wwPDB EM Validation Summary Report (i)

Feb 3, 2024 – 06:29 am GMT

PDB ID	:	8C06
EMDB ID	:	EMD-16355
Title	:	Structure of Dimeric HECT E3 Ubiquitin Ligase UBR5
Authors	:	Hehl, L.A.; Prabu, J.R.; Schulman, B.A.
Deposited on	:	2022-12-16
Resolution	:	2.70 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:

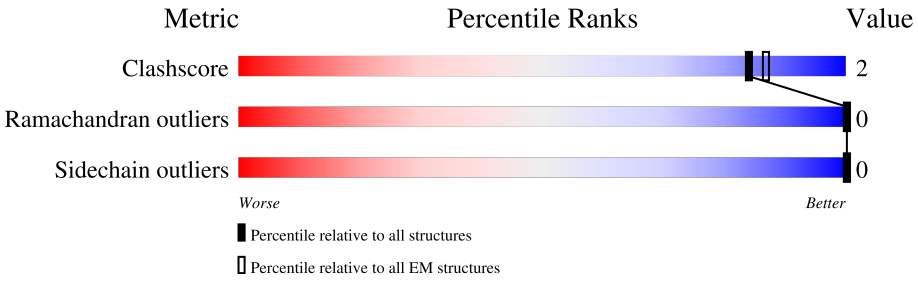
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.70 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	2806	10% 31% 67%
1	B	2806	7% 23% 75%
1	D	2806	11% 31% 67%
1	E	2806	7% 23% 75%
1	F	2806	99%
1	G	2806	99%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 25324 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 UBR5.

Mol	Chain	Residues	Atoms	AltConf	Trace
1	A	925	Total C N O S 7080 4480 1226 1317 57	0	0
1	B	694	Total C N O S 5353 3407 941 974 31	0	0
1	D	925	Total C N O S 7080 4480 1226 1317 57	0	0
1	E	694	Total C N O S 5353 3407 941 974 31	0	0
1	F	30	Total C N O S 226 135 46 44 1	0	0
1	G	30	Total C N O S 226 135 46 44 1	0	0

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP O95071
A	-5	SER	-	expression tag	UNP O95071
A	-4	GLY	-	expression tag	UNP O95071
A	-3	SER	-	expression tag	UNP O95071
A	-2	GLY	-	expression tag	UNP O95071
A	-1	ALA	-	expression tag	UNP O95071
A	0	PRO	-	expression tag	UNP O95071
A	503	ARG	LYS	engineered mutation	UNP O95071
A	710	ASP	LEU	engineered mutation	UNP O95071
B	-6	GLY	-	expression tag	UNP O95071
B	-5	SER	-	expression tag	UNP O95071
B	-4	GLY	-	expression tag	UNP O95071
B	-3	SER	-	expression tag	UNP O95071
B	-2	GLY	-	expression tag	UNP O95071
B	-1	ALA	-	expression tag	UNP O95071
B	0	PRO	-	expression tag	UNP O95071
B	503	ARG	LYS	engineered mutation	UNP O95071
B	710	ASP	LEU	engineered mutation	UNP O95071

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	GLY	-	expression tag	UNP O95071
D	-5	SER	-	expression tag	UNP O95071
D	-4	GLY	-	expression tag	UNP O95071
D	-3	SER	-	expression tag	UNP O95071
D	-2	GLY	-	expression tag	UNP O95071
D	-1	ALA	-	expression tag	UNP O95071
D	0	PRO	-	expression tag	UNP O95071
D	503	ARG	LYS	engineered mutation	UNP O95071
D	710	ASP	LEU	engineered mutation	UNP O95071
E	-6	GLY	-	expression tag	UNP O95071
E	-5	SER	-	expression tag	UNP O95071
E	-4	GLY	-	expression tag	UNP O95071
E	-3	SER	-	expression tag	UNP O95071
E	-2	GLY	-	expression tag	UNP O95071
E	-1	ALA	-	expression tag	UNP O95071
E	0	PRO	-	expression tag	UNP O95071
E	503	ARG	LYS	engineered mutation	UNP O95071
E	710	ASP	LEU	engineered mutation	UNP O95071
F	-6	GLY	-	expression tag	UNP O95071
F	-5	SER	-	expression tag	UNP O95071
F	-4	GLY	-	expression tag	UNP O95071
F	-3	SER	-	expression tag	UNP O95071
F	-2	GLY	-	expression tag	UNP O95071
F	-1	ALA	-	expression tag	UNP O95071
F	0	PRO	-	expression tag	UNP O95071
F	503	ARG	LYS	engineered mutation	UNP O95071
F	710	ASP	LEU	engineered mutation	UNP O95071
G	-6	GLY	-	expression tag	UNP O95071
G	-5	SER	-	expression tag	UNP O95071
G	-4	GLY	-	expression tag	UNP O95071
G	-3	SER	-	expression tag	UNP O95071
G	-2	GLY	-	expression tag	UNP O95071
G	-1	ALA	-	expression tag	UNP O95071
G	0	PRO	-	expression tag	UNP O95071
G	503	ARG	LYS	engineered mutation	UNP O95071
G	710	ASP	LEU	engineered mutation	UNP O95071

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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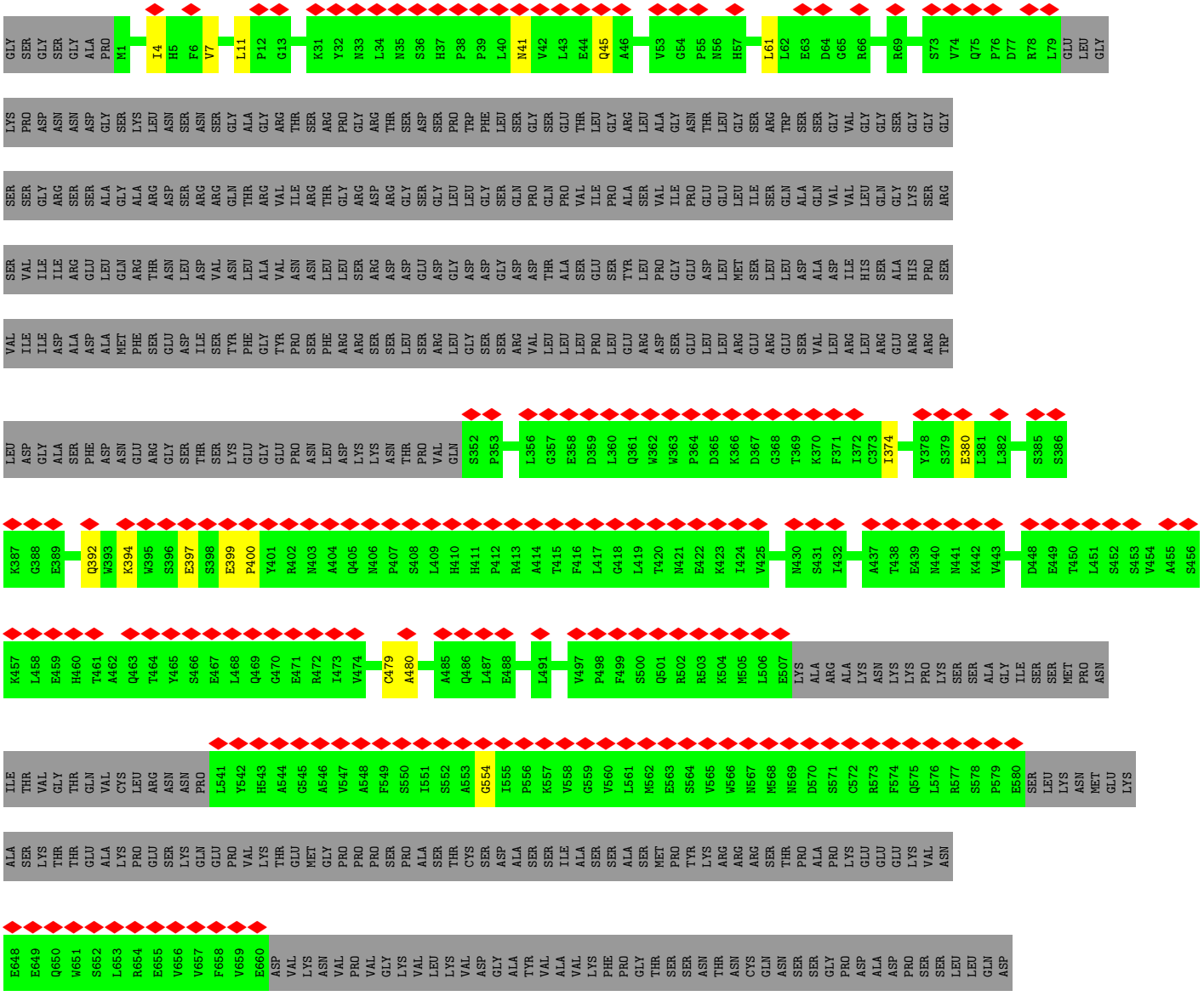
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
2	D	3	3	3	0

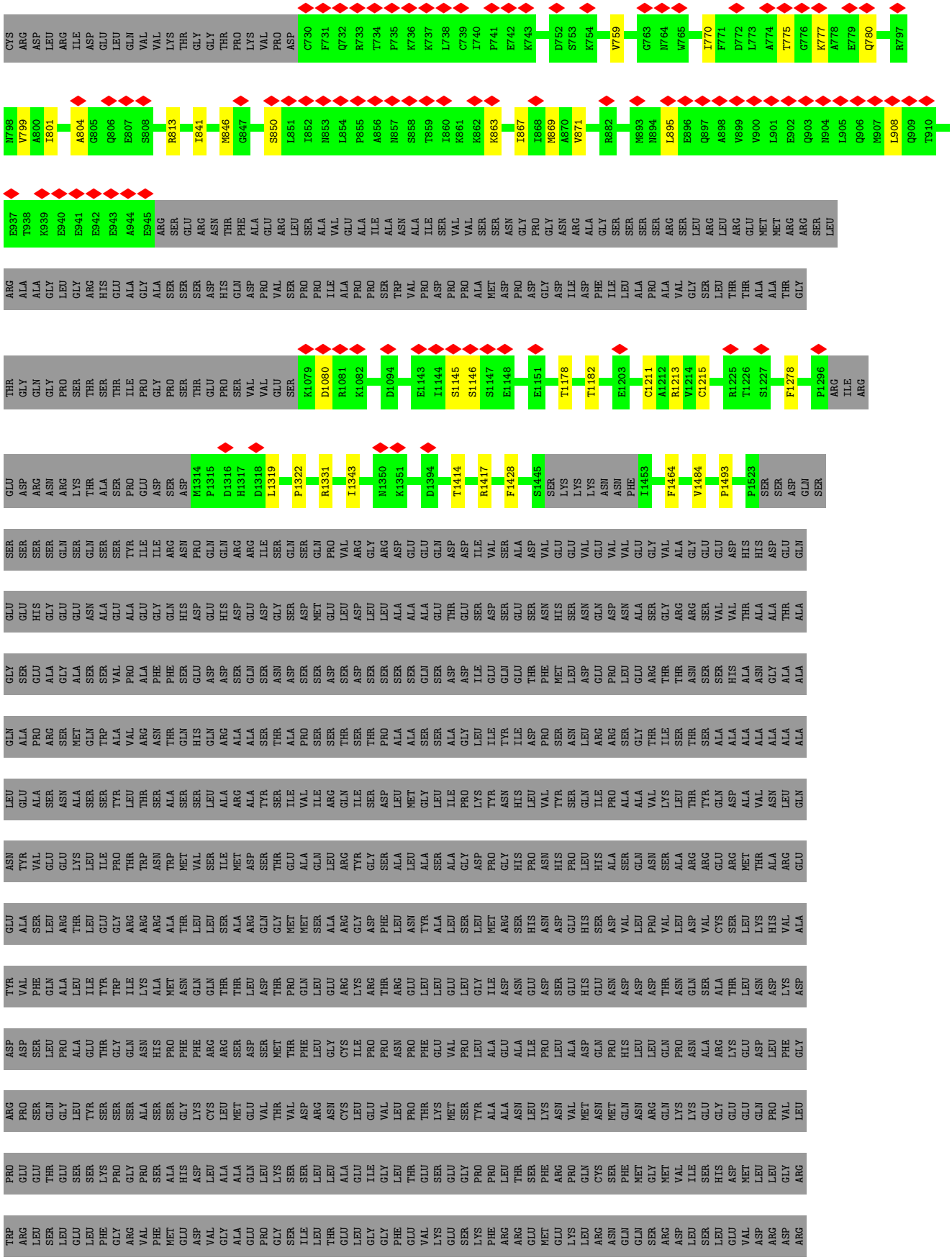
3 Residue-property plots (i)

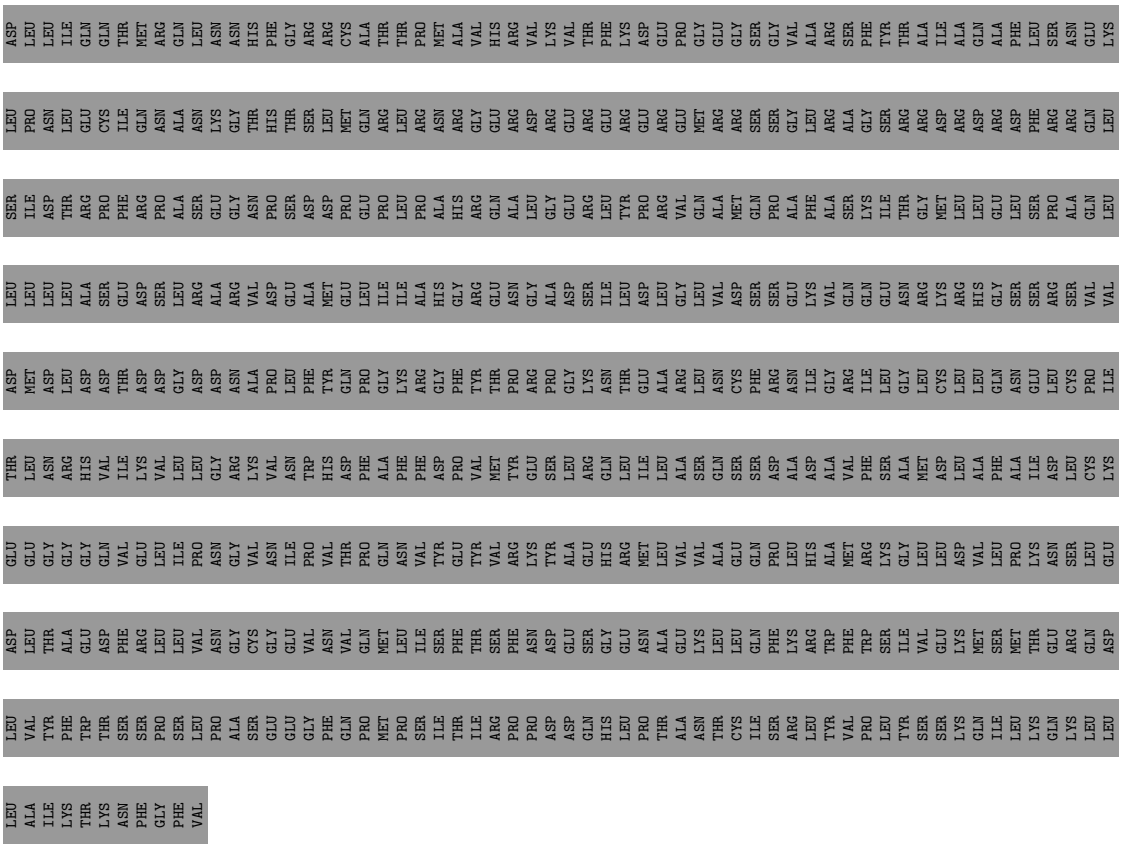
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 UBR5

