Full wwPDB EM Validation Report ⓘ

Feb 22, 2025 – 01:55 PM EST

PDB ID	:	9EA7
EMDB ID	:	EMD-47801
Title	:	The Structure of ApoB100 from Human Low-Density Lipoprotein
Authors	:	Berndsen, Z.T.; Cassidy, C.K.
Deposited on	:	2024-11-10
Resolution	:	9.00 Å(reported)
Based on initial model	:	.

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:

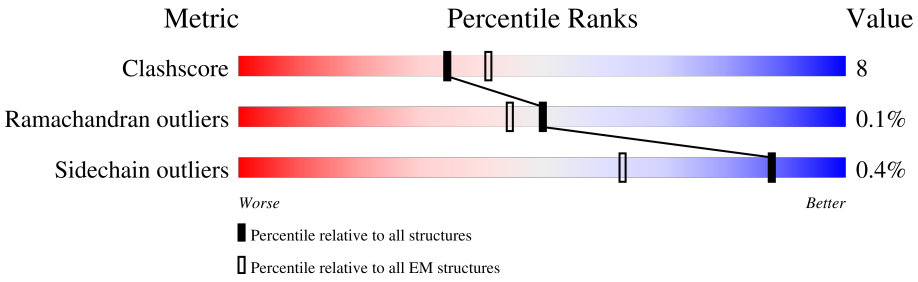
EMDB validation analysis	:	0.0.1.dev117
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

1 Overall quality at a glance (i)

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

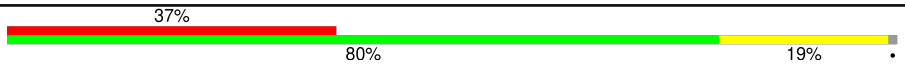
The reported resolution of this entry is 9.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	4563	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 72328 atoms, of which 36245 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 Apolipoprotein B 100.

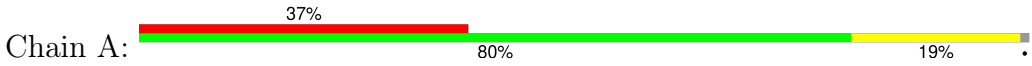
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	4526	72328	23018	36245	6066	6897	102	0	0

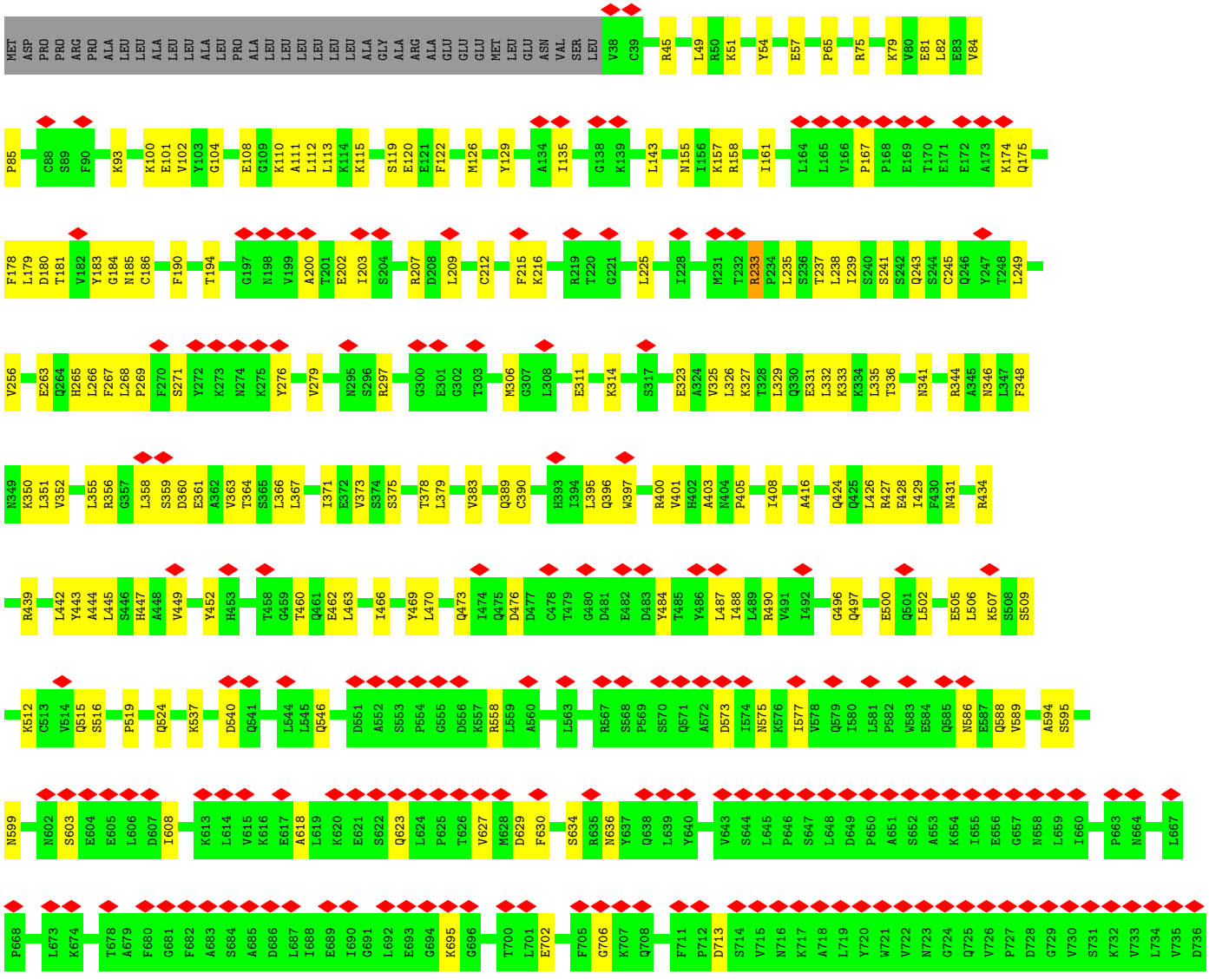
3 Residue-property plots (i)

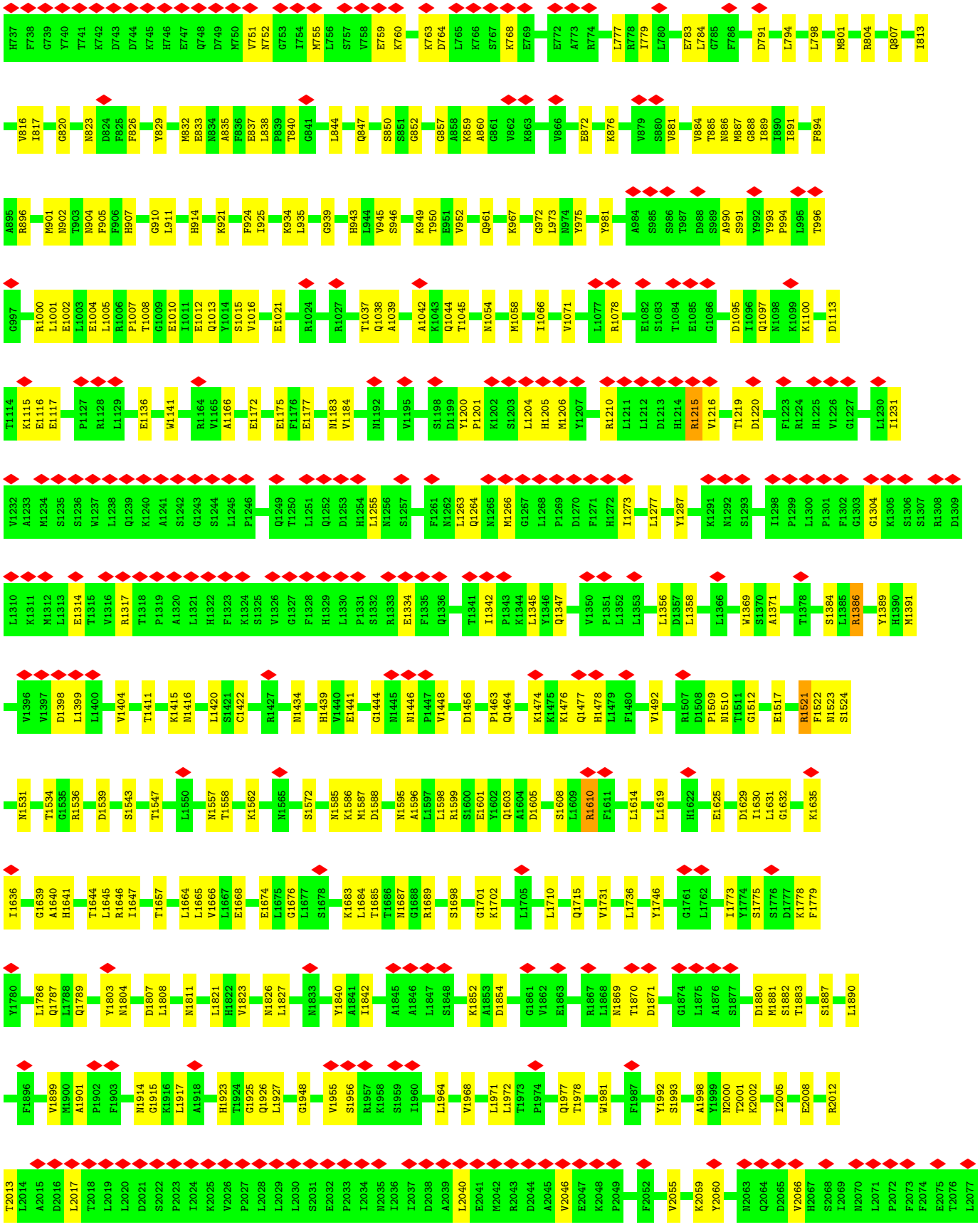
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Apolipoprotein B 100

Chain A:



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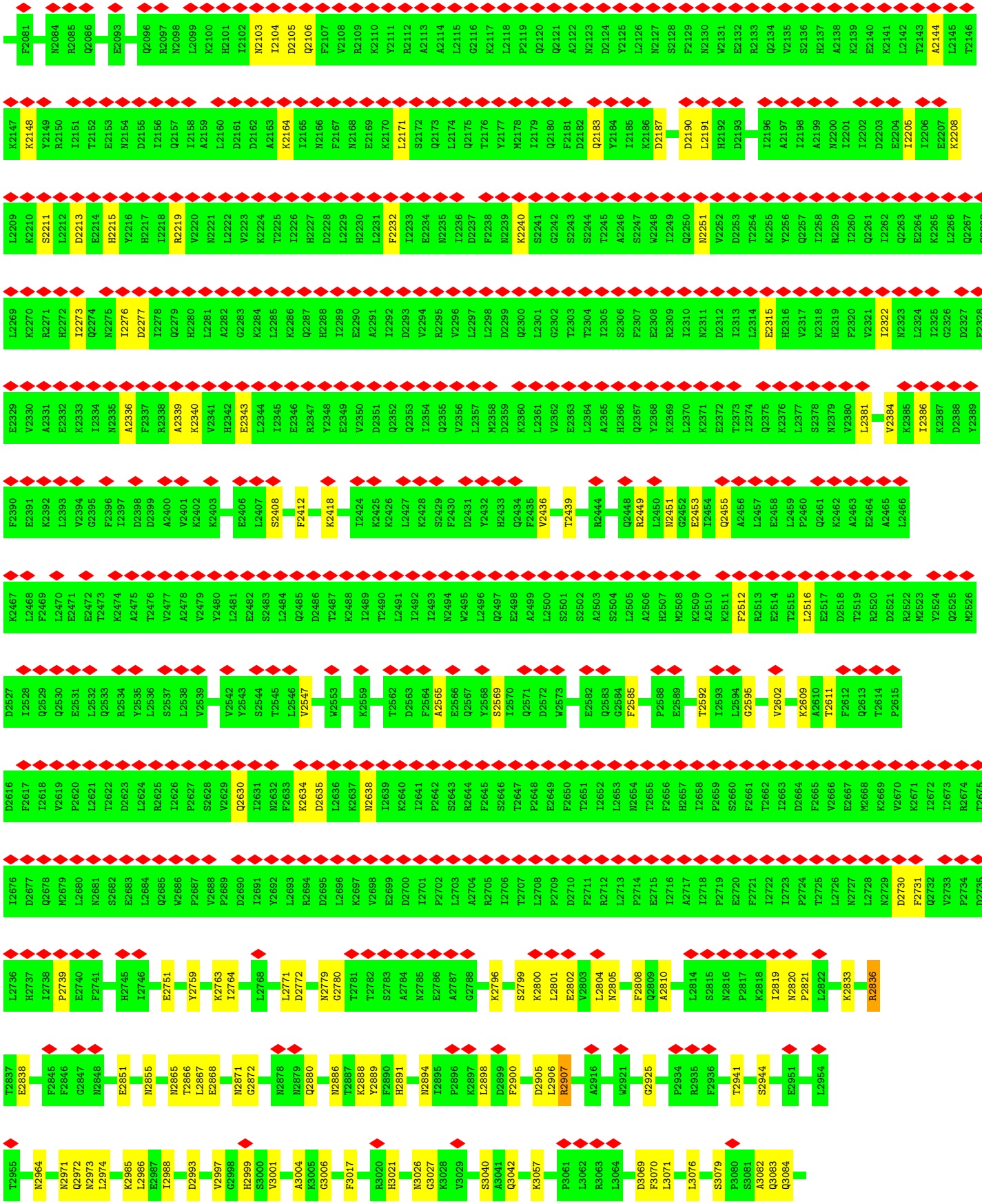
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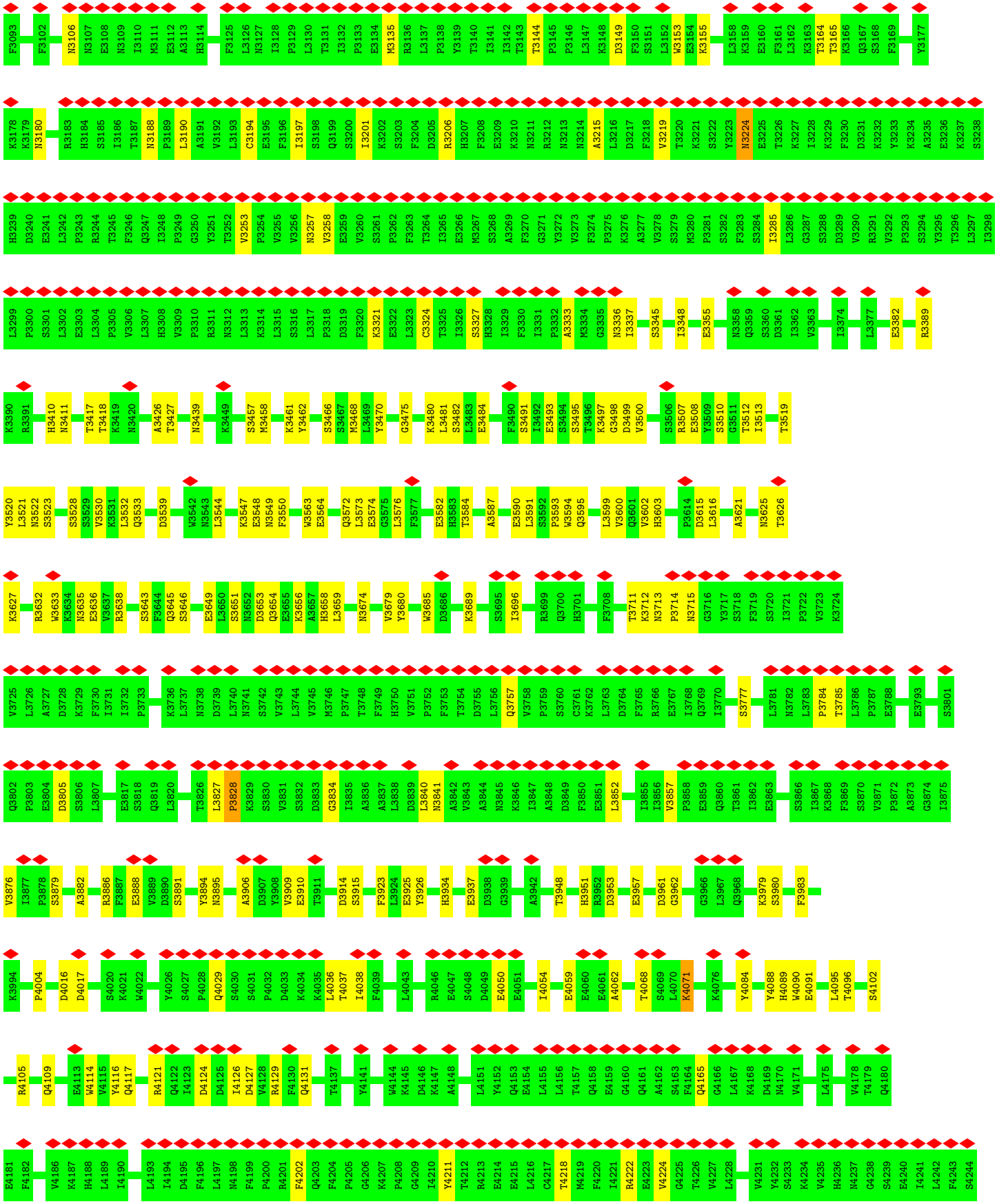
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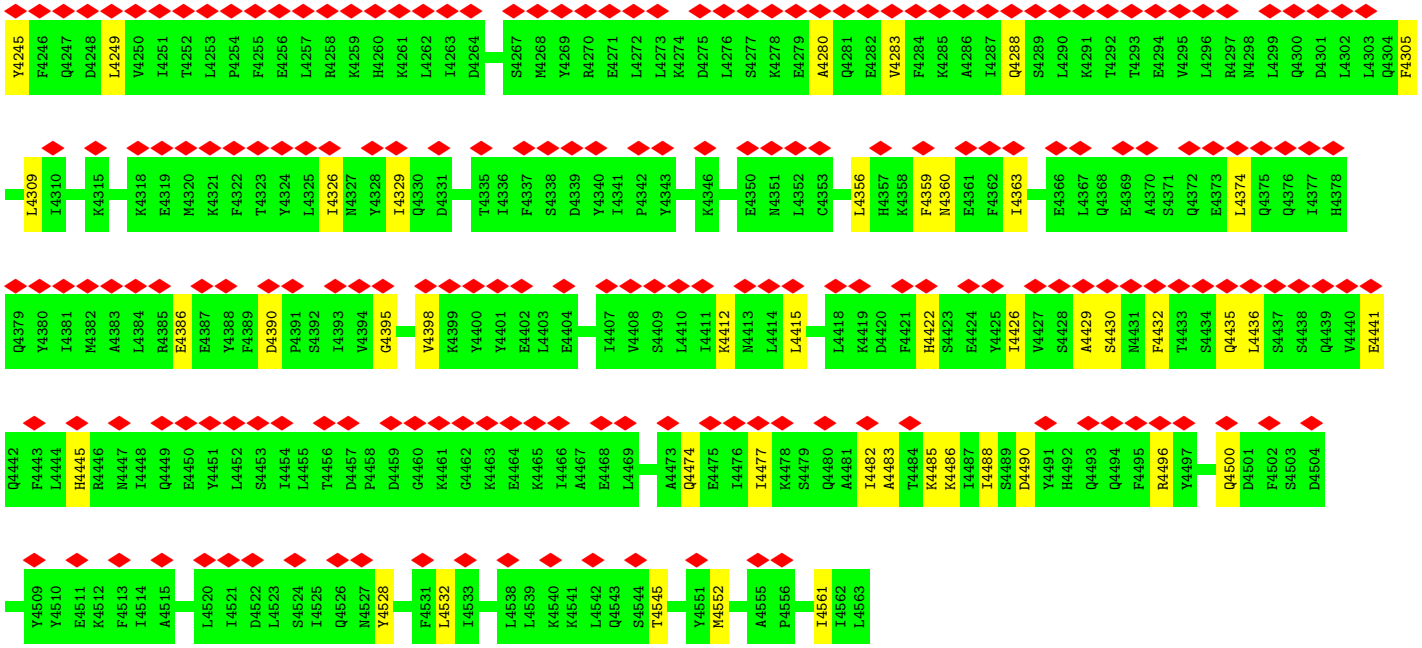
Y4245 F4246 Q4247 D4248 L4249 V4250 I4251 T4252 L4253 P4254 F4255 E4256 L4257 R4258 K4259 H4260 K4261 L4262 I4263 D4264
S4267 M4268 Y4269 R4270 E4271 L4272 L4273 K4274 D4275 L4276 S4277 K4278 E4279 A4280 Q4281 E4282 V4283 F4284 K4285 A4286 I4287 Q4288 S4289 L4290 K4291 T4292 T4293 E4294 V4295 L4296 R4297 M4298 L4299 Q4300 D4301 L4302 L4303 Q4304 F4305
L4309 I4310 K4315 K4318 E4319 M4320 K4321 F4322 T4323 Y4324 L4325 I4326 N4327 Y4328 I4329 Q4330 D4331 T4335 I4336 F4337 S4338 D4339 Y4340 I4341 P4342 Y4343 K4346 E4350 N4351 L4352 C4353 L4356 H4357 K4358 F4359 N4360 E4361 F4362 I4363 E4366 L4367 Q4368 E4369 A4370 S4371 Q4372 E4373 L4374 Q4375 Q4376 I4377 H4378
Q4379 Y4380 I4381 M4382 A4383 L4384 R4385 E4386 E4387 Y4388 F4389 D4390 P4391 S4392 I4393 V4394 G4395 V4398 K4399 Y4400 Y4401 E4402 L4403 E4404 I4407 V4408 S4409 L4410 I4411 K4412 N4413 L4414 L4415 L4418 K4419 D4420 F4421 H4422 S4423 E4424 Y4425 I4426 V4427 S4428 A4429 S4430 N4431 F4432 T4433 S4434 Q4435 L4436 S4437 S4438 Q4439 V4440 E4441
Q4442 F4443 L4444 H4445 R4446 N4447 I4448 Q4449 E4450 Y4451 L4452 S4453 I4454 L4455 T4456 D4457 P4458 D4459 G4460 K4461 G4462 K4463 E4464 K4465 I4466 A4467 E4468 L4469 A4473 Q4474 E4475 I4476 I4477 K4478 S4479 Q4480 A4481 I4482 A4483 T4484 K4485 K4486 I4487 I4488 S4489 D4490 Y4491 H4492 Q4493 Q4494 F4495 R4496 Y4497 Q4500 D4501 F4502 S4503 D4504
Y4509 Y4510 E4511 K4512 F4513 I4514 A4515 L4520 I4521 D4522 L4523 S4524 I4525 Q4526 N4527 Y4528 F4531 L4532 I4533 L4538 L4539 K4540 K4541 L4542 Q4543 S4544 T4545 Y4551 M4552 A4555 P4556 I4561 I4562 L4563

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	52843	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.148	Depositor
Minimum map value	-0.560	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.182	Depositor
Map size (Å)	490.5, 490.5, 490.5	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	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	0.25	0/36813	0.46	0/49814

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2820	ASN	Peptide

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	36083	36245	36243	573	0
All	All	36083	36245	36243	573	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 8.

