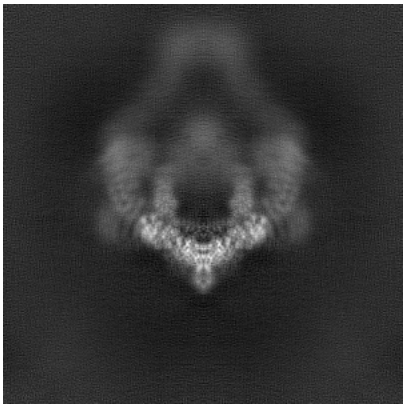


Z

6.1.2 Raw map



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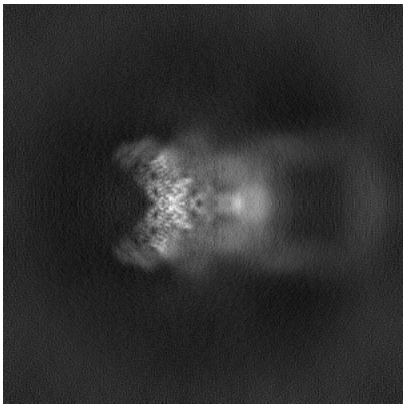

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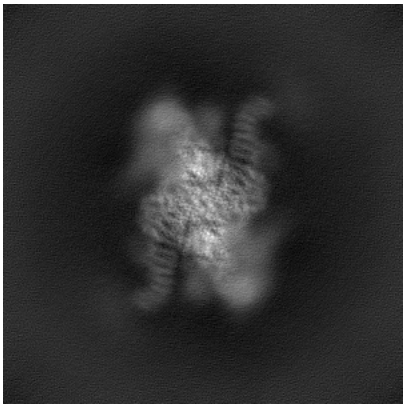
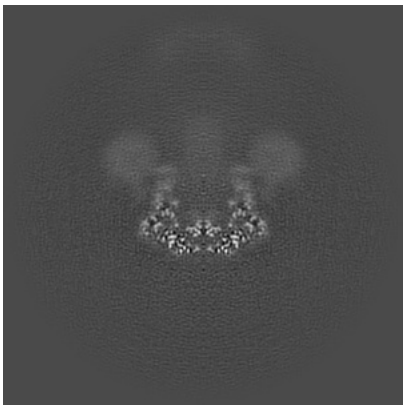


Z

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

6.2 Central slices (i)

6.2.1 Primary map



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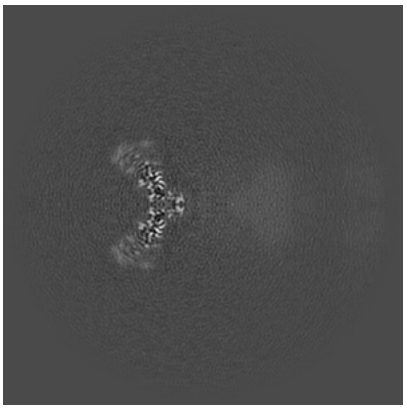

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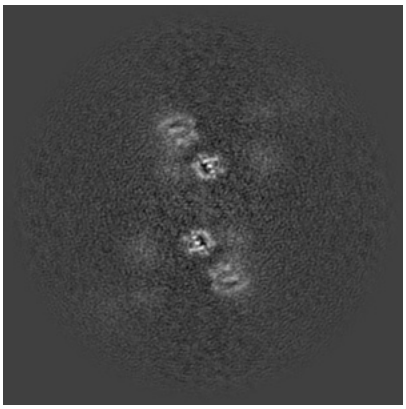
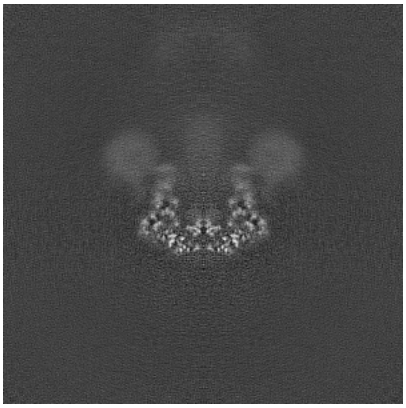


Z Index: 200

6.2.2 Raw map



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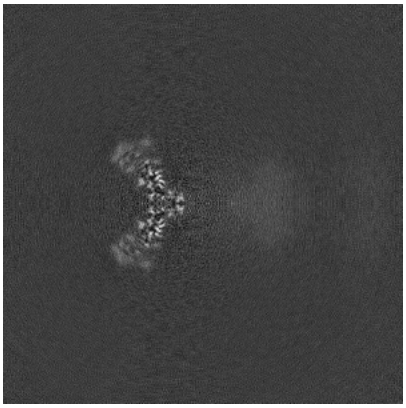

