wwPDB EM Validation Summary Report

Dec 30, 2024 – 03:46 PM EST

PDB ID	:	8E2I
EMDB ID	:	EMD-27837
Title	:	Cryo-EM structure of BIRC6/Smac
Authors	:	Hunkeler, M.; Fischer, E.S.
Deposited on	:	2022-08-15
Resolution	:	3.04 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 ⓘ 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:

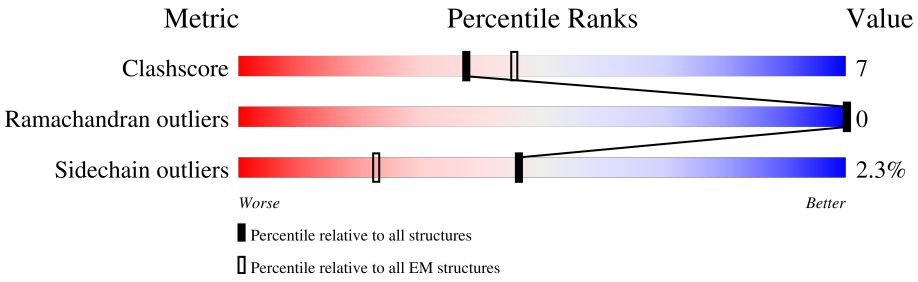
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 3.04 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	4888	22% 45% 11% 44%
1	B	4888	21% 45% 11% 44%
2	E	194	39% 72% 15% • 11%
2	F	194	43% 76% 13% • 11%
3	C	57	37% 98% •
3	D	57	39% 96% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 93130 atoms, of which 46956 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 Baculoviral IAP repeat-containing protein 6.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	2745	Total	C	H	N	O	S	23	0
			43333	13715	21905	3644	3919	150		
1	B	2745	Total	C	H	N	O	S	23	0
			43331	13715	21903	3644	3919	150		

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-30	MET	-	expression tag	UNP Q9NR09
A	-29	ASP	-	expression tag	UNP Q9NR09
A	-28	TYR	-	expression tag	UNP Q9NR09
A	-27	LYS	-	expression tag	UNP Q9NR09
A	-26	ASP	-	expression tag	UNP Q9NR09
A	-25	ASP	-	expression tag	UNP Q9NR09
A	-24	ASP	-	expression tag	UNP Q9NR09
A	-23	ASP	-	expression tag	UNP Q9NR09
A	-22	LYS	-	expression tag	UNP Q9NR09
A	-21	LEU	-	expression tag	UNP Q9NR09
A	-20	ALA	-	expression tag	UNP Q9NR09
A	-19	ALA	-	expression tag	UNP Q9NR09
A	-18	ALA	-	expression tag	UNP Q9NR09
A	-17	ASN	-	expression tag	UNP Q9NR09
A	-16	SER	-	expression tag	UNP Q9NR09
A	-15	SER	-	expression tag	UNP Q9NR09
A	-14	ILE	-	expression tag	UNP Q9NR09
A	-13	ASP	-	expression tag	UNP Q9NR09
A	-12	LEU	-	expression tag	UNP Q9NR09
A	-11	ILE	-	expression tag	UNP Q9NR09
A	-10	SER	-	expression tag	UNP Q9NR09
A	-9	THR	-	expression tag	UNP Q9NR09
A	-8	SER	-	expression tag	UNP Q9NR09
A	-7	LEU	-	expression tag	UNP Q9NR09
A	-6	TYR	-	expression tag	UNP Q9NR09
A	-5	LYS	-	expression tag	UNP Q9NR09

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	LYS	-	expression tag	UNP Q9NR09
A	-3	ALA	-	expression tag	UNP Q9NR09
A	-2	GLY	-	expression tag	UNP Q9NR09
A	-1	LEU	-	expression tag	UNP Q9NR09
A	0	THR	-	expression tag	UNP Q9NR09
A	1332	VAL	LEU	conflict	UNP Q9NR09
B	-30	MET	-	expression tag	UNP Q9NR09
B	-29	ASP	-	expression tag	UNP Q9NR09
B	-28	TYR	-	expression tag	UNP Q9NR09
B	-27	LYS	-	expression tag	UNP Q9NR09
B	-26	ASP	-	expression tag	UNP Q9NR09
B	-25	ASP	-	expression tag	UNP Q9NR09
B	-24	ASP	-	expression tag	UNP Q9NR09
B	-23	ASP	-	expression tag	UNP Q9NR09
B	-22	LYS	-	expression tag	UNP Q9NR09
B	-21	LEU	-	expression tag	UNP Q9NR09
B	-20	ALA	-	expression tag	UNP Q9NR09
B	-19	ALA	-	expression tag	UNP Q9NR09
B	-18	ALA	-	expression tag	UNP Q9NR09
B	-17	ASN	-	expression tag	UNP Q9NR09
B	-16	SER	-	expression tag	UNP Q9NR09
B	-15	SER	-	expression tag	UNP Q9NR09
B	-14	ILE	-	expression tag	UNP Q9NR09
B	-13	ASP	-	expression tag	UNP Q9NR09
B	-12	LEU	-	expression tag	UNP Q9NR09
B	-11	ILE	-	expression tag	UNP Q9NR09
B	-10	SER	-	expression tag	UNP Q9NR09
B	-9	THR	-	expression tag	UNP Q9NR09
B	-8	SER	-	expression tag	UNP Q9NR09
B	-7	LEU	-	expression tag	UNP Q9NR09
B	-6	TYR	-	expression tag	UNP Q9NR09
B	-5	LYS	-	expression tag	UNP Q9NR09
B	-4	LYS	-	expression tag	UNP Q9NR09
B	-3	ALA	-	expression tag	UNP Q9NR09
B	-2	GLY	-	expression tag	UNP Q9NR09
B	-1	LEU	-	expression tag	UNP Q9NR09
B	0	THR	-	expression tag	UNP Q9NR09
B	1332	VAL	LEU	conflict	UNP Q9NR09

- Molecule 2 is a protein called Diablo IAP-binding mitochondrial protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	F	173	Total	C	H	N	O	S	0	0
			2721	849	1347	231	289	5		
2	E	173	Total	C	H	N	O	S	0	0
			2721	849	1347	231	289	5		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	0	MET	-	initiating methionine	UNP Q9NR28
F	185	HIS	-	expression tag	UNP Q9NR28
F	186	HIS	-	expression tag	UNP Q9NR28
F	187	HIS	-	expression tag	UNP Q9NR28
F	188	HIS	-	expression tag	UNP Q9NR28
F	189	HIS	-	expression tag	UNP Q9NR28
F	190	HIS	-	expression tag	UNP Q9NR28
F	191	HIS	-	expression tag	UNP Q9NR28
F	192	HIS	-	expression tag	UNP Q9NR28
F	193	HIS	-	expression tag	UNP Q9NR28
E	0	MET	-	initiating methionine	UNP Q9NR28
E	185	HIS	-	expression tag	UNP Q9NR28
E	186	HIS	-	expression tag	UNP Q9NR28
E	187	HIS	-	expression tag	UNP Q9NR28
E	188	HIS	-	expression tag	UNP Q9NR28
E	189	HIS	-	expression tag	UNP Q9NR28
E	190	HIS	-	expression tag	UNP Q9NR28
E	191	HIS	-	expression tag	UNP Q9NR28
E	192	HIS	-	expression tag	UNP Q9NR28
E	193	HIS	-	expression tag	UNP Q9NR28

- Molecule 3 is a protein called Baculoviral IAP repeat-containing protein 6.

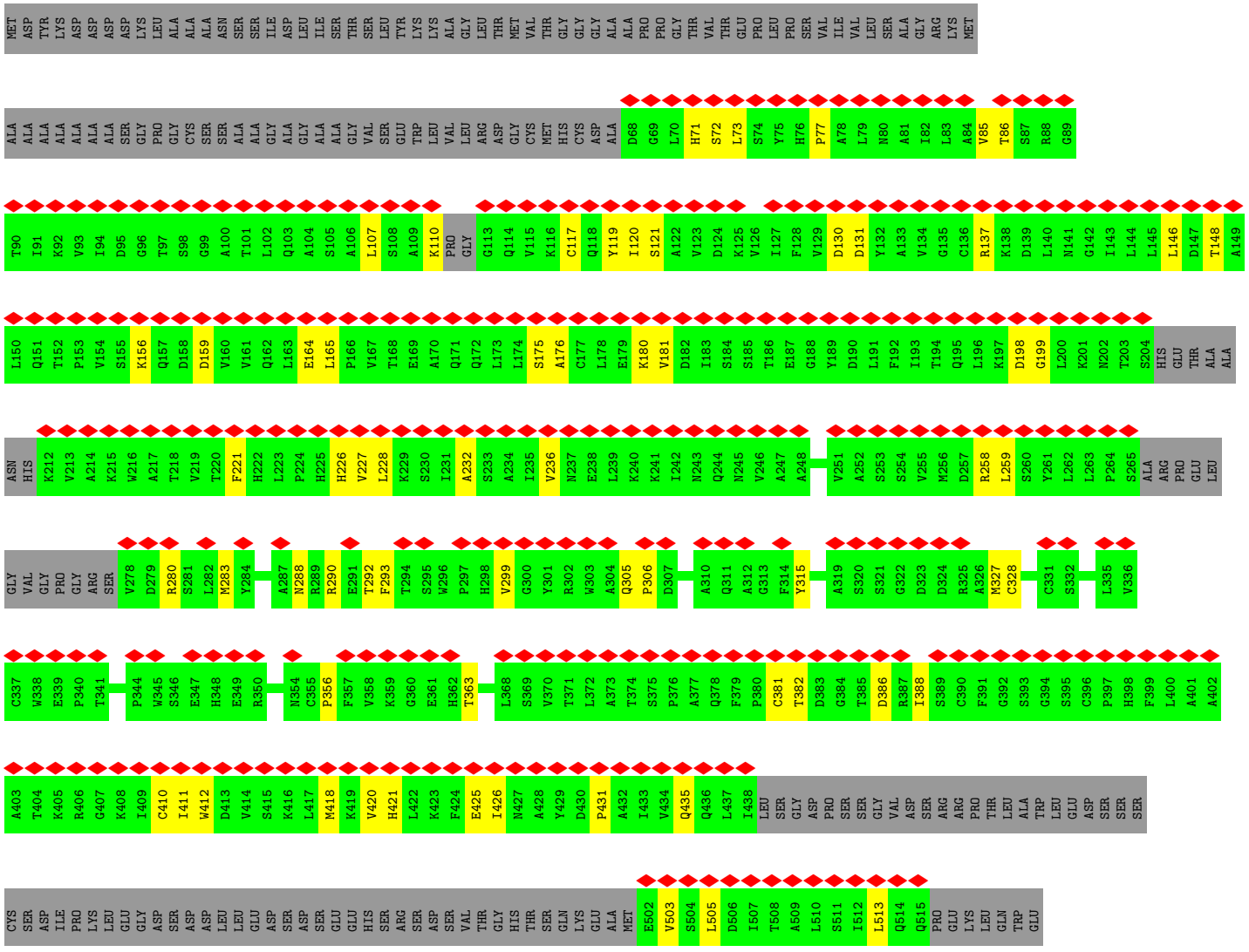
Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	57	Total	C	H	N	O	0	0
			512	171	227	57	57		
3	D	57	Total	C	H	N	O	0	0
			512	171	227	57	57		