All (573) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:GLU:OE2	1:A:537:LYS:NZ	1.96	0.98
1:A:325:VAL:HG13	1:A:351:LEU:HD11	1.46	0.95
1:A:323:GLU:OE1	1:A:327:LYS:NZ	2.03	0.92
1:A:3632:ARG:NH1	1:A:3633:TRP:O	2.03	0.92
1:A:3482:SER:OG	1:A:3484:GLU:OE2	1.90	0.89
1:A:243:GLN:NE2	1:A:245:CYS:SG	2.48	0.86
1:A:3491:SER:OG	1:A:3493:GLU:OE2	1.93	0.84
1:A:3135:MET:SD	1:A:3144:THR:OG1	2.35	0.84
1:A:332:LEU:O	1:A:344:ARG:NH2	2.11	0.84
1:A:3649:GLU:OE2	1:A:3651:SER:OG	1.95	0.83
1:A:1038:GLN:NE2	1:A:1044:GLN:OE1	2.12	0.83
1:A:1684:LEU:O	1:A:1698:SER:OG	1.97	0.82
1:A:1608:SER:O	1:A:1610:ARG:NH1	2.13	0.81
1:A:57:GLU:N	1:A:57:GLU:OE1	2.14	0.80
1:A:2833:LYS:O	1:A:2836:ARG:NH1	2.15	0.80
1:A:907:HIS:ND1	1:A:935:LEU:O	2.14	0.80
1:A:2802:GLU:N	1:A:2802:GLU:OE1	2.15	0.80
1:A:1521:ARG:NH1	1:A:1522:PHE:O	2.15	0.80
1:A:336:THR:O	1:A:859:LYS:NZ	2.15	0.79
1:A:847:GLN:N	1:A:888:GLY:O	2.15	0.79
1:A:54:TYR:OH	1:A:256:VAL:O	2.00	0.79
1:A:79:LYS:NZ	1:A:81:GLU:OE2	2.15	0.79
1:A:4109:GLN:O	1:A:4496:ARG:NH2	2.17	0.78
1:A:1386:ARG:O	1:A:1386:ARG:NH1	2.17	0.77
1:A:143:LEU:N	1:A:306:MET:O	2.16	0.77
1:A:1881:MET:SD	1:A:1883:THR:OG1	2.42	0.76
1:A:3636:GLU:N	1:A:3636:GLU:OE1	2.18	0.76
1:A:1603:GLN:OE1	1:A:1605:ASP:N	2.19	0.76
1:A:271:SER:OG	1:A:276:TYR:N	2.20	0.75
1:A:1012:GLU:N	1:A:1012:GLU:OE1	2.20	0.75
1:A:1668:GLU:OE2	1:A:1687:ASN:N	2.20	0.74
1:A:460:THR:OG1	1:A:462:GLU:OE1	2.04	0.74
1:A:1978:THR:OG1	1:A:1998:ALA:O	2.04	0.74
1:A:1789:GLN:OE1	1:A:1789:GLN:N	2.20	0.73
1:A:3888:GLU:OE2	1:A:3895:ASN:ND2	2.21	0.73
1:A:1531:ASN:ND2	1:A:1547:THR:O	2.22	0.72
1:A:2183:GLN:NE2	1:A:2187:ASP:OD2	2.22	0.72
1:A:949:LYS:NZ	1:A:950:THR:O	2.22	0.72
1:A:120:GLU:N	1:A:120:GLU:OE1	2.23	0.72
1:A:3953:ASP:OD2	1:A:4088:TYR:OH	2.08	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ASP:OD1	1:A:181:THR:N	2.23	0.71
1:A:3784:PRO:O	1:A:3785:THR:OG1	2.06	0.71
1:A:352:VAL:HG23	1:A:356:ARG:HH22	1.56	0.71
1:A:429:ILE:HG22	1:A:445:LEU:HD13	1.73	0.71
1:A:1977:GLN:OE1	1:A:2000:ASN:ND2	2.24	0.71
1:A:158:ARG:NH2	1:A:311:GLU:OE1	2.23	0.70
1:A:2855:ASN:ND2	1:A:2871:ASN:O	2.25	0.70
1:A:896:ARG:NH2	1:A:946:SER:O	2.23	0.70
1:A:4102:SER:OG	1:A:4105:ARG:NH2	2.24	0.70
1:A:991:SER:N	1:A:996:THR:OG1	2.24	0.69
1:A:389:GLN:NE2	1:A:390:CYS:SG	2.66	0.69
1:A:1039:ALA:N	1:A:1045:THR:OG1	2.26	0.69
1:A:3654:GLN:NE2	1:A:3805:ASP:O	2.25	0.69
1:A:1586:LYS:N	1:A:1601:GLU:OE2	2.26	0.69
1:A:186:CYS:SG	1:A:207:ARG:NH1	2.65	0.69
1:A:1715:GLN:OE1	1:A:1715:GLN:N	2.26	0.69
1:A:558:ARG:NH2	1:A:586:ASN:OD1	2.27	0.68
1:A:603:SER:HB3	1:A:608:ILE:HG21	1.75	0.68
1:A:1586:LYS:O	1:A:1599:ARG:NH1	2.25	0.68
1:A:1664:LEU:O	1:A:1689:ARG:NH1	2.26	0.68
1:A:4037:THR:N	1:A:4059:GLU:OE2	2.24	0.67
1:A:3480:LYS:NZ	1:A:3481:LEU:O	2.27	0.67
1:A:1915:GLY:N	1:A:1925:GLY:O	2.26	0.67
1:A:1869:ASN:ND2	1:A:1880:ASP:OD1	2.27	0.67
1:A:85:PRO:O	1:A:297:ARG:NH1	2.27	0.66
1:A:375:SER:O	1:A:378:THR:OG1	2.13	0.66
1:A:3180:ASN:ND2	1:A:3333:ALA:O	2.27	0.66
1:A:3508:GLU:OE1	1:A:3510:SER:OG	2.14	0.66
1:A:443:TYR:O	1:A:447:HIS:ND1	2.29	0.66
1:A:1314:GLU:N	1:A:1314:GLU:OE1	2.28	0.66
1:A:599:ASN:ND2	1:A:636:ASN:OD1	2.29	0.65
1:A:497:GLN:N	1:A:497:GLN:OE1	2.30	0.65
1:A:3355:GLU:N	1:A:3355:GLU:OE1	2.29	0.65
1:A:314:LYS:NZ	1:A:358:LEU:O	2.30	0.64
1:A:3548:GLU:N	1:A:3548:GLU:OE1	2.30	0.64
1:A:4004:PRO:O	1:A:4029:GLN:NE2	2.30	0.64
1:A:1172:GLU:N	1:A:1172:GLU:OE1	2.30	0.64
1:A:431:ASN:OD1	1:A:434:ARG:NH2	2.30	0.64
1:A:586:ASN:O	1:A:589:VAL:N	2.31	0.64
1:A:1632:GLY:O	1:A:1639:GLY:N	2.30	0.64
1:A:2925:GLY:N	1:A:2944:SER:O	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3582:GLU:OE1	1:A:3582:GLU:N	2.30	0.64
1:A:4124:ASP:OD1	1:A:4485:LYS:NZ	2.27	0.63
1:A:967:LYS:O	1:A:975:TYR:N	2.31	0.63
1:A:3522:ASN:OD1	1:A:3523:SER:N	2.31	0.63
1:A:1585:ASN:ND2	1:A:1601:GLU:O	2.31	0.63
1:A:3079:SER:OG	1:A:3082:ALA:O	2.14	0.63
1:A:3602:VAL:HG23	1:A:3603:HIS:ND1	2.14	0.63
1:A:1955:VAL:O	1:A:1956:SER:OG	2.07	0.63
1:A:396:GLN:N	1:A:396:GLN:OE1	2.29	0.63
1:A:764:ASP:O	1:A:768:LYS:NZ	2.30	0.62
1:A:2512:PHE:CZ	1:A:2516:LEU:HD11	2.34	0.62
1:A:967:LYS:NZ	1:A:4050:GLU:OE2	2.33	0.62
1:A:2867:LEU:HD23	1:A:2868:GLU:N	2.13	0.62
1:A:1334:GLU:OE1	1:A:1334:GLU:N	2.33	0.62
1:A:2888:LYS:NZ	1:A:2889:TYR:O	2.33	0.61
1:A:1273:ILE:HD12	1:A:1277:LEU:HD11	1.82	0.61
1:A:777:LEU:O	1:A:784:LEU:N	2.31	0.61
1:A:3004:ALA:HB1	1:A:3017:PHE:CZ	2.36	0.61
1:A:2017:LEU:N	1:A:2046:VAL:O	2.32	0.61
1:A:2889:TYR:OH	1:A:2891:HIS:ND1	2.30	0.61
1:A:3689:LYS:NZ	1:A:4091:GLU:OE2	2.32	0.61
1:A:181:THR:HG22	1:A:184:GLY:O	2.01	0.61
1:A:3001:VAL:O	1:A:3021:HIS:ND1	2.33	0.61
1:A:3040:SER:OG	1:A:3042:GLN:NE2	2.34	0.61
1:A:325:VAL:HG13	1:A:351:LEU:CD1	2.28	0.60
1:A:1595:ASN:ND2	1:A:1619:LEU:O	2.34	0.60
1:A:462:GLU:O	1:A:466:ILE:HD12	2.00	0.60
1:A:194:THR:OG1	1:A:202:GLU:OE1	2.18	0.60
1:A:961:GLN:N	1:A:981:TYR:O	2.34	0.60
1:A:1523:ASN:OD1	1:A:1524:SER:N	2.35	0.60
1:A:3417:THR:O	1:A:3418:THR:OG1	2.18	0.60
1:A:179:LEU:O	1:A:186:CYS:N	2.35	0.59
1:A:424:GLN:O	1:A:428:GLU:OE1	2.20	0.59
1:A:623:GLN:OE1	1:A:623:GLN:N	2.34	0.59
1:A:1701:GLY:HA2	1:A:1710:LEU:HD23	1.82	0.59
1:A:4038:ILE:HD13	1:A:4062:ALA:HB1	1.84	0.59
1:A:2339:ALA:O	1:A:2343:GLU:OE1	2.19	0.59
1:A:3891:SER:OG	1:A:3894:TYR:O	2.14	0.59
1:A:844:LEU:HD22	1:A:891:ILE:HG13	1.84	0.59
1:A:2838:GLU:N	1:A:2838:GLU:OE1	2.36	0.59
1:A:505:GLU:OE1	1:A:505:GLU:N	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1852:LYS:NZ	1:A:1854:ASP:OD2	2.34	0.59
1:A:2144:ALA:O	1:A:2148:LYS:N	2.36	0.59
1:A:3149:ASP:O	1:A:3155:LYS:NZ	2.34	0.59
1:A:2801:LEU:O	1:A:2804:LEU:N	2.30	0.59
1:A:2008:GLU:OE1	1:A:2008:GLU:N	2.35	0.59
1:A:155:ASN:OD1	1:A:158:ARG:NH1	2.35	0.58
1:A:2005:ILE:HG22	1:A:2060:TYR:HD2	1.68	0.58
1:A:233:ARG:NH1	1:A:237:THR:OG1	2.36	0.58
1:A:3153:TRP:NE1	1:A:3164:THR:O	2.36	0.58
1:A:3411:ASN:ND2	1:A:3426:ALA:O	2.34	0.58
1:A:990:ALA:HB1	1:A:996:THR:HG21	1.84	0.58
1:A:1683:LYS:NZ	1:A:1698:SER:OG	2.31	0.58
1:A:1512:GLY:O	1:A:1539:ASP:N	2.31	0.58
1:A:135:ILE:O	1:A:135:ILE:HG23	2.04	0.58
1:A:1175:GLU:N	1:A:1175:GLU:OE1	2.36	0.58
1:A:445:LEU:O	1:A:449:VAL:HG23	2.03	0.58
1:A:901:MET:SD	1:A:901:MET:N	2.77	0.58
1:A:1948:GLY:O	1:A:1964:LEU:N	2.36	0.58
1:A:3345:SER:OG	1:A:3348:ILE:O	2.19	0.57
1:A:801:MET:HE3	1:A:801:MET:O	2.03	0.57
1:A:1314:GLU:OE2	1:A:1317:ARG:NH2	2.38	0.57
1:A:891:ILE:HG22	1:A:894:PHE:HB2	1.87	0.57
1:A:4090:TRP:HE1	1:A:4096:THR:HG22	1.69	0.57
1:A:2451:ASN:OD1	1:A:2455:GLN:NE2	2.38	0.57
1:A:359:SER:O	1:A:363:VAL:HG23	2.05	0.56
1:A:4435:GLN:OE1	1:A:4436:LEU:HD22	2.05	0.56
1:A:515:GLN:NE2	1:A:546:GLN:OE1	2.36	0.56
1:A:1666:VAL:HG23	1:A:1689:ARG:HH21	1.70	0.56
1:A:2986:LEU:O	1:A:3006:GLY:N	2.34	0.56
1:A:3532:LEU:N	1:A:3549:ASN:OD1	2.33	0.56
1:A:4114:TRP:O	1:A:4117:GLN:NE2	2.38	0.56
1:A:3643:SER:OG	1:A:3645:GLN:NE2	2.39	0.56
1:A:826:PHE:HA	1:A:857:GLY:HA3	1.88	0.56
1:A:329:LEU:HG	1:A:373:VAL:HG11	1.88	0.56
1:A:1887:SER:OG	1:A:1890:LEU:O	2.13	0.56
1:A:3711:THR:OG1	1:A:3882:ALA:N	2.39	0.56
1:A:1206:MET:SD	1:A:4545:THR:HG23	2.46	0.56
1:A:1992:TYR:HD1	1:A:2013:THR:HG1	1.52	0.56
1:A:914:HIS:O	1:A:925:ILE:N	2.30	0.55
1:A:2449:ARG:O	1:A:2453:GLU:OE1	2.24	0.55
1:A:2764:ILE:HD13	1:A:2771:LEU:HD23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ARG:CB	1:A:113:LEU:HD13	2.37	0.55
1:A:3253:VAL:O	1:A:3257:ASN:N	2.40	0.55
1:A:239:ILE:HD13	1:A:267:PHE:HD1	1.71	0.55
1:A:3439:ASN:OD1	1:A:3461:LYS:NZ	2.26	0.55
1:A:395:LEU:HD22	1:A:428:GLU:HB3	1.89	0.55
1:A:1016:VAL:HG23	1:A:1037:THR:HG22	1.90	0.54
1:A:1881:MET:SD	1:A:1882:SER:N	2.80	0.54
1:A:1478:HIS:CE1	1:A:1509:PRO:HG2	2.42	0.54
1:A:3714:PRO:O	1:A:3876:VAL:HG11	2.07	0.54
1:A:476:ASP:OD1	1:A:509:SER:OG	2.18	0.54
1:A:973:LEU:HD13	1:A:1007:PRO:HA	1.88	0.54
1:A:2973:ASN:O	1:A:2974:LEU:HD22	2.07	0.54
1:A:1746:TYR:OH	1:A:4390:ASP:OD1	2.22	0.54
1:A:2779:ASN:OD1	1:A:2780:GLY:N	2.41	0.54
1:A:4386:GLU:N	1:A:4386:GLU:OE1	2.41	0.54
1:A:3961:ASP:OD1	1:A:3962:GLY:N	2.41	0.54
1:A:1420:LEU:HD11	1:A:1422:CYS:SG	2.48	0.54
1:A:2040:LEU:HD21	1:A:2800:LYS:NZ	2.22	0.54
1:A:352:VAL:HG23	1:A:356:ARG:NH2	2.22	0.53
1:A:397:TRP:CZ2	1:A:401:VAL:HG11	2.43	0.53
1:A:881:VAL:N	1:A:905:PHE:O	2.41	0.53
1:A:3057:LYS:NZ	1:A:3069:ASP:OD1	2.38	0.53
1:A:837:GLU:O	1:A:838:LEU:HD22	2.08	0.53
1:A:1826:ASN:OD1	1:A:1827:LEU:N	2.42	0.53
1:A:4165:GLN:OE1	1:A:4165:GLN:N	2.36	0.53
1:A:3206:ARG:NH2	1:A:3834:GLY:O	2.37	0.53
1:A:3914:ASP:OD1	1:A:3915:SER:N	2.42	0.53
1:A:466:ILE:O	1:A:470:LEU:HD23	2.09	0.53
1:A:910:GLY:C	1:A:911:LEU:HD22	2.29	0.53
1:A:1078:ARG:NH1	1:A:1095:ASP:OD2	2.38	0.53
