Full wwPDB EM Validation Report ⓘ

Mar 18, 2023 – 07:02 am GMT

PDB ID	:	8ATM
EMDB ID	:	EMD-15653
Title	:	Structure of the giant inhibitor of apoptosis, BIRC6 (composite map)
Authors	:	Dietz, L.; Elliott, P.R.
Deposited on	:	2022-08-23
Resolution	:	3.30 Å(reported)

This is a Full wwPDB EM Validation 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:

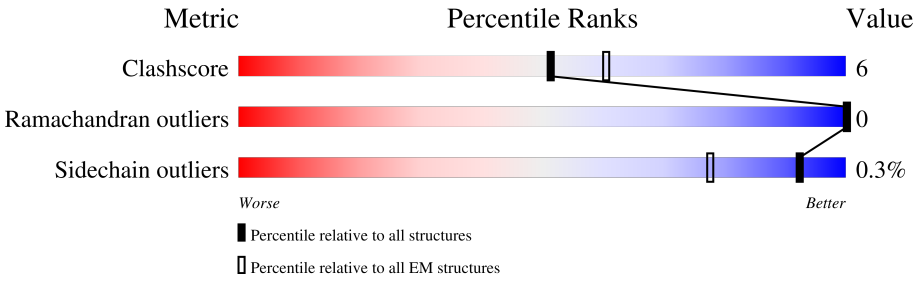
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

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 3.30 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	4859	36% 6% 58%
1	B	4859	35% 6% 60%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 30885 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 Baculoviral IAP repeat-containing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2035	Total	C	N	O	S	0	0
			15729	10066	2671	2876	116		
1	B	1963	Total	C	N	O	S	0	0
			15156	9705	2568	2772	111		

There are 4 discrepancies between the modelled and reference sequences:

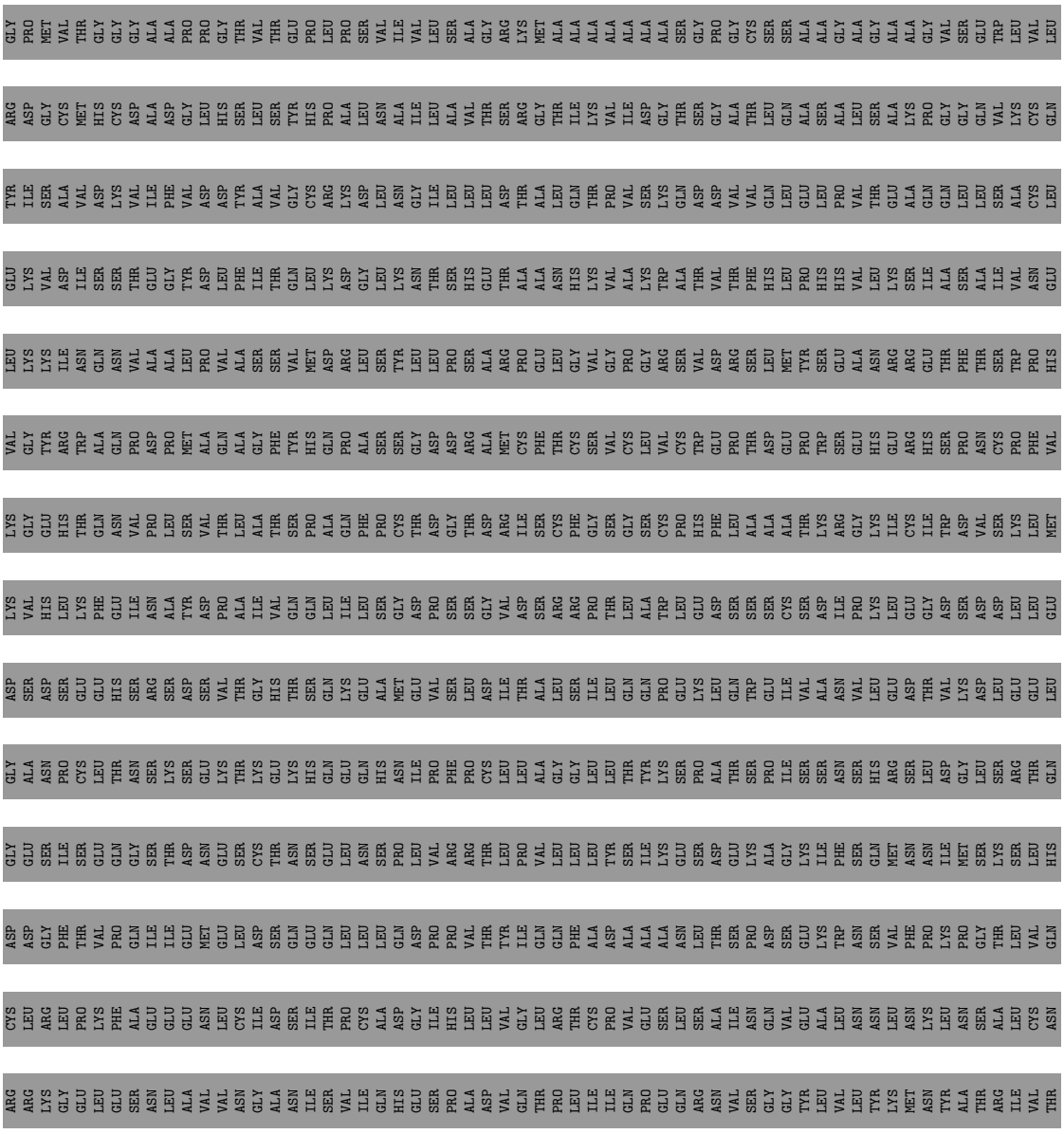
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q9NR09
A	0	PRO	-	expression tag	UNP Q9NR09
B	-1	GLY	-	expression tag	UNP Q9NR09
B	0	PRO	-	expression tag	UNP Q9NR09

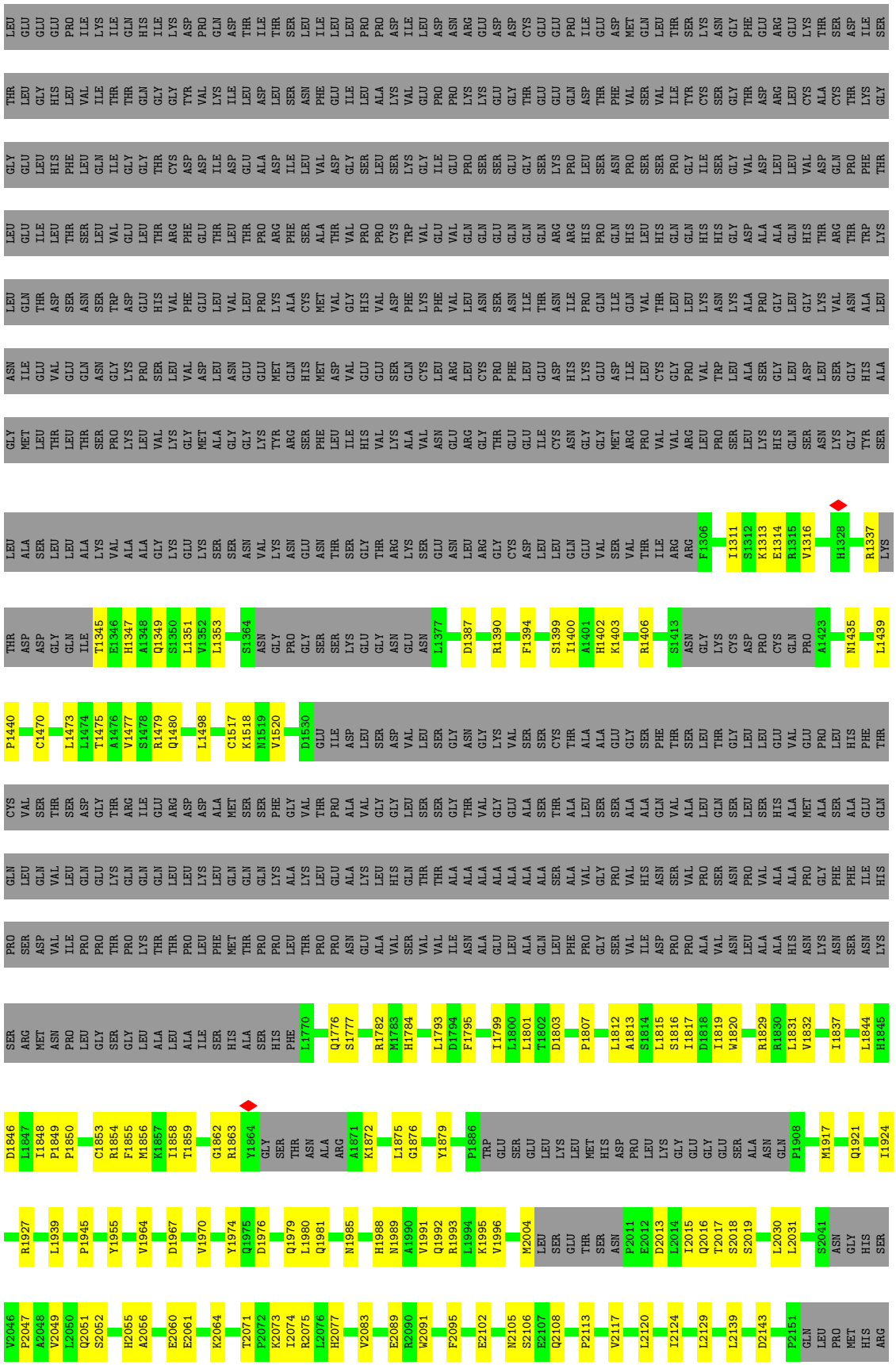
3 Residue-property plots (i)

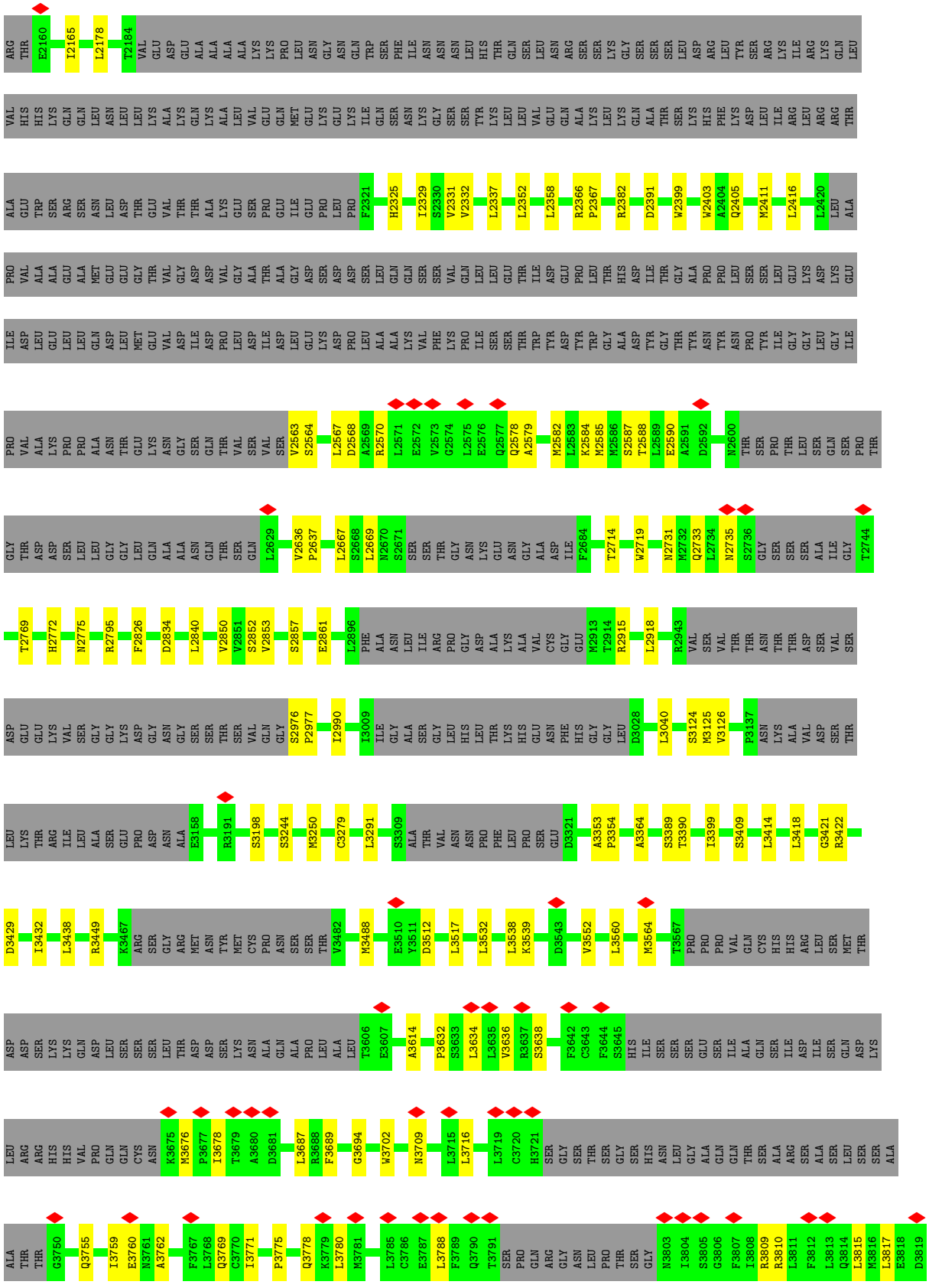
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

