Full wwPDB EM Validation Report ⓘ

Mar 25, 2024 – 05:51 PM JST

PDB ID	:	7YUW
EMDB ID	:	EMD-34113
Title	:	MtaLon-ADP for the spiral oligomers of pentamer
Authors	:	Li, S.; Hsieh, K.; Kuo, C.; Lee, S.; Ho, M.; Wang, C.; Zhang, K.; Chang, C.I.
Deposited on	:	2022-08-18
Resolution	:	3.60 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

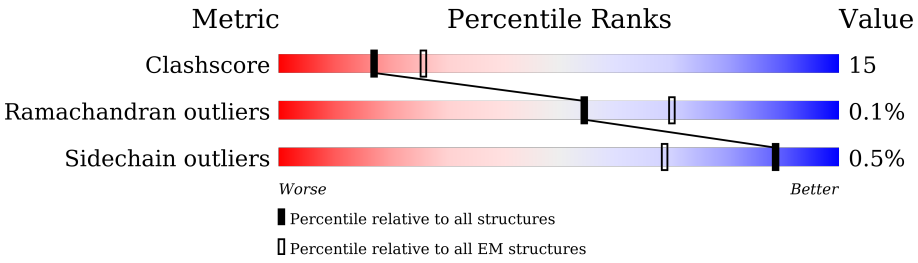
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	793	38% 64% 34% ·
1	B	793	32% 62% 35% ·
1	C	793	29% 63% 34% ·
1	D	793	30% 64% 33% · ·
1	E	793	42% 60% 37% ·

2 Entry composition

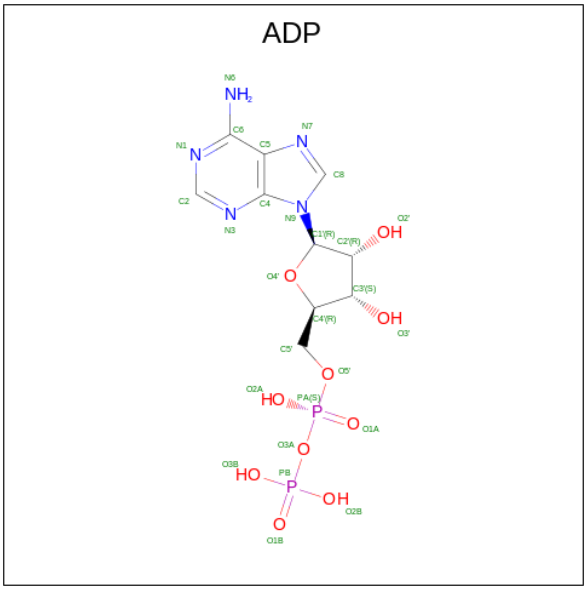
There are 2 unique types of molecules in this entry. The entry contains 30483 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Lon protease.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	773	Total	C	N	O	S	0	0
			6075	3838	1067	1149	21		
1	B	773	Total	C	N	O	S	0	0
			6075	3838	1067	1149	21		
1	C	773	Total	C	N	O	S	0	0
			6075	3838	1067	1149	21		
1	D	773	Total	C	N	O	S	0	0
			6075	3838	1067	1149	21		
1	E	773	Total	C	N	O	S	0	0
			6075	3838	1067	1149	21		

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

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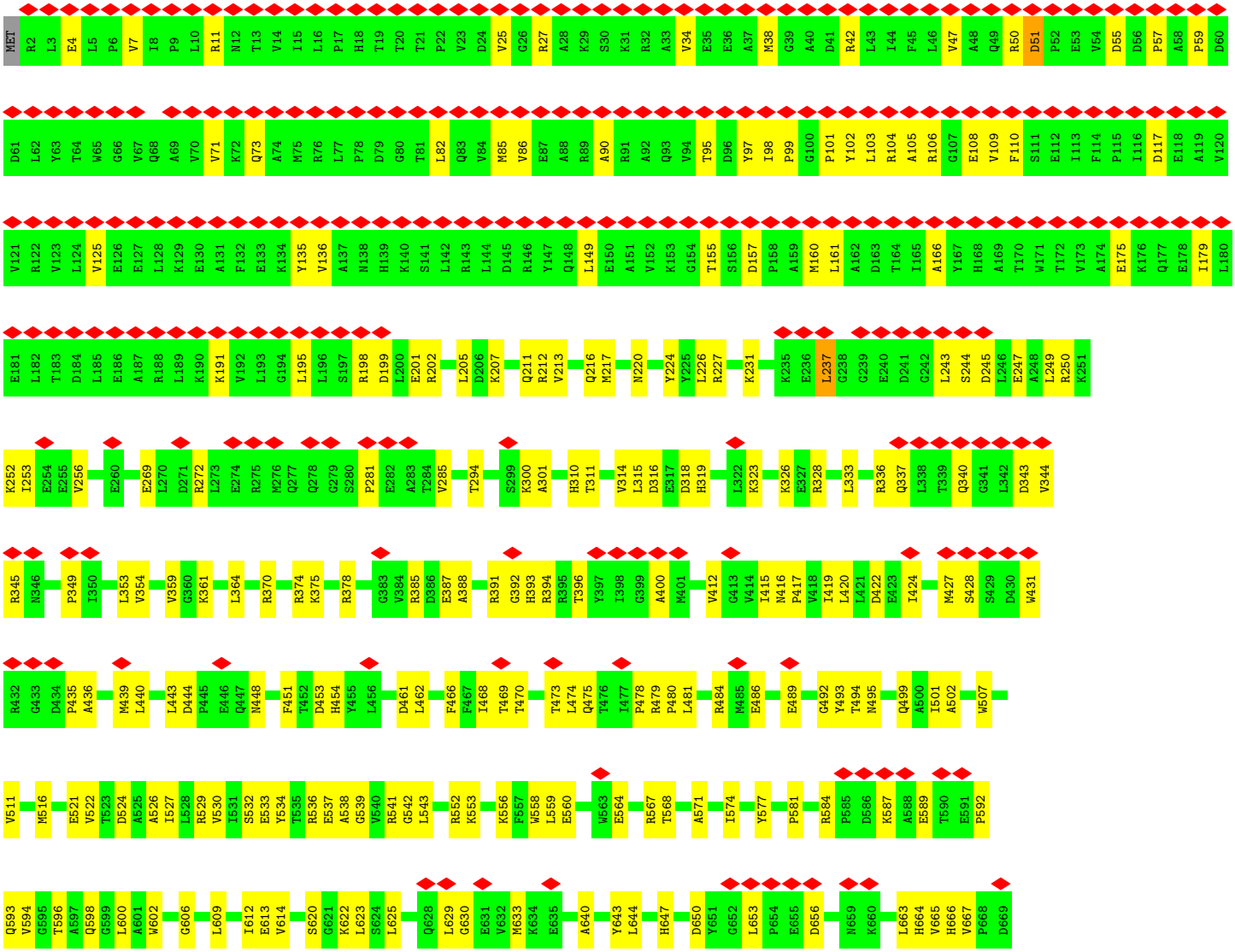
Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	D	1	Total	C	N	O	P	0
			27	10	5	10	2	

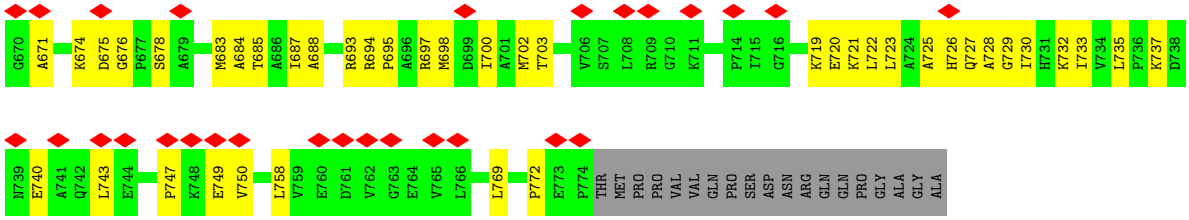
3 Residue-property plots (i)

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: Lon protease

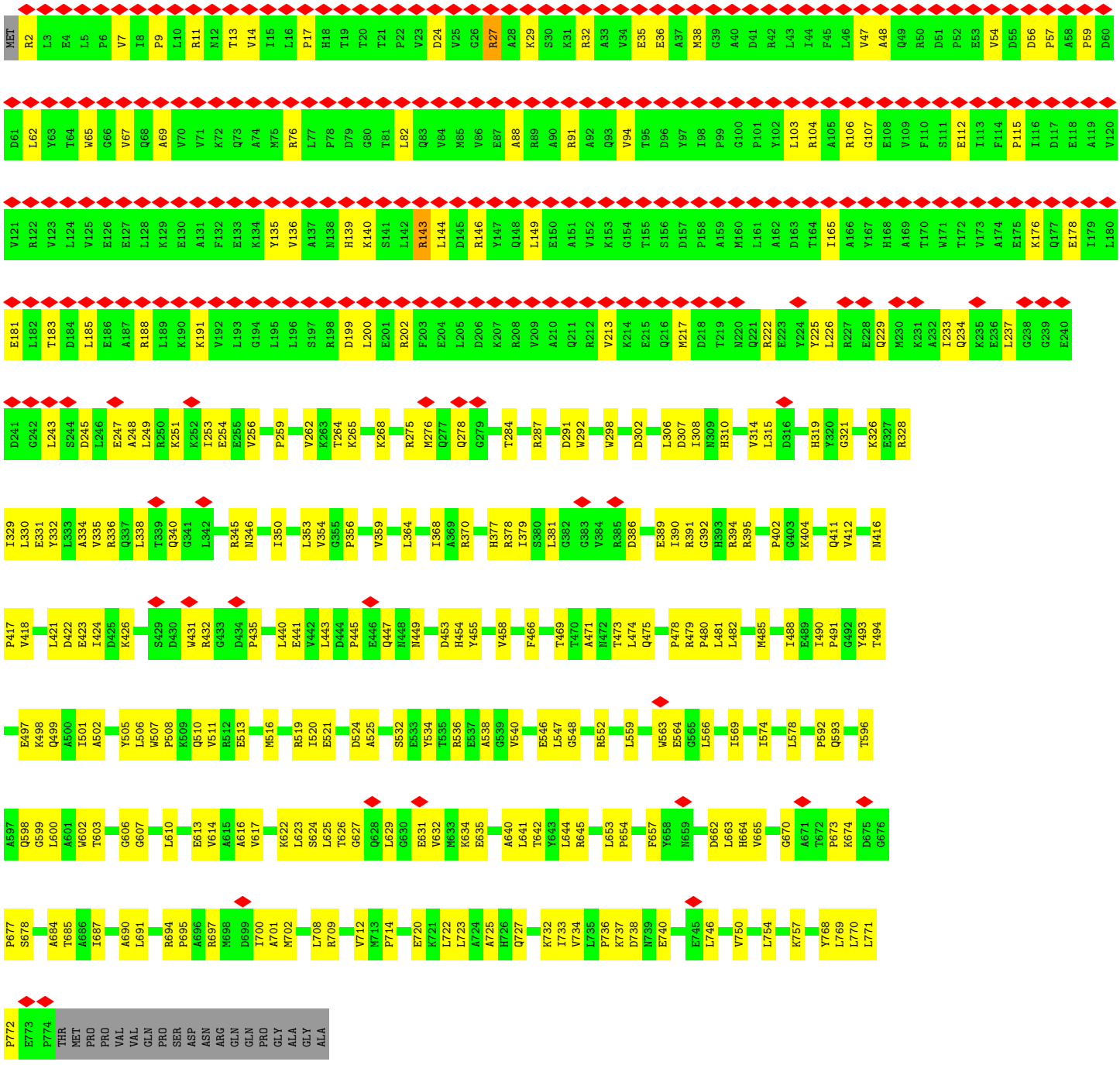
Chain A:





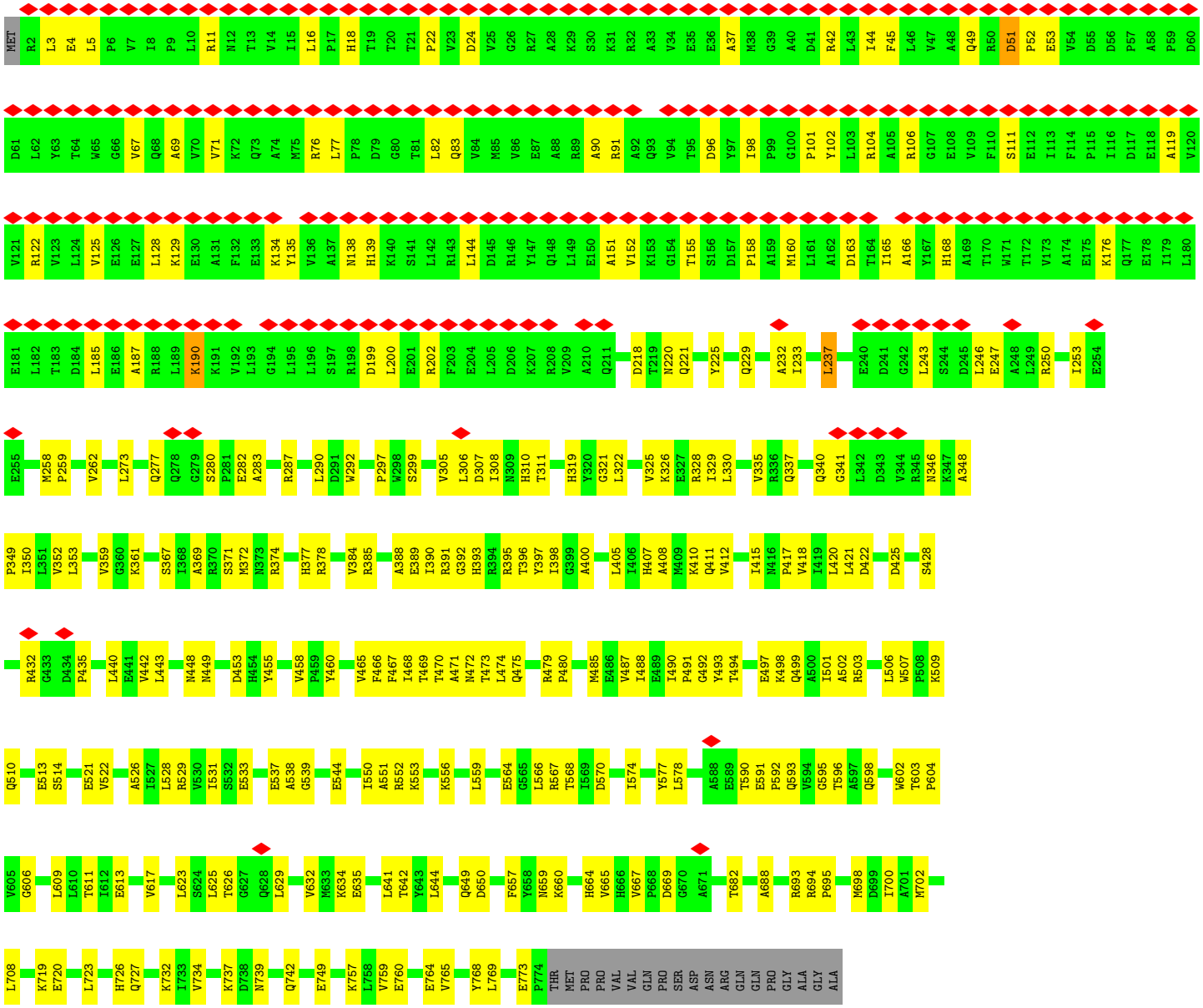
- Molecule 1: Lon protease

Chain B:



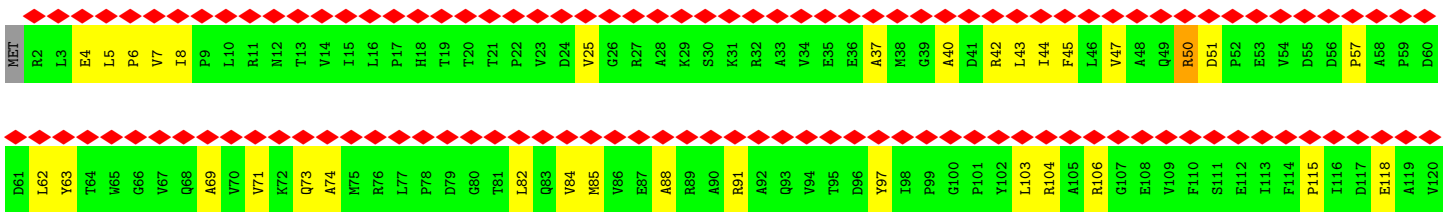
• Molecule 1: Lon protease

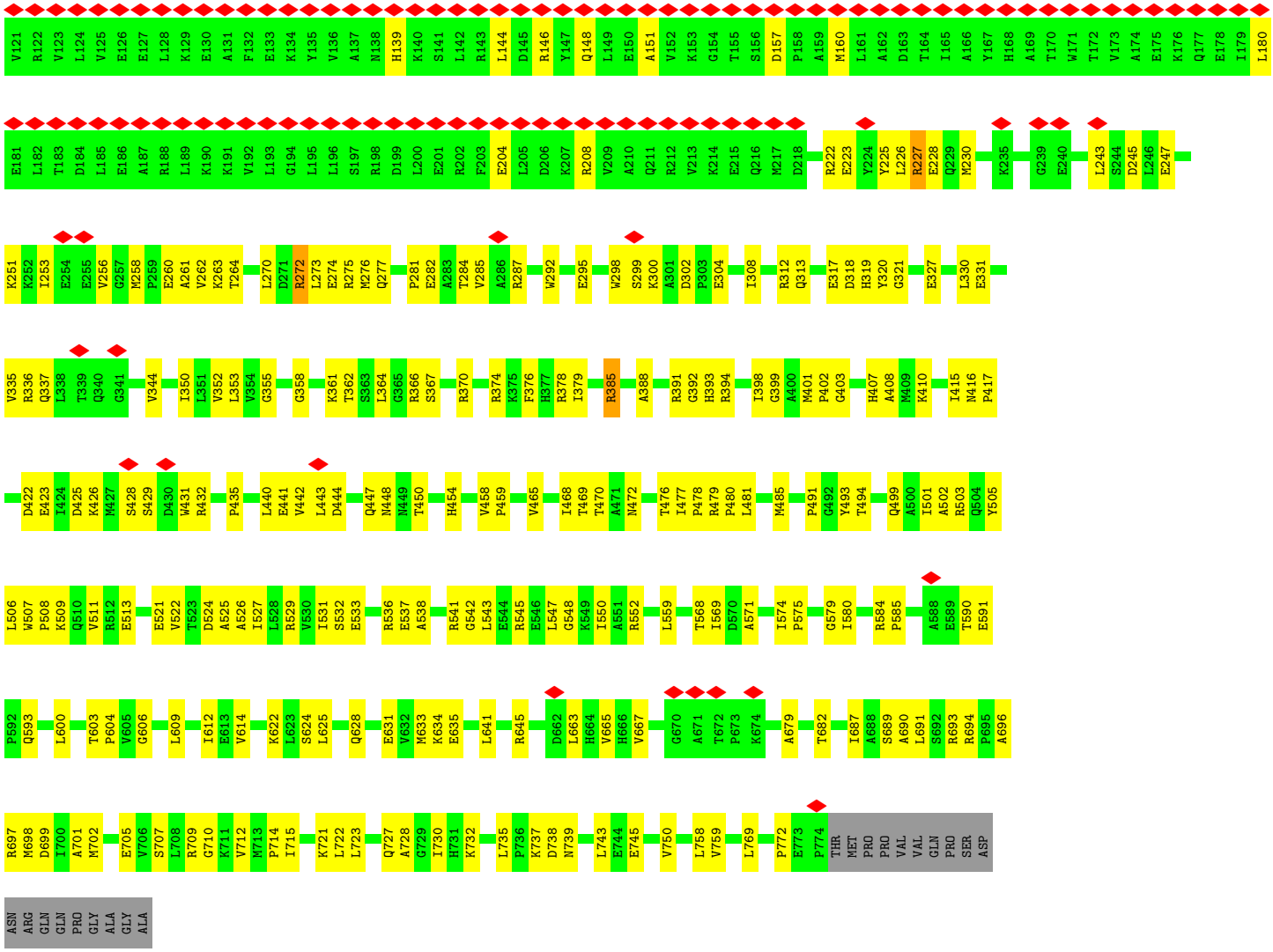
Chain C:



• Molecule 1: Lon protease

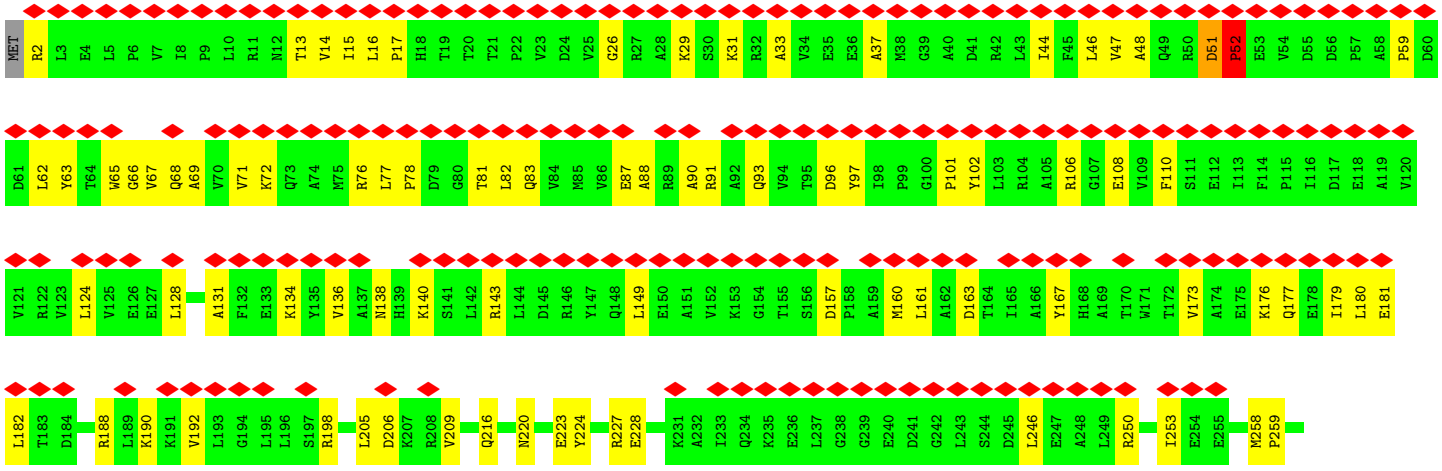
Chain D:

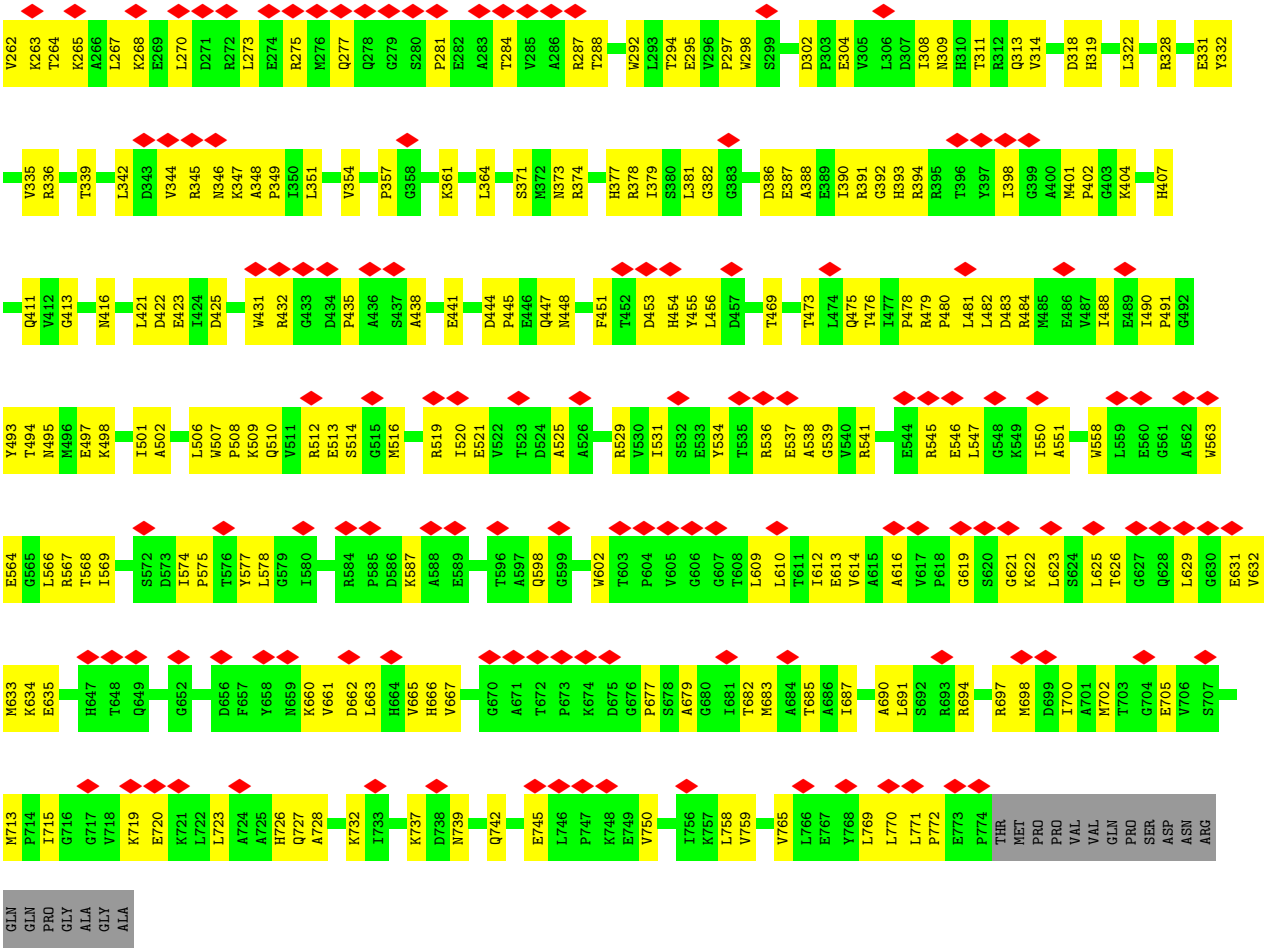




• Molecule 1: Lon protease

Chain E:




V262 K263 T264 K265 A266 L267 K268 E269 L270 D271 R272 L273 E274 R275 M276 Q277 Q278 G279 S280 P281 E282 A283 T284 V285 A286 R287 T288 W292 L293 T294 E295 V296 P297 W298 S299 D302 P303 E304 V305 L306 D307 I308 N309 H310 T311 R312 Q313 V314 D318 H319 L322 R328 E331 Y332
V335 R336 T339 L342 D343 V344 R345 N346 K347 A348 P349 I350 L351 V354 P357 G358 K361 L364 S371 M372 N373 R374 H377 R378 I379 S380 L381 G382 G383 D386 E387 A388 E389 I390 R391 G392 H393 R394 R395 T396 Y397 I398 G399 A400 M401 P402 G403 K404 H407
Q411 V412 G413 N416 L421 D422 E423 T424 D425 W431 R432 G433 D434 P435 A436 S437 A438 E441 D444 P445 E446 Q447 N448 F451 T452 D453 H454 Y455 L456 D457 T469 T473 L474 Q475 T476 I477 P478 R479 P480 L481 L482 D483 R484 M485 E486 V487 I488 E489 I490 P491 G492
Y493 T494 N495 M496 E497 K498 I501 A502 L506 W507 P508 K509 Q510 V511 R512 E513 S514 G515 M516 R519 I520 E521 V522 T523 D524 A525 A526 R529 V530 I531 S532 E533 Y534 T535 R536 E537 A538 G539 V540 R541 E544 R545 E546 L547 G548 K549 I550 A551 W558 L559 E560 G561 A562 W563
E564 G565 L566 R567 T568 I569 S572 D573 I574 P575 T576 Y577 L578 G579 I580 R584 P585 D586 K587 A588 E589 T596 A597 Q598 G599 W602 T603 P604 V605 G606 G607 T608 L609 L610 T611 I612 E613 V614 A615 A616 V617 P618 G619 S620 G621 K622 L623 S624 L625 T626 G627 Q628 L629 G630 E631 V632
M633 K634 E635 H647 T648 Q649 G652 D656 F657 Y658 N659 K660 V661 D662 L663 H664 V665 H666 V667 G670 A671 T672 P673 K674 D675 G676 P677 S678 A679 G680 I681 T682 M683 A684 T685 A686 I687 A690 L691 S692 R693 R694 R697 M698 D699 I700 A701 M702 T703 G704 E705 V706 S707
M713 P714 I715 G716 G717 V718 K719 E720 K721 L722 L723 A724 A725 H726 Q727 A728 K732 I733 K737 D738 N739 Q742 E745 L746 P747 K748 E749 V750 I756 K757 L758 V759 V765 L766 E767 Y768 L769 L770 L771 P772 E773 P774 THR MET PRO PRO VAL VAL GLN PRO SER ASP ASN ARG
GLN GLN PRO GLY ALA GLY ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	253989	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	48	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.669	Depositor
Minimum map value	-1.316	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.17	Depositor
Map size (Å)	275.52, 275.52, 275.52	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.26	0/6184	0.53	0/8380
1	B	0.27	0/6184	0.54	0/8380
1	C	0.28	0/6184	0.55	0/8380
1	D	0.27	0/6184	0.54	0/8380
1	E	0.26	0/6184	0.53	0/8380
All	All	0.27	0/30920	0.54	0/41900

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	E	0	2
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	51	ASP	Peptide
1	C	51	ASP	Peptide
1	E	51	ASP	Peptide
1	E	52	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	A	6075	0	6188	187	0
1	B	6075	0	6188	202	0
1	C	6075	0	6188	195	0
1	D	6075	0	6188	198	0
1	E	6075	0	6188	212	0
2	A	27	0	12	1	0
2	B	27	0	12	1	0
2	C	27	0	12	3	0
2	D	27	0	12	3	0
All	All	30483	0	30988	946	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 15.

