Full wwPDB EM Validation Report ⓘ

Apr 22, 2024 – 04:47 pm BST

PDB ID	:	7BLN
EMDB ID	:	EMD-12220
Title	:	VPS35/VPS29 arch of metazoan membrane-assembled retromer:SNX3 complex modelled with human proteins
Authors	:	Leneva, N.; Kovtun, O.; Morado, D.R.; Briggs, J.A.G.; Owen, D.J.
Deposited on	:	2021-01-18
Resolution	:	8.90 Å(reported)
Based on initial models	:	5F0L, 2R17

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:

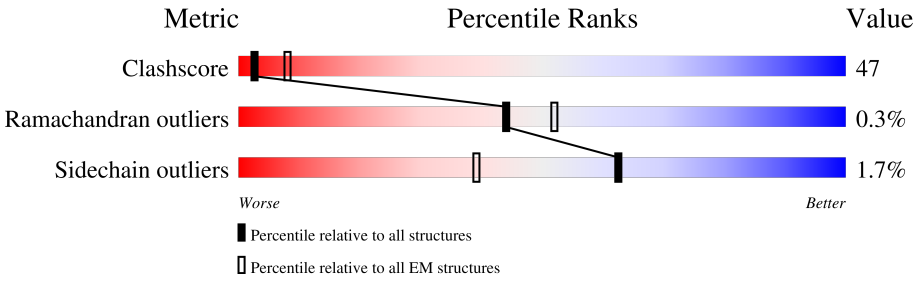
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 8.90 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	B	182	60% 57% 38% 5%
1	D	182	58% 54% 42% .
2	A	796	32% 29% 65% . .
2	C	796	34% 30% 64% . .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15364 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 Vacuolar protein sorting-associated protein 29.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	182	Total	C	N	O	S	0	0
			1447	936	242	263	6		
1	D	182	Total	C	N	O	S	0	0
			1447	936	242	263	6		

- Molecule 2 is a protein called Vacuolar protein sorting-associated protein 35.

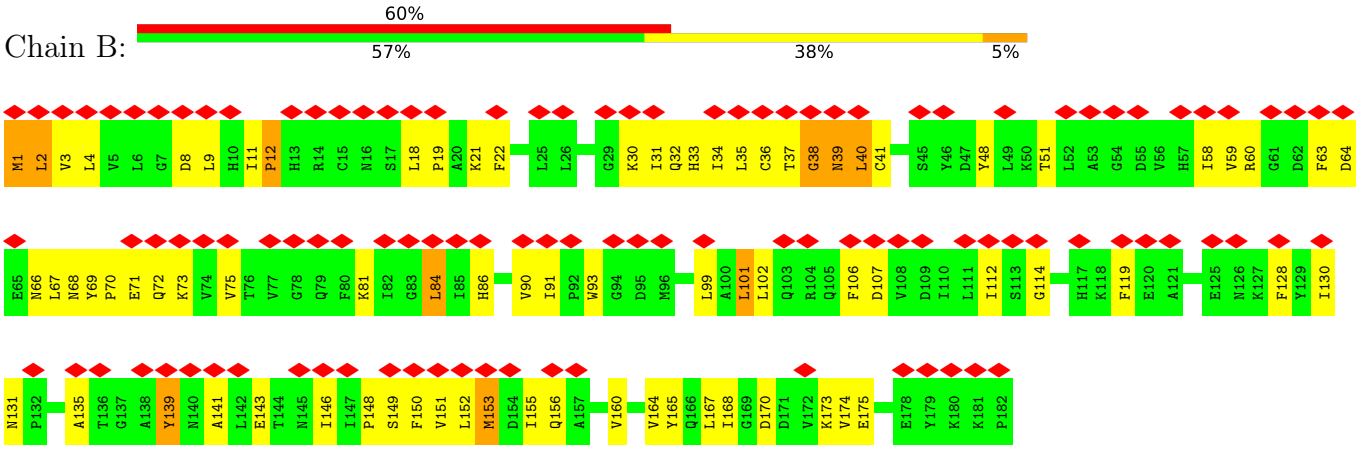
Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	769	Total	C	N	O	S	0	0
			6235	3959	1069	1175	32		
2	C	769	Total	C	N	O	S	0	0
			6235	3959	1069	1175	32		

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.

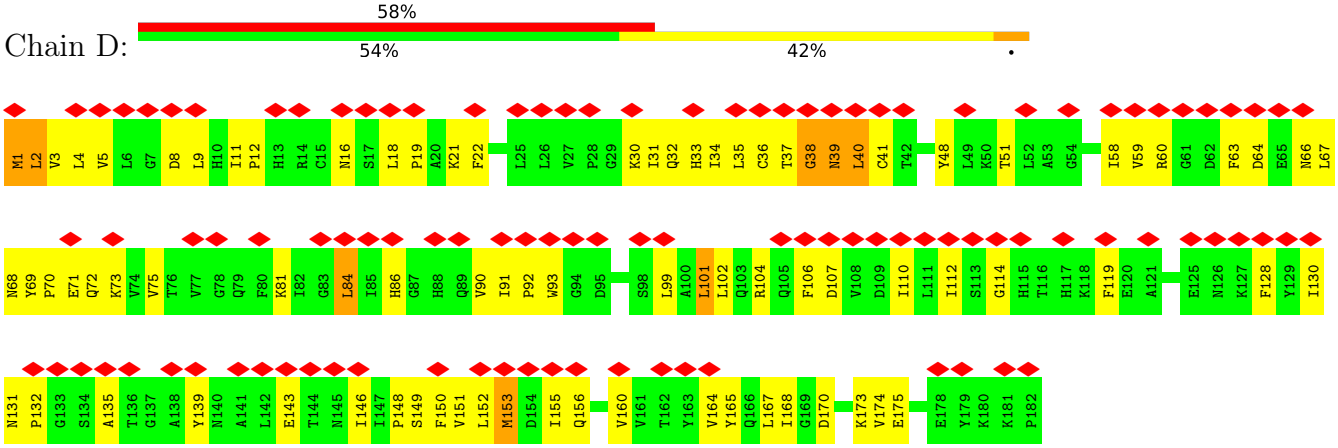
• Molecule 1: Vacuolar protein sorting-associated protein 29

Chain B:



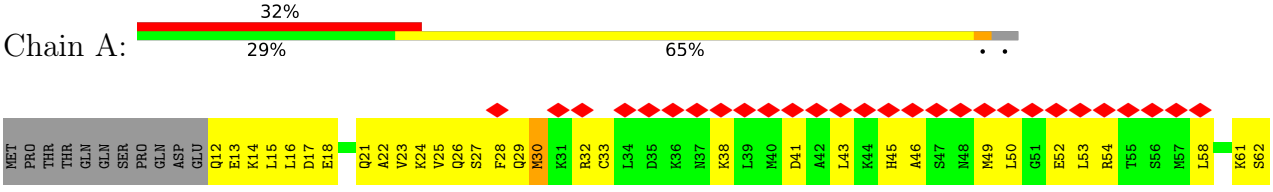
• Molecule 1: Vacuolar protein sorting-associated protein 29

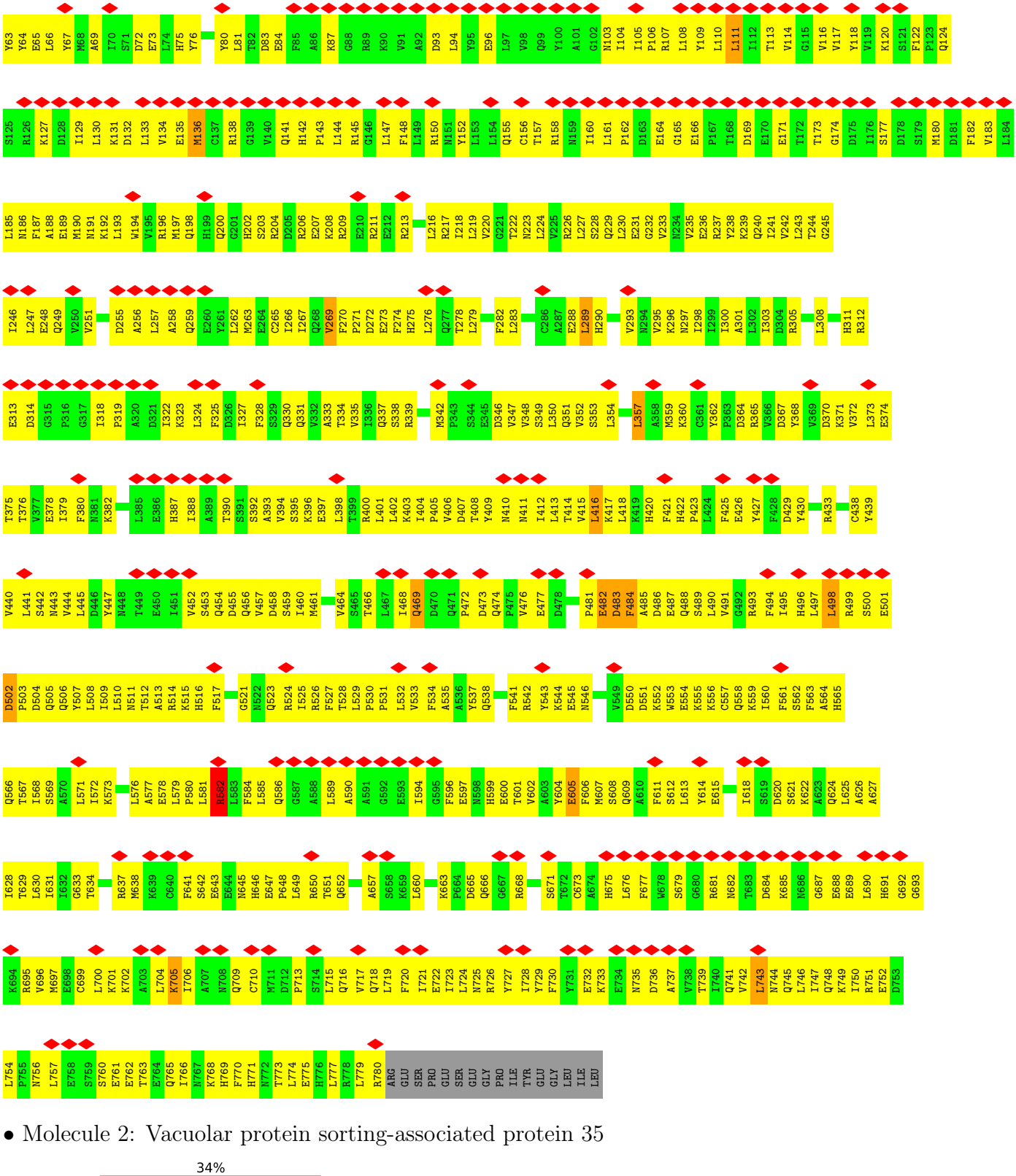
Chain D:



• Molecule 2: Vacuolar protein sorting-associated protein 35

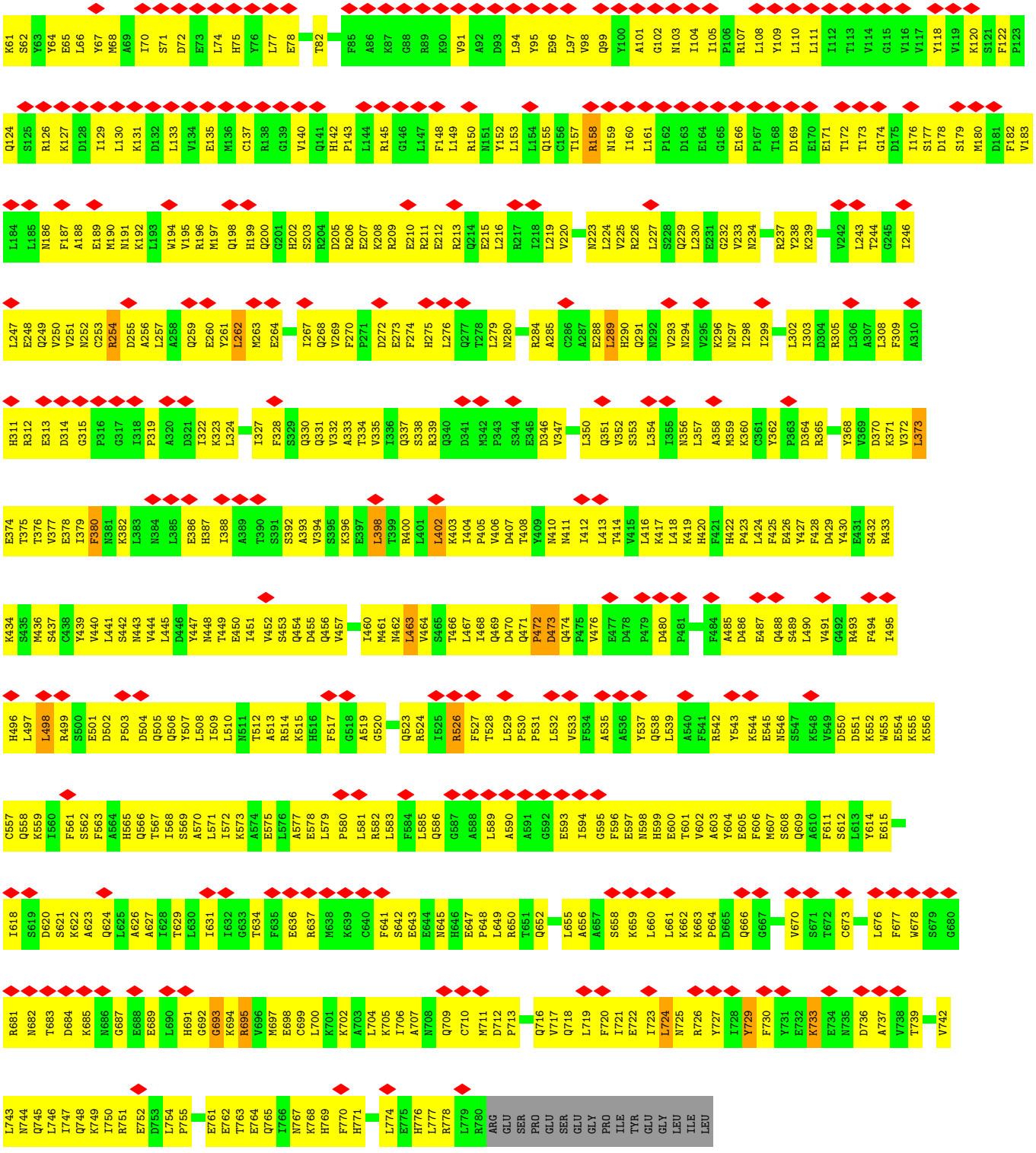
Chain A:





• Molecule 2: Vacuolar protein sorting-associated protein 35

Chain C:


K61 S62 Y63 Y64 E65 L66 Y67 M68 A69 I70 S71 D72 E73 L74 H75 Y76 L77 E78 T82 F85 A86 K87 G88 R89 K90 V91 A92 D93 L94 Y95 E96 L97 V98 Q99 Y100 A101 G102 N103 I104 I105 P106 R107 L108 Y109 L110 L111 I112 T113 V114 G115 V116 V117 Y118 V119 K120 S121 F122 P123
Q124 S125 R126 K127 D128 I129 L130 K131 D132 L133 V134 E135 M136 C137 R138 G139 V140 Q141 H142 P143 L144 R145 G146 L147 F148 L149 R150 N151 Y152 L153 L154 Q155 C156 T157 R158 N159 I160 L161 P162 D163 E164 G165 E166 P167 T168 D169 E170 E171 T172 T173 G174 D175 I176 S177 D178 S179 M180 D181 F182 V183
L184 L185 N186 F187 A188 E189 M190 N191 K192 L193 W194 V195 R196 M197 Q198 H199 Q200 G201 H202 S203 R204 D205 R206 E207 K208 R209 E210 R211 E212 R213 Q214 E215 L216 R217 I218 L219 V220 N223 L224 V225 R226 L227 S228 Q229 L230 E231 G232 V233 N234 R237 Y238 K239 V242 L243 T244 G245 I246
L247 E248 Q249 V250 V251 N252 C253 R254 D255 A256 L257 A258 Q259 E260 Y261 L262 M263 E264 I267 Q268 V269 P270 P271 D272 E273 F274 H275 L276 Q277 T278 L279 N280 R284 A285 C286 A287 E288 L289 H290 Q291 N292 V293 N294 V295 K296 N297 I298 I299 L302 I303 D304 R305 L306 A307 L308 F309 A310
H311 R312 E313 D314 G315 P316 G317 I318 P319 A320 D321 I322 K323 L324 I327 F328 S329 Q330 Q331 V332 A333 T334 V335 I336 Q337 S338 R339 Q340 D341 M342 P343 S344 E345 D346 V347 L350 Q351 V352 S353 L354 I355 N356 L357 A358 M359 K360 C361 Y362 P363 D364 R365 Y368 V369 D370 K371 V372 L373
E374 T375 T376 V377 E378 I379 F380 N381 K382 L383 N384 L385 E386 H387 I388 A389 T390 S391 S392 A393 V394 S395 K396 E397 L398 T399 R400 L401 L402 K403 I404 P405 V406 D407 T408 Y409 N410 N411 I412 L413 T414 V415 L416 K417 L418 K419 H420 F421 H422 P423 L424 F425 E426 Y427 F428 D429 Y430 E431 S432 R433
K434 S435 M436 S437 C438 Y439 V440 L441 S442 N443 V444 L445 D446 Y447 N448 T449 E450 I451 V452 S453 Q454 D455 Q456 V457 I460 M461 N462 L463 V464 S465 T466 L467 I468 Q469 D470 Q471 P472 D473 Q474 P475 V476 E477 D478 P479 D480 P481 F484 A485 D486 E487 Q488 S489 L490 V491 G492 R493 F494 I495
H496 L497 L498 R499 S500 E501 D502 P503 D504 Q505 Q506 Y507 L508 I509 L510 N511 T512 A513 R514 K515 H516 F517 G518 A519 G520 Q523 R524 I525 R526 F527 T528 L529 P530 P531 L532 V533 P534 A535 A536 Y537 Q538 L539 A540 F541 R542 Y543 K544 E545 N546 S547 K548 V549 D550 D551 K552 W553 E554 K555 K556
C557 Q558 K559 I560 F561 S562 F563 A564 H565 Q566 T567 I568 S569 A570 L571 I572 K573 A574 E575 L576 A577 E578 L579 P580 L581 R582 L583 F584 L585 Q586 G587 A588 L589 A590 A591 G592 E593 I594 G595 F596 E597 N598 H599 E600 T601 V602 A603 Y604 E605 F606 M607 S608 Q609 A610 F611 S612 L613 Y614 E615
I618 S619 D620 S621 K622 A623 Q624 L625 A626 A627 I628 T629 L630 I631 I632 G633 T634 F635 E636 R637 M638 K639 C640 F641 S642 E643 E644 N645 H646 E647 P648 L649 R650 T651 Q652 L655 A656 A657 S658 K659 L660 L661 K662 K663 P664 D665 Q666 G667 V670 S671 T672 C673 L676 F677 W678 S679 G680
R681 N682 T683 D684 K685 N686 G687 E688 E689 L690 H691 G692 G693 K694 R695 V696 M697 E698 C699 L700 K701 K702 A703 L704 K705 I706 A707 N708 Q709 C710 M711 D712 P713 Q716 V717 Q718 L719 F720 I721 E722 I723 L724 N725 R726 Y727 I728 Y729 F730 Y731 E732 K733 E734 N735 D736 A737 V738 T739 V742
L743 N744 Q745 L746 I747 Q748 K749 I750 R751 E752 D753 L754 P755 E761 E762 T763 E764 Q765 Y766 N767 K768 H769 F770 H771 L774 E775 H776 L777 R778 L779 R780 ARG GLU SER PRO GLU SER GLU GLY PRO ILE TYR GLU GLY LEU ILE LEU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	89313	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	3	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.068	Depositor
Minimum map value	-0.047	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.021	Depositor
Map size (Å)	285.768, 285.768, 285.768	wwPDB
Map dimensions	168, 168, 168	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.701, 1.701, 1.701	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	B	0.46	2/1481 (0.1%)	0.68	0/2008
1	D	0.46	2/1481 (0.1%)	0.68	0/2008
2	A	0.53	0/6348	0.82	10/8578 (0.1%)
2	C	0.49	2/6348 (0.0%)	0.79	11/8578 (0.1%)
All	All	0.50	6/15658 (0.0%)	0.78	21/21172 (0.1%)

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
2	A	0	5
2	C	0	1
All	All	0	6

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	729	TYR	CD1-CE1	-6.78	1.29	1.39
1	B	1	MET	CG-SD	5.86	1.96	1.81
1	D	1	MET	CG-SD	5.85	1.96	1.81
1	D	153	MET	CG-SD	5.76	1.96	1.81
1	B	153	MET	CG-SD	5.75	1.96	1.81
2	C	380	PHE	CB-CG	-5.22	1.42	1.51

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	724	LEU	CB-CG-CD1	-10.12	93.80	111.00
2	A	30	MET	CA-CB-CG	8.15	127.15	113.30
2	C	398	LEU	CB-CG-CD2	-7.39	98.43	111.00
2	C	402	LEU	CA-CB-CG	-7.30	98.52	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	136	MET	CA-CB-CG	7.25	125.62	113.30
2	A	269	VAL	C-N-CA	-6.56	105.31	121.70
2	C	463	LEU	CA-CB-CG	-6.04	101.41	115.30
2	C	729	TYR	CB-CG-CD1	-5.95	117.43	121.00
2	C	373	LEU	CA-CB-CG	5.92	128.91	115.30
2	A	498	LEU	CA-CB-CG	5.85	128.76	115.30
2	C	262	LEU	CA-CB-CG	-5.82	101.91	115.30
2	C	424	LEU	CA-CB-CG	-5.80	101.96	115.30
2	C	269	VAL	C-N-CA	-5.79	107.22	121.70
2	A	111	LEU	CA-CB-CG	5.76	128.55	115.30
2	C	289	LEU	CA-CB-CG	-5.53	102.58	115.30
2	A	743	LEU	CB-CG-CD2	-5.46	101.72	111.00
2	A	416	LEU	CA-CB-CG	-5.33	103.04	115.30
2	A	289	LEU	CA-CB-CG	-5.20	103.35	115.30
2	C	498	LEU	CA-CB-CG	-5.17	103.41	115.30
2	A	357	LEU	CB-CG-CD1	5.08	119.63	111.00
2	A	582	ARG	NE-CZ-NH1	-5.04	117.78	120.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	469	GLN	Peptide
2	A	482	GLU	Peptide
2	A	483	ASP	Peptide
2	A	502	ASP	Peptide
2	A	605	GLU	Mainchain
2	C	472	PRO	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1447	0	1459	90	0
1	D	1447	0	1459	89	0
2	A	6235	0	6251	675	0
2	C	6235	0	6251	622	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	15364	0	15420	1437	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 47.