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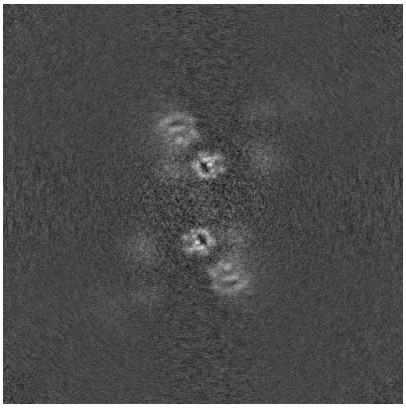
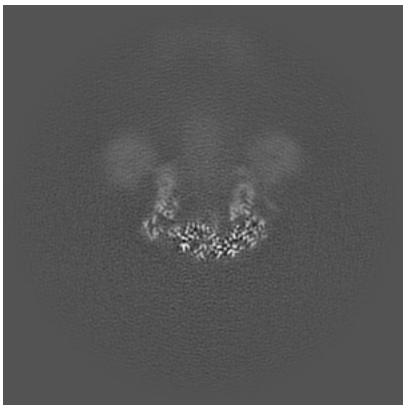


Z Index: 200

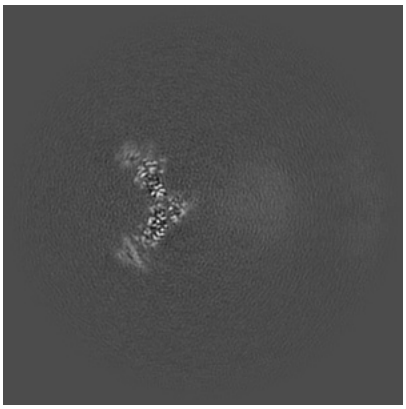
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

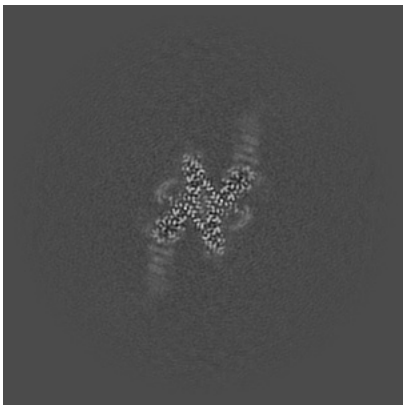
6.3.1 Primary map



X Index: 195

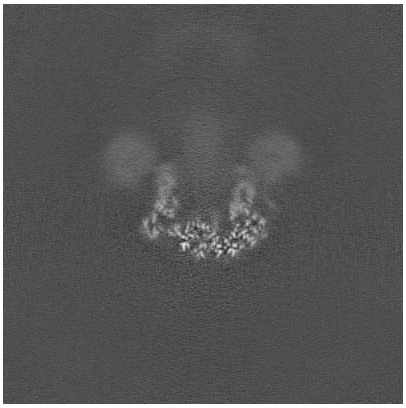


Y Index: 194

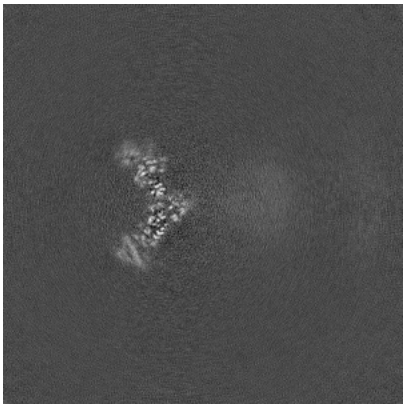


Z Index: 158

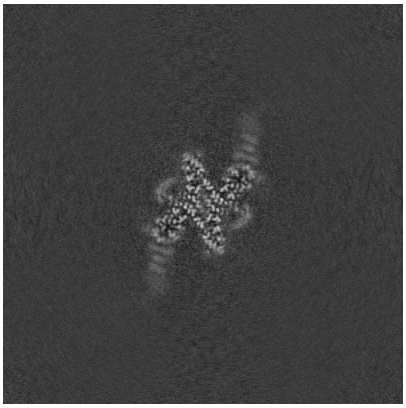
6.3.2 Raw map



X Index: 195



Y Index: 194

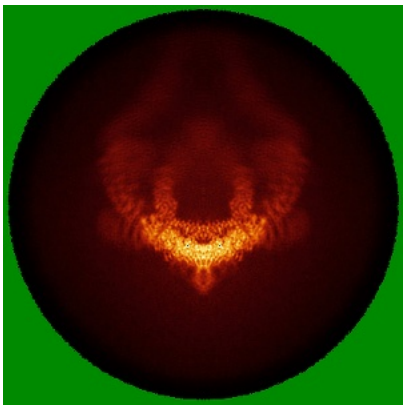


Z Index: 158

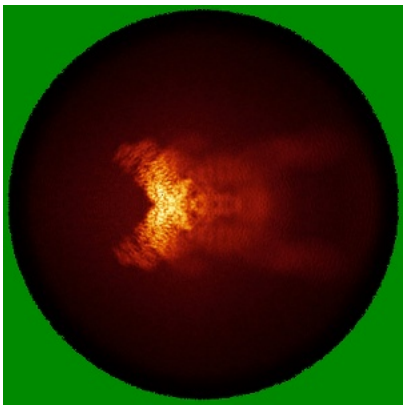
The images above show the largest variance slices of the map in three orthogonal directions.