All (946) 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:502:ALA:HA	1:D:506:LEU:HB2	1.61	0.83
1:C:502:ALA:HA	1:C:506:LEU:HB2	1.62	0.81
1:C:243:LEU:HA	1:C:247:GLU:HB2	1.60	0.80
1:E:14:VAL:HG21	1:E:177:GLN:HB2	1.64	0.80
1:B:502:ALA:HA	1:B:506:LEU:HB2	1.65	0.79
1:C:277:GLN:HB3	1:C:283:ALA:HB3	1.63	0.79
1:A:663:LEU:HD21	1:A:687:ILE:HD12	1.65	0.78
1:A:644:LEU:HD12	1:A:653:LEU:HD11	1.64	0.78
1:D:538:ALA:HA	1:D:727:GLN:HG2	1.65	0.77
1:B:600:LEU:HD22	1:B:725:ALA:HB2	1.65	0.77
1:B:135:TYR:HA	1:B:200:LEU:HD13	1.66	0.76
1:B:402:PRO:O	1:C:432:ARG:NH2	2.18	0.76
1:B:412:VAL:HG11	1:B:417:PRO:HB3	1.69	0.75
1:C:306:LEU:O	1:C:337:GLN:NE2	2.20	0.75
1:D:285:VAL:HA	1:D:398:ILE:HD13	1.70	0.74
1:D:281:PRO:HG3	1:D:398:ILE:HG22	1.69	0.74
1:E:525:ALA:HB1	1:E:529:ARG:HH12	1.52	0.74
1:B:491:PRO:HB2	1:B:723:LEU:HD12	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:LEU:HB3	1:B:326:LYS:HD2	1.70	0.73
1:C:625:LEU:HD11	1:C:634:LYS:HB2	1.68	0.73
1:C:328:ARG:HB3	1:C:488:ILE:HD12	1.69	0.73
1:E:441:GLU:HG3	1:E:447:GLN:HG2	1.69	0.73
1:E:502:ALA:HA	1:E:506:LEU:HB2	1.70	0.73
1:A:629:LEU:HD21	1:A:667:VAL:HB	1.71	0.73
1:C:501:ILE:HD11	2:C:801:ADP:C5	2.23	0.73
1:B:421:LEU:HB2	1:B:469:THR:HG22	1.70	0.73
1:B:524:ASP:OD1	1:B:525:ALA:N	2.22	0.72
1:A:125:VAL:HG13	1:A:161:LEU:HD22	1.71	0.72
1:D:472:ASN:ND2	1:D:604:PRO:O	2.23	0.72
1:A:117:ASP:OD1	1:D:146:ARG:NH2	2.23	0.72
1:E:759:VAL:HG21	1:E:765:VAL:HG23	1.72	0.72
1:E:157:ASP:HB3	1:E:160:MET:HG2	1.72	0.72
1:A:448:ASN:HB2	1:A:462:LEU:HB2	1.72	0.71
1:B:532:SER:O	1:B:536:ARG:NH2	2.24	0.70
1:E:16:LEU:HD12	1:E:167:TYR:HB2	1.74	0.70
1:C:220:ASN:ND2	1:E:228:GLU:OE2	2.23	0.69
1:D:737:LYS:N	1:D:759:VAL:O	2.24	0.69
1:B:506:LEU:HD11	1:B:540:VAL:HB	1.73	0.69
1:E:13:THR:HA	1:E:173:VAL:HG21	1.74	0.69
1:A:529:ARG:NH1	1:A:571:ALA:O	2.26	0.69
1:C:700:ILE:HG12	1:C:732:LYS:HB2	1.75	0.69
1:E:72:LYS:NZ	1:E:87:GLU:OE1	2.26	0.69
1:A:614:VAL:HG22	1:A:665:VAL:HG22	1.74	0.69
1:D:222:ARG:HH22	1:D:225:TYR:HD2	1.37	0.69
1:D:391:ARG:NH1	1:D:441:GLU:OE1	2.26	0.68
1:D:715:ILE:HD12	1:D:721:LYS:HG3	1.75	0.68
1:E:131:ALA:HA	1:E:134:LYS:HE2	1.74	0.68
1:C:16:LEU:HB3	1:C:163:ASP:HB3	1.75	0.68
1:D:350:ILE:H	1:D:485:MET:HE3	1.58	0.68
1:E:694:ARG:HD2	1:E:770:LEU:HD13	1.76	0.68
1:E:739:ASN:ND2	1:E:742:GLN:OE1	2.23	0.68
1:D:355:GLY:O	1:D:361:LYS:NZ	2.24	0.68
1:B:654:PRO:HG2	1:B:657:PHE:HB3	1.75	0.68
1:C:353:LEU:HD22	1:C:490:ILE:HD11	1.76	0.68
1:D:378:ARG:NH2	1:D:422:ASP:OD2	2.26	0.68
1:E:140:LYS:HD3	1:E:143:ARG:HH12	1.56	0.68
1:B:143:ARG:HG2	1:B:144:LEU:H	1.57	0.67
1:D:401:MET:HE3	1:E:432:ARG:HB3	1.76	0.67
1:E:281:PRO:HB3	1:E:398:ILE:HB	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:TRP:HD1	1:A:567:ARG:HE	1.42	0.67
1:E:253:ILE:O	1:E:263:LYS:NZ	2.27	0.67
1:E:663:LEU:HD13	1:E:687:ILE:HD12	1.77	0.67
1:A:333:LEU:O	1:A:337:GLN:N	2.27	0.67
1:B:702:MET:HG2	1:B:734:VAL:HB	1.77	0.67
1:C:417:PRO:HD2	1:C:465:VAL:HG22	1.77	0.67
1:C:491:PRO:HB2	1:C:723:LEU:HG	1.76	0.67
1:E:623:LEU:HD23	1:E:634:LYS:HD3	1.76	0.67
1:A:559:LEU:HD12	1:B:334:ALA:HB1	1.77	0.67
1:A:424:ILE:HG21	1:A:469:THR:HB	1.77	0.66
1:C:739:ASN:ND2	1:C:742:GLN:OE1	2.27	0.66
1:C:398:ILE:HD11	1:D:394:ARG:HB3	1.77	0.66
1:E:304:GLU:HG2	1:E:374:ARG:HH22	1.60	0.66
1:D:442:VAL:O	1:D:448:ASN:ND2	2.29	0.66
1:D:493:TYR:O	1:D:727:GLN:NE2	2.29	0.66
1:C:501:ILE:HD11	2:C:801:ADP:C6	2.31	0.66
1:E:265:LYS:HA	1:E:268:LYS:HE2	1.76	0.66
1:B:149:LEU:HD13	1:B:165:ILE:HG12	1.77	0.66
1:D:477:ILE:O	1:D:479:ARG:NH2	2.29	0.66
1:C:377:HIS:NE2	1:C:411:GLN:OE1	2.23	0.66
1:C:473:THR:HG22	1:C:475:GLN:H	1.61	0.66
1:E:444:ASP:OD1	1:E:484:ARG:NH1	2.28	0.66
1:B:478:PRO:HD2	1:B:481:LEU:HD12	1.77	0.65
1:B:592:PRO:HB3	1:B:697:ARG:HA	1.77	0.65
1:E:182:LEU:O	1:E:188:ARG:NH2	2.29	0.65
1:E:525:ALA:HB1	1:E:529:ARG:NH1	2.11	0.65
1:A:475:GLN:HG3	1:A:675:ASP:H	1.61	0.65
1:E:381:LEU:HD22	1:E:390:ILE:HG12	1.78	0.65
1:D:276:MET:HG2	1:D:282:GLU:HB3	1.77	0.65
1:E:685:THR:HG21	1:E:769:LEU:HB3	1.79	0.65
1:B:723:LEU:HD21	1:B:750:VAL:HG22	1.78	0.65
1:C:262:VAL:HG22	1:C:458:VAL:HG11	1.77	0.65
1:A:359:VAL:HG21	1:A:539:GLY:HA3	1.77	0.65
1:A:612:ILE:HG12	1:A:667:VAL:HG22	1.77	0.65
1:D:745:GLU:N	1:D:745:GLU:OE2	2.30	0.65
1:E:96:ASP:HB3	1:E:106:ARG:HB3	1.79	0.65
1:A:600:LEU:HB2	1:A:703:THR:HB	1.78	0.64
1:C:625:LEU:HD13	1:C:629:LEU:HB2	1.79	0.64
1:D:318:ASP:OD1	1:D:319:HIS:N	2.30	0.64
1:A:532:SER:O	1:A:536:ARG:NH2	2.30	0.64
1:A:564:GLU:OE1	1:A:567:ARG:NH1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:694:ARG:NE	1:C:773:GLU:O	2.30	0.64
1:D:318:ASP:OD2	1:D:370:ARG:NH2	2.30	0.64
1:D:443:LEU:HD22	1:D:481:LEU:HD23	1.78	0.64
1:E:445:PRO:HD3	1:E:484:ARG:HH22	1.61	0.64
1:D:444:ASP:HB2	1:D:447:GLN:HE22	1.62	0.64
1:A:417:PRO:HG2	1:A:419:ILE:HD11	1.79	0.64
1:D:503:ARG:HH22	1:D:524:ASP:HA	1.62	0.64
1:E:47:VAL:HG22	1:E:66:GLY:HA3	1.79	0.64
1:E:37:ALA:HB1	1:E:44:ILE:HG12	1.79	0.64
1:A:502:ALA:HB2	1:A:543:LEU:HD21	1.80	0.64
1:C:322:LEU:H	1:C:326:LYS:HE3	1.62	0.64
1:A:443:LEU:HD11	1:A:481:LEU:HD23	1.79	0.64
1:B:510:GLN:NE2	1:B:513:GLU:OE1	2.31	0.63
1:C:253:ILE:HD11	1:C:290:LEU:HD12	1.79	0.63
1:C:388:ALA:HB1	1:C:393:HIS:HA	1.81	0.63
1:D:299:SER:HA	1:D:415:ILE:HD13	1.80	0.63
1:B:714:PRO:HG3	1:B:738:ASP:HB3	1.79	0.63
1:E:173:VAL:HG23	1:E:176:LYS:HD2	1.79	0.63
1:D:336:ARG:HA	1:D:344:VAL:HG11	1.81	0.62
1:B:278:GLN:HA	1:C:397:TYR:HB2	1.80	0.62
1:C:166:ALA:O	1:C:176:LYS:NZ	2.32	0.62
1:E:357:PRO:O	1:E:361:LYS:NZ	2.31	0.62
1:A:59:PRO:HB2	1:A:97:TYR:HB2	1.80	0.62
1:E:332:TYR:OH	1:E:336:ARG:NH2	2.31	0.62
1:A:556:LYS:HD3	1:B:331:GLU:HB3	1.81	0.62
1:B:287:ARG:NH1	1:B:291:ASP:OD1	2.32	0.62
1:E:264:THR:HG22	1:E:268:LYS:HZ3	1.63	0.62
1:E:382:GLY:HA3	1:E:423:GLU:HB3	1.80	0.62
1:E:425:ASP:HB2	1:E:476:THR:HG23	1.80	0.62
1:C:361:LYS:HD3	1:C:470:THR:HG23	1.81	0.62
1:D:503:ARG:HH21	1:D:527:ILE:HG13	1.65	0.62
1:E:393:HIS:HA	1:E:454:HIS:HB2	1.80	0.62
1:A:501:ILE:HD13	2:A:801:ADP:C2	2.35	0.62
1:E:493:TYR:O	1:E:727:GLN:NE2	2.32	0.62
1:B:559:LEU:HD21	1:C:337:GLN:OE1	1.99	0.62
1:A:336:ARG:HH22	1:A:344:VAL:HA	1.63	0.61
1:E:598:GLN:NE2	1:E:610:LEU:O	2.32	0.61
1:A:73:GLN:HB2	1:A:85:MET:HB2	1.82	0.61
1:C:391:ARG:HG2	1:C:453:ASP:HA	1.81	0.61
1:D:444:ASP:HB2	1:D:447:GLN:NE2	2.14	0.61
1:E:720:GLU:HA	1:E:723:LEU:HD12	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:ASN:ND2	1:A:726:HIS:O	2.32	0.61
1:B:391:ARG:HH21	1:B:454:HIS:CD2	2.18	0.61
1:B:498:LYS:HA	1:B:501:ILE:HD12	1.83	0.61
1:A:494:THR:HG21	1:A:750:VAL:HG22	1.82	0.61
1:B:479:ARG:HD2	1:B:482:LEU:HD12	1.83	0.61
1:A:440:LEU:HD11	1:A:480:PRO:HB2	1.81	0.61
1:B:359:VAL:HG13	1:B:493:TYR:CE2	2.36	0.61
1:B:378:ARG:NH1	1:B:422:ASP:OD2	2.33	0.61
1:C:51:ASP:HB3	1:C:52:PRO:HD3	1.82	0.61
1:E:93:GLN:NE2	1:E:108:GLU:OE1	2.34	0.61
1:E:136:VAL:O	1:E:143:ARG:NH2	2.24	0.61
1:C:378:ARG:NH1	1:C:422:ASP:OD2	2.33	0.61
1:E:626:THR:OG1	1:E:665:VAL:O	2.17	0.61
1:E:29:LYS:HD3	1:E:101:PRO:HG2	1.83	0.60
1:E:444:ASP:O	1:E:448:ASN:N	2.32	0.60
1:E:479:ARG:HD2	1:E:482:LEU:HD12	1.82	0.60
1:C:98:ILE:HG13	1:C:106:ARG:HH12	1.66	0.60
1:E:76:ARG:HG3	1:E:78:PRO:HD3	1.83	0.60
1:A:202:ARG:HA	1:D:222:ARG:NH1	2.16	0.60
1:B:392:GLY:N	1:B:453:ASP:OD1	2.34	0.60
1:D:256:VAL:HG13	1:D:300:LYS:HZ1	1.67	0.60
1:D:694:ARG:HE	1:D:772:PRO:HB2	1.65	0.60
1:E:179:ILE:HG13	1:E:182:LEU:HD12	1.83	0.60
1:C:493:TYR:O	1:C:494:THR:OG1	2.14	0.60
1:A:499:GLN:HE21	1:A:524:ASP:HB3	1.67	0.60
1:B:59:PRO:HD3	1:B:103:LEU:HG	1.82	0.60
1:C:305:VAL:HB	1:C:372:MET:HA	1.84	0.60