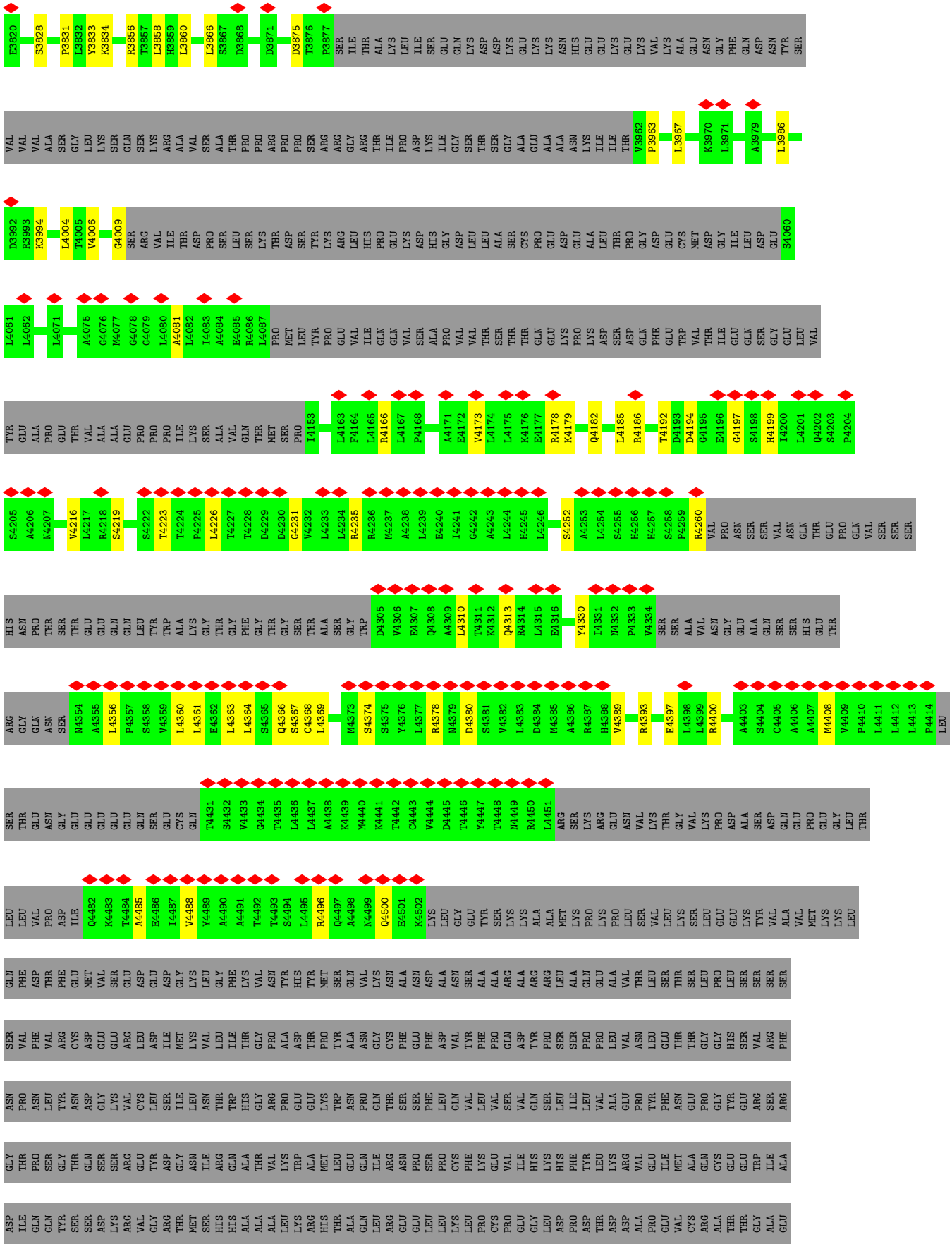
- Molecule 1: Baculoviral IAP repeat-containing protein 6

Chain A:






ARG THR E2160 I2165 L2178 T2184 VAL GLU ASP GLU ALA ALA ALA ALA LYS LYS PRO LEU ASN GLY ASN GLN TRP SER PHE ILE ASN ASN ASN LEU HIS THR GLN SER LEU ASN ARG SER SER LYS GLY SER SER SER LEU ASP ARG LEU TYR SER ARG LYS ILE ARG LYS GLN LEU
VAL HIS HIS LYS GLN GLN LEU ASN LEU LEU LYS ALA LYS GLN LYS ALA LEU VAL GLU GLN MET GLU LYS GLU LYS ILE GLN SER ASN LYS GLY SER SER TYR LYS LEU LEU VAL GLU GLN ALA LYS LEU LYS GLN ALA THR SER LYS HIS PHE LYS ASP LEU ILE ARG LEU ARG THR
ALA GLU TRP SER ARG SER ASN LEU ASP THR GLU VAL THR THR ALA LYS GLU SER PRO GLU ILE GLU PRO LEU PRO F2321 H2325 I2329 S2330 V2331 V2332 L2337 L2352 L2358 R2366 P2367 R2382 D2391 W2399 W2403 A2404 Q2405 M2411 L2416 L2420 LEU ALA
PRO VAL ALA ALA GLU ALA MET GLU GLU GLY THR VAL GLY ASP ASP VAL GLY ALA THR ALA GLY ASP SER ASP ASP SER LEU GLN GLN SER SER VAL GLN LEU LEU GLU THR ILE ASP GLU PRO LEU THR HIS ASP ILE THR GLY ALA PRO PRO LEU SER SER LEU GLU GLU LYS ASP LYS GLU
ILE ASP LEU GLU LEU LEU GLN ASP LEU MET GLU VAL ASP ILE ASP PRO LEU ASP ILE ASP LEU GLU LYS ASP PRO LEU ALA ALA LYS VAL PHE LYS PRO ILE SER SER THR TRP TYR ASP TYR TRP GLY ALA ASP TYR GLY THR TYR ASN TYR ASN PRO TYR ILE GLY GLY LEU GLY ILE
PRO VAL ALA LYS PRO PRO ALA ASN THR GLU LYS ASN GLY SER GLN THR VAL SER VAL SER V2563 S2564 L2567 D2568 A2569 R2570 L2571 E2572 V2573 G2574 L2575 E2576 Q2577 Q2578 A2579 M2582 L2583 K2584 M2585 M2586 S2587 T2588 L2589 E2590 A2591 D2592 N2600 THR SER PRO THR LEU SER GLN SER PRO THR
GLY THR ASP ASP SER LEU LEU GLY GLY LEU GLN ALA ALA ASN GLN THR SER GLN L2629 V2636 P2637 L2667 S2668 L2669 N2670 S2671 SER SER THR GLY ASN LYS GLU ASN GLY ALA ASP ILE F2684 T2714 W2719 N2731 N2732 Q2733 L2734 N2735 S2736 GLY SER SER SER ALA ILE GLY T2744
T2769 H2772 N2775 R2795 F2826 D2834 L2840 V2850 V2851 S2852 V2853 S2857 E2861 L2896 PHE ALA ASN LEU ILE ARG PRO GLY ASP ALA LYS ALA VAL CYS GLY GLU M2913 T2914 R2915 L2918 R2943 VAL SER VAL THR THR ASN THR THR ASP SER VAL SER
ASP GLU GLU LYS VAL SER GLY GLY LYS ASP GLY ASN GLY SER SER THR SER VAL GLN GLY S2976 P2977 I2990 I3009 ILE GLY ALA SER GLY LEU HIS LEU THR LYS HIS GLU ASN PHE HIS GLY GLY LEU D3028 L3040 S3124 M3125 V3126 P3137 ASN LYS ALA VAL ASP SER THR
LEU LYS THR ARG ILE LEU ALA SER GLU PRO ASP ASN ALA E3158 R3191 S3198 S3244 M3250 C3279 L3291 S3309 ALA THR VAL ASN ASN PRO PHE LEU PRO SER GLU D3321 A3353 P3354 A3364 S3389 T3390 I3399 S3409 L3414 L3418 G3421 R3422
D3429 I3432 L3438 R3449 K3467 ARG SER GLY ARG MET ASN TYR MET CYS PRO ASN SER SER THR V3482 M3488 E3510 Y3511 D3512 L3517 L3532 L3538 K3539 D3543 V3552 L3560 M3564 T3567 PRO PRO PRO VAL GLN CYS HIS HIS ARG LEU SER MET THR
ASP ASP SER LYS LYS GLN ASP LEU SER SER LEU THR ASP ASP SER LYS ASN ALA GLN ALA PRO LEU ALA LEU T3606 E3607 A3614 P3632 S3633 L3634 L3635 V3636 R3637 S3638 F3642 C3643 F3644 S3645 HIS ILE SER SER SER GLU SER ILE ALA GLN SER ILE ASP ILE SER GLN ASP LYS
LEU ARG ARG HIS HIS VAL PRO GLN GLN CYS ASN K3675 M3676 P3677 I3678 T3679 A3680 D3681 L3687 R3688 F3689 G3694 W3702 N3709 L3715 L3716 L3719 C3720 H3721 SER GLY SER THR SER GLY SER HIS ASN LEU GLY ALA GLN GLN THR SER LYS HIS PHE LYS ASP LEU ILE ARG LEU ARG THR
ALA THR THR G3750 Q3755 I3759 E3760 N3761 A3762 F3767 L3768 Q3769 C3770 I3771 P3775 Q3778 K3779 L3780 M3781 L3785 C3786 E3787 L3788 F3789 Q3790 T3791 SER PRO GLN ARG GLY ASN LEU PRO THR SER GLY N3803 I3804 S3805 G3806 F3807 I3808 R3809 R3810 L3811 F3812 L3813 Q3814 L3815 M3816 L3817 E3818 D3819


E3820 S3828 P3831 L3832 V3833 K3834 R3856 T3857 L3858 H3859 L3860 L3866 S3867 D3868 D3871 D3875 T3876 P3877 SER ILE THR ALA LYS LEU ILE SER 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 GLU ALA ALA ASN LYS ILE ILE THR V3962 P3963 L3967 K3970 L3971 A3979 L3986
D3992 R3993 K3994 L4004 T4005 V4006 G4009 SER ARG VAL ILE THR ASP PRO SER LEU SER LYS THR ASP SER TYR LYS ARG LEU HIS PRO GLU GLN LYS ASP HIS GLY ASP LEU LEU ALA SER CYS PRO GLU GLU ASP GLU ALA LEU THR PRO GLY ASP GLU CYS MET ASP GLY ILE LEU ASP GLU S4060
L4061 L4062 L4071 A4075 G4076 M4077 G4078 G4079 L4080 A4081 L4082 I4083 A4084 E4085 R4086 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 CYS TRP VAL THR ILE GLU GLN SER GLY GLU LEU VAL
TYR GLU ALA PRO GLU THR VAL ALA ALA GLU PRO PRO PRO ILE LYS SER ALA VAL GLN THR MET SER PRO I4153 L4163 F4164 L4165 R4166 L4167 P4168 A4171 E4172 V4173 L4174 L4175 K4176 E4177 R4178 K4179 Q4182 L4185 R4186 T4192 D4193 D4194 G4195 E4196 G4197 S4198 H4199 I4200 L4201 Q4202 S4203 P4204
S4205 A4206 N4207 V4216 L4217 R4218 S4219 S4222 T4223 T4224 P4225 L4226 T4227 T4228 D4229 D4230 G4231 V4232 L4233 L4234 R4235 R4236 M4237 A4238 L4239 E4240 I4241 G4242 A4243 L4244 H4245 L4246 S4252 A4253 L4254 S4255 H4256 H4257 S4258 P4259 R4260 VAL PRO ASN SER SER VAL ASN GLN THR GLU PRO GLN VAL SER SER SER
HIS ASN PRO THR SER THR GLU 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 Y4330 I4331 N4332 P4333 V4334 SER SER ALA VAL ASN GLY GLU ALA GLN SER SER HIS GLU THR
ARG GLY GLN ASN SER N4354 A4355 L4356 P4357 S4358 V4359 L4360 L4361 E4362 L4363 L4364 S4365 Q4366 S4367 C4368 L4369 M4373 S4374 S4375 Y4376 L4377 R4378 N4379 D4380 S4381 V4382 L4383 D4384 M4385 A4386 R4387 H4388 V4389 R4393 E4397 L4398 L4399 R4400 A4403 S4404 C4405 A4406 A4407 M4408 V4409 P4410 L4411 L4412 L4413 P4414 LEU
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 ARG SER LYS ARG GLU ASN VAL LYS THR GLY VAL LYS PRO ASP ALA SER ASP GLN GLU PRO GLU GLY LEU THR
LEU LEU VAL PRO ASP ILE Q4482 K4483 T4484 A4485 E4486 I4487 V4488 Y4489 A4490 A4491 T4492 T4493 S4494 L4495 R4496 Q4497 A4498 N4499 Q4500 E4501 K4502 LYS LEU GLY GLU TYR SER LYS LYS ALA ALA MET LYS PRO LYS PRO LEU SER VAL LEU LEU LYS SER LEU GLU GLU LYS 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 ASN ASP ALA ASN SER ALA ALA ARG ALA ALA ARG ARG LEU ALA GLN GLU ALA VAL THR LEU LEU SER THR SER LEU PRO LEU LEU SER SER SER SER
SER VAL PHE VAL ARG CYS ASP GLU GLU ARG LEU ASP ILE MET LYS VAL 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 GLY 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 ASN PRO GLN THR SER SER PHE LEU GLN VAL 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 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 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
WORLDWIDE PDB PROTEIN DATA BANK