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

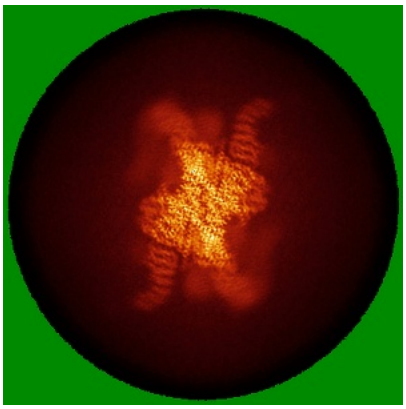
6.4.1 Primary map



X

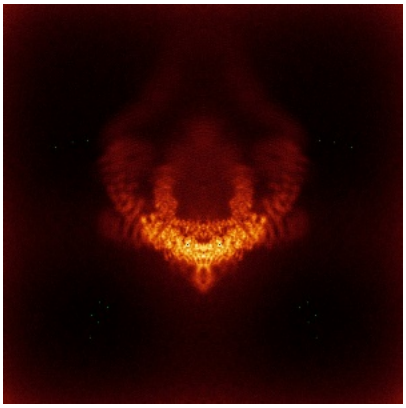


Y

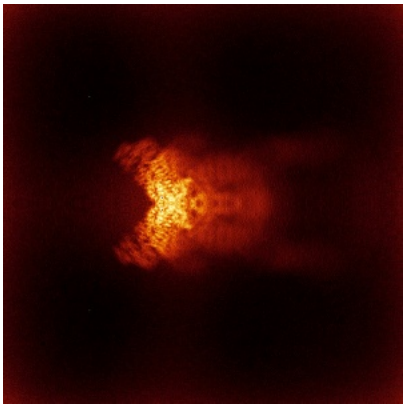


Z

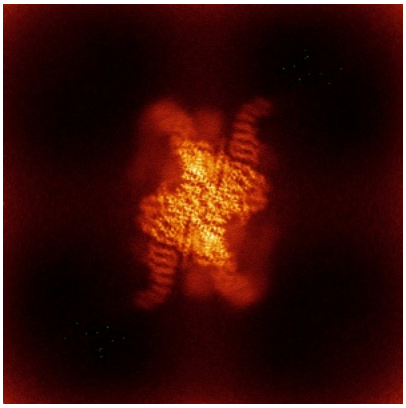
6.4.2 Raw map



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 0.146. 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.

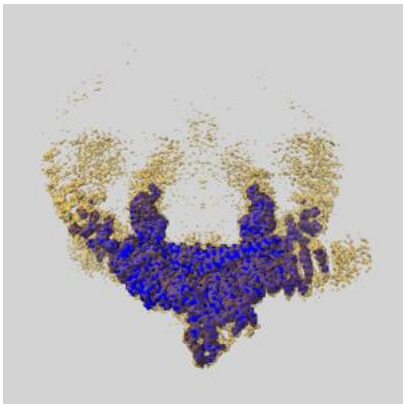
6.6 Mask visualisation (i)

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

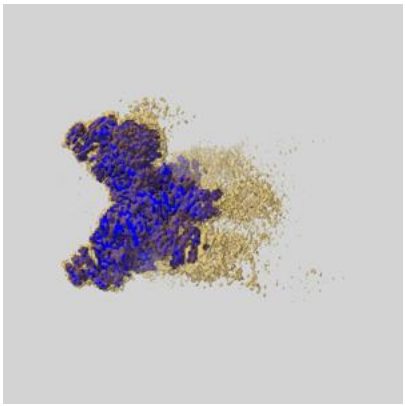
A mask typically either:

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

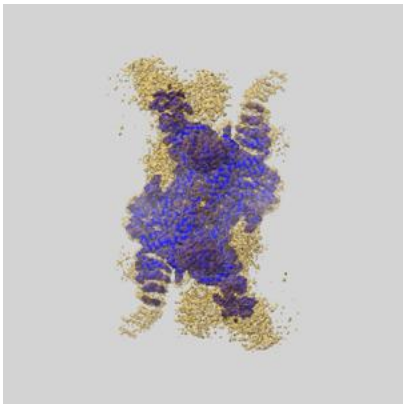
6.6.1 emd_49876_msk_1.map (i)