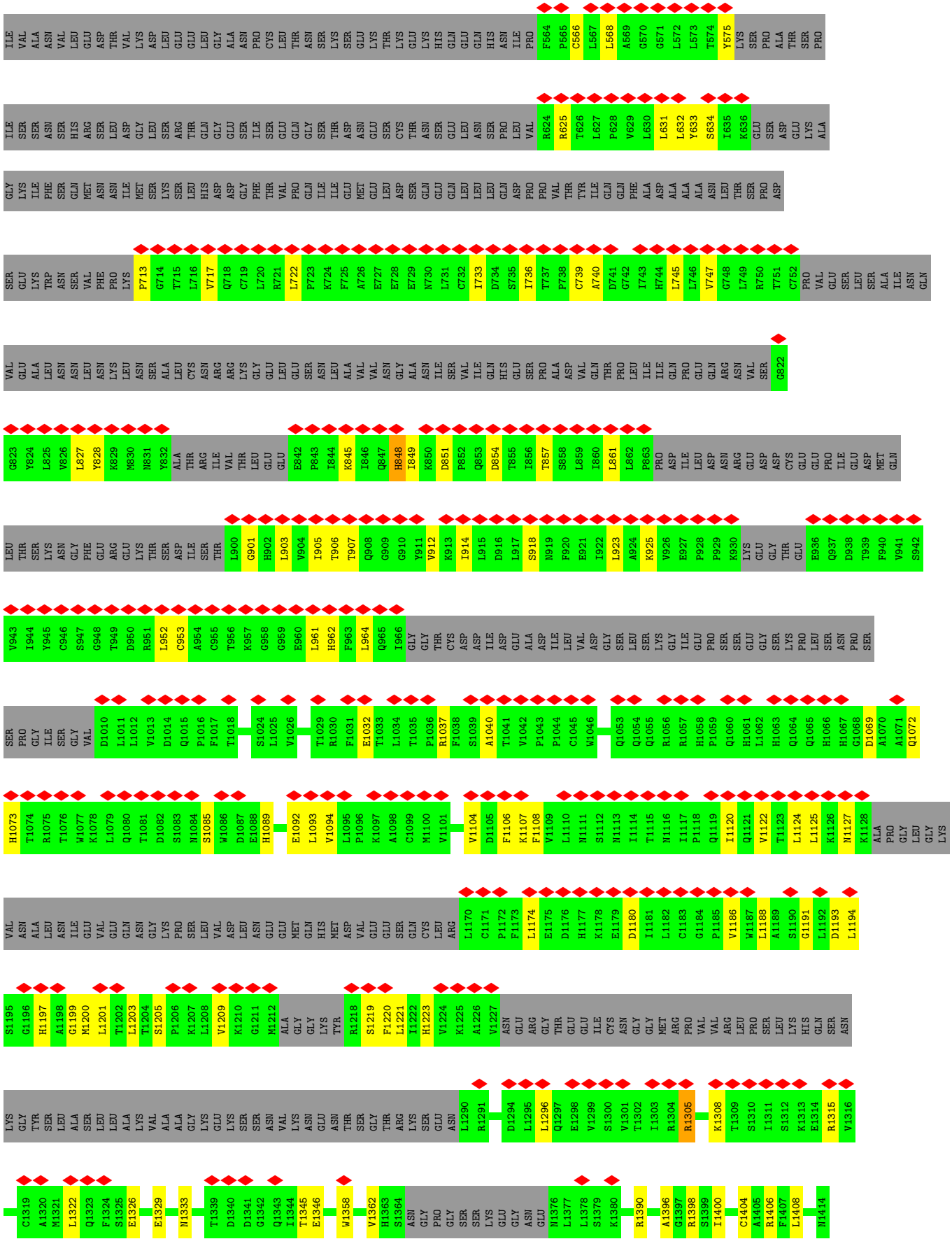
3 Residue-property plots (i)

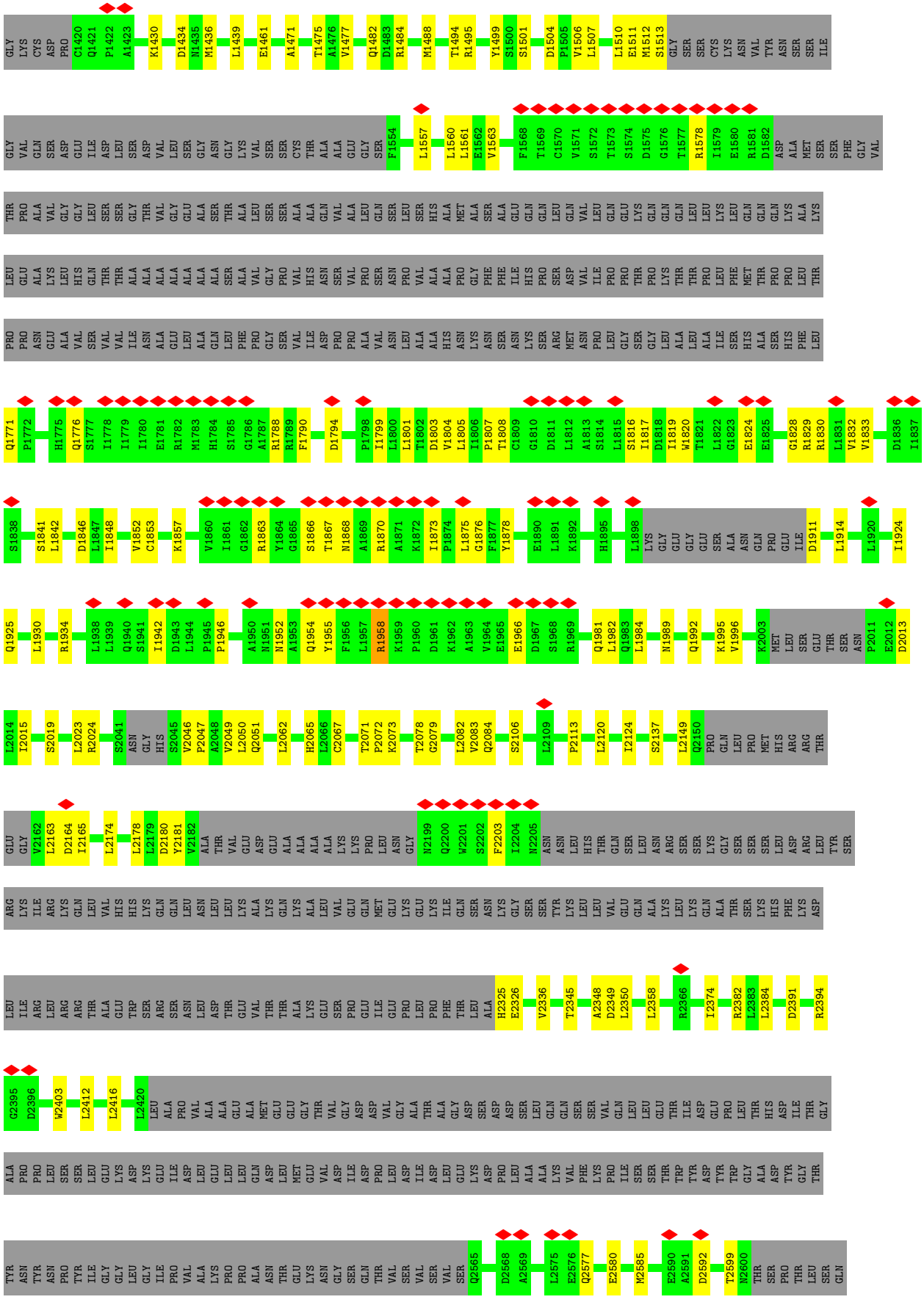
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

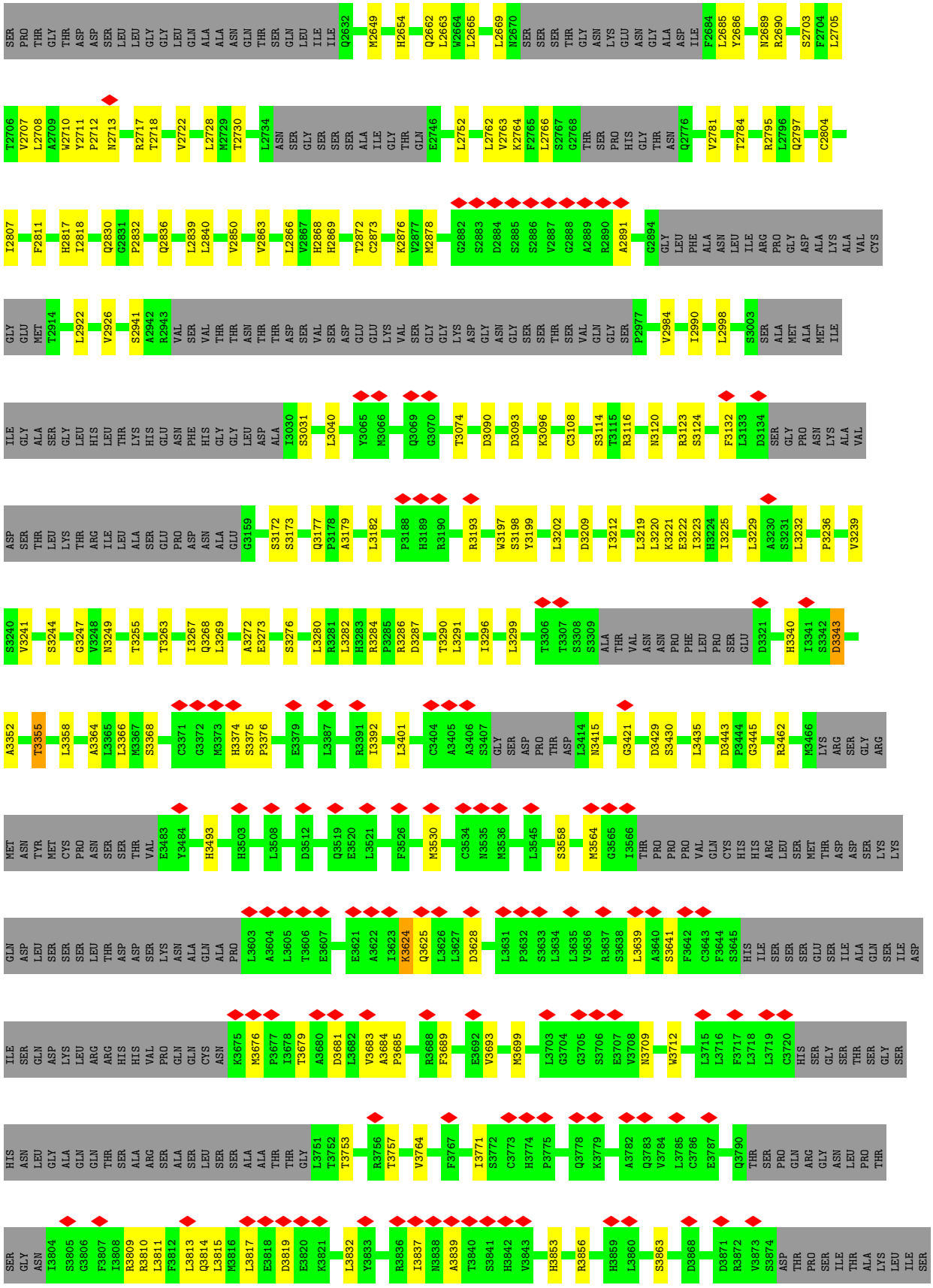
- Molecule 1: Baculoviral IAP repeat-containing protein 6

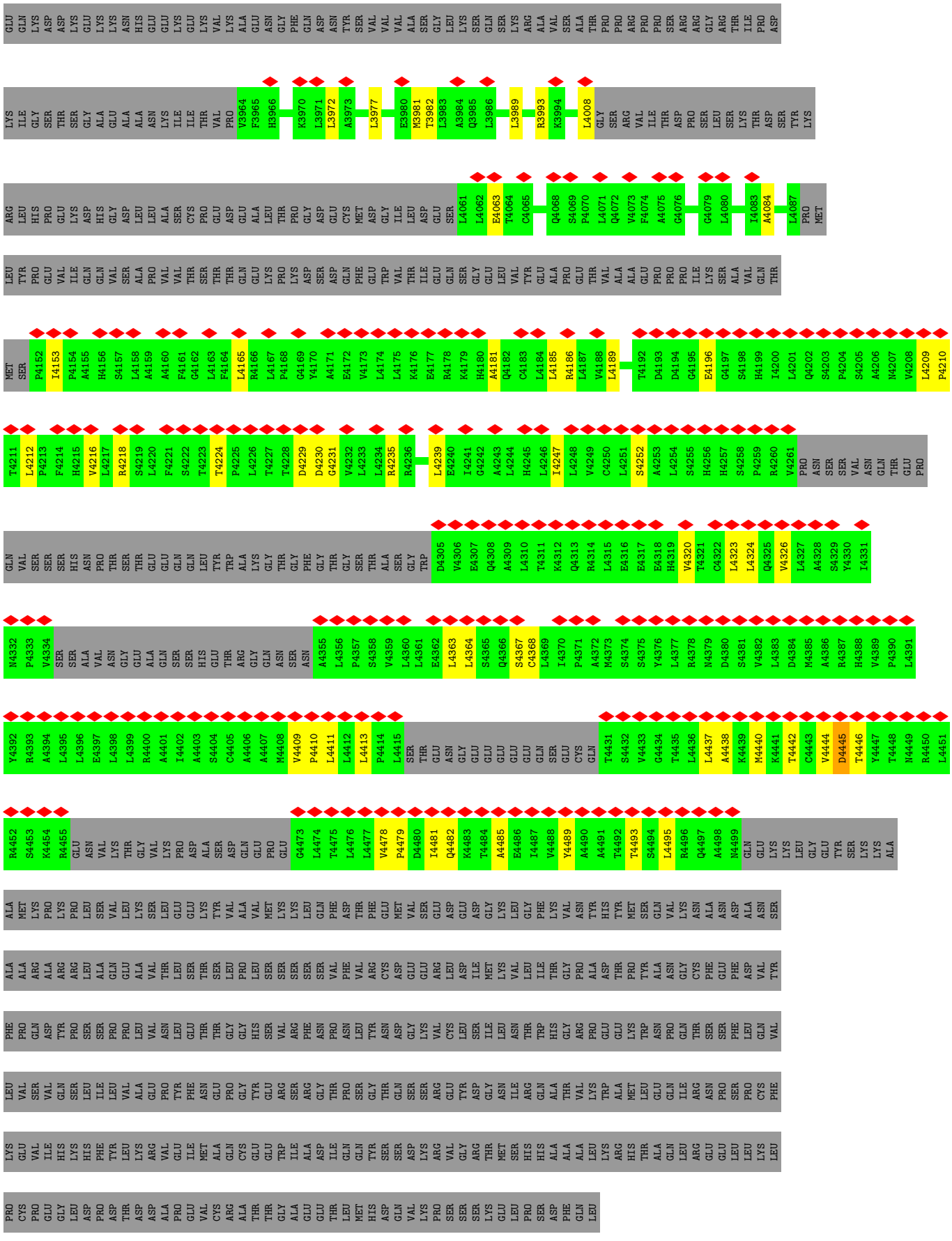
Chain A:





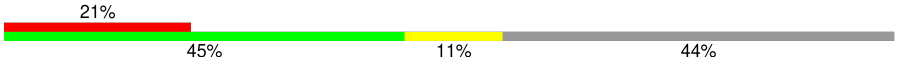


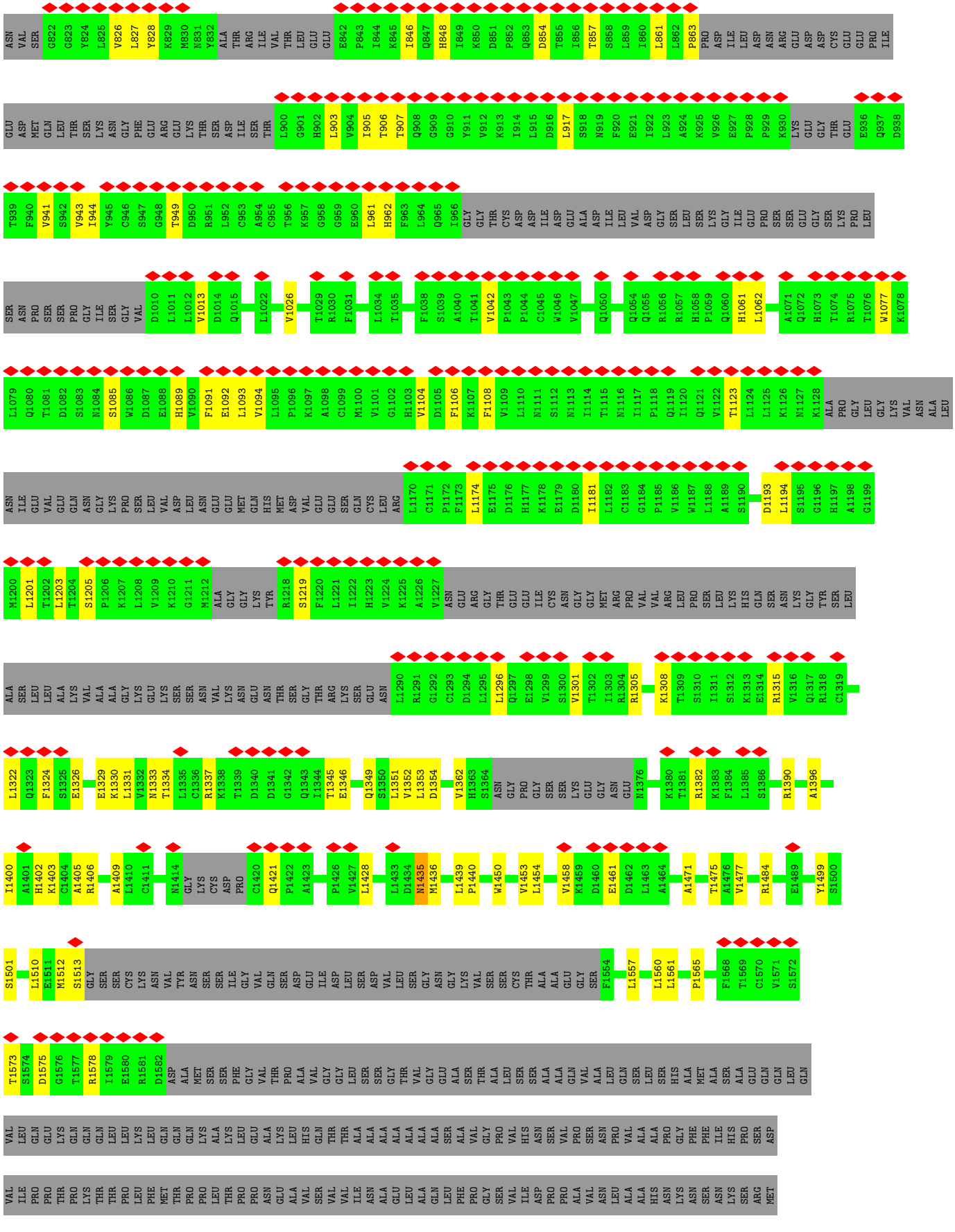


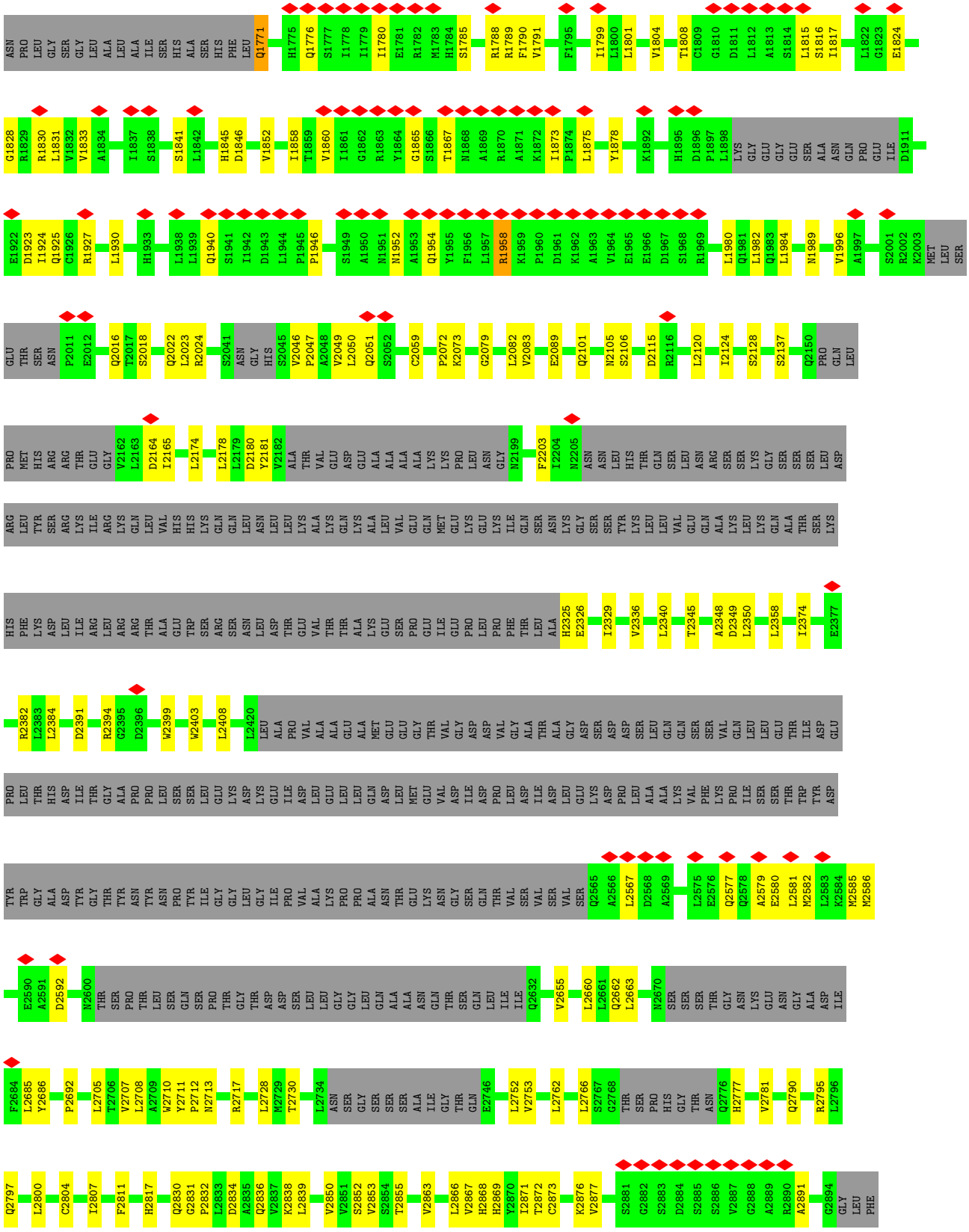

GLU GLN LYS ASP ASP LYS GLU LYS LYS ASN HIS GLU GLU LYS GLU LYS VAL LYS ALA GLU ASN GLY PHE GLN ASP ASN TYR SER VAL VAL VAL ALA SER GLY LEU LYS SER GLN SER LYS ARG ALA VAL SER ALA THR PRO PRO ARG PRO PRO SER ARG ARG GLY ARG THR ILE PRO ASP
LYS ILE GLY SER THR SER GLY ALA ALA ASN LYS ILE ILE THR VAL PRO V3964 F3965 H3966 K3970 L3971 L3972 A3973 L3977 E3980 M3981 T3982 L3983 A3984 Q3985 L3986 L3989 R3993 K3994 L4008 GLY SER ARG VAL ILE THR ASP PRO SER LEU SER LYS THR ASP SER TYR LYS
ARG LEU HIS PRO GLU LYS ASP HIS GLY ASP LEU LEU ALA SER CYS PRO GLU ASP GLU ALA LEU THR PRO GLY ASP GLU CYS MET ASP GLY ILE LEU ASP GLU SER L4061 L4062 E4063 T4064 C4065 Q4068 S4069 P4070 L4071 Q4072 V4073 F4074 A4075 G4076 G4079 L4080 I4083 A4084 L4087 PRO MET
LEU TYR PRO GLU VAL ILE GLN GLN VAL SER ALA PRO VAL VAL THR SER THR THR GLN GLU LYS PRO LYS ASP SER ASP GLN PHE GLU TRP VAL THR ILE GLU GLN SER GLY GLU LEU VAL TYR GLU ALA PRO GLU THR VAL ALA ALA GLU PRO PRO ILE LYS SER ALA VAL GLN THR
MET SER P4152 I4153 P4154 A4155 H4156 S4157 L4158 A4159 A4160 F4161 G4162 L4163 F4164 L4165 R4166 L4167 P4168 G4169 Y4170 A4171 E4172 V4173 L4174 L4175 K4176 E4177 R4178 K4179 H4180 A4181 Q4182 C4183 L4184 L4185 R4186 L4187 V4188 L4189 T4192 D4193 D4194 G4195 E4196 G4197 S4198 H4199 I4200 L4201 Q4202 S4203 P4204 S4205 A4206 N4207 V4208 L4209 P4210
T4211 L4212 P4213 F4214 H4215 V4216 L4217 R4218 S4219 L4220 F4221 S4222 T4223 T4224 P4225 L4226 T4227 T4228 D4229 D4230 G4231 V4232 L4233 L4234 R4235 R4236 L4239 E4240 I4241 G4242 A4243 L4244 H4245 L4246 I4247 L4248 V4249 C4250 L4251 S4252 A4253 L4254 S4255 H4256 H4257 S4258 P4259 R4260 V4261 PRO ASN SER SER VAL ASN GLN THR GLU PRO
GLN VAL SER SER HIS ASN PRO THR SER THR GLU GLN GLN LEU TYR TRP ALA LYS GLY THR GLY PHE GLY THR GLY SER THR ALA SER GLY TRP D4305 V4306 E4307 Q4308 A4309 L4310 T4311 K4312 Q4313 R4314 L4315 E4316 E4317 E4318 H4319 V4320 T4321 C4322 L4323 L4324 Q4325 V4326 L4327 A4328 S4329 Y4330 I4331
N4332 P4333 V4334 SER SER ALA VAL ASN GLY GLU ALA GLN SER SER HIS GLU THR ARG GLY GLN ASN SER ASN A4355 L4356 P4357 S4358 S4359 L4360 L4361 E4362 L4363 L4364 S4365 Q4366 S4367 C4368 L4369 I4370 P4371 A4372 M4373 S4374 S4375 Y4376 L4377 R4378 N4379 D4380 S4381 V4382 L4383 D4384 M4385 A4386 R4387 H4388 V4389 P4390 L4391
Y4392 R4393 A4394 L4395 L4396 E4397 L4398 L4399 R4400 A4401 I4402 A4403 S4404 C4405 A4406 A4407 M4408 V4409 P4410 L4411 L4412 L4413 P4414 L4415 SER THR GLU ASN GLY GLU GLU GLU GLU GLU GLN SER GLU CYS GLN T4431 S4432 V4433 G4434 T4435 L4436 L4437 A4438 K4439 M4440 K4441 T4442 C4443 V4444 D4445 T4446 Y4447 T4448 N4449 R4450 L4451
R4452 S4453 K4454 R4455 GLU ASN VAL LYS THR GLY VAL LYS PRO ASP ALA SER ASP GLN GLU PRO GLU G4473 L4474 T4475 L4476 L4477 V4478 P4479 D4480 I4481 Q4482 K4483 T4484 A4485 E4486 I4487 V4488 Y4489 A4490 A4491 T4492 T4493 S4494 L4495 R4496 Q4497 A4498 N4499 GLN GLU LYS LYS LEU GLY GLU TYR SER LYS ALA
ALA MET LYS PRO LYS PRO LEU SER VAL LEU LYS SER LEU GLU GLU LYS TYR VAL ALA VAL MET LYS LYS LEU GLN PHE ASP THR PHE GLU MET VAL SER GLU ASP GLU ASP GLY LYS LEU GLY PHE LYS VAL ASN TYR HIS TYR MET SER GLN VAL LYS ASN ALA ASP ALA ASN SER
ALA ALA ARG ALA ARG LEU GLU ALA VAL THR LEU SER THR SER LEU PRO LEU SER SER SER SER SER VAL PHE VAL ARG CYS ASP GLU GLU ARG LEU ASP ILE MET LYS VAL LEU LEU ILE THR GLY PRO ALA ASP THR PRO TYR ALA ASN GLY CYS PHE GLU PHE ASP VAL TYR
PHE PRO GLN ASP TYR PRO SER SER PRO PRO LEU VAL ASN LEU GLU THR THR SER LEU PRO GLY HIS SER VAL ARG PHE ASN PRO ASN LEU TYR ASN ASP GLY LYS VAL CYS LEU SER ILE LEU ASN THR TRP HIS GLY ARG PRO GLU GLU LYS TRP ASP GLY GLU PHE GLU PHE ASP ALA ASN SER
LEU VAL SER VAL GLN SER LEU ILE LEU VAL ALA GLU PRO TYR PHE ASN GLU PRO GLY TYR GLU ARG SER ARG GLY THR PRO SER GLY THR GLN SER SER ARG GLU TYR ASP GLY ASN ILE ARG GLN ALA THR VAL LYS TRP ALA MET LEU GLU GLN ILE ARG ASN PRO SER PRO CYS PHE
LYS GLU VAL ILE HIS LYS HIS PHE TYR LEU LYS ARG VAL GLU ILE MET ALA GLN CYS GLU GLU TRP ILE ALA ASP ILE GLN GLN TYR SER SER ASP LYS ARG VAL GLY ARG THR MET SER HIS HIS ALA ALA ALA LEU LYS ARG HIS THR ALA GLN LEU ARG GLU GLU LEU LEU LYS LEU
PRO CYS PRO GLU GLY LEU ASP PRO ASP THR ASP ASP ALA PRO GLU VAL CYS ARG ALA THR THR GLY ALA GLU GLU THR LEU MET HIS ASP GLN VAL LYS PRO SER SER SER LYS GLU LEU PRO SER ASP PHE GLN LEU