1:D:115:PRO:HB2	1:D:118:GLU:HG2	1.83	0.60
1:D:358:GLY:N	2:D:801:ADP:O3B	2.33	0.60
1:D:379:ILE:HG21	1:D:408:ALA:HB2	1.83	0.60
1:C:667:VAL:HG12	1:C:669:ASP:H	1.67	0.60
1:D:603:THR:OG1	1:D:606:GLY:O	2.20	0.60
1:E:521:GLU:HB3	1:E:568:THR:HA	1.84	0.60
1:D:42:ARG:HB3	1:D:71:VAL:HB	1.83	0.59
1:E:59:PRO:HB3	1:E:97:TYR:HB3	1.83	0.59
1:E:65:TRP:HB2	1:E:181:GLU:HG2	1.84	0.59
1:E:311:THR:HA	1:E:371:SER:HB2	1.84	0.59
1:D:272:ARG:HG2	1:D:275:ARG:HH21	1.67	0.59
1:E:679:ALA:HB1	1:E:682:THR:HB	1.84	0.59
1:A:552:ARG:HD3	1:B:335:VAL:HG11	1.85	0.59
1:B:346:ASN:ND2	1:B:443:LEU:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:493:TYR:O	1:B:494:THR:OG1	2.19	0.59
1:C:590:THR:O	1:C:591:GLU:HG2	2.02	0.59
1:D:63:TYR:O	1:D:97:TYR:OH	2.20	0.59
1:B:771:LEU:HB2	1:B:772:PRO:HD3	1.83	0.59
1:E:15:ILE:HG13	1:E:46:LEU:HD13	1.83	0.59
1:E:537:GLU:HG3	1:E:539:GLY:H	1.67	0.59
1:A:493:TYR:O	1:A:727:GLN:NE2	2.35	0.59
1:E:619:GLY:N	1:E:660:LYS:O	2.36	0.59
1:B:520:ILE:HD11	1:B:569:ILE:HD11	1.83	0.59
1:D:304:GLU:OE1	1:D:374:ARG:NH2	2.35	0.59
1:A:328:ARG:HH22	1:A:489:GLU:H	1.50	0.59
1:D:614:VAL:HG12	1:D:665:VAL:HG12	1.85	0.59
1:A:747:PRO:HB2	1:A:749:GLU:HG2	1.83	0.59
1:E:614:VAL:HG22	1:E:665:VAL:HG22	1.85	0.59
1:E:737:LYS:HA	1:E:758:LEU:HD12	1.85	0.59
1:D:422:ASP:HA	1:D:470:THR:HB	1.85	0.58
1:A:440:LEU:HD13	1:A:443:LEU:HD12	1.84	0.58
1:B:226:LEU:HD21	1:E:205:LEU:HD21	1.84	0.58
1:C:440:LEU:HD22	1:C:480:PRO:HB2	1.83	0.58
1:E:494:THR:HG21	1:E:750:VAL:HG13	1.85	0.58
1:E:277:GLN:HG3	1:E:287:ARG:HD2	1.84	0.58
1:B:319:HIS:O	1:B:321:GLY:N	2.36	0.58
1:E:264:THR:HA	1:E:267:LEU:HD12	1.85	0.58
1:B:2:ARG:HB3	1:B:106:ARG:HG3	1.85	0.58
1:B:757:LYS:HD2	1:B:768:TYR:HD2	1.66	0.58
1:D:73:GLN:HG3	1:D:85:MET:HE3	1.85	0.58
1:E:602:TRP:NE1	1:E:720:GLU:OE1	2.37	0.58
1:A:422:ASP:HA	1:A:470:THR:HB	1.86	0.58
1:C:37:ALA:HB1	1:C:44:ILE:HG12	1.86	0.58
1:C:552:ARG:HD3	1:D:335:VAL:HG21	1.85	0.58
1:D:537:GLU:OE2	1:D:542:GLY:N	2.36	0.58
1:A:59:PRO:HG3	1:A:99:PRO:HA	1.83	0.58
1:A:427:MET:HG3	1:A:436:ALA:HB2	1.84	0.58
1:D:532:SER:O	1:D:536:ARG:NH2	2.37	0.58
1:C:499:GLN:HE21	1:C:528:LEU:HB2	1.69	0.58
1:B:340:GLN:O	1:B:345:ARG:NH1	2.37	0.58
1:C:299:SER:HA	1:C:415:ILE:HD13	1.85	0.58
1:E:62:LEU:HB2	1:E:97:TYR:HE2	1.69	0.58
1:A:25:VAL:HG22	1:A:82:LEU:H	1.68	0.57
1:A:175:GLU:OE1	1:A:198:ARG:NH2	2.37	0.57
1:B:332:TYR:HE1	1:B:466:PHE:HE1	1.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:644:LEU:HD21	1:C:688:ALA:HA	1.84	0.57
1:E:17:PRO:HB3	1:E:90:ALA:HA	1.86	0.57
1:A:643:TYR:HD2	1:A:644:LEU:HD22	1.68	0.57
1:D:401:MET:HG2	1:D:402:PRO:O	2.04	0.57
1:B:292:TRP:CE3	1:B:402:PRO:HG2	2.39	0.57
1:B:499:GLN:NE2	1:B:524:ASP:HB2	2.19	0.57
1:D:417:PRO:HD2	1:D:465:VAL:HG22	1.86	0.57
1:B:418:VAL:HG22	1:B:466:PHE:HD2	1.68	0.57
1:E:558:TRP:HD1	1:E:567:ARG:HH12	1.50	0.57
1:B:307:ASP:OD1	1:B:308:ILE:N	2.37	0.57
1:A:375:LYS:HG3	1:A:412:VAL:HG21	1.85	0.57
1:A:587:LYS:HG3	1:A:728:ALA:HB1	1.85	0.57
1:B:632:VAL:HB	1:B:677:PRO:HD3	1.87	0.57
1:E:378:ARG:NH2	1:E:422:ASP:OD2	2.38	0.57
1:A:387:GLU:HG2	1:A:431:TRP:HD1	1.68	0.57
1:D:350:ILE:HD11	1:D:443:LEU:HD12	1.87	0.57
1:E:514:SER:HB2	1:E:551:ALA:HB1	1.87	0.57
1:B:722:LEU:HD12	1:B:746:LEU:HD12	1.87	0.57
1:D:722:LEU:HD21	1:D:735:LEU:HD11	1.86	0.57
1:E:377:HIS:ND1	1:E:411:GLN:OE1	2.37	0.57
1:D:6:PRO:HA	1:D:104:ARG:HD2	1.87	0.56
1:A:530:VAL:HA	1:A:534:TYR:HD2	1.70	0.56
1:B:614:VAL:HG21	1:B:687:ILE:HD13	1.87	0.56
1:B:662:ASP:O	1:B:663:LEU:HD23	2.06	0.56
1:E:26:GLY:HA2	1:E:81:THR:HA	1.87	0.56
1:B:663:LEU:HD21	1:B:691:LEU:HD21	1.86	0.56
1:C:393:HIS:CE1	1:D:432:ARG:HE	2.23	0.56
1:C:421:LEU:HD12	1:C:469:THR:HG22	1.86	0.56
1:E:16:LEU:HD23	1:E:180:LEU:HD12	1.87	0.56
1:E:510:GLN:HA	1:E:513:GLU:HB2	1.86	0.56
1:A:533:GLU:HB3	1:A:581:PRO:HB3	1.86	0.56
1:D:47:VAL:HG11	1:D:62:LEU:HB3	1.88	0.56
1:D:631:GLU:O	1:D:635:GLU:HG2	2.05	0.56
1:B:377:HIS:NE2	1:B:411:GLN:OE1	2.29	0.56
1:B:473:THR:HG23	1:B:673:PRO:HB3	1.88	0.56
1:C:67:VAL:HG23	1:C:91:ARG:HA	1.88	0.56
1:D:401:MET:CE	1:E:432:ARG:HB3	2.36	0.56
1:A:4:GLU:O	1:A:104:ARG:NH1	2.38	0.56
1:C:574:ILE:O	1:C:578:LEU:N	2.28	0.56
1:D:552:ARG:HG2	1:E:335:VAL:HG21	1.85	0.56
1:A:340:GLN:NE2	1:A:343:ASP:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:705:GLU:O	1:D:712:VAL:HA	2.06	0.56
1:A:300:LYS:H	1:A:415:ILE:HG12	1.71	0.56
1:A:394:ARG:HH11	1:A:396:THR:HG22	1.71	0.56
1:D:4:GLU:HG2	1:D:106:ARG:HG2	1.88	0.56
1:B:614:VAL:HG23	1:B:665:VAL:HG22	1.88	0.56
1:C:307:ASP:OD1	1:C:310:HIS:N	2.30	0.56
1:E:391:ARG:NE	1:E:438:ALA:HB2	2.21	0.56
1:A:640:ALA:HB1	1:A:684:ALA:HA	1.88	0.55
1:B:245:ASP:C	1:B:247:GLU:H	2.09	0.55
1:C:259:PRO:HB2	1:C:262:VAL:HG23	1.87	0.55
1:B:499:GLN:HE21	1:B:524:ASP:HB2	1.71	0.55
1:C:537:GLU:CG	1:C:538:ALA:H	2.18	0.55
1:A:444:ASP:OD1	1:A:484:ARG:NH1	2.40	0.55
1:B:354:VAL:HG21	1:B:474:LEU:HB3	1.87	0.55
1:C:737:LYS:HB3	1:C:760:GLU:HG2	1.89	0.55
1:A:213:VAL:O	1:A:217:MET:HG2	2.06	0.55
1:B:629:LEU:HD13	1:B:670:GLY:HA3	1.88	0.55
1:C:139:HIS:ND1	1:C:144:LEU:HB2	2.21	0.55
1:C:492:GLY:HA3	1:C:727:GLN:NE2	2.20	0.55
1:E:336:ARG:HD2	1:E:344:VAL:HG13	1.88	0.55
1:A:393:HIS:HD2	1:A:400:ALA:HA	1.71	0.55
1:A:630:GLY:H	1:A:671:ALA:HB2	1.71	0.55
1:B:626:THR:HG22	1:B:627:GLY:H	1.72	0.55
1:E:77:LEU:HD12	1:E:83:GLN:HB3	1.88	0.55
1:A:559:LEU:HD11	1:B:338:LEU:HG	1.89	0.55
1:A:719:LYS:O	1:A:723:LEU:HG	2.06	0.55
1:B:256:VAL:HG12	1:B:298:TRP:HB2	1.89	0.55
1:E:483:ASP:OD1	1:E:484:ARG:N	2.40	0.55
1:B:222:ARG:HB2	1:E:198:ARG:HH12	1.72	0.55
1:C:499:GLN:NE2	1:C:528:LEU:HB2	2.22	0.55
1:D:529:ARG:NH1	1:D:571:ALA:O	2.40	0.55
1:A:249:LEU:O	1:A:253:ILE:HG13	2.07	0.55
1:A:388:ALA:HB1	1:A:393:HIS:HA	1.89	0.55
1:A:584:ARG:NH2	1:A:589:GLU:OE2	2.39	0.55
1:A:202:ARG:HA	1:D:222:ARG:HH12	1.72	0.54
1:A:537:GLU:OE1	1:A:542:GLY:N	2.31	0.54
1:A:730:ILE:HB	1:A:733:ILE:HD11	1.89	0.54
1:B:319:HIS:HE1	1:B:364:LEU:HA	1.72	0.54
1:D:590:THR:O	1:D:591:GLU:HG3	2.07	0.54
1:A:205:LEU:HB3	1:D:222:ARG:NH1	2.22	0.54
1:B:199:ASP:OD1	1:B:202:ARG:NH2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:757:LYS:HD2	1:B:768:TYR:CD2	2.42	0.54
1:C:559:LEU:HD21	1:D:337:GLN:OE1	2.07	0.54
1:D:7:VAL:HG22	1:D:45:PHE:HB2	1.89	0.54
1:D:478:PRO:HD2	1:D:481:LEU:HD12	1.88	0.54
1:A:227:ARG:O	1:A:231:LYS:HG2	2.07	0.54
1:A:333:LEU:HA	1:A:336:ARG:HG2	1.89	0.54
1:A:427:MET:HG2	1:A:435:PRO:HG2	1.90	0.54
1:B:185:LEU:HD22	1:B:188:ARG:HH21	1.71	0.54
1:B:402:PRO:HG3	1:B:455:TYR:CD1	2.41	0.54
1:B:445:PRO:O	1:B:449:ASN:ND2	2.23	0.54
1:D:699:ASP:OD2	1:D:732:LYS:NZ	2.39	0.54
1:E:354:VAL:O	1:E:490:ILE:N	2.36	0.54
1:E:541:ARG:HB3	1:E:545:ARG:HH12	1.71	0.54
1:B:136:VAL:HG21	1:B:146:ARG:HG3	1.89	0.54
1:D:522:VAL:HG22	1:D:569:ILE:HB	1.89	0.54
1:D:701:ALA:H	1:D:730:ILE:HG21	1.71	0.54
1:C:5:LEU:HB2	1:C:45:PHE:CD2	2.42	0.54
1:E:134:LYS:O	1:E:138:ASN:HB2	2.08	0.54
1:E:516:MET:HB2	1:E:519:ARG:HD3	1.90	0.54
1:B:593:GLN:HE21	1:B:596:THR:HB	1.71	0.54
1:E:538:ALA:HA	1:E:727:GLN:HE22	1.73	0.54
1:A:226:LEU:HD22	1:B:233:ILE:HG23	1.89	0.54
1:A:526:ALA:HB1	1:A:574:ILE:HD11	1.90	0.54
1:D:295:GLU:OE1	1:D:410:LYS:NZ	2.28	0.54
1:E:705:GLU:HB2	1:E:713:MET:HB2	1.90	0.54
1:A:478:PRO:HD2	1:A:481:LEU:HD12	1.89	0.54
1:C:503:ARG:NH1	1:C:522:VAL:O	2.40	0.54
1:D:507:TRP:HH2	1:D:521:GLU:HA	1.73	0.54
1:E:14:VAL:HG22	1:E:48:ALA:HB3	1.89	0.54
1:E:68:GLN:NE2	1:E:108:GLU:O	2.40	0.54
1:A:191:LYS:HE2	1:A:195:LEU:HD11	1.90	0.53
1:D:74:ALA:HB1	1:D:84:VAL:HG22	1.88	0.53
1:A:387:GLU:HG2	1:A:431:TRP:CD1	2.43	0.53