X



Y

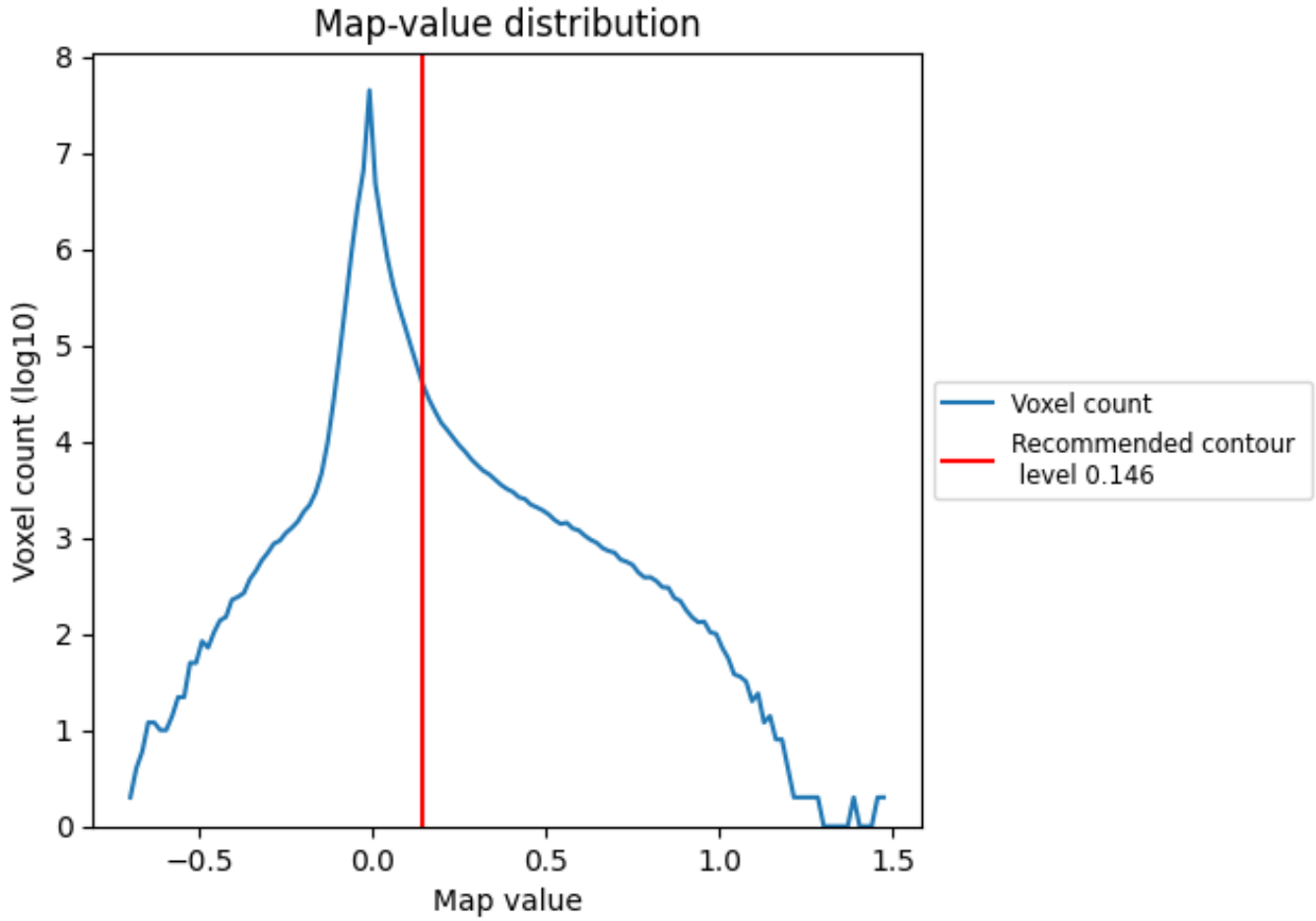


Z

7 Map analysis

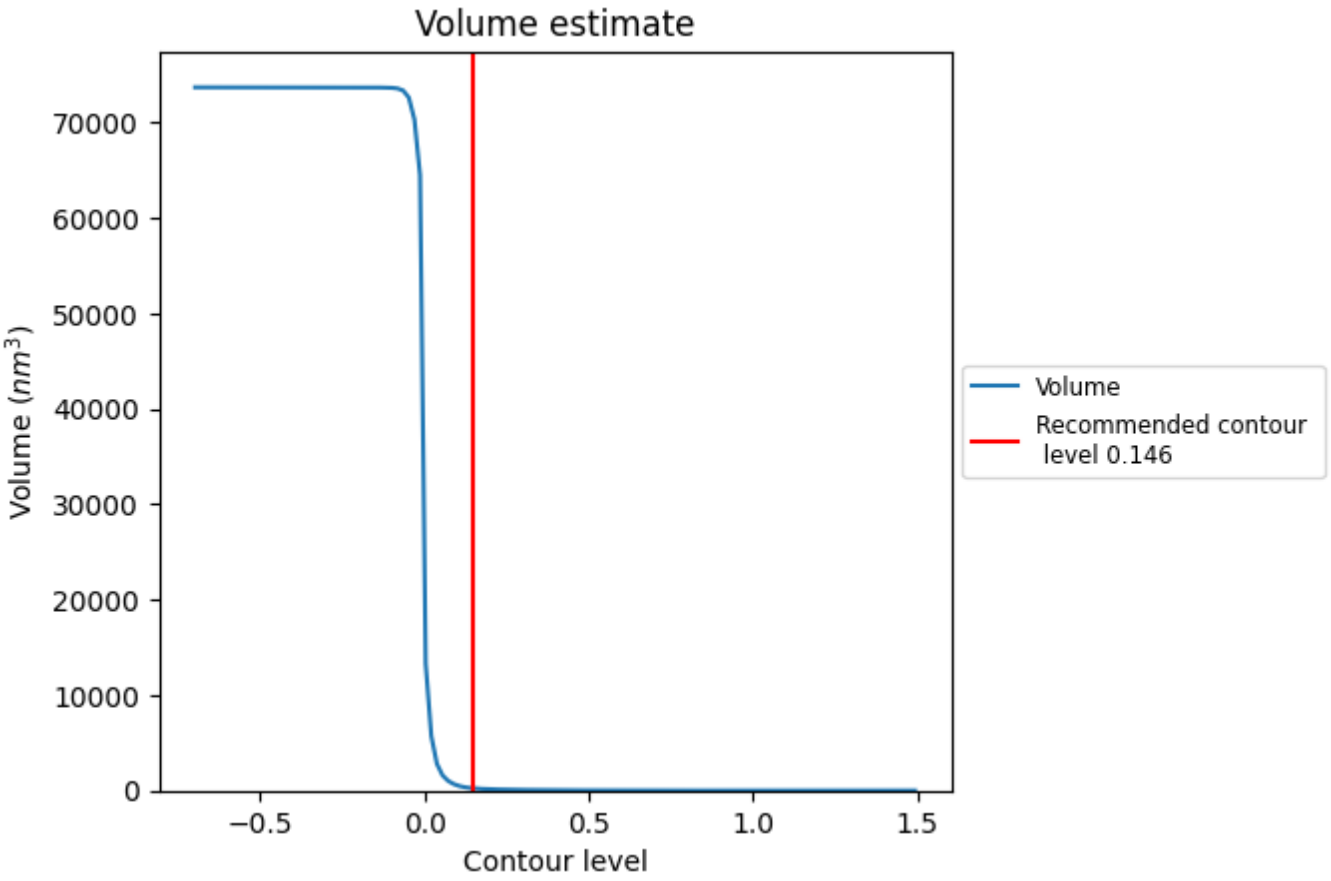
This section contains the results of