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:

GLY PRO MET VAL THR GLY GLY GLY ALA ALA PRO PRO GLY THR VAL THR GLU PRO LEU PRO SER VAL ILE VAL LEU SER ALA GLY ARG LYS MET ALA ALA ALA ALA ALA ALA ALA SER GLY PRO GLY CYS SER SER ALA ALA GLY ALA GLY ALA ALA GLY VAL SER GLU TRP LEU VAL LEU

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

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

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

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

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

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

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

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

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

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

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

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

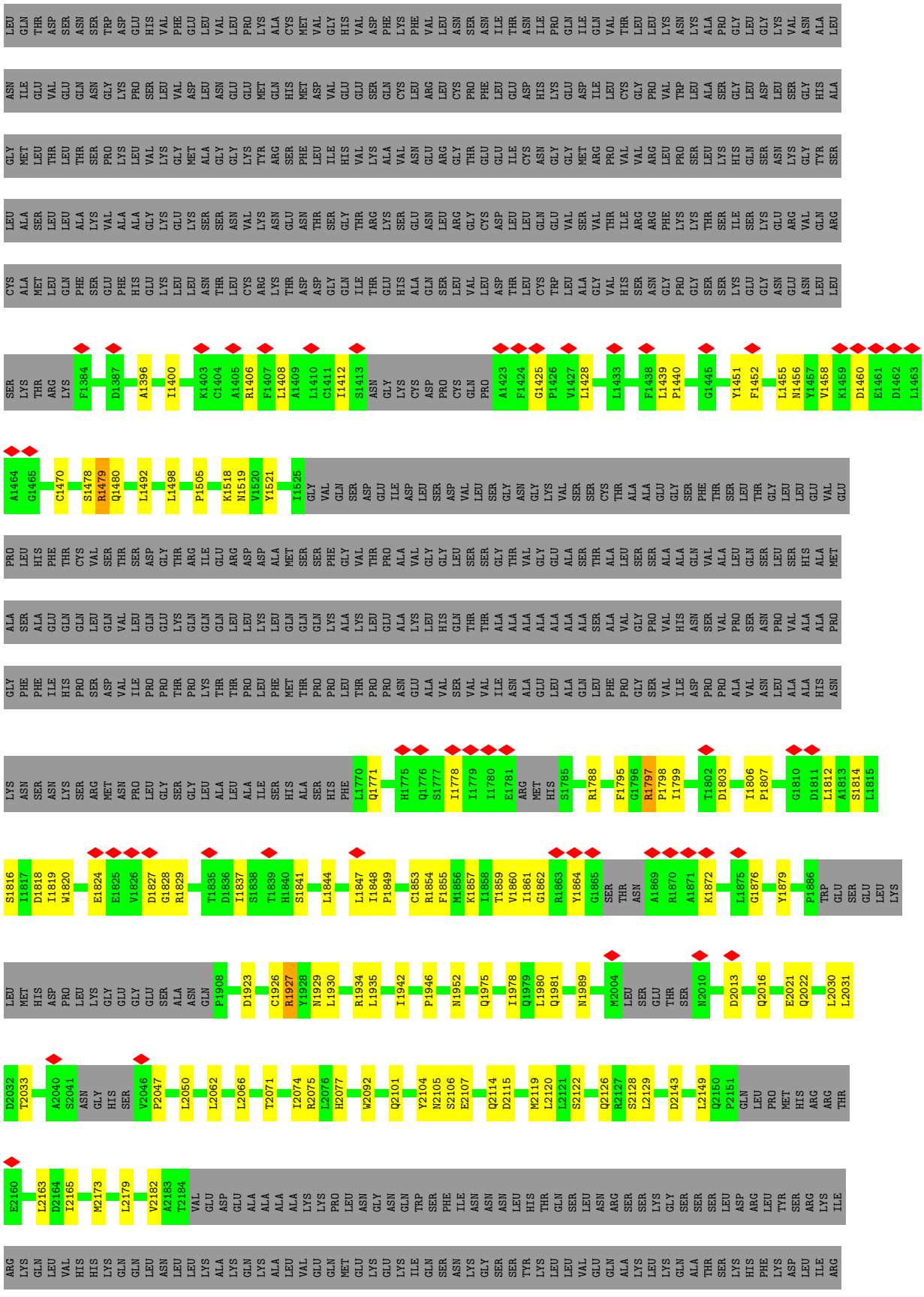
ARG ARG LYS GLY GLU LEU GLU SER ASN LEU ALA VAL VAL ASN GLY ALA ASN ILE SER VAL ILE GLN HIS GLU SER PRO ALA ASP VAL GLN THR PRO LEU ILE ILE GLN PRO GLU GLN ARG ASN VAL SER GLY GLY TYR LEU VAL LEU TYR LYS MET ASN TYR ALA THR ARG ILE VAL THR

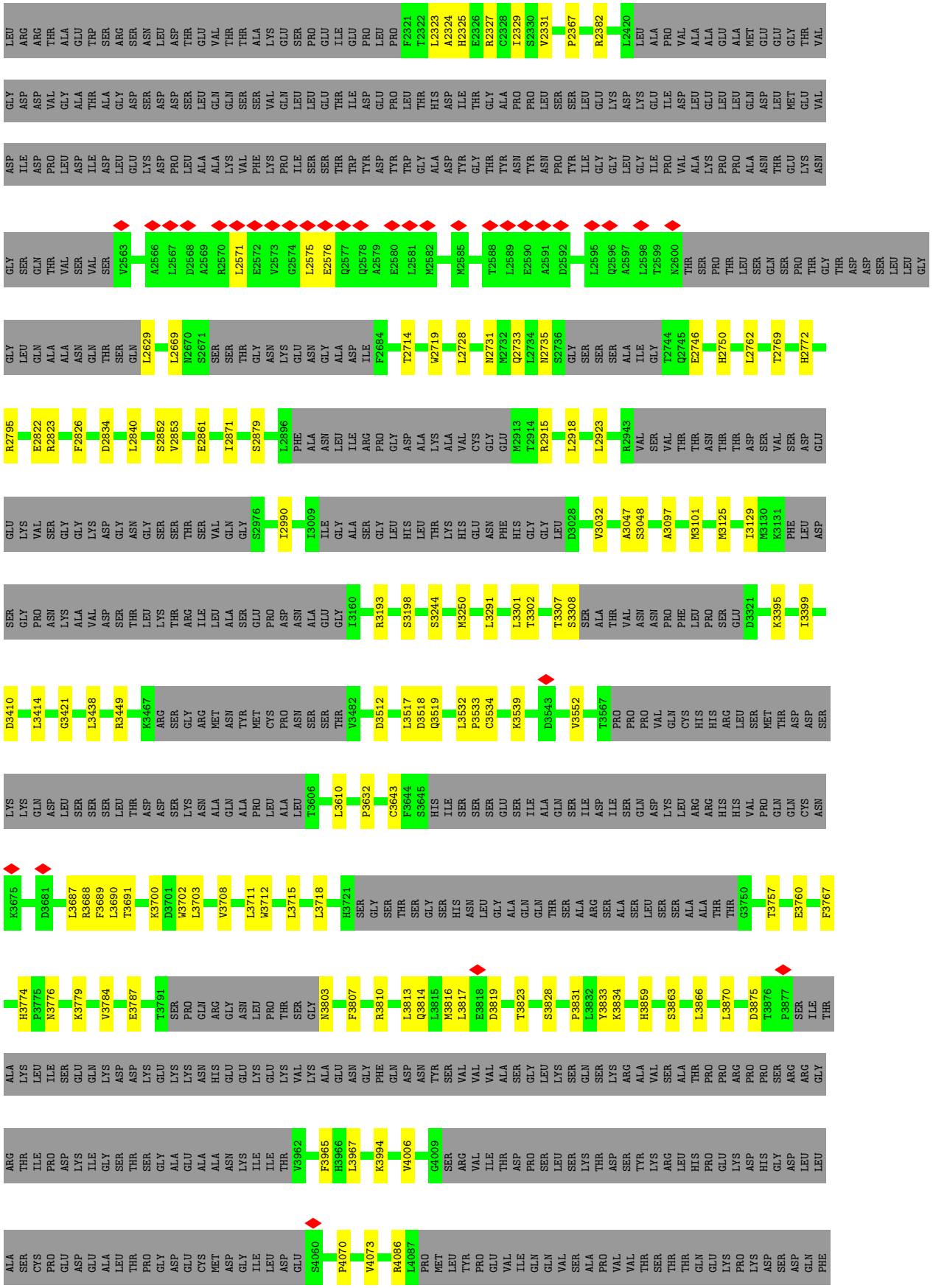
LEU GLU GLU GLU PRO ILE LYS ILE GLN HIS ILE LYS ASP PRO GLN ASP THR ILE THR SER LEU ILE LEU LEU PRO PRO ASP ILE LEU ASP ASN ARG GLU ASP ASP CYS GLU GLU PRO ILE GLU ASP MET GLN LEU THR SER LYS ASN GLY PHE GLU ARG GLU LYS THR SER ASP ILE SER

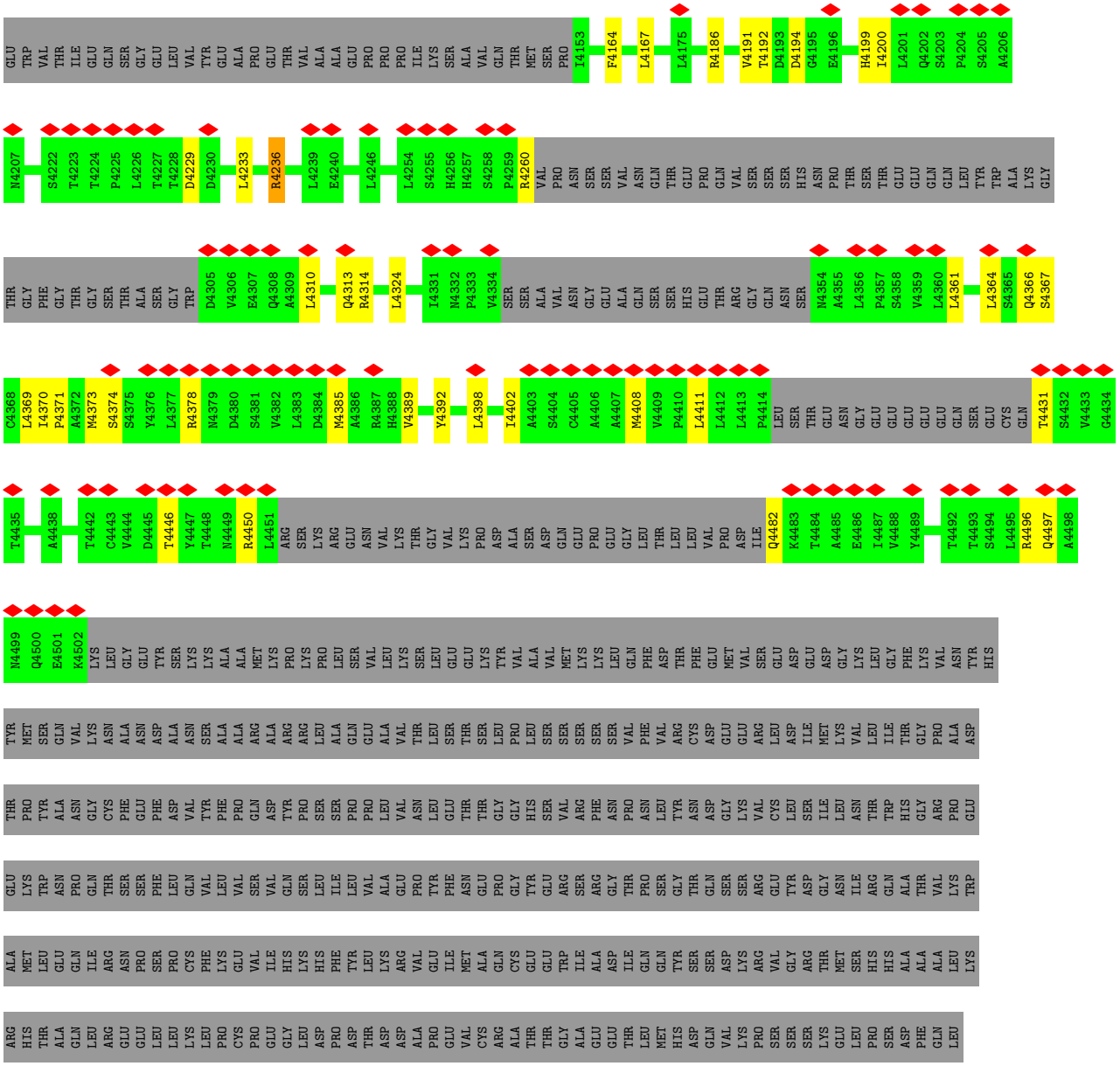
THR LEU GLY HIS LEU VAL ILE THR THR GLN GLY GLY TYR VAL LYS ILE LEU ASP LEU SER ASN PHE GLU ILE LEU ALA LYS VAL GLU PRO PRO LYS LYS GLU GLY THR GLU GLU GLN ASP THR PHE VAL SER VAL ILE TYR CYS SER GLY THR ASP ARG LEU CYS ALA CYS THR LYS GLY