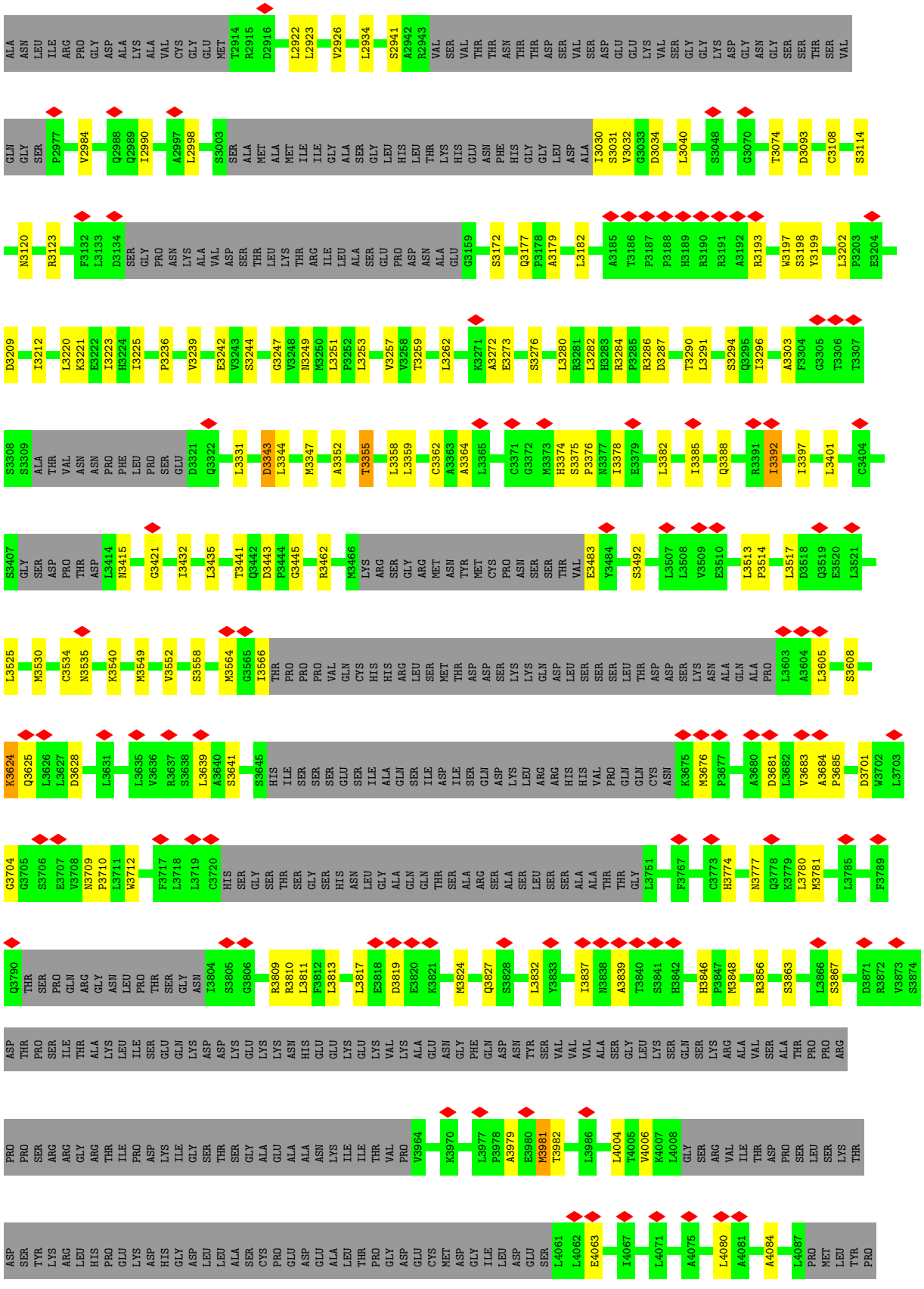
• Molecule 1: Baculoviral IAP repeat-containing protein 6

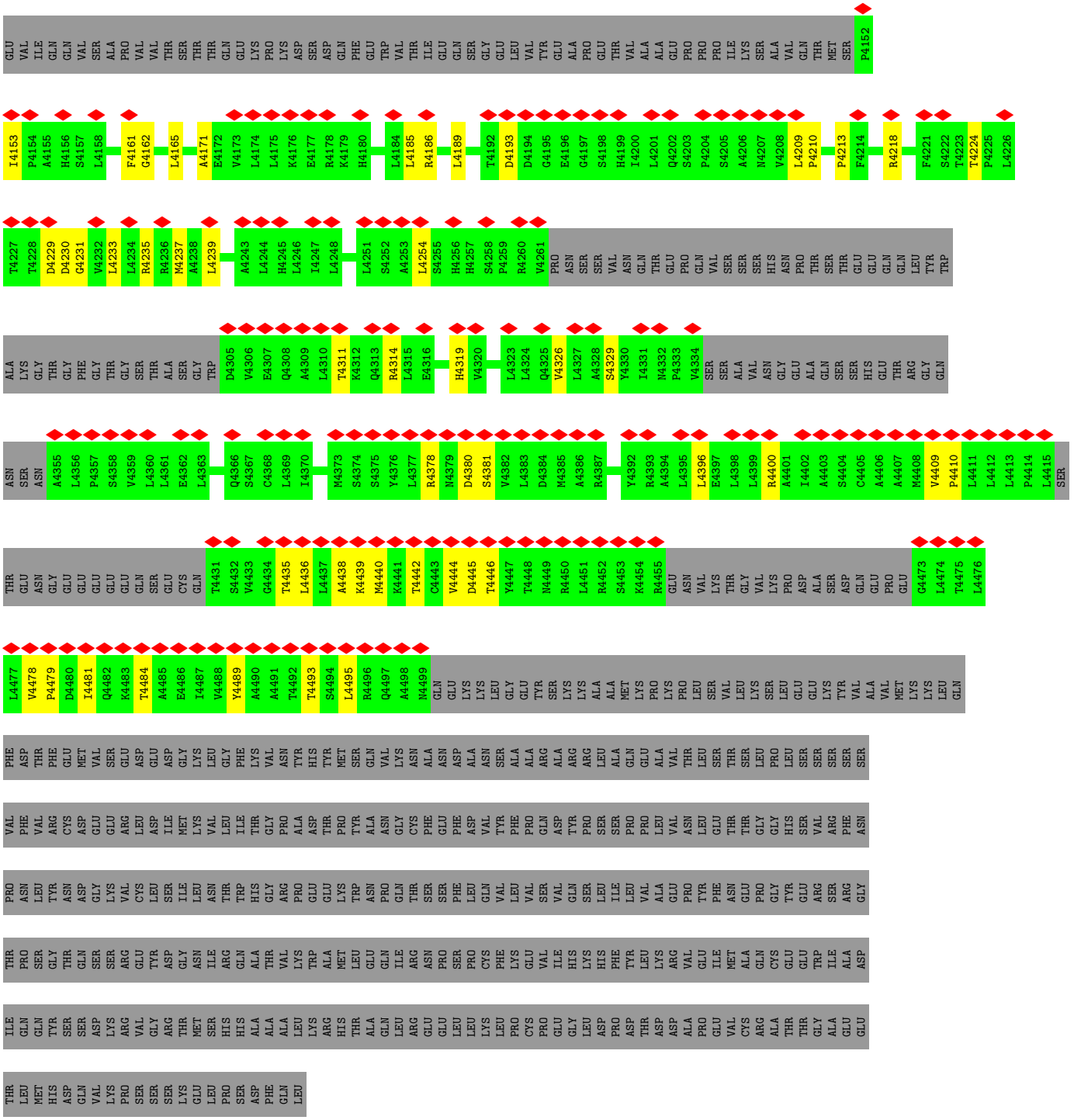
Chain B:




ASN VAL SER G822 G823 Y824 L825 V826 L827 Y828 K829 M830 N831 Y832 ALA THR ARG ILE VAL THR LEU GLU GLU E842 P843 I844 K845 I846 Q847 H848 I849 K850 D851 P852 Q853 D854 T855 I856 T857 S858 L859 I860 L861 L862 P863 PRO ASP ILE LEU ASP ASN ARG GLU ASP ASP CYS GLU GLU PRO ILE
GLU ASP MET GLN LEU THR SER LYS ASN GLY PHE GLU ARG GLU LYS THR SER ASP ILE SER THR L900 G901 H902 L903 V904 I905 T906 T907 Q908 G909 G910 Y911 V912 K913 I914 L915 D916 L917 S918 N919 F920 E921 I922 L923 A924 K925 V926 E927 P928 P929 K930 LYS GLU GLY THR GLU E936 Q937 D938
T939 F940 V941 S942 V943 I944 Y945 C946 S947 G948 T949 D950 R951 L952 C953 A954 C955 T956 K957 G958 G959 E960 L961 H962 F963 L964 Q965 I966 GLY GLY THR CYS ASP ASP ILE ASP GLU ALA ASP ILE LEU VAL ASP GLY SER LEU SER LYS GLY ILE GLU PRO SER SER GLU GLY SER LYS PRO LEU
SER ASN PRO SER SER PRO GLY ILE SER GLY VAL D1010 L1011 L1012 V1013 D1014 Q1015 L1022 V1026 T1029 R1030 F1031 L1034 T1035 F1038 S1039 A1040 T1041 V1042 P1043 P1044 C1045 W1046 V1047 Q1050 Q1054 Q1055 R1056 R1057 H1058 P1059 Q1060 H1061 L1062 A1071 Q1072 H1073 T1074 R1075 T1076 W1077 K1078
L1079 Q1080 T1081 D1082 S1083 N1084 S1085 W1086 D1087 E1088 H1089 V1090 F1091 E1092 L1093 V1094 L1095 P1096 K1097 A1098 C1099 M1100 V1101 G1102 H1103 V1104 D1105 F1106 K1107 F1108 V1109 L1110 N1111 S1112 N1113 I1114 T1115 N1116 I1117 P1118 Q1119 I1120 Q1121 V1122 T1123 L1124 L1125 K1126 N1127 K1128 ALA PRO GLY LEU GLY LYS VAL ASN ALA LEU
ASN ILE GLU VAL GLU GLN ASN GLY LYS PRO SER LEU VAL ASP LEU ASN GLU GLU MET GLN HIS MET ASP VAL GLU GLU SER GLN CYS LEU ARG L1170 C1171 P1172 F1173 L1174 E1175 D1176 H1177 K1178 E1179 D1180 I1181 L1182 C1183 G1184 P1185 V1186 W1187 L1188 A1189 S1190 D1193 L1194 S1195 G1196 H1197 A1198 G1199
M1200 L1201 T1202 L1203 T1204 S1205 P1206 K1207 L1208 V1209 K1210 G1211 M1212 ALA GLY GLY LYS TYR R1218 S1219 F1220 L1221 I1222 H1223 V1224 K1225 A1226 V1227 ASN GLU ARG GLY THR GLU GLU ILE CYS ASN GLY GLY MET ARG PRO VAL VAL ARG LEU PRO SER LEU LYS HIS GLN SER ASN LYS GLY TYR SER LEU
ALA SER LEU LEU ALA LYS VAL ALA ALA GLY LYS GLU LYS SER SER ASN VAL LYS ASN GLU ASN THR SER GLY THR ARG LYS SER GLU ASN L1290 R1291 G1292 C1293 D1294 L1295 L1296 Q1297 E1298 V1299 S1300 V1301 T1302 I1303 R1304 R1305 K1308 T1309 S1310 I1311 S1312 K1313 E1314 R1315 V1316 Q1317 R1318 C1319
L1322 Q1323 F1324 S1325 E1326 E1329 K1330 L1331 V1332 N1333 T1334 L1335 C1336 R1337 K1338 T1339 D1340 D1341 G1342 Q1343 T1344 T1345 E1346 Q1349 S1350 L1351 V1352 L1353 D1354 V1362 H1363 S1364 ASN GLY PRO GLY SER SER LYS GLU GLY ASN GLU N1376 K1380 T1381 R1382 K1383 F1384 L1385 S1386 R1390 A1396
I1400 A1401 H1402 K1403 C1404 A1405 R1406 A1409 L1410 C1411 N1414 GLY LYS CYS ASP PRO C1420 Q1421 P1422 A1423 P1426 V1427 L1428 L1433 D1434 N1435 M1436 L1439 P1440 W1450 V1453 L1454 V1458 K1459 D1460 E1461 D1462 L1463 A1464 A1471 T1475 A1476 V1477 R1484 E1489 Y1499 S1500
S1501 L1510 E1511 M1512 S1513 GLY SER SER CYS LYS ASN VAL TYR ASN SER SER ILE GLY VAL GLN SER ASP GLU ILE ASP LEU SER ASP VAL LEU SER GLY ASN GLY LYS VAL SER SER CYS THR ALA ALA GLU GLY SER F1554 L1557 L1560 L1561 P1565 F1568 T1569 C1570 V1571 S1572
T1573 S1574 D1575 G1576 T1577 R1578 I1579 E1580 R1581 D1582 ASP ALA MET SER SER PHE GLY VAL THR PRO ALA VAL GLY GLY LEU SER SER GLY THR VAL GLY GLU ALA SER THR ALA LEU SER SER ALA ALA GLN VAL ALA LEU GLN SER LEU SER HIS ALA MET ALA SER ALA GLU GLN GLN LEU GLN
VAL LEU GLN GLU LYS GLN GLN LEU LEU LYS LEU GLN GLN LYS ALA LYS LEU GLU ALA LYS LEU HIS GLN THR THR ALA ALA ALA ALA ALA ALA SER ALA SER VAL PRO SER ASN PRO VAL ALA ALA PRO GLY PHE PHE ILE HIS PRO SER ASP
VAL ILE PRO PRO THR PRO LYS THR THR PRO LEU PHE MET THR PRO PRO LEU THR PRO PRO ASN GLU ALA VAL SER VAL VAL ILE ALA GLU LEU ALA LEU GLN LEU PHE PRO GLY SER VAL ILE ASP PRO PRO ALA VAL ASN LEU ALA ALA HIS ASN LYS LYS ASN SER ASN LYS SER ARG MET

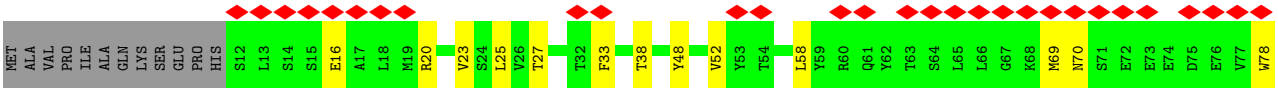


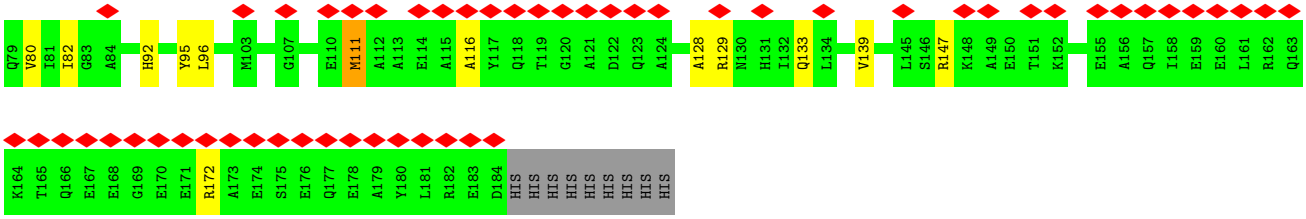




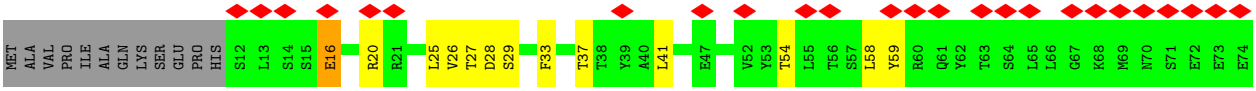
• Molecule 2: Diablo IAP-binding mitochondrial protein

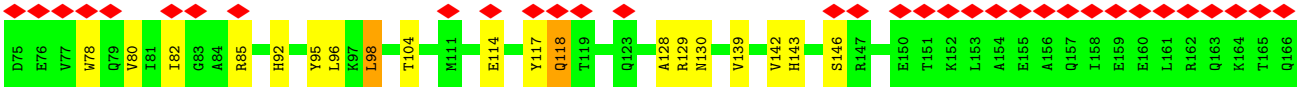
Chain F:

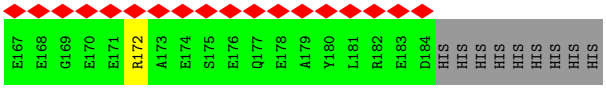




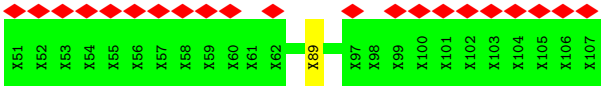
• Molecule 2: Diablo IAP-binding mitochondrial protein



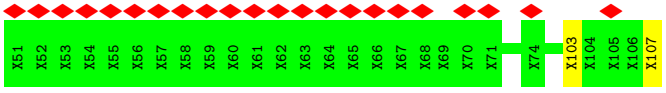




• Molecule 3: Baculoviral IAP repeat-containing protein 6



• Molecule 3: Baculoviral IAP repeat-containing protein 6



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	192025	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	56.379	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.614	Depositor
Minimum map value	-0.931	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.049	Depositor
Recommended contour level	0.284	Depositor
Map size (Å)	422.224, 422.224, 422.224	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1995, 1.1995, 1.1995	Depositor

5 Model quality

5.1 Standard geometry

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	0.28	0/21907	0.49	0/29741
1	B	0.28	0/21907	0.49	0/29741
2	E	0.26	0/1389	0.48	0/1876
2	F	0.25	0/1389	0.47	0/1876
All	All	0.28	0/46592	0.49	0/63234

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	21428	21905	21819	329	0
1	B	21428	21903	21819	349	0
2	E	1374	1347	1347	24	0
2	F	1374	1347	1347	15	0
3	C	285	227	59	1	0
3	D	285	227	59	1	0
All	All	46174	46956	46450	677	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 677 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:280:ARG:NH2	1:B:328:CYS:O	2.03	0.91
1:B:1946:PRO:O	1:B:1952:ASN:ND2	2.09	0.85
1:A:3172:SER:OG	1:A:3209:ASP:OD2	1.92	0.84
1:B:3172:SER:OG	1:B:3209:ASP:OD2	1.93	0.84
1:A:164:GLU:OE1	1:A:258:ARG:NH2	2.12	0.82

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	2670/4888 (55%)	2620 (98%)	50 (2%)	0	100	100
1	B	2670/4888 (55%)	2624 (98%)	46 (2%)	0	100	100
2	E	171/194 (88%)	167 (98%)	4 (2%)	0	100	100
2	F	171/194 (88%)	167 (98%)	4 (2%)	0	100	100
All	All	5682/10164 (56%)	5578 (98%)	104 (2%)	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	2442/4242 (58%)	2387 (98%)	55 (2%)	45	72
1	B	2442/4242 (58%)	2391 (98%)	51 (2%)	48	74

Continued on next page...

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	E	148/167 (89%)	140 (95%)	8 (5%)	18 47
2	F	148/167 (89%)	142 (96%)	6 (4%)	26 57
All	All	5180/8818 (59%)	5060 (98%)	120 (2%)	46 72

5 of 120 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	180	LYS
2	F	147	ARG
1	B	1435	ASN
2	F	133	GLN
2	E	146	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	244	GLN
1	B	1067	HIS
1	B	3283	HIS
1	B	351	HIS
1	B	1845	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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.

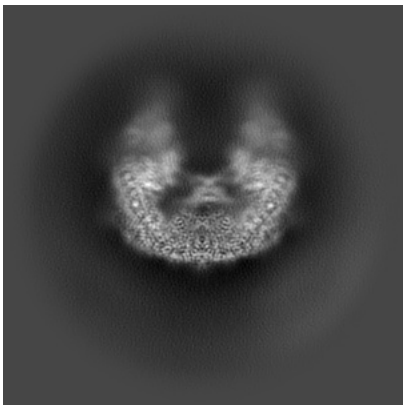
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-27837. These allow visual inspection of the internal detail of the map and identification of artifacts.