Chain A:

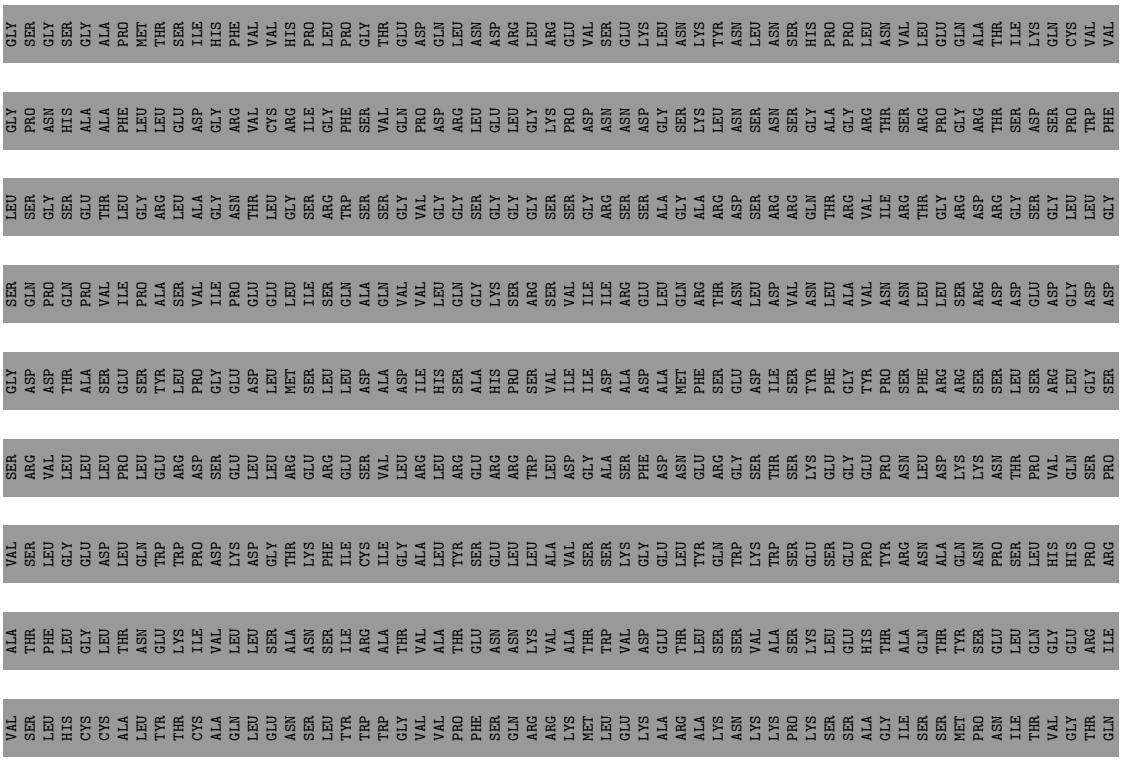



CYS ARG ASP LEU ARG ILE ASP GLU LEU GLN VAL VAL LYS THR GLY GLY THR PRO LYS VAL PRO ASP C730 F731 Q732 R733 T734 P735 K736 K737 L738 C739 I740 P741 E742 K743 D752 S763 K754 V759 G763 N764 W765 I770 F771 D772 L773 A774 T775 G776 K777 A778 E779 Q780 R797
N798 V799 A800 I801 A804 G805 Q806 E807 S808 R813 I841 M846 G847 S850 L851 I852 N853 L854 P855 A856 N857 S858 T859 I860 K861 K862 K863 I867 I868 M869 A870 V871 R882 M893 N894 L895 E896 Q897 A898 V899 V900 L901 E902 Q903 N904 L905 Q906 M907 L908 Q909 T910
E937 T938 K939 E940 E941 E942 E943 A944 E945 ARG SER GLU ARG ASN THR PHE ALA GLU ARG LEU SER ALA VAL GLU ALA ILE ALA ASN ALA ILE SER VAL VAL SER SER ASN GLY PRO GLY ASN ARG ALA GLY SER SER SER ARG SER LEU ARG LEU ARG GLU MET MET ARG ARG SER LEU
ARG ALA ALA GLY LEU GLY ARG HIS GLU ALA GLY ALA SER SER SER ASP HIS GLN ASP PRO VAL SER PRO PRO PRO ILE ALA PRO PRO SER TRP VAL PRO ASP PRO PRO ALA MET ASP PRO ASP PRO GLY ASP ILE ASP PHE ILE LEU ALA PRO ALA VAL GLY SER LEU THR THR ALA ALA THR GLY
THR GLY GLN GLY PRO SER THR SER THR ILE PRO GLY PRO SER THR GLU PRO SER VAL VAL GLU SER K1079 D1080 R1081 K1082 D1094 E1143 I1144 S1145 S1146 S1147 E1148 E1151 T1178 T1182 E1203 C1211 A1212 R1213 V1214 C1215 R1225 T1226 S1227 F1278 P1296 ARG ILE ARG
GLU ASP ARG ASN ARG LYS THR ALA SER PRO GLU ASP SER ASP M1314 P1315 D1316 H1317 D1318 L1319 P1322 R1331 I1343 N1350 K1351 D1394 T1414 R1417 F1428 S1445 SER LYS LYS LYS ASN ASN PHE I1453 F1464 V1484 P1493 P1523 SER SER ASP GLN SER
SER SER SER GLN SER GLN SER SER TYR ILE ILE ARG ASN PRO GLN GLN ARG ARG ILE SER GLN SER GLN PRO VAL ARG GLY ARG ASP GLU GLU GLN ASP ASP ILE VAL SER ALA ASP VAL GLU GLU VAL GLU VAL VAL GLU GLY VAL ALA GLY GLU GLU ASP HIS HIS ASP GLU GLN
GLU GLU HIS GLY GLU GLU ASN ALA GLU GLY GLN HIS ASP GLU HIS ASP GLU ASP GLY SER ASP MET GLU LEU ASP LEU LEU ALA ALA ALA GLU THR GLU SER ASN HIS SER ASN GLN ASP ASN ALA SER GLY ARG ARG SER VAL VAL THR ALA ALA THR ALA
GLY SER GLU ALA GLY ALA SER SER VAL PRO ALA PHE PHE SER GLU ASP ASP SER GLN SER ASN ASP SER SER SER SER ASP SER SER GLN SER ASP ASP ILE GLU GLN GLN GLU THR PHE MET LEU ASP GLU PRO LEU GLU ARG THR THR ASN SER SER HIS ALA ASN GLY ALA ALA
GLN ALA PRO ARG SER MET GLN TRP ALA VAL ARG ASN THR GLN HIS GLN ARG ARG ALA ALA SER THR ALA PRO SER SER THR SER THR PRO ALA ALA SER SER GLN ILE ILE TYR ILE ASP PRO SER ASN LEU LEU ARG ARG SER GLY THR ILE ILE SER THR SER ALA ALA ALA ALA ALA ALA
LEU GLU ALA SER ASN ALA SER SER TYR LEU THR SER ALA SER SER LEU ALA ARG ALA TYR SER ILE VAL ILE ARG GLN ILE SER ASP LEU MET GLY LEU ILE PRO ALA ALA SER SER GLY LEU ILE PRO LYS TYR ASN HIS LEU VAL TYR SER GLN ILE PRO ALA ALA VAL LYS LEU THR TYR GLN ASP ALA ALA VAL ASN LEU GLN
ASN TYR VAL GLU GLU LYS LEU ILE PRO THR TRP ASN TRP MET VAL SER ILE MET ASP SER THR GLU ALA GLN LEU ARG GLY TYR GLY SER ALA LEU ALA SER ALA ASN ASP PHE LEU ASN TYR ALA SER ALA ASN ASP VAL LEU PRO VAL LEU ASP ARG GLU ARG MET THR ALA ARG GLU
GLU ALA SER LEU ARG THR LEU GLU GLY ARG ARG ALA THR LEU LEU SER ILE MET ALA ARG GLN GLY MET MET SER ALA ARG GLY ASP PHE LEU ASN TYR ALA LEU GLU ARG SER LEU MET ARG SER HIS ASN ASP GLU HIS SER ASP VAL LEU PRO VAL LEU ASP ARG ARG GLU ASP ALA VAL CYS SER LEU LYS HIS VAL ALA
TYR VAL PHE GLN ALA LEU ILE TYR TRP ILE LYS ALA MET ASN GLN GLN THR LEU ASP THR PRO GLN GLU LEU GLU ARG LYS ARG THR ARG GLU LEU LEU GLU LEU GLY ILE ASP ASN GLU ASP SER GLU HIS SER GLU ASN ASP ASP THR ASN GLN SER ALA THR LEU ASN ASP LYS ASP
ASP ASP SER LEU PRO ALA GLU THR GLY GLN ASN HIS PRO PHE PHE ARG ARG SER ASP SER MET THR PHE LEU GLY CYS ILE PRO PRO PRO ASN PRO PHE GLU VAL PRO LEU ALA GLU ALA ILE PRO LEU ALA ASP GLN PRO HIS LEU LEU GLN PRO ASN ALA ARG LYS GLU ASP LEU PHE GLY
ARG PRO SER GLN GLY LEU TYR SER SER SER ALA SER SER GLY LYS CYS LEU MET VAL THR VAL ASP ARG ASN CYS LEU GLU VAL LEU PRO THR LYS MET SER TYR ALA ALA ASN LEU LYS ASN VAL MET ASN MET GLN ASN ARG GLN LYS LYS GLU GLY GLU GLU GLN PRO VAL LEU
PRO GLU GLU THR GLU SER LYS PRO GLY PRO SER ALA HIS ASP LEU ALA ALA GLN LEU LYS SER SER LEU LEU ALA GLU ILE GLY LEU THR GLU SER GLU GLY PRO PRO LEU THR SER PHE ARG PRO GLN CYS SER PHE MET GLY MET GLN ASN ARG GLN LYS GLU ASP LEU PHE GLY
TRP ARG LEU SER LEU GLU PHE GLY VAL ARG PHE MET GLU ASP VAL GLY ALA GLU PRO ARG ARG GLU MET GLU LYS LEU ARG ASN GLN GLN SER ARG ASP LEU SER LEU GLU VAL ASP ARG ASP GLN



• Molecule 1: E3 ubiquitin-protein ligase UBR5

Chain B: 7% 23% 75%



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

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

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

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

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

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

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

GLU ARG LEU SER ALA VAL GLU ALA ILE ALA ASN ALA ILE SER VAL VAL SER SER ASN GLY PRO GLY ASN ARG ALA GLY SER SER SER ARG SER LEU ARG LEU ARG GLU MET MET ARG ARG SER LEU ARG ALA ALA GLY LEU GLY ARG HIS GLU ALA GLY ALA SER SER SER ASP HIS

GLN ASP PRO VAL SER PRO PRO ILE ALA PRO PRO SER TRP VAL PRO ASP PRO PRO ALA MET ASP PRO ASP GLY ASP ILE ASP PHE ILE LEU ALA PRO ALA VAL GLY SER LEU THR THR ALA ALA THR GLY THR GLY GLN GLY PRO SER THR SER THR ILE PRO GLY PRO SER THR GLU PRO

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

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

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

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

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

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

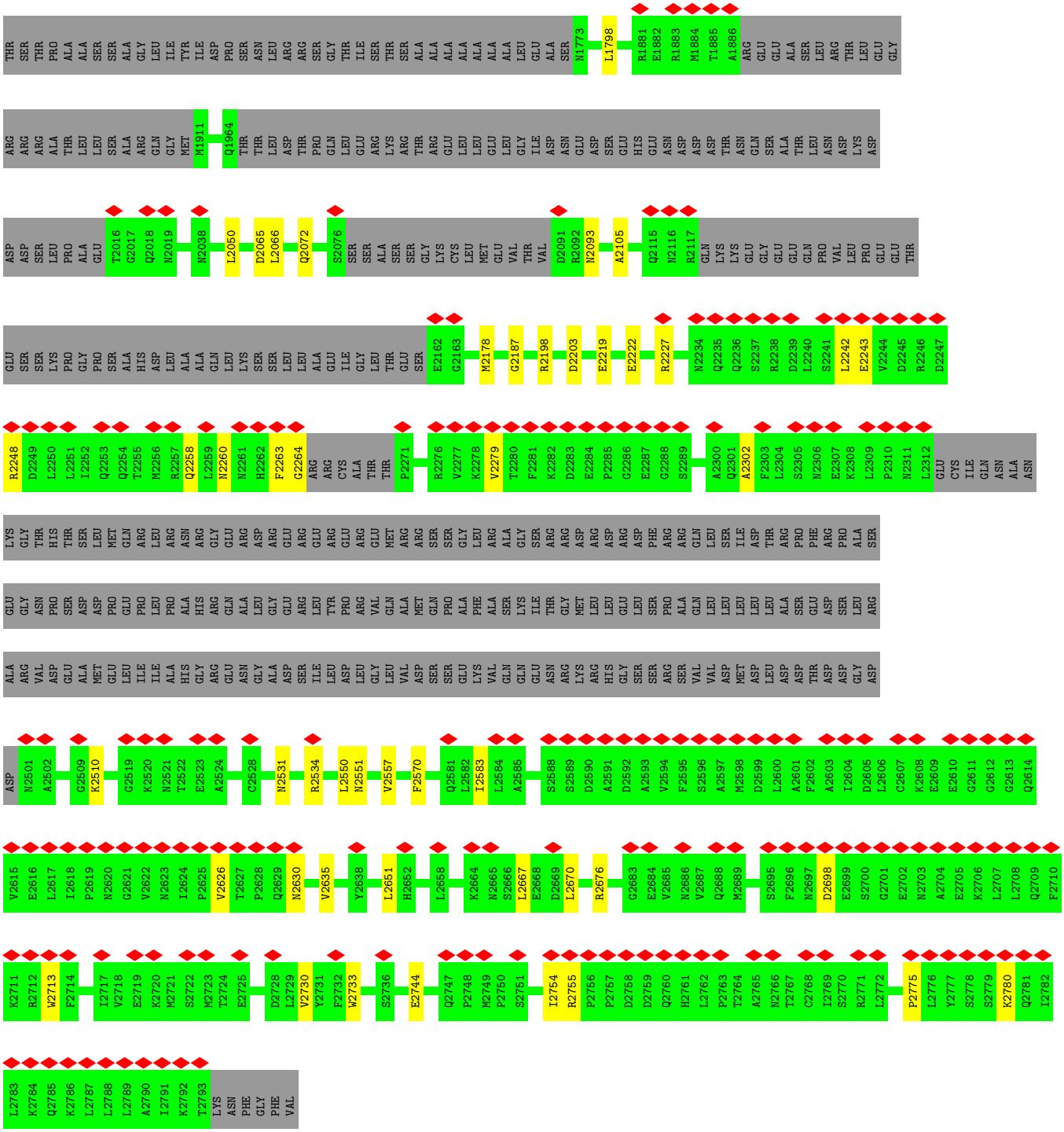
ARG VAL PHE VAL ILE LEU SER VAL GLU MET ALA SER SER LYS LYS LYS ASN ASN PHE ILE PRO GLN PRO ILE GLY LYS CYS LYS ARG VAL PHE GLN ALA LEU LEU PRO TYR ALA VAL GLU GLU LEU CYS ASN VAL ALA GLU SER LEU ILE VAL PRO VAL ARG MET GLY ILE ALA ARG PRO