GLY GLU LEU HIS PHE LEU GLN ILE 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 ASP LEU LEU VAL ASP GLN PRO PHE THR

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






GLU TRP VAL THR ILE GLU GLN SER GLY GLU LEU VAL TYR GLU ALA PRO GLU THR VAL ALA ALA GLU PRO PRO PRO ILE LYS SER ALA VAL GLN THR MET SER PRO I4153 F4164 L4167 L4175 R4186 V4191 T4192 D4193 D4194 G4195 E4196 H4199 I4200 L4201 Q4202 S4203 P4204 S4205 A4206
N4207 S4222 T4223 T4224 P4225 L4226 T4227 T4228 D4229 D4230 L4233 R4236 L4239 E4240 L4246 L4254 S4255 H4256 H4257 S4258 P4259 R4260 VAL PRO ASN SER SER VAL ASN GLN THR GLU PRO GLN VAL SER SER SER HIS ASN PRO THR SER THR GLU 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 Q4313 R4314 L4324 I4331 N4332 P4333 V4334 SER SER ALA VAL ASN GLY GLU ALA GLN SER SER HIS GLU THR ARG GLY GLN ASN SER N4354 A4355 L4356 P4357 S4358 V4359 L4360 L4361 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 Y4392 L4398 I4402 A4403 S4404 C4405 A4406 A4407 M4408 V4409 P4410 L4411 L4412 L4413 P4414 LEU SER THR GLU ASN GLY GLU GLU GLU GLU GLU GLN SER GLU CYS GLN T4431 S4432 V4433 G4434
T4435 A4438 T4442 C4443 V4444 D4445 T4446 Y4447 T4448 N4449 R4450 L4451 ARG SER LYS ARG GLU ASN VAL LYS THR GLY VAL LYS PRO ASP ALA SER ASP GLN GLU PRO GLU GLY LEU THR LEU LEU VAL PRO ASP ILE Q4482 K4483 T4484 A4485 E4486 I4487 V4488 Y4489 T4492 T4493 S4494 L4495 R4496 Q4497 A4498
N4499 Q4500 E4501 K4502 LYS LEU GLY GLU TYR SER LYS LYS ALA ALA MET LYS PRO LYS PRO LEU SER VAL LEU LYS SER LEU GLU GLU LYS TYR VAL ALA 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 ASN ASP ALA ASN SER ALA ALA ARG ALA ARG ARG LEU ALA GLN GLU ALA VAL THR LEU SER THR SER LEU PRO LEU SER SER SER SER VAL PHE VAL ARG CYS ASP GLU GLU ARG LEU ASP ILE MET LYS VAL 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 GLY 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 ASN PRO GLN THR SER SER PHE LEU GLN VAL 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

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	127710	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	49.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	18.896	Depositor
Minimum map value	-7.641	Depositor
Average map value	-0.020	Depositor
Map value standard deviation	0.841	Depositor
Recommended contour level	2.5	Depositor
Map size (Å)	258.0, 258.0, 258.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	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	0.26	0/16012	0.47	0/21743
1	B	0.27	0/15429	0.48	0/20963
All	All	0.26	0/31441	0.47	0/42706

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	15729	0	16117	199	0
1	B	15156	0	15536	177	0
All	All	30885	0	31653	362	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 6.