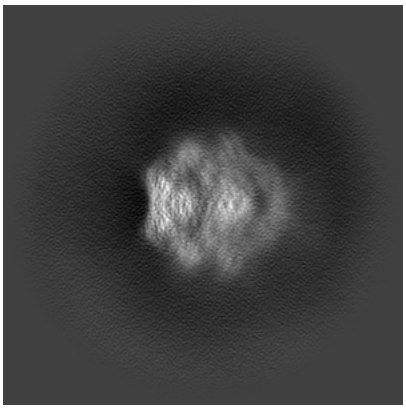
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

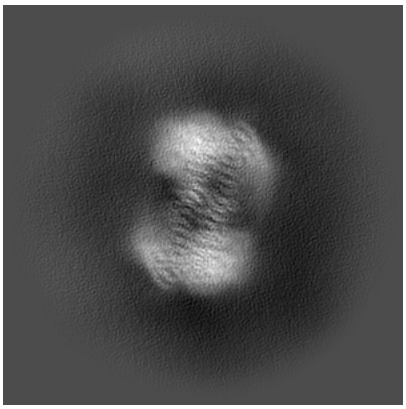
6.1.1 Primary map



X

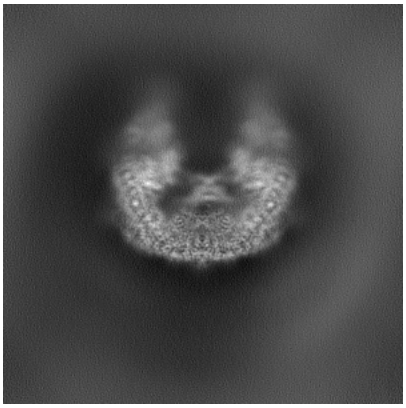


Y

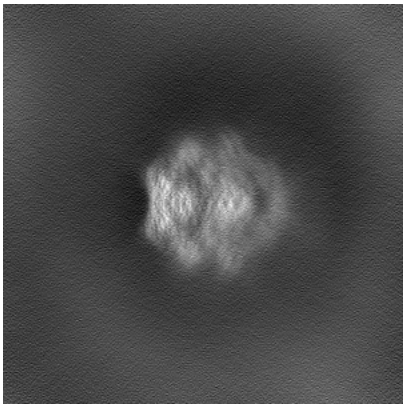


Z

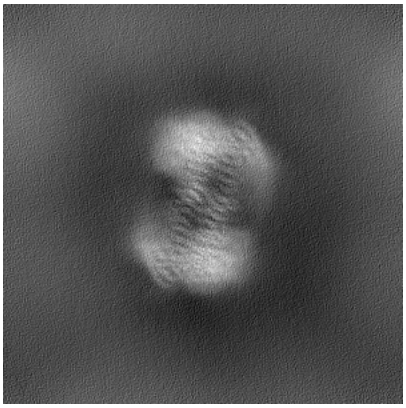
6.1.2 Raw map



X



Y

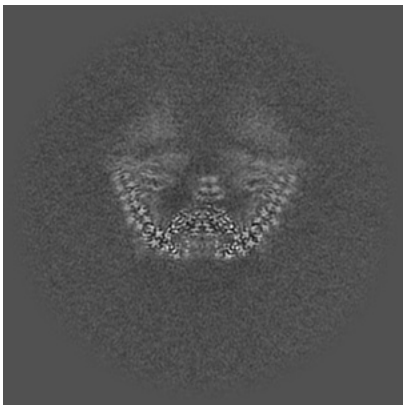


Z

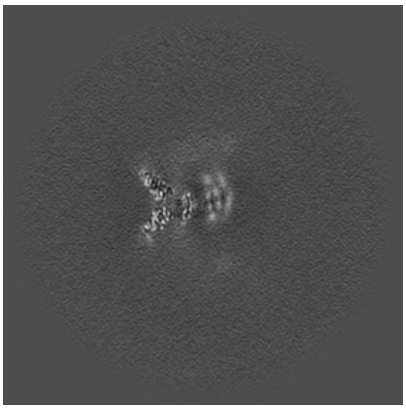
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

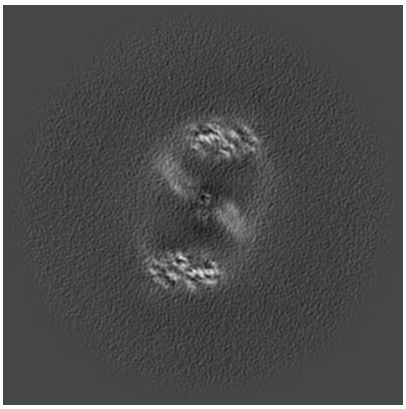
6.2.1 Primary map



X Index: 176

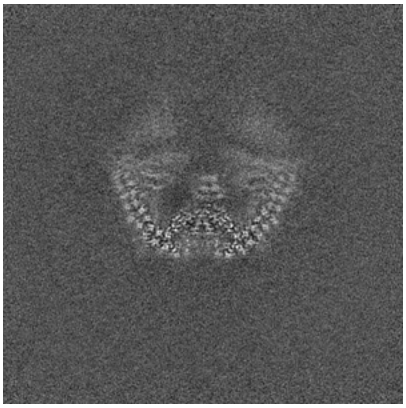


Y Index: 176

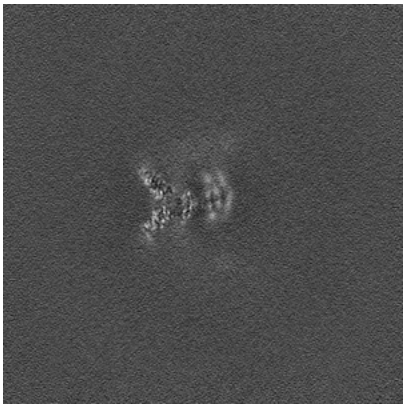


Z Index: 176

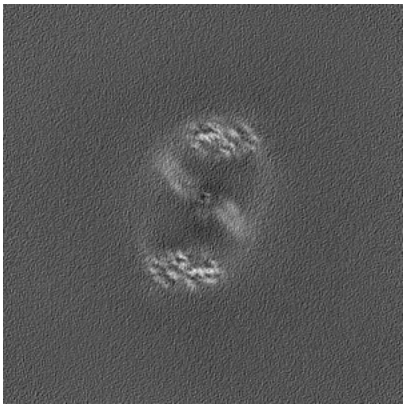
6.2.2 Raw map



X Index: 176



Y Index: 176

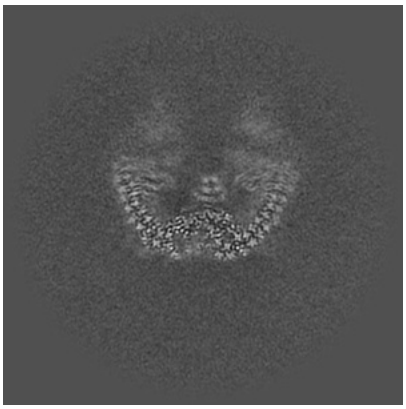


Z Index: 176

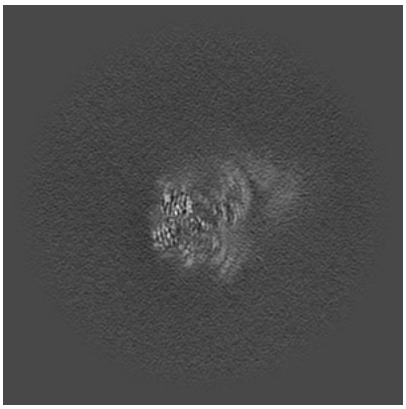
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

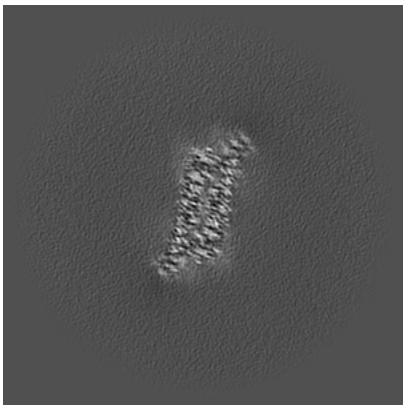
6.3.1 Primary map



X Index: 174

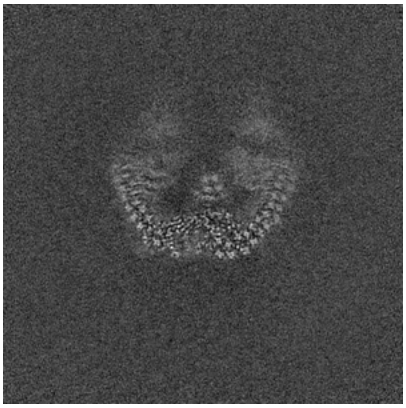


Y Index: 128

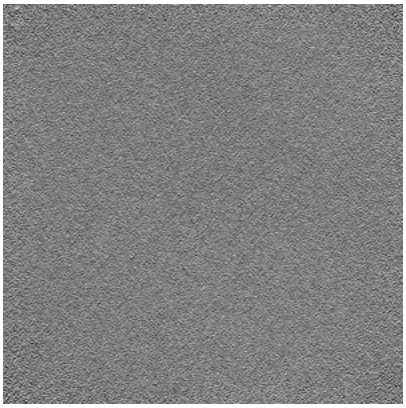


Z Index: 141

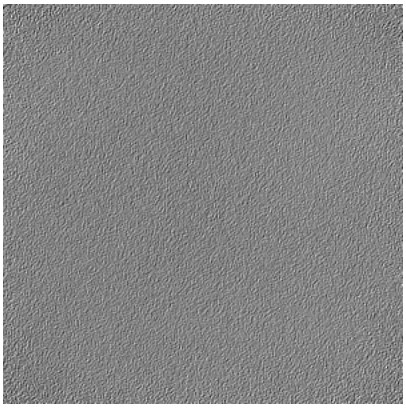
6.3.2 Raw map



X Index: 173



Y Index: 0

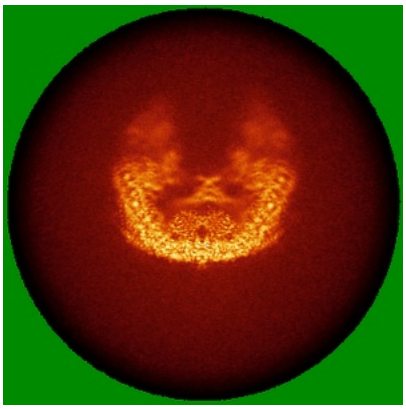


Z Index: 0

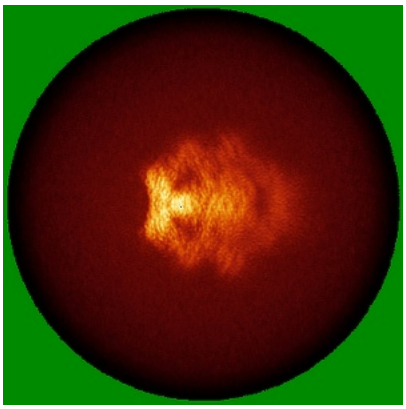
The images above show the largest variance slices of the map in three orthogonal directions.

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

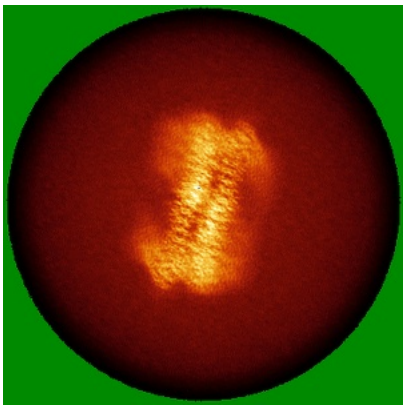
6.4.1 Primary map



X

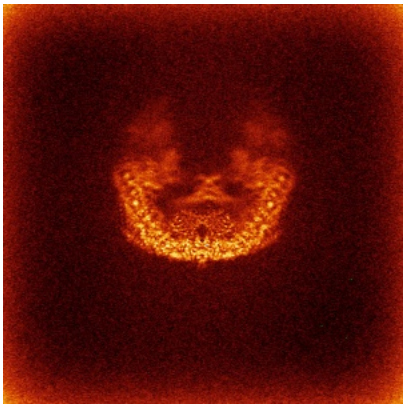


Y

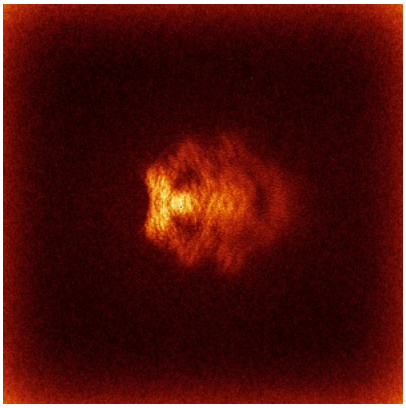


Z

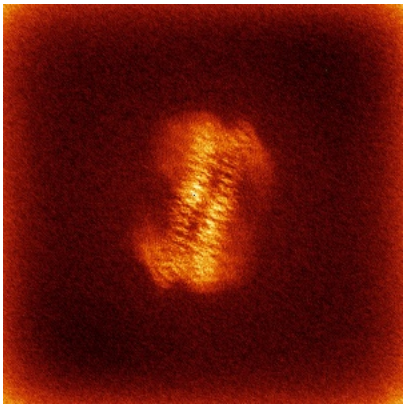
6.4.2 Raw map



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 0.284. 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.