statistical analysis of the map.

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.

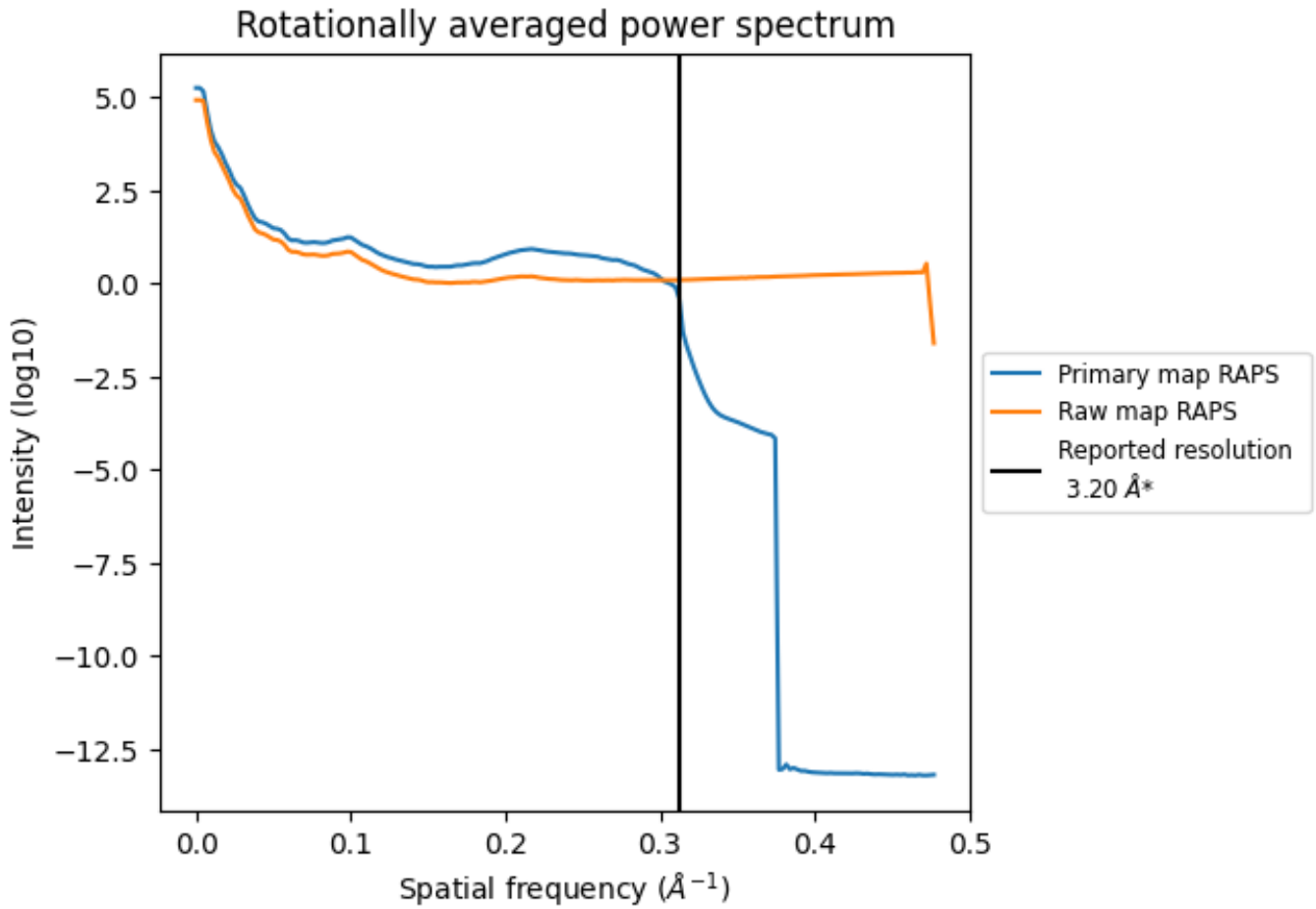
7.2 Volume estimate (i)