1:B:328:ARG:O	1:B:331:GLU:HG2	2.09	0.53
1:C:625:LEU:HB3	1:C:629:LEU:HD12	1.91	0.53
1:B:115:PRO:HG2	1:B:185:LEU:HB2	1.90	0.53
1:E:275:ARG:O	1:E:277:GLN:NE2	2.42	0.53
1:E:421:LEU:HB2	1:E:469:THR:HG23	1.90	0.53
1:B:616:ALA:HB2	1:B:690:ALA:HB1	1.91	0.53
1:C:42:ARG:HD2	1:C:71:VAL:HB	1.91	0.53
1:D:358:GLY:H	2:D:801:ADP:PB	2.31	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:179:ILE:O	1:E:188:ARG:NH1	2.41	0.53
1:E:625:LEU:HD22	1:E:629:LEU:HD12	1.90	0.53
1:C:129:LYS:HE2	1:C:152:VAL:HG23	1.90	0.53
1:C:425:ASP:OD2	1:C:471:ALA:HB1	2.08	0.53
1:D:714:PRO:HB3	1:D:738:ASP:HB2	1.91	0.53
1:A:108:GLU:HG2	1:A:109:VAL:H	1.73	0.53
1:D:227:ARG:HA	1:D:230:MET:HG3	1.91	0.53
1:B:143:ARG:HG2	1:B:144:LEU:N	2.23	0.53
1:D:276:MET:SD	1:D:277:GLN:N	2.81	0.53
1:E:510:GLN:HG3	1:E:547:LEU:HB3	1.90	0.53
1:B:440:LEU:HD13	1:B:480:PRO:HB2	1.90	0.53
1:C:412:VAL:HG21	1:C:417:PRO:HB3	1.89	0.53
1:A:614:VAL:HG11	1:A:687:ILE:HD13	1.91	0.53
1:E:33:ALA:HB2	1:E:102:TYR:HB2	1.89	0.53
1:B:140:LYS:HD2	1:E:190:LYS:HG3	1.91	0.52
1:C:321:GLY:HA2	1:C:326:LYS:NZ	2.23	0.52
1:D:247:GLU:OE2	1:D:251:LYS:NZ	2.33	0.52
1:D:491:PRO:HB2	1:D:723:LEU:HD12	1.91	0.52
1:B:302:ASP:H	1:B:416:ASN:HD21	1.57	0.52
1:B:626:THR:OG1	1:B:664:HIS:NE2	2.41	0.52
1:C:393:HIS:HE2	1:C:397:TYR:HH	1.47	0.52
1:E:44:ILE:O	1:E:69:ALA:N	2.42	0.52
1:A:354:VAL:HG11	1:A:474:LEU:HB3	1.92	0.52
1:B:390:ILE:HD13	1:B:435:PRO:HB3	1.90	0.52
1:D:702:MET:HE3	1:D:769:LEU:HD21	1.91	0.52
1:E:51:ASP:HB3	1:E:52:PRO:HD3	1.91	0.52
1:E:302:ASP:HB3	1:E:373:ASN:O	2.10	0.52
1:A:473:THR:HG22	1:A:475:GLN:H	1.74	0.52
1:C:98:ILE:HB	1:C:104:ARG:HB2	1.92	0.52
1:E:314:VAL:HB	1:E:371:SER:HB3	1.92	0.52
1:A:594:VAL:HG22	1:A:695:PRO:HA	1.92	0.52
1:C:521:GLU:HG2	1:C:566:LEU:HD11	1.92	0.52
1:E:381:LEU:HD12	1:E:421:LEU:HB3	1.91	0.52
1:D:222:ARG:NH2	1:D:225:TYR:HD2	2.07	0.52
1:D:580:ILE:HD13	1:E:745:GLU:HG2	1.92	0.52
1:C:526:ALA:HB2	1:C:570:ASP:HA	1.92	0.52
1:D:37:ALA:HA	1:D:40:ALA:HB3	1.92	0.52
1:B:389:GLU:O	1:B:404:LYS:N	2.31	0.52
1:D:547:LEU:HD23	1:D:550:ILE:HD12	1.90	0.52
1:E:223:GLU:HB3	1:E:227:ARG:HH21	1.75	0.52
1:E:391:ARG:HD2	1:E:435:PRO:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:659:ASN:OD1	1:C:660:LYS:N	2.43	0.51
1:D:628:GLN:HE22	1:E:631:GLU:HG2	1.74	0.51
1:B:737:LYS:O	1:B:740:GLU:HB2	2.11	0.51
1:C:125:VAL:HG21	1:C:158:PRO:HB3	1.92	0.51
1:C:135:TYR:HA	1:C:200:LEU:HD21	1.92	0.51
1:E:67:VAL:HG13	1:E:180:LEU:HD11	1.93	0.51
1:A:349:PRO:HB3	1:A:486:GLU:N	2.26	0.51
1:A:700:ILE:HD12	1:A:732:LYS:HD3	1.93	0.51
1:C:277:GLN:NE2	1:C:287:ARG:HE	2.08	0.51
1:E:264:THR:HG22	1:E:268:LYS:NZ	2.25	0.51
1:E:347:LYS:H	1:E:445:PRO:HG3	1.75	0.51
1:B:353:LEU:HD23	1:B:488:ILE:HB	1.92	0.51
1:D:663:LEU:HD11	1:D:691:LEU:HD11	1.91	0.51
1:D:261:ALA:O	1:D:264:THR:OG1	2.20	0.51
1:D:440:LEU:HD11	1:D:480:PRO:HB2	1.93	0.51
1:D:689:SER:O	1:D:693:ARG:N	2.44	0.51
1:D:707:SER:O	1:D:710:GLY:N	2.37	0.51
1:E:91:ARG:NH2	1:E:163:ASP:OD2	2.38	0.51
1:E:473:THR:HG22	1:E:475:GLN:H	1.76	0.51
1:C:393:HIS:O	1:C:395:ARG:N	2.44	0.51
1:C:567:ARG:HG2	1:C:568:THR:H	1.76	0.51
1:D:284:THR:HG22	1:D:287:ARG:HH12	1.74	0.51
1:E:322:LEU:HD11	1:E:364:LEU:HD21	1.91	0.51
1:E:602:TRP:CD1	1:E:720:GLU:HB3	2.46	0.51
1:B:136:VAL:HA	1:B:139:HIS:CD2	2.45	0.51
1:B:265:LYS:HD2	1:B:458:VAL:HG22	1.92	0.51
1:B:329:ILE:HG21	1:B:368:ILE:HD11	1.92	0.51
1:B:599:GLY:O	1:B:610:LEU:N	2.44	0.51
1:D:319:HIS:O	1:D:321:GLY:N	2.43	0.51
1:C:759:VAL:HG23	1:C:764:GLU:HB2	1.93	0.51
1:A:538:ALA:HB2	1:A:606:GLY:HA3	1.93	0.51
1:A:552:ARG:HE	1:B:335:VAL:HG21	1.76	0.51
1:A:737:LYS:HA	1:A:758:LEU:HD22	1.93	0.51
1:B:381:LEU:HD11	1:B:421:LEU:HD22	1.93	0.51
1:C:361:LYS:N	2:C:801:ADP:O1A	2.44	0.51
1:C:510:GLN:HE21	1:C:544:GLU:HG2	1.76	0.51
1:E:661:VAL:HG11	1:E:691:LEU:HD21	1.93	0.51
1:A:725:ALA:O	1:A:729:GLY:N	2.44	0.51
1:B:47:VAL:HB	1:B:62:LEU:HD22	1.93	0.51
1:C:24:ASP:OD1	1:C:83:GLN:NE2	2.35	0.51
1:B:9:PRO:HG2	1:B:27:ARG:HH22	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:ASP:HB2	1:C:106:ARG:HG3	1.93	0.50
1:C:507:TRP:HH2	1:C:521:GLU:HA	1.76	0.50
1:E:124:LEU:HD21	1:E:190:LYS:HG2	1.92	0.50
1:E:339:THR:H	1:E:342:LEU:HA	1.76	0.50
1:E:478:PRO:HD2	1:E:481:LEU:HD12	1.91	0.50
1:E:574:ILE:HG22	1:E:575:PRO:HD3	1.92	0.50
1:E:302:ASP:O	1:E:416:ASN:ND2	2.41	0.50
1:E:509:LYS:HA	1:E:512:ARG:HH21	1.76	0.50
1:B:76:ARG:HD3	1:B:82:LEU:HD22	1.93	0.50
1:C:352:VAL:HG13	1:C:487:VAL:HA	1.92	0.50
1:C:499:GLN:HE21	1:C:528:LEU:HD13	1.75	0.50
1:E:386:ASP:HA	1:E:431:TRP:HD1	1.77	0.50
1:A:250:ARG:HA	1:A:253:ILE:HD12	1.93	0.50
1:B:603:THR:OG1	1:B:606:GLY:O	2.25	0.50
1:A:353:LEU:HB3	1:A:361:LYS:HG2	1.92	0.50
1:D:429:SER:HB2	1:D:435:PRO:HD2	1.93	0.50
1:D:609:LEU:HD23	1:D:728:ALA:HB1	1.93	0.50
1:E:258:MET:SD	1:E:298:TRP:NE1	2.77	0.50
1:A:439:MET:O	1:A:443:LEU:HG	2.11	0.50
1:B:481:LEU:HB3	1:B:485:MET:HE1	1.93	0.50
1:B:534:TYR:HB3	1:B:546:GLU:OE1	2.12	0.50
1:A:135:TYR:HE1	1:A:199:ASP:HB3	1.76	0.50
1:A:136:VAL:HB	1:A:149:LEU:HD11	1.94	0.50
1:B:538:ALA:HB2	1:B:607:GLY:H	1.76	0.50
1:B:563:TRP:HD1	1:B:564:GLU:HG3	1.77	0.50
1:C:11:ARG:NH1	1:C:22:PRO:O	2.43	0.50
1:D:69:ALA:HA	1:D:88:ALA:HA	1.93	0.50
1:D:501:ILE:HG22	1:D:506:LEU:HG	1.93	0.50
1:C:570:ASP:OD1	1:C:570:ASP:N	2.45	0.50
1:D:531:ILE:HG12	1:D:543:LEU:HD11	1.94	0.50
1:A:301:ALA:HA	1:A:416:ASN:HD21	1.77	0.50
1:C:708:LEU:HD12	1:C:708:LEU:H	1.76	0.50
1:D:702:MET:HE1	1:D:769:LEU:HD11	1.93	0.50
1:A:7:VAL:HG13	1:A:47:VAL:H	1.76	0.49
1:A:598:GLN:HE22	1:A:609:LEU:HD12	1.77	0.49
1:D:352:VAL:HA	1:D:469:THR:HB	1.94	0.49
1:E:250:ARG:HH21	1:E:270:LEU:HB3	1.77	0.49
1:A:95:THR:HB	1:A:106:ARG:HB2	1.94	0.49
1:A:391:ARG:HB3	1:A:453:ASP:HA	1.93	0.49
1:A:552:ARG:NE	1:B:335:VAL:HG21	2.27	0.49
1:B:391:ARG:NH1	1:B:441:GLU:OE2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:614:VAL:HG23	1:D:690:ALA:HB2	1.93	0.49
1:E:498:LYS:HA	1:E:501:ILE:HG12	1.94	0.49
1:A:323:LYS:HA	1:A:326:LYS:HD3	1.95	0.49
1:B:178:GLU:HG2	1:B:191:LYS:HZ2	1.76	0.49
1:D:25:VAL:HB	1:D:82:LEU:HB2	1.95	0.49
1:D:302:ASP:HB2	1:D:416:ASN:HD21	1.76	0.49
1:E:569:ILE:HG12	1:E:577:TYR:CE2	2.47	0.49
1:E:621:GLY:N	1:E:662:ASP:OD1	2.45	0.49
1:E:694:ARG:HG3	1:E:770:LEU:HD22	1.95	0.49
1:A:700:ILE:HB	1:A:769:LEU:HD13	1.94	0.49
1:B:13:THR:HB	1:B:176:LYS:HG3	1.94	0.49
1:C:308:ILE:HD11	1:C:330:LEU:HB3	1.94	0.49
1:D:148:GLN:HA	1:D:151:ALA:HB3	1.94	0.49
1:D:679:ALA:HB1	1:D:682:THR:HB	1.94	0.49
1:E:2:ARG:HH21	1:E:108:GLU:HG2	1.77	0.49
1:A:269:GLU:OE1	1:A:272:ARG:NH1	2.45	0.49
1:C:529:ARG:NH1	1:C:533:GLU:OE2	2.45	0.49
1:D:575:PRO:O	1:D:579:GLY:N	2.46	0.49
1:E:69:ALA:HA	1:E:88:ALA:HA	1.94	0.49
1:D:253:ILE:O	1:D:263:LYS:NZ	2.45	0.49
1:B:7:VAL:HB	1:B:103:LEU:HB3	1.94	0.49
1:C:702:MET:HE1	1:C:769:LEU:HD13	1.95	0.49
1:E:349:PRO:HB2	1:E:351:LEU:HD23	1.94	0.49
1:A:666:HIS:HB2	1:B:708:LEU:HD12	1.95	0.49
1:C:629:LEU:HD21	1:C:667:VAL:HB	1.94	0.49
1:D:223:GLU:HG2	1:D:227:ARG:NE	2.28	0.49
1:D:548:GLY:O	1:D:552:ARG:HG3	2.12	0.49
1:E:702:MET:SD	1:E:769:LEU:HD22	2.52	0.49
1:B:441:GLU:HA	1:B:447:GLN:HG2	1.94	0.49
1:B:642:THR:HA	1:B:645:ARG:HG2	1.94	0.49
1:C:392:GLY:HA3	1:C:455:TYR:H	1.77	0.49
1:E:31:LYS:HZ2	1:E:82:LEU:HB2	1.78	0.49
1:A:492:GLY:H	1:A:720:GLU:HG2	1.77	0.48
1:B:284:THR:HA	1:C:396:THR:HG21	1.95	0.48
1:E:328:ARG:HA	1:E:331:GLU:HG3	1.95	0.48
1:A:629:LEU:HD22	1:A:633:MET:HG3	1.95	0.48
1:B:602:TRP:CD1	1:B:720:GLU:HG2	2.47	0.48
1:E:277:GLN:O	1:E:284:THR:OG1	2.19	0.48
1:E:297:PRO:HG2	1:E:413:GLY:HA3	1.95	0.48