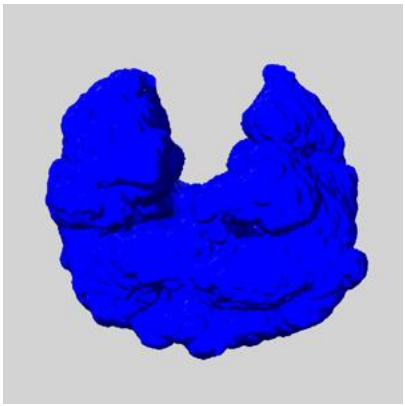
6.6 Mask visualisation

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

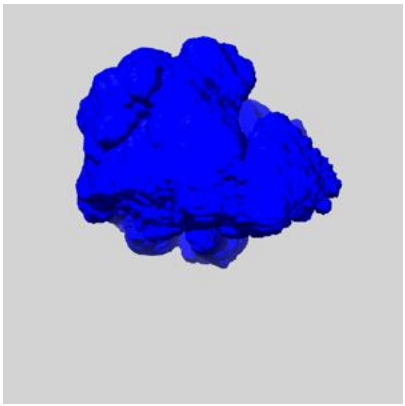
A mask typically either:

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

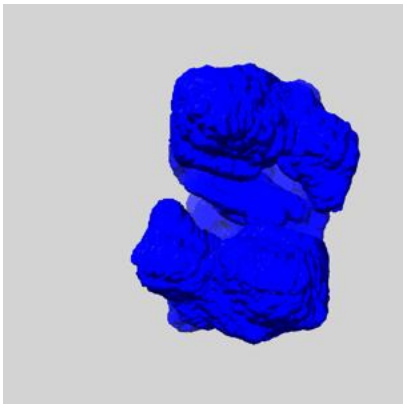
6.6.1 emd_27837_msk_1.map



X



Y

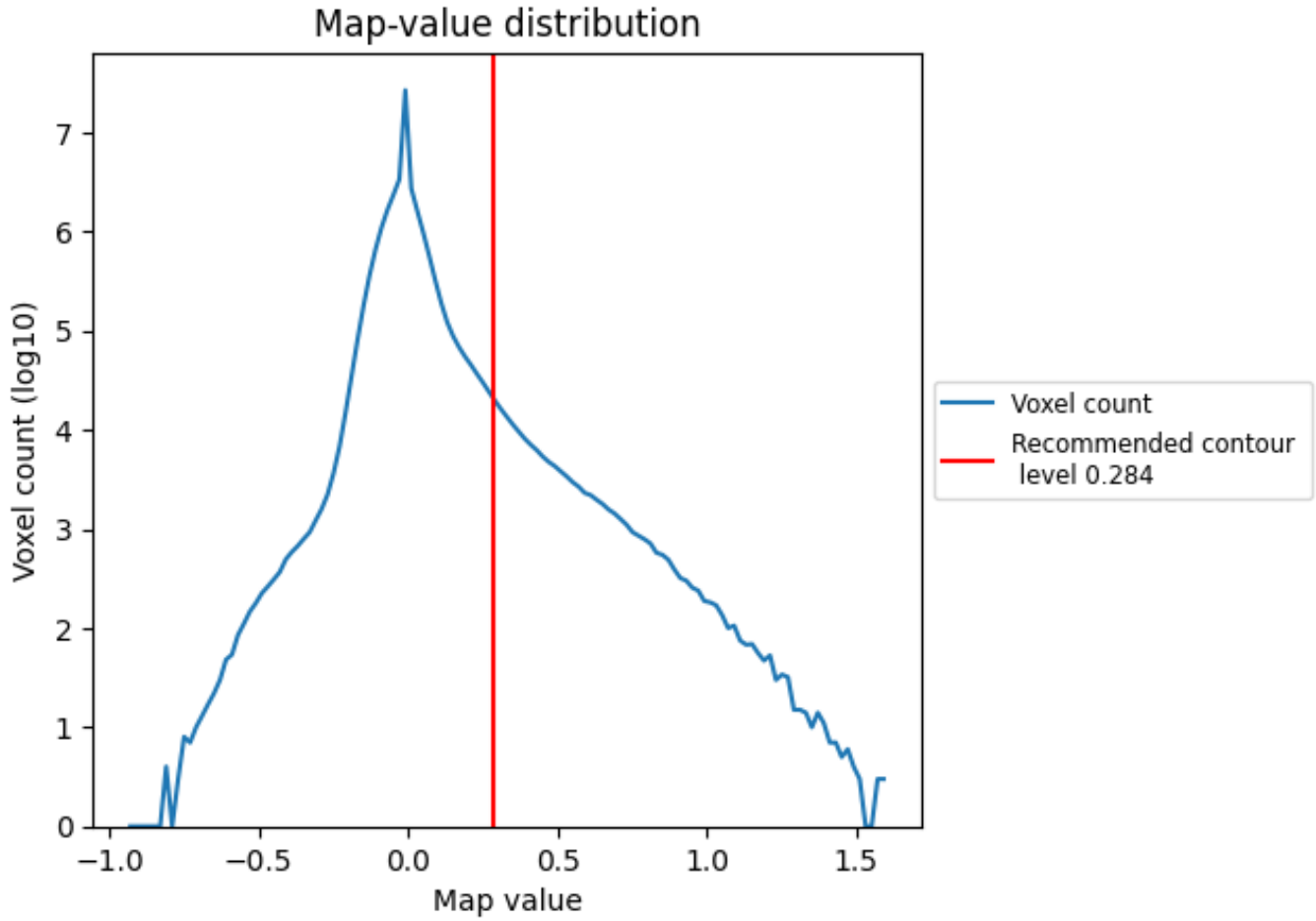


Z

7 Map analysis

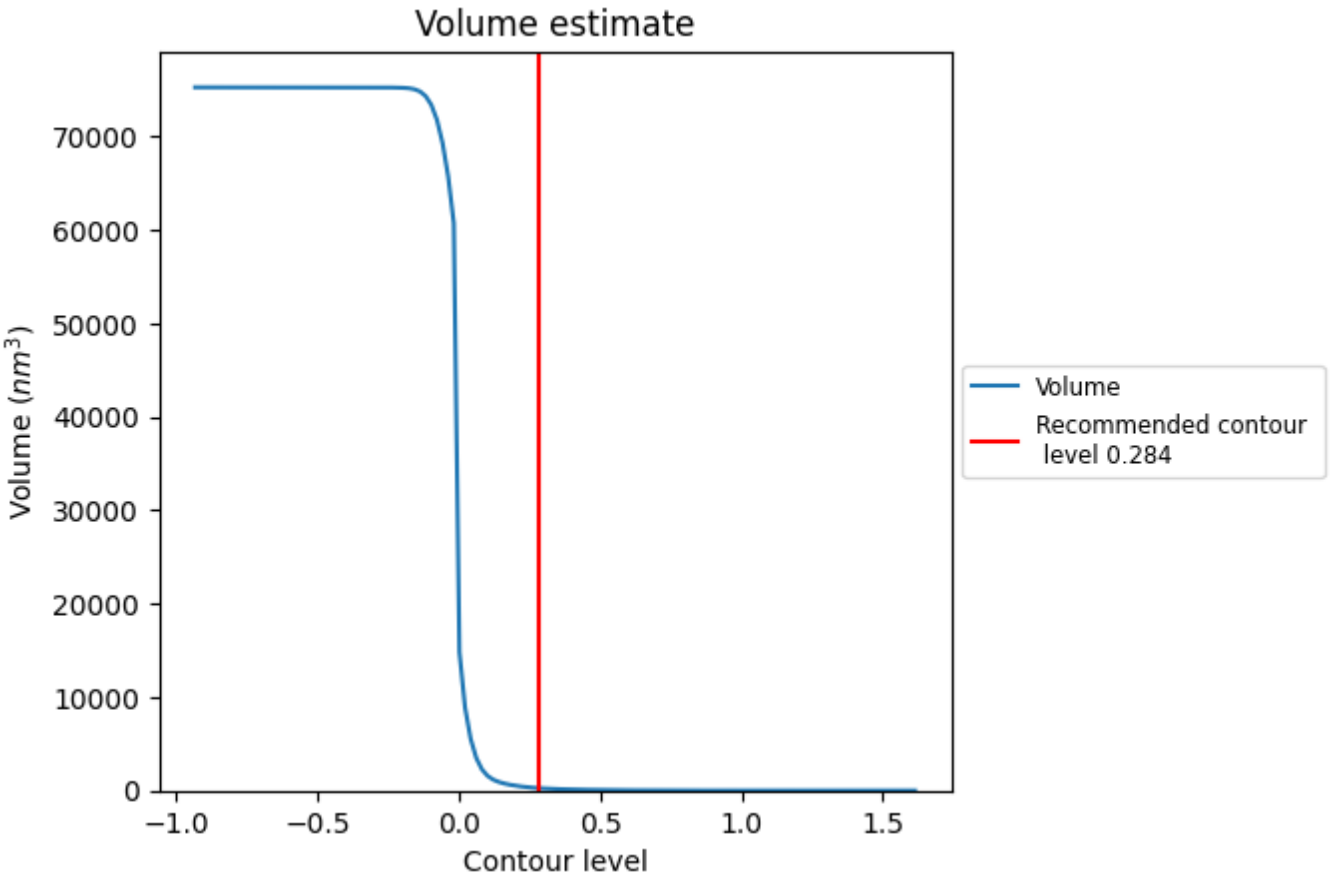
This section contains the results of statistical analysis of the map.

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.

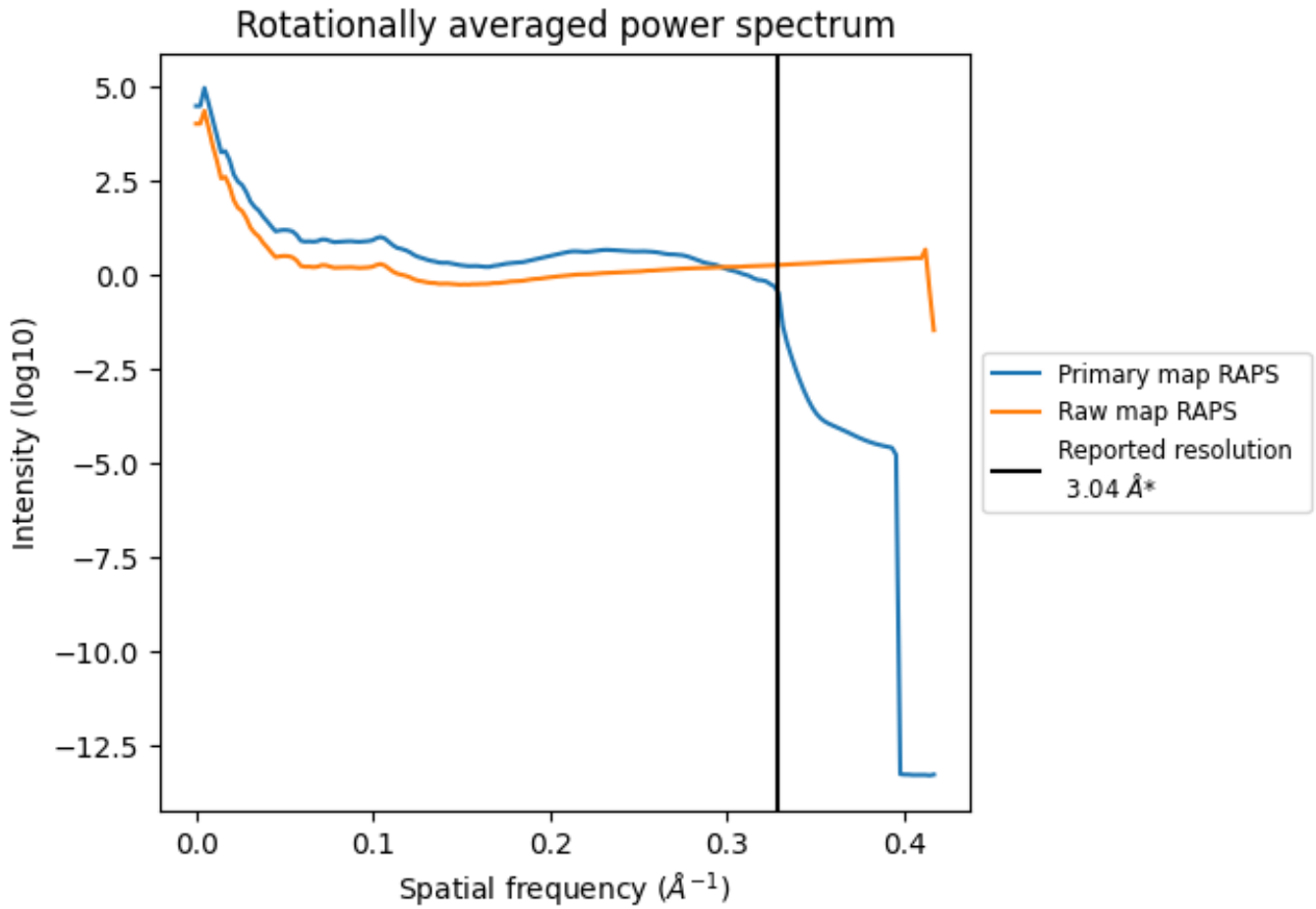
7.2 Volume estimate (i)



The volume at the recommended contour level is 257 nm^3; this corresponds to an approximate mass of 232 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)