All (1437) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:92:PRO:HB3	2:C:637:ARG:NH2	1.58	1.15
2:A:647:GLU:HA	2:A:650:ARG:HE	1.17	1.10
1:B:8:ASP:H	1:B:38:GLY:HA3	1.15	1.10
1:D:8:ASP:H	1:D:38:GLY:HA3	1.15	1.09
2:C:471:GLN:HB2	2:C:476:VAL:H	1.28	0.96
2:A:633:GLY:O	2:A:637:ARG:NH1	1.99	0.96
2:C:673:CYS:HA	2:C:676:LEU:HD13	1.48	0.95
2:C:196:ARG:O	2:C:196:ARG:NH1	2.01	0.94
2:A:445:LEU:HB3	2:A:493:ARG:HH11	1.33	0.92
2:C:398:LEU:HD23	2:C:428:PHE:HE1	1.34	0.91
2:A:150:ARG:NH2	2:A:189:GLU:OE1	2.04	0.90
2:A:501:GLU:O	2:A:506:GLN:NE2	2.05	0.89
2:A:296:LYS:NZ	2:A:346:ASP:O	2.07	0.88
2:C:663:LYS:NZ	2:C:706:ILE:O	2.09	0.86
2:C:430:TYR:OH	2:C:434:LYS:NZ	2.08	0.85
1:D:40:LEU:H	1:D:40:LEU:CD2	1.89	0.85
2:A:491:VAL:HA	2:A:494:PHE:HD2	1.40	0.85
2:A:665:ASP:OD1	2:A:668:ARG:NH1	2.09	0.85
2:A:296:LYS:HD2	2:A:346:ASP:HB3	1.57	0.85
2:C:454:GLN:HE22	2:C:509:ILE:HG12	1.39	0.85
1:B:141:ALA:HB1	2:A:589:LEU:HD22	1.56	0.85
2:C:677:PHE:O	2:C:695:ARG:NH2	2.08	0.85
1:B:40:LEU:H	1:B:40:LEU:CD2	1.89	0.84
2:C:105:ILE:HG23	2:C:109:TYR:HE2	1.42	0.84
2:A:23:VAL:HG21	2:A:66:LEU:HD11	1.60	0.84
2:A:50:LEU:O	2:A:54:ARG:NH1	2.11	0.84
1:D:38:GLY:HA2	1:D:86:HIS:CD2	2.14	0.83
2:C:529:LEU:HD13	2:C:532:LEU:HD12	1.60	0.83
2:A:17:ASP:O	2:A:21:GLN:NE2	2.12	0.83
2:C:124:GLN:HA	2:C:172:THR:HA	1.58	0.83
2:C:303:ILE:HG21	2:C:353:SER:HB2	1.61	0.83
1:B:3:VAL:HG22	1:B:33:HIS:HB2	1.61	0.82
1:B:38:GLY:HA2	1:B:86:HIS:CD2	2.14	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:150:ARG:NE	2:C:189:GLU:OE1	2.12	0.82
2:C:767:ASN:O	2:C:771:HIS:ND1	2.10	0.82
1:B:139:TYR:OH	2:A:586:GLN:NE2	2.12	0.82
2:C:250:VAL:O	2:C:259:GLN:NE2	2.13	0.82
2:C:636:GLU:HG3	2:C:637:ARG:HD2	1.59	0.82
2:C:523:GLN:O	2:C:526:ARG:NH1	2.13	0.81
2:A:578:GLU:N	2:A:578:GLU:OE1	2.13	0.81
2:A:108:LEU:HA	2:A:111:LEU:HG	1.62	0.81
2:C:333:ALA:O	2:C:337:GLN:NE2	2.13	0.81
2:A:72:ASP:HA	2:A:75:HIS:CD2	2.16	0.81
2:C:491:VAL:HA	2:C:494:PHE:CD2	2.16	0.80
2:A:541:PHE:HA	2:A:544:LYS:HZ3	1.46	0.80
1:D:3:VAL:HG22	1:D:33:HIS:HB2	1.61	0.80
2:A:534:PHE:HA	2:A:537:TYR:CD2	2.15	0.80
1:D:151:VAL:HG22	1:D:164:VAL:HA	1.64	0.80
2:A:529:LEU:HD12	2:A:571:LEU:HD21	1.62	0.80
2:A:685:LYS:HB3	2:A:688:GLU:HB3	1.63	0.80
1:B:151:VAL:HG22	1:B:164:VAL:HA	1.64	0.80
1:D:92:PRO:HB3	2:C:637:ARG:HH22	1.44	0.80
2:A:569:SER:HA	2:A:572:ILE:HD12	1.63	0.80
2:C:724:LEU:HD11	2:C:746:LEU:HD11	1.63	0.79
2:A:456:GLN:HE21	2:A:460:ILE:HG13	1.45	0.79
2:C:105:ILE:HG23	2:C:109:TYR:CE2	2.18	0.78
2:A:682:ASN:HD21	2:A:685:LYS:HG3	1.49	0.78
2:C:41:ASP:HA	2:C:44:LYS:HE3	1.65	0.78
2:A:523:GLN:O	2:A:526:ARG:NH1	2.18	0.77
2:A:688:GLU:OE2	2:A:691:HIS:NE2	2.17	0.77
2:C:183:VAL:HA	2:C:186:ASN:HD21	1.47	0.77
2:A:578:GLU:HB2	2:A:582:ARG:HH12	1.47	0.77
2:A:390:THR:O	2:A:396:LYS:NZ	2.12	0.77
2:A:557:CYS:O	2:A:561:PHE:HD1	1.68	0.77
2:C:284:ARG:HG3	2:C:331:GLN:HE22	1.49	0.77
2:C:370:ASP:HA	2:C:373:LEU:HD12	1.67	0.77
2:A:155:GLN:NE2	2:A:156:CYS:SG	2.59	0.76
2:C:29:GLN:HA	2:C:32:ARG:HE	1.48	0.76
1:B:141:ALA:HB1	2:A:589:LEU:CD2	2.14	0.76
2:A:647:GLU:HA	2:A:650:ARG:NE	1.98	0.76
2:A:744:ASN:O	2:A:748:GLN:NE2	2.17	0.76
2:C:451:ILE:HD11	2:C:501:GLU:HG2	1.66	0.76
2:C:312:ARG:HH22	2:C:315:GLY:HA3	1.51	0.76
2:C:188:ALA:HA	2:C:191:ASN:HD21	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:PHE:CZ	2:C:582:ARG:HD3	2.21	0.75
2:A:368:TYR:HA	2:A:371:LYS:HE2	1.67	0.75
2:A:324:LEU:HB3	2:A:328:PHE:HE2	1.51	0.75
2:C:445:LEU:HD11	2:C:490:LEU:HD23	1.67	0.75
2:C:763:THR:O	2:C:767:ASN:ND2	2.17	0.75
2:A:238:TYR:HA	2:A:242:VAL:HB	1.67	0.74
2:A:725:ASN:HB2	2:A:726:ARG:HH12	1.49	0.74
2:C:188:ALA:HA	2:C:191:ASN:ND2	2.02	0.74
2:A:324:LEU:HB3	2:A:328:PHE:CE2	2.22	0.74
2:C:441:LEU:HD21	2:C:494:PHE:HZ	1.51	0.74
2:C:223:ASN:OD1	2:C:224:LEU:N	2.21	0.74
2:A:12:GLN:HE21	2:A:15:LEU:HB2	1.52	0.74
2:C:190:MET:HE1	2:C:220:VAL:HA	1.70	0.74
1:B:139:TYR:OH	2:A:586:GLN:CD	2.26	0.74
2:A:445:LEU:HB3	2:A:493:ARG:NH1	2.03	0.74
2:C:692:GLY:H	2:C:695:ARG:NH1	1.86	0.74
2:A:263:MET:HA	2:A:266:ILE:HD12	1.70	0.73
2:A:775:GLU:HB2	2:A:780:ARG:HH11	1.54	0.73
2:A:164:GLU:HG3	2:A:232:GLY:HA2	1.69	0.73
2:A:308:LEU:O	2:A:312:ARG:HB2	1.89	0.73
1:D:40:LEU:H	1:D:40:LEU:HD23	1.54	0.73
2:A:531:PRO:HA	2:A:534:PHE:HD2	1.54	0.73
2:A:267:ILE:HD13	2:A:301:ALA:HB3	1.69	0.73
2:C:471:GLN:HB3	2:C:472:PRO:HD2	1.71	0.73
2:C:244:THR:O	2:C:248:GLU:HG3	1.89	0.73
2:A:182:PHE:O	2:A:186:ASN:ND2	2.20	0.72
2:A:352:VAL:HG13	2:A:404:ILE:HD11	1.71	0.72
2:C:291:GLN:NE2	2:C:338:SER:O	2.13	0.72
2:A:266:ILE:HG23	2:A:270:PHE:CE2	2.23	0.72
2:C:570:ALA:HA	2:C:573:LYS:NZ	2.05	0.72
2:C:725:ASN:HB3	2:C:729:TYR:OH	1.88	0.72
2:A:543:TYR:CE2	2:A:556:LYS:HB3	2.25	0.72
2:C:95:TYR:HE1	2:C:111:LEU:HB2	1.54	0.72
2:C:724:LEU:HA	2:C:727:TYR:HD2	1.54	0.72
2:C:733:LYS:HD2	2:C:733:LYS:O	1.89	0.72
1:B:40:LEU:H	1:B:40:LEU:HD23	1.54	0.72
2:C:354:LEU:HD23	2:C:357:LEU:HD21	1.71	0.72
1:D:92:PRO:HB3	2:C:637:ARG:HH21	1.50	0.72
2:C:312:ARG:NH1	2:C:313:GLU:O	2.23	0.72
2:C:718:GLN:NE2	2:C:722:GLU:OE2	2.23	0.71
2:A:429:ASP:O	2:A:433:ARG:N	2.18	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:29:GLN:HA	2:A:32:ARG:HG3	1.70	0.71
2:A:207:GLU:OE1	2:A:211:ARG:NH1	2.20	0.71
2:A:17:ASP:OD1	2:A:18:GLU:N	2.23	0.71
2:C:605:GLU:OE2	2:C:609:GLN:NE2	2.24	0.71
2:C:50:LEU:O	2:C:54:ARG:NH1	2.23	0.71
1:D:107:ASP:OD1	2:C:768:LYS:HE3	1.91	0.71
2:A:272:ASP:N	2:A:305:ARG:HH12	1.89	0.71
2:A:741:GLN:OE1	2:A:745:GLN:NE2	2.22	0.71
2:C:23:VAL:HG21	2:C:66:LEU:HD11	1.72	0.71
2:C:198:GLN:HE21	2:C:213:ARG:HH12	1.38	0.71
2:C:202:HIS:O	2:C:209:ARG:NH2	2.21	0.70
2:A:608:SER:HA	2:A:611:PHE:HD2	1.57	0.70
2:C:224:LEU:HA	2:C:227:LEU:HD12	1.72	0.70
2:C:685:LYS:NZ	2:C:689:GLU:O	2.23	0.70
1:D:18:LEU:HD12	1:D:18:LEU:H	1.56	0.70
2:C:96:GLU:O	2:C:99:GLN:HG2	1.89	0.70
2:A:646:HIS:O	2:A:650:ARG:HG3	1.90	0.70
1:D:16:ASN:HB2	2:C:493:ARG:NH2	2.07	0.70
2:A:485:ALA:O	2:A:488:GLN:NE2	2.24	0.70
2:A:535:ALA:O	2:A:538:GLN:HG3	1.91	0.70
2:C:681:ARG:NE	2:C:687:GLY:O	2.25	0.70
2:A:681:ARG:HG2	2:A:689:GLU:HA	1.74	0.70
2:C:29:GLN:HB2	2:C:32:ARG:HH21	1.55	0.70
2:C:137:CYS:SG	2:C:150:ARG:NH2	2.64	0.69
2:C:681:ARG:HB2	2:C:687:GLY:O	1.93	0.69
2:A:550:ASP:OD1	2:A:553:TRP:N	2.24	0.69
2:A:496:HIS:HA	2:A:499:ARG:NH1	2.07	0.69
2:C:205:ASP:HB2	2:C:209:ARG:NH1	2.07	0.69
2:A:194:TRP:CZ3	2:A:258:ALA:HB2	2.27	0.69
2:A:267:ILE:HG21	2:A:301:ALA:HB1	1.75	0.69
2:A:483:ASP:HB2	2:A:486:ASP:HB3	1.74	0.69
2:C:751:ARG:HH21	2:C:754:LEU:HD22	1.56	0.69
2:A:403:LYS:HZ3	2:A:406:VAL:HG11	1.58	0.69
1:B:18:LEU:HD12	1:B:18:LEU:H	1.56	0.69
2:A:67:TYR:CE2	2:A:148:PHE:HB3	2.28	0.69
2:C:662:LYS:HG2	2:C:664:PRO:HD2	1.73	0.69
2:A:58:LEU:HB2	2:A:63:TYR:CE2	2.28	0.69
2:A:233:VAL:HA	2:A:237:ARG:HH12	1.58	0.69
2:A:236:GLU:HA	2:A:239:LYS:HG2	1.75	0.69
2:C:368:TYR:HA	2:C:371:LYS:HE2	1.75	0.69
2:A:12:GLN:HG2	2:A:13:GLU:N	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:724:LEU:HD11	2:C:746:LEU:CD1	2.22	0.68
2:A:206:ARG:NH2	2:A:209:ARG:HE	1.91	0.68
2:C:373:LEU:HB3	2:C:420:HIS:HD2	1.56	0.68
2:A:710:CYS:HB2	2:A:716:GLN:HG3	1.74	0.68
2:C:499:ARG:HD3	2:C:535:ALA:HA	1.75	0.68
2:A:481:PRO:HD2	2:A:484:PHE:CE1	2.29	0.68
2:C:373:LEU:HD13	2:C:420:HIS:HB3	1.75	0.68
2:A:319:PRO:HD2	2:A:322:ILE:HD11	1.75	0.68
2:C:26:GLN:NE2	2:C:52:GLU:OE2	2.20	0.68
1:D:39:ASN:HD22	1:D:63:PHE:H	1.41	0.68
2:A:556:LYS:HA	2:A:559:LYS:HE3	1.76	0.68
2:C:689:GLU:HB2	2:C:691:HIS:CE1	2.28	0.68
1:B:9:LEU:CD2	1:B:135:ALA:HB3	2.24	0.68
2:A:226:ARG:HD2	2:A:229:GLN:NE2	2.08	0.68
2:A:455:ASP:OD1	2:A:456:GLN:N	2.27	0.68
2:C:183:VAL:HA	2:C:186:ASN:ND2	2.08	0.68
2:C:243:LEU:HA	2:C:246:ILE:HG12	1.74	0.68
1:D:9:LEU:CD2	1:D:135:ALA:HB3	2.24	0.67
2:C:71:SER:O	2:C:75:HIS:ND1	2.26	0.67
2:A:461:MET:HB3	2:A:516:HIS:CD2	2.30	0.67
2:A:552:LYS:HA	2:A:555:LYS:HE2	1.77	0.67
2:A:689:GLU:HB2	2:A:691:HIS:CE1	2.30	0.67
1:D:8:ASP:N	1:D:38:GLY:HA3	2.00	0.67
2:C:176:ILE:HG12	2:C:232:GLY:HA3	1.77	0.67
2:C:718:GLN:O	2:C:721:ILE:HG22	1.93	0.67
1:B:39:ASN:HD22	1:B:63:PHE:H	1.41	0.67
1:D:112:ILE:HD13	1:D:130:ILE:HB	1.76	0.67
2:A:375:THR:HA	2:A:378:GLU:OE1	1.95	0.67
2:C:702:LYS:HA	2:C:705:LYS:HE3	1.74	0.67
2:A:495:ILE:O	2:A:498:LEU:HG	1.94	0.67
2:A:745:GLN:O	2:A:749:LYS:HG3	1.95	0.67
2:C:362:TYR:HB3	2:C:365:ARG:HG2	1.76	0.67
2:C:569:SER:HA	2:C:572:ILE:HD12	1.77	0.67
1:B:112:ILE:HD13	1:B:130:ILE:HB	1.76	0.67
2:A:647:GLU:OE1	2:A:695:ARG:NH1	2.28	0.67
2:A:722:GLU:O	2:A:726:ARG:NH1	2.27	0.67
2:A:702:LYS:O	2:A:705:LYS:HG3	1.95	0.67
1:B:38:GLY:HA2	1:B:86:HIS:HD2	1.58	0.67
1:D:38:GLY:HA2	1:D:86:HIS:HD2	1.57	0.67
2:A:246:ILE:HD13	2:A:249:GLN:HE22	1.58	0.67
2:A:296:LYS:NZ	2:A:350:LEU:HG	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:99:GLN:HA	2:C:107:ARG:HG2	1.77	0.67
2:C:582:ARG:O	2:C:586:GLN:HG2	1.95	0.67
2:A:505:GLN:O	2:A:509:ILE:HG13	1.96	0.66
2:C:118:TYR:O	2:C:122:PHE:N	2.25	0.66
2:C:495:ILE:HG22	2:C:499:ARG:HH22	1.60	0.66
2:A:224:LEU:HD23	2:A:265:CYS:SG	2.35	0.66
2:A:233:VAL:HA	2:A:237:ARG:NH1	2.11	0.66
2:A:725:ASN:HB2	2:A:726:ARG:NH1	2.10	0.66
1:B:93:TRP:CZ3	2:A:637:ARG:NH2	2.63	0.66
2:A:13:GLU:HA	2:A:16:LEU:HD12	1.76	0.66
2:A:303:ILE:HG23	2:A:357:LEU:HD21	1.77	0.66
2:A:577:ALA:HA	2:A:613:LEU:HD21	1.77	0.66
2:A:93:ASP:HB3	2:A:96:GLU:OE2	1.96	0.66
2:A:333:ALA:O	2:A:337:GLN:HG2	1.95	0.66
2:A:487:GLU:HA	2:A:490:LEU:HD13	1.76	0.66
2:C:205:ASP:HB3	2:C:208:LYS:HE3	1.77	0.66
1:B:63:PHE:HZ	2:A:582:ARG:HB3	1.60	0.66
2:C:238:TYR:CE2	2:C:274:PHE:HB3	2.30	0.66
2:C:264:GLU:HA	2:C:267:ILE:HD12	1.78	0.66
2:A:116:VAL:O	2:A:120:LYS:NZ	2.27	0.66
2:A:483:ASP:O	2:A:485:ALA:N	2.29	0.66
2:A:660:LEU:O	2:A:666:GLN:NE2	2.29	0.66
2:A:730:PHE:HB3	2:A:735:ASN:HD22	1.61	0.66
2:C:387:HIS:HB3	2:C:429:ASP:HA	1.76	0.66
2:A:158:ARG:HA	2:A:226:ARG:NE	2.11	0.66
2:C:101:ALA:O	2:C:107:ARG:NH1	2.29	0.66
2:A:46:ALA:HA	2:A:49:MET:CE	2.26	0.65
2:A:138:ARG:NH1	2:A:189:GLU:OE2	2.20	0.65
2:A:503:PRO:HG3	2:A:542:ARG:HG2	1.79	0.65
2:C:296:LYS:HG3	2:C:350:LEU:HD21	1.76	0.65
2:C:685:LYS:HG2	2:C:685:LYS:O	1.95	0.65
2:A:627:ALA:O	2:A:631:ILE:HG13	1.96	0.65
2:C:145:ARG:O	2:C:149:LEU:HD23	1.97	0.65
2:A:270:PHE:HB2	2:A:275:HIS:NE2	2.10	0.65
2:C:660:LEU:HD21	2:C:666:GLN:HA	1.77	0.65
2:A:46:ALA:HA	2:A:49:MET:HE1	1.79	0.65
2:C:745:GLN:O	2:C:749:LYS:HG3	1.97	0.65
2:A:609:GLN:O	2:A:612:SER:OG	2.12	0.65
2:C:723:ILE:HG12	2:C:727:TYR:CE2	2.32	0.65
1:B:141:ALA:HB2	2:A:586:GLN:HE22	1.61	0.65
2:A:648:PRO:HB2	2:A:649:LEU:HD12	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:523:GLN:HG3	2:C:524:ARG:HG3	1.79	0.65
2:C:726:ARG:HA	2:C:729:TYR:CD2	2.32	0.65
2:A:296:LYS:HZ2	2:A:350:LEU:HG	1.61	0.64
2:C:705:LYS:O	2:C:709:GLN:HG2	1.97	0.64
2:A:513:ALA:HB1	2:A:517:PHE:HE2	1.62	0.64
2:A:538:GLN:HA	2:A:541:PHE:CD2	2.32	0.64
2:A:727:TYR:CB	2:A:743:LEU:HD21	2.27	0.64
2:A:750:ILE:HG22	2:A:751:ARG:HH22	1.62	0.64
2:C:297:ASN:OD1	2:C:298:ILE:N	2.29	0.64
2:C:533:VAL:HG11	2:C:583:LEU:HD22	1.79	0.64
2:C:494:PHE:O	2:C:498:LEU:HG	1.97	0.64
2:C:596:PHE:O	2:C:599:HIS:ND1	2.30	0.64
1:D:104:ARG:HB3	2:C:769:HIS:ND1	2.12	0.64
1:B:8:ASP:N	1:B:38:GLY:HA3	2.00	0.64
1:D:4:LEU:HB3	1:D:34:ILE:HG12	1.79	0.64
2:A:342:MET:SD	2:A:346:ASP:HB2	2.37	0.64
2:A:393:ALA:HA	2:A:396:LYS:HG2	1.80	0.64
2:C:224:LEU:HD11	2:C:270:PHE:CZ	2.32	0.64
2:A:183:VAL:HG11	2:A:227:LEU:HD21	1.78	0.64
2:A:474:GLN:HE22	2:A:477:GLU:H	1.45	0.64
2:C:206:ARG:HD3	2:C:209:ARG:HE	1.61	0.64
2:C:474:GLN:HG2	2:C:476:VAL:HG13	1.78	0.64
2:C:626:ALA:O	2:C:629:THR:HG22	1.98	0.64
1:B:4:LEU:HB3	1:B:34:ILE:HG12	1.79	0.64
2:A:403:LYS:HD2	2:A:439:TYR:HE2	1.62	0.64
1:B:164:VAL:CG1	1:B:175:GLU:HB3	2.28	0.63
2:C:98:VAL:HB	2:C:110:LEU:HD13	1.79	0.63
2:C:505:GLN:O	2:C:509:ILE:HG13	1.99	0.63
2:A:327:ILE:O	2:A:330:GLN:HG3	1.99	0.63
2:A:650:ARG:HB2	2:A:650:ARG:CZ	2.28	0.63
2:A:224:LEU:HD12	2:A:227:LEU:HB2	1.81	0.63
2:C:469:GLN:NE2	2:C:519:ALA:O	2.31	0.63
2:A:545:GLU:OE1	2:A:546:ASN:ND2	2.32	0.63
2:C:620:ASP:OD1	2:C:622:LYS:NZ	2.31	0.63
2:A:489:SER:OG	2:A:493:ARG:NH1	2.31	0.63
1:B:19:PRO:HG2	1:B:22:PHE:HB2	1.81	0.63
1:D:164:VAL:CG1	1:D:175:GLU:HB3	2.28	0.63
2:C:249:GLN:NE2	2:C:250:VAL:HG23	2.14	0.63
2:C:347:VAL:O	2:C:351:GLN:HG2	1.99	0.63
2:C:692:GLY:N	2:C:695:ARG:NH1	2.47	0.63
2:A:645:ASN:O	2:A:649:LEU:HD13	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:535:ALA:O	2:C:538:GLN:NE2	2.31	0.63
2:A:295:VAL:HA	2:A:298:ILE:HD12	1.81	0.63
2:A:775:GLU:HB2	2:A:780:ARG:NH1	2.12	0.63
2:C:359:MET:HE3	2:C:405:PRO:HA	1.81	0.63
2:A:541:PHE:HA	2:A:544:LYS:NZ	2.13	0.62
2:A:665:ASP:O	2:A:668:ARG:HG2	1.99	0.62
2:C:323:LYS:NZ	2:C:365:ARG:HH12	1.97	0.62
2:C:394:VAL:O	2:C:398:LEU:HD13	1.99	0.62
2:C:487:GLU:HA	2:C:490:LEU:HD12	1.79	0.62
2:A:766:ILE:HA	2:A:769:HIS:ND1	2.13	0.62
2:C:371:LYS:O	2:C:374:GLU:HG3	1.99	0.62
2:C:726:ARG:HH21	2:C:729:TYR:HB2	1.64	0.62
1:D:104:ARG:HB3	2:C:769:HIS:HD1	1.64	0.62
2:C:496:HIS:HA	2:C:499:ARG:NH2	2.14	0.62
2:C:776:HIS:O	2:C:778:ARG:NH1	2.32	0.62
2:C:311:HIS:CE1	2:C:360:LYS:HB2	2.34	0.62
2:A:27:SER:HA	2:A:30:MET:HG2	1.82	0.62
2:A:297:ASN:HA	2:A:300:ILE:HG12	1.81	0.62
2:A:365:ARG:HB2	2:A:368:TYR:CD1	2.34	0.62
2:A:412:ILE:HD13	2:A:444:VAL:HG13	1.82	0.62
2:C:545:GLU:OE1	2:C:546:ASN:ND2	2.33	0.62
2:C:655:LEU:O	2:C:659:LYS:HG2	1.99	0.62
2:A:403:LYS:HA	2:A:406:VAL:HB	1.80	0.62
1:D:19:PRO:HG2	1:D:22:PHE:HB2	1.81	0.62
1:D:48:TYR:O	1:D:51:THR:HB	2.00	0.62
2:A:134:VAL:HG22	2:A:185:LEU:HD23	1.81	0.62
2:A:198:GLN:OE1	2:A:213:ARG:HD2	2.00	0.62
2:C:585:LEU:HD13	2:C:634:THR:HG21	1.80	0.62
2:A:513:ALA:O	2:A:517:PHE:CD2	2.53	0.62
2:A:534:PHE:HA	2:A:537:TYR:CE2	2.35	0.62
2:A:585:LEU:HD13	2:A:634:THR:HG21	1.82	0.62
2:A:750:ILE:HG22	2:A:751:ARG:NH2	2.15	0.62
2:C:526:ARG:HG2	2:C:527:PHE:CD1	2.35	0.62
1:D:150:PHE:HE2	1:D:152:LEU:HD22	1.65	0.62
2:A:380:PHE:HB3	2:A:427:TYR:CZ	2.35	0.62
2:C:12:GLN:HG3	2:C:14:LYS:HE2	1.82	0.62
2:C:95:TYR:CD1	2:C:111:LEU:HD13	2.35	0.62
2:A:104:ILE:HA	2:A:107:ARG:HH11	1.65	0.61
2:A:607:MET:SD	2:A:649:LEU:HD23	2.39	0.61
2:A:677:PHE:HB2	2:A:696:VAL:HG22	1.82	0.61
1:B:48:TYR:O	1:B:51:THR:HB	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:102:GLY:C	2:C:107:ARG:HH12	2.03	0.61
2:C:226:ARG:HD2	2:C:229:GLN:HE22	1.66	0.61
2:C:604:TYR:HB2	2:C:641:PHE:HE1	1.65	0.61
2:C:682:ASN:ND2	2:C:684:ASP:OD2	2.34	0.61
2:A:183:VAL:HG21	2:A:227:LEU:HD11	1.81	0.61
2:A:271:PRO:HA	2:A:305:ARG:HH22	1.65	0.61
2:A:456:GLN:NE2	2:A:460:ILE:HG13	2.15	0.61
2:A:468:ILE:HG13	2:A:469:GLN:N	2.15	0.61
2:C:718:GLN:O	2:C:722:GLU:OE1	2.17	0.61
2:A:50:LEU:HD13	2:A:105:ILE:HG22	1.81	0.61
2:A:474:GLN:NE2	2:A:476:VAL:HA	2.16	0.61
2:C:378:GLU:OE1	2:C:382:LYS:NZ	2.28	0.61
2:A:296:LYS:HZ3	2:A:349:SER:HB2	1.64	0.61
2:A:543:TYR:HE2	2:A:556:LYS:HB3	1.64	0.61
2:C:499:ARG:HH11	2:C:499:ARG:HG3	1.66	0.61
2:C:748:GLN:O	2:C:752:GLU:HG3	2.00	0.61
1:D:16:ASN:HB2	2:C:493:ARG:CZ	2.31	0.61
2:A:114:VAL:HG22	2:A:118:TYR:CE1	2.35	0.61
2:A:308:LEU:HB2	2:A:312:ARG:HH22	1.64	0.61
2:A:438:CYS:O	2:A:442:SER:OG	2.13	0.61
2:A:506:GLN:O	2:A:510:LEU:HG	2.00	0.61
2:A:713:PRO:HB3	2:A:757:LEU:HD22	1.83	0.61
2:A:751:ARG:HA	2:A:751:ARG:NE	2.16	0.61
2:C:226:ARG:HD2	2:C:229:GLN:NE2	2.15	0.61
1:B:141:ALA:CB	2:A:589:LEU:HD13	2.31	0.61
2:A:568:ILE:HD12	2:A:584:PHE:CE1	2.35	0.61
2:A:528:THR:O	2:A:531:PRO:HD2	2.01	0.61
2:A:727:TYR:HB2	2:A:743:LEU:HD21	1.82	0.61
2:C:238:TYR:CD2	2:C:274:PHE:HB3	2.36	0.61
2:C:762:GLU:N	2:C:762:GLU:OE1	2.34	0.61
1:B:36:CYS:HB3	1:B:58:ILE:HG12	1.82	0.60
2:C:31:LYS:HD3	2:C:34:LEU:HD12	1.83	0.60
2:C:70:ILE:O	2:C:74:LEU:HD23	2.00	0.60
1:B:63:PHE:HZ	2:A:582:ARG:CB	2.14	0.60
2:A:275:HIS:O	2:A:279:LEU:HG	2.01	0.60
2:A:751:ARG:HH21	2:A:754:LEU:HD22	1.66	0.60
1:D:92:PRO:CB	2:C:637:ARG:NH2	2.51	0.60
2:A:620:ASP:OD1	2:A:622:LYS:N	2.35	0.60
2:C:196:ARG:HH12	2:C:200:GLN:N	1.98	0.60
1:B:39:ASN:HD22	1:B:63:PHE:N	2.00	0.60