1:A:203:ILE:HD12	1:A:249:LEU:HD11	1.90	0.53
1:A:397:TRP:CE2	1:A:401:VAL:HG11	2.43	0.53
1:A:573:ASP:O	1:A:577:ILE:HG13	2.09	0.53
1:A:519:PRO:O	1:A:524:GLN:NE2	2.39	0.53
1:A:1446:ASN:O	1:A:1448:VAL:N	2.42	0.53
1:A:2105:ASP:OD1	1:A:2106:GLN:N	2.42	0.53
1:A:3757:GLN:N	1:A:3777:SER:OG	2.36	0.53
1:A:837:GLU:C	1:A:838:LEU:HD22	2.29	0.53
1:A:2988:ILE:HD11	1:A:3004:ALA:HB3	1.91	0.53
1:A:3194:CYS:O	1:A:3321:LYS:NZ	2.41	0.53
1:A:3715:ASN:O	1:A:3876:VAL:HG13	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3948:THR:HG23	1:A:3957:GLU:HG3	1.91	0.52
1:A:1870:THR:HG22	1:A:1871:ASP:N	2.24	0.52
1:A:2941:THR:N	1:A:2964:ASN:OD1	2.39	0.52
1:A:327:LYS:O	1:A:331:GLU:HG2	2.10	0.52
1:A:595:SER:N	1:A:627:VAL:HG11	2.25	0.52
1:A:3910:GLU:N	1:A:3910:GLU:OE1	2.42	0.52
1:A:4360:ASN:HB2	1:A:4426:ILE:HG21	1.92	0.52
1:A:813:ILE:HD12	1:A:2240:LYS:HE3	1.92	0.52
1:A:934:LYS:HA	1:A:1004:GLU:HG2	1.91	0.52
1:A:1386:ARG:O	1:A:1386:ARG:HG2	2.10	0.52
1:A:1463:PRO:O	1:A:1464:GLN:NE2	2.43	0.52
1:A:212:CYS:O	1:A:215:PHE:HD1	1.93	0.51
1:A:235:LEU:O	1:A:238:LEU:N	2.42	0.51
1:A:325:VAL:CG1	1:A:351:LEU:HD11	2.31	0.51
1:A:2799:SER:O	1:A:2805:ASN:ND2	2.41	0.51
1:A:921:LYS:NZ	1:A:1021:GLU:OE2	2.41	0.51
1:A:1968:VAL:HG13	1:A:1981:TRP:CD1	2.45	0.51
1:A:3626:THR:OG1	1:A:3627:LYS:N	2.38	0.51
1:A:2585:PHE:O	1:A:2602:VAL:HG22	2.10	0.51
1:A:2997:VAL:O	1:A:3026:ASN:N	2.42	0.51
1:A:336:THR:HB	1:A:344:ARG:HH22	1.75	0.51
1:A:713:ASP:OD2	1:A:760:LYS:NZ	2.33	0.51
1:A:794:LEU:O	1:A:798:LEU:HG	2.11	0.51
1:A:101:GLU:N	1:A:101:GLU:OE1	2.44	0.51
1:A:3468:MET:SD	1:A:3468:MET:N	2.83	0.51
1:A:833:GLU:OE2	1:A:835:ALA:HB2	2.09	0.51
1:A:2547:VAL:HG11	1:A:2634:LYS:HD3	1.93	0.51
1:A:3564:GLU:OE1	1:A:3584:THR:HG21	2.11	0.51
1:A:3674:ASN:ND2	1:A:3696:ILE:O	2.40	0.51
1:A:4305:PHE:CE2	1:A:4309:LEU:HD11	2.45	0.51
1:A:702:GLU:O	1:A:706:GLY:N	2.40	0.51
1:A:1625:GLU:OE1	1:A:1625:GLU:N	2.43	0.51
1:A:850:SER:HB2	1:A:885:THR:HG23	1.93	0.51
1:A:3507:ARG:NH2	1:A:3539:ASP:O	2.41	0.51
1:A:3512:THR:HG23	1:A:3512:THR:O	2.11	0.51
1:A:3625:ASN:O	1:A:3626:THR:OG1	2.20	0.51
1:A:4202:PHE:N	1:A:4211:TYR:O	2.39	0.51
1:A:1304:GLY:N	1:A:1342:ILE:O	2.36	0.51
1:A:4117:GLN:OE1	1:A:4121:ARG:NH1	2.43	0.51
1:A:175:GLN:O	1:A:190:PHE:N	2.38	0.50
1:A:3925:GLU:O	1:A:3951:HIS:ND1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:881:VAL:O	1:A:905:PHE:N	2.43	0.50
1:A:1993:SER:OG	1:A:2012:ARG:NH2	2.43	0.50
1:A:75:ARG:HB3	1:A:113:LEU:HD13	1.92	0.50
1:A:3544:LEU:HD23	1:A:3544:LEU:O	2.11	0.50
1:A:490:ARG:NH1	1:A:783:GLU:OE2	2.37	0.50
1:A:847:GLN:OE1	1:A:888:GLY:N	2.45	0.50
1:A:1369:TRP:CH2	1:A:1371:ALA:HB2	2.46	0.50
1:A:2008:GLU:OE2	1:A:2059:LYS:NZ	2.40	0.50
1:A:3190:LEU:N	1:A:3324:CYS:O	2.45	0.50
1:A:3083:GLN:OE1	1:A:3106:ASN:ND2	2.44	0.49
1:A:3533:GLN:OE1	1:A:3547:LYS:N	2.40	0.49
1:A:3595:GLN:OE1	1:A:3625:ASN:ND2	2.45	0.49
1:A:3653:ASP:OD1	1:A:3656:LYS:N	2.40	0.49
1:A:3498:GLY:N	1:A:3513:ILE:O	2.44	0.49
1:A:3633:TRP:HZ3	1:A:3646:SER:HG	1.58	0.49
1:A:2894:ASN:ND2	1:A:2900:PHE:O	2.45	0.49
1:A:266:LEU:HD13	1:A:279:VAL:HA	1.93	0.49
1:A:816:VAL:O	1:A:820:GLY:N	2.40	0.49
1:A:1917:LEU:O	1:A:1923:HIS:N	2.42	0.49
1:A:3520:TYR:O	1:A:3521:LEU:HD22	2.13	0.49
1:A:4109:GLN:NE2	1:A:4500:GLN:OE1	2.45	0.49
1:A:1398:ASP:OD1	1:A:1399:LEU:N	2.44	0.49
1:A:1915:GLY:O	1:A:1925:GLY:N	2.41	0.49
1:A:225:LEU:O	1:A:829:TYR:OH	2.23	0.49
1:A:943:HIS:ND1	1:A:952:VAL:HA	2.27	0.49
1:A:817:ILE:HD13	1:A:2240:LYS:HB3	1.94	0.49
1:A:1646:ARG:NH1	1:A:1647:ILE:O	2.46	0.49
1:A:3572:GLN:OE1	1:A:3574:GLU:N	2.46	0.49
1:A:3599:LEU:HD13	1:A:3621:ALA:HA	1.93	0.49
1:A:1266:MET:SD	1:A:1266:MET:N	2.86	0.48
1:A:4359:PHE:O	1:A:4363:ILE:HG23	2.13	0.48
1:A:209:LEU:HD11	1:A:263:GLU:OE1	2.13	0.48
1:A:333:LYS:O	1:A:336:THR:HG22	2.13	0.48
1:A:884:VAL:HG23	1:A:902:ASN:OD1	2.12	0.48
1:A:2592:THR:OG1	1:A:2595:GLY:O	2.17	0.48
1:A:2609:LYS:O	1:A:2634:LYS:NZ	2.46	0.48
1:A:840:THR:HG21	1:A:889:ILE:HD13	1.94	0.48
1:A:3576:LEU:O	1:A:3576:LEU:HD12	2.13	0.48
1:A:2213:ASP:OD2	1:A:2219:ARG:HD3	2.14	0.48
1:A:2219:ARG:NH2	1:A:2277:ASP:OD2	2.46	0.48
1:A:1448:VAL:HG13	1:A:1474:LYS:HG2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:594:ALA:HB3	1:A:627:VAL:HG12	1.94	0.48
1:A:872:GLU:OE1	1:A:872:GLU:N	2.46	0.48
1:A:4068:THR:O	1:A:4071:LYS:HG3	2.13	0.48
1:A:4374:LEU:HD11	1:A:4415:LEU:HD12	1.95	0.48
1:A:331:GLU:O	1:A:335:LEU:HG	2.14	0.48
1:A:1345:LEU:O	1:A:1347:GLN:NE2	2.44	0.48
1:A:1439:HIS:NE2	1:A:1441:GLU:OE2	2.47	0.48
1:A:104:GLY:O	1:A:112:LEU:N	2.47	0.48
1:A:1811:ASN:O	1:A:1840:TYR:OH	2.28	0.48
1:A:914:HIS:N	1:A:925:ILE:O	2.42	0.48
1:A:1166:ALA:N	1:A:1177:GLU:OE2	2.46	0.48
1:A:945:VAL:HG22	1:A:950:THR:HG23	1.96	0.47
1:A:2066:VAL:HG21	1:A:2751:GLU:HB3	1.96	0.47
1:A:3827:LEU:HD12	1:A:3857:VAL:HG23	1.96	0.47
1:A:1731:VAL:HG22	1:A:1736:LEU:HD13	1.95	0.47
1:A:3550:PHE:HB3	1:A:3563:TRP:O	2.14	0.47
1:A:183:TYR:CE2	1:A:212:CYS:HB2	2.49	0.47
1:A:3713:ASN:ND2	1:A:3879:SER:OG	2.47	0.47
1:A:326:LEU:HD21	1:A:366:LEU:HD11	1.96	0.47
1:A:348:PHE:O	1:A:352:VAL:HG22	2.14	0.47
1:A:804:ARG:O	1:A:807:GLN:HG3	2.15	0.47
1:A:2103:ASN:OD1	1:A:2104:ILE:N	2.48	0.47
1:A:2905:ASP:O	1:A:2907:ARG:NH1	2.47	0.47
1:A:3572:GLN:OE1	1:A:3573:LEU:N	2.47	0.47
1:A:4245:TYR:CZ	1:A:4249:LEU:HD11	2.49	0.47
1:A:1899:VAL:HG12	1:A:1901:ALA:H	1.80	0.47
1:A:2384:VAL:HG23	1:A:2386:ILE:HG23	1.96	0.47
1:A:3563:TRP:CZ2	1:A:3587:ALA:HB3	2.49	0.47
1:A:1201:PRO:O	1:A:1205:HIS:ND1	2.43	0.47
1:A:2905:ASP:O	1:A:2905:ASP:OD1	2.32	0.47
1:A:4552:MET:CE	1:A:4561:ILE:HG23	2.45	0.47
1:A:122:PHE:CD2	1:A:126:MET:HE1	2.50	0.47
1:A:505:GLU:HG2	1:A:506:LEU:HD12	1.97	0.47
1:A:1415:LYS:O	1:A:1416:ASN:HB2	2.15	0.47
1:A:1572:SER:N	1:A:1587:MET:O	2.39	0.47
1:A:3026:ASN:OD1	1:A:3027:GLY:N	2.48	0.47
1:A:3827:LEU:HB3	1:A:3828:PRO:HD2	1.97	0.47
1:A:1264:GLN:N	1:A:1264:GLN:OE1	2.47	0.47
1:A:1476:LYS:O	1:A:1478:HIS:N	2.49	0.47
1:A:2040:LEU:HG	1:A:2800:LYS:HE3	1.96	0.47
1:A:3462:TYR:OH	1:A:3499:ASP:O	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3658:HIS:C	1:A:3659:LEU:HD22	2.36	0.47
1:A:239:ILE:HD13	1:A:267:PHE:CD1	2.51	0.46
1:A:1968:VAL:HG13	1:A:1981:TRP:NE1	2.30	0.46
1:A:102:VAL:HG22	1:A:111:ALA:HB1	1.96	0.46
1:A:1644:THR:C	1:A:1645:LEU:HD22	2.36	0.46
1:A:1183:ASN:OD1	1:A:1184:VAL:N	2.49	0.46
1:A:2868:GLU:N	1:A:2868:GLU:OE1	2.48	0.46
1:A:934:LYS:O	1:A:934:LYS:HG3	2.14	0.46
1:A:1391:MET:N	1:A:1404:VAL:O	2.42	0.46
1:A:1478:HIS:CE1	1:A:1510:ASN:OD1	2.69	0.46
1:A:1775:SER:N	1:A:1778:LYS:O	2.43	0.46
1:A:2851:GLU:N	1:A:2851:GLU:OE1	2.48	0.46
1:A:367:LEU:HD23	1:A:371:ILE:HD13	1.97	0.46
1:A:1010:GLU:O	1:A:1042:ALA:N	2.49	0.46
1:A:2451:ASN:O	1:A:2455:GLN:OE1	2.33	0.46
1:A:442:LEU:HD12	1:A:487:LEU:HD21	1.97	0.46
1:A:813:ILE:O	1:A:817:ILE:HD12	2.15	0.46
1:A:2381:LEU:O	1:A:2384:VAL:HG22	2.16	0.46
1:A:764:ASP:HB3	1:A:768:LYS:HZ1	1.81	0.46
1:A:1356:LEU:HD21	1:A:1358:LEU:HD11	1.98	0.46
1:A:3382:GLU:N	1:A:3382:GLU:OE1	2.49	0.46
1:A:4127:ASP:O	1:A:4131:GLN:HG2	2.16	0.46
1:A:4441:GLU:O	1:A:4445:HIS:ND1	2.49	0.46
1:A:178:PHE:HA	1:A:186:CYS:O	2.15	0.45
1:A:1536:ARG:HA	1:A:1536:ARG:NE	2.31	0.45
1:A:1557:ASN:OD1	1:A:1558:THR:N	2.48	0.45
1:A:2512:PHE:CE2	1:A:2516:LEU:HD11	2.51	0.45
1:A:2898:LEU:H	1:A:2898:LEU:HD23	1.81	0.45
1:A:2993:ASP:OD1	1:A:2999:HIS:NE2	2.50	0.45
1:A:3615:ASP:C	1:A:3616:LEU:HD22	2.37	0.45
1:A:507:LYS:NZ	1:A:540:ASP:OD2	2.39	0.45
1:A:886:ASN:OD1	1:A:887:MET:N	2.50	0.45
1:A:1210:ARG:NH2	1:A:4545:THR:OG1	2.46	0.45
1:A:2880:GLN:OE1	1:A:2880:GLN:N	2.44	0.45
1:A:426:LEU:HD11	1:A:452:TYR:CG	2.50	0.45
1:A:2273:ILE:HD13	1:A:2276:ILE:HD12	1.98	0.45
1:A:3923:PHE:O	1:A:3951:HIS:NE2	2.49	0.45
1:A:3957:GLU:N	1:A:3957:GLU:OE1	2.49	0.45
1:A:371:ILE:H	1:A:371:ILE:HD12	1.81	0.45
1:A:1113:ASP:N	1:A:1117:GLU:O	2.50	0.45
1:A:1206:MET:SD	1:A:1210:ARG:NH2	2.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1674:GLU:OE1	1:A:1676:GLY:N	2.50	0.45
1:A:1683:LYS:NZ	1:A:1685:THR:OG1	2.49	0.45
1:A:157:LYS:O	1:A:161:ILE:HG12	2.16	0.45
1:A:463:LEU:HD12	1:A:463:LEU:H	1.82	0.45
1:A:1807:ASP:OD1	1:A:1808:LEU:N	2.49	0.45
1:A:45:ARG:NH2	1:A:167:PRO:O	2.37	0.45
1:A:346:ASN:O	1:A:350:LYS:HE3	2.15	0.45
1:A:462:GLU:O	1:A:466:ILE:CD1	2.65	0.45
1:A:972:GLY:O	1:A:1008:THR:OG1	2.29	0.45
1:A:2808:PHE:CZ	1:A:2810:ALA:HB2	2.52	0.45
1:A:3915:SER:OG	1:A:3926:TYR:OH	2.29	0.45
1:A:844:LEU:CB	1:A:889:ILE:HD11	2.46	0.45
1:A:1002:GLU:N	1:A:1002:GLU:OE1	2.49	0.45
1:A:4016:ASP:OD1	1:A:4017:ASP:N	2.46	0.45
1:A:1821:LEU:HD11	1:A:1823:VAL:CG2	2.46	0.45
1:A:1823:VAL:O	1:A:1842:ILE:N	2.45	0.45
1:A:4054:ILE:HB	1:A:4561:ILE:HB	1.99	0.45