All (362) 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:1820:TRP:O	1:B:1855:PHE:HB2	1.66	0.96
1:A:2031:LEU:HD22	1:A:2077:HIS:HB3	1.56	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1927:ARG:HB3	1:B:1980:LEU:HD11	1.62	0.81
1:A:2332:VAL:HG13	1:A:2358:LEU:HD11	1.68	0.73
1:B:3828:SER:HB3	1:B:4006:VAL:HB	1.71	0.72
1:A:1817:ILE:HB	1:A:1832:VAL:HG12	1.72	0.71
1:A:1795:PHE:HB3	1:A:1799:ILE:HD12	1.73	0.70
1:A:1992:GLN:HA	1:A:1995:LYS:HG2	1.73	0.70
1:A:3421:GLY:HA2	1:B:2165:ILE:HG13	1.74	0.70
1:B:1818:ASP:HB2	1:B:1857:LYS:HB3	1.74	0.68
1:A:3775:PRO:HA	1:A:3778:GLN:HG3	1.75	0.68
1:B:4260:ARG:HE	1:B:4366:GLN:HA	1.57	0.67
1:B:1812:LEU:HA	1:B:1862:GLY:HA2	1.77	0.67
1:B:1406:ARG:NH1	1:B:2576:GLU:OE1	2.27	0.67
1:B:2324:ALA:HB3	1:B:2327:ARG:HD3	1.78	0.66
1:B:3803:ASN:N	1:B:4086:ARG:O	2.27	0.66
1:B:2746:GLU:OE1	1:B:2750:HIS:ND1	2.28	0.66
1:B:4186:ARG:HD2	1:B:4200:ILE:HD11	1.78	0.65
1:A:2733:GLN:NE2	1:A:2735:ASN:OD1	2.29	0.65
1:A:1817:ILE:HD13	1:A:1858:ILE:HG12	1.79	0.65
1:B:1946:PRO:O	1:B:1952:ASN:ND2	2.30	0.64
1:B:2013:ASP:HA	1:B:2016:GLN:HE21	1.62	0.64
1:B:3834:LYS:HD2	1:B:3875:ASP:HB3	1.79	0.64
1:B:2861:GLU:HG2	1:B:2990:ILE:HD11	1.79	0.64
1:A:3716:LEU:HD13	1:A:3788:LEU:HD22	1.79	0.63
1:B:4446:THR:HG22	1:B:4450:ARG:HE	1.64	0.63
1:A:1776:GLN:HG3	1:A:1875:LEU:HD21	1.81	0.63
1:A:2102:GLU:O	1:A:2108:GLN:NE2	2.31	0.63
1:B:2769:THR:HG1	1:B:2772:HIS:HE2	1.43	0.63
1:A:3817:LEU:HD22	1:A:4186:ARG:HG3	1.82	0.62
1:A:2714:THR:OG1	1:A:2719:TRP:NE1	2.30	0.62
1:A:2826:PHE:O	1:A:2915:ARG:NH2	2.32	0.62
1:A:3532:LEU:HD22	1:A:3539:LYS:HB2	1.80	0.62
1:A:4226:LEU:HD11	1:A:4235:ARG:HH21	1.65	0.62
1:B:3816:MET:HE1	1:B:4070:PRO:HB2	1.80	0.62
1:B:1844:LEU:HD21	1:B:1847:LEU:HD21	1.80	0.62
1:A:2120:LEU:O	1:A:2124:ILE:HG12	1.99	0.61
1:B:2714:THR:OG1	1:B:2719:TRP:NE1	2.31	0.61
1:A:1848:ILE:HD12	1:A:1850:PRO:HD3	1.82	0.61
1:B:3301:LEU:HD22	1:B:3308:SER:HB2	1.82	0.61
1:A:1399:SER:HB3	1:A:1403:LYS:HZ1	1.66	0.61
1:B:2733:GLN:OE1	1:B:2735:ASN:ND2	2.32	0.61
1:A:1517:CYS:SG	1:A:1518:LYS:N	2.71	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3632:PRO:HB3	1:B:3702:TRP:HZ2	1.66	0.60
1:B:3708:VAL:HG13	1:B:3711:LEU:HD12	1.83	0.60
1:A:1848:ILE:HD12	1:A:1849:PRO:HA	1.83	0.60
1:A:3709:ASN:HD21	1:A:3780:LEU:HD23	1.67	0.60
1:B:2822:GLU:OE2	1:B:2823:ARG:NH1	2.33	0.60
1:B:1440:PRO:O	1:B:2022:GLN:NE2	2.35	0.59
1:A:1988:HIS:CD2	1:A:1992:GLN:HE22	2.21	0.59
1:B:1848:ILE:HD12	1:B:1849:PRO:HA	1.82	0.59
1:B:3438:LEU:O	1:B:3449:ARG:NH1	2.34	0.59
1:A:2013:ASP:HA	1:A:2016:GLN:HB3	1.85	0.59
1:B:1807:PRO:HD3	1:B:1876:GLY:HA2	1.85	0.59
1:A:1803:ASP:HB3	1:A:1879:TYR:HB2	1.84	0.59
1:B:2104:TYR:OH	1:B:2114:GLN:O	2.20	0.59
1:A:2861:GLU:HG2	1:A:2990:ILE:HD11	1.83	0.59
1:A:1981:GLN:NE2	1:A:1985:ASN:OD1	2.31	0.58
1:A:1777:SER:HB2	1:A:1872:LYS:HE3	1.86	0.58
1:A:1815:LEU:HB2	1:A:1837:ILE:HD13	1.85	0.58
1:A:2071:THR:H	1:A:2074:ILE:HG22	1.68	0.58
1:B:1505:PRO:O	1:B:1981:GLN:NE2	2.28	0.58
1:B:1428:LEU:HD11	1:B:1458:VAL:HG11	1.85	0.58
1:B:4361:LEU:HA	1:B:4411:LEU:HD11	1.86	0.58
1:A:3638:SER:HB3	1:A:3678:ILE:HG13	1.86	0.58
1:B:1812:LEU:HD23	1:B:1837:ILE:HG21	1.85	0.58
1:B:3712:TRP:CD1	1:B:3767:PHE:HE2	2.21	0.58
1:A:4179:LYS:HD2	1:A:4182:GLN:HE21	1.68	0.58
1:A:2139:LEU:HD12	1:A:2331:VAL:HG11	1.85	0.57
1:A:1403:LYS:HD2	1:A:1848:ILE:HG12	1.86	0.57
1:A:1480:GLN:HG2	1:A:2015:ILE:HG12	1.86	0.57
1:B:1797:ARG:NH1	1:B:1798:PRO:O	2.37	0.57
1:B:3774:HIS:CE1	1:B:3776:ASN:HB2	2.39	0.57
1:A:1917:MET:HB3	1:A:1991:VAL:HG22	1.87	0.56
1:A:1819:ILE:HD12	1:A:1853:CYS:HB2	1.87	0.56
1:B:1806:ILE:O	1:B:1841:SER:OG	2.23	0.56
1:A:4235:ARG:NH2	1:A:4330:TYR:O	2.38	0.56
1:B:3517:LEU:HD12	1:B:3552:VAL:HG11	1.88	0.56
1:B:4374:SER:O	1:B:4378:ARG:HB2	2.05	0.56
1:B:1452:PHE:O	1:B:1456:ASN:ND2	2.36	0.56
1:B:1812:LEU:HD11	1:B:1860:VAL:HB	1.88	0.56
1:A:3694:GLY:O	1:A:3769:GLN:NE2	2.39	0.56
1:A:1311:ILE:HG23	1:A:1314:GLU:HG2	1.87	0.55
1:B:2071:THR:HG22	1:B:2074:ILE:HG22	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2143:ASP:HB2	1:A:2331:VAL:HG22	1.88	0.55
1:A:3389:SER:OG	1:A:3390:THR:N	2.38	0.55
1:A:4393:ARG:HE	1:A:4488:VAL:HG21	1.72	0.55
1:A:1813:ALA:HB2	1:A:1863:ARG:HA	1.89	0.55
1:B:3779:LYS:HZ3	1:B:4073:VAL:HG13	1.72	0.55
1:A:4364:LEU:HD22	1:A:4369:LEU:HD22	1.89	0.55
1:B:1853:CYS:SG	1:B:1854:ARG:N	2.80	0.54
1:A:3817:LEU:HD21	1:A:4185:LEU:HB3	1.89	0.54
1:A:3687:LEU:HD22	1:A:3762:ALA:HB1	1.89	0.54
1:B:3097:ALA:O	1:B:3101:MET:HG3	2.08	0.54
1:A:3517:LEU:HD12	1:A:3552:VAL:HG11	1.90	0.54
1:A:2031:LEU:CD2	1:A:2077:HIS:HB3	2.35	0.54
1:A:3866:LEU:HD11	1:A:3986:LEU:HD11	1.89	0.54
1:B:2826:PHE:O	1:B:2915:ARG:NH2	2.40	0.53
1:B:1479:ARG:HG3	1:B:1480:GLN:N	2.22	0.53
1:A:1812:LEU:HD13	1:A:1862:GLY:HA2	1.88	0.53
1:A:2915:ARG:NH1	1:B:2772:HIS:HB2	2.24	0.53
1:B:2769:THR:OG1	1:B:2772:HIS:NE2	2.37	0.53
1:B:3532:LEU:HD12	1:B:3533:PRO:HD2	1.91	0.53
1:A:2013:ASP:O	1:A:2017:THR:OG1	2.24	0.53
1:A:1967:ASP:HA	1:A:1970:VAL:HG12	1.91	0.53
1:B:2179:LEU:HA	1:B:2182:VAL:HG12	1.91	0.53
1:A:2018:SER:OG	1:A:2019:SER:N	2.40	0.53
1:B:2021:GLU:N	1:B:2021:GLU:OE1	2.41	0.53
1:A:1313:LYS:HB3	1:A:1316:VAL:HB	1.91	0.53
1:A:2358:LEU:HD23	1:A:2411:MET:SD	2.49	0.53
1:A:2564:SER:O	1:A:2584:LYS:NZ	2.36	0.53
1:A:3614:ALA:HB2	1:A:3689:PHE:HD1	1.73	0.52
1:B:1788:ARG:HD3	1:B:1861:ILE:HG23	1.90	0.52
1:A:1782:ARG:HG2	1:A:1784:HIS:H	1.73	0.52
1:A:3244:SER:HB2	1:A:3250:MET:HG2	1.91	0.52
1:A:4361:LEU:HD13	1:A:4408:MET:HA	1.92	0.52
1:A:3124:SER:OG	1:A:3125:MET:N	2.41	0.52
1:A:3771:ILE:HG21	1:A:3815:LEU:HD21	1.92	0.52
1:A:3488:MET:CE	1:B:2107:GLU:HA	2.40	0.52
1:B:4378:ARG:NH2	1:B:4431:THR:OG1	2.43	0.52
1:A:2004:MET:SD	1:A:2004:MET:N	2.78	0.51
1:A:3634:LEU:HD12	1:A:3676:MET:HG2	1.92	0.51
1:A:3438:LEU:O	1:A:3449:ARG:NH1	2.42	0.51
1:A:2075:ARG:HG2	1:A:2120:LEU:HD22	1.92	0.51
1:A:2636:VAL:HG23	1:A:2637:PRO:HD3	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3687:LEU:HA	1:B:3690:LEU:HD12	1.91	0.51
1:A:3834:LYS:HD2	1:A:3875:ASP:HB3	1.92	0.51
1:B:2149:LEU:HD23	1:B:2163:LEU:HD11	1.93	0.51
1:A:1399:SER:HB3	1:A:1403:LYS:NZ	2.26	0.51
1:B:2101:GLN:O	1:B:2105:ASN:HB2	2.10	0.51
1:B:2129:LEU:HD21	1:B:2182:VAL:HB	1.93	0.51
1:B:2031:LEU:HD21	1:B:2077:HIS:HB3	1.94	0.50
1:B:2325:HIS:HB2	1:B:2367:PRO:HG2	1.93	0.50
1:A:3429:ASP:HA	1:A:3432:ILE:HD12	1.92	0.50
1:A:3632:PRO:HB3	1:A:3702:TRP:CZ2	2.45	0.50
1:A:4397:GLU:OE1	1:A:4400:ARG:NH1	2.43	0.50
1:A:2051:GLN:N	1:A:2051:GLN:OE1	2.43	0.50
1:A:2047:PRO:O	1:A:2051:GLN:NE2	2.37	0.50
1:A:1353:LEU:HD11	1:A:1400:ILE:HG23	1.92	0.50
1:A:3760:GLU:OE2	1:B:1929:ASN:ND2	2.45	0.50
1:B:2571:LEU:HD23	1:B:2575:LEU:HD13	1.94	0.50
1:B:3244:SER:HB2	1:B:3250:MET:HG2	1.94	0.50
1:A:4310:LEU:O	1:A:4313:GLN:HG3	2.11	0.50
1:B:2115:ASP:OD1	1:B:2115:ASP:N	2.44	0.49
1:A:1816:SER:HB2	1:A:1859:THR:OG1	2.13	0.49
1:B:3410:ASP:OD1	1:B:3410:ASP:N	2.44	0.49
1:B:3688:ARG:O	1:B:3691:THR:OG1	2.22	0.49
1:B:3816:MET:HG3	1:B:3817:LEU:H	1.77	0.49
1:A:2769:THR:OG1	1:A:2772:HIS:NE2	2.40	0.49
1:B:3632:PRO:HB3	1:B:3702:TRP:CZ2	2.47	0.49
1:A:1817:ILE:HG23	1:A:1856:MET:CE	2.43	0.49
1:A:4226:LEU:HD21	1:A:4235:ARG:HE	1.77	0.49
1:A:2834:ASP:OD1	1:A:2834:ASP:N	2.45	0.49
1:A:2775:ASN:HD21	1:B:2879:SER:HB3	1.78	0.49
1:B:1819:ILE:HG23	1:B:1829:ARG:HB2	1.95	0.49
1:A:1807:PRO:HD3	1:A:1876:GLY:HA2	1.94	0.49
1:A:2366:ARG:HB2	1:A:2367:PRO:HD3	1.95	0.49
1:A:3250:MET:SD	1:A:3279:CYS:HB2	2.53	0.48
1:B:3125:MET:O	1:B:3129:ILE:HG12	2.13	0.48
1:B:2834:ASP:OD1	1:B:2834:ASP:N	2.43	0.48
1:B:3534:CYS:HA	1:B:3539:LYS:HD3	1.94	0.48
1:A:1991:VAL:HG12	1:A:1995:LYS:NZ	2.28	0.48
1:A:2129:LEU:HD21	1:A:2178:LEU:HG	1.94	0.48
1:A:3967:LEU:HD23	1:A:4004:LEU:HD22	1.95	0.48
1:B:3810:ARG:NH1	1:B:3814:GLN:OE1	2.44	0.48
1:A:2382:ARG:NH2	1:B:3414:LEU:O	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1824:GLU:N	1:B:1824:GLU:OE1	2.46	0.48
1:B:2325:HIS:CD2	1:B:2329:ILE:HD11	2.49	0.48
1:B:4370:ILE:HB	1:B:4371:PRO:HD3	1.95	0.48
1:A:1793:LEU:HB2	1:A:1856:MET:HB3	1.95	0.48
1:B:1492:LEU:HG	1:B:1498:LEU:HB2	1.96	0.48
1:B:3760:GLU:HB2	1:B:3807:PHE:CE1	2.49	0.48
1:B:2115:ASP:O	1:B:2119:MET:HG3	2.13	0.47
1:B:3687:LEU:O	1:B:3691:THR:HG23	2.13	0.47
1:B:1816:SER:HB2	1:B:1859:THR:OG1	2.13	0.47
1:A:1799:ILE:HG22	1:A:1801:LEU:HD12	1.97	0.47
1:A:3963:PRO:HA	1:A:4009:GLY:O	2.13	0.47
1:B:1519:ASN:OD1	1:B:1989:ASN:ND2	2.41	0.47
1:A:2073:LYS:O	1:A:2077:HIS:ND1	2.48	0.47
1:B:1479:ARG:HE	1:B:1479:ARG:HB2	1.51	0.47
1:B:3823:THR:HG22	1:B:3859:HIS:ND1	2.29	0.47
1:A:2587:SER:O	1:A:2590:GLU:HG3	2.15	0.47
1:A:3429:ASP:OD1	1:A:3429:ASP:N	2.48	0.47
1:A:4081:ALA:HB1	1:A:4166:ARG:HH12	1.78	0.47
1:B:4233:LEU:O	1:B:4236:ARG:HD3	2.15	0.47
1:A:4231:GLY:O	1:A:4235:ARG:HG2	2.14	0.47
1:B:1778:ILE:HD11	1:B:1872:LYS:HA	1.97	0.47
1:A:1520:VAL:HG22	1:A:1879:TYR:HB3	1.95	0.47
1:B:2852:SER:OG	1:B:2853:VAL:N	2.48	0.47
1:B:3198:SER:HA	1:B:3291:LEU:O	2.15	0.47
1:A:1820:TRP:O	1:A:1855:PHE:HB2	2.15	0.47
1:B:4402:ILE:HG23	1:B:4408:MET:HG3	1.96	0.46
1:A:3409:SER:HB2	1:A:3418:LEU:HD23	1.97	0.46
1:B:3700:LYS:HA	1:B:3703:LEU:HD12	1.96	0.46
1:A:2840:LEU:HD12	1:A:2918:LEU:HD12	1.98	0.46
1:B:3047:ALA:O	1:B:3048:SER:OG	2.28	0.46
1:B:3819:ASP:OD2	1:B:3863:SER:OG	2.28	0.46
1:A:1939:LEU:HD13	1:A:1970:VAL:HG21	1.96	0.46
1:B:2840:LEU:HD12	1:B:2918:LEU:HD12	1.98	0.46
1:A:2416:LEU:HD12	1:A:2667:LEU:HD22	1.97	0.46
1:A:4374:SER:O	1:A:4378:ARG:HB2	2.16	0.46
1:B:1521:TYR:HB2	1:B:1771:GLN:HG2	1.97	0.46
1:B:2323:LEU:HA	1:B:2327:ARG:NH2	2.31	0.46
1:A:2582:MET:O	1:A:2585:MET:HG3	2.15	0.46
1:A:3810:ARG:HD3	1:B:1926:CYS:O	2.15	0.46
1:B:3610:LEU:HD12	1:B:3689:PHE:CG	2.51	0.45
1:A:1498:LEU:HD13	1:A:1974:TYR:CD2	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1819:ILE:HG13	1:B:1853:CYS:SG	2.56	0.45
1:A:1387:ASP:HA	1:A:1390:ARG:HG2	1.99	0.45
1:B:2075:ARG:HG2	1:B:2120:LEU:HD22	1.99	0.45
1:B:2143:ASP:HB2	1:B:2331:VAL:HG22	1.98	0.45
1:B:2325:HIS:NE2	1:B:2329:ILE:HD11	2.32	0.45
1:B:2575:LEU:H	1:B:2575:LEU:HD23	1.82	0.45
1:A:2568:ASP:HB3	1:A:2570:ARG:HH12	1.82	0.45
1:B:1451:TYR:O	1:B:1455:LEU:HD23	2.17	0.45
1:B:3870:LEU:HD21	1:B:3965:PHE:HB2	1.98	0.45
1:A:3809:ARG:HH22	1:B:1923:ASP:HA	1.82	0.45
1:B:3302:THR:OG1	1:B:3307:THR:OG1	2.21	0.45
1:A:2061:GLU:HA	1:A:2064:LYS:HG2	1.99	0.44
1:B:2822:GLU:HG3	1:B:2823:ARG:HG2	1.98	0.44
1:B:1819:ILE:HD11	1:B:1853:CYS:HB2	1.98	0.44
1:B:3813:LEU:HD21	1:B:4191:VAL:HG21	1.99	0.44
1:B:3831:PRO:HB2	1:B:3833:TYR:CZ	2.52	0.44
1:B:4496:ARG:HG3	1:B:4497:GLN:N	2.31	0.44
1:B:1975:GLN:HA	1:B:1978:ILE:HG12	1.99	0.44
1:A:3198:SER:HA	1:A:3291:LEU:O	2.18	0.44
1:A:2976:SER:HA	1:A:2977:PRO:HD3	1.84	0.44
1:B:2030:LEU:O	1:B:2033:THR:OG1	2.30	0.44
1:B:3512:ASP:OD1	1:B:3512:ASP:N	2.45	0.44
1:A:1844:LEU:HD23	1:A:1844:LEU:HA	1.85	0.44
1:B:1788:ARG:HH12	1:B:1864:TYR:HD1	1.66	0.44
1:B:2031:LEU:CD2	1:B:2077:HIS:HB3	2.48	0.44
1:B:3643:CYS:HA	1:B:3718:LEU:HD12	1.98	0.44
1:B:4186:ARG:NE	1:B:4194:ASP:HA	2.33	0.44
1:A:2352:LEU:HD21	1:A:2403:TRP:HB3	2.00	0.44
1:A:4356:LEU:HD12	1:A:4360:LEU:HD23	1.98	0.44
1:A:4363:LEU:O	1:A:4367:SER:HB3	2.17	0.44
1:A:4389:VAL:HG13	1:A:4485:ALA:HB2	2.00	0.44
1:A:1817:ILE:HG22	1:A:1831:LEU:HB2	1.99	0.44
1:A:2731:ASN:OD1	1:A:2795:ARG:NH2	2.47	0.44
1:B:2324:ALA:H	1:B:2327:ARG:CZ	2.31	0.44
1:B:2871:ILE:HD11	1:B:3032:VAL:HG11	2.00	0.44
1:A:1945:PRO:HG2	1:A:1955:TYR:CD2	2.52	0.44
1:A:3560:LEU:O	1:A:3564:MET:HG2	2.18	0.44
1:A:3771:ILE:HD11	1:A:3778:GLN:HA	2.00	0.44
1:B:4310:LEU:O	1:B:4313:GLN:HG3	2.18	0.44
1:B:4369:LEU:HG	1:B:4373:MET:HE2	2.00	0.44
1:A:1473:LEU:HD23	1:A:2030:LEU:HD12	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2083:VAL:HG23	1:A:2124:ILE:HD12	2.00	0.43
1:A:2165:ILE:HG13	1:B:3421:GLY:HA2	2.00	0.43
1:A:4178:ARG:HH12	1:A:4182:GLN:HB3	1.83	0.43
1:A:4197:GLY:HA2	1:B:1934:ARG:NH2	2.33	0.43
1:B:3518:ASP:OD1	1:B:3519:GLN:N	2.47	0.43
1:A:2055:HIS:ND1	1:A:2056:ALA:O	2.51	0.43
1:A:2049:VAL:O	1:A:2052:SER:OG	2.28	0.43
1:A:2563:VAL:HG11	1:A:2588:THR:HG22	2.00	0.43
1:A:3532:LEU:HD11	1:A:3538:LEU:HD23	1.98	0.43
1:A:3771:ILE:HG13	1:A:3771:ILE:O	2.19	0.43
1:B:1460:ASP:OD1	1:B:1460:ASP:N	2.51	0.43
1:A:3512:ASP:OD1	1:A:3512:ASP:N	2.44	0.43
1:A:3858:LEU:HB3	1:A:3860:LEU:HD23	2.00	0.43
1:B:2669:LEU:HD23	1:B:2669:LEU:HA	1.84	0.43
1:A:1964:VAL:HA	1:A:1967:ASP:OD2	2.18	0.43
1:A:3755:GLN:O	1:A:3759:ILE:HG12	2.18	0.43
1:A:4260:ARG:C	1:A:4366:GLN:HE21	2.22	0.43
1:B:4364:LEU:O	1:B:4367:SER:OG	2.27	0.43
1:B:2731:ASN:OD1	1:B:2795:ARG:NH2	2.46	0.43
1:A:1475:THR:O	1:A:1479:ARG:NH1	2.52	0.43
1:A:2060:GLU:HA	1:A:2095:PHE:HE1	1.84	0.43
1:A:2578:GLN:O	1:A:2582:MET:HG2	2.18	0.43
1:A:1832:VAL:HG23	1:A:2567:LEU:O	2.19	0.43
1:B:4310:LEU:HB3	1:B:4314:ARG:HH21	1.82	0.43
1:A:2399:TRP:HB3	1:A:2405:GLN:OE1	2.19	0.43
1:A:2850:VAL:HG12	1:A:2850:VAL:O	2.19	0.43
1:A:4192:THR:HB	1:A:4199:HIS:CE1	2.54	0.43
1:A:3414:LEU:O	1:B:2382:ARG:NH2	2.49	0.43
1:A:3632:PRO:O	1:A:3636:VAL:HG22	2.18	0.43
1:B:3784:VAL:O	1:B:3787:GLU:HG3	2.18	0.43
1:A:1992:GLN:HG3	1:A:1995:LYS:HZ3	1.84	0.42
1:A:3040:LEU:HD23	1:A:3040:LEU:HA	1.93	0.42
1:A:1402:HIS:CE1	1:A:1846:ASP:HB3	2.52	0.42
1:A:3831:PRO:HB2	1:A:3833:TYR:CZ	2.55	0.42
1:B:1425:GLY:O	1:B:1428:LEU:HG	2.19	0.42
1:B:1470:CYS:SG	1:B:2030:LEU:HG	2.60	0.42
1:A:1924:ILE:HA	1:A:1927:ARG:HE	1.82	0.42
1:A:2089:GLU:HG3	1:A:2091:TRP:NE1	2.35	0.42
1:A:2105:ASN:OD1	1:A:2106:SER:N	2.53	0.42
1:B:1788:ARG:CD	1:B:1861:ILE:HG23	2.49	0.42
1:A:2391:ASP:OD1	1:A:2391:ASP:N	2.46	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3809:ARG:NH1	1:B:1923:ASP:OD1	2.44	0.42
1:B:1814:SER:HB3	1:B:1861:ILE:HB	2.02	0.42
1:A:3126:VAL:HG13	1:B:2173:MET:SD	2.60	0.42
1:A:4186:ARG:NE	1:A:4194:ASP:HA	2.35	0.42
1:B:2105:ASN:OD1	1:B:2106:SER:N	2.52	0.42
1:A:2669:LEU:HD23	1:A:2669:LEU:HA	1.82	0.42
1:A:3614:ALA:HB2	1:A:3689:PHE:CD1	2.53	0.42
1:A:4173:VAL:HG12	1:A:4216:VAL:HG23	2.02	0.42
1:A:1817:ILE:HG23	1:A:1856:MET:HE3	2.00	0.41
1:A:1993:ARG:O	1:A:1996:VAL:HG12	2.20	0.41
1:A:3828:SER:HB3	1:A:4006:VAL:HB	2.03	0.41
1:B:1820:TRP:HA	1:B:1829:ARG:HH21	1.84	0.41
1:B:1942:ILE:HD12	1:B:1942:ILE:HA	1.92	0.41
1:B:2923:LEU:HD23	1:B:2923:LEU:HA	1.85	0.41
1:B:4192:THR:HB	1:B:4199:HIS:CE1	2.55	0.41
1:A:2325:HIS:O	1:A:2329:ILE:HG23	2.20	0.41
1:A:3834:LYS:O	1:A:3856:ARG:NH2	2.47	0.41
1:B:2105:ASN:ND2	1:B:2107:GLU:HB2	2.35	0.41
1:B:2762:LEU:HD23	1:B:2762:LEU:HA	1.82	0.41
1:A:1347:HIS:O	1:A:1351:LEU:HG	2.20	0.41
1:B:1827:ASP:OD1	1:B:1827:ASP:N	2.53	0.41
1:B:2122:SER:O	1:B:2126:GLN:HG3	2.20	0.41
1:B:3395:LYS:O	1:B:3399:ILE:HG12	2.21	0.41
1:B:4229:ASP:N	1:B:4229:ASP:OD1	2.54	0.41
1:A:1345:THR:O	1:A:1349:GLN:HG2	2.20	0.41
1:A:2113:PRO:O	1:A:2117:VAL:HG23	2.20	0.41
1:B:1795:PHE:HB3	1:B:1799:ILE:HD12	2.03	0.41
1:B:2092:TRP:NE1	1:B:2128:SER:OG	2.51	0.41
1:B:4389:VAL:HG22	1:B:4482:GLN:HE22	1.85	0.41
1:A:1853:CYS:SG	1:A:1854:ARG:N	2.93	0.41
1:A:2178:LEU:HD12	1:A:2178:LEU:HA	1.96	0.41
1:A:2337:LEU:HD12	1:A:2337:LEU:HA	1.92	0.41
1:B:1518:LYS:HD3	1:B:1519:ASN:H	1.85	0.41
1:B:1812:LEU:HD12	1:B:1862:GLY:HA2	2.02	0.41
1:B:2728:LEU:HD23	1:B:2728:LEU:HA	1.92	0.41
1:B:1935:LEU:HD12	1:B:1935:LEU:HA	1.90	0.41
1:B:3715:LEU:HD23	1:B:3715:LEU:HA	1.91	0.41
1:A:1470:CYS:HB3	1:A:2030:LEU:HD21	2.03	0.41
1:A:3364:ALA:HA	1:A:3422:ARG:NH1	2.36	0.41
1:B:1408:LEU:O	1:B:1412:ILE:HG12	2.20	0.41
1:B:1439:LEU:N	1:B:1440:PRO:HD2	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1820:TRP:HB3	1:B:1828:GLY:HA2	2.03	0.41
1:B:3757:THR:HA	1:B:3760:GLU:HG2	2.03	0.41
1:A:1394:PHE:HE2	1:A:1435:ASN:HD21	1.68	0.41
1:A:2071:THR:HG22	1:A:2074:ILE:HG22	2.02	0.41
1:A:3399:ILE:HD13	1:A:3399:ILE:HA	1.91	0.41
1:A:3810:ARG:NH1	1:B:1930:LEU:HA	2.35	0.41
1:B:1803:ASP:HB3	1:B:1879:TYR:HD2	1.86	0.41
1:B:2840:LEU:HD23	1:B:2840:LEU:HA	1.91	0.41
1:B:4324:LEU:HG	1:B:4398:LEU:HD13	2.02	0.41
1:A:1976:ASP:O	1:A:1979:GLN:HG3	2.21	0.41
1:A:1979:GLN:NE2	1:A:1980:LEU:HG	2.36	0.41
1:A:4219:SER:O	1:A:4223:THR:OG1	2.27	0.41
1:A:2165:ILE:HD13	1:A:2165:ILE:HA	1.86	0.40
1:B:2047:PRO:HB2	1:B:2050:LEU:HB3	2.03	0.40
1:B:2629:LEU:HD23	1:B:2629:LEU:HA	1.97	0.40
1:B:4385:MET:HG2	1:B:4392:TYR:CE2	2.56	0.40
1:A:4496:ARG:O	1:A:4500:GLN:HB2	2.21	0.40
1:A:1406:ARG:HG3	1:A:2579:ALA:CB	2.51	0.40
1:A:2852:SER:OG	1:A:2853:VAL:N	2.55	0.40
1:A:2857:SER:O	1:A:2861:GLU:HG3	2.22	0.40
1:A:4252:SER:HB2	1:A:4368:CYS:SG	2.61	0.40
1:B:2062:LEU:HD11	1:B:2066:LEU:HD12	2.04	0.40
1:B:3866:LEU:HD23	1:B:3967:LEU:HD12	2.04	0.40
1:A:1921:GLN:HE22	1:A:1988:HIS:HD2	1.68	0.40
1:A:3353:ALA:N	1:A:3354:PRO:HD2	2.36	0.40
1:B:1396:ALA:HB1	1:B:1400:ILE:HG21	2.03	0.40
1:A:1439:LEU:N	1:A:1440:PRO:HD2	2.37	0.40
1:A:1473:LEU:O	1:A:1477:VAL:HG23	2.22	0.40
1:A:1988:HIS:NE2	1:A:1992:GLN:NE2	2.70	0.40
1:A:4260:ARG:O	1:A:4366:GLN:NE2	2.47	0.40
1:A:4380:ASP:N	1:A:4380:ASP:OD1	2.54	0.40
1:B:4164:PHE:HA	1:B:4167:LEU:HD13	2.03	0.40