1:D:148:PRO:O	1:D:149:SER:HB3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:142:HIS:HE1	2:A:144:LEU:HB3	1.67	0.60
2:A:514:ARG:HH12	2:A:566:GLN:CG	2.14	0.60
2:C:440:VAL:O	2:C:444:VAL:HG23	2.02	0.60
1:B:150:PHE:HE2	1:B:152:LEU:HD22	1.65	0.60
1:D:36:CYS:HB3	1:D:58:ILE:HG12	1.82	0.60
2:A:81:LEU:HD22	2:A:117:VAL:HG21	1.84	0.60
2:A:311:HIS:CE1	2:A:360:LYS:HB2	2.36	0.60
2:C:253:CYS:SG	2:C:259:GLN:NE2	2.72	0.60
2:C:550:ASP:OD1	2:C:552:LYS:N	2.35	0.60
1:D:39:ASN:HD22	1:D:63:PHE:N	2.00	0.60
2:A:606:PHE:HA	2:A:609:GLN:NE2	2.17	0.60
2:C:611:PHE:CE2	2:C:649:LEU:HD22	2.36	0.60
2:C:403:LYS:O	2:C:407:ASP:N	2.27	0.60
2:C:426:GLU:H	2:C:426:GLU:CD	2.06	0.60
2:A:445:LEU:HD21	2:A:490:LEU:HA	1.84	0.59
2:C:33:CYS:HA	2:C:36:LYS:HG2	1.84	0.59
2:A:487:GLU:OE1	2:A:487:GLU:N	2.35	0.59
2:C:169:ASP:O	2:C:172:THR:N	2.34	0.59
2:C:194:TRP:O	2:C:197:MET:HB2	2.02	0.59
2:C:17:ASP:OD1	2:C:18:GLU:N	2.35	0.59
2:C:503:PRO:HB3	2:C:543:TYR:CE1	2.37	0.59
1:B:148:PRO:O	1:B:149:SER:HB3	2.01	0.59
2:A:359:MET:HE1	2:A:405:PRO:HA	1.83	0.59
2:A:550:ASP:OD1	2:A:552:LYS:N	2.36	0.59
2:A:469:GLN:OE1	2:A:524:ARG:NH2	2.29	0.59
2:A:647:GLU:HG3	2:A:650:ARG:HH21	1.68	0.59
2:C:537:TYR:OH	2:C:586:GLN:HG3	2.03	0.59
1:B:93:TRP:CH2	2:A:637:ARG:NH2	2.70	0.59
2:C:468:ILE:HG13	2:C:469:GLN:OE1	2.02	0.59
2:A:255:ASP:OD1	2:A:256:ALA:N	2.33	0.59
2:A:577:ALA:O	2:A:581:LEU:HG	2.02	0.59
2:A:673:CYS:HA	2:A:676:LEU:HD23	1.85	0.59
2:A:775:GLU:HA	2:A:780:ARG:HB3	1.82	0.59
2:C:506:GLN:HE22	2:C:510:LEU:HD22	1.67	0.59
2:C:621:SER:HA	2:C:624:GLN:OE1	2.02	0.59
2:A:150:ARG:NH1	2:A:186:ASN:OD1	2.36	0.59
2:A:194:TRP:HZ3	2:A:258:ALA:HB2	1.68	0.59
2:C:378:GLU:OE2	2:C:379:ILE:HG13	2.03	0.59
2:C:730:PHE:HA	2:C:733:LYS:HB3	1.84	0.59
2:C:746:LEU:HD12	2:C:747:ILE:N	2.18	0.59
2:A:347:VAL:O	2:A:351:GLN:HG2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:495:ILE:O	2:C:499:ARG:NH1	2.36	0.59
2:C:512:THR:O	2:C:515:LYS:HG2	2.03	0.59
2:C:606:PHE:HA	2:C:609:GLN:NE2	2.18	0.59
1:D:104:ARG:HD2	2:C:769:HIS:CE1	2.38	0.58
2:A:62:SER:O	2:A:65:GLU:HG3	2.02	0.58
2:C:268:GLN:O	2:C:305:ARG:NH2	2.28	0.58
2:C:563:PHE:O	2:C:567:THR:HG23	2.03	0.58
1:D:4:LEU:HB2	1:D:31:ILE:HD13	1.85	0.58
2:A:605:GLU:O	2:A:609:GLN:OE1	2.21	0.58
2:A:648:PRO:C	2:A:652:GLN:HE22	2.07	0.58
2:C:198:GLN:HG2	2:C:213:ARG:HH11	1.68	0.58
2:C:450:GLU:HA	2:C:497:LEU:HD22	1.84	0.58
2:C:717:VAL:HA	2:C:720:PHE:CD2	2.38	0.58
1:B:71:GLU:HB3	1:B:72:GLN:OE1	2.04	0.58
1:D:71:GLU:HB3	1:D:72:GLN:OE1	2.04	0.58
2:A:127:LYS:O	2:A:131:LYS:HG2	2.04	0.58
2:A:529:LEU:HD23	2:A:532:LEU:HD12	1.84	0.58
2:C:60:PRO:HG2	2:C:61:LYS:HD2	1.85	0.58
2:C:330:GLN:O	2:C:334:THR:HG23	2.03	0.58
2:C:412:ILE:HB	2:C:449:THR:HG21	1.84	0.58
1:B:18:LEU:HD12	1:B:18:LEU:N	2.18	0.58
2:A:169:ASP:OD2	2:A:171:GLU:HB2	2.02	0.58
2:A:270:PHE:HB2	2:A:275:HIS:CE1	2.39	0.58
2:C:433:ARG:NH2	2:C:473:ASP:OD2	2.37	0.58
2:C:468:ILE:O	2:C:524:ARG:NH2	2.37	0.58
2:C:230:LEU:O	2:C:233:VAL:HG22	2.02	0.58
2:C:323:LYS:HZ3	2:C:365:ARG:HH12	1.48	0.58
2:C:503:PRO:HB3	2:C:543:TYR:HE1	1.69	0.58
2:C:583:LEU:HD23	2:C:586:GLN:NE2	2.19	0.58
1:B:4:LEU:HB2	1:B:31:ILE:HD13	1.85	0.58
2:A:197:MET:HG2	2:A:200:GLN:HE21	1.67	0.58
2:C:514:ARG:CZ	2:C:567:THR:HG22	2.34	0.58
2:A:138:ARG:HA	2:A:138:ARG:NE	2.19	0.58
2:A:700:LEU:HD11	2:A:723:ILE:HG23	1.84	0.58
2:C:471:GLN:CB	2:C:476:VAL:H	2.08	0.58
2:A:26:GLN:HB3	2:A:49:MET:SD	2.43	0.58
2:A:353:SER:O	2:A:357:LEU:HD13	2.04	0.58
2:A:362:TYR:HB3	2:A:365:ARG:HH11	1.68	0.58
2:A:541:PHE:HD1	2:A:544:LYS:HZ1	1.51	0.58
2:A:718:GLN:O	2:A:722:GLU:OE1	2.21	0.58
2:C:486:ASP:OD1	2:C:487:GLU:HG3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:29:GLN:HA	2:A:32:ARG:CG	2.34	0.58
2:C:375:THR:O	2:C:378:GLU:HG3	2.04	0.58
2:A:452:VAL:HB	2:A:497:LEU:HD13	1.86	0.57
2:C:75:HIS:O	2:C:78:GLU:HG3	2.04	0.57
1:D:18:LEU:HD12	1:D:18:LEU:N	2.18	0.57
2:A:114:VAL:HG22	2:A:118:TYR:HE1	1.68	0.57
2:A:681:ARG:HG2	2:A:689:GLU:HG2	1.87	0.57
2:A:673:CYS:O	2:A:676:LEU:HB2	2.04	0.57
2:C:590:ALA:O	2:C:593:GLU:HG3	2.03	0.57
1:B:67:LEU:HD23	1:B:67:LEU:O	2.05	0.57
1:D:67:LEU:HD23	1:D:67:LEU:O	2.05	0.57
2:A:638:MET:HB3	2:A:641:PHE:CE2	2.38	0.57
2:A:760:SER:O	2:A:763:THR:HG22	2.04	0.57
2:C:253:CYS:C	2:C:254:ARG:HD3	2.24	0.57
2:C:256:ALA:O	2:C:260:GLU:HG3	2.05	0.57
2:A:158:ARG:HA	2:A:226:ARG:HE	1.70	0.57
2:A:297:ASN:OD1	2:A:298:ILE:N	2.37	0.57
2:A:723:ILE:O	2:A:727:TYR:HD1	1.88	0.57
2:C:707:ALA:O	2:C:716:GLN:NE2	2.38	0.57
1:B:40:LEU:H	1:B:40:LEU:HD22	1.68	0.57
1:B:152:LEU:HD21	1:B:165:TYR:CE2	2.40	0.57
2:A:122:PHE:HD1	2:A:124:GLN:HE22	1.53	0.57
2:A:715:LEU:HA	2:A:718:GLN:HG3	1.87	0.57
2:C:131:LYS:NZ	2:C:135:GLU:OE2	2.37	0.57
2:C:354:LEU:O	2:C:357:LEU:HG	2.04	0.57
2:A:311:HIS:NE2	2:A:360:LYS:HB2	2.20	0.57
2:A:422:HIS:O	2:A:425:PHE:HB2	2.05	0.57
2:C:198:GLN:NE2	2:C:255:ASP:OD2	2.37	0.57
2:C:319:PRO:HB2	2:C:322:ILE:HG12	1.85	0.57
1:B:2:LEU:HD11	1:B:152:LEU:HD12	1.87	0.56
2:A:563:PHE:O	2:A:567:THR:HG23	2.05	0.56
2:C:643:GLU:CD	2:C:650:ARG:HH22	2.08	0.56
2:A:305:ARG:O	2:A:308:LEU:HG	2.05	0.56
2:A:612:SER:HA	2:A:615:GLU:OE1	2.05	0.56
2:C:39:LEU:HD12	2:C:40:MET:N	2.20	0.56
2:C:192:LYS:HE2	2:C:192:LYS:HA	1.87	0.56
2:C:412:ILE:HG12	2:C:444:VAL:HG22	1.86	0.56
2:C:445:LEU:CD1	2:C:490:LEU:HD23	2.35	0.56
2:C:517:PHE:CD2	2:C:532:LEU:HD11	2.40	0.56
2:C:570:ALA:HA	2:C:573:LYS:HZ1	1.68	0.56
2:A:94:LEU:HD13	2:A:114:VAL:HG21	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:577:ALA:O	2:A:580:PRO:HD2	2.05	0.56
2:C:182:PHE:O	2:C:186:ASN:ND2	2.37	0.56
2:A:32:ARG:NH1	2:A:41:ASP:OD2	2.38	0.56
2:A:713:PRO:O	2:A:717:VAL:HG22	2.05	0.56
2:A:719:LEU:HA	2:A:722:GLU:OE1	2.05	0.56
2:A:739:THR:OG1	2:A:742:VAL:HG23	2.04	0.56
2:A:749:LYS:HA	2:A:752:GLU:HG3	1.87	0.56
2:C:563:PHE:HA	2:C:566:GLN:OE1	2.05	0.56
2:A:218:ILE:O	2:A:222:THR:HG23	2.04	0.56
2:A:296:LYS:NZ	2:A:349:SER:HB2	2.21	0.56
2:C:155:GLN:O	2:C:158:ARG:HD2	2.04	0.56
2:C:454:GLN:HE22	2:C:509:ILE:CG1	2.15	0.56
1:D:152:LEU:HD21	1:D:165:TYR:CE2	2.40	0.56
2:A:647:GLU:CA	2:A:650:ARG:HE	2.05	0.56
2:C:95:TYR:HA	2:C:98:VAL:HG22	1.88	0.56
2:C:743:LEU:HD13	2:C:746:LEU:HD21	1.87	0.56
2:A:279:LEU:O	2:A:283:LEU:HG	2.06	0.56
2:A:561:PHE:O	2:A:565:HIS:ND1	2.38	0.56
2:A:705:LYS:O	2:A:709:GLN:HG3	2.06	0.56
2:A:718:GLN:HA	2:A:721:ILE:HD12	1.87	0.56
2:C:512:THR:OG1	2:C:515:LYS:HE3	2.06	0.56
2:C:663:LYS:NZ	2:C:710:CYS:SG	2.67	0.56
2:A:50:LEU:HD22	2:A:105:ILE:HG21	1.88	0.56
2:C:65:GLU:HA	2:C:68:MET:HG2	1.88	0.56
2:C:290:HIS:O	2:C:339:ARG:NH1	2.38	0.56
2:A:230:LEU:HB2	2:A:233:VAL:HG23	1.87	0.56
2:A:348:VAL:HG13	2:A:401:LEU:HD12	1.88	0.56
1:B:63:PHE:CZ	2:A:582:ARG:HG2	2.40	0.56
1:B:152:LEU:HD21	1:B:165:TYR:HE2	1.71	0.56
2:A:374:GLU:O	2:A:378:GLU:OE1	2.24	0.56
2:A:682:ASN:ND2	2:A:685:LYS:HG3	2.18	0.56
2:A:722:GLU:O	2:A:726:ARG:HG2	2.06	0.56
2:C:232:GLY:O	2:C:237:ARG:NH1	2.28	0.56
2:A:387:HIS:NE2	2:A:426:GLU:O	2.38	0.55
2:A:514:ARG:HH12	2:A:566:GLN:HE21	1.54	0.55
2:C:52:GLU:O	2:C:55:THR:HG22	2.06	0.55
2:C:105:ILE:O	2:C:109:TYR:HD2	1.89	0.55
2:C:126:ARG:NH1	2:C:166:GLU:OE2	2.36	0.55
2:C:563:PHE:HA	2:C:566:GLN:NE2	2.21	0.55
2:C:605:GLU:O	2:C:609:GLN:NE2	2.39	0.55
2:A:642:SER:O	2:A:646:HIS:N	2.28	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:648:PRO:O	2:A:652:GLN:NE2	2.39	0.55
2:A:761:GLU:OE1	2:A:761:GLU:N	2.39	0.55
2:A:190:MET:SD	2:A:191:ASN:N	2.79	0.55
2:C:330:GLN:NE2	2:C:331:GLN:HG2	2.22	0.55
2:C:739:THR:OG1	2:C:742:VAL:HG23	2.07	0.55
2:A:430:TYR:HA	2:A:433:ARG:HE	1.72	0.55
2:C:206:ARG:HH11	2:C:209:ARG:CZ	2.19	0.55
2:C:243:LEU:HD12	2:C:244:THR:N	2.22	0.55
2:C:246:ILE:HG13	2:C:247:LEU:N	2.22	0.55
2:C:430:TYR:HB2	2:C:473:ASP:HA	1.88	0.55
2:A:213:ARG:NH1	2:A:257:LEU:HD22	2.21	0.55
2:C:359:MET:HE1	2:C:408:THR:HB	1.87	0.55
2:C:742:VAL:O	2:C:745:GLN:HG2	2.07	0.55
2:A:638:MET:HB3	2:A:641:PHE:HE2	1.70	0.55
2:A:697:MET:O	2:A:701:LYS:HG2	2.06	0.55
2:A:716:GLN:HG2	2:A:720:PHE:CE2	2.41	0.55
2:C:346:ASP:O	2:C:350:LEU:HD23	2.06	0.55
2:C:356:ASN:C	2:C:360:LYS:HZ1	2.10	0.55
2:C:398:LEU:HD23	2:C:428:PHE:CE1	2.27	0.55
2:C:524:ARG:HA	2:C:526:ARG:NH1	2.22	0.55
2:C:609:GLN:O	2:C:612:SER:OG	2.22	0.55
2:A:165:GLY:N	2:A:231:GLU:OE1	2.39	0.55
2:A:330:GLN:NE2	2:A:331:GLN:HG2	2.22	0.55
2:A:530:PRO:HB2	2:A:531:PRO:HD3	1.89	0.55
2:A:577:ALA:CA	2:A:613:LEU:HD21	2.37	0.55
2:A:279:LEU:O	2:A:283:LEU:N	2.38	0.55
2:A:739:THR:OG1	2:A:741:GLN:NE2	2.39	0.55
2:C:528:THR:O	2:C:531:PRO:HD2	2.06	0.55
2:C:662:LYS:O	2:C:666:GLN:HB2	2.07	0.55
2:C:751:ARG:HA	2:C:751:ARG:NE	2.22	0.55
1:D:2:LEU:HD11	1:D:152:LEU:HD12	1.87	0.55
2:A:200:GLN:O	2:A:209:ARG:NH1	2.39	0.55
2:A:335:VAL:O	2:A:339:ARG:HG2	2.07	0.55
2:A:581:LEU:HD21	2:A:613:LEU:HD23	1.89	0.55
2:C:187:PHE:HE1	2:C:220:VAL:HG13	1.72	0.55
2:C:299:ILE:HA	2:C:302:LEU:HD12	1.89	0.55
2:C:711:MET:H	2:C:716:GLN:NE2	2.05	0.55
2:A:414:THR:HA	2:A:417:LYS:HE2	1.89	0.54
2:C:95:TYR:CE1	2:C:111:LEU:HB2	2.40	0.54
2:C:702:LYS:HA	2:C:705:LYS:CE	2.36	0.54
1:B:2:LEU:O	1:B:2:LEU:HD23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:152:LEU:HD21	1:D:165:TYR:HE2	1.71	0.54
2:A:180:MET:HE1	2:A:237:ARG:HE	1.72	0.54
2:A:226:ARG:HD2	2:A:229:GLN:HE22	1.72	0.54
2:A:452:VAL:HG13	2:A:456:GLN:HB3	1.89	0.54
2:C:493:ARG:HA	2:C:496:HIS:ND1	2.22	0.54
2:C:597:GLU:OE1	2:C:597:GLU:N	2.38	0.54
2:C:710:CYS:HB2	2:C:716:GLN:HE21	1.72	0.54
2:A:330:GLN:O	2:A:334:THR:HG23	2.08	0.54
2:C:495:ILE:HG22	2:C:499:ARG:NH2	2.21	0.54
2:C:517:PHE:CE2	2:C:532:LEU:HD11	2.43	0.54
2:A:162:PRO:HA	2:A:166:GLU:OE1	2.08	0.54
2:A:526:ARG:HD2	2:A:527:PHE:CZ	2.42	0.54
2:A:627:ALA:O	2:A:630:LEU:HG	2.07	0.54
2:C:103:ASN:OD1	2:C:104:ILE:N	2.39	0.54
2:C:206:ARG:HG2	2:C:209:ARG:HH21	1.71	0.54
2:A:504:ASP:N	2:A:504:ASP:OD1	2.38	0.54
2:A:190:MET:HE1	2:A:220:VAL:HG22	1.89	0.54
2:A:514:ARG:CZ	2:A:567:THR:HG22	2.38	0.54
2:A:622:LYS:O	2:A:625:LEU:HG	2.08	0.54
2:A:692:GLY:O	2:A:696:VAL:HG23	2.06	0.54
2:C:380:PHE:CE1	2:C:398:LEU:HD21	2.42	0.54
2:C:454:GLN:NE2	2:C:508:LEU:HD22	2.22	0.54
2:C:570:ALA:HA	2:C:573:LYS:HZ2	1.72	0.54
2:C:692:GLY:O	2:C:695:ARG:HD3	2.07	0.54
2:C:122:PHE:HD1	2:C:124:GLN:NE2	2.06	0.54
2:C:377:VAL:HG13	2:C:427:TYR:OH	2.07	0.54
2:C:495:ILE:HG22	2:C:499:ARG:HH12	1.73	0.54
2:C:678:TRP:O	2:C:689:GLU:HG2	2.07	0.54
2:C:695:ARG:HA	2:C:698:GLU:HG2	1.89	0.54
2:A:33:CYS:HB3	2:A:38:LYS:O	2.07	0.54
2:A:675:HIS:O	2:A:679:SER:OG	2.22	0.54
2:C:410:ASN:OD1	2:C:411:ASN:N	2.40	0.54
2:C:454:GLN:NE2	2:C:509:ILE:HG12	2.17	0.54
2:C:655:LEU:O	2:C:659:LYS:HE2	2.08	0.54
2:A:726:ARG:O	2:A:730:PHE:HD2	1.91	0.54
2:C:416:LEU:HD13	2:C:456:GLN:HB3	1.88	0.54
2:C:670:VAL:HG11	2:C:706:ILE:HD12	1.90	0.54
2:C:704:LEU:HD21	2:C:727:TYR:OH	2.08	0.54
1:D:63:PHE:HZ	2:C:582:ARG:HD3	1.72	0.54
2:A:681:ARG:HE	2:A:689:GLU:HG2	1.73	0.54
2:C:507:TYR:OH	2:C:556:LYS:O	2.24	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:69:ALA:O	2:A:72:ASP:OD1	2.26	0.53
2:A:143:PRO:HD3	2:A:196:ARG:HH22	1.72	0.53
2:A:251:VAL:HG12	2:A:289:LEU:HD21	1.90	0.53
2:A:380:PHE:HZ	2:A:398:LEU:HD21	1.72	0.53
2:A:526:ARG:HD2	2:A:527:PHE:CE1	2.43	0.53
2:A:556:LYS:HA	2:A:559:LYS:CE	2.38	0.53
2:C:716:GLN:HB3	2:C:720:PHE:CZ	2.43	0.53
1:D:2:LEU:O	1:D:2:LEU:HD23	2.07	0.53
2:A:496:HIS:HA	2:A:499:ARG:CZ	2.38	0.53
2:A:430:TYR:CG	2:A:473:ASP:HB2	2.43	0.53
2:A:491:VAL:O	2:A:495:ILE:HG12	2.09	0.53
2:A:590:ALA:O	2:A:594:ILE:HG12	2.09	0.53
2:A:763:THR:HA	2:A:766:ILE:HD12	1.89	0.53
2:C:393:ALA:HA	2:C:396:LYS:HG2	1.91	0.53
2:C:579:LEU:HA	2:C:582:ARG:HG2	1.90	0.53
1:B:141:ALA:HB2	2:A:586:GLN:NE2	2.23	0.53
2:A:469:GLN:HB2	2:A:524:ARG:NH2	2.24	0.53
2:A:602:VAL:HA	2:A:605:GLU:OE1	2.09	0.53
2:C:224:LEU:HD11	2:C:270:PHE:HZ	1.73	0.53
1:D:92:PRO:CB	2:C:637:ARG:HH22	2.16	0.53
2:A:238:TYR:CE2	2:A:274:PHE:HB3	2.43	0.53
2:A:496:HIS:HA	2:A:499:ARG:HH12	1.73	0.53
2:C:30:MET:HG3	2:C:46:ALA:HB2	1.91	0.53
2:C:227:LEU:HA	2:C:230:LEU:HD12	1.89	0.53
2:C:412:ILE:HD13	2:C:444:VAL:HA	1.91	0.53
2:C:437:SER:HA	2:C:440:VAL:HG22	1.91	0.53
2:C:563:PHE:HA	2:C:566:GLN:HE22	1.73	0.53
2:C:643:GLU:OE1	2:C:682:ASN:ND2	2.42	0.53
2:A:105:ILE:HG23	2:A:109:TYR:CE2	2.44	0.53
2:A:323:LYS:HE3	2:A:368:TYR:CE2	2.44	0.53
2:A:491:VAL:HA	2:A:494:PHE:CD2	2.32	0.53
2:C:206:ARG:HH11	2:C:209:ARG:NH2	2.07	0.53
2:C:333:ALA:C	2:C:337:GLN:HE22	2.12	0.53
2:A:495:ILE:HG22	2:A:499:ARG:HH21	1.73	0.53
2:A:525:ILE:HA	2:A:528:THR:OG1	2.09	0.53
2:A:557:CYS:HA	2:A:560:ILE:HG12	1.91	0.53
2:A:663:LYS:NZ	2:A:706:ILE:O	2.25	0.53
2:A:769:HIS:O	2:A:773:THR:OG1	2.22	0.53
2:C:570:ALA:O	2:C:573:LYS:HG2	2.09	0.53
2:A:701:LYS:HD3	2:A:701:LYS:N	2.24	0.53
2:C:413:LEU:HD21	2:C:452:VAL:HG22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:198:GLN:NE2	2:C:213:ARG:HH12	2.03	0.52
2:C:578:GLU:CD	2:C:578:GLU:H	2.11	0.52
1:B:101:LEU:HD12	1:B:101:LEU:O	2.09	0.52
2:A:247:LEU:O	2:A:251:VAL:HG22	2.08	0.52
2:C:297:ASN:OD1	2:C:298:ILE:HG13	2.09	0.52
2:C:643:GLU:OE2	2:C:650:ARG:NH1	2.31	0.52
1:B:39:ASN:HA	1:B:64:ASP:OD2	2.10	0.52
1:B:63:PHE:CZ	2:A:582:ARG:CB	2.92	0.52
2:A:233:VAL:HG12	2:A:274:PHE:CE2	2.44	0.52
2:A:323:LYS:NZ	2:A:325:PHE:HB3	2.24	0.52
1:B:174:VAL:HG12	1:B:175:GLU:N	2.24	0.52
1:D:40:LEU:H	1:D:40:LEU:HD22	1.69	0.52
2:A:403:LYS:NZ	2:A:406:VAL:HG11	2.24	0.52
2:A:495:ILE:HG22	2:A:499:ARG:NH2	2.23	0.52
2:C:26:GLN:HG2	2:C:48:ASN:OD1	2.09	0.52
2:C:267:ILE:HG12	2:C:302:LEU:HD21	1.90	0.52
1:B:141:ALA:HB3	2:A:589:LEU:HD13	1.91	0.52
1:D:9:LEU:HD22	1:D:135:ALA:HB3	1.92	0.52
1:D:174:VAL:HG12	1:D:175:GLU:N	2.24	0.52
2:C:252:ASN:O	2:C:254:ARG:NH1	2.35	0.52
2:C:767:ASN:C	2:C:771:HIS:HD1	2.08	0.52
1:B:164:VAL:HG13	1:B:175:GLU:HB3	1.91	0.52
2:A:501:GLU:OE2	2:A:505:GLN:HB2	2.10	0.52
2:C:26:GLN:HB2	2:C:49:MET:HB2	1.92	0.52
2:C:72:ASP:HA	2:C:75:HIS:HD1	1.75	0.52
2:C:191:ASN:O	2:C:195:VAL:HG22	2.09	0.52
2:C:506:GLN:NE2	2:C:510:LEU:HB2	2.25	0.52
2:C:620:ASP:O	2:C:624:GLN:N	2.38	0.52
2:A:563:PHE:HA	2:A:566:GLN:NE2	2.25	0.52
1:D:40:LEU:HD23	1:D:40:LEU:N	2.24	0.52
2:C:158:ARG:HG2	2:C:159:ASN:CG	2.30	0.52
1:B:3:VAL:HG22	1:B:33:HIS:CB	2.38	0.52
2:A:127:LYS:O	2:A:130:LEU:HG	2.10	0.52
2:A:241:ILE:HG13	2:A:242:VAL:N	2.23	0.52
2:A:645:ASN:O	2:A:648:PRO:HD2	2.10	0.52
2:A:716:GLN:HG2	2:A:720:PHE:HE2	1.73	0.52
1:D:164:VAL:HG13	1:D:175:GLU:HB3	1.91	0.52
2:A:650:ARG:HH12	2:A:695:ARG:NH2	2.07	0.52
2:A:741:GLN:NE2	2:A:742:VAL:HG23	2.25	0.52
2:C:29:GLN:HA	2:C:32:ARG:NE	2.22	0.52
2:C:439:TYR:O	2:C:442:SER:OG	2.26	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:598:ASN:O	2:C:601:THR:OG1	2.26	0.52
1:D:39:ASN:HA	1:D:64:ASP:OD2	2.10	0.51
2:A:124:GLN:HA	2:A:171:GLU:O	2.09	0.51
2:A:202:HIS:O	2:A:209:ARG:NH2	2.39	0.51
2:A:533:VAL:HG12	2:A:537:TYR:CZ	2.44	0.51
2:C:96:GLU:OE1	2:C:96:GLU:N	2.39	0.51
1:B:35:LEU:HD21	1:B:75:VAL:HG11	1.92	0.51
1:B:40:LEU:HD23	1:B:40:LEU:N	2.24	0.51
1:D:101:LEU:HD12	1:D:101:LEU:O	2.09	0.51
2:A:578:GLU:HA	2:A:581:LEU:HD12	1.91	0.51
2:A:770:PHE:O	2:A:774:LEU:HD23	2.10	0.51
2:A:775:GLU:HG2	2:A:780:ARG:HG2	1.92	0.51
2:C:176:ILE:HG21	2:C:237:ARG:CZ	2.40	0.51
2:C:744:ASN:HA	2:C:747:ILE:HG12	1.92	0.51
2:A:374:GLU:HG3	2:A:420:HIS:CE1	2.45	0.51
2:A:638:MET:O	2:A:646:HIS:HE1	1.93	0.51
2:A:648:PRO:C	2:A:652:GLN:NE2	2.64	0.51
2:A:704:LEU:HD11	2:A:727:TYR:OH	2.09	0.51
2:C:489:SER:O	2:C:493:ARG:NH1	2.42	0.51
1:D:168:ILE:HD12	1:D:173:LYS:HD2	1.93	0.51
2:A:238:TYR:HE2	2:A:278:THR:OG1	1.93	0.51
2:A:452:VAL:HG11	2:A:460:ILE:HD12	1.92	0.51
2:A:725:ASN:HB3	2:A:726:ARG:HH22	1.76	0.51
2:A:747:ILE:O	2:A:751:ARG:HG2	2.11	0.51
2:A:760:SER:HB3	2:A:761:GLU:OE1	2.10	0.51
2:C:195:VAL:O	2:C:198:GLN:HG3	2.10	0.51
2:C:410:ASN:HB2	2:C:447:TYR:CE1	2.45	0.51
1:B:168:ILE:HD12	1:B:173:LYS:HD2	1.93	0.51
2:A:577:ALA:C	2:A:580:PRO:HD2	2.30	0.51
2:C:324:LEU:HD22	2:C:328:PHE:HE2	1.75	0.51
2:C:558:GLN:NE2	2:C:598:ASN:HB3	2.26	0.51