1:A:209:LEU:HD12	1:A:241:SER:HB2	1.99	0.45
1:A:1803:TYR:CG	1:A:1803:TYR:O	2.70	0.45
1:A:2730:ASP:OD1	1:A:2731:PHE:N	2.49	0.45
1:A:2865:ASN:OD1	1:A:2866:THR:N	2.50	0.45
1:A:1534:THR:HG23	1:A:1534:THR:O	2.17	0.45
1:A:3658:HIS:O	1:A:3659:LEU:HD22	2.17	0.45
1:A:3909:VAL:N	1:A:3934:HIS:O	2.44	0.45
1:A:3594:TRP:CZ3	1:A:3626:THR:HG21	2.52	0.44
1:A:3828:PRO:HA	1:A:3840:LEU:HD12	1.99	0.44
1:A:49:LEU:N	1:A:84:VAL:O	2.51	0.44
1:A:268:LEU:HB2	1:A:269:PRO:HD3	1.98	0.44
1:A:1517:GLU:N	1:A:1517:GLU:OE1	2.49	0.44
1:A:2635:ASP:OD1	1:A:2638:ASN:ND2	2.50	0.44
1:A:1463:PRO:HG3	1:A:1492:VAL:HG13	1.97	0.44
1:A:3564:GLU:CD	1:A:3564:GLU:O	2.56	0.44
1:A:924:PHE:O	1:A:1015:SER:HA	2.17	0.44
1:A:1635:LYS:HG3	1:A:1636:ILE:HD12	1.99	0.44
1:A:1641:HIS:ND1	1:A:1657:THR:O	2.50	0.44
1:A:183:TYR:HE2	1:A:212:CYS:HB2	1.81	0.44
1:A:813:ILE:HD12	1:A:2240:LYS:CE	2.47	0.44
1:A:925:ILE:HG23	1:A:1013:GLN:NE2	2.33	0.44
1:A:3653:ASP:O	1:A:3712:LYS:NZ	2.44	0.44
1:A:416:ALA:HB2	1:A:444:ALA:HB1	1.98	0.44
1:A:3188:ASN:N	1:A:3327:SER:O	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3530:VAL:HB	1:A:3550:PHE:CE1	2.53	0.44
1:A:400:ARG:HA	1:A:400:ARG:NE	2.33	0.44
1:A:2171:LEU:HD13	1:A:2315:GLU:HB2	1.98	0.44
1:A:4036:LEU:HB3	1:A:4062:ALA:HB2	2.00	0.44
1:A:405:PRO:HA	1:A:408:ILE:HD12	2.00	0.43
1:A:629:ASP:OD1	1:A:630:PHE:N	2.51	0.43
1:A:755:MET:SD	1:A:2205:ILE:HG13	2.58	0.43
1:A:1971:LEU:C	1:A:1972:LEU:HD22	2.38	0.43
1:A:3258:VAL:HG13	1:A:3285:ILE:HG22	1.99	0.43
1:A:379:LEU:HD21	1:A:397:TRP:CE2	2.54	0.43
1:A:3153:TRP:NE1	1:A:3165:THR:HA	2.34	0.43
1:A:4395:GLY:O	1:A:4398:VAL:HG22	2.18	0.43
1:A:603:SER:CB	1:A:608:ILE:HG21	2.47	0.43
1:A:627:VAL:O	1:A:627:VAL:HG23	2.17	0.43
1:A:904:ASN:N	1:A:939:GLY:O	2.51	0.43
1:A:1231:ILE:HG23	1:A:1255:LEU:HB3	2.00	0.43
1:A:1630:ILE:O	1:A:1631:LEU:HD22	2.18	0.43
1:A:1631:LEU:HD13	1:A:1640:ALA:HA	2.00	0.43
1:A:1890:LEU:HD12	1:A:1914:ASN:O	2.18	0.43
1:A:1955:VAL:HG12	1:A:1956:SER:N	2.33	0.43
1:A:1971:LEU:HD12	1:A:2739:PRO:HD3	2.00	0.43
1:A:3685:TRP:O	1:A:3689:LYS:N	2.52	0.43
1:A:3937:GLU:N	1:A:3937:GLU:OE1	2.51	0.43
1:A:1773:ILE:HD13	1:A:1779:PHE:HB2	2.00	0.43
1:A:4432:PHE:O	1:A:4436:LEU:HD23	2.18	0.43
1:A:424:GLN:O	1:A:427:ARG:N	2.51	0.43
1:A:993:TYR:N	1:A:994:PRO:HD2	2.34	0.43
1:A:1971:LEU:HD12	1:A:2739:PRO:CD	2.48	0.43
1:A:1216:VAL:HG23	1:A:1219:THR:HG22	1.99	0.43
1:A:1614:LEU:N	1:A:1629:ASP:O	2.44	0.43
1:A:2001:THR:HG22	1:A:2002:LYS:N	2.34	0.43
1:A:3495:SER:OG	1:A:3497:LYS:NZ	2.51	0.43
1:A:360:ASP:OD1	1:A:389:GLN:HB3	2.18	0.43
1:A:1136:GLU:N	1:A:1136:GLU:OE1	2.52	0.43
1:A:1588:ASP:N	1:A:1588:ASP:OD1	2.51	0.43
1:A:2872:GLY:N	1:A:2886:ASN:OD1	2.41	0.43
1:A:326:LEU:HD21	1:A:366:LEU:HD21	2.01	0.43
1:A:588:GLN:NE2	1:A:589:VAL:HG23	2.33	0.43
1:A:1926:GLN:OE1	1:A:1927:LEU:N	2.52	0.43
1:A:2565:ALA:O	1:A:2569:SER:N	2.52	0.43
1:A:2905:ASP:O	1:A:2906:LEU:HD22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3197:ILE:O	1:A:3201:ILE:HG12	2.19	0.43
1:A:3410:HIS:ND1	1:A:3427:THR:HG23	2.33	0.43
1:A:4089:HIS:HB3	1:A:4095:LEU:O	2.18	0.43
1:A:65:PRO:HD3	1:A:279:VAL:HG12	2.01	0.43
1:A:2211:SER:O	1:A:2215:HIS:ND1	2.52	0.43
1:A:4422:HIS:O	1:A:4426:ILE:HG12	2.19	0.43
1:A:763:LYS:HE2	1:A:2208:LYS:HE3	2.01	0.43
1:A:2772:ASP:OD1	1:A:2796:LYS:HB2	2.19	0.43
1:A:3587:ALA:HB1	1:A:3600:VAL:HA	1.99	0.43
1:A:3602:VAL:HG23	1:A:3603:HIS:CE1	2.54	0.43
1:A:1384:SER:HB3	1:A:1411:THR:HG23	2.00	0.42
1:A:1786:LEU:O	1:A:1787:GLN:NE2	2.52	0.42
1:A:3466:SER:O	1:A:3470:TYR:N	2.52	0.42
1:A:876:LYS:HA	1:A:910:GLY:HA3	2.02	0.42
1:A:2973:ASN:C	1:A:2974:LEU:HD22	2.39	0.42
1:A:3841:ASN:OD1	1:A:3852:LEU:N	2.53	0.42
1:A:4280:ALA:HA	1:A:4283:VAL:HG12	2.01	0.42
1:A:93:LYS:NZ	1:A:129:TYR:O	2.47	0.42
1:A:361:GLU:HA	1:A:364:THR:HG22	2.01	0.42
1:A:367:LEU:O	1:A:371:ILE:HD12	2.20	0.42
1:A:2988:ILE:CD1	1:A:3004:ALA:HB3	2.50	0.42
1:A:751:VAL:HG23	1:A:752:ASN:N	2.35	0.42
1:A:1775:SER:HB3	1:A:1778:LYS:HB3	2.01	0.42
1:A:2819:ILE:HG13	1:A:2821:PRO:HD3	2.01	0.42
1:A:496:GLY:O	1:A:500:GLU:HG3	2.19	0.42
1:A:2436:VAL:O	1:A:2439:THR:OG1	2.29	0.42
1:A:3679:VAL:HG23	1:A:3680:TYR:N	2.35	0.42
1:A:4116:TYR:CD1	1:A:4488:ILE:HG22	2.54	0.42
1:A:200:ALA:HB3	1:A:203:ILE:HD11	2.02	0.42
1:A:403:ALA:O	1:A:408:ILE:HD11	2.20	0.42
1:A:588:GLN:HB2	1:A:634:SER:H	1.84	0.42
1:A:755:MET:CG	1:A:2205:ILE:HG13	2.50	0.42
1:A:759:GLU:HG2	1:A:2208:LYS:HE2	2.02	0.42
1:A:1543:SER:OG	1:A:1562:LYS:NZ	2.45	0.42
1:A:4474:GLN:O	1:A:4477:ILE:HG22	2.19	0.42
1:A:363:VAL:O	1:A:367:LEU:N	2.50	0.42
1:A:512:LYS:O	1:A:516:SER:N	2.53	0.42
1:A:910:GLY:O	1:A:911:LEU:HD22	2.19	0.42
1:A:108:GLU:HG2	1:A:110:LYS:HG2	2.02	0.42
1:A:779:ILE:CG1	1:A:784:LEU:HD11	2.50	0.42
1:A:823:ASN:O	1:A:860:ALA:N	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:993:TYR:CG	1:A:994:PRO:HD3	2.54	0.42
1:A:4356:LEU:HD23	1:A:4430:SER:HB2	2.00	0.42
1:A:3336:ASN:OD1	1:A:3337:ILE:N	2.53	0.41
1:A:3590:GLU:O	1:A:3591:LEU:HD22	2.20	0.41
1:A:174:LYS:O	1:A:174:LYS:HD3	2.20	0.41
1:A:1054:ASN:O	1:A:1058:MET:N	2.53	0.41
1:A:1204:LEU:HD13	1:A:1263:LEU:HB2	2.01	0.41
1:A:2190:ASP:OD1	1:A:2191:LEU:HD12	2.20	0.41
1:A:1115:LYS:NZ	1:A:1116:GLU:OE1	2.37	0.41
1:A:1587:MET:CE	1:A:1598:LEU:HD12	2.51	0.41
1:A:4126:ILE:O	1:A:4129:ARG:HG2	2.20	0.41
1:A:4356:LEU:HD21	1:A:4429:ALA:HB3	2.03	0.41
1:A:379:LEU:O	1:A:383:VAL:HG22	2.19	0.41
1:A:807:GLN:HA	1:A:2232:PHE:CD1	2.55	0.41
1:A:4218:THR:O	1:A:4222:ARG:HG2	2.20	0.41
1:A:4326:ILE:O	1:A:4329:ILE:HG22	2.20	0.41
1:A:185:ASN:O	1:A:186:CYS:SG	2.79	0.41
1:A:439:ARG:NH2	1:A:791:ASP:OD1	2.53	0.41
1:A:972:GLY:O	1:A:973:LEU:HD22	2.20	0.41
1:A:1066:ILE:HB	1:A:1071:VAL:HB	2.03	0.41
1:A:1200:TYR:CZ	1:A:1204:LEU:HD11	2.56	0.41
1:A:1415:LYS:O	1:A:1415:LYS:HD3	2.20	0.41
1:A:3070:PHE:C	1:A:3071:LEU:HD22	2.41	0.41
1:A:3635:ASN:OD1	1:A:3636:GLU:N	2.54	0.41
1:A:341:ASN:HA	1:A:344:ARG:HG2	2.03	0.41
1:A:1215:ARG:HE	1:A:1220:ASP:HA	1.86	0.41
1:A:2611:THR:HG22	1:A:2630:GLN:NE2	2.35	0.41
1:A:3076:LEU:HD12	1:A:3084:GLN:O	2.21	0.41
1:A:3475:GLY:HA3	1:A:3500:VAL:HA	2.02	0.41
1:A:975:TYR:HA	1:A:1005:LEU:HD13	2.02	0.41
1:A:1587:MET:HE1	1:A:1598:LEU:HD12	2.02	0.41
1:A:3508:GLU:O	1:A:3539:ASP:N	2.49	0.41
1:A:3937:GLU:HG2	1:A:3937:GLU:O	2.21	0.41
1:A:4528:TYR:CE1	1:A:4532:LEU:HD11	2.56	0.41
1:A:341:ASN:OD1	1:A:341:ASN:O	2.39	0.41
1:A:352:VAL:O	1:A:355:LEU:HB3	2.21	0.41
1:A:416:ALA:CB	1:A:444:ALA:HB1	2.50	0.41
1:A:1000:ARG:C	1:A:1001:LEU:HD22	2.41	0.41
1:A:1097:GLN:HB3	1:A:1100:LYS:HA	2.03	0.41
1:A:1116:GLU:O	1:A:1141:TRP:N	2.45	0.41
1:A:1200:TYR:HB3	1:A:1201:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1596:ALA:HB3	1:A:1619:LEU:HD21	2.02	0.41
1:A:1665:LEU:HD12	1:A:1689:ARG:O	2.20	0.41
1:A:2764:ILE:HD13	1:A:2771:LEU:HB3	2.02	0.41
1:A:3564:GLU:OE1	1:A:3584:THR:CG2	2.69	0.41
1:A:4482:ILE:HG23	1:A:4483:ALA:N	2.36	0.41
1:A:4486:LYS:NZ	1:A:4490:ASP:OD2	2.44	0.41
1:A:115:LYS:NZ	1:A:119:SER:OG	2.42	0.41
1:A:885:THR:HB	1:A:901:MET:HB2	2.01	0.41
1:A:1416:ASN:O	1:A:1444:GLY:N	2.53	0.41
1:A:3004:ALA:HB1	1:A:3017:PHE:CE2	2.56	0.41
1:A:4038:ILE:HD13	1:A:4062:ALA:CB	2.48	0.41
1:A:4224:VAL:HG21	1:A:4288:GLN:OE1	2.21	0.41
1:A:265:HIS:C	1:A:266:LEU:HD22	2.42	0.40
1:A:463:LEU:HB3	1:A:502:LEU:CD1	2.51	0.40
1:A:2336:ALA:O	1:A:2340:LYS:HG2	2.21	0.40
1:A:3215:ALA:O	1:A:3219:VAL:HG23	2.21	0.40
1:A:3224:ASN:C	1:A:3224:ASN:HD22	2.23	0.40
1:A:3593:PRO:O	1:A:3594:TRP:HB3	2.21	0.40
1:A:469:TYR:O	1:A:473:GLN:HG2	2.22	0.40
1:A:833:GLU:OE2	1:A:835:ALA:N	2.55	0.40
1:A:1389:TYR:HE2	1:A:1404:VAL:HG12	1.86	0.40
1:A:3980:SER:O	1:A:3983:PHE:O	2.40	0.40
1:A:1287:TYR:HD1	1:A:1356:LEU:HA	1.86	0.40
1:A:1644:THR:O	1:A:1645:LEU:HD22	2.22	0.40
1:A:2164:LYS:HB2	1:A:2322:ILE:HD13	2.01	0.40
1:A:2800:LYS:HD3	1:A:2800:LYS:N	2.36	0.40
1:A:51:LYS:HA	1:A:82:LEU:O	2.22	0.40
1:A:832:MET:SD	1:A:852:GLY:N	2.95	0.40
1:A:2055:VAL:O	1:A:2763:LYS:N	2.51	0.40
1:A:2408:SER:O	1:A:2412:PHE:N	2.40	0.40
1:A:4084:TYR:CE1	1:A:4088:TYR:HE2	2.38	0.40
1:A:100:LYS:HB3	1:A:113:LEU:HB3	2.02	0.40
1:A:484:TYR:O	1:A:488:ILE:HG12	2.22	0.40
1:A:575:ASN:HA	1:A:618:ALA:HB1	2.03	0.40
1:A:1434:ASN:N	1:A:1456:ASP:O	2.44	0.40
1:A:2059:LYS:HB2	1:A:2759:TYR:CZ	2.56	0.40
1:A:2971:ASN:OD1	1:A:2972:GLN:N	2.55	0.40
1:A:2985:LYS:C	1:A:2986:LEU:HD22	2.41	0.40
1:A:3457:SER:O	1:A:3458:MET:HE2	2.22	0.40
1:A:3519:THR:HG23	1:A:3528:SER:OG	2.21	0.40
1:A:3957:GLU:OE1	1:A:3979:LYS:NZ	2.50	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	4524/4563 (99%)	4338 (96%)	182 (4%)	4 (0%)	48 83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3828	PRO
1	A	1477	GLN
1	A	3906	ALA
1	A	1804	ASN