The volume at the recommended contour level is 247 nm^3; this corresponds to an approximate mass of 223 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)

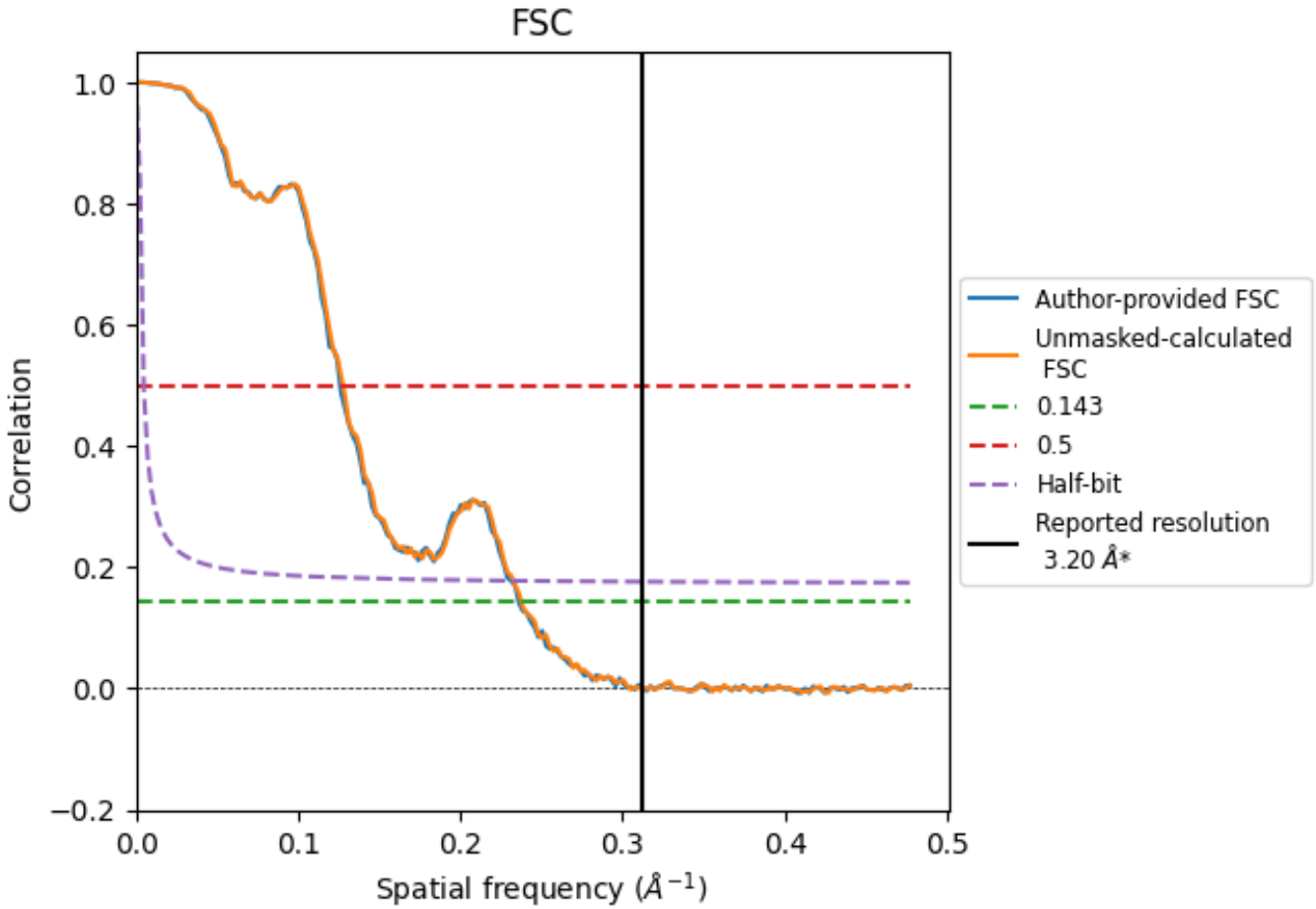


*Reported resolution corresponds to spatial frequency of 0.312 $Å^{-1}$

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	4.24	7.94	4.33
Unmasked-calculated*	4.21	7.84	4.30