2:A:26:GLN:O	2:A:30:MET:HE3	2.10	0.51
2:A:244:THR:O	2:A:248:GLU:OE1	2.29	0.51
2:A:416:LEU:HB3	2:A:456:GLN:OE1	2.11	0.51
2:A:563:PHE:HA	2:A:566:GLN:OE1	2.11	0.51
2:A:572:ILE:HD11	2:A:584:PHE:HZ	1.74	0.51
2:A:620:ASP:O	2:A:624:GLN:HG3	2.11	0.51
2:A:771:HIS:O	2:A:780:ARG:NH1	2.44	0.51
2:A:142:HIS:CE1	2:A:144:LEU:HB3	2.46	0.51
2:A:552:LYS:HD3	2:A:556:LYS:HZ1	1.76	0.51
2:C:375:THR:HA	2:C:378:GLU:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:533:VAL:HG12	2:C:537:TYR:CE2	2.46	0.51
2:C:535:ALA:O	2:C:538:GLN:HG3	2.11	0.51
2:A:80:TYR:O	2:A:84:GLU:OE1	2.29	0.51
2:A:364:ASP:OD1	2:A:365:ARG:HG2	2.11	0.51
2:C:67:TYR:CE1	2:C:148:PHE:HB3	2.46	0.51
2:C:750:ILE:HG22	2:C:751:ARG:HH22	1.75	0.51
1:B:9:LEU:HD22	1:B:135:ALA:HB3	1.92	0.51
2:A:127:LYS:HZ1	2:A:174:GLY:H	1.59	0.51
2:A:194:TRP:CH2	2:A:258:ALA:HB2	2.46	0.51
2:C:468:ILE:HG13	2:C:469:GLN:CD	2.31	0.51
2:C:578:GLU:HB3	2:C:582:ARG:HH22	1.74	0.51
2:A:403:LYS:O	2:A:407:ASP:N	2.27	0.51
2:A:454:GLN:OE1	2:A:509:ILE:HG12	2.11	0.51
2:A:578:GLU:HG2	2:A:582:ARG:HH22	1.76	0.51
2:A:581:LEU:CD2	2:A:613:LEU:HD23	2.40	0.51
2:C:16:LEU:HD13	2:C:62:SER:HB3	1.93	0.51
2:C:285:ALA:O	2:C:288:GLU:HG3	2.11	0.51
2:A:228:SER:HB3	2:A:269:VAL:HG13	1.94	0.50
2:C:472:PRO:O	2:C:474:GLN:N	2.44	0.50
2:C:495:ILE:CG2	2:C:499:ARG:HH12	2.23	0.50
2:C:729:TYR:O	2:C:733:LYS:HB2	2.11	0.50
2:A:682:ASN:ND2	2:A:684:ASP:HB2	2.26	0.50
2:A:113:THR:HG22	2:A:152:TYR:OH	2.12	0.50
2:A:236:GLU:OE2	2:A:240:GLN:NE2	2.45	0.50
2:A:387:HIS:HE1	2:A:433:ARG:NH1	2.09	0.50
2:A:579:LEU:HB3	2:A:580:PRO:HD3	1.94	0.50
2:A:733:LYS:CE	2:A:735:ASN:HD21	2.24	0.50
2:C:471:GLN:HB3	2:C:472:PRO:CD	2.42	0.50
2:C:530:PRO:HB2	2:C:531:PRO:HD3	1.93	0.50
2:C:614:TYR:O	2:C:618:ILE:HB	2.11	0.50
2:A:370:ASP:O	2:A:374:GLU:OE1	2.30	0.50
2:A:460:ILE:O	2:A:464:VAL:HG23	2.11	0.50
2:A:554:GLU:O	2:A:558:GLN:HG3	2.12	0.50
2:C:177:SER:HA	2:C:180:MET:CE	2.42	0.50
2:C:552:LYS:HA	2:C:555:LYS:HG2	1.94	0.50
2:C:662:LYS:CG	2:C:664:PRO:HD2	2.41	0.50
2:A:624:GLN:O	2:A:628:ILE:HG12	2.11	0.50
2:C:196:ARG:NH1	2:C:199:HIS:HB3	2.27	0.50
2:C:463:LEU:O	2:C:466:THR:OG1	2.21	0.50
2:C:655:LEU:HD12	2:C:656:ALA:N	2.26	0.50
2:A:193:LEU:HA	2:A:196:ARG:HE	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:105:ILE:HD11	2:C:145:ARG:HD2	1.94	0.50
1:D:35:LEU:HD21	1:D:75:VAL:HG11	1.92	0.50
2:A:404:ILE:HB	2:A:405:PRO:HD3	1.93	0.50
2:A:657:ALA:O	2:A:660:LEU:HD23	2.12	0.50
2:C:124:GLN:HA	2:C:172:THR:CA	2.35	0.50
2:C:190:MET:SD	2:C:191:ASN:N	2.84	0.50
2:C:308:LEU:O	2:C:312:ARG:HB2	2.12	0.50
2:C:471:GLN:HB2	2:C:476:VAL:N	2.10	0.50
2:C:643:GLU:HB2	2:C:684:ASP:OD2	2.11	0.50
1:D:104:ARG:HB3	2:C:769:HIS:CE1	2.47	0.50
2:A:177:SER:O	2:A:180:MET:HG2	2.11	0.50
2:A:388:ILE:HG21	2:A:395:SER:HB2	1.93	0.50
2:A:690:LEU:HD12	2:A:692:GLY:H	1.76	0.50
2:C:60:PRO:HG3	2:C:211:ARG:HH12	1.77	0.50
2:C:327:ILE:O	2:C:330:GLN:HG3	2.12	0.50
2:A:116:VAL:HG23	2:A:160:ILE:HD13	1.94	0.49
2:A:718:GLN:O	2:A:721:ILE:HB	2.12	0.49
2:C:143:PRO:HG2	2:C:200:GLN:OE1	2.11	0.49
2:C:289:LEU:O	2:C:339:ARG:NH2	2.34	0.49
2:C:524:ARG:HA	2:C:526:ARG:HH11	1.76	0.49
1:B:141:ALA:CB	2:A:586:GLN:HE22	2.24	0.49
1:D:3:VAL:HG22	1:D:33:HIS:CB	2.37	0.49
2:A:502:ASP:N	2:A:502:ASP:OD1	2.46	0.49
2:A:508:LEU:HA	2:A:511:ASN:OD1	2.13	0.49
2:A:538:GLN:O	2:A:541:PHE:HB2	2.13	0.49
2:C:216:LEU:HA	2:C:219:LEU:HD13	1.94	0.49
2:C:328:PHE:O	2:C:332:VAL:HG22	2.12	0.49
1:D:70:PRO:HG2	1:D:73:LYS:HE3	1.95	0.49
2:A:359:MET:SD	2:A:404:ILE:HG22	2.51	0.49
2:A:685:LYS:HD2	2:A:689:GLU:O	2.12	0.49
2:A:749:LYS:HA	2:A:752:GLU:CG	2.43	0.49
2:C:261:TYR:HA	2:C:264:GLU:OE1	2.11	0.49
2:C:677:PHE:O	2:C:695:ARG:CZ	2.60	0.49
2:A:43:LEU:HD22	2:A:110:LEU:HD21	1.94	0.49
2:A:72:ASP:HA	2:A:75:HIS:HD2	1.75	0.49
2:A:368:TYR:HA	2:A:371:LYS:CE	2.40	0.49
2:C:198:GLN:NE2	2:C:257:LEU:HD21	2.27	0.49
2:C:595:GLY:HA2	2:C:599:HIS:CD2	2.48	0.49
2:C:276:LEU:HD11	2:C:309:PHE:CE2	2.48	0.49
2:A:400:ARG:O	2:A:404:ILE:HD12	2.13	0.49
2:A:578:GLU:O	2:A:581:LEU:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:681:ARG:HD3	2:A:687:GLY:O	2.13	0.49
2:C:14:LYS:O	2:C:17:ASP:OD1	2.31	0.49
2:C:604:TYR:HB2	2:C:641:PHE:CE1	2.48	0.49
2:A:127:LYS:HG2	2:A:131:LYS:HE3	1.95	0.49
2:A:217:ARG:CZ	2:A:217:ARG:HB3	2.43	0.49
2:C:61:LYS:O	2:C:64:TYR:HB3	2.13	0.49
2:C:196:ARG:NH1	2:C:200:GLN:HG3	2.27	0.49
2:C:553:TRP:CE2	2:C:554:GLU:HG3	2.47	0.49
2:A:103:ASN:HB3	2:A:106:PRO:HD2	1.94	0.49
2:A:525:ILE:HD12	2:A:525:ILE:H	1.78	0.49
2:A:765:GLN:C	2:A:769:HIS:CE1	2.86	0.49
2:C:713:PRO:O	2:C:717:VAL:HG22	2.13	0.49
2:A:259:GLN:O	2:A:262:LEU:HG	2.13	0.49
1:B:112:ILE:CD1	1:B:130:ILE:HB	2.43	0.48
2:A:562:SER:O	2:A:566:GLN:OE1	2.31	0.48
2:A:741:GLN:O	2:A:745:GLN:HG3	2.13	0.48
2:C:312:ARG:NH2	2:C:315:GLY:HA3	2.25	0.48
2:C:422:HIS:HD2	2:C:463:LEU:HD11	1.78	0.48
2:C:441:LEU:HD11	2:C:494:PHE:CE1	2.49	0.48
2:C:463:LEU:O	2:C:467:LEU:HD23	2.13	0.48
2:C:558:GLN:OE1	2:C:602:VAL:HG21	2.13	0.48
2:A:700:LEU:HD21	2:A:727:TYR:CE1	2.48	0.48
2:C:376:THR:O	2:C:380:PHE:HD2	1.96	0.48
2:C:455:ASP:OD1	2:C:455:ASP:N	2.44	0.48
2:C:764:GLU:HG3	2:C:765:GLN:N	2.28	0.48
2:A:272:ASP:O	2:A:276:LEU:HD23	2.12	0.48
2:C:161:LEU:HB3	2:C:179:SER:OG	2.13	0.48
2:A:331:GLN:O	2:A:334:THR:OG1	2.26	0.48
2:A:422:HIS:HB3	2:A:423:PRO:HD3	1.95	0.48
2:A:553:TRP:CE2	2:A:554:GLU:HG3	2.48	0.48
2:A:599:HIS:NE2	2:A:600:GLU:HG2	2.28	0.48
2:A:736:ASP:OD1	2:A:737:ALA:N	2.47	0.48
2:A:114:VAL:O	2:A:118:TYR:HD1	1.96	0.48
2:A:392:SER:O	2:A:396:LYS:HE2	2.13	0.48
2:C:577:ALA:O	2:C:580:PRO:HD2	2.14	0.48
2:A:104:ILE:HG13	2:A:105:ILE:N	2.28	0.48
2:A:373:LEU:O	2:A:376:THR:OG1	2.30	0.48
2:A:715:LEU:HA	2:A:718:GLN:CG	2.43	0.48
2:C:12:GLN:NE2	2:C:15:LEU:HG	2.29	0.48
1:B:37:THR:CG2	1:B:112:ILE:HG22	2.43	0.48
1:D:37:THR:CG2	1:D:112:ILE:HG22	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:403:LYS:NZ	2:A:443:ASN:OD1	2.46	0.48
2:A:723:ILE:HG22	2:A:727:TYR:HE1	1.79	0.48
2:A:726:ARG:HG2	2:A:726:ARG:HH11	1.79	0.48
2:C:78:GLU:O	2:C:82:THR:OG1	2.26	0.48
2:C:351:GLN:HA	2:C:354:LEU:HD12	1.95	0.48
2:C:379:ILE:HA	2:C:382:LYS:NZ	2.29	0.48
2:C:723:ILE:O	2:C:727:TYR:CD2	2.66	0.48
1:D:22:PHE:CE1	1:D:167:LEU:HB2	2.48	0.48
1:D:104:ARG:CB	2:C:769:HIS:CE1	2.96	0.48
2:A:193:LEU:HA	2:A:196:ARG:NE	2.29	0.48
2:A:660:LEU:C	2:A:666:GLN:HE21	2.17	0.48
2:C:365:ARG:HD2	2:C:368:TYR:CE1	2.49	0.48
2:C:411:ASN:ND2	2:C:413:LEU:HB2	2.28	0.48
2:C:568:ILE:O	2:C:572:ILE:HG13	2.13	0.48
1:D:112:ILE:CD1	1:D:130:ILE:HB	2.42	0.48
2:A:16:LEU:CD2	2:A:62:SER:HB3	2.44	0.48
2:A:697:MET:HB3	2:A:701:LYS:HZ3	1.79	0.48
2:A:721:ILE:HD11	2:A:766:ILE:HG23	1.95	0.48
2:C:352:VAL:HG13	2:C:404:ILE:CD1	2.44	0.48
2:C:386:GLU:OE2	2:C:387:HIS:HB2	2.13	0.48
2:C:451:ILE:HA	2:C:497:LEU:HD13	1.96	0.48
2:A:288:GLU:OE1	2:A:288:GLU:N	2.41	0.48
2:A:552:LYS:HA	2:A:555:LYS:CE	2.43	0.48
2:A:556:LYS:O	2:A:559:LYS:HG2	2.13	0.48
2:A:602:VAL:HA	2:A:605:GLU:CD	2.34	0.48
2:A:650:ARG:NH2	2:A:651:THR:HG23	2.28	0.48
2:A:700:LEU:O	2:A:704:LEU:HG	2.13	0.48
2:C:61:LYS:O	2:C:65:GLU:OE1	2.31	0.48
2:C:191:ASN:OD1	2:C:192:LYS:N	2.47	0.48
2:C:352:VAL:HG11	2:C:400:ARG:NH1	2.29	0.48
2:C:647:GLU:HB3	2:C:648:PRO:HD3	1.96	0.48
1:B:139:TYR:HH	2:A:586:GLN:NE2	2.08	0.47
2:A:147:LEU:HB3	2:A:219:LEU:HD23	1.96	0.47
2:A:188:ALA:O	2:A:192:LYS:HG2	2.13	0.47
2:A:193:LEU:HD12	2:A:194:TRP:N	2.29	0.47
2:A:550:ASP:OD1	2:A:551:ASP:N	2.46	0.47
2:A:566:GLN:HG2	2:A:567:THR:N	2.29	0.47
2:C:198:GLN:HG2	2:C:213:ARG:NH1	2.29	0.47
2:C:255:ASP:OD1	2:C:256:ALA:N	2.44	0.47
2:C:441:LEU:HD12	2:C:444:VAL:HB	1.95	0.47
2:C:485:ALA:HA	2:C:488:GLN:OE1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:660:LEU:HD11	2:C:666:GLN:CA	2.44	0.47
2:C:660:LEU:HD11	2:C:666:GLN:CB	2.44	0.47
2:A:50:LEU:HA	2:A:53:LEU:HD23	1.97	0.47
2:A:141:GLN:O	2:A:196:ARG:NH2	2.47	0.47
2:A:376:THR:HA	2:A:379:ILE:HD12	1.96	0.47
2:C:335:VAL:O	2:C:339:ARG:HG2	2.15	0.47
2:C:464:VAL:O	2:C:468:ILE:HG12	2.14	0.47
2:C:636:GLU:HG3	2:C:637:ARG:CD	2.38	0.47
2:C:685:LYS:HZ1	2:C:689:GLU:C	2.14	0.47
1:B:22:PHE:CE1	1:B:167:LEU:HB2	2.48	0.47
2:A:580:PRO:O	2:A:584:PHE:CD2	2.66	0.47
2:A:739:THR:HG1	2:A:742:VAL:HG23	1.78	0.47
2:C:212:GLU:HA	2:C:215:GLU:OE1	2.14	0.47
2:C:593:GLU:OE2	2:C:594:ILE:HG13	2.14	0.47
2:A:416:LEU:HD22	2:A:456:GLN:NE2	2.28	0.47
2:A:497:LEU:O	2:A:500:SER:OG	2.32	0.47
2:A:507:TYR:HE2	2:A:559:LYS:HG3	1.80	0.47
2:C:174:GLY:HA2	2:C:178:ASP:OD2	2.15	0.47
2:C:645:ASN:O	2:C:648:PRO:HD2	2.14	0.47
2:C:663:LYS:CE	2:C:709:GLN:HB2	2.44	0.47
1:B:70:PRO:HG2	1:B:73:LYS:HE3	1.95	0.47
2:A:12:GLN:NE2	2:A:15:LEU:HD12	2.29	0.47
2:A:110:LEU:O	2:A:114:VAL:HG12	2.13	0.47
2:C:373:LEU:HB3	2:C:420:HIS:CD2	2.42	0.47
2:C:495:ILE:HD13	2:C:531:PRO:HB2	1.96	0.47
2:C:750:ILE:HG22	2:C:751:ARG:NH2	2.29	0.47
2:A:164:GLU:HB2	2:A:231:GLU:CB	2.45	0.47
2:C:108:LEU:HD12	2:C:109:TYR:N	2.30	0.47
2:C:463:LEU:HD23	2:C:463:LEU:HA	1.66	0.47
2:C:495:ILE:HG22	2:C:499:ARG:NH1	2.30	0.47
2:A:131:LYS:O	2:A:135:GLU:HG3	2.15	0.47
2:A:192:LYS:HE2	2:A:192:LYS:HA	1.96	0.47
2:A:235:VAL:HG13	2:A:239:LYS:NZ	2.30	0.47
2:A:367:ASP:O	2:A:371:LYS:HG3	2.14	0.47
2:A:403:LYS:HB3	2:A:407:ASP:OD2	2.15	0.47
2:A:494:PHE:O	2:A:497:LEU:HG	2.15	0.47
2:A:733:LYS:HE3	2:A:735:ASN:HD21	1.79	0.47
2:C:187:PHE:CD1	2:C:223:ASN:ND2	2.82	0.47
2:C:260:GLU:O	2:C:264:GLU:OE1	2.33	0.47
2:C:270:PHE:HB2	2:C:275:HIS:NE2	2.30	0.47
2:C:354:LEU:HA	2:C:357:LEU:CD2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:451:ILE:CD1	2:C:501:GLU:HG2	2.42	0.47
2:C:537:TYR:HE2	2:C:586:GLN:OE1	1.98	0.47
2:C:565:HIS:HD2	2:C:606:PHE:CE1	2.32	0.47
1:D:60:ARG:HB2	1:D:69:TYR:HB2	1.96	0.47
1:D:119:PHE:CE1	1:D:164:VAL:HB	2.50	0.47
2:A:25:VAL:O	2:A:28:PHE:HB2	2.14	0.47
2:A:388:ILE:HG22	2:A:392:SER:HB3	1.95	0.47
2:A:409:TYR:HB3	2:A:411:ASN:OD1	2.14	0.47
2:A:604:TYR:HA	2:A:607:MET:HG2	1.95	0.47
2:A:724:LEU:HD11	2:A:747:ILE:HG22	1.96	0.47
2:C:280:ASN:OD1	2:C:331:GLN:NE2	2.48	0.47
2:C:411:ASN:HD21	2:C:413:LEU:HB2	1.80	0.47
2:C:762:GLU:O	2:C:765:GLN:N	2.48	0.47
2:A:430:TYR:CZ	2:A:472:PRO:HA	2.50	0.47
2:A:455:ASP:HA	2:A:458:ASP:OD2	2.15	0.47
2:A:532:LEU:O	2:A:535:ALA:HB3	2.14	0.47
2:A:576:LEU:HD11	2:A:578:GLU:OE2	2.15	0.47
2:A:604:TYR:O	2:A:607:MET:HG2	2.14	0.47
2:C:196:ARG:HD2	2:C:196:ARG:HA	1.65	0.47
2:C:411:ASN:HA	2:C:447:TYR:CE2	2.50	0.47
2:C:620:ASP:H	2:C:623:ALA:HB3	1.80	0.47
2:C:627:ALA:O	2:C:631:ILE:HG13	2.15	0.47
2:C:725:ASN:HB3	2:C:729:TYR:CZ	2.50	0.47
1:D:155:ILE:HG13	1:D:160:VAL:HG23	1.97	0.47
2:A:495:ILE:HA	2:A:498:LEU:CD2	2.45	0.47
2:A:621:SER:O	2:A:624:GLN:HB2	2.15	0.47
2:C:643:GLU:O	2:C:647:GLU:CB	2.63	0.47
2:A:414:THR:HA	2:A:417:LYS:CE	2.44	0.46
2:A:490:LEU:O	2:A:494:PHE:CD2	2.68	0.46
2:C:305:ARG:O	2:C:308:LEU:HG	2.16	0.46
2:C:720:PHE:O	2:C:724:LEU:HD23	2.15	0.46
2:A:127:LYS:HG2	2:A:131:LYS:CE	2.46	0.46
2:A:164:GLU:HG3	2:A:232:GLY:CA	2.42	0.46
2:A:270:PHE:O	2:A:305:ARG:NH2	2.48	0.46
2:A:308:LEU:HD13	2:A:312:ARG:HH12	1.79	0.46
2:A:380:PHE:HB3	2:A:427:TYR:OH	2.15	0.46
2:C:29:GLN:HB2	2:C:32:ARG:NH2	2.26	0.46
2:C:40:MET:H	2:C:40:MET:HE3	1.79	0.46
2:C:276:LEU:HA	2:C:279:LEU:HG	1.96	0.46
2:C:357:LEU:HD12	2:C:358:ALA:N	2.30	0.46
2:C:695:ARG:O	2:C:698:GLU:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:ILE:HG13	1:B:160:VAL:HG23	1.96	0.46
2:A:16:LEU:HD22	2:A:62:SER:HB3	1.97	0.46
2:A:127:LYS:HB2	2:A:173:THR:HB	1.98	0.46
2:A:372:VAL:O	2:A:376:THR:HG23	2.15	0.46
2:A:422:HIS:NE2	2:A:466:THR:HG21	2.31	0.46
2:A:730:PHE:CB	2:A:735:ASN:HD22	2.26	0.46
2:C:26:GLN:CB	2:C:49:MET:HB2	2.45	0.46
2:C:29:GLN:HG3	2:C:45:HIS:CD2	2.50	0.46
2:C:262:LEU:HA	2:C:262:LEU:HD23	1.68	0.46
2:C:562:SER:O	2:C:566:GLN:OE1	2.33	0.46
2:C:563:PHE:HA	2:C:566:GLN:CD	2.36	0.46
2:C:751:ARG:NH2	2:C:754:LEU:HD22	2.27	0.46
1:B:141:ALA:HB2	2:A:586:GLN:OE1	2.15	0.46
2:A:464:VAL:O	2:A:468:ILE:HG12	2.16	0.46
2:C:514:ARG:HH12	2:C:566:GLN:CG	2.27	0.46
2:C:566:GLN:HG2	2:C:567:THR:N	2.31	0.46
2:A:130:LEU:HD12	2:A:131:LYS:N	2.30	0.46
2:A:508:LEU:O	2:A:512:THR:HG23	2.16	0.46
2:A:556:LYS:O	2:A:560:ILE:HG23	2.16	0.46
2:A:765:GLN:O	2:A:769:HIS:ND1	2.48	0.46
2:C:450:GLU:N	2:C:450:GLU:OE1	2.48	0.46
2:C:457:VAL:HA	2:C:460:ILE:HG12	1.96	0.46
2:C:770:PHE:CZ	2:C:774:LEU:HD11	2.51	0.46
1:B:60:ARG:HB2	1:B:69:TYR:HB2	1.97	0.46
1:B:119:PHE:CE1	1:B:164:VAL:HB	2.50	0.46
2:A:461:MET:O	2:A:516:HIS:NE2	2.44	0.46
2:A:531:PRO:HA	2:A:534:PHE:CD2	2.42	0.46
2:C:403:LYS:HD3	2:C:439:TYR:CE1	2.50	0.46
2:C:441:LEU:HD21	2:C:490:LEU:HB3	1.98	0.46
1:B:91:ILE:N	1:B:91:ILE:HD12	2.31	0.46
2:A:415:VAL:HA	2:A:418:LEU:HD12	1.98	0.46
2:A:422:HIS:HA	2:A:425:PHE:CD2	2.50	0.46
2:A:563:PHE:HA	2:A:566:GLN:CD	2.36	0.46
2:C:61:LYS:HD2	2:C:61:LYS:H	1.81	0.46
2:C:470:ASP:OD1	2:C:471:GLN:N	2.49	0.46
2:C:539:LEU:HD12	2:C:542:ARG:HB3	1.97	0.46
2:C:694:LYS:HG3	2:C:695:ARG:N	2.31	0.46
2:A:180:MET:SD	2:A:241:ILE:HD12	2.56	0.46
2:A:482:GLU:HB3	2:A:486:ASP:OD2	2.16	0.46
2:C:294:ASN:OD1	2:C:296:LYS:HB3	2.16	0.46
2:C:402:LEU:HD12	2:C:428:PHE:HZ	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:736:ASP:OD1	2:C:737:ALA:N	2.49	0.46
1:D:91:ILE:HD12	1:D:91:ILE:N	2.31	0.46
2:A:352:VAL:HG11	2:A:400:ARG:NH1	2.31	0.46
2:C:451:ILE:HB	2:C:497:LEU:O	2.15	0.46
2:C:499:ARG:HG3	2:C:499:ARG:NH1	2.31	0.46
2:C:502:ASP:OD1	2:C:502:ASP:N	2.49	0.46
2:C:660:LEU:HD11	2:C:666:GLN:HB2	1.98	0.46
1:B:37:THR:OG1	1:B:38:GLY:N	2.49	0.46
2:A:227:LEU:HA	2:A:230:LEU:HD12	1.98	0.46
2:A:271:PRO:HB2	2:A:273:GLU:OE1	2.15	0.46
2:A:382:LYS:HB3	2:A:382:LYS:HE3	1.64	0.46
2:A:474:GLN:HE22	2:A:477:GLU:HG2	1.81	0.46
2:A:668:ARG:O	2:A:671:SER:OG	2.26	0.46
2:A:726:ARG:HA	2:A:726:ARG:NE	2.31	0.46
2:A:777:LEU:C	2:A:779:LEU:H	2.19	0.46
2:C:550:ASP:OD1	2:C:551:ASP:N	2.49	0.46
2:C:577:ALA:HB3	2:C:578:GLU:OE1	2.15	0.46
2:C:596:PHE:HD2	2:C:597:GLU:O	1.99	0.46
2:A:233:VAL:HG12	2:A:274:PHE:HE2	1.80	0.45
2:A:456:GLN:NE2	2:A:459:SER:HB2	2.31	0.45
2:A:756:ASN:O	2:A:757:LEU:HD23	2.16	0.45
2:C:17:ASP:O	2:C:21:GLN:HG3	2.16	0.45
2:C:457:VAL:O	2:C:461:MET:HG3	2.15	0.45
2:C:761:GLU:O	2:C:765:GLN:HG3	2.16	0.45
1:D:143:GLU:HG3	1:D:146:ILE:HD13	1.99	0.45
2:A:14:LYS:O	2:A:17:ASP:N	2.49	0.45
2:A:46:ALA:HA	2:A:49:MET:HE2	1.98	0.45
2:A:413:LEU:HG	2:A:414:THR:N	2.30	0.45
2:A:625:LEU:HD12	2:A:626:ALA:N	2.31	0.45
2:A:728:ILE:O	2:A:732:GLU:HG3	2.16	0.45
2:C:127:LYS:HB2	2:C:173:THR:C	2.37	0.45
1:B:150:PHE:CE2	1:B:152:LEU:HD22	2.50	0.45
1:D:63:PHE:CE1	2:C:582:ARG:HD3	2.51	0.45
2:A:568:ILE:HD12	2:A:584:PHE:HE1	1.81	0.45
2:C:441:LEU:HD12	2:C:441:LEU:HA	1.70	0.45
2:C:751:ARG:HG2	2:C:751:ARG:HH11	1.81	0.45
2:A:246:ILE:HA	2:A:249:GLN:NE2	2.30	0.45
2:A:472:PRO:HB3	2:A:476:VAL:HB	1.98	0.45
2:A:626:ALA:O	2:A:629:THR:HG22	2.16	0.45
2:C:422:HIS:O	2:C:425:PHE:HD2	1.99	0.45
2:C:430:TYR:CB	2:C:473:ASP:HA	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:460:ILE:HG13	2:C:461:MET:N	2.31	0.45
1:B:59:VAL:HG13	1:B:84:LEU:HD13	1.99	0.45
1:B:81:LYS:HD3	1:B:107:ASP:O	2.16	0.45
1:D:59:VAL:HG13	1:D:84:LEU:HD13	1.99	0.45
2:A:530:PRO:O	2:A:533:VAL:HB	2.17	0.45
2:A:705:LYS:NZ	2:A:706:ILE:HD11	2.31	0.45
2:A:777:LEU:HD13	2:A:779:LEU:HD12	1.98	0.45
2:C:544:LYS:NZ	2:C:593:GLU:O	2.48	0.45
2:C:700:LEU:O	2:C:704:LEU:HG	2.17	0.45
2:C:712:ASP:H	2:C:716:GLN:CG	2.29	0.45
2:A:177:SER:HA	2:A:180:MET:HG2	1.97	0.45
2:C:324:LEU:HD22	2:C:328:PHE:CE2	2.51	0.45
2:C:359:MET:CE	2:C:405:PRO:HA	2.46	0.45
1:D:81:LYS:HD3	1:D:107:ASP:O	2.16	0.45
2:A:142:HIS:CG	2:A:145:ARG:NH1	2.84	0.45
2:A:216:LEU:HD22	2:A:219:LEU:HD22	1.99	0.45
2:A:412:ILE:HG21	2:A:444:VAL:HG13	1.99	0.45
2:A:568:ILE:HG13	2:A:569:SER:N	2.32	0.45
2:A:699:CYS:HA	2:A:702:LYS:HE2	1.99	0.45
2:C:47:SER:O	2:C:50:LEU:HG	2.16	0.45
1:B:18:LEU:H	1:B:18:LEU:CD1	2.29	0.45
1:D:37:THR:OG1	1:D:38:GLY:N	2.50	0.45
2:A:116:VAL:HG22	2:A:120:LYS:NZ	2.32	0.45