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	4051/4080 (99%)	4033 (100%)	18 (0%)	89 91

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	216	LYS
1	A	233	ARG
1	A	695	LYS
1	A	1215	ARG

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Mol	Chain	Res	Type
1	A	1386	ARG
1	A	1521	ARG
1	A	1610	ARG
1	A	1702	LYS
1	A	2251	ASN
1	A	2418	LYS
1	A	2836	ARG
1	A	2907	ARG
1	A	3224	ASN
1	A	3389	ARG
1	A	3638	ARG
1	A	3886	ARG
1	A	4071	LYS
1	A	4412	LYS

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	255	HIS
1	A	1013	GLN
1	A	1478	HIS
1	A	3051	ASN
1	A	3207	HIS
1	A	3224	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (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.

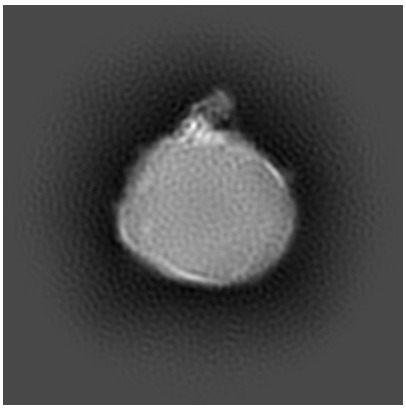
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-47801. These allow visual inspection of the internal detail of the map and identification of artifacts.

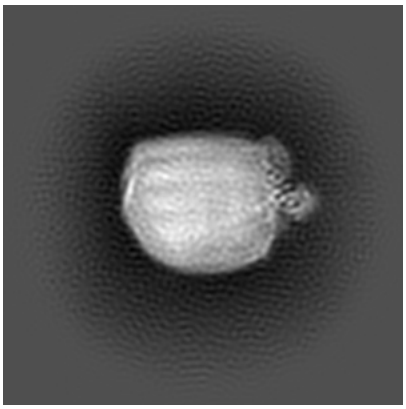
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

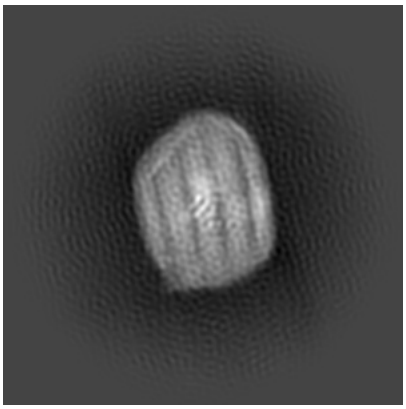
6.1.1 Primary map



X

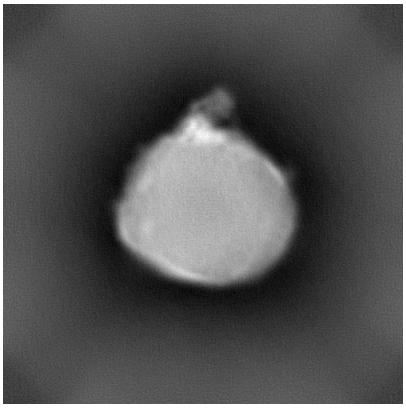


Y

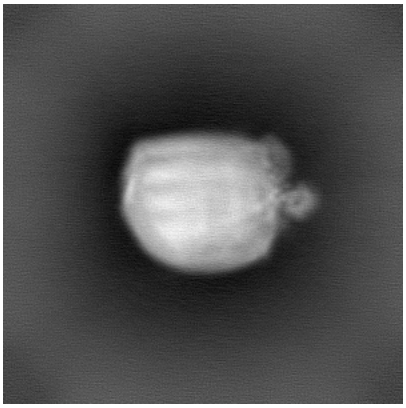


Z

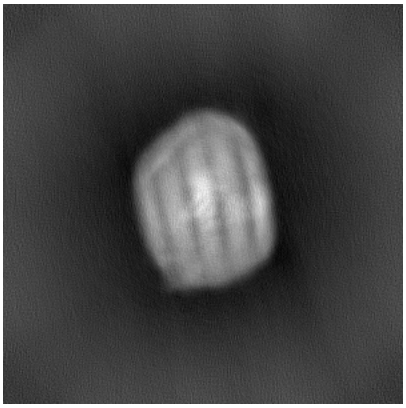
6.1.2 Raw map



X



Y

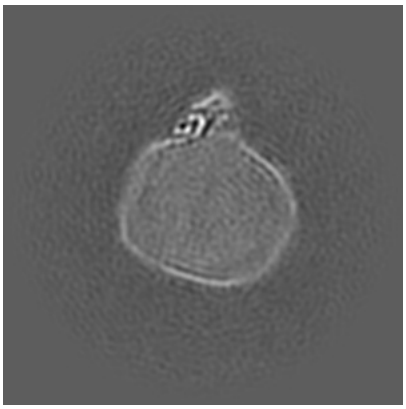


Z

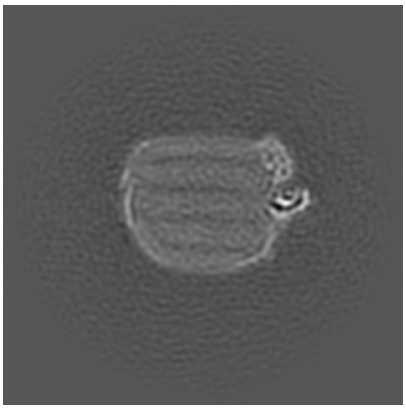
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

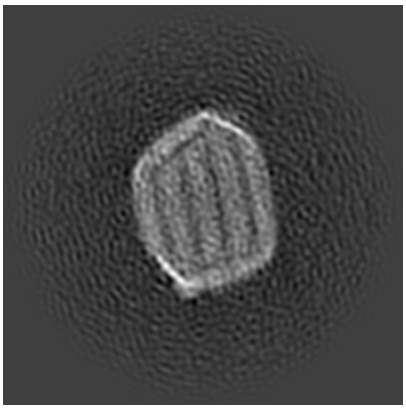
6.2.1 Primary map



X Index: 225

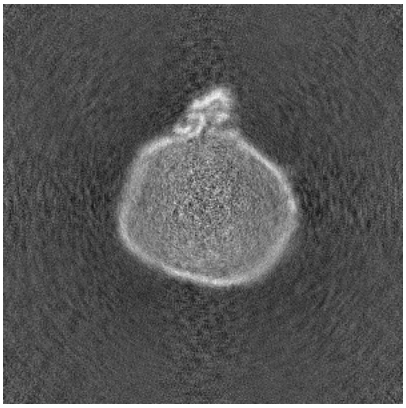


Y Index: 225

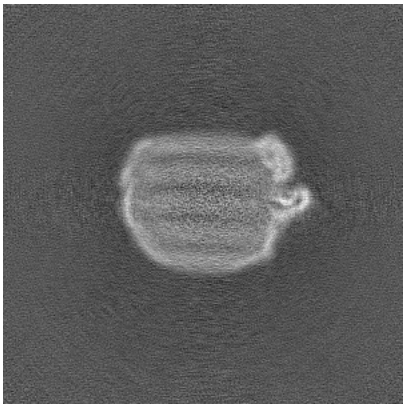


Z Index: 225

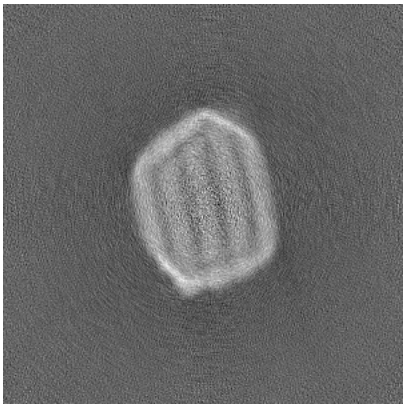
6.2.2 Raw map



X Index: 225



Y Index: 225

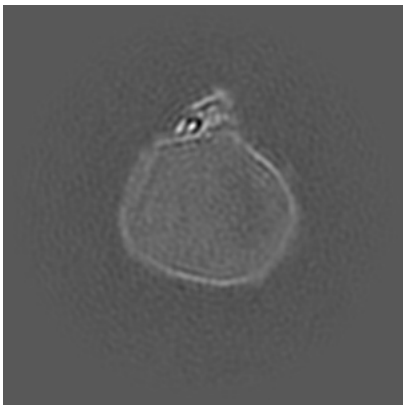


Z Index: 225

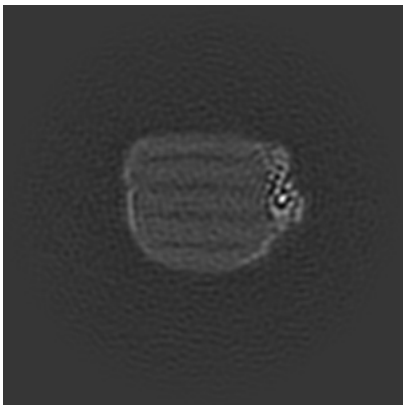
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

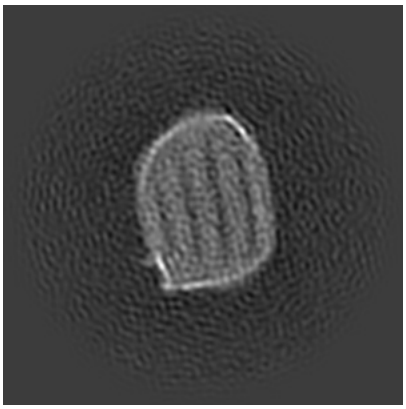
6.3.1 Primary map



X Index: 230

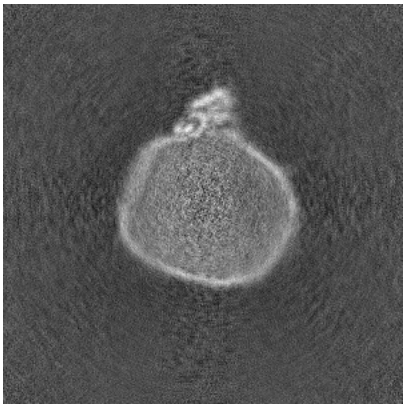


Y Index: 213

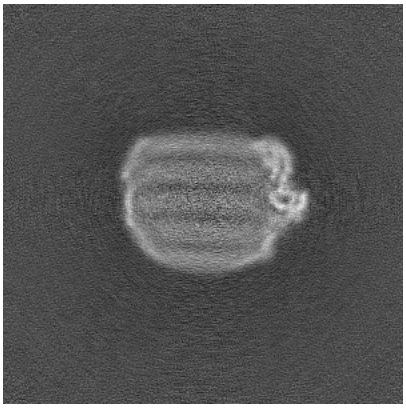


Z Index: 196

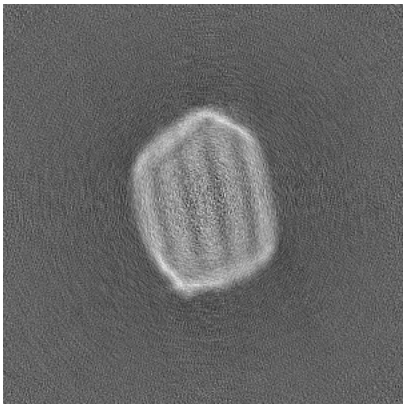
6.3.2 Raw map



X Index: 227



Y Index: 219

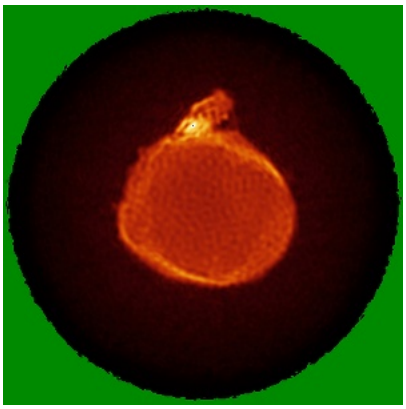


Z Index: 219

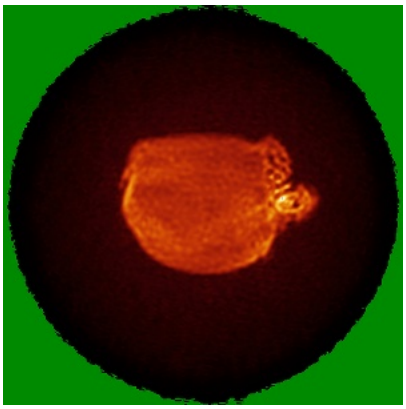
The images above show the largest variance slices of the map in three orthogonal directions.