1:A:166:ALA:HB1	1:A:179:ILE:HD13	1.94	0.48
1:A:245:ASP:HB2	1:B:275:ARG:HH12	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:622:LYS:HG2	1:B:623:LEU:H	1.78	0.48
1:C:311:THR:HA	1:C:371:SER:HB2	1.95	0.48
1:C:393:HIS:NE2	1:C:397:TYR:OH	2.33	0.48
1:D:522:VAL:HG13	1:D:526:ALA:HB3	1.96	0.48
1:C:273:LEU:HD23	1:C:273:LEU:HA	1.74	0.48
1:D:743:LEU:HD11	1:D:758:LEU:HD21	1.95	0.48
1:E:149:LEU:HD11	1:E:161:LEU:HD22	1.95	0.48
1:A:224:TYR:HA	1:A:227:ARG:HG2	1.96	0.48
1:D:590:THR:H	1:D:698:MET:HE1	1.78	0.48
1:E:534:TYR:HB3	1:E:546:GLU:CD	2.32	0.48
1:A:656:ASP:OD1	1:A:656:ASP:N	2.47	0.48
1:C:280:SER:OG	1:C:282:GLU:OE2	2.31	0.48
1:B:424:ILE:HG22	1:B:471:ALA:HB2	1.96	0.48
1:C:510:GLN:NE2	1:C:544:GLU:O	2.47	0.48
1:C:592:PRO:HB2	1:C:695:PRO:HB2	1.96	0.48
1:D:401:MET:HE1	1:E:432:ARG:HD2	1.95	0.48
1:E:516:MET:HG3	1:E:519:ARG:HB2	1.95	0.48
1:A:319:HIS:CE1	1:A:364:LEU:HD22	2.49	0.48
1:C:44:ILE:O	1:C:69:ALA:N	2.47	0.48
1:C:702:MET:CE	1:C:769:LEU:HD13	2.44	0.48
1:D:57:PRO:HB2	1:D:103:LEU:HG	1.96	0.48
1:E:379:ILE:HB	1:E:404:LYS:HB3	1.96	0.48
1:A:602:TRP:CD1	1:A:674:LYS:HD3	2.49	0.48
1:B:723:LEU:O	1:B:727:GLN:HG2	2.14	0.48
1:B:733:ILE:HD11	1:B:754:LEU:HD23	1.96	0.48
1:E:246:LEU:HD13	1:E:273:LEU:HB2	1.95	0.48
1:A:596:THR:HG22	1:A:613:GLU:HA	1.95	0.47
1:B:663:LEU:HD13	1:B:687:ILE:HD12	1.96	0.47
1:B:17:PRO:HG3	1:B:91:ARG:HH21	1.79	0.47
1:C:325:VAL:O	1:C:329:ILE:HD12	2.14	0.47
1:D:5:LEU:HD13	1:D:43:LEU:HB3	1.97	0.47
1:E:345:ARG:HH21	1:E:347:LYS:HD3	1.79	0.47
1:E:394:ARG:HA	1:E:455:TYR:HA	1.94	0.47
1:B:253:ILE:HG22	1:B:254:GLU:HG3	1.97	0.47
1:B:275:ARG:HG2	1:B:276:MET:SD	2.55	0.47
1:A:11:ARG:NH2	1:A:27:ARG:HE	2.12	0.47
1:A:50:ARG:HG2	1:A:51:ASP:N	2.29	0.47
1:A:683:MET:O	1:A:687:ILE:HG12	2.15	0.47
1:B:511:VAL:HG12	1:B:516:MET:O	2.15	0.47
1:C:498:LYS:O	1:C:501:ILE:HG22	2.14	0.47
1:D:379:ILE:O	1:D:379:ILE:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:62:LEU:HB2	1:E:97:TYR:CE2	2.48	0.47
1:A:522:VAL:HG12	1:A:527:ILE:HG12	1.95	0.47
1:C:187:ALA:O	1:C:190:LYS:HG3	2.14	0.47
1:D:694:ARG:HB3	1:D:772:PRO:HG2	1.95	0.47
1:C:49:GLN:NE2	1:C:53:GLU:OE2	2.30	0.47
1:C:359:VAL:O	1:C:361:LYS:N	2.46	0.47
1:C:526:ALA:HA	1:C:574:ILE:HD11	1.95	0.47
1:C:757:LYS:NZ	1:C:768:TYR:O	2.48	0.47
1:D:91:ARG:HE	1:D:180:LEU:HD12	1.78	0.47
1:D:308:ILE:HB	1:D:330:LEU:HD22	1.96	0.47
1:D:723:LEU:HD23	1:D:723:LEU:HA	1.75	0.47
1:E:302:ASP:N	1:E:416:ASN:OD1	2.38	0.47
1:A:205:LEU:HD22	1:D:222:ARG:NH2	2.30	0.47
1:A:474:LEU:HD23	1:A:474:LEU:H	1.80	0.47
1:B:54:VAL:HG12	1:B:56:ASP:H	1.79	0.47
1:B:640:ALA:HB1	1:B:684:ALA:HA	1.97	0.47
1:B:685:THR:HG21	1:B:702:MET:HE1	1.96	0.47
1:D:697:ARG:HB2	1:D:769:LEU:HA	1.95	0.47
1:C:292:TRP:HH2	1:C:407:HIS:CD2	2.33	0.47
1:C:641:LEU:HD12	1:C:657:PHE:HE1	1.80	0.47
1:E:292:TRP:HE1	1:E:407:HIS:HA	1.80	0.47
1:C:151:ALA:O	1:C:155:THR:OG1	2.32	0.47
1:C:649:GLN:NE2	1:C:650:ASP:OD1	2.48	0.47
1:A:212:ARG:O	1:A:216:GLN:HG2	2.15	0.47
1:D:507:TRP:CH2	1:D:521:GLU:HA	2.50	0.47
1:E:31:LYS:HZ1	1:E:82:LEU:HD12	1.78	0.47
1:E:224:TYR:O	1:E:227:ARG:HG2	2.15	0.47
1:E:697:ARG:HB3	1:E:700:ILE:HD12	1.95	0.47
1:A:420:LEU:HA	1:A:468:ILE:HG23	1.98	0.46
1:A:479:ARG:O	1:A:479:ARG:NH1	2.40	0.46
1:B:769:LEU:O	1:B:770:LEU:HD23	2.15	0.46
1:C:529:ARG:O	1:C:533:GLU:HB2	2.15	0.46
1:E:700:ILE:HA	1:E:732:LYS:HB2	1.97	0.46
1:A:461:ASP:OD1	1:A:461:ASP:N	2.48	0.46
1:B:631:GLU:O	1:B:634:LYS:N	2.48	0.46
1:C:262:VAL:HG22	1:C:458:VAL:CG1	2.45	0.46
1:C:384:VAL:HG13	1:C:389:GLU:OE2	2.16	0.46
1:C:595:GLY:HA3	1:D:709:ARG:HD2	1.98	0.46
1:D:361:LYS:HD2	1:D:470:THR:HG23	1.97	0.46
1:D:388:ALA:HB1	1:D:393:HIS:CD2	2.49	0.46
1:D:590:THR:OG1	1:D:591:GLU:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:ASN:HB2	1:A:726:HIS:CE1	2.51	0.46
1:B:65:TRP:CE2	1:B:181:GLU:HA	2.49	0.46
1:B:722:LEU:HA	1:B:722:LEU:HD23	1.77	0.46
1:C:498:LYS:HB3	1:C:531:ILE:HD13	1.97	0.46
1:A:98:ILE:HB	1:A:104:ARG:HB2	1.96	0.46
1:A:318:ASP:OD1	1:A:370:ARG:NH2	2.48	0.46
1:B:234:GLN:HA	1:B:237:LEU:HB2	1.97	0.46
1:C:514:SER:OG	1:C:551:ALA:HB1	2.15	0.46
1:D:494:THR:HG21	1:D:750:VAL:HA	1.98	0.46
1:E:609:LEU:HD11	1:E:728:ALA:HB2	1.97	0.46
1:B:262:VAL:HA	1:B:265:LYS:HG2	1.97	0.46
1:B:346:ASN:HB2	1:B:445:PRO:HB3	1.96	0.46
1:C:247:GLU:HG2	1:C:250:ARG:HE	1.81	0.46
1:C:393:HIS:HD2	1:C:400:ALA:HA	1.81	0.46
1:D:625:LEU:HD11	1:D:634:LYS:NZ	2.31	0.46
1:E:494:THR:HB	1:E:726:HIS:CD2	2.51	0.46
1:A:71:VAL:HG22	1:A:86:VAL:HG12	1.97	0.46
1:B:14:VAL:HG13	1:B:48:ALA:HB2	1.96	0.46
1:B:386:ASP:OD1	1:B:432:ARG:NH2	2.42	0.46
1:C:719:LYS:O	1:C:723:LEU:HD23	2.15	0.46
1:E:284:THR:O	1:E:288:THR:HG23	2.16	0.46
1:D:625:LEU:HD11	1:D:634:LYS:HZ2	1.79	0.46
1:E:336:ARG:NH1	1:E:346:ASN:OD1	2.43	0.46
1:A:392:GLY:H	1:A:453:ASP:HB2	1.81	0.46
1:B:350:ILE:HG12	1:B:485:MET:HG2	1.98	0.46
1:D:298:TRP:H	1:D:300:LYS:NZ	2.13	0.46
1:E:262:VAL:HG13	1:E:265:LYS:HE2	1.98	0.46
1:E:631:GLU:O	1:E:634:LYS:HB3	2.15	0.46
1:A:157:ASP:O	1:A:160:MET:HG3	2.15	0.46
1:A:326:LYS:H	1:A:326:LYS:HD2	1.80	0.46
1:A:623:LEU:HD13	1:A:663:LEU:HD23	1.98	0.46
1:B:685:THR:HG21	1:B:702:MET:CE	2.46	0.46
1:A:310:HIS:O	1:A:314:VAL:HG23	2.16	0.45
1:D:423:GLU:HB3	1:D:426:LYS:HE2	1.98	0.45
1:D:533:GLU:HG2	1:D:585:PRO:HA	1.97	0.45
1:A:587:LYS:CG	1:A:728:ALA:HB1	2.47	0.45
1:B:259:PRO:HB2	1:B:262:VAL:HG23	1.96	0.45
1:B:306:LEU:HD13	1:B:336:ARG:HG3	1.98	0.45
1:D:600:LEU:HG	1:D:701:ALA:HB1	1.97	0.45
1:A:90:ALA:HB3	1:A:110:PHE:HB3	1.98	0.45
1:A:553:LYS:HD2	1:A:577:TYR:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:GLU:OE1	1:B:104:ARG:NH2	2.49	0.45
1:B:507:TRP:CZ2	1:B:511:VAL:HG21	2.52	0.45
1:B:507:TRP:CH2	1:B:521:GLU:HA	2.51	0.45
1:B:625:LEU:HD13	1:B:634:LYS:HG2	1.97	0.45
1:B:7:VAL:HG11	1:B:62:LEU:HD21	1.99	0.45
1:B:308:ILE:HG23	1:B:330:LEU:HD11	1.97	0.45
1:C:682:THR:HA	1:C:702:MET:SD	2.57	0.45
1:E:401:MET:SD	1:E:402:PRO:HD2	2.57	0.45
1:E:491:PRO:HG3	1:E:719:LYS:NZ	2.32	0.45
1:A:392:GLY:O	1:A:454:HIS:HB2	2.17	0.45
1:B:9:PRO:HG2	1:B:27:ARG:NH2	2.31	0.45
1:E:67:VAL:HB	1:E:88:ALA:HB1	1.99	0.45
1:E:318:ASP:OD1	1:E:319:HIS:N	2.48	0.45
1:E:616:ALA:HB2	1:E:690:ALA:HB1	1.97	0.45
1:B:264:THR:HB	1:B:268:LYS:NZ	2.31	0.45
1:B:624:SER:OG	1:B:625:LEU:N	2.50	0.45
1:C:90:ALA:HB1	1:C:111:SER:H	1.81	0.45
1:C:494:THR:HB	1:C:726:HIS:CE1	2.52	0.45
1:E:494:THR:HB	1:E:726:HIS:HD2	1.81	0.45
1:E:17:PRO:HA	1:E:88:ALA:HB3	1.98	0.45
1:E:354:VAL:N	1:E:488:ILE:O	2.46	0.45
1:E:388:ALA:HA	1:E:392:GLY:HA2	1.99	0.45
1:E:441:GLU:HG2	1:E:451:PHE:HA	1.99	0.45
1:A:625:LEU:HG	1:A:665:VAL:HB	1.98	0.45
1:A:644:LEU:HD11	1:A:688:ALA:HB2	1.98	0.45
1:C:405:LEU:HD11	1:C:442:VAL:HG11	1.98	0.45
1:D:298:TRP:H	1:D:300:LYS:HZ3	1.64	0.45
1:D:319:HIS:NE2	1:D:364:LEU:HA	2.32	0.45
1:D:531:ILE:HA	1:D:543:LEU:HD21	1.99	0.45
1:A:492:GLY:N	1:A:720:GLU:HG2	2.32	0.45
1:A:697:ARG:HB3	1:A:698:MET:H	1.68	0.45
1:B:314:VAL:HG13	1:B:370:ARG:HH21	1.82	0.45
1:C:626:THR:N	1:C:665:VAL:O	2.45	0.45
1:D:521:GLU:HG2	1:D:568:THR:HA	1.97	0.45
1:A:316:ASP:OD1	1:A:323:LYS:NZ	2.50	0.44
1:A:740:GLU:HG2	1:A:743:LEU:HD12	1.99	0.44
1:B:29:LYS:HE3	1:B:57:PRO:HD2	1.99	0.44
1:D:624:SER:O	1:D:665:VAL:HG22	2.17	0.44
1:D:701:ALA:N	1:D:730:ILE:HG21	2.31	0.44
1:E:294:THR:OG1	1:E:295:GLU:OE1	2.30	0.44
1:A:34:VAL:O	1:A:38:MET:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:548:GLY:O	1:B:552:ARG:HG3	2.17	0.44
1:D:50:ARG:NH1	1:D:51:ASP:OD2	2.51	0.44
1:E:262:VAL:HA	1:E:265:LYS:HE2	2.00	0.44
1:A:201:GLU:OE1	1:D:222:ARG:HD2	2.16	0.44
1:B:222:ARG:HG3	1:E:198:ARG:HH22	1.82	0.44