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

VAL ARG GLY ARG ASP GLU GLU GLN ASP ASP ILE VAL SER ALA ASP VAL GLU GLU VAL GLU VAL VAL GLU GLY VAL ALA GLY GLU GLU ASP HIS HIS ASP GLU GLN GLU GLU HIS GLY GLU GLU ASN ALA GLU ALA GLU GLY GLN HIS ASP GLU HIS ASP GLU ASP GLY SER ASP MET GLU

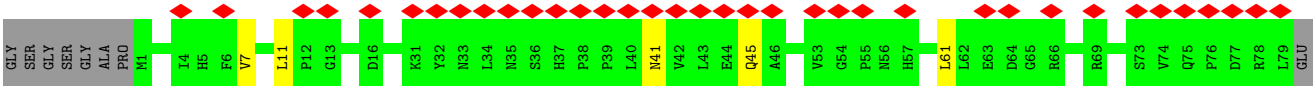
LEU ASP LEU LEU ALA ALA ALA GLU THR GLU SER ASP SER GLU SER ASN HIS SER ASN GLN ASP ASN ALA SER GLY ARG ARG SER VAL VAL THR ALA ALA THR ALA GLY SER GLU ALA GLY ALA SER SER VAL PRO ALA PHE PHE SER GLU ASP ASP SER GLN SER ASN ASP SER SER ASP

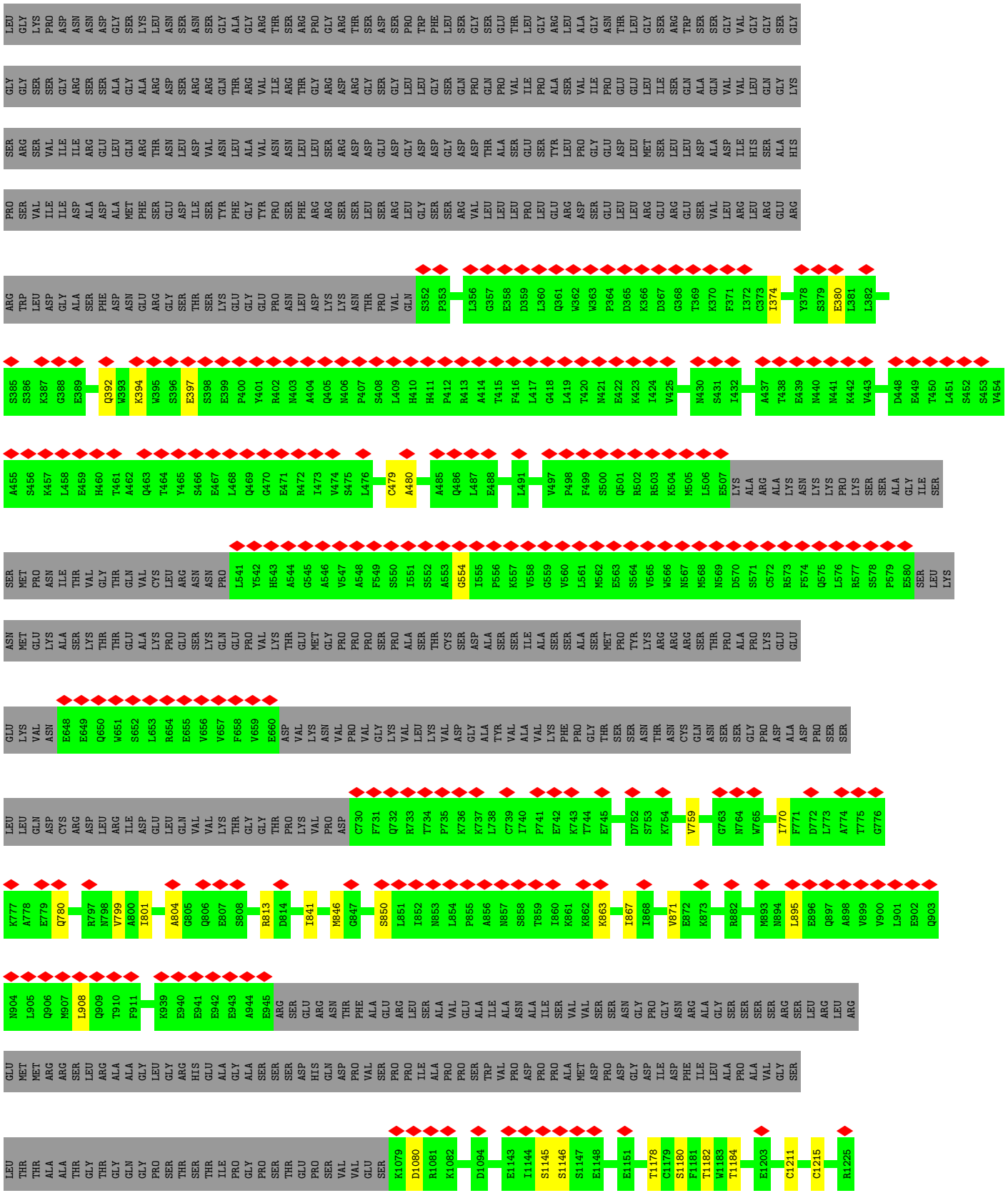
SER ASP SER SER SER SER GLN SER ASP ASP ILE GLU GLN GLN THR PHE MET LEU ASP GLU PRO LEU GLU ARG THR THR ASN SER SER HIS ALA ASN GLY ALA ALA GLN ALA PRO ARG SER MET GLN TRP ALA VAL ARG ASN THR GLN HIS GLN ARG ALA ALA SER THR ALA PRO SER SER



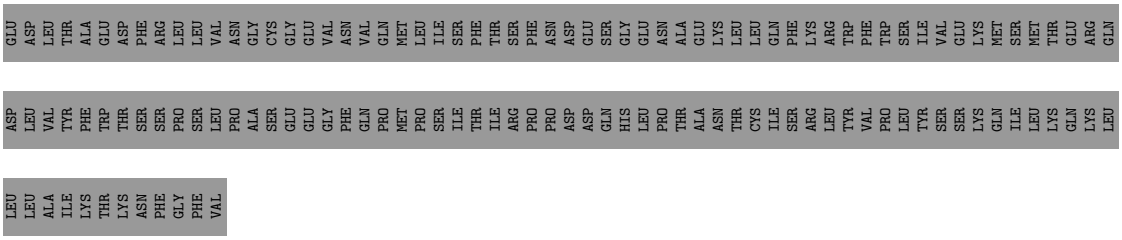
• Molecule 1: E3 ubiquitin-protein ligase UBR5

Chain D:



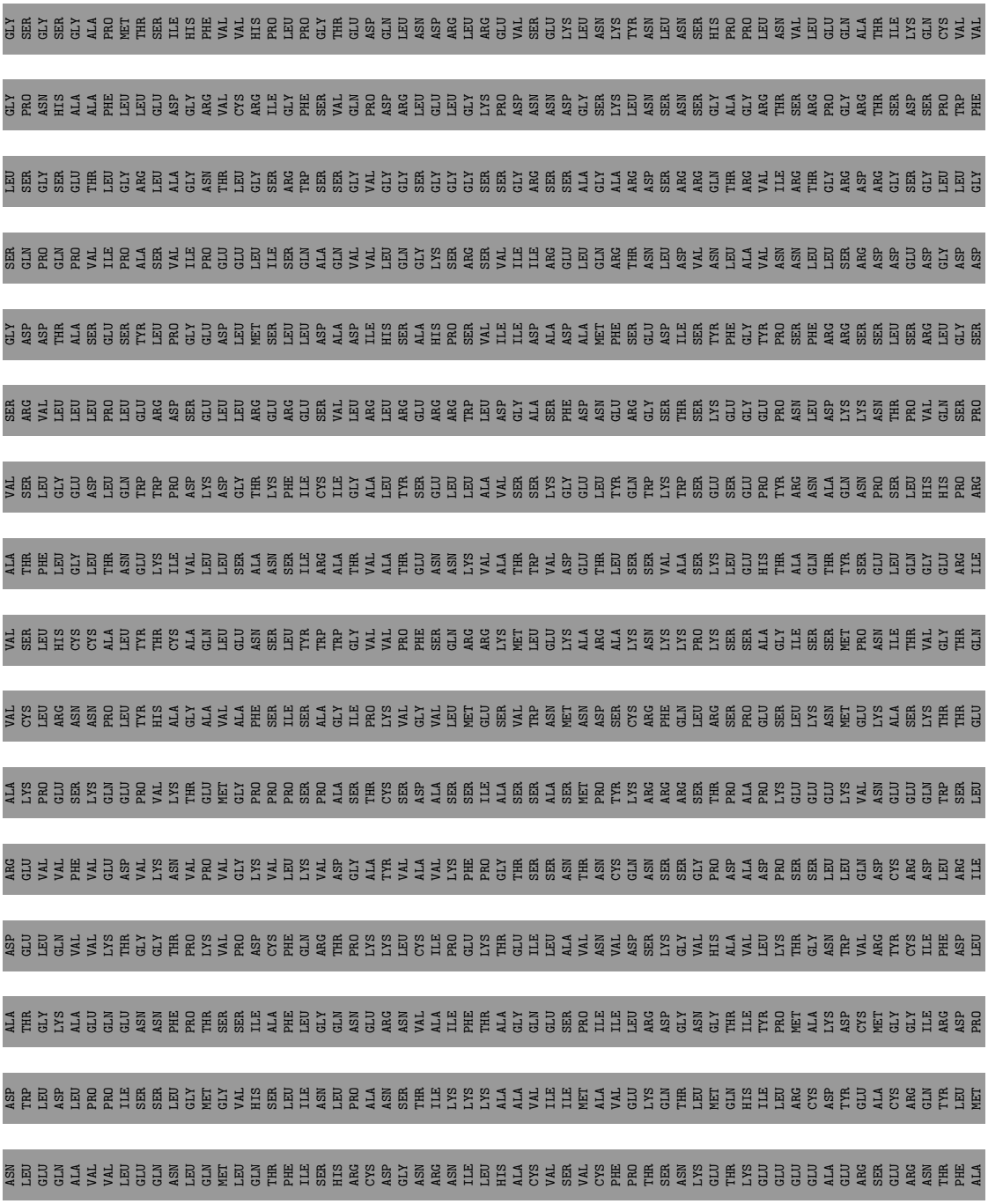

LEU GLY LYS PRO ASP ASN ASN ASP GLY SER LYS LEU ASN SER ASN SER GLY ALA GLY ARG THR SER ARG PRO GLY ARG THR SER ASP SER PRO TRP PHE LEU SER GLY SER GLU THR LEU GLY ARG LEU ALA GLY ASN THR LEU GLY SER ARG TRP SER SER GLY VAL GLY GLY SER
GLY GLY SER SER GLY ARG SER SER ALA GLY ALA ARG ASP SER ARG ARG GLN THR ARG VAL ILE ARG THR GLY ARG ASP ARG GLY SER GLY LEU LEU GLY SER GLN PRO GLN PRO VAL ILE PRO GLU GLU LEU ILE SER GLN ALA GLN VAL VAL LEU GLN GLY LYS
SER ARG SER VAL ILE ILE ARG GLU LEU GLN ARG THR ASN LEU ASP VAL ASN LEU ALA VAL ASN ASN LEU LEU SER ARG ASP ASP GLU ASP GLY ASP ASP ASP GLY ASP ASP THR ALA SER GLU SER TYR LEU PRO GLY GLU ASP LEU MET SER LEU LEU ARG GLU ARG GLU LEU ILE HIS SER ALA HIS
PRO SER VAL ILE ILE ASP ALA ASP ALA MET PHE SER GLU ASP ILE SER TYR PHE GLY TYR PRO SER PHE ARG ARG SER SER LEU SER ARG LEU GLY SER SER ARG VAL LEU LEU LEU PRO LEU GLU ARG ASP SER GLU LEU LEU ARG GLU ARG GLU SER VAL LEU ARG LEU ARG GLU ARG
ARG TRP LEU ASP GLY ALA SER PHE ASP ASN GLU ARG GLY SER THR SER LYS GLU GLY GLU PRO ASN LEU ASP LYS LYS ASN THR PRO VAL GLN S352 P353 L356 G357 E358 D359 L360 Q361 W362 W363 P364 D365 K366 D367 G368 T369 K370 F371 I372 C373 I374 Y378 S379 E380 L381 L382
S385 S386 K387 G388 E389 Q392 W393 K394 W395 S396 E397 S398 E399 P400 Y401 R402 N403 A404 Q405 N406 P407 S408 L409 H410 H411 P412 R413 A414 T415 F416 L417 G418 L419 T420 N421 E422 K423 I424 V425 N430 S431 I432 A437 T438 E439 N440 N441 K442 V443 D448 E449 T450 L451 S452 S453 V454
A455 S456 K457 L458 E459 H460 T461 A462 Q463 T464 Y465 S466 E467 L468 Q469 G470 E471 R472 I473 V474 S475 L476 C479 A480 A485 Q486 L487 E488 L491 V497 P498 F499 S500 Q501 R502 R503 K504 M505 L506 E507 LYS ALA ARG ALA LYS ASN LYS LYS PRO LYS SER SER ALA GLY ILE SER
SER MET PRO ASN ILE THR VAL GLY THR GLN VAL CYS LEU ARG ASN ASN PRO L541 Y542 H543 A544 G545 A546 V547 A548 F549 S550 I551 S552 A553 Q554 I555 P556 K557 V558 G559 V560 L561 M562 E563 S564 V565 W566 N567 M568 N569 D570 S571 C572 R573 F574 Q575 L576 R577 S578 P579 E580 SER LEU LYS
ASN MET GLU LYS ALA SER LYS THR THR GLU ALA LYS PRO GLU SER LYS GLN GLU PRO VAL LYS THR GLU MET GLY PRO PRO PRO SER PRO ALA SER THR CYS SER ASP ALA SER SER ILE ALA SER SER ALA SER MET PRO TYR LYS ARG ARG SER THR PRO ALA PRO LYS GLU GLU
GLU LYS VAL ASN E648 E649 Q650 W651 S652 L653 R654 E655 V656 V657 F658 V659 E660 ASP VAL LYS ASN VAL PRO VAL GLY LYS VAL LEU LYS VAL ASP GLY ALA TYR VAL ALA VAL LYS PHE PRO GLY THR SER SER ASN THR ASN CYS GLN ASN SER SER GLY PRO ASP ALA ASP PRO SER SER
LEU LEU GLN ASP CYS ARG ASP LEU ARG ILE ASP GLU LEU GLN VAL VAL LYS THR GLY GLY THR PRO LYS VAL PRO ASP C730 F731 Q732 R733 T734 P735 K736 K737 L738 C739 I740 P741 E742 K743 T744 E745 D752 S753 K754 V759 G763 N764 W765 I770 F771 D772 L773 A774 T775 G776
K777 A778 E779 Q780 R797 N798 V799 A800 I801 A804 G805 Q806 E807 S808 R813 D814 I841 M846 G847 S850 L851 I852 N853 L854 P855 A856 N857 S858 T859 I860 K861 K862 K863 I867 I868 V871 E872 K873 R882 M893 N894 L895 E896 Q897 A898 V899 V900 L901 E902 Q903
N904 L905 Q906 M907 L908 Q909 T910 F911 K939 E940 E941 E942 E943 A944 E945 ARG SER GLU ARG ASN THR PHE ALA GLU ARG LEU SER ALA VAL GLU ALA ILE ALA ASN ALA ILE SER VAL VAL SER SER ASN GLY PRO GLY ASN ARG ALA ALA GLY SER SER SER ARG SER LEU ARG LEU ARG
GLU MET MET ARG SER LEU ARG ALA ALA GLY LEU GLY ARG GLY HIS GLU ALA GLY ALA SER SER ASP HIS GLN ASP PRO VAL SER PRO PRO ILE ALA PRO PRO SER TRP VAL PRO ASP PRO PRO ALA MET ASP PRO ASP GLY ASP ILE ASP PHE ILE LEU ALA PRO PRO ALA VAL GLY SER
LEU THR THR ALA ALA THR GLY THR THR GLY GLN GLY PRO SER THR SER THR ILE PRO GLY PRO SER THR GLU PRO SER VAL VAL GLU SER K1079 D1080 R1081 K1082 D1094 E1143 I1144 S1145 S1146 S1147 E1148 E1151 T1178 C1179 S1180 F1181 T1182 W1183 T1184 E1203 C1211 C1215 R1225

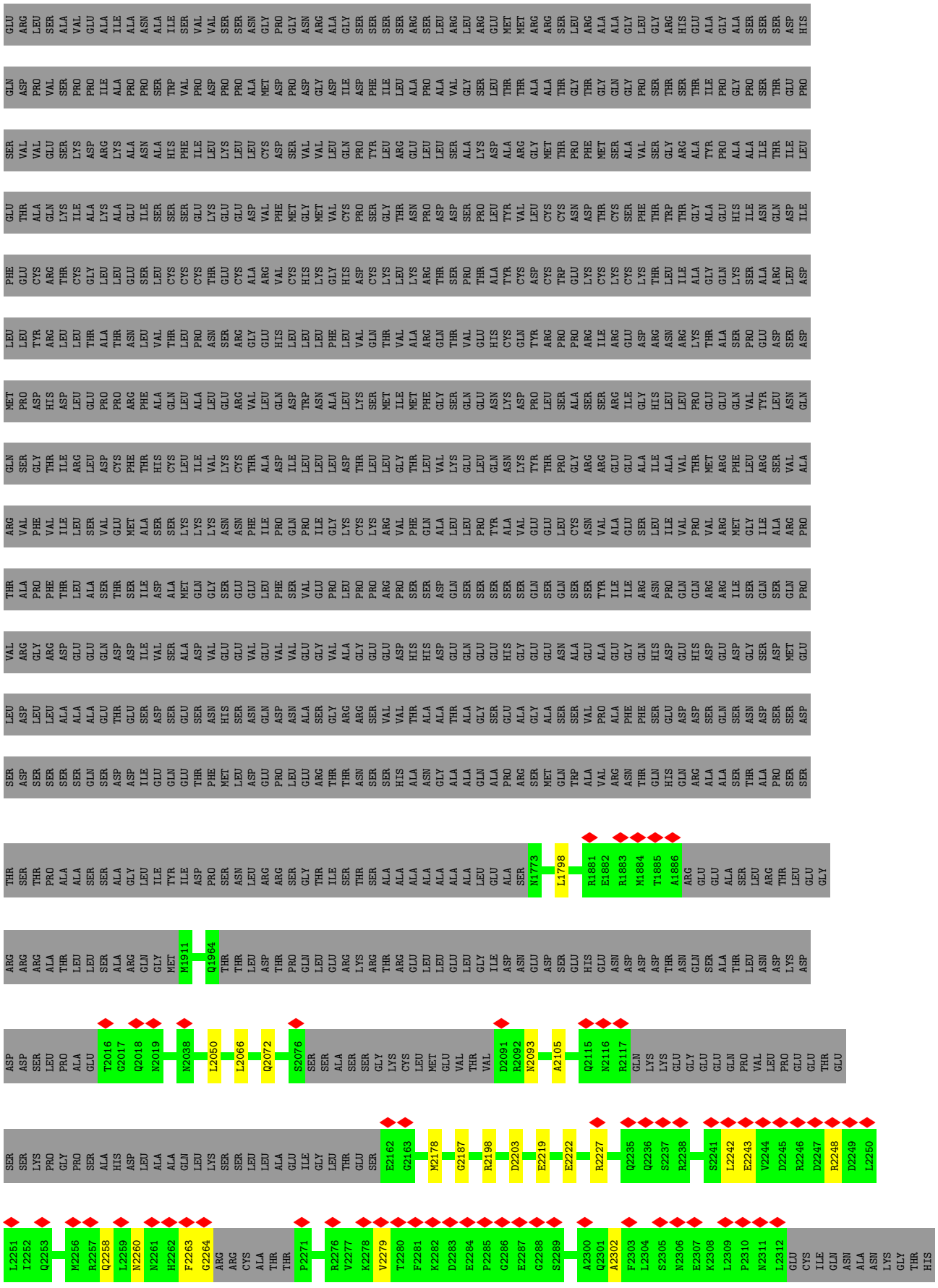
T1226
S1227
P1296
M1314
P1315
D1316
H1317
D1318
L1319
P1322
I1343
N1350
K1351
D1394
F1428
S1445
I1453
F1464
V1484
P1493
P1523

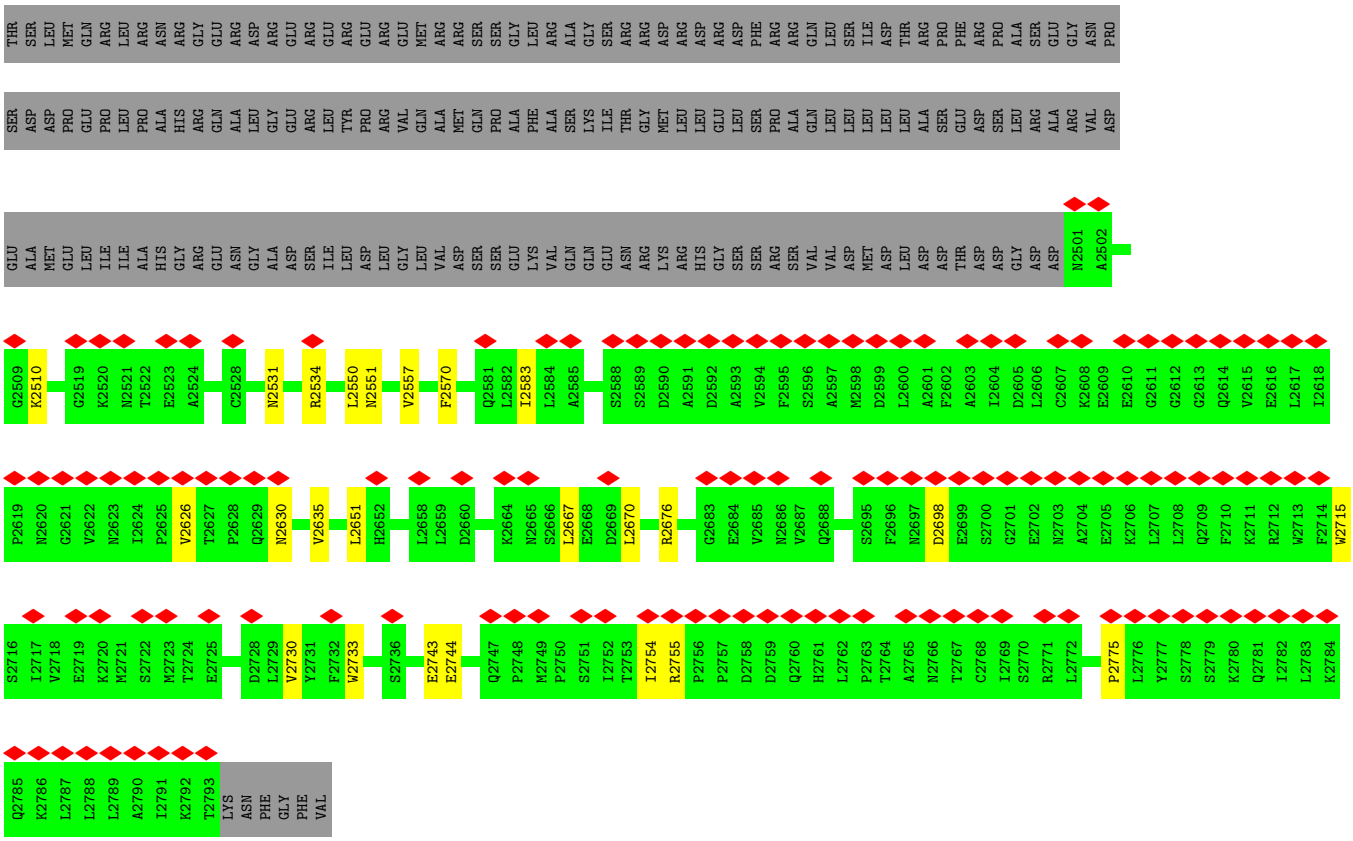


• Molecule 1: E3 ubiquitin-protein ligase UBR5

Chain E:

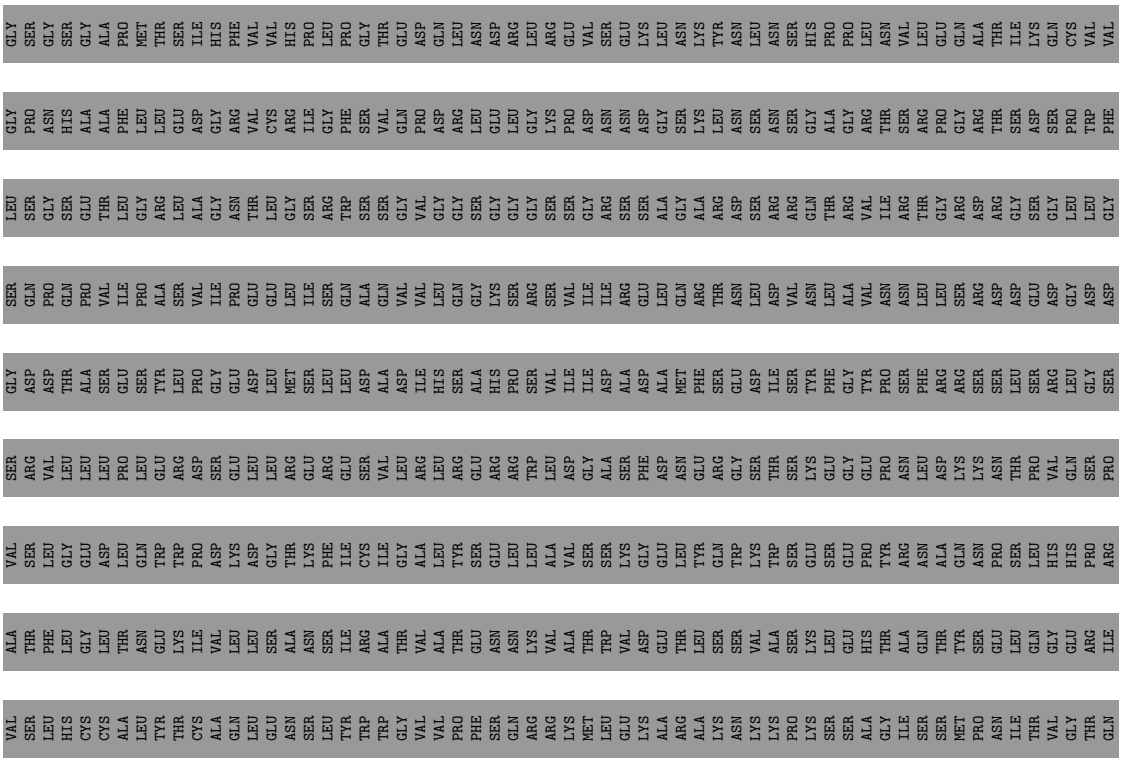


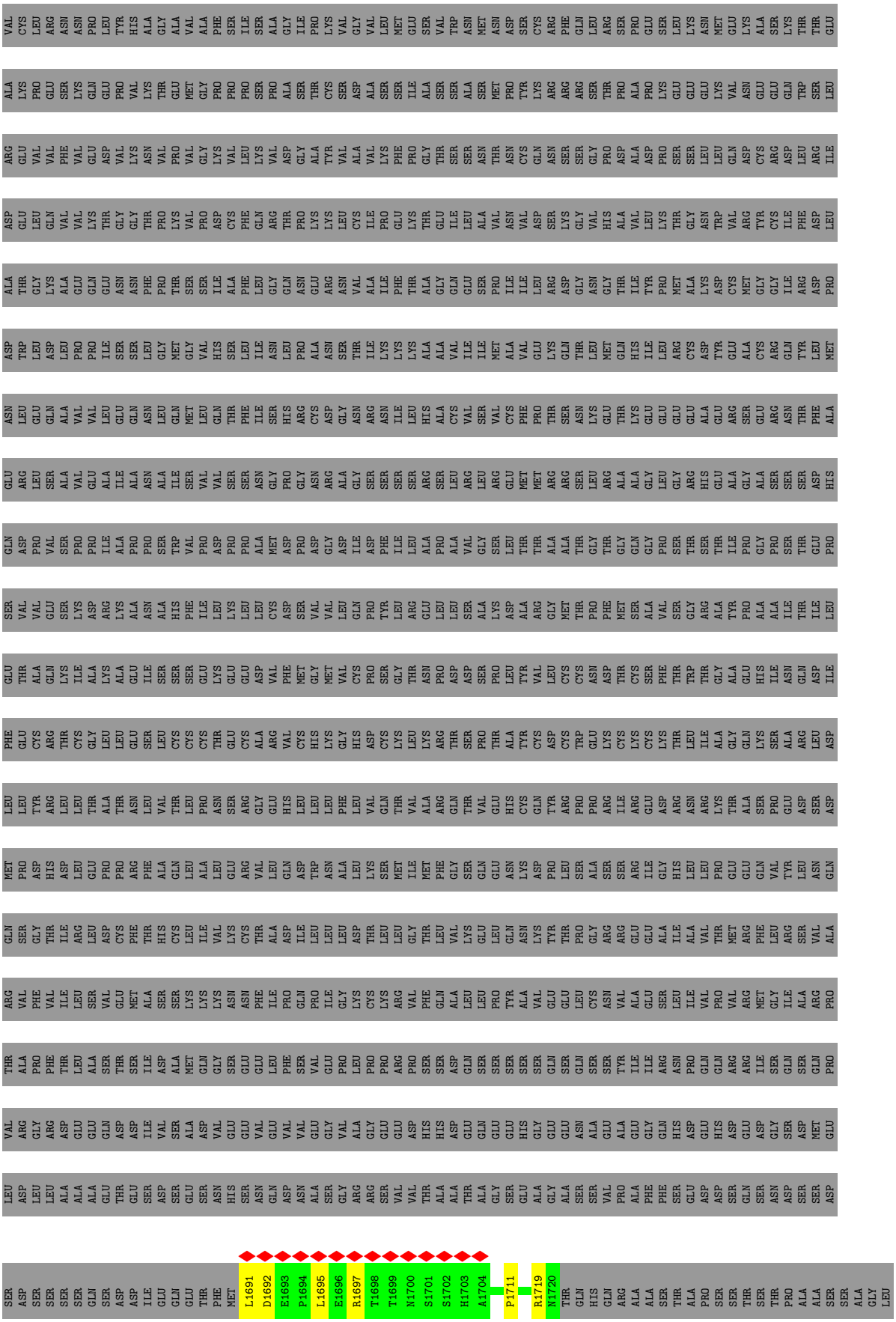


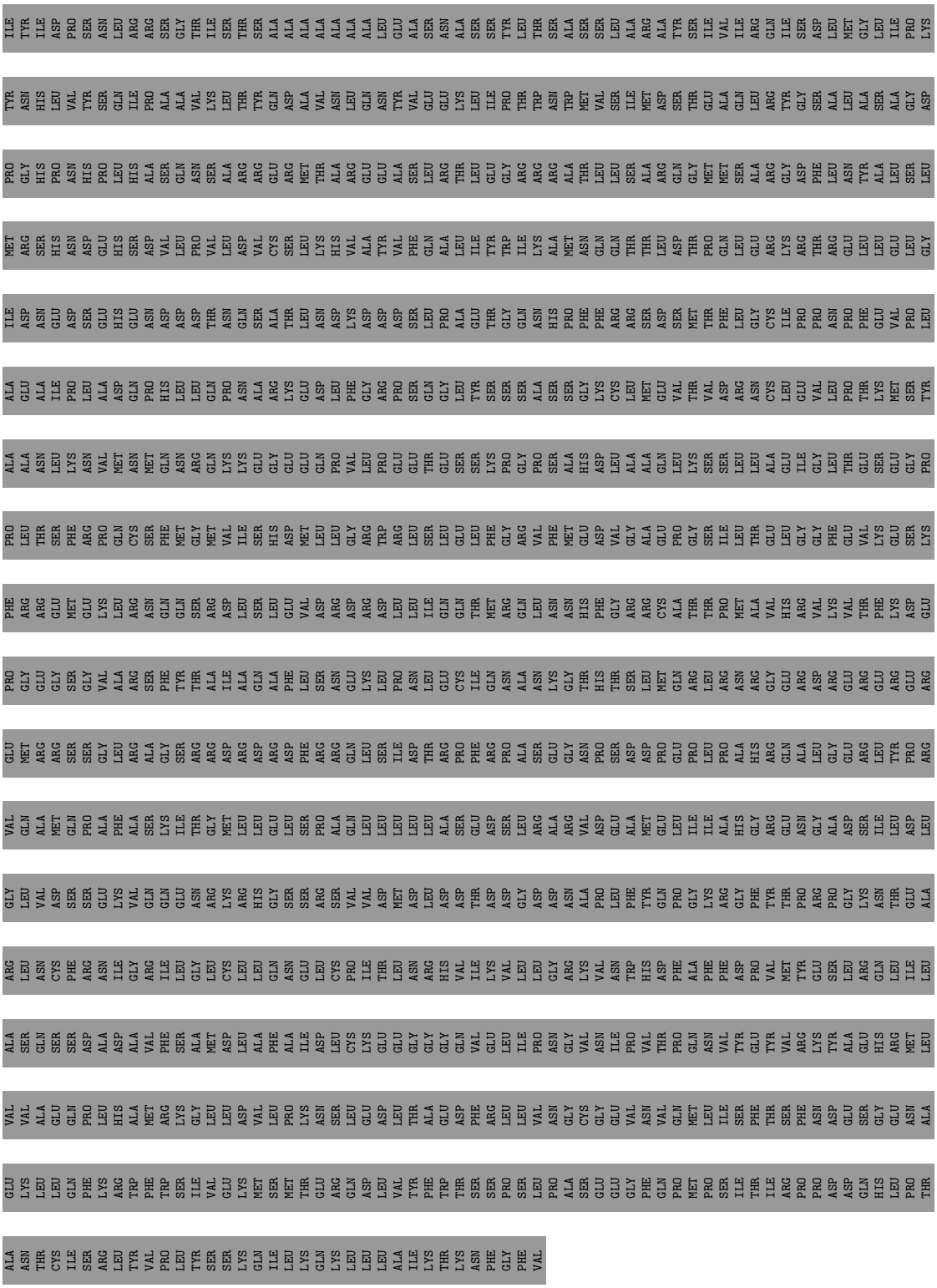


• Molecule 1: E3 ubiquitin-protein ligase UBR5

Chain F: 99%

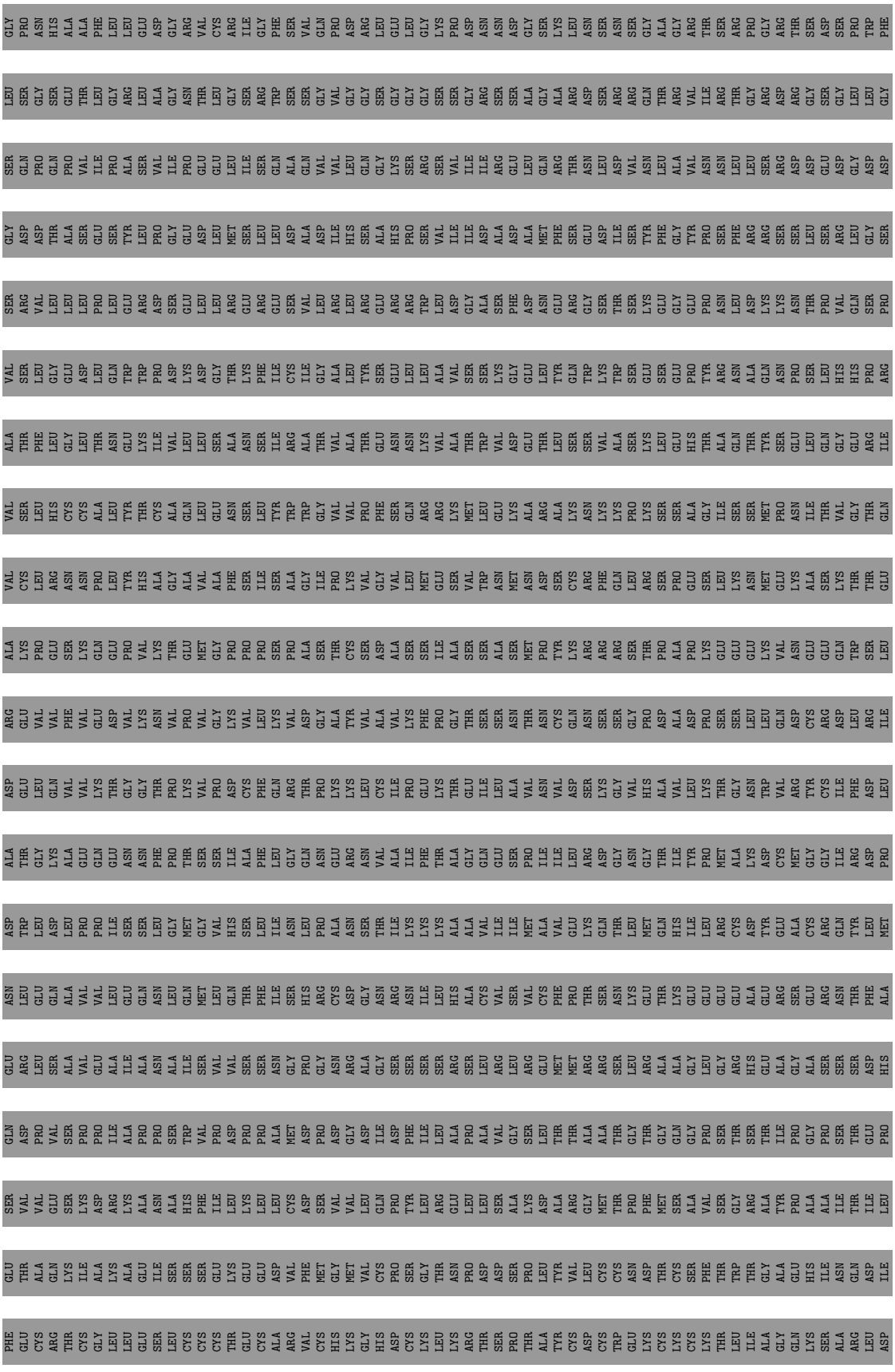


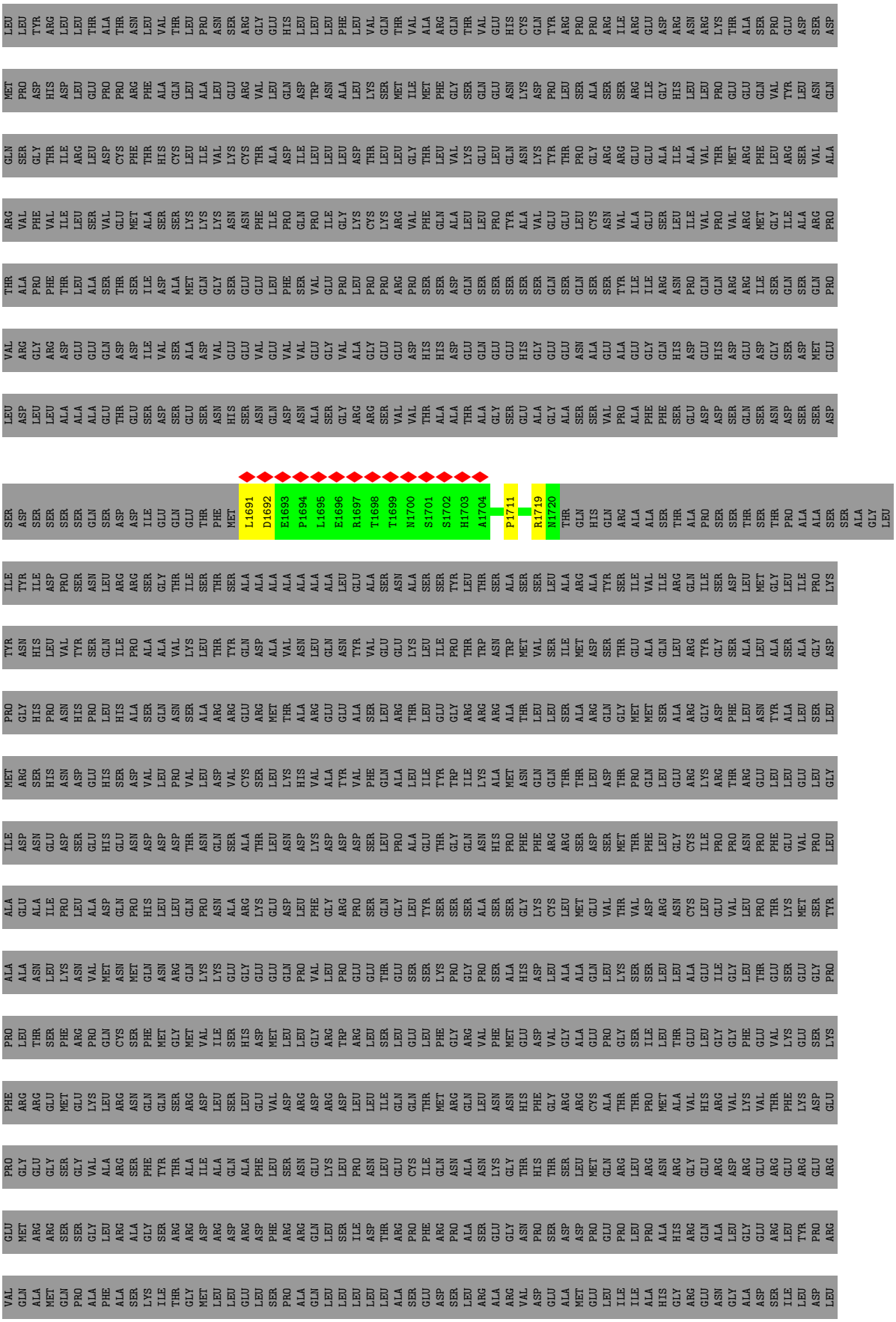

L1691
D1692
E1693
P1694
L1695
E1696
R1697
T1698
T1699
N1700
S1701
S1702
H1703
A1704
P1711
R1719
N1720

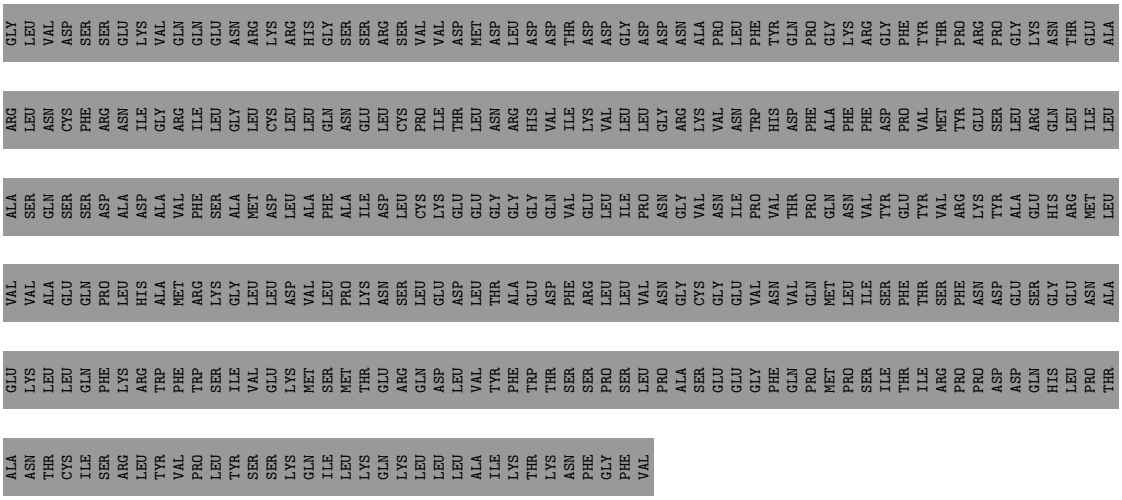


• Molecule 1: E3 ubiquitin-protein ligase UBR5

Chain G: 99%




L1691
D1692
E1693
P1694
L1695
E1696
R1697
T1698
T1699
N1700
S1701
S1702
H1703
A1704
P1711
R1719
N1720


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

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	226919	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 ($e^-/Å^2$)	67.8	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.091	Depositor
Minimum map value	-0.050	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0101	Depositor
Map size (Å)	326.86078, 326.86078, 326.86078	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8511999, 0.8511999, 0.8511999	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.27	0/7223	0.55	0/9821
1	B	0.26	0/5476	0.53	0/7439
1	D	0.27	0/7223	0.55	0/9821
1	E	0.26	0/5476	0.54	0/7439
1	F	0.25	0/230	0.62	0/312
1	G	0.25	0/230	0.62	0/312
All	All	0.27	0/25858	0.54	0/35144

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	7080	0	6948	30	0
1	B	5353	0	5187	29	0
1	D	7080	0	6948	26	0
1	E	5353	0	5187	30	0
1	F	226	0	207	5	0
1	G	226	0	207	3	0
2	A	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3	0	0	0	0
All	All	25324	0	24684	113	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 2.

The worst 5 of 113 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:D:1211:CYS:O	1:D:1215:CYS:HB2	1.77	0.84
1:A:1211:CYS:O	1:A:1215:CYS:HB2	1.77	0.82
1:E:2531:ASN:OD1	1:E:2534:ARG:NH2	2.33	0.61
1:B:2531:ASN:OD1	1:B:2534:ARG:NH2	2.33	0.60
1:A:804:ALA:HB2	1:A:846:MET:HG3	1.82	0.60

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	909/2806 (32%)	860 (95%)	49 (5%)	0	100	100
1	B	680/2806 (24%)	643 (95%)	37 (5%)	0	100	100
1	D	909/2806 (32%)	859 (94%)	50 (6%)	0	100	100
1	E	680/2806 (24%)	643 (95%)	37 (5%)	0	100	100
1	F	28/2806 (1%)	25 (89%)	3 (11%)	0	100	100