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	1971/4859 (41%)	1901 (96%)	70 (4%)	0	100 100
1	B	1901/4859 (39%)	1835 (96%)	66 (4%)	0	100 100
All	All	3872/9718 (40%)	3736 (96%)	136 (4%)	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	1783/4217 (42%)	1779 (100%)	4 (0%)	93 97
1	B	1717/4217 (41%)	1710 (100%)	7 (0%)	91 95
All	All	3500/8434 (42%)	3489 (100%)	11 (0%)	92 96

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1337	ARG
1	A	1829	ARG
1	A	1989	ASN
1	A	3994	LYS
1	B	1478	SER
1	B	1479	ARG
1	B	1797	ARG
1	B	1927	ARG
1	B	3193	ARG
1	B	3994	LYS
1	B	4236	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1921	GLN
1	B	1480	GLN
1	B	1929	ASN
1	B	2016	GLN
1	B	2022	GLN
1	B	2735	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 monosaccharides 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.

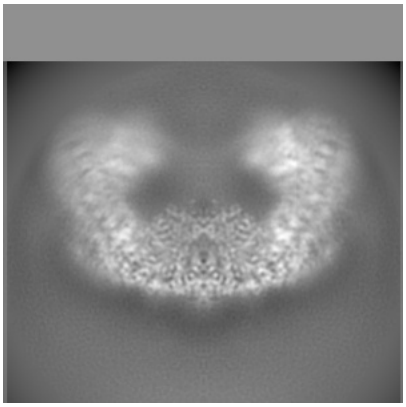
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-15653. These allow visual inspection of the internal detail of the map and identification of artifacts.