2:A:202:HIS:HD2	2:A:204:ARG:H	1.64	0.45
2:C:243:LEU:HA	2:C:246:ILE:CG1	2.42	0.45
2:C:372:VAL:O	2:C:376:THR:HG23	2.17	0.45
2:C:433:ARG:HA	2:C:436:MET:HG2	1.98	0.45
1:D:2:LEU:CD1	1:D:152:LEU:HD12	2.47	0.44
2:A:762:GLU:H	2:A:762:GLU:HG3	1.60	0.44
2:C:403:LYS:HA	2:C:406:VAL:HB	1.98	0.44
2:C:461:MET:HE3	2:C:513:ALA:HA	1.99	0.44
2:C:776:HIS:ND1	2:C:777:LEU:HD22	2.32	0.44
1:D:128:PHE:CE2	1:D:130:ILE:HD11	2.53	0.44
2:A:26:GLN:CB	2:A:49:MET:SD	3.05	0.44
2:C:196:ARG:HH12	2:C:199:HIS:C	2.21	0.44
2:C:203:SER:O	2:C:206:ARG:HG2	2.17	0.44
2:C:208:LYS:HD3	2:C:212:GLU:OE2	2.18	0.44
2:C:480:ASP:OD1	2:C:480:ASP:N	2.48	0.44
2:C:724:LEU:HD21	2:C:746:LEU:HD13	1.99	0.44
2:C:412:ILE:HG21	2:C:444:VAL:HG22	1.99	0.44
2:C:603:ALA:O	2:C:607:MET:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:LEU:CD1	1:B:152:LEU:HD12	2.47	0.44
1:B:90:VAL:O	1:B:93:TRP:HA	2.18	0.44
2:A:227:LEU:O	2:A:233:VAL:HG21	2.18	0.44
2:A:649:LEU:HD12	2:A:649:LEU:N	2.33	0.44
2:C:364:ASP:OD1	2:C:365:ARG:N	2.49	0.44
1:B:90:VAL:C	1:B:91:ILE:HD12	2.38	0.44
1:D:150:PHE:O	1:D:151:VAL:HG23	2.18	0.44
2:A:104:ILE:CA	2:A:107:ARG:HH11	2.30	0.44
2:A:241:ILE:HG13	2:A:242:VAL:HG23	2.00	0.44
2:A:365:ARG:HD3	2:A:368:TYR:CD1	2.53	0.44
2:A:374:GLU:OE1	2:A:374:GLU:N	2.50	0.44
2:A:396:LYS:HD3	2:A:396:LYS:N	2.32	0.44
2:A:514:ARG:NE	2:A:567:THR:HG22	2.33	0.44
2:C:129:ILE:O	2:C:133:LEU:HG	2.18	0.44
2:C:373:LEU:HD11	2:C:418:LEU:HD23	1.99	0.44
2:C:692:GLY:H	2:C:695:ARG:HH12	1.64	0.44
1:B:143:GLU:HG3	1:B:146:ILE:HD13	1.99	0.44
2:A:388:ILE:CG2	2:A:395:SER:HB2	2.48	0.44
2:C:137:CYS:O	2:C:140:VAL:HG23	2.18	0.44
2:C:413:LEU:O	2:C:417:LYS:NZ	2.23	0.44
2:C:157:THR:HG21	2:C:182:PHE:CZ	2.53	0.44
2:C:600:GLU:OE2	2:C:641:PHE:HA	2.17	0.44
2:A:84:GLU:HA	2:A:87:LYS:HD2	2.00	0.44
2:A:127:LYS:NZ	2:A:174:GLY:H	2.16	0.44
2:A:359:MET:HE1	2:A:408:THR:HB	1.99	0.44
2:A:650:ARG:HH22	2:A:695:ARG:HH22	1.65	0.44
2:A:729:TYR:CZ	2:A:733:LYS:HD3	2.52	0.44
2:C:253:CYS:O	2:C:254:ARG:HD3	2.17	0.44
2:C:537:TYR:CE2	2:C:586:GLN:HB2	2.53	0.44
1:D:11:ILE:O	1:D:41:CYS:HB2	2.18	0.44
2:A:529:LEU:O	2:A:533:VAL:HG23	2.17	0.44
2:A:568:ILE:O	2:A:572:ILE:HG13	2.18	0.44
2:A:710:CYS:HB2	2:A:716:GLN:CG	2.46	0.44
1:B:30:LYS:O	1:B:32:GLN:NE2	2.51	0.43
1:B:66:ASN:OD1	1:B:68:ASN:HB2	2.18	0.43
1:B:141:ALA:HB1	2:A:589:LEU:CD1	2.48	0.43
2:A:81:LEU:CD2	2:A:117:VAL:HG21	2.47	0.43
2:A:495:ILE:HD11	2:A:532:LEU:HD23	1.99	0.43
2:C:226:ARG:HA	2:C:229:GLN:OE1	2.18	0.43
2:C:561:PHE:HE2	2:C:596:PHE:CE1	2.36	0.43
1:D:16:ASN:CB	2:C:493:ARG:NH2	2.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:83:ASP:O	2:A:87:LYS:HG3	2.17	0.43
2:A:303:ILE:HG23	2:A:357:LEU:CD2	2.44	0.43
2:A:313:GLU:HG2	2:A:314:ASP:H	1.82	0.43
2:A:404:ILE:O	2:A:408:THR:CB	2.66	0.43
2:C:158:ARG:HG2	2:C:159:ASN:N	2.32	0.43
2:C:289:LEU:HD23	2:C:289:LEU:HA	1.70	0.43
2:C:555:LYS:HD3	2:C:555:LYS:N	2.33	0.43
1:B:150:PHE:O	1:B:151:VAL:HG23	2.18	0.43
1:D:104:ARG:CD	2:C:769:HIS:CE1	3.01	0.43
2:A:157:THR:HB	2:A:161:LEU:HG	1.99	0.43
2:A:194:TRP:O	2:A:197:MET:HB3	2.18	0.43
2:A:270:PHE:O	2:A:305:ARG:CZ	2.65	0.43
2:A:550:ASP:CG	2:A:553:TRP:HB3	2.38	0.43
2:C:32:ARG:O	2:C:35:ASP:OD1	2.36	0.43
2:C:152:TYR:O	2:C:155:GLN:HG3	2.18	0.43
2:C:160:ILE:H	2:C:160:ILE:HD12	1.83	0.43
2:C:555:LYS:O	2:C:559:LYS:NZ	2.48	0.43
2:C:565:HIS:CD2	2:C:606:PHE:CE1	3.06	0.43
2:C:658:SER:HG	2:C:659:LYS:HE2	1.83	0.43
1:D:90:VAL:C	1:D:91:ILE:HD12	2.38	0.43
2:A:105:ILE:O	2:A:109:TYR:HD2	2.02	0.43
2:A:650:ARG:HB2	2:A:650:ARG:NH1	2.34	0.43
2:A:665:ASP:HA	2:A:668:ARG:CD	2.49	0.43
2:C:40:MET:H	2:C:40:MET:CE	2.31	0.43
2:C:652:GLN:O	2:C:655:LEU:HG	2.18	0.43
1:B:11:ILE:O	1:B:41:CYS:HB2	2.18	0.43
1:B:106:PHE:O	1:B:107:ASP:HB3	2.19	0.43
1:D:66:ASN:OD1	1:D:68:ASN:HB2	2.18	0.43
2:A:601:THR:O	2:A:605:GLU:OE1	2.37	0.43
2:C:21:GLN:O	2:C:25:VAL:HG23	2.18	0.43
2:C:234:ASN:ND2	2:C:237:ARG:HD2	2.33	0.43
2:C:290:HIS:HB3	2:C:293:VAL:HG23	2.00	0.43
2:C:554:GLU:HB2	2:C:555:LYS:NZ	2.32	0.43
2:C:697:MET:O	2:C:700:LEU:HG	2.19	0.43
2:A:394:VAL:O	2:A:398:LEU:HG	2.18	0.43
2:A:693:GLY:O	2:A:697:MET:HG2	2.18	0.43
2:A:765:GLN:HA	2:A:768:LYS:HE2	1.99	0.43
2:C:207:GLU:HA	2:C:210:GLU:HG3	2.00	0.43
2:A:245:GLY:O	2:A:249:GLN:OE1	2.37	0.43
2:A:511:ASN:HB3	2:A:515:LYS:NZ	2.34	0.43
2:A:521:GLY:HA3	2:A:524:ARG:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:746:LEU:HD13	2:A:746:LEU:HA	1.81	0.43
2:C:247:LEU:O	2:C:251:VAL:HG12	2.18	0.43
2:C:411:ASN:HB3	2:C:414:THR:HG23	2.00	0.43
1:D:21:LYS:HZ2	1:D:170:ASP:C	2.21	0.43
1:D:30:LYS:O	1:D:32:GLN:NE2	2.51	0.43
2:A:206:ARG:NH1	2:A:209:ARG:HH21	2.16	0.43
2:A:514:ARG:NH1	2:A:566:GLN:HE21	2.15	0.43
2:A:681:ARG:HA	2:A:689:GLU:HA	2.01	0.43
2:C:18:GLU:HA	2:C:21:GLN:OE1	2.18	0.43
2:C:462:ASN:O	2:C:466:THR:HG23	2.19	0.43
2:C:514:ARG:NE	2:C:567:THR:HG22	2.34	0.43
2:C:542:ARG:NH1	2:C:546:ASN:OD1	2.50	0.43
2:C:550:ASP:OD1	2:C:553:TRP:N	2.51	0.43
2:C:585:LEU:HA	2:C:585:LEU:HD23	1.70	0.43
2:C:611:PHE:O	2:C:615:GLU:OE1	2.37	0.43
2:C:720:PHE:HA	2:C:723:ILE:HG22	2.00	0.43
2:A:12:GLN:OE1	2:A:12:GLN:N	2.51	0.43
2:A:22:ALA:O	2:A:26:GLN:HG2	2.19	0.43
2:A:322:ILE:HG13	2:A:322:ILE:O	2.19	0.43
2:A:456:GLN:O	2:A:460:ILE:HG13	2.18	0.43
2:C:142:HIS:CG	2:C:145:ARG:NH1	2.87	0.43
2:C:272:ASP:HB2	2:C:309:PHE:CE1	2.53	0.43
2:C:432:SER:O	2:C:436:MET:HG2	2.18	0.43
2:C:448:ASN:HB3	2:C:450:GLU:OE2	2.19	0.43
2:C:726:ARG:NH2	2:C:729:TYR:HB2	2.31	0.43
1:D:90:VAL:O	1:D:93:TRP:HA	2.18	0.43
2:A:73:GLU:HA	2:A:76:TYR:HD2	1.84	0.43
2:A:681:ARG:HG2	2:A:689:GLU:CA	2.45	0.43
2:C:719:LEU:HA	2:C:722:GLU:OE1	2.19	0.43
1:B:128:PHE:CE2	1:B:130:ILE:HD11	2.53	0.42
1:D:152:LEU:HD23	1:D:152:LEU:H	1.84	0.42
2:A:208:LYS:HD2	2:A:208:LYS:HA	1.76	0.42
2:A:442:SER:HA	2:A:445:LEU:HD12	2.00	0.42
2:A:461:MET:HE1	2:A:512:THR:C	2.39	0.42
2:C:91:VAL:HB	2:C:94:LEU:HD21	2.01	0.42
2:C:130:LEU:HD12	2:C:131:LYS:N	2.34	0.42
2:C:216:LEU:O	2:C:219:LEU:HB2	2.19	0.42
2:C:441:LEU:HD11	2:C:494:PHE:CZ	2.54	0.42
2:C:498:LEU:HD23	2:C:498:LEU:HA	1.71	0.42
2:A:203:SER:O	2:A:206:ARG:HG2	2.19	0.42
2:A:296:LYS:O	2:A:300:ILE:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:324:LEU:HD23	2:A:324:LEU:HA	1.85	0.42
2:A:452:VAL:HG12	2:A:457:VAL:HG23	2.01	0.42
2:A:690:LEU:HD12	2:A:692:GLY:N	2.34	0.42
2:A:765:GLN:HA	2:A:768:LYS:NZ	2.34	0.42
2:C:441:LEU:HD23	2:C:490:LEU:HD13	2.01	0.42
2:A:197:MET:HG2	2:A:200:GLN:NE2	2.33	0.42
2:A:235:VAL:HG23	2:A:274:PHE:HA	2.01	0.42
2:A:243:LEU:HD21	2:A:282:PHE:HB2	2.01	0.42
2:A:300:ILE:HG13	2:A:301:ALA:N	2.35	0.42
2:A:441:LEU:HD23	2:A:441:LEU:HA	1.86	0.42
2:A:602:VAL:HA	2:A:605:GLU:OE2	2.19	0.42
2:A:765:GLN:O	2:A:769:HIS:CE1	2.72	0.42
2:C:377:VAL:HG21	2:C:420:HIS:NE2	2.34	0.42
2:C:524:ARG:CA	2:C:526:ARG:HH11	2.32	0.42
2:C:571:LEU:CD2	2:C:580:PRO:HG3	2.49	0.42
2:C:608:SER:HA	2:C:611:PHE:HD2	1.82	0.42
2:C:620:ASP:OD1	2:C:621:SER:N	2.52	0.42
2:C:726:ARG:HA	2:C:729:TYR:HD2	1.79	0.42
2:A:132:ASP:O	2:A:136:MET:HG2	2.18	0.42
2:A:185:LEU:O	2:A:189:GLU:HG3	2.20	0.42
2:A:308:LEU:HB2	2:A:312:ARG:NH2	2.34	0.42
2:A:318:ILE:HG12	2:A:324:LEU:HD12	2.01	0.42
2:A:677:PHE:CB	2:A:696:VAL:HG22	2.47	0.42
2:C:171:GLU:HG3	2:C:172:THR:N	2.35	0.42
2:C:453:SER:O	2:C:457:VAL:HG23	2.19	0.42
2:C:467:LEU:HD13	2:C:467:LEU:HA	1.79	0.42
2:C:557:CYS:HB3	2:C:561:PHE:CE2	2.54	0.42
2:C:577:ALA:O	2:C:581:LEU:HG	2.19	0.42
2:C:725:ASN:C	2:C:729:TYR:CE2	2.93	0.42
2:A:142:HIS:HB3	2:A:145:ARG:HG2	2.02	0.42
2:A:197:MET:HE1	2:A:213:ARG:HG2	2.02	0.42
2:C:233:VAL:HG23	2:C:233:VAL:O	2.20	0.42
1:B:19:PRO:HG2	1:B:22:PHE:CG	2.55	0.42
2:A:338:SER:CB	2:A:339:ARG:HH21	2.33	0.42
2:C:14:LYS:O	2:C:15:LEU:C	2.57	0.42
2:C:450:GLU:HB3	2:C:451:ILE:H	1.70	0.42
2:A:453:SER:HB3	2:A:455:ASP:OD1	2.20	0.42
2:A:511:ASN:O	2:A:514:ARG:HB3	2.20	0.42
2:A:596:PHE:HD2	2:A:597:GLU:O	2.02	0.42
2:A:652:GLN:CG	2:C:661:LEU:HD23	2.50	0.42
2:C:24:LYS:HA	2:C:24:LYS:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:250:VAL:HG21	2:C:263:MET:HE3	2.02	0.42
2:C:642:SER:HB3	2:C:683:THR:OG1	2.19	0.42
2:C:645:ASN:C	2:C:648:PRO:HD2	2.40	0.42
2:A:24:LYS:O	2:A:28:PHE:CG	2.73	0.42
2:A:456:GLN:HE21	2:A:460:ILE:CG1	2.25	0.42
2:A:542:ARG:NH1	2:A:546:ASN:OD1	2.53	0.42
2:A:706:ILE:HD13	2:A:706:ILE:HA	1.83	0.42
2:A:743:LEU:HA	2:A:743:LEU:HD23	1.60	0.42
2:A:760:SER:HB2	2:A:762:GLU:OE2	2.20	0.42
2:C:419:LYS:HD3	2:C:419:LYS:N	2.34	0.42
2:C:460:ILE:O	2:C:464:VAL:HG23	2.20	0.42
2:C:543:TYR:CE2	2:C:556:LYS:HB3	2.54	0.42
2:C:729:TYR:CD1	2:C:729:TYR:N	2.82	0.42
1:D:22:PHE:CE2	1:D:150:PHE:HD1	2.38	0.42
2:A:12:GLN:CG	2:A:13:GLU:N	2.81	0.42
2:A:404:ILE:O	2:A:408:THR:HB	2.20	0.42
2:A:416:LEU:HD22	2:A:456:GLN:HE22	1.84	0.42
2:A:456:GLN:HE22	2:A:459:SER:HB2	1.85	0.42
2:A:483:ASP:O	2:A:486:ASP:N	2.49	0.42
2:C:94:LEU:HD23	2:C:97:LEU:HD21	2.02	0.42
2:C:171:GLU:HG3	2:C:172:THR:HG23	2.01	0.42
2:C:471:GLN:O	2:C:472:PRO:C	2.57	0.42
2:C:712:ASP:H	2:C:716:GLN:HG3	1.85	0.42
1:D:18:LEU:H	1:D:18:LEU:CD1	2.29	0.42
1:D:106:PHE:O	1:D:107:ASP:HB3	2.19	0.42
1:D:149:SER:HA	1:D:165:TYR:O	2.19	0.42
2:A:14:LYS:O	2:A:15:LEU:C	2.59	0.42
2:A:226:ARG:HH22	2:A:230:LEU:HD21	1.85	0.42
2:A:245:GLY:HA2	2:A:248:GLU:OE1	2.18	0.42
2:A:324:LEU:HD22	2:A:328:PHE:CZ	2.55	0.42
2:A:410:ASN:HA	2:A:447:TYR:CE2	2.55	0.42
2:A:564:ALA:O	2:A:568:ILE:HG23	2.20	0.42
2:A:643:GLU:OE1	2:A:682:ASN:HB3	2.20	0.42
2:A:647:GLU:HB3	2:A:648:PRO:HD3	2.02	0.42
2:C:234:ASN:OD1	2:C:237:ARG:N	2.42	0.42
2:C:375:THR:HA	2:C:378:GLU:CG	2.49	0.42
2:C:663:LYS:HZ3	2:C:706:ILE:HG23	1.84	0.42
1:B:21:LYS:HZ2	1:B:170:ASP:C	2.22	0.41
1:B:22:PHE:CE2	1:B:150:PHE:HD1	2.38	0.41
1:B:149:SER:HA	1:B:165:TYR:O	2.19	0.41
1:D:19:PRO:HG2	1:D:22:PHE:CG	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:193:LEU:CB	2:A:196:ARG:HH21	2.33	0.41
2:A:397:GLU:OE1	2:A:400:ARG:NH2	2.34	0.41
2:C:12:GLN:HG3	2:C:14:LYS:CE	2.49	0.41
2:C:380:PHE:HB3	2:C:427:TYR:CE1	2.55	0.41
2:C:388:ILE:O	2:C:429:ASP:HB2	2.20	0.41
2:C:422:HIS:HA	2:C:425:PHE:CD2	2.55	0.41
2:C:678:TRP:CH2	2:C:691:HIS:ND1	2.88	0.41
2:A:26:GLN:O	2:A:30:MET:CE	2.68	0.41
2:A:164:GLU:HB2	2:A:231:GLU:HB2	2.02	0.41
2:A:177:SER:HA	2:A:180:MET:CE	2.50	0.41
2:A:552:LYS:HG3	2:A:556:LYS:HE2	2.01	0.41
2:A:571:LEU:HD23	2:A:571:LEU:HA	1.82	0.41
2:A:614:TYR:O	2:A:618:ILE:HB	2.20	0.41
2:A:652:GLN:HG2	2:C:661:LEU:HD23	2.02	0.41
2:A:730:PHE:HD1	2:A:735:ASN:ND2	2.19	0.41
2:C:454:GLN:O	2:C:457:VAL:HB	2.20	0.41
2:A:14:LYS:HD3	2:A:14:LYS:N	2.35	0.41
2:A:118:TYR:O	2:A:122:PHE:N	2.45	0.41
2:A:514:ARG:HH12	2:A:566:GLN:NE2	2.18	0.41
2:C:34:LEU:HD11	2:C:77:LEU:HD13	2.01	0.41
2:C:54:ARG:HA	2:C:54:ARG:NE	2.35	0.41
2:C:169:ASP:HB2	2:C:172:THR:HG23	2.02	0.41
2:C:187:PHE:HA	2:C:190:MET:HG3	2.02	0.41
2:C:544:LYS:CD	2:C:594:ILE:HA	2.51	0.41
1:B:99:LEU:O	1:B:102:LEU:HB3	2.19	0.41
1:D:99:LEU:O	1:D:102:LEU:HB3	2.19	0.41
2:A:116:VAL:HG22	2:A:120:LYS:HZ2	1.85	0.41
2:A:202:HIS:CD2	2:A:204:ARG:HG3	2.54	0.41
2:A:387:HIS:HE1	2:A:433:ARG:CZ	2.34	0.41
2:C:198:GLN:CG	2:C:213:ARG:NH1	2.83	0.41
1:D:110:ILE:HG12	1:D:128:PHE:HB3	2.03	0.41
2:A:129:ILE:O	2:A:133:LEU:HG	2.21	0.41
2:A:247:LEU:HD21	2:A:282:PHE:CD1	2.55	0.41
2:A:645:ASN:C	2:A:648:PRO:HD2	2.40	0.41
2:C:82:THR:HG23	2:C:120:LYS:HD3	2.02	0.41
2:C:579:LEU:O	2:C:583:LEU:HG	2.21	0.41
2:C:693:GLY:O	2:C:697:MET:HG2	2.20	0.41
1:B:58:ILE:O	1:B:70:PRO:HD2	2.21	0.41
1:B:141:ALA:CB	2:A:589:LEU:CD1	2.98	0.41
1:D:5:VAL:HG12	1:D:132:PRO:HB3	2.03	0.41
2:A:29:GLN:OE1	2:A:45:HIS:CE1	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:420:HIS:C	2:C:423:PRO:HD2	2.40	0.41
2:C:605:GLU:CD	2:C:609:GLN:HE22	2.23	0.41
2:C:743:LEU:HD13	2:C:743:LEU:HA	1.94	0.41
2:A:213:ARG:NH2	2:A:257:LEU:HB2	2.36	0.41
2:A:453:SER:O	2:A:457:VAL:HG23	2.21	0.41
2:C:177:SER:HA	2:C:180:MET:HE2	2.02	0.41
2:C:177:SER:HA	2:C:180:MET:HE3	2.02	0.41
2:C:290:HIS:C	2:C:339:ARG:HH12	2.24	0.41
2:C:333:ALA:C	2:C:337:GLN:NE2	2.73	0.41
2:C:388:ILE:HG22	2:C:392:SER:HB3	2.01	0.41
2:C:724:LEU:HA	2:C:724:LEU:HD13	1.64	0.41
1:B:114:GLY:HA2	1:B:131:ASN:OD1	2.21	0.41
1:D:58:ILE:O	1:D:70:PRO:HD2	2.21	0.41
2:C:573:LYS:C	2:C:575:GLU:H	2.23	0.41
2:C:681:ARG:HB3	2:C:689:GLU:OE2	2.21	0.41
2:C:692:GLY:N	2:C:695:ARG:HH11	2.17	0.41
2:A:54:ARG:HA	2:A:54:ARG:NE	2.36	0.41
2:A:61:LYS:O	2:A:64:TYR:HB3	2.21	0.41
2:A:226:ARG:HA	2:A:229:GLN:OE1	2.21	0.41
2:A:262:LEU:O	2:A:266:ILE:HG13	2.20	0.41
2:A:403:LYS:NZ	2:A:440:VAL:HA	2.35	0.41
2:A:483:ASP:HB2	2:A:486:ASP:OD2	2.20	0.41
2:A:485:ALA:O	2:A:487:GLU:N	2.54	0.41
2:A:498:LEU:HD22	2:A:510:LEU:HD21	2.03	0.41
2:A:563:PHE:CE1	2:A:567:THR:HG21	2.55	0.41
2:A:596:PHE:CZ	2:A:599:HIS:HA	2.55	0.41
2:C:50:LEU:HD13	2:C:105:ILE:HG22	2.03	0.41
2:C:205:ASP:HB2	2:C:209:ARG:HH12	1.84	0.41
2:C:257:LEU:H	2:C:257:LEU:HD23	1.86	0.41
2:C:273:GLU:OE1	2:C:273:GLU:N	2.49	0.41
2:C:402:LEU:HA	2:C:402:LEU:HD23	1.80	0.41
2:C:469:GLN:NE2	2:C:520:GLY:O	2.54	0.41
2:C:559:LYS:HE3	2:C:559:LYS:HB3	1.82	0.41
1:B:11:ILE:HA	1:B:12:PRO:HA	1.88	0.41
1:B:152:LEU:HD23	1:B:152:LEU:H	1.85	0.41
1:D:114:GLY:HA2	1:D:131:ASN:OD1	2.21	0.41
2:A:354:LEU:HD23	2:A:354:LEU:HA	1.90	0.41
2:A:398:LEU:HD23	2:A:398:LEU:HA	1.82	0.41
2:A:457:VAL:O	2:A:461:MET:HG3	2.20	0.41
2:C:190:MET:CE	2:C:220:VAL:HG22	2.51	0.41
2:C:312:ARG:HH12	2:C:314:ASP:C	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:469:GLN:HE22	2:C:520:GLY:HA2	1.85	0.41
2:A:49:MET:O	2:A:52:GLU:HB2	2.21	0.40
2:A:208:LYS:HD3	2:A:211:ARG:NH2	2.36	0.40
2:A:362:TYR:CB	2:A:365:ARG:HH11	2.33	0.40
2:C:296:LYS:HG3	2:C:350:LEU:CD2	2.47	0.40
2:C:439:TYR:O	2:C:443:ASN:ND2	2.55	0.40
2:C:604:TYR:CE1	2:C:649:LEU:HD11	2.55	0.40
1:B:22:PHE:CD2	1:B:150:PHE:HD1	2.40	0.40
2:A:183:VAL:HG23	2:A:223:ASN:OD1	2.21	0.40
2:A:216:LEU:O	2:A:219:LEU:HB2	2.21	0.40
2:A:563:PHE:HA	2:A:566:GLN:HE22	1.86	0.40
2:A:717:VAL:HG23	2:A:718:GLN:N	2.36	0.40
2:A:733:LYS:HE2	2:A:733:LYS:HB3	1.82	0.40
2:C:270:PHE:HB2	2:C:275:HIS:CE1	2.57	0.40
2:C:589:LEU:HD23	2:C:589:LEU:HA	1.81	0.40
2:C:663:LYS:HE3	2:C:709:GLN:HB2	2.03	0.40
2:C:681:ARG:CZ	2:C:687:GLY:O	2.69	0.40
2:A:187:PHE:O	2:A:190:MET:HG3	2.20	0.40
2:A:296:LYS:HG2	2:A:350:LEU:HD21	2.03	0.40
2:A:402:LEU:HD22	2:A:421:PHE:CZ	2.57	0.40
2:A:555:LYS:HD3	2:A:555:LYS:N	2.36	0.40
2:A:607:MET:O	2:A:611:PHE:CD2	2.75	0.40
2:A:730:PHE:HE1	2:A:733:LYS:HZ1	1.62	0.40
2:A:760:SER:H	2:A:763:THR:HG22	1.86	0.40
2:C:150:ARG:O	2:C:153:LEU:HB3	2.21	0.40
2:C:368:TYR:HA	2:C:371:LYS:CE	2.48	0.40
2:C:583:LEU:HA	2:C:586:GLN:CG	2.50	0.40
2:C:606:PHE:HA	2:C:609:GLN:HE21	1.83	0.40
2:C:751:ARG:O	2:C:755:PRO:HD3	2.21	0.40
2:A:230:LEU:HD23	2:A:230:LEU:HA	1.89	0.40
2:A:290:HIS:O	2:A:293:VAL:HG12	2.21	0.40
2:A:507:TYR:CE2	2:A:559:LYS:HG3	2.56	0.40
2:A:761:GLU:HG2	2:A:762:GLU:N	2.37	0.40
2:C:124:GLN:N	2:C:172:THR:HG22	2.36	0.40
2:C:187:PHE:O	2:C:190:MET:HG3	2.20	0.40
2:C:425:PHE:O	2:C:433:ARG:HD3	2.21	0.40
2:C:504:ASP:OD1	2:C:504:ASP:N	2.54	0.40
2:C:677:PHE:CD2	2:C:699:CYS:HB2	2.56	0.40
1:D:22:PHE:CD2	1:D:150:PHE:HD1	2.40	0.40
2:A:236:GLU:HA	2:A:239:LYS:NZ	2.37	0.40
2:A:367:ASP:N	2:A:367:ASP:OD1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:388:ILE:CG2	2:A:392:SER:HB3	2.52	0.40
2:A:454:GLN:HE22	2:A:509:ILE:HA	1.86	0.40
2:A:557:CYS:O	2:A:561:PHE:CD1	2.60	0.40
2:A:564:ALA:O	2:A:568:ILE:HG12	2.21	0.40
2:A:668:ARG:HE	2:A:668:ARG:HB3	1.50	0.40
2:A:713:PRO:HB3	2:A:757:LEU:CD2	2.51	0.40
2:C:225:VAL:O	2:C:229:GLN:OE1	2.39	0.40
2:C:230:LEU:HA	2:C:230:LEU:HD23	1.75	0.40
2:C:403:LYS:HA	2:C:403:LYS:HE2	2.04	0.40
2:C:643:GLU:O	2:C:647:GLU:HB2	2.21	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	B	180/182 (99%)	157 (87%)	22 (12%)	1 (1%)	25	66
1	D	180/182 (99%)	157 (87%)	22 (12%)	1 (1%)	25	66
2	A	767/796 (96%)	726 (95%)	40 (5%)	1 (0%)	51	86
2	C	767/796 (96%)	723 (94%)	42 (6%)	2 (0%)	41	77
All	All	1894/1956 (97%)	1763 (93%)	126 (7%)	5 (0%)	44	77