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

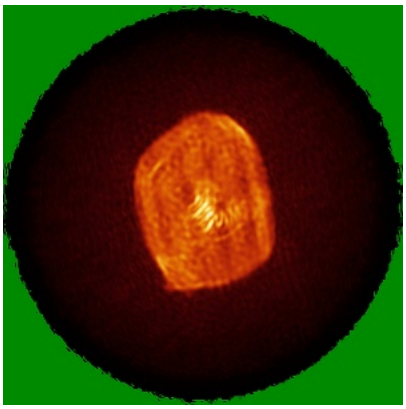
6.4.1 Primary map



X

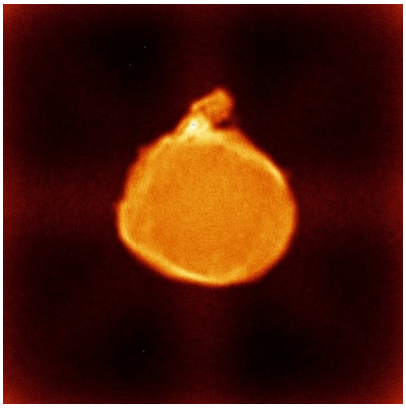


Y

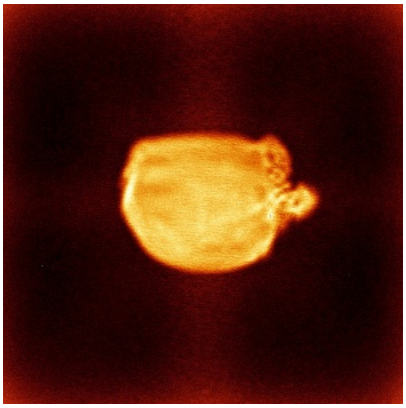


Z

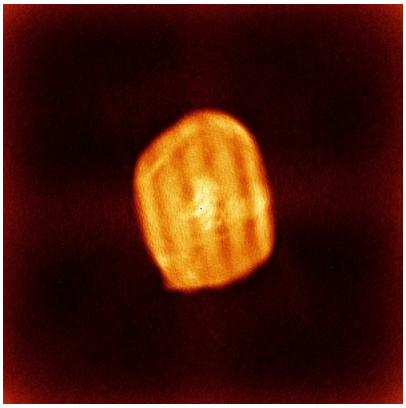
6.4.2 Raw map



X



Y

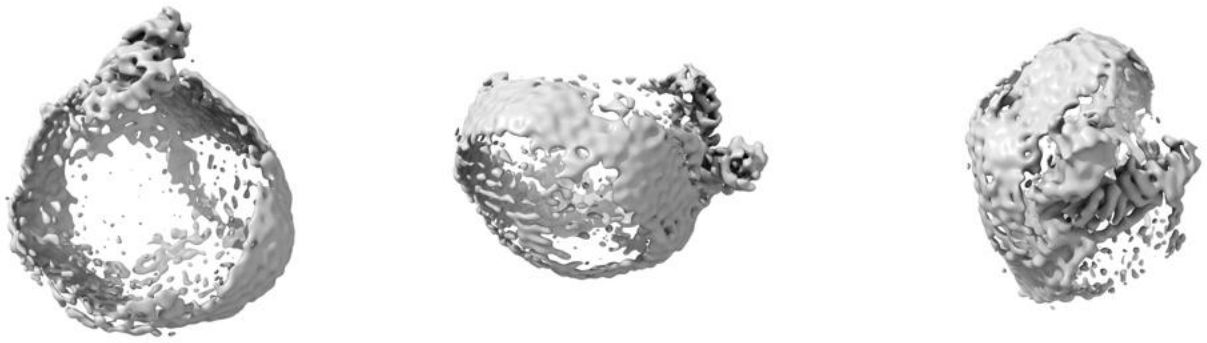


Z

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 0.182. 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.

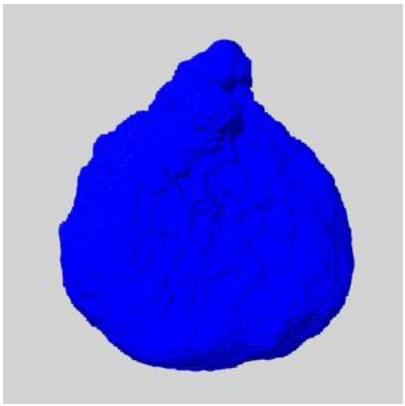
6.6 Mask visualisation (i)

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

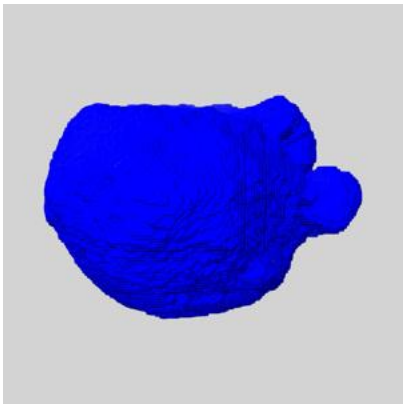
A mask typically either:

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

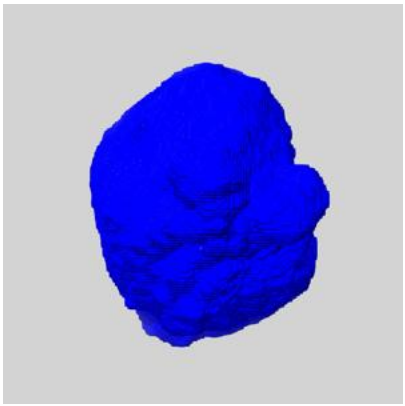
6.6.1 emd_47801_msk_1.map (i)



X



Y

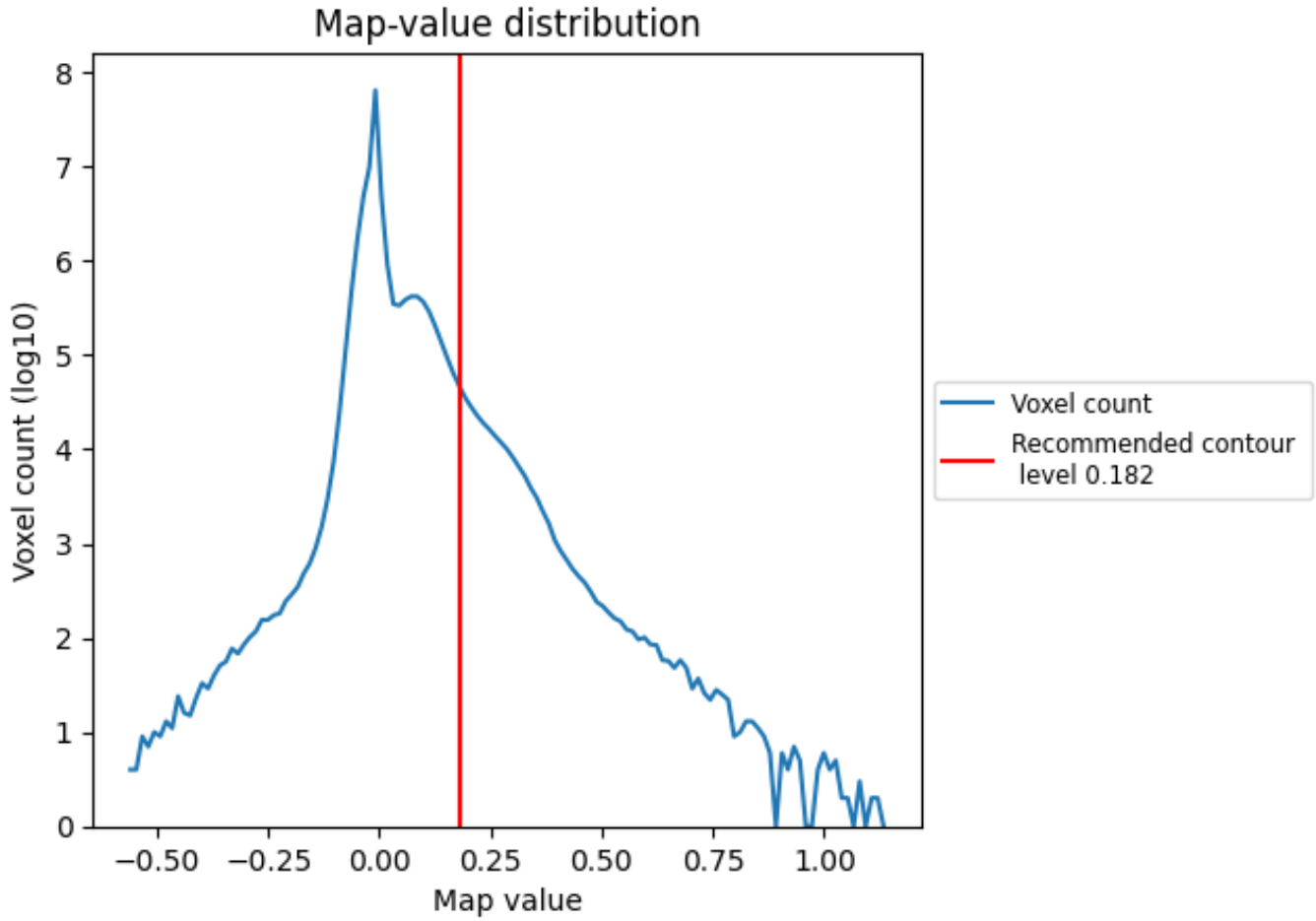


Z

7 Map analysis

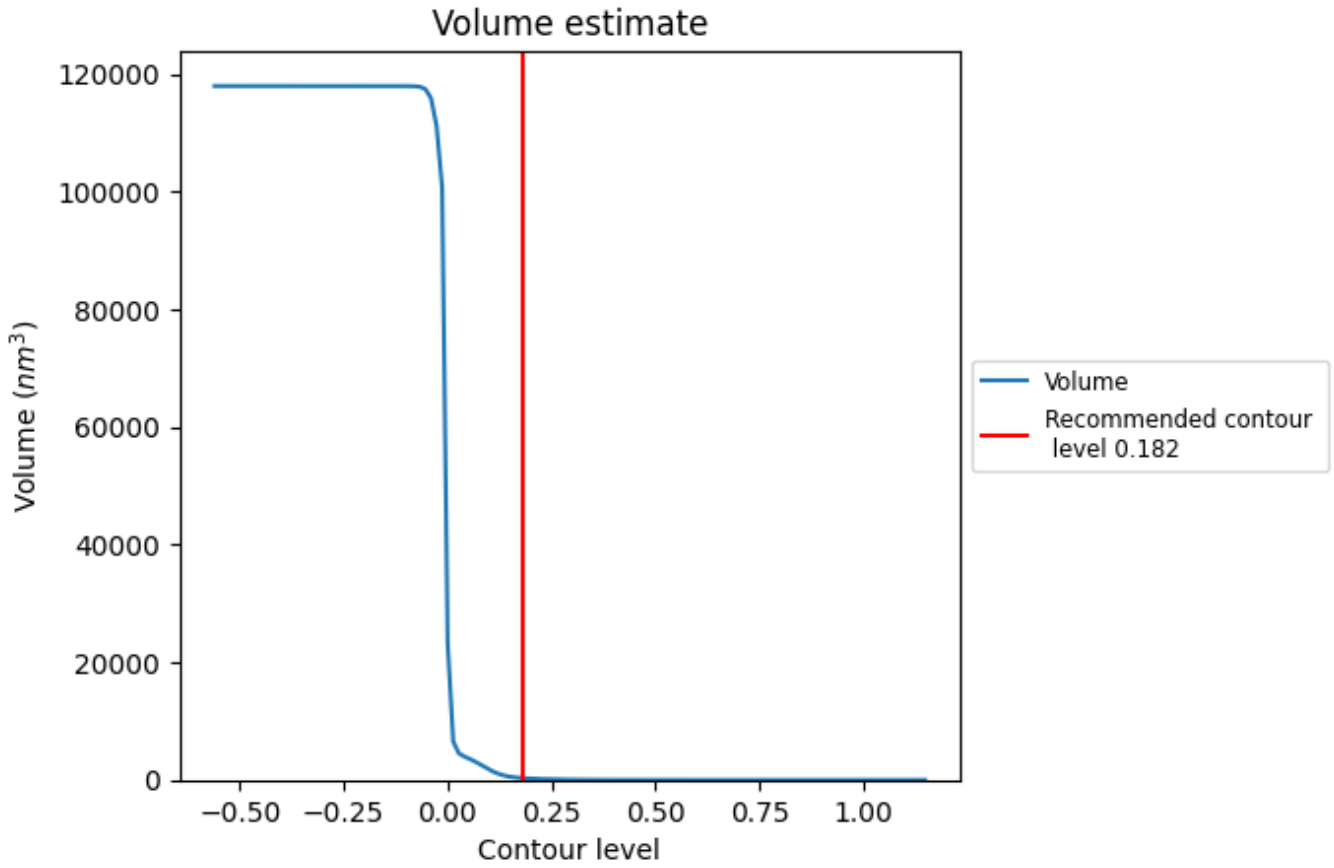
This section contains the results of statistical analysis of the map.

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.

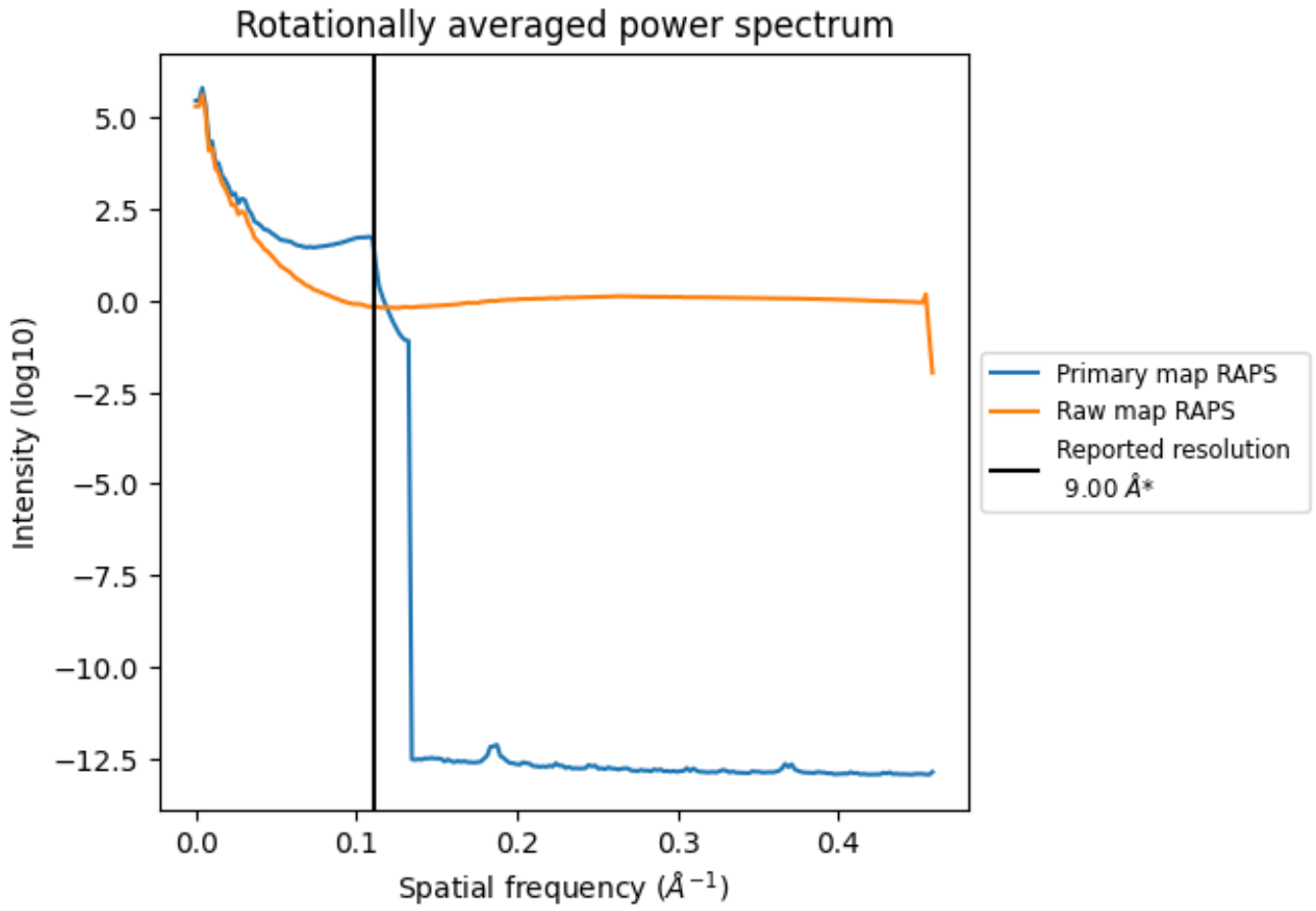
7.2 Volume estimate



The volume at the recommended contour level is 304 nm^3; this corresponds to an approximate mass of 275 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)