1	G	28/2806 (1%)	25 (89%)	3 (11%)	0	100	100
All	All	3234/16836 (19%)	3055 (94%)	179 (6%)	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	766/2422 (32%)	766 (100%)	0	100	100
1	B	564/2422 (23%)	564 (100%)	0	100	100
1	D	766/2422 (32%)	766 (100%)	0	100	100
1	E	564/2422 (23%)	564 (100%)	0	100	100
1	F	22/2422 (1%)	22 (100%)	0	100	100
1	G	22/2422 (1%)	22 (100%)	0	100	100
All	All	2704/14532 (19%)	2704 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	2258	GLN
1	E	2258	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 6 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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

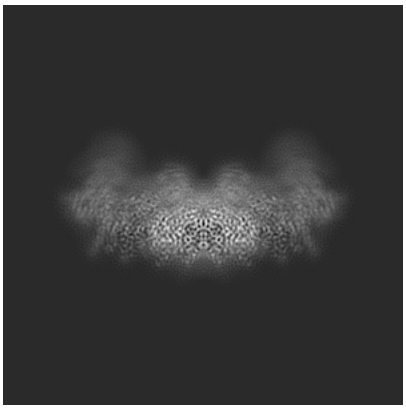
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-16355. These allow visual inspection of the internal detail of the map and identification of artifacts.

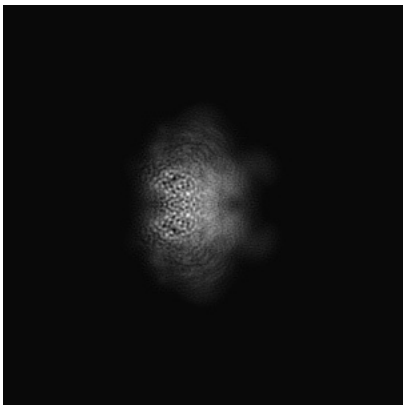
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

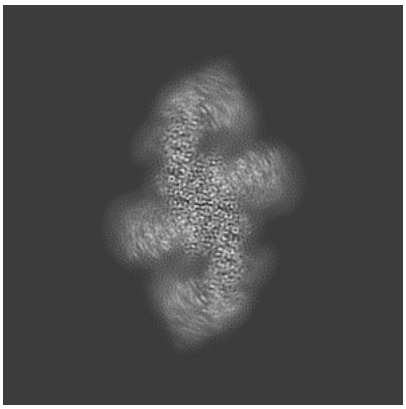
6.1.1 Primary map



X

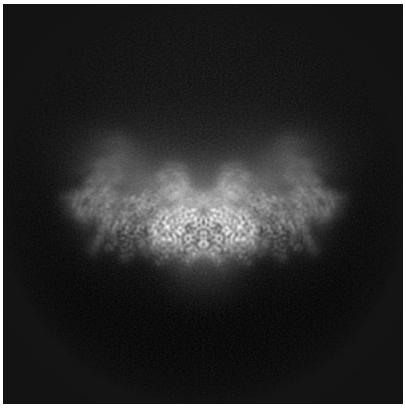


Y

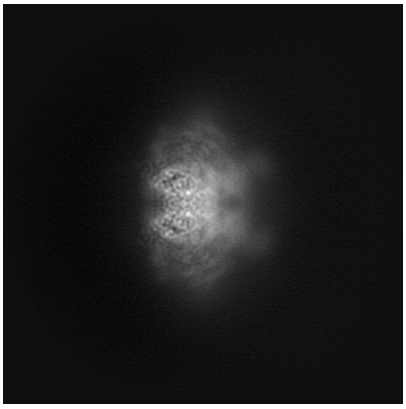


Z

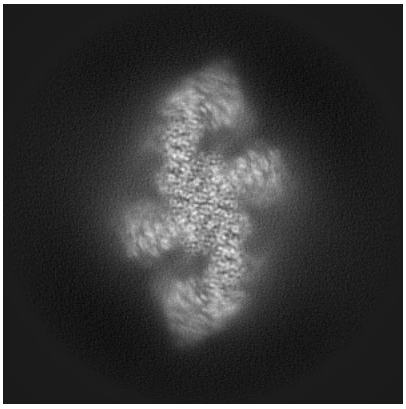
6.1.2 Raw map



X



Y



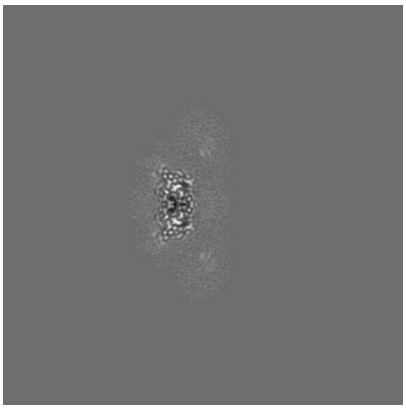
Z

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

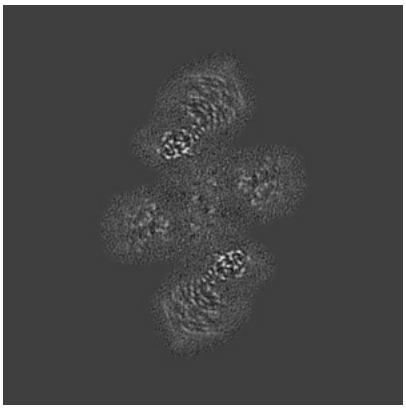
6.2 Central slices (i)

6.2.1 Primary map

X Index: 192

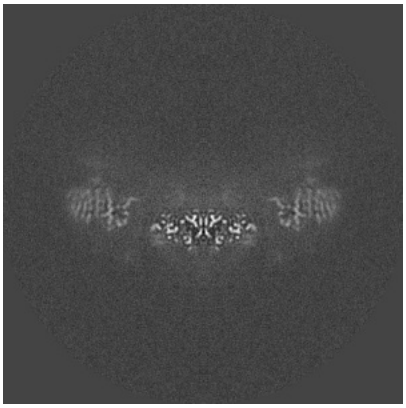


Y Index: 192

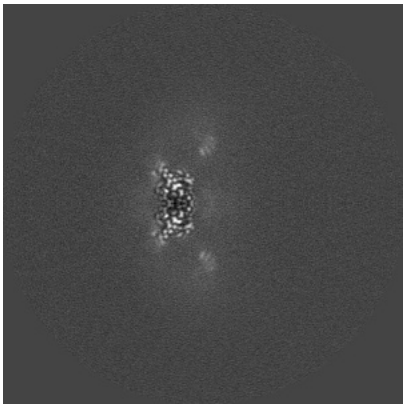


Z Index: 192

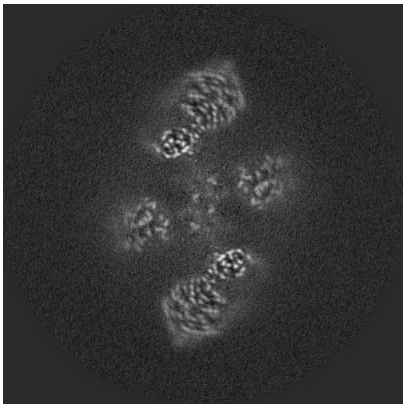
6.2.2 Raw map



X Index: 192



Y Index: 192



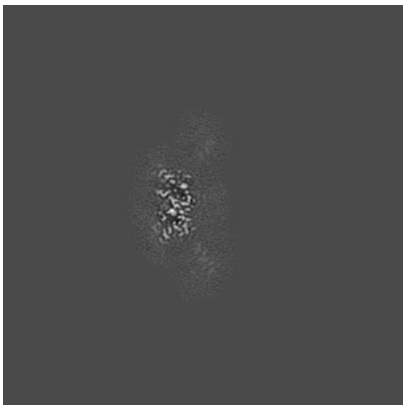
Z Index: 192

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

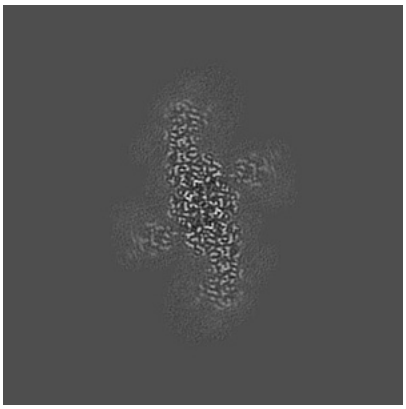
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 204

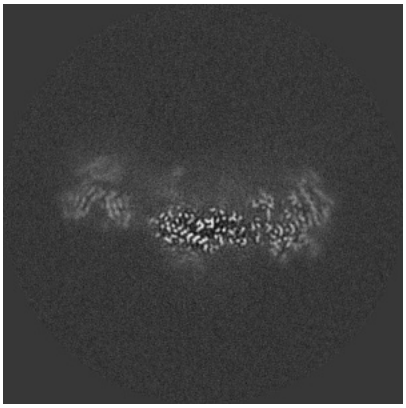


Y Index: 190

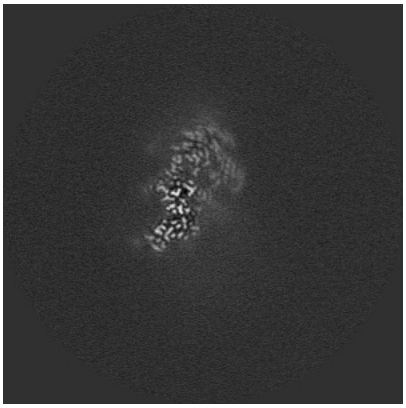


Z Index: 170

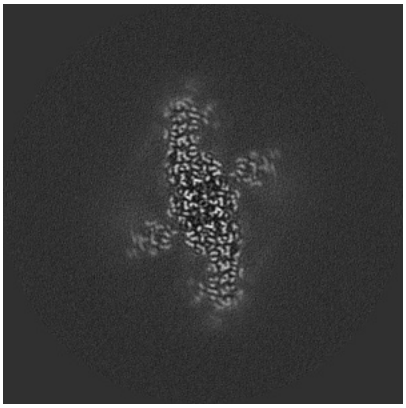
6.3.2 Raw map



X Index: 180



Y Index: 214

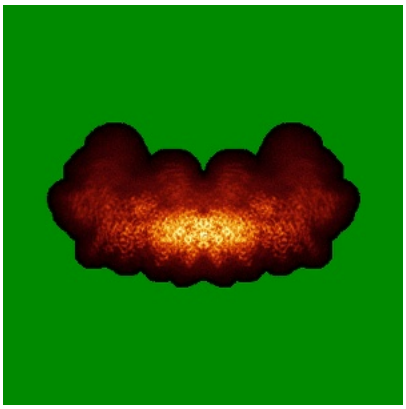


Z Index: 170

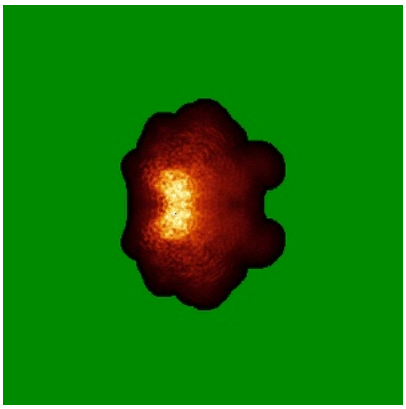
The images above show the largest variance slices of the map in three orthogonal directions.