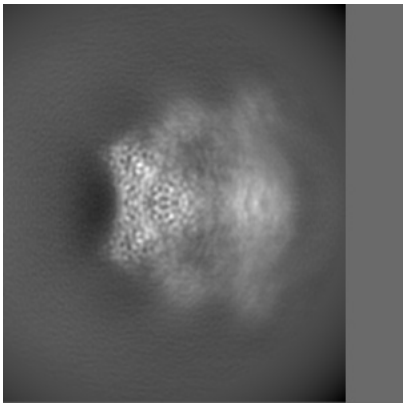
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

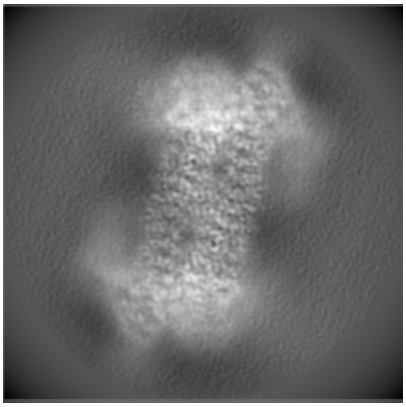
6.1.1 Primary map



X



Y

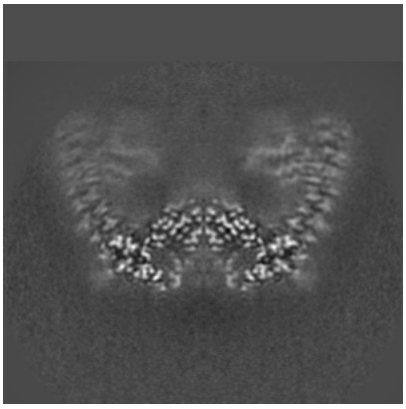


Z

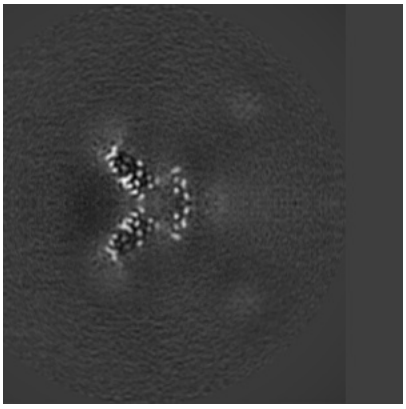
The images above show the map projected in three orthogonal directions.

6.2 Central slices

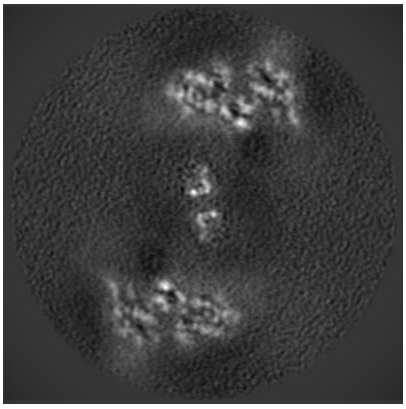
6.2.1 Primary map



X Index: 150



Y Index: 150

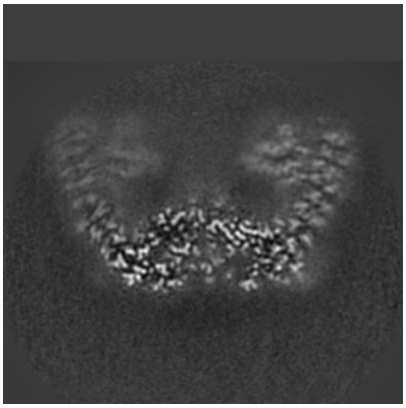


Z Index: 150

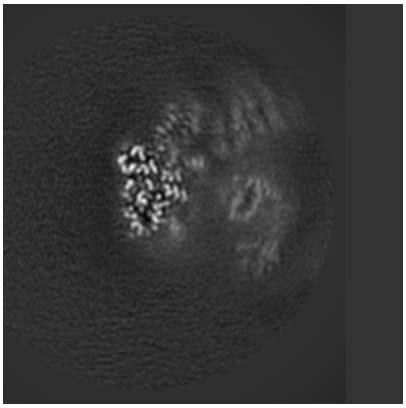
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

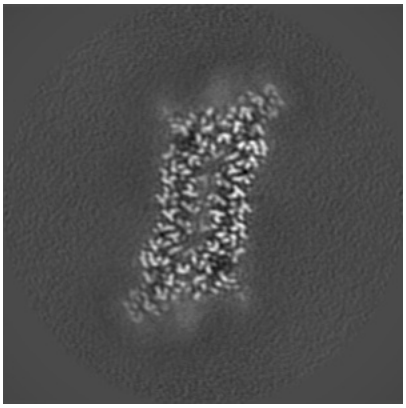
6.3.1 Primary map



X Index: 154



Y Index: 207



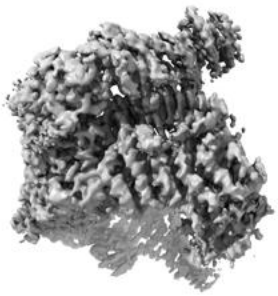
Z Index: 101

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 2.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

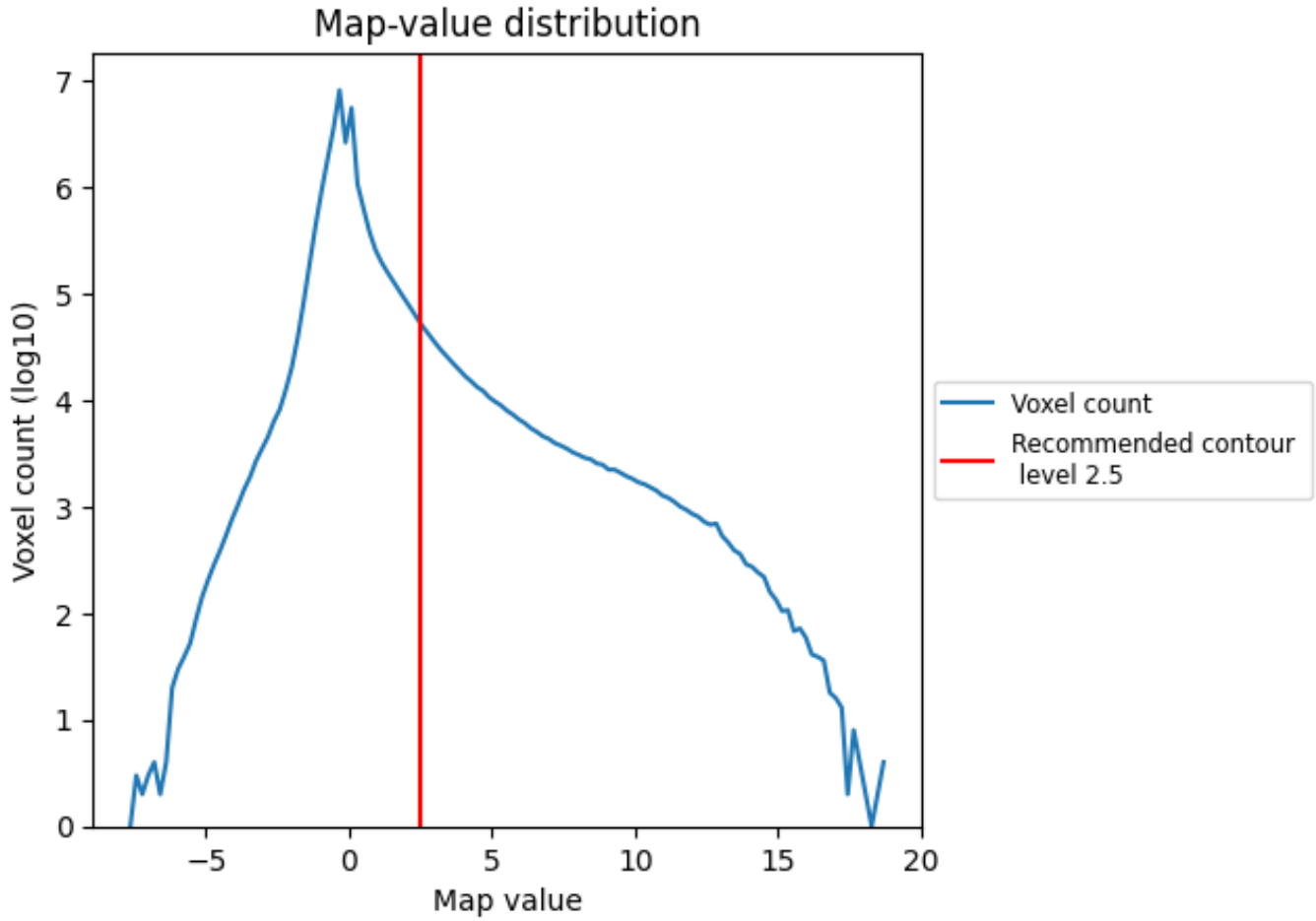
6.5 Mask visualisation (i)

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

7 Map analysis

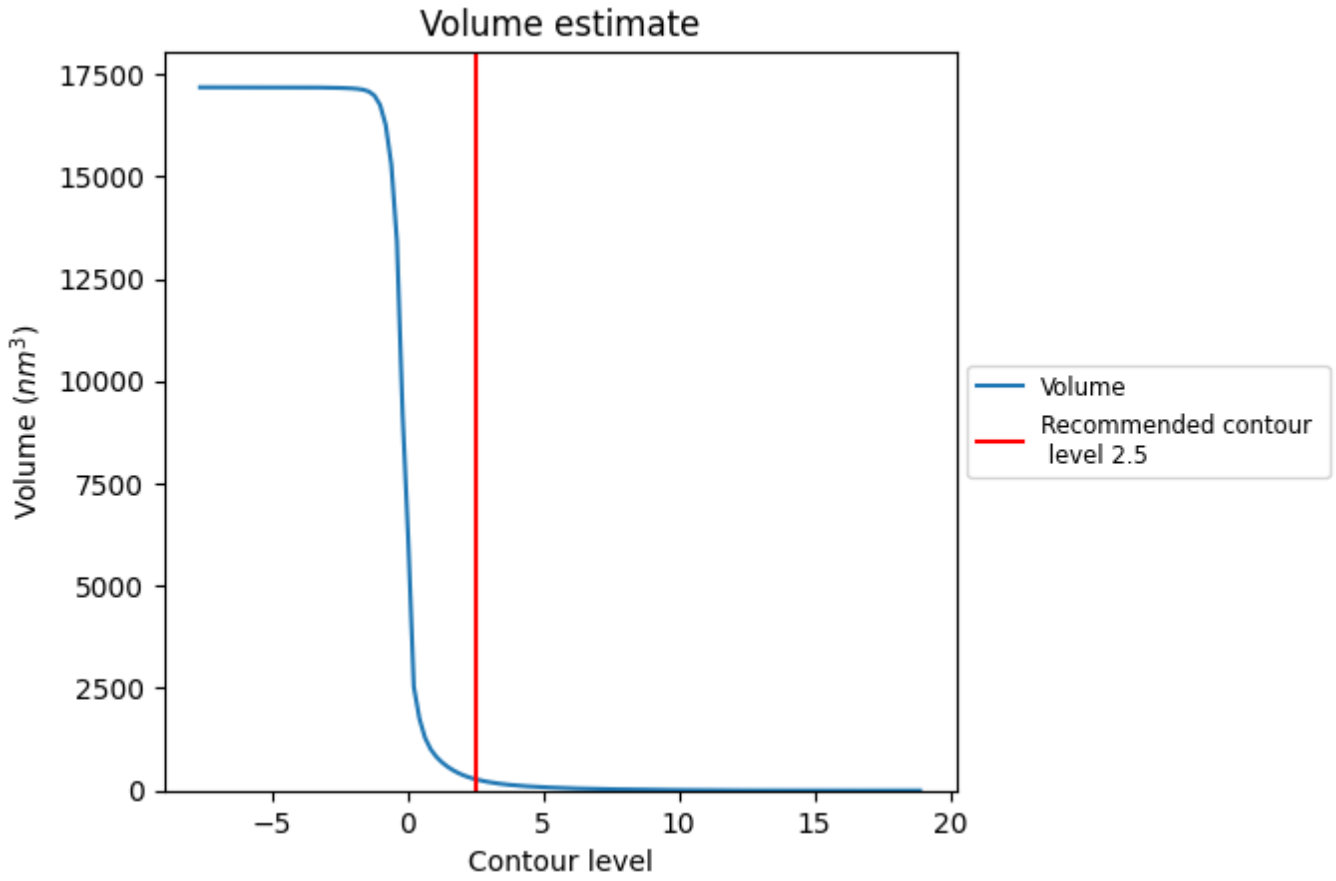
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