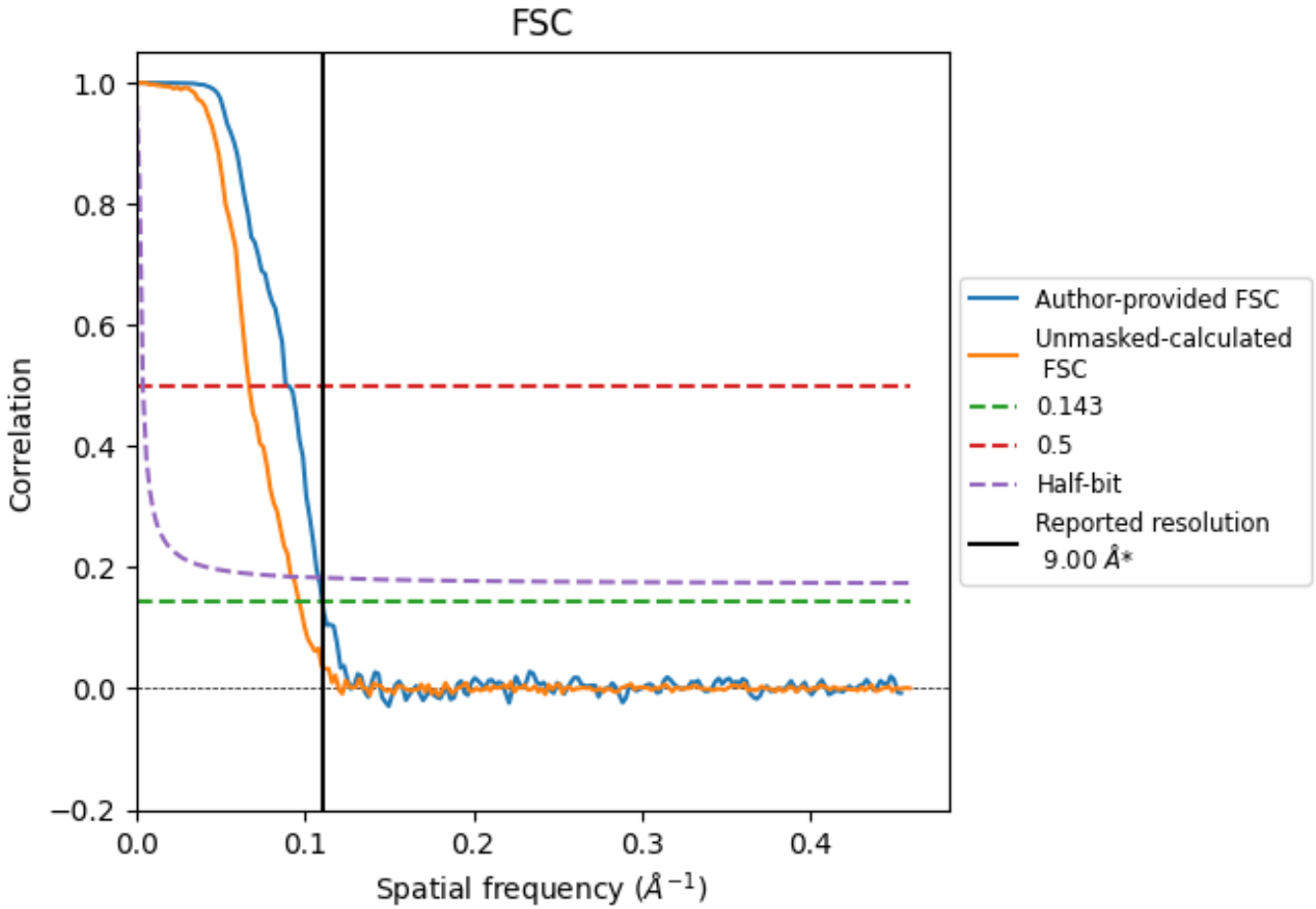


*Reported resolution corresponds to spatial frequency of 0.111 $Å^{-1}$

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 0.111 Å^{-1}

8.2 Resolution estimates (i)

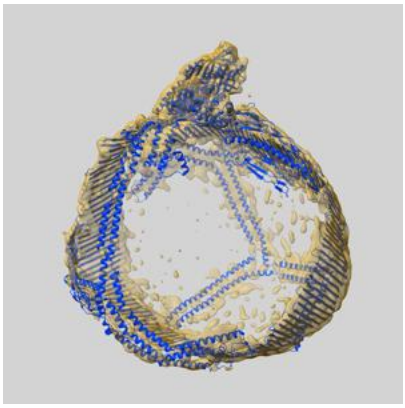
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	9.00	-	-
Author-provided FSC curve	9.06	11.27	9.24
Unmasked-calculated*	10.34	14.93	10.85

*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 10.34 differs from the reported value 9.0 by more than 10 %

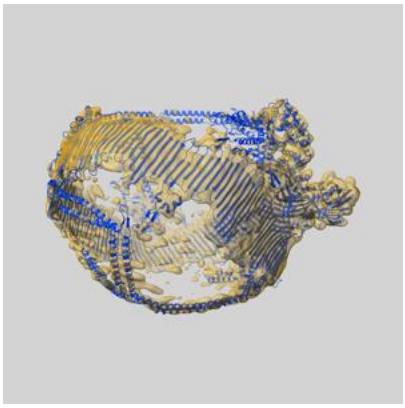
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-47801 and PDB model 9EA7. Per-residue inclusion information can be found in section 3 on page 4.

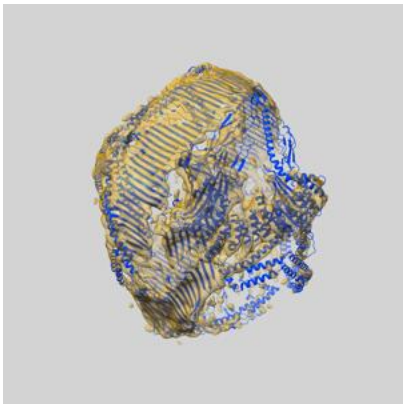
9.1 Map-model overlay



X



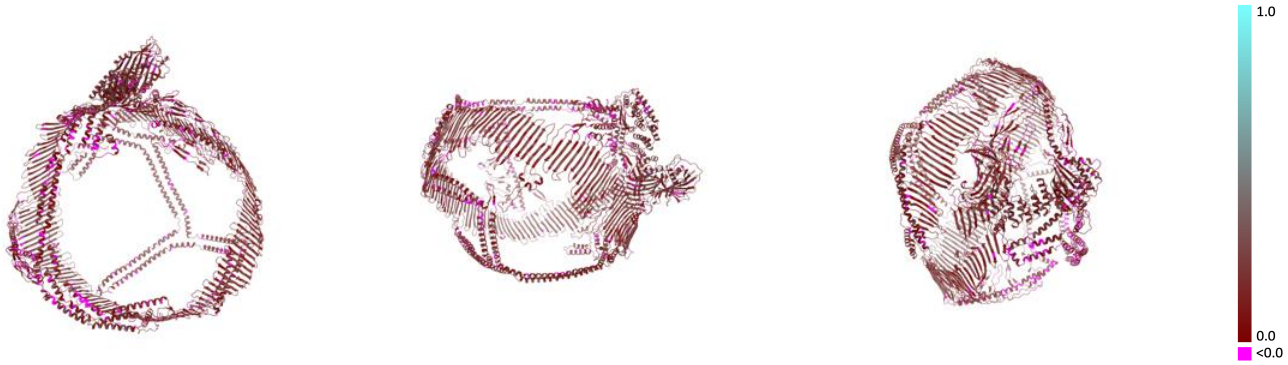
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.182 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.

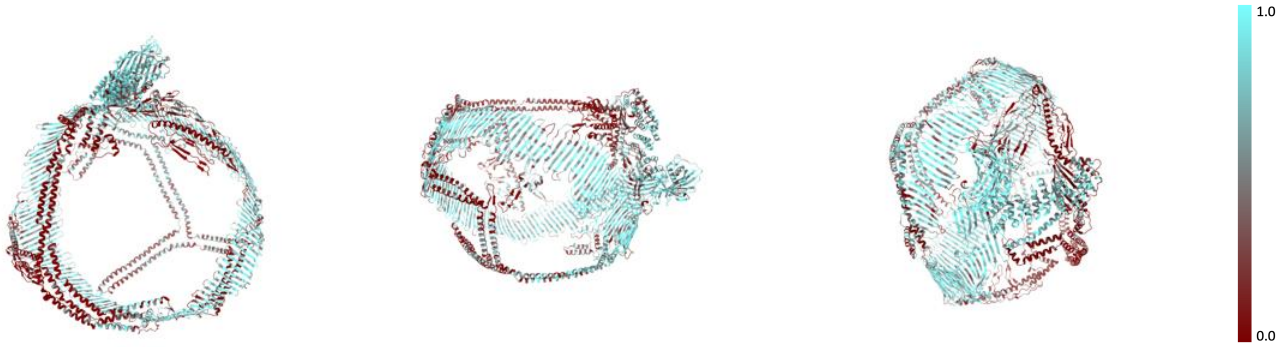
9.2 Q-score mapped to coordinate model



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.

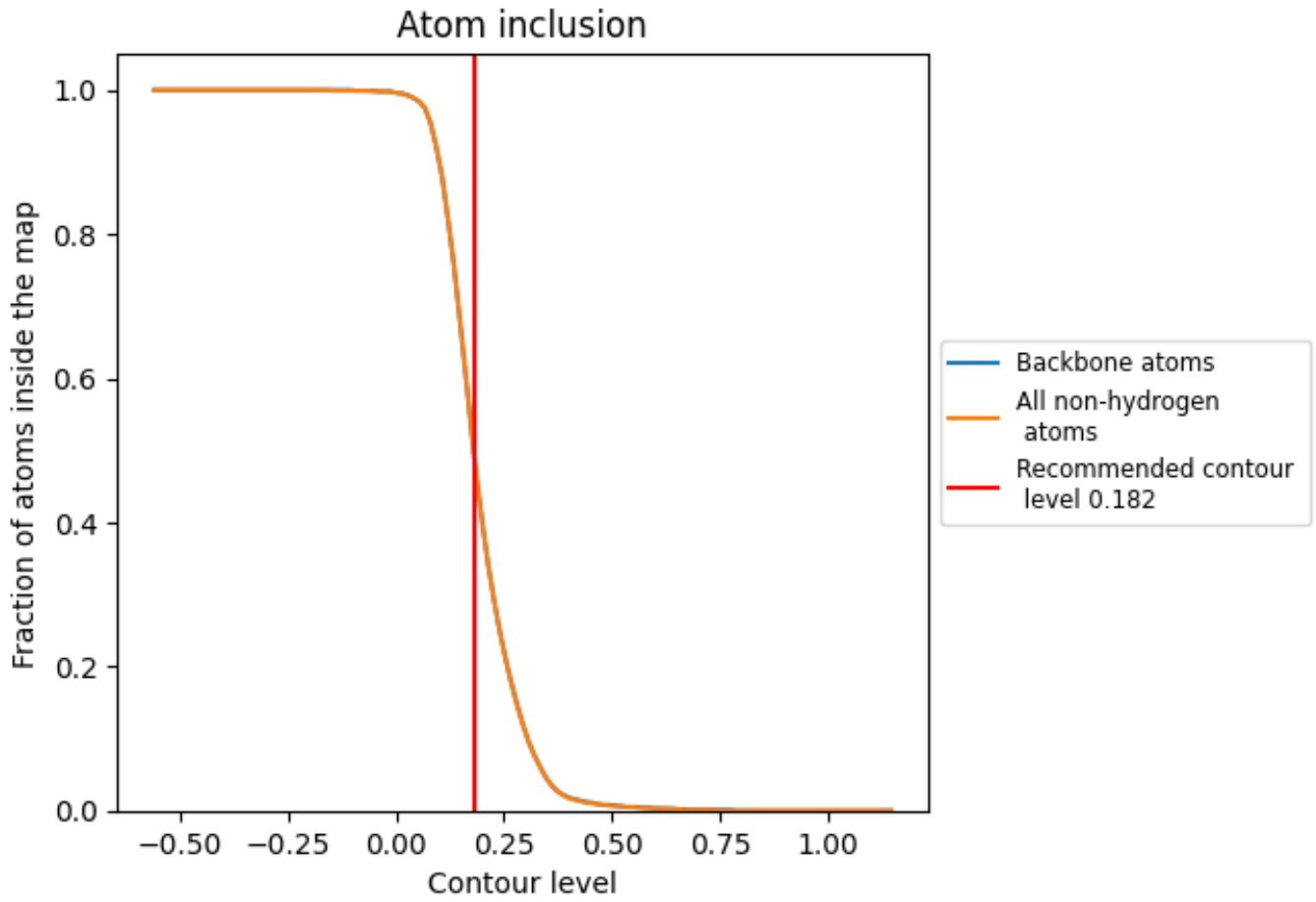
9.3 Atom inclusion mapped to coordinate model



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 (0.182).

9.4 Atom inclusion (i)



At the recommended contour level, 49% of all backbone atoms, 49% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.182) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4860	0.1580
A	0.4930	0.1580