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

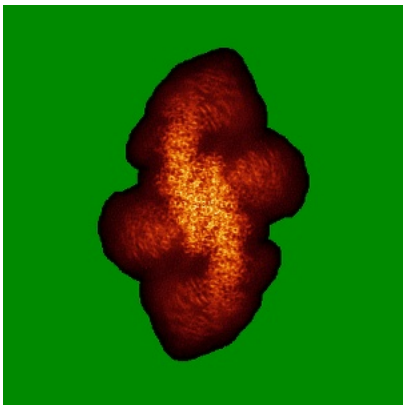
6.4.1 Primary map



X

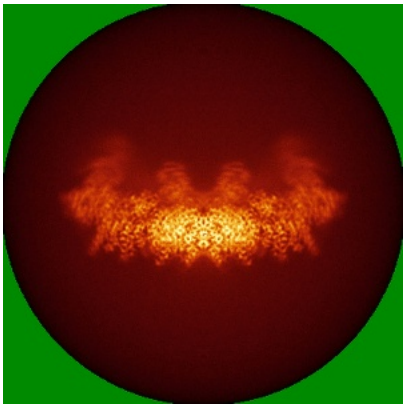


Y

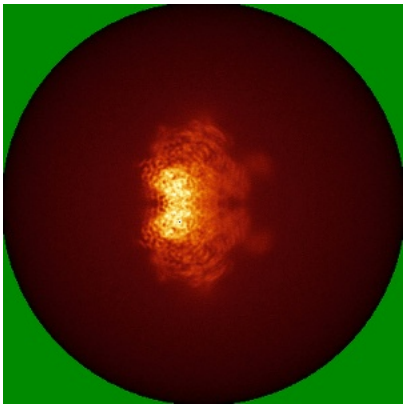


Z

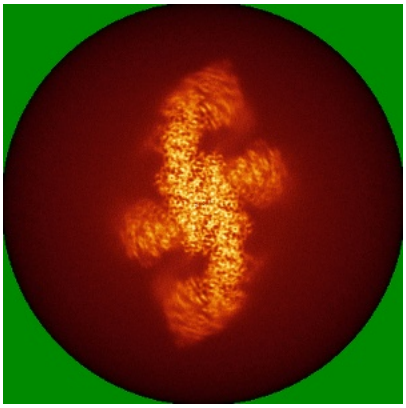
6.4.2 Raw map



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 0.0101. 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.

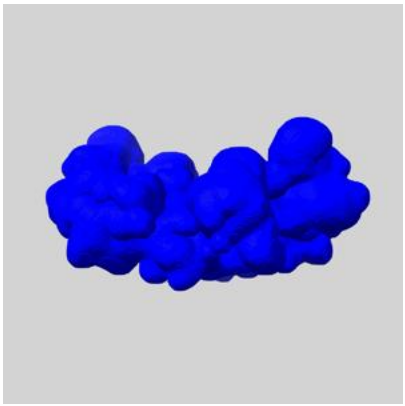
6.6 Mask visualisation (i)

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

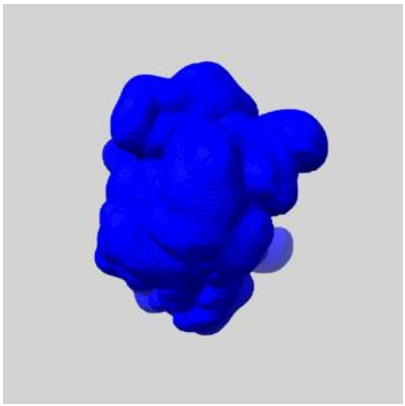
A mask typically either:

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

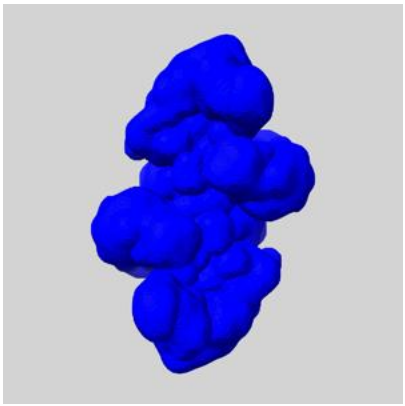
6.6.1 emd_16355_msk_1.map (i)



X



Y

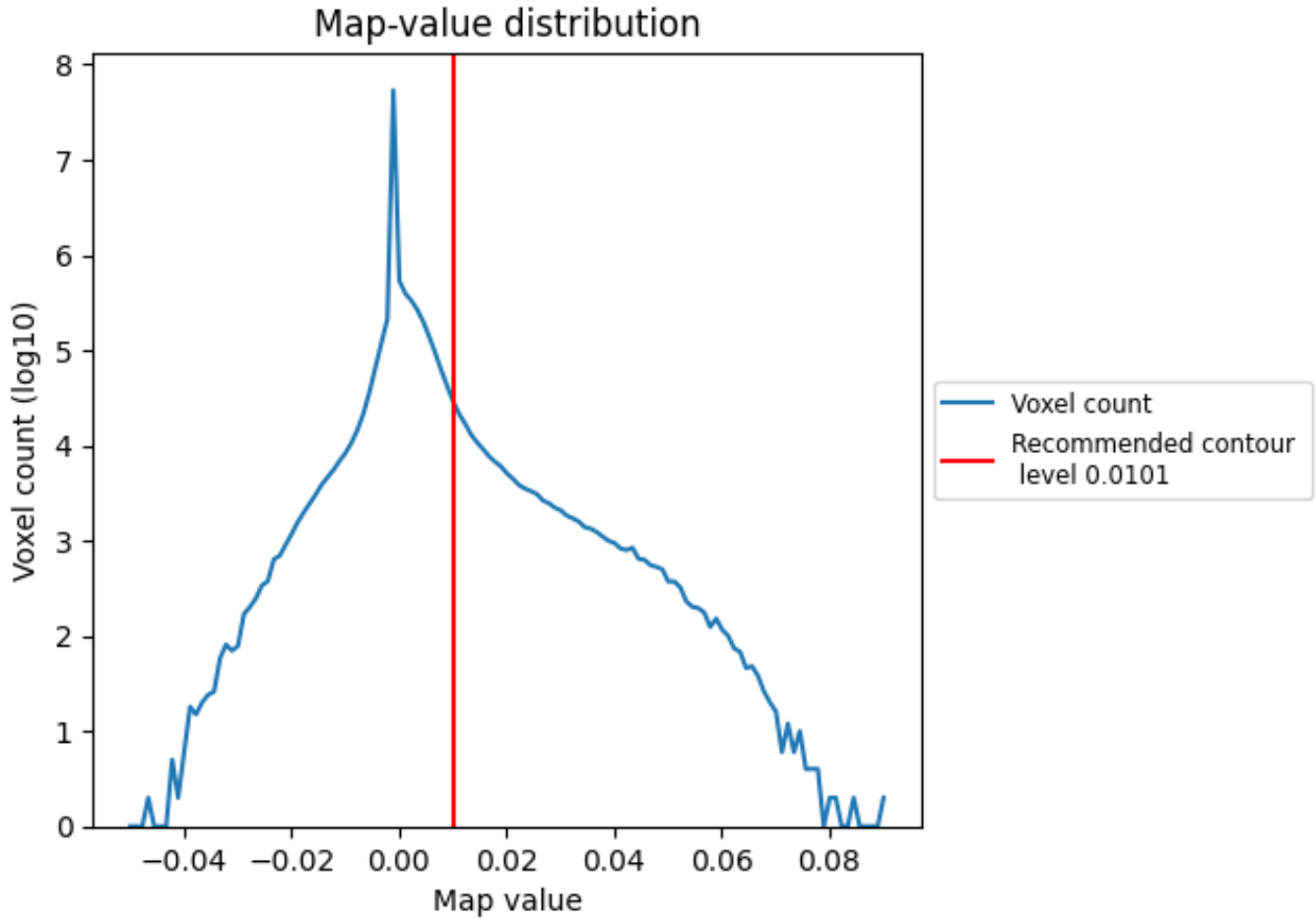


Z

7 Map analysis

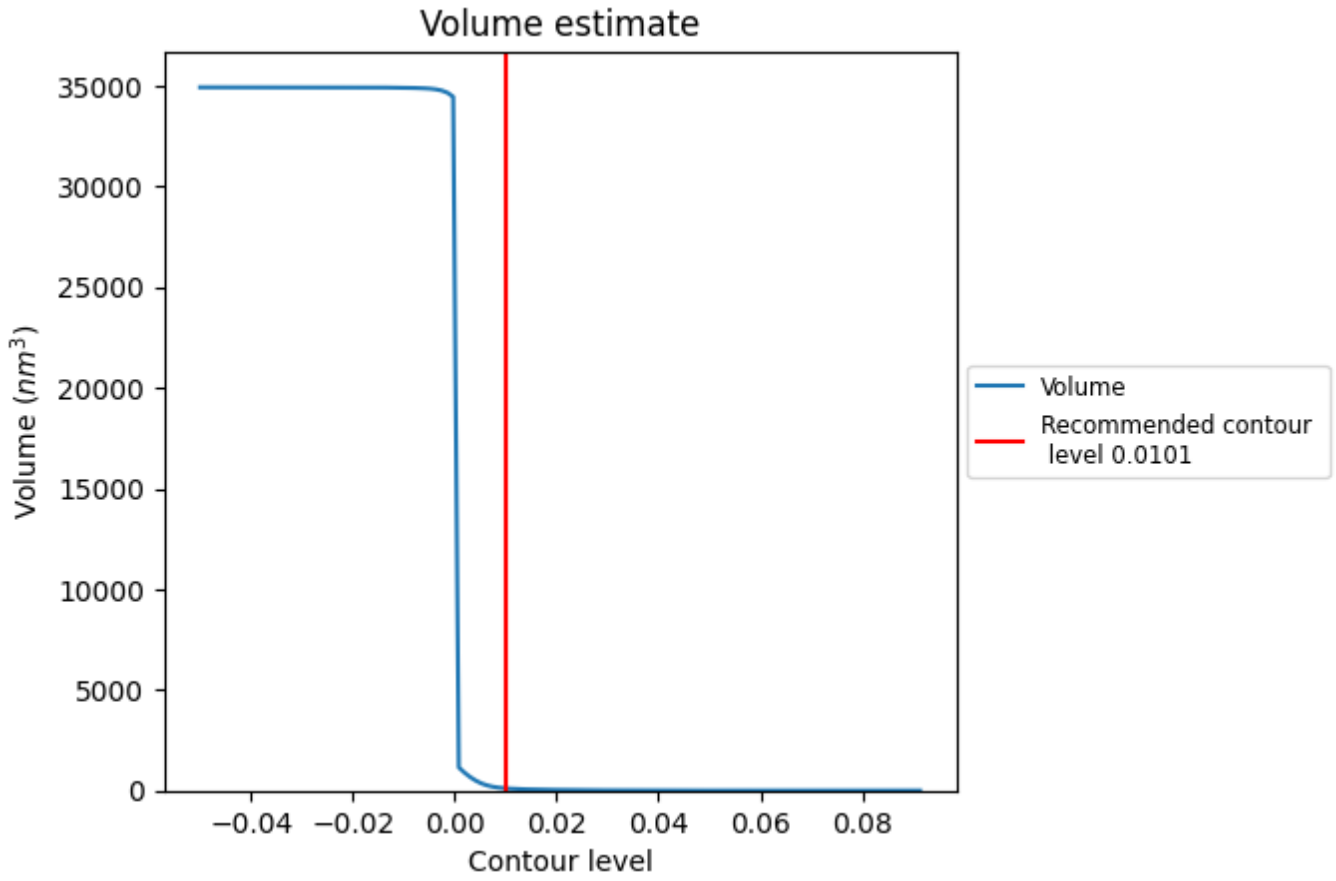
This section contains the results of statistical analysis of the map.

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.

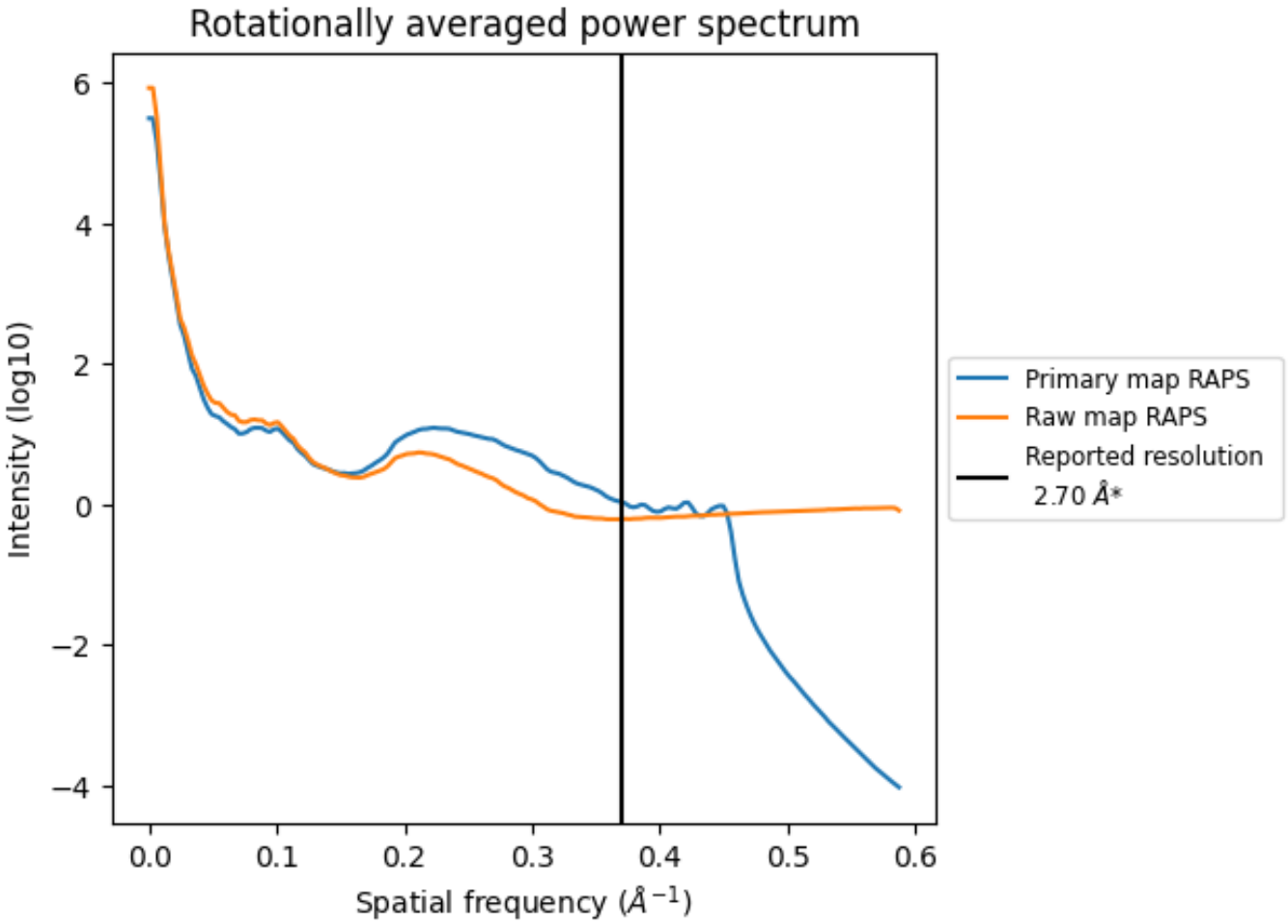
7.2 Volume estimate (i)