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	484	PHE
2	C	473	ASP
2	C	693	GLY
1	B	38	GLY
1	D	38	GLY

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	B	160/160 (100%)	150 (94%)	10 (6%)	18 43
1	D	160/160 (100%)	150 (94%)	10 (6%)	18 43
2	A	695/720 (96%)	692 (100%)	3 (0%)	91 94
2	C	695/720 (96%)	689 (99%)	6 (1%)	78 87
All	All	1710/1760 (97%)	1681 (98%)	29 (2%)	62 78

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1	MET
1	B	2	LEU
1	B	12	PRO
1	B	39	ASN
1	B	40	LEU
1	B	84	LEU
1	B	101	LEU
1	B	139	TYR
1	B	153	MET
1	B	156	GLN
1	D	1	MET
1	D	2	LEU
1	D	12	PRO
1	D	39	ASN
1	D	40	LEU
1	D	84	LEU
1	D	101	LEU
1	D	139	TYR
1	D	153	MET
1	D	156	GLN
2	A	573	LYS
2	A	582	ARG
2	A	705	LYS
2	C	158	ARG

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Mol	Chain	Res	Type
2	C	239	LYS
2	C	254	ARG
2	C	526	ARG
2	C	695	ARG
2	C	733	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	12	GLN
2	A	21	GLN
2	A	75	HIS
2	A	155	GLN
2	A	200	GLN
2	A	202	HIS
2	A	456	GLN
2	A	474	GLN
2	A	586	GLN
2	A	599	HIS
2	A	646	HIS
2	A	652	GLN
2	A	666	GLN
2	A	735	ASN
2	A	741	GLN
2	A	745	GLN
2	A	748	GLN
2	C	29	GLN
2	C	45	HIS
2	C	99	GLN
2	C	186	ASN
2	C	198	GLN
2	C	259	GLN
2	C	331	GLN
2	C	337	GLN
2	C	454	GLN
2	C	506	GLN
2	C	586	GLN
2	C	609	GLN
2	C	716	GLN
2	C	725	ASN
2	C	769	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Map visualisation