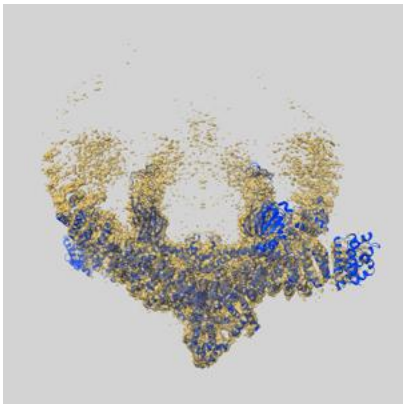
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.24 differs from the reported value 3.2 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.21 differs from the reported value 3.2 by more than 10 %

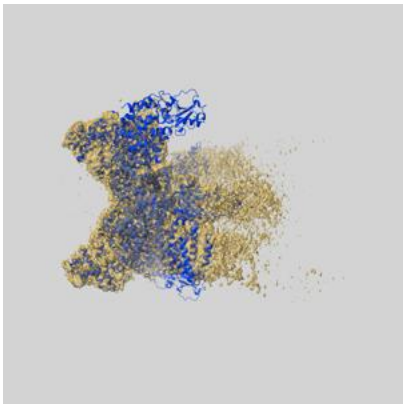
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-49876 and PDB model 9NWE. Per-residue inclusion information can be found in section 3 on page 7.

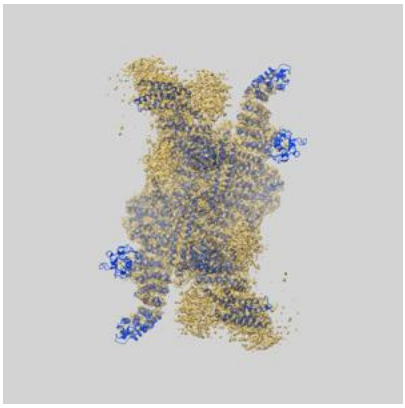
9.1 Map-model overlay



X



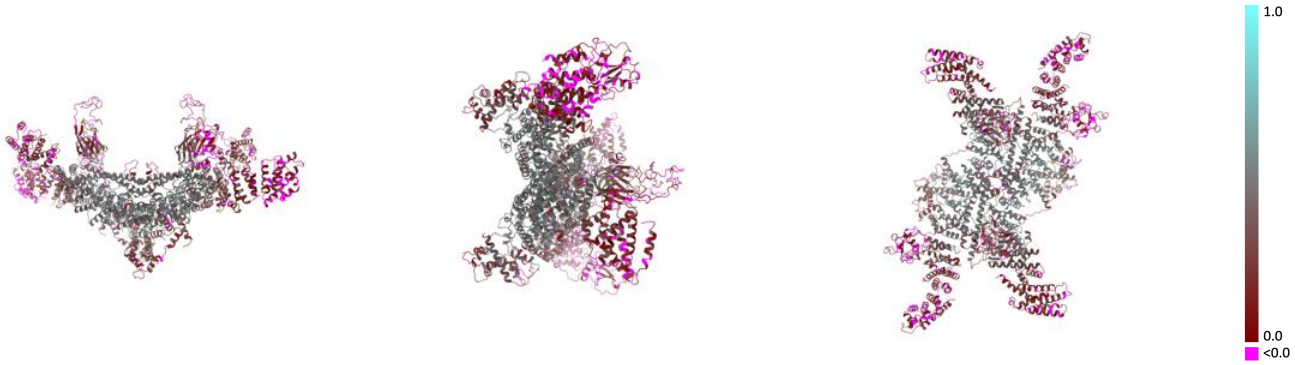
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.146 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.