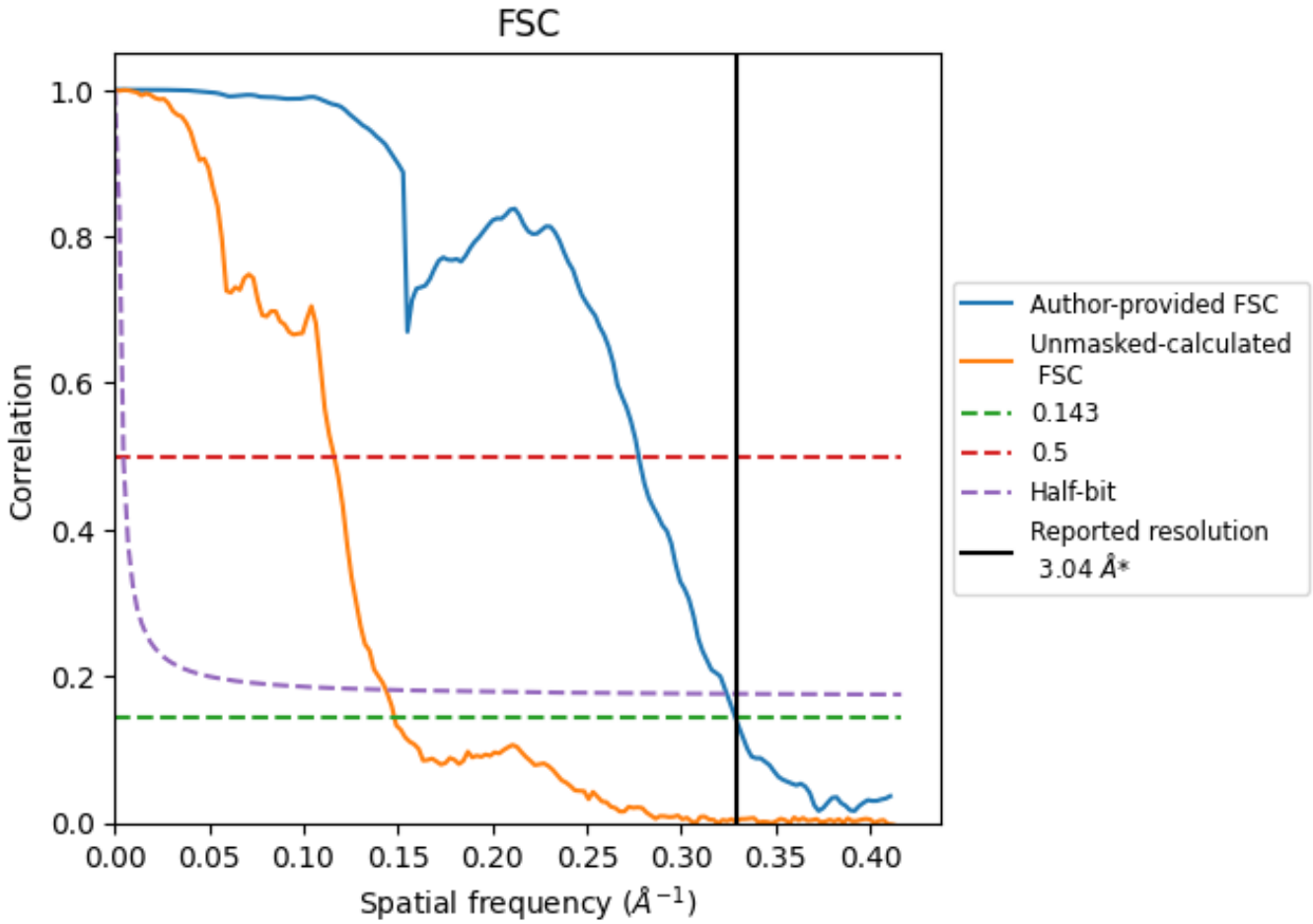


*Reported resolution corresponds to spatial frequency of 0.329 $Å^{-1}$

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 0.329 Å^{-1}

8.2 Resolution estimates (i)

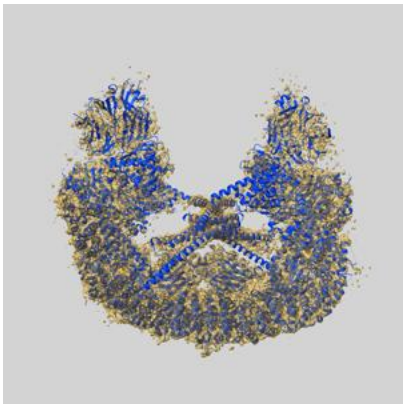
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.04	-	-
Author-provided FSC curve	3.04	3.60	3.08
Unmasked-calculated*	6.74	8.61	6.96

*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 6.74 differs from the reported value 3.04 by more than 10 %

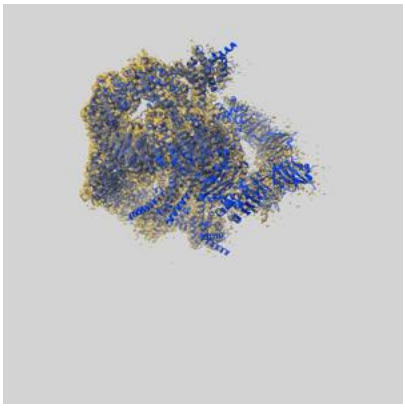
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-27837 and PDB model 8E2I. Per-residue inclusion information can be found in section 3 on page 6.

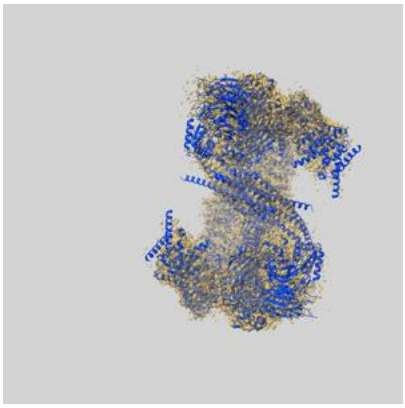
9.1 Map-model overlay



X



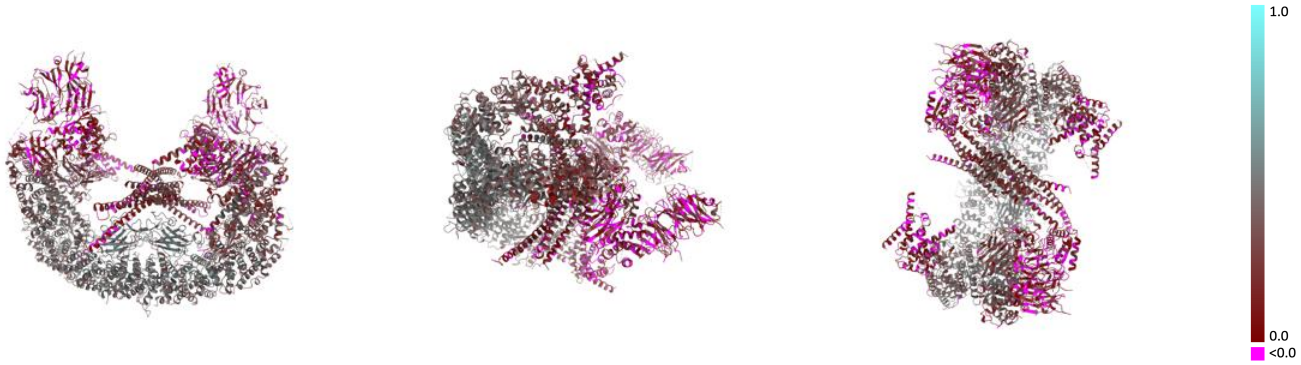
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.284 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.

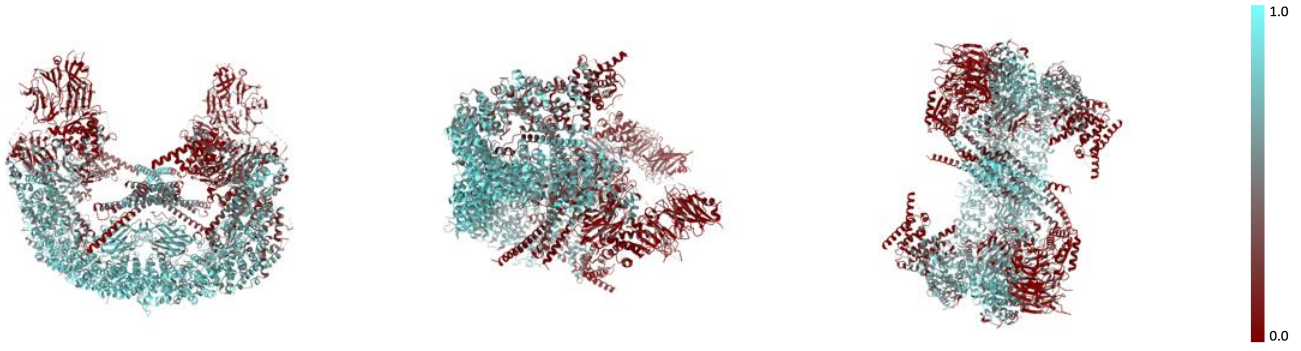
9.2 Q-score mapped to coordinate model



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.

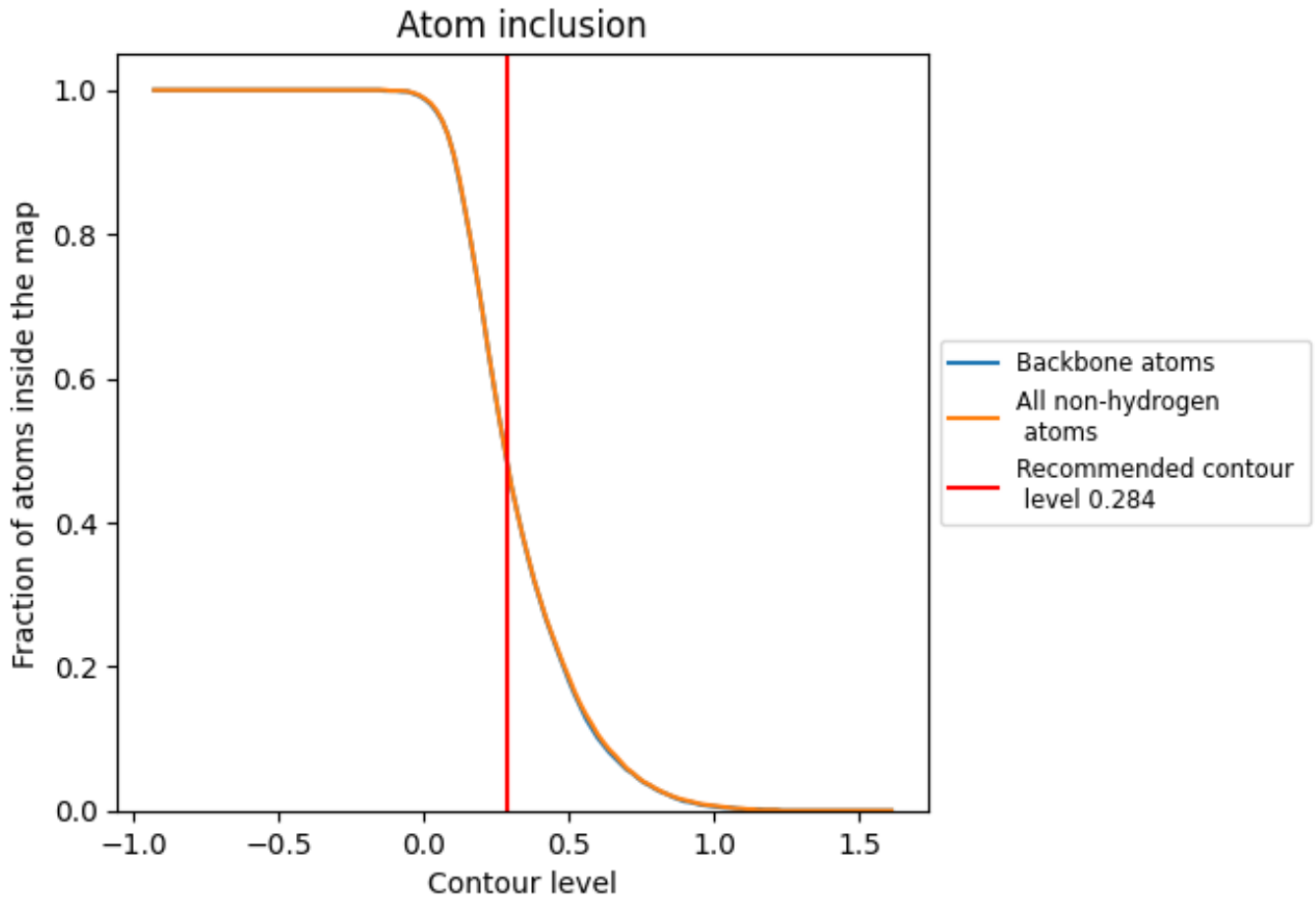
9.3 Atom inclusion mapped to coordinate model



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 (0.284).

9.4 Atom inclusion (i)



At the recommended contour level, 49% of all backbone atoms, 49% 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 (0.284) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4910	0.2900
A	0.5010	0.3040
B	0.5080	0.2940
C	0.5510	0.2120
D	0.5230	0.2010
E	0.4290	0.1880
F	0.3970	0.1590