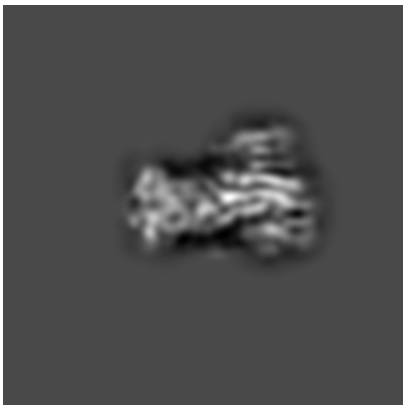
This section contains visualisations of the EMDB entry EMD-12220. These allow visual inspection of the internal detail of the map and identification of artifacts.

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.

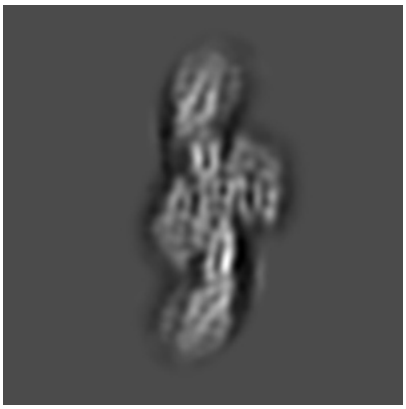
6.1 Orthogonal projections

6.1.1 Primary map

X

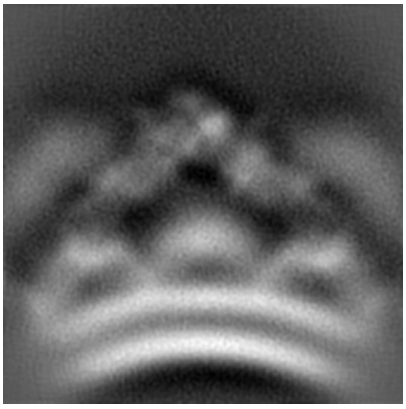


Y

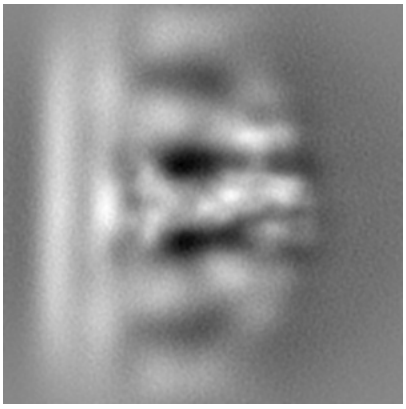


Z

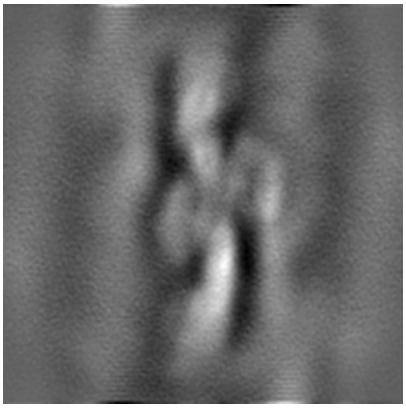
6.1.2 Raw map



X



Y



Z

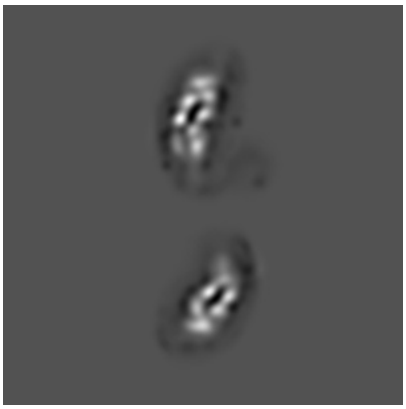
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map

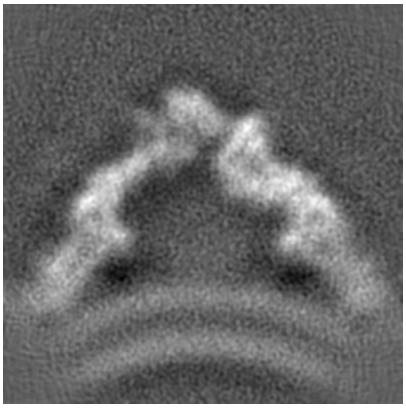
X Index: 84

Y Index: 84

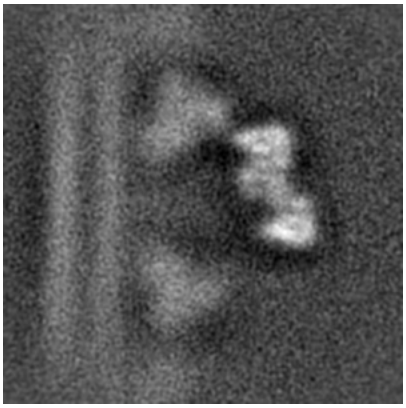


Z Index: 84

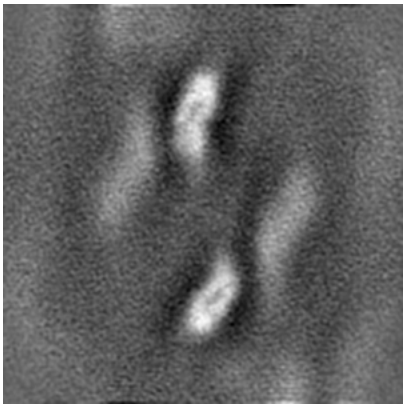
6.2.2 Raw map



X Index: 84



Y Index: 84



Z Index: 84

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

6.3 Largest variance slices (i)

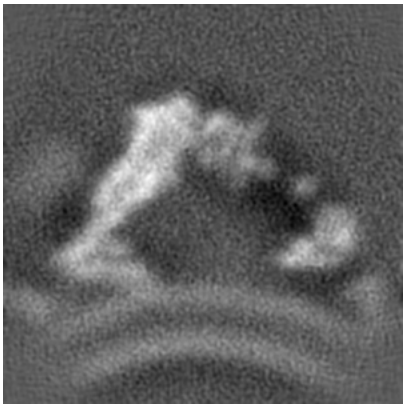
6.3.1 Primary map

X Index: 88

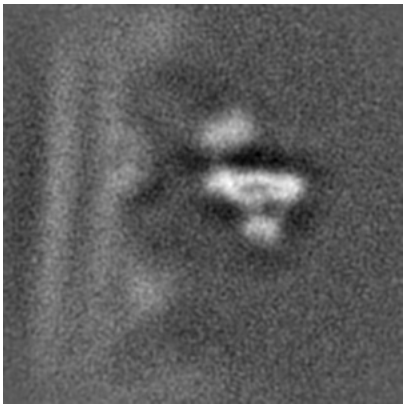
Y Index: 86

Z Index: 107

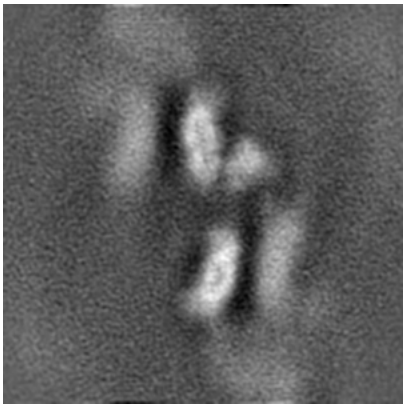
6.3.2 Raw map



X Index: 92



Y Index: 61

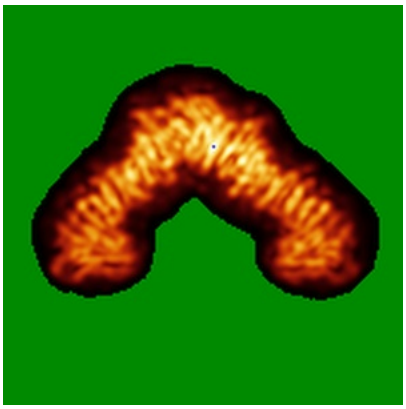


Z Index: 95

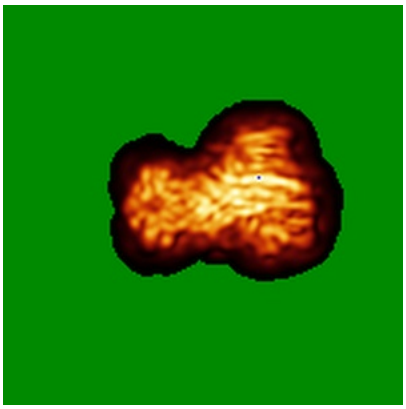
The images above show the largest variance slices of the map in three orthogonal directions.

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

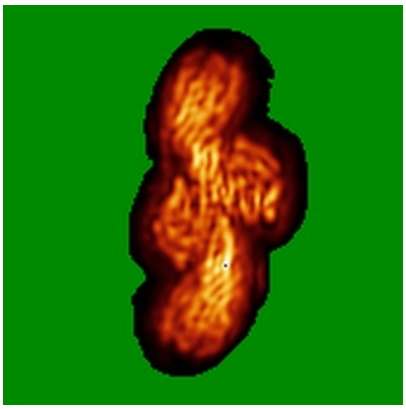
6.4.1 Primary map



X

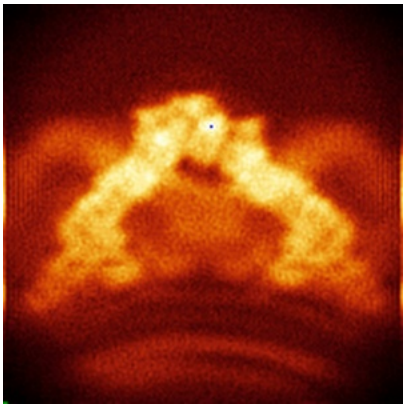


Y

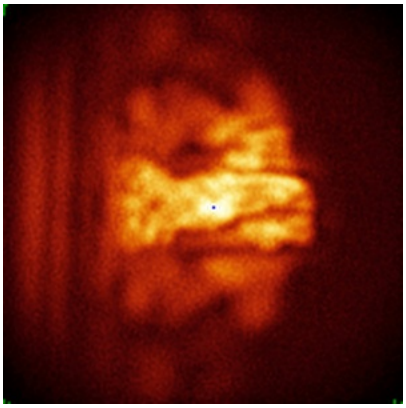


Z

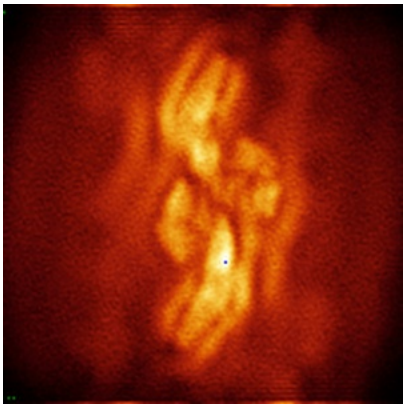
6.4.2 Raw map



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 0.021. 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.

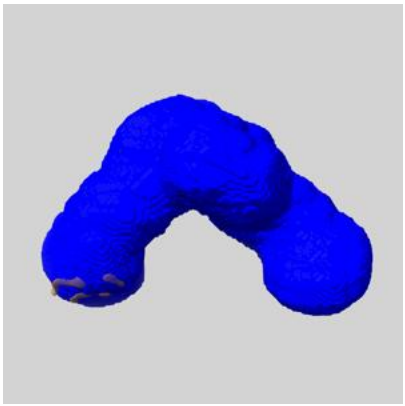
6.6 Mask visualisation (i)

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

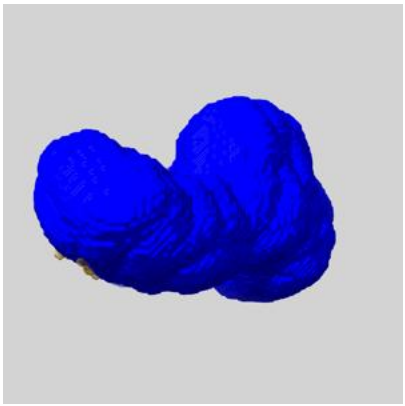
A mask typically either:

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

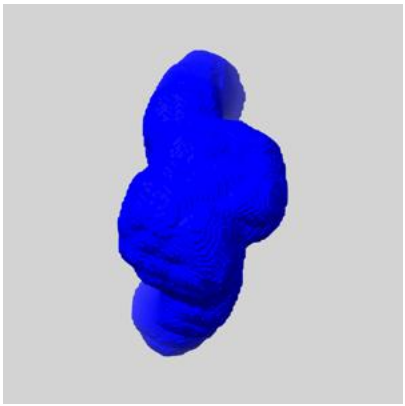
6.6.1 emd_12220_msk_1.map (i)