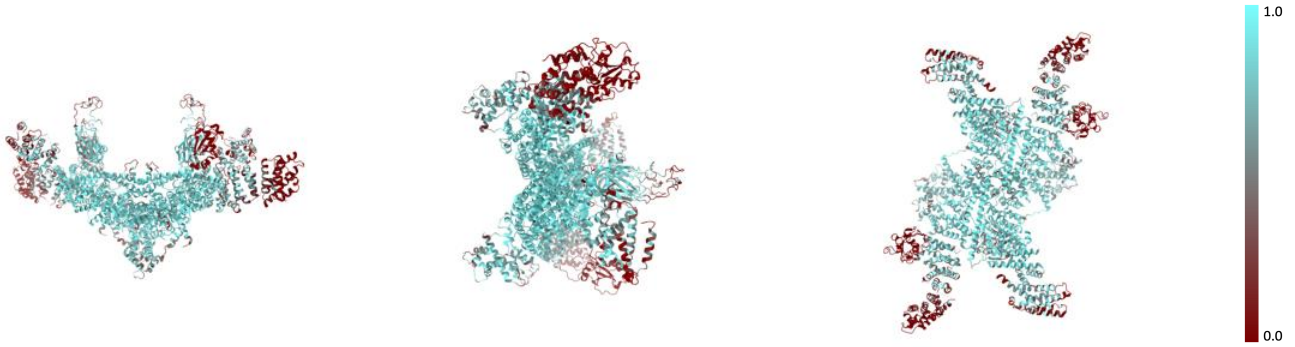
9.2 Q-score mapped to coordinate model



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.

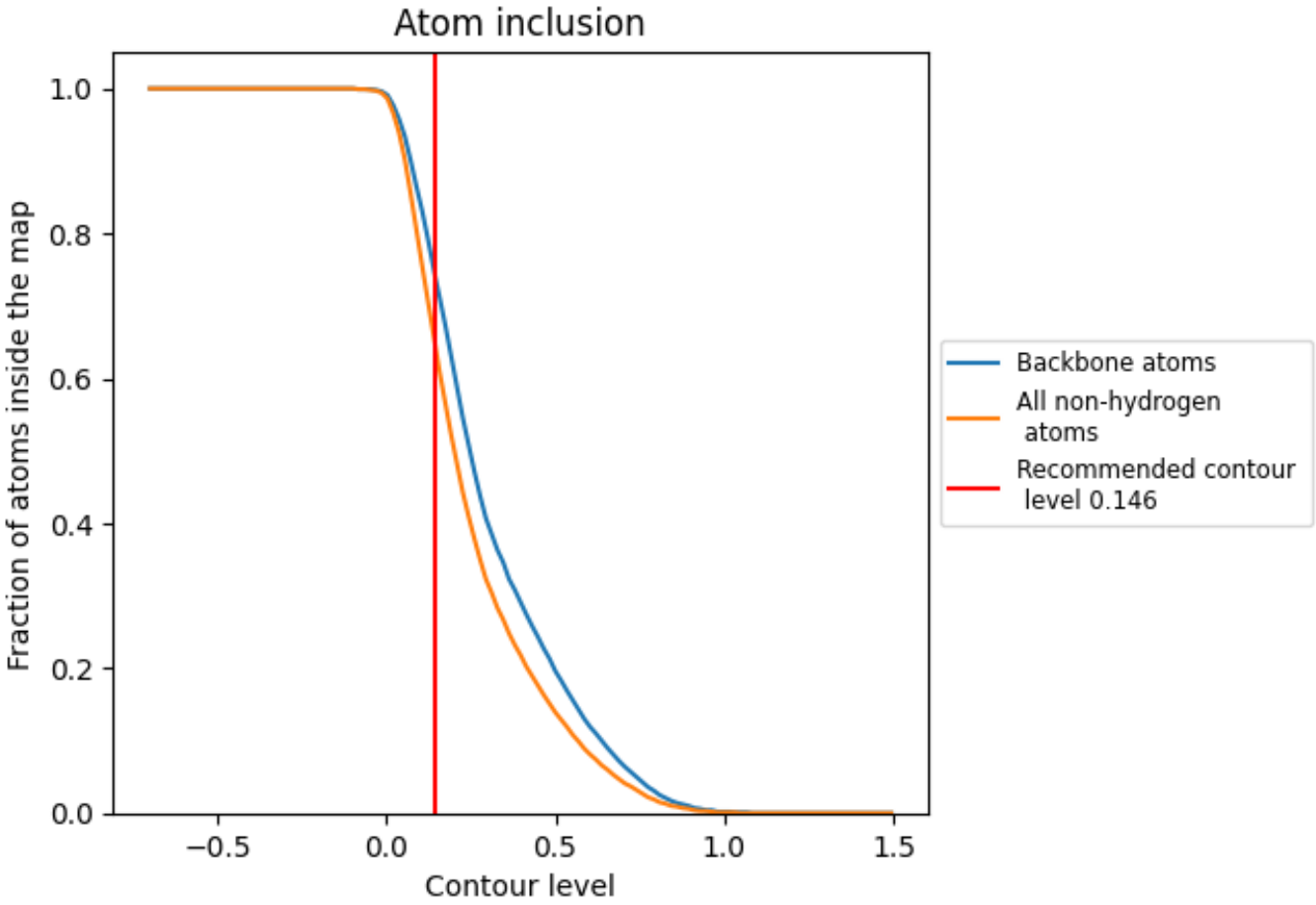
9.3 Atom inclusion mapped to coordinate model



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 (0.146).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 64% 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 (0.146) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6410	0.2850
A	0.6370	0.2880
B	0.6360	0.2870
C	0.6210	0.2260
D	0.6390	0.2360
E	0.8160	0.3900
F	0.8230	0.3850