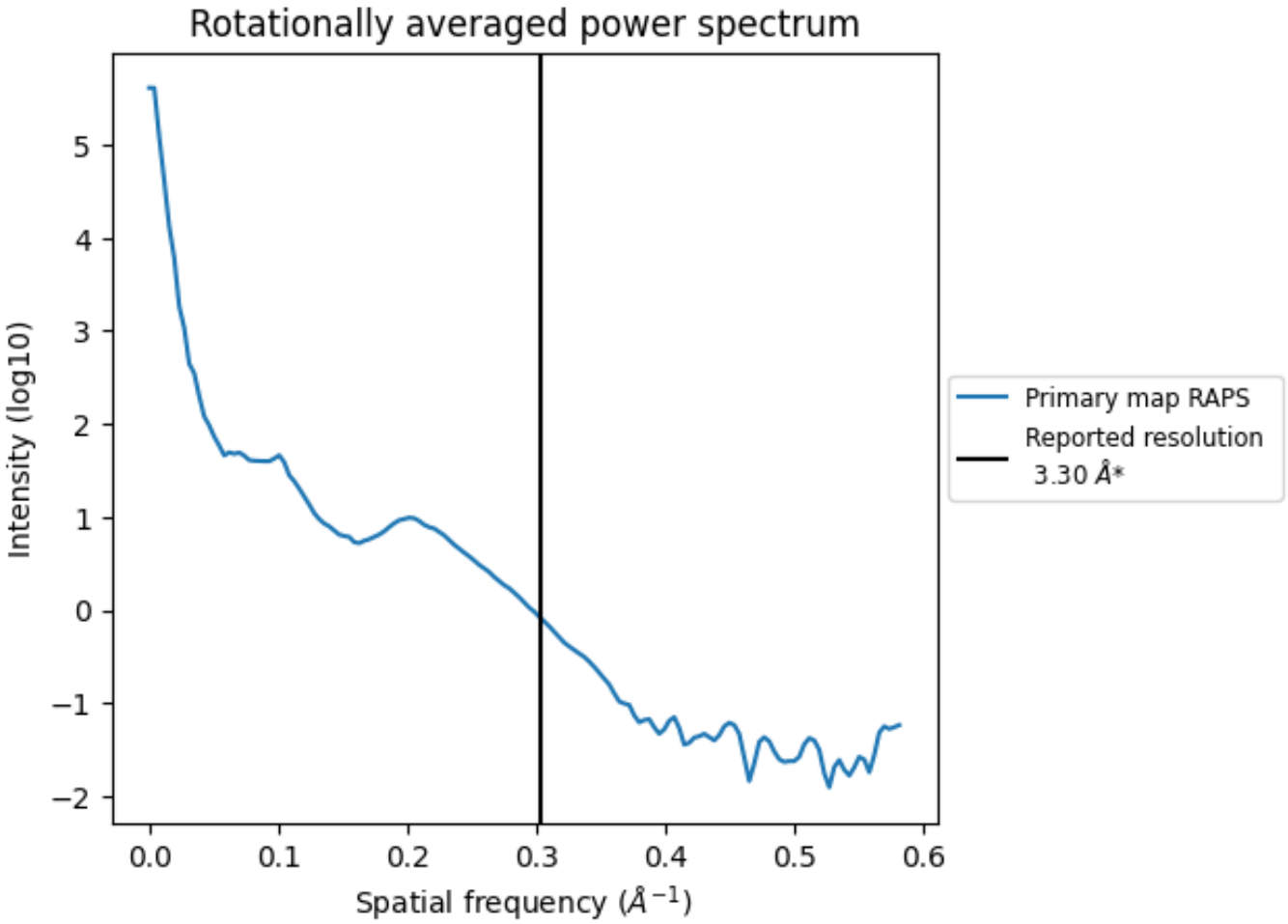
7.2 Volume estimate



The volume at the recommended contour level is 279 nm^3; this corresponds to an approximate mass of 252 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 0.303 Å^{-1}

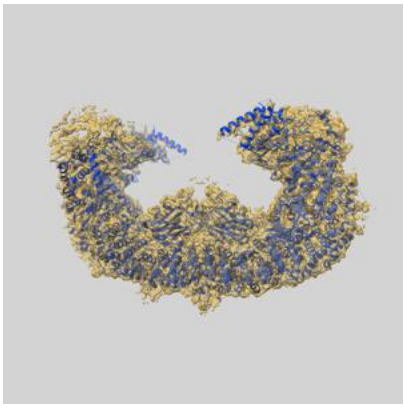
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

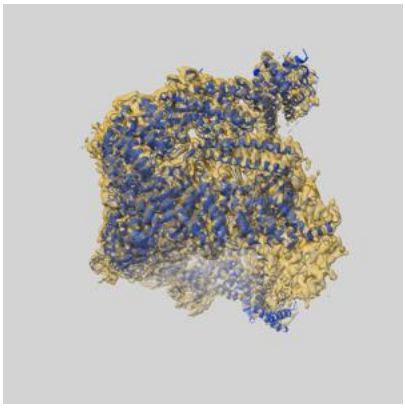
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-15653 and PDB model 8ATM. Per-residue inclusion information can be found in section 3 on page 4.

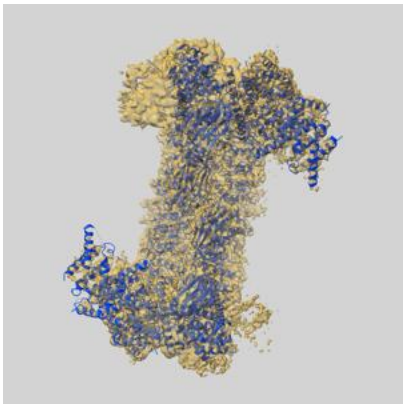
9.1 Map-model overlay



X



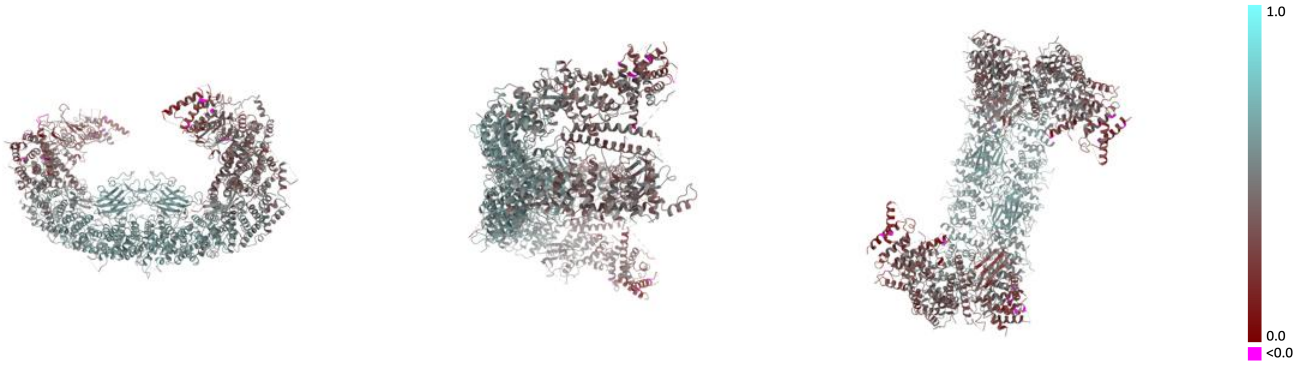
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.5 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.

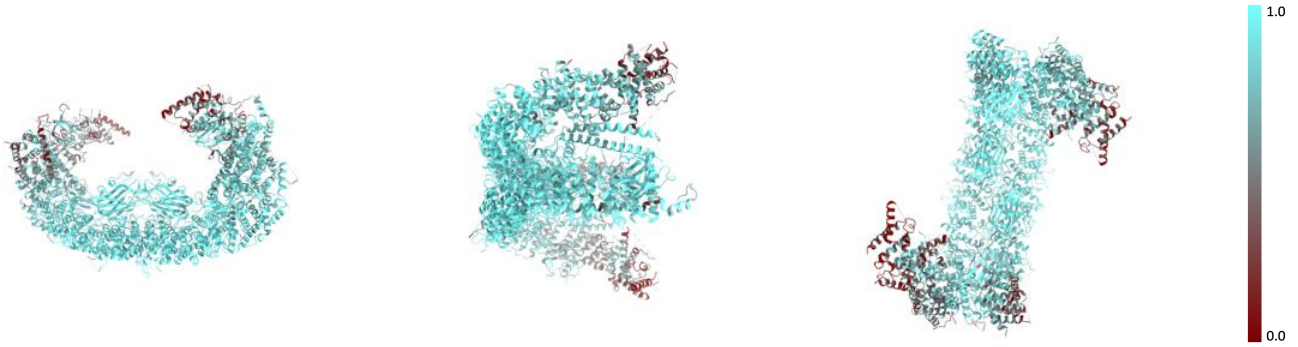
9.2 Q-score mapped to coordinate model



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.

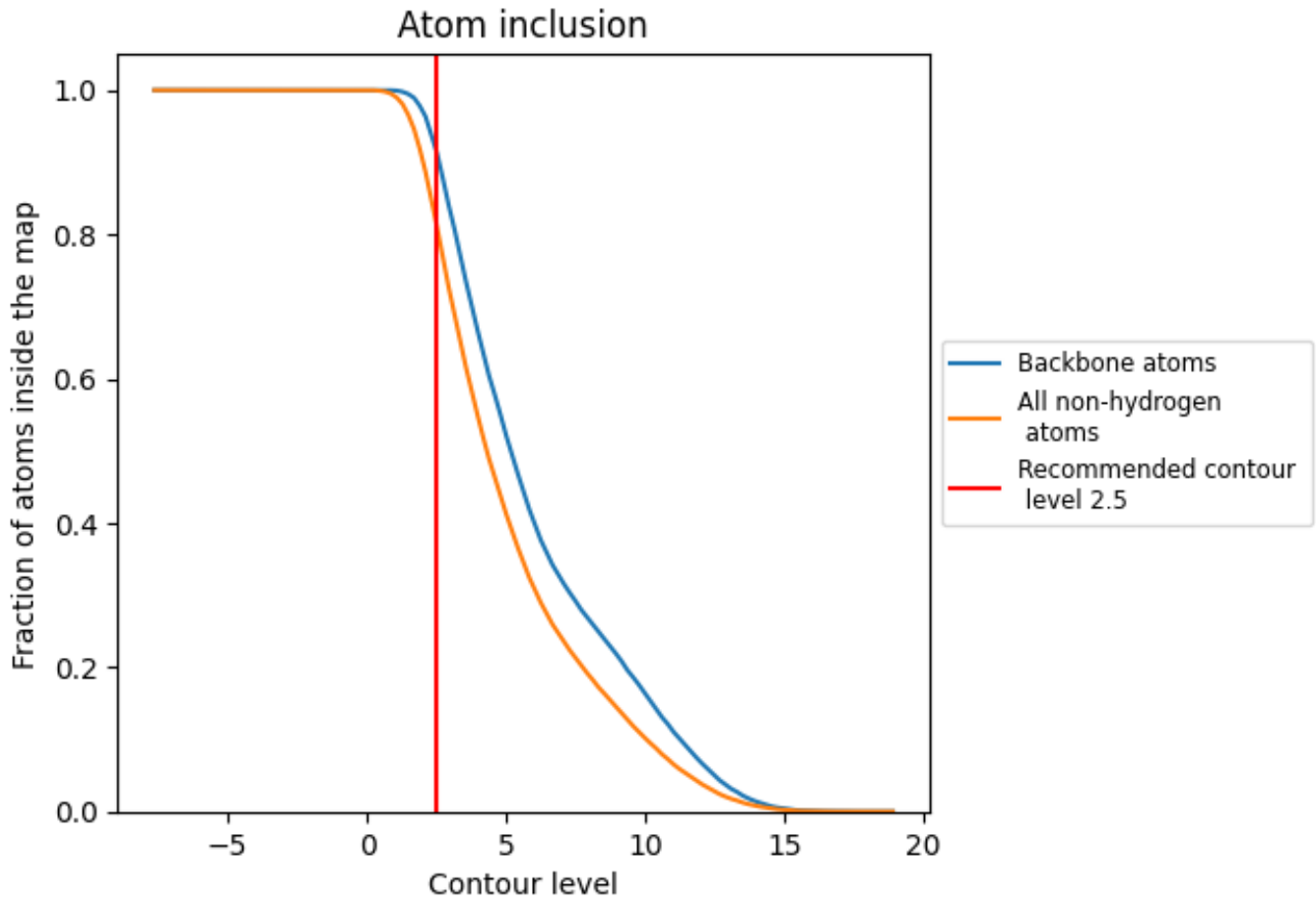
9.3 Atom inclusion mapped to coordinate model



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 (2.5).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 81% 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 (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8132	0.4680
A	0.8097	0.4680
B	0.8168	0.4670