The volume at the recommended contour level is 109 nm^3; this corresponds to an approximate mass of 98 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)

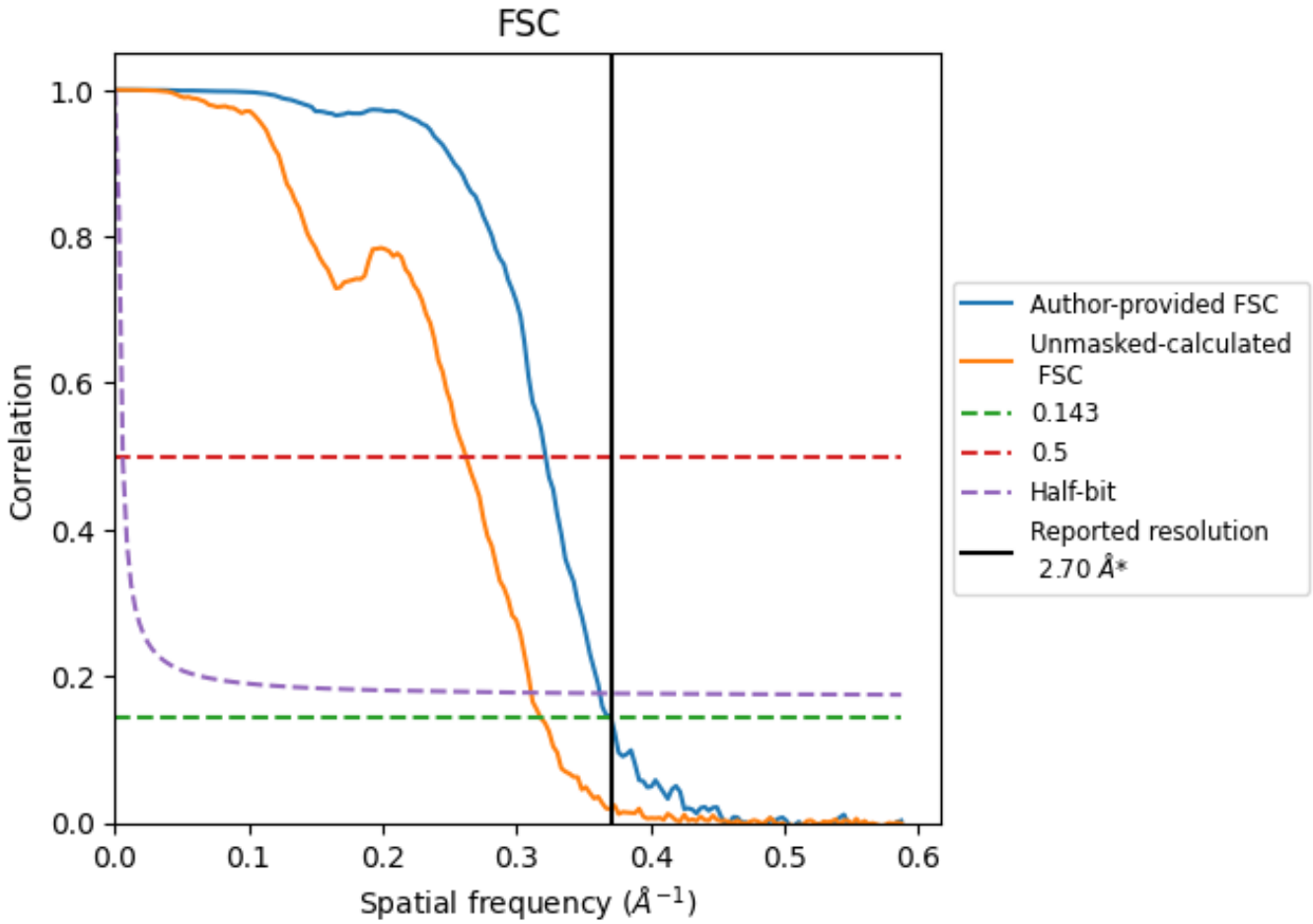


*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

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 0.370 Å^{-1}

8.2 Resolution estimates (i)

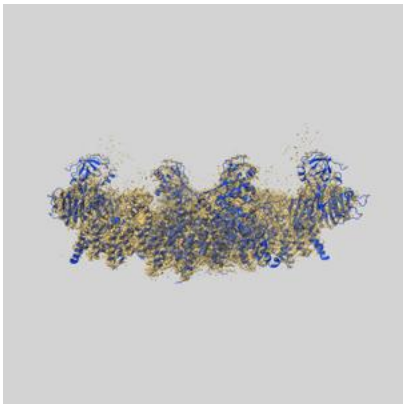
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.70	3.11	2.76
Unmasked-calculated*	3.14	3.82	3.22

*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 3.14 differs from the reported value 2.7 by more than 10 %

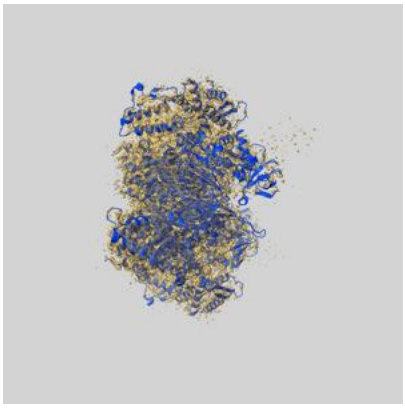
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-16355 and PDB model 8C06. Per-residue inclusion information can be found in section 3 on page 6.

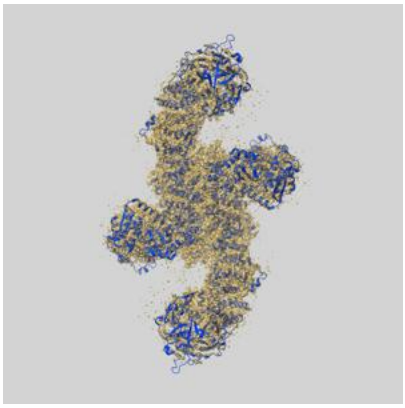
9.1 Map-model overlay



X



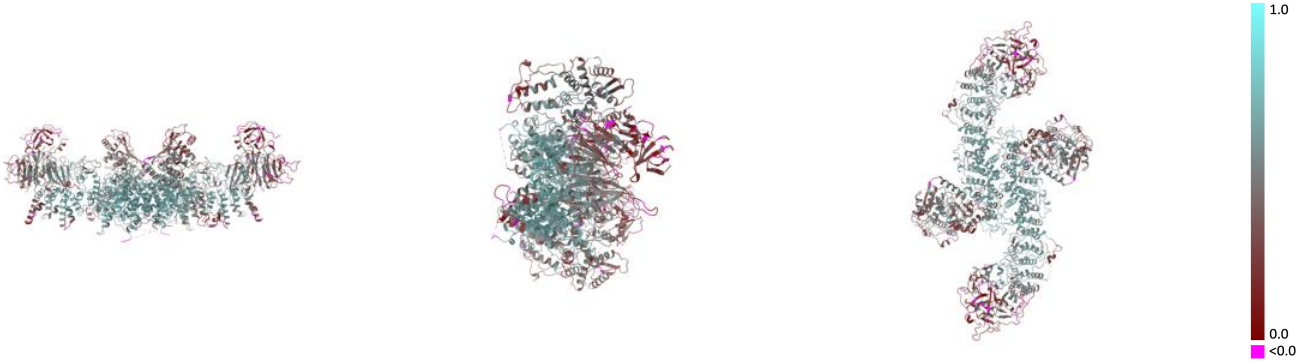
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0101 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.

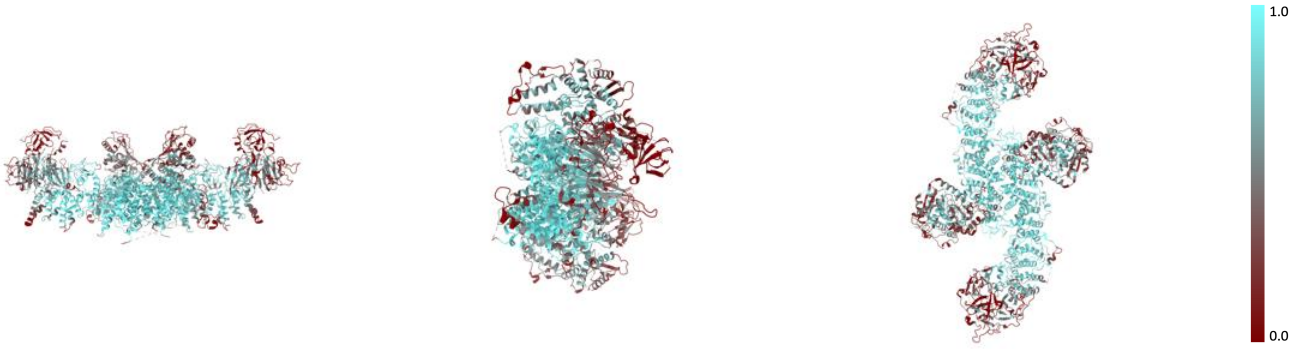
9.2 Q-score mapped to coordinate model



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.

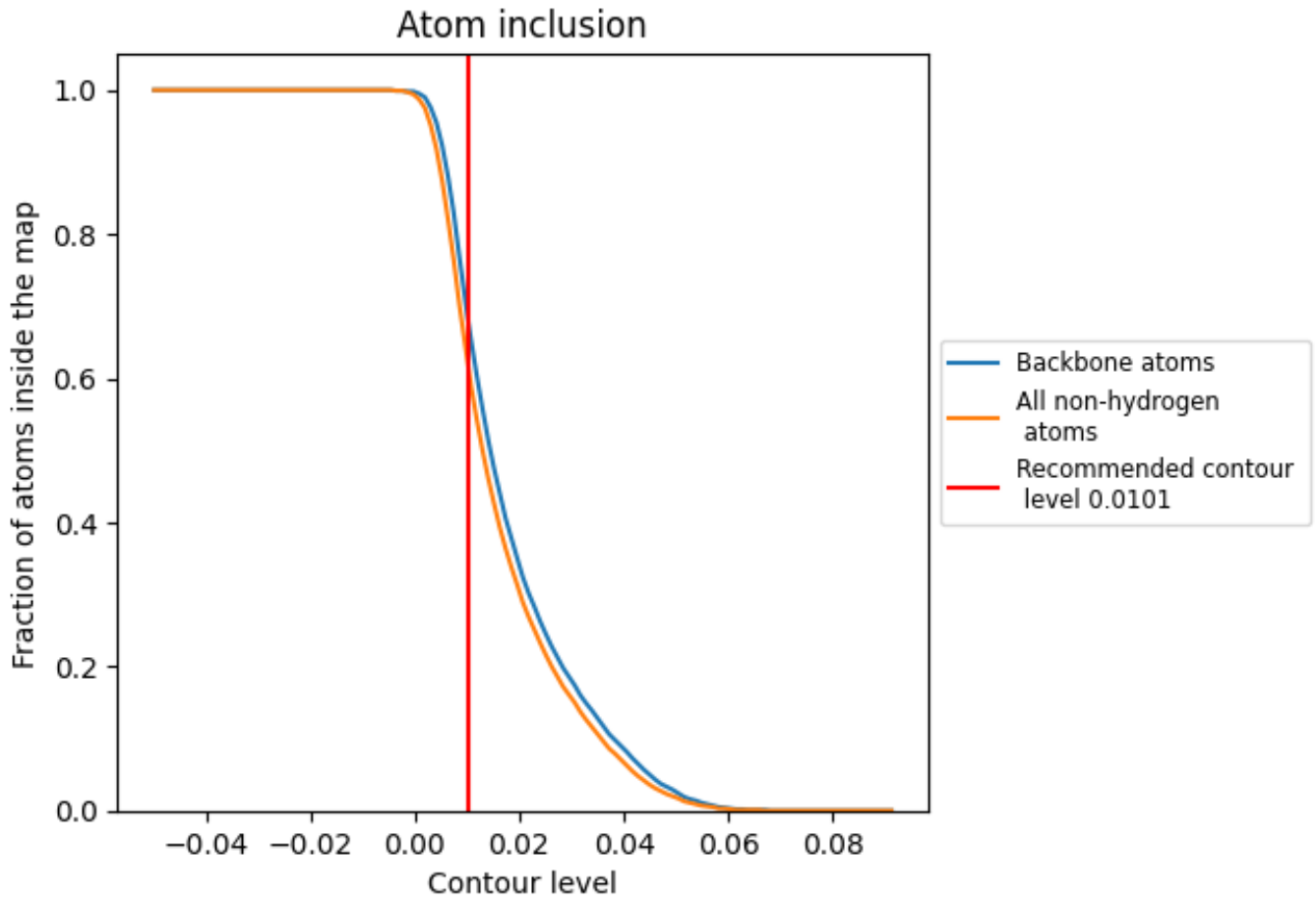
9.3 Atom inclusion mapped to coordinate model



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 (0.0101).

9.4 Atom inclusion (i)



At the recommended contour level, 68% of all backbone atoms, 62% 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 (0.0101) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6220	0.4780
A	0.6070	0.4650
B	0.6460	0.4990
D	0.6060	0.4640
E	0.6470	0.4970
F	0.5390	0.4430
G	0.5340	0.4410