X



Y

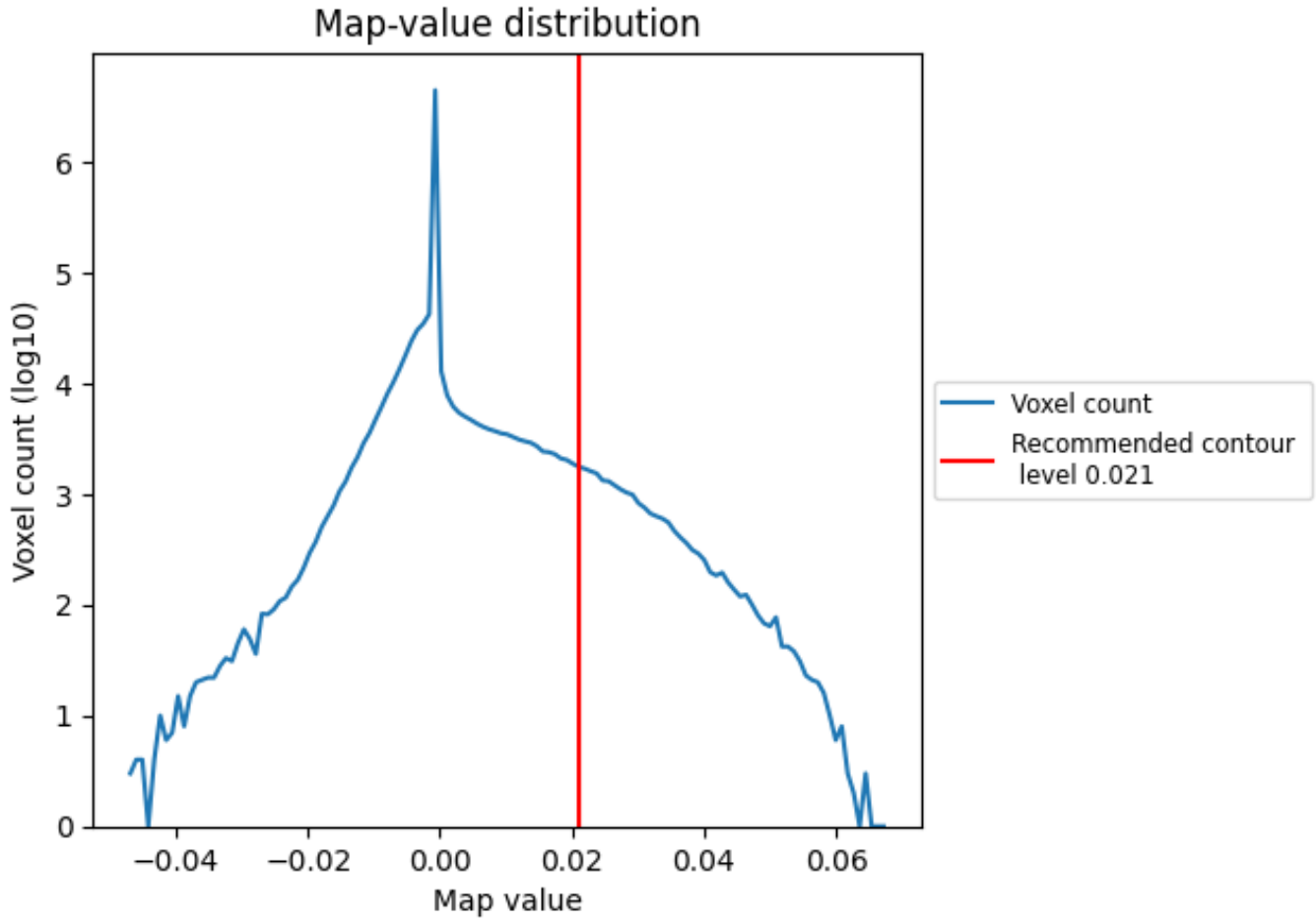


Z

7 Map analysis

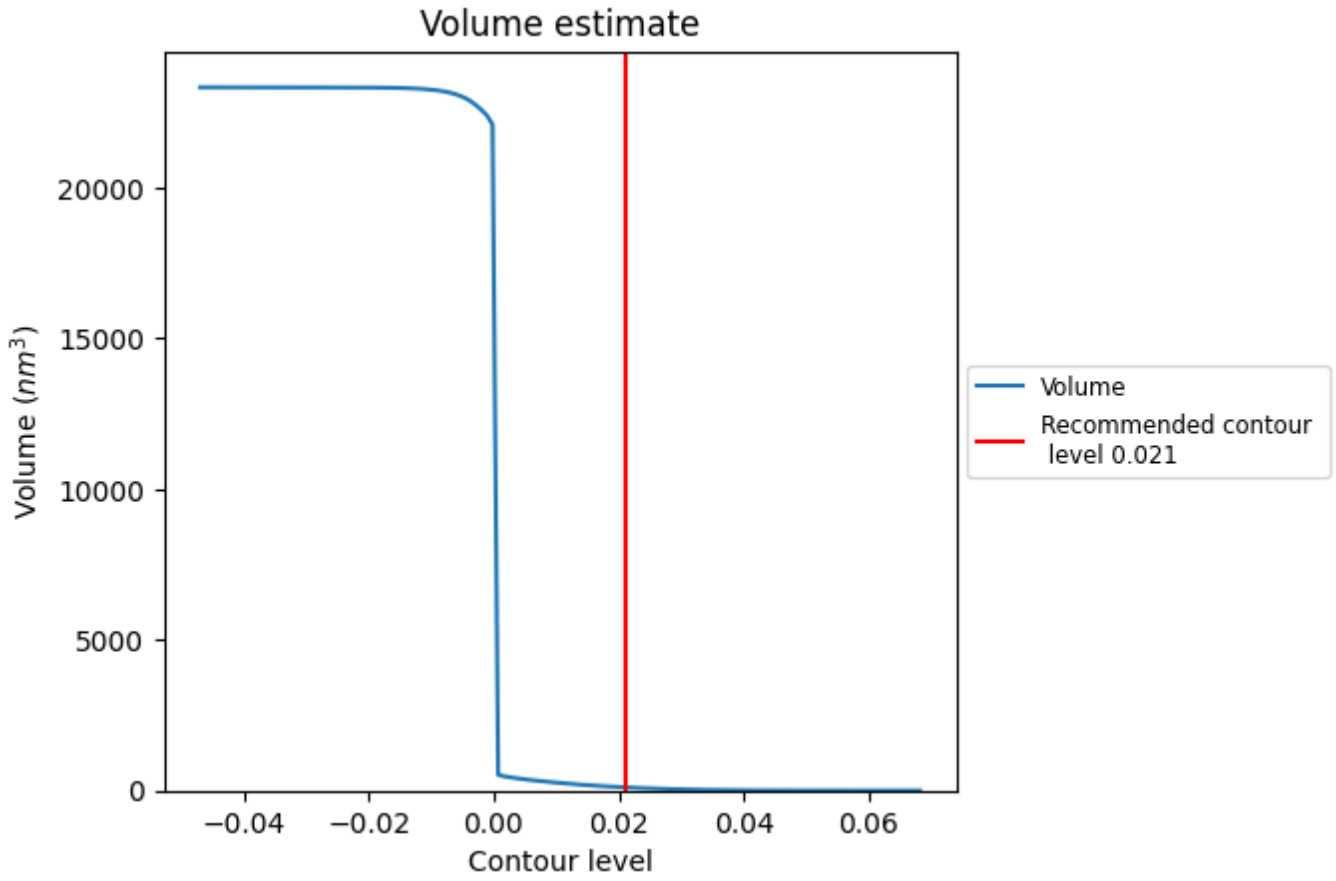
This section contains the results of statistical analysis of the map.

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.

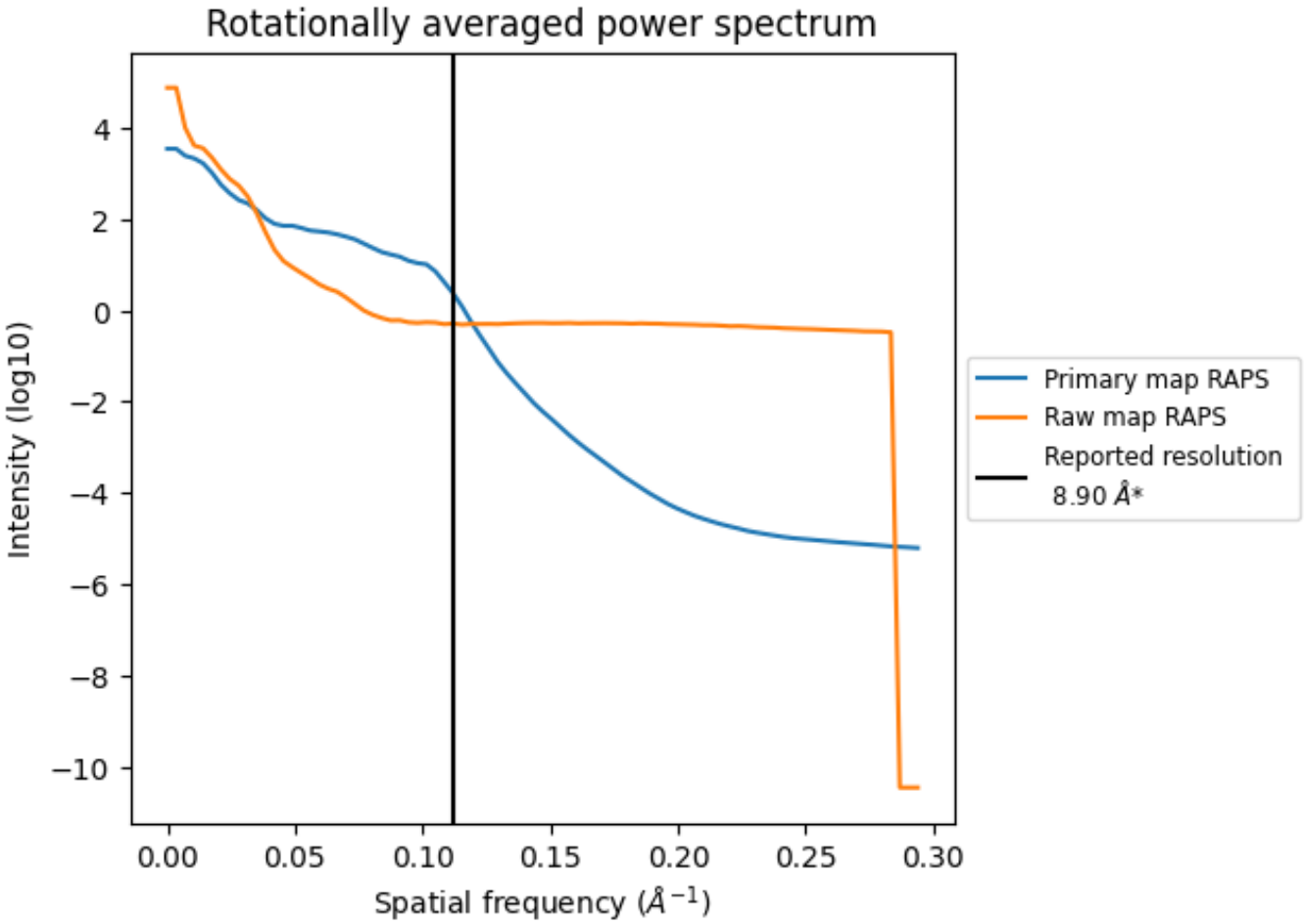
7.2 Volume estimate



The volume at the recommended contour level is 106 nm^3; this corresponds to an approximate mass of 96 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)

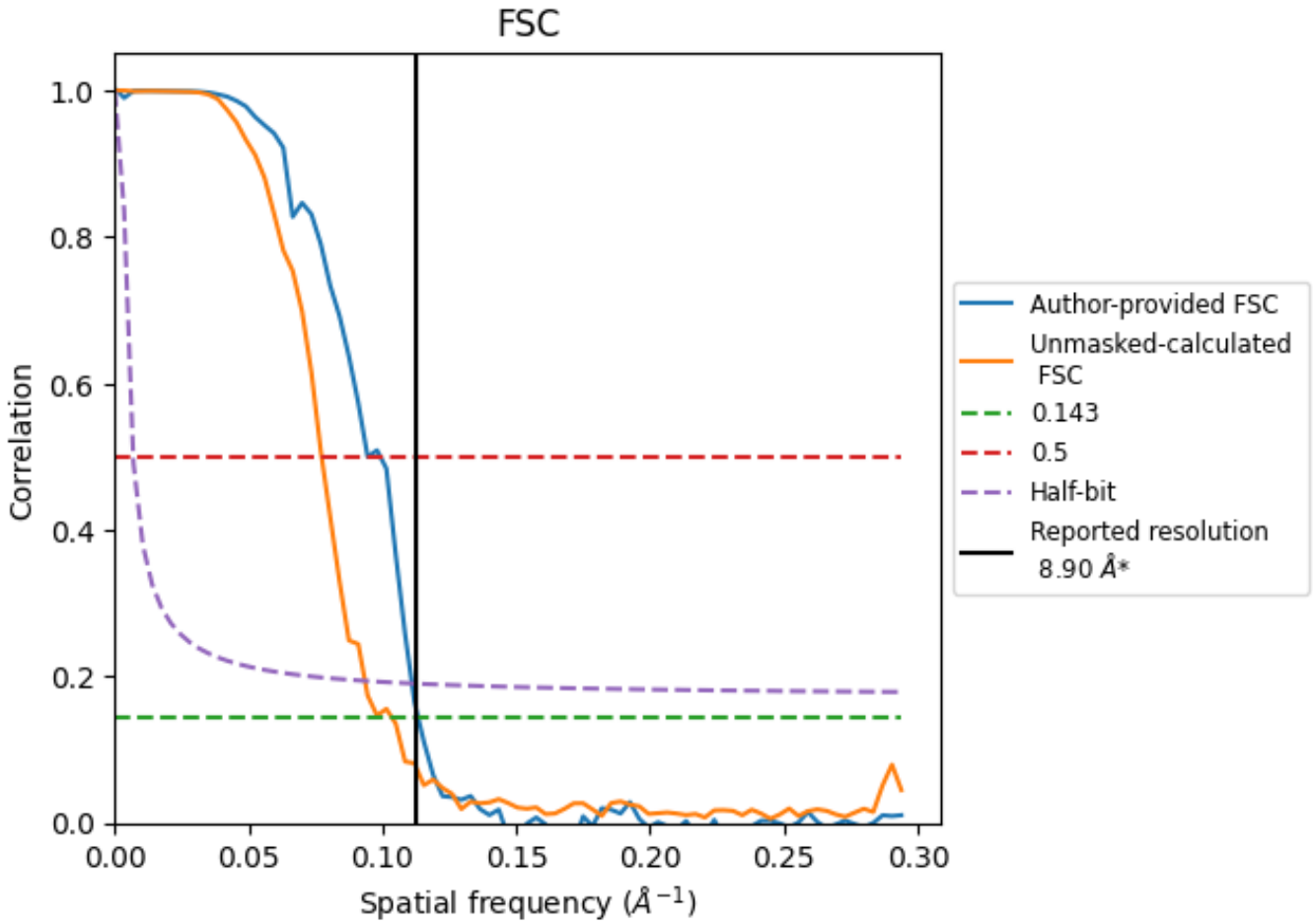


*Reported resolution corresponds to spatial frequency of 0.112 Å^{-1}

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 0.112 Å^{-1}

8.2 Resolution estimates (i)

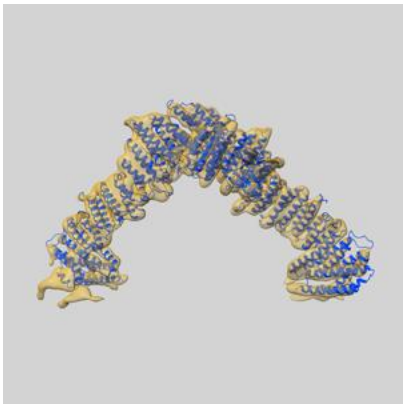
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.90	-	-
Author-provided FSC curve	8.82	10.58	9.01
Unmasked-calculated*	9.65	12.94	10.70

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

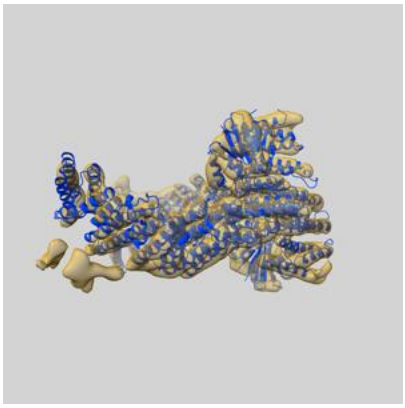
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12220 and PDB model 7BLN. Per-residue inclusion information can be found in section 3 on page 4.

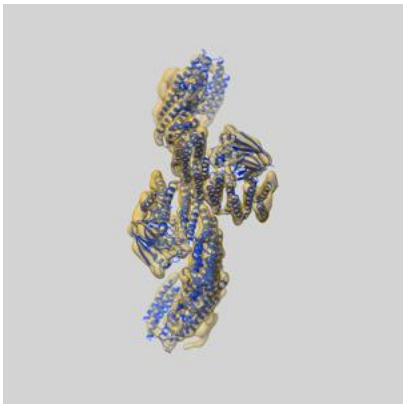
9.1 Map-model overlay



X



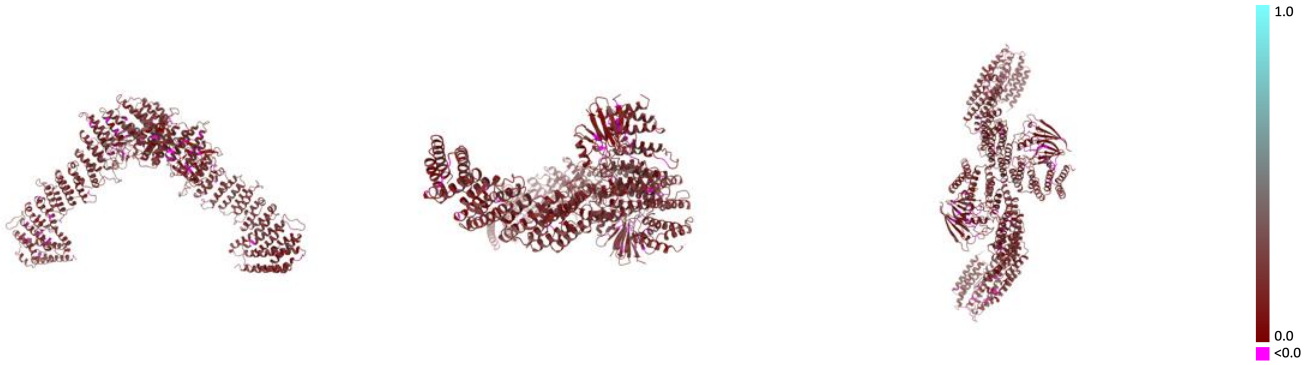
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.021 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.

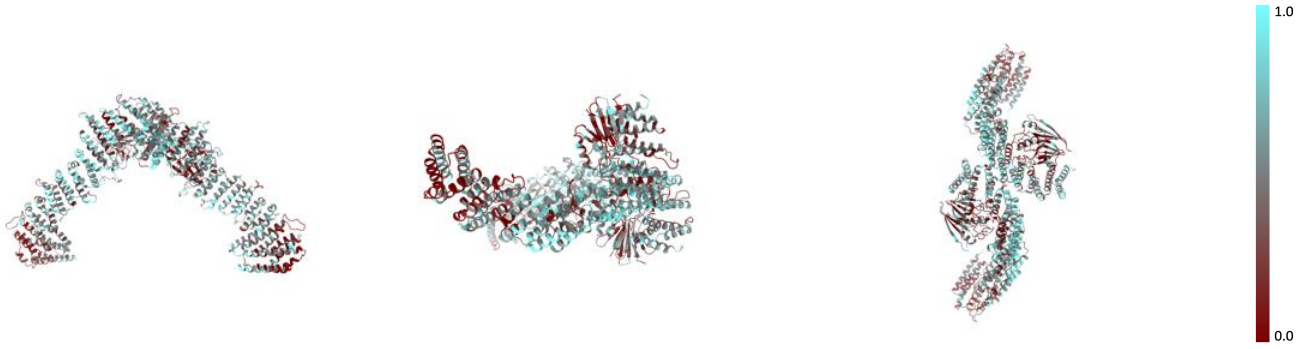
9.2 Q-score mapped to coordinate model (i)



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.

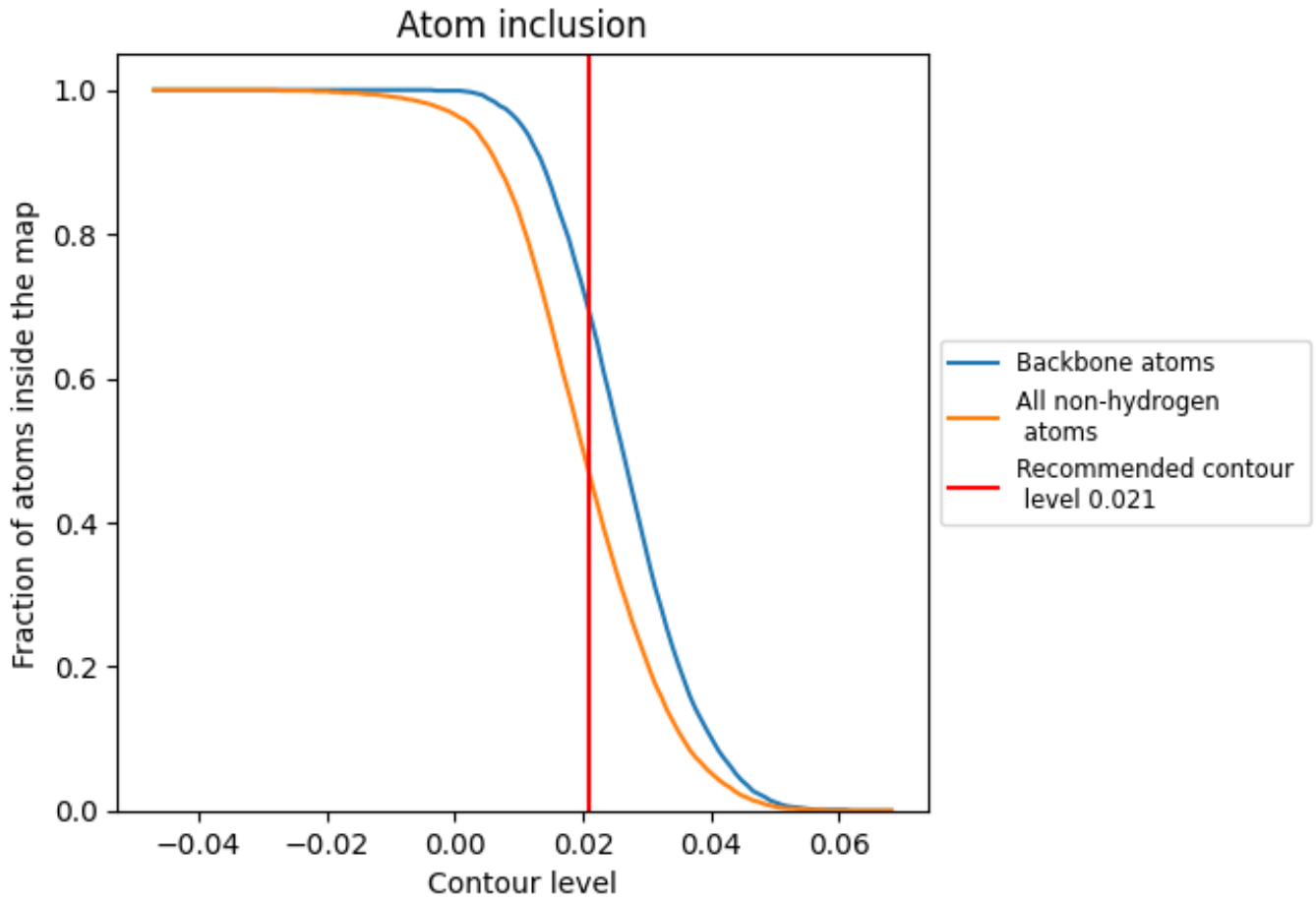
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.021).

9.4 Atom inclusion (i)



At the recommended contour level, 69% of all backbone atoms, 47% 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 (0.021) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4660	0.1800
A	0.4960	0.1890
B	0.3170	0.1270
C	0.5020	0.1910
D	0.3340	0.1380