1:B:479:ARG:N	1:B:480:PRO:HD2	2.33	0.44
1:C:18:HIS:ND1	1:C:160:MET:HG2	2.32	0.44
1:C:218:ASP:O	1:C:221:GLN:HG3	2.18	0.44
1:C:593:GLN:HB2	1:C:698:MET:CE	2.47	0.44
1:D:425:ASP:OD1	1:D:426:LYS:HD3	2.17	0.44
1:D:641:LEU:O	1:D:645:ARG:HG3	2.17	0.44
1:E:216:GLN:NE2	1:E:220:ASN:OD1	2.41	0.44
1:E:563:TRP:CD1	1:E:564:GLU:HG3	2.53	0.44
1:A:252:LYS:HG2	1:A:294:THR:HB	2.00	0.44
1:A:385:ARG:HG2	1:A:428:SER:HB3	2.00	0.44
1:A:647:HIS:HB3	1:A:650:ASP:HB2	2.00	0.44
1:A:685:THR:OG1	1:A:769:LEU:HD23	2.18	0.44
1:C:4:GLU:HG2	1:C:106:ARG:CZ	2.47	0.44
1:C:185:LEU:HD23	1:C:185:LEU:H	1.82	0.44
1:C:353:LEU:HD11	1:C:468:ILE:HD11	1.99	0.44
1:D:139:HIS:CE1	1:D:144:LEU:HB2	2.52	0.44
1:D:157:ASP:HB2	1:D:160:MET:SD	2.58	0.44
1:E:770:LEU:HD23	1:E:770:LEU:HA	1.83	0.44
1:A:593:GLN:NE2	1:A:596:THR:HG21	2.33	0.44
1:B:307:ASP:HB3	1:B:310:HIS:HB3	1.99	0.44
1:B:394:ARG:HH21	1:B:395:ARG:HB3	1.83	0.44
1:C:734:VAL:HG11	1:C:765:VAL:HG22	2.00	0.44
1:B:674:LYS:HG2	1:B:678:SER:HB3	1.99	0.44
1:C:98:ILE:HD12	1:C:104:ARG:HB2	1.99	0.44
1:C:199:ASP:HA	1:C:202:ARG:HG2	2.00	0.44
1:C:598:GLN:HB2	1:C:609:LEU:HD22	2.00	0.44
1:D:352:VAL:HG23	1:D:485:MET:CE	2.48	0.44
1:B:593:GLN:OE1	1:B:593:GLN:N	2.50	0.44
1:D:440:LEU:HG	1:D:481:LEU:HG	1.99	0.44
1:E:258:MET:SD	1:E:259:PRO:HD2	2.58	0.44
1:A:499:GLN:NE2	1:A:524:ASP:O	2.50	0.44
1:B:497:GLU:O	1:B:501:ILE:HG13	2.18	0.44
1:B:700:ILE:HA	1:B:732:LYS:O	2.17	0.44
1:C:408:ALA:O	1:C:412:VAL:HG12	2.17	0.44
1:C:623:LEU:HD22	1:C:634:LYS:HG3	1.99	0.44
1:D:468:ILE:HG22	1:D:469:THR:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:51:ASP:OD2	1:E:63:TYR:OH	2.32	0.44
1:E:612:ILE:HG13	1:E:667:VAL:HG22	2.00	0.44
1:A:448:ASN:HA	1:A:451:PHE:HB2	2.00	0.43
1:C:77:LEU:HB2	1:C:83:GLN:HB3	2.00	0.43
1:C:421:LEU:HD11	1:C:467:PHE:HD2	1.83	0.43
1:D:507:TRP:O	1:D:511:VAL:HG22	2.19	0.43
1:B:67:VAL:HA	1:B:91:ARG:HA	2.00	0.43
1:B:213:VAL:O	1:B:217:MET:HE2	2.18	0.43
1:B:356:PRO:HG2	1:B:359:VAL:HG23	2.01	0.43
1:D:526:ALA:HB1	1:D:574:ILE:HD11	2.00	0.43
1:A:511:VAL:HG13	1:A:516:MET:HB2	1.99	0.43
1:A:620:SER:HB2	1:A:622:LYS:NZ	2.32	0.43
1:B:379:ILE:HG23	1:B:379:ILE:O	2.19	0.43
1:C:537:GLU:HG2	1:C:539:GLY:H	1.81	0.43
1:D:593:GLN:O	1:D:696:ALA:N	2.51	0.43
1:A:244:SER:HB2	1:A:247:GLU:HB2	2.01	0.43
1:A:359:VAL:HG22	1:A:541:ARG:HG3	2.00	0.43
1:A:602:TRP:HB2	1:A:721:LYS:NZ	2.32	0.43
1:A:609:LEU:H	1:A:609:LEU:HD23	1.83	0.43
1:D:225:TYR:HA	1:D:228:GLU:HB2	2.00	0.43
1:B:265:LYS:HA	1:B:268:LYS:HE2	2.01	0.43
1:B:632:VAL:HA	1:B:635:GLU:OE2	2.18	0.43
1:B:642:THR:O	1:B:645:ARG:HG2	2.18	0.43
1:C:350:ILE:HD13	1:C:443:LEU:HB3	1.99	0.43
1:A:55:ASP:OD1	1:A:55:ASP:N	2.52	0.43
1:B:359:VAL:HG11	1:B:490:ILE:HG22	1.99	0.43
1:C:479:ARG:N	1:C:480:PRO:HD2	2.33	0.43
1:C:552:ARG:HD3	1:D:335:VAL:CG2	2.49	0.43
1:C:564:GLU:HG3	1:C:566:LEU:H	1.84	0.43
1:D:663:LEU:HD21	1:D:687:ILE:HG23	2.01	0.43
1:E:677:PRO:O	1:E:705:GLU:HG2	2.19	0.43
1:A:311:THR:O	1:A:315:LEU:HG	2.18	0.43
1:C:390:ILE:HD12	1:C:435:PRO:HB2	2.00	0.43
1:D:401:MET:HB2	1:D:407:HIS:CE1	2.53	0.43
1:E:771:LEU:HB3	1:E:772:PRO:HD3	2.01	0.43
1:A:103:LEU:HD23	1:A:103:LEU:H	1.84	0.43
1:E:393:HIS:O	1:E:455:TYR:HD1	2.02	0.43
1:C:392:GLY:HA3	1:C:453:ASP:HB3	2.01	0.43
1:C:497:GLU:OE2	1:C:749:GLU:HG3	2.18	0.43
1:C:509:LYS:HE2	1:C:513:GLU:HG3	2.00	0.43
1:D:425:ASP:HB2	1:D:476:THR:OG1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:THR:HG23	1:A:160:MET:SD	2.59	0.43
1:A:598:GLN:NE2	1:A:609:LEU:HD12	2.34	0.43
1:A:674:LYS:NZ	1:A:676:GLY:O	2.36	0.43
1:B:94:VAL:HG22	1:B:107:GLY:HA2	1.99	0.43
1:C:420:LEU:HA	1:C:468:ILE:HG23	2.00	0.43
1:C:632:VAL:HA	1:C:635:GLU:HG3	2.00	0.43
1:E:494:THR:H	1:E:497:GLU:HB2	1.84	0.43
1:E:633:MET:HG3	1:E:683:MET:SD	2.59	0.43
1:A:336:ARG:HA	1:A:345:ARG:HG3	2.01	0.42
1:A:374:ARG:HD3	1:A:374:ARG:HA	1.64	0.42
1:B:144:LEU:HD23	1:B:146:ARG:NH2	2.34	0.42
1:E:715:ILE:H	1:E:739:ASN:HD21	1.67	0.42
1:B:32:ARG:HA	1:B:35:GLU:HB2	2.00	0.42
1:B:248:ALA:HA	1:B:251:LYS:HE3	2.01	0.42
1:B:505:TYR:HB2	2:B:801:ADP:H2	1.83	0.42
1:C:593:GLN:HB2	1:C:698:MET:HE3	2.01	0.42
1:D:260:GLU:O	1:D:264:THR:HG23	2.19	0.42
1:E:715:ILE:N	1:E:739:ASN:HD21	2.17	0.42
1:C:16:LEU:HD22	1:C:163:ASP:HA	2.01	0.42
1:C:553:LYS:HG3	1:C:577:TYR:O	2.19	0.42
1:C:596:THR:HG21	1:C:613:GLU:HG2	2.00	0.42
1:D:392:GLY:HA3	1:D:402:PRO:HA	2.01	0.42
1:D:524:ASP:OD1	1:D:525:ALA:N	2.52	0.42
1:E:258:MET:O	1:E:263:LYS:HE2	2.19	0.42
1:E:479:ARG:N	1:E:480:PRO:HD2	2.34	0.42
1:E:541:ARG:HB3	1:E:545:ARG:NH1	2.34	0.42
1:A:592:PRO:HG3	1:A:698:MET:HE2	2.02	0.42
1:B:178:GLU:HG2	1:B:191:LYS:NZ	2.34	0.42
1:B:394:ARG:HE	1:B:395:ARG:N	2.18	0.42
1:C:319:HIS:HE1	1:C:367:SER:OG	2.02	0.42
1:C:598:GLN:HA	1:C:611:THR:HA	2.00	0.42
1:D:317:GLU:O	1:D:505:TYR:OH	2.21	0.42
1:B:507:TRP:CE2	1:B:511:VAL:HG21	2.54	0.42
1:B:566:LEU:HD12	1:B:566:LEU:HA	1.88	0.42
1:C:233:ILE:HG13	1:C:237:LEU:HD23	2.02	0.42
1:C:448:ASN:OD1	1:C:449:ASN:N	2.52	0.42
1:D:350:ILE:HG13	1:D:485:MET:HE1	2.00	0.42
1:D:431:TRP:CG	1:D:432:ARG:N	2.87	0.42
1:D:499:GLN:NE2	1:D:524:ASP:HB2	2.34	0.42
1:D:715:ILE:H	1:D:739:ASN:HD21	1.68	0.42
1:D:737:LYS:HA	1:D:737:LYS:HD3	1.95	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:VAL:HG23	1:A:300:LYS:HZ1	1.84	0.42
1:B:136:VAL:HA	1:B:139:HIS:HD2	1.85	0.42
1:B:249:LEU:HD21	1:B:287:ARG:NH1	2.35	0.42
1:B:359:VAL:HG13	1:B:493:TYR:HE2	1.82	0.42
1:C:76:ARG:HD3	1:C:82:LEU:HD22	2.02	0.42
1:C:128:LEU:HG	1:C:165:ILE:HD13	2.02	0.42
1:C:297:PRO:O	1:C:460:TYR:OH	2.30	0.42
1:C:340:GLN:HG3	1:C:341:GLY:H	1.84	0.42
1:D:362:THR:HG22	2:D:801:ADP:PA	2.59	0.42
1:D:450:THR:HB	1:D:459:PRO:HB3	2.02	0.42
1:D:559:LEU:HD23	1:E:308:ILE:HG23	2.01	0.42
1:A:160:MET:SD	1:A:161:LEU:N	2.93	0.42
1:A:205:LEU:HD22	1:D:222:ARG:CZ	2.50	0.42
1:A:594:VAL:O	1:B:709:ARG:HD2	2.19	0.42
1:A:678:SER:HB3	1:A:721:LYS:HE2	2.02	0.42
1:C:407:HIS:O	1:C:410:LYS:HB3	2.20	0.42
1:D:399:GLY:C	1:E:432:ARG:HB2	2.39	0.42
1:A:663:LEU:O	1:A:664:HIS:ND1	2.50	0.42
1:B:35:GLU:O	1:B:38:MET:HG2	2.20	0.42
1:B:473:THR:HG22	1:B:475:GLN:H	1.85	0.42
1:C:553:LYS:HE3	1:D:331:GLU:OE2	2.20	0.42
1:E:550:ILE:HG12	1:E:578:LEU:HD11	2.02	0.42
1:A:101:PRO:HA	1:A:102:TYR:HA	1.77	0.42
1:A:117:ASP:HA	1:D:146:ARG:HE	1.85	0.42
1:D:243:LEU:HG	1:D:245:ASP:HB2	2.02	0.42
1:D:313:GLN:O	1:D:317:GLU:HG2	2.20	0.42
1:A:693:ARG:HD3	1:A:693:ARG:HA	1.86	0.42
1:B:332:TYR:CE1	1:B:466:PHE:HE1	2.35	0.42
1:B:423:GLU:HB3	1:B:426:LYS:HB2	2.01	0.42
1:B:626:THR:HG22	1:B:627:GLY:N	2.35	0.42
1:C:556:LYS:NZ	1:D:327:GLU:OE2	2.40	0.42
1:D:8:ILE:HD12	1:D:44:ILE:HD13	2.02	0.42
1:E:453:ASP:H	1:E:456:LEU:HB2	1.84	0.42
1:A:466:PHE:HE2	1:A:468:ILE:HB	1.84	0.41
1:B:510:GLN:HG2	1:B:547:LEU:C	2.40	0.41
1:C:603:THR:OG1	1:C:606:GLY:O	2.38	0.41
1:D:353:LEU:HD11	1:D:364:LEU:HD22	2.02	0.41
1:E:44:ILE:HD11	1:E:71:VAL:HG22	2.01	0.41
1:E:176:LYS:HA	1:E:179:ILE:HG22	2.02	0.41
1:A:521:GLU:HB2	1:A:568:THR:HA	2.03	0.41
1:B:507:TRP:HB3	1:B:508:PRO:HD3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:516:MET:CE	1:B:519:ARG:HB2	2.50	0.41
1:C:101:PRO:HA	1:C:102:TYR:HA	1.51	0.41
1:C:550:ILE:HD11	1:C:578:LEU:HG	2.01	0.41
1:C:625:LEU:HD22	1:C:629:LEU:HD12	2.01	0.41
1:D:403:GLY:O	1:D:407:HIS:ND1	2.50	0.41
1:E:521:GLU:HB2	1:E:566:LEU:HG	2.02	0.41
1:A:38:MET:SD	1:A:42:ARG:NE	2.92	0.41
1:A:378:ARG:HG3	1:A:378:ARG:HH11	1.85	0.41
1:B:712:VAL:HG12	1:B:736:PRO:HB3	2.01	0.41
1:C:134:LYS:O	1:C:138:ASN:ND2	2.53	0.41
1:C:349:PRO:HB3	1:C:485:MET:C	2.41	0.41
1:C:474:LEU:H	1:C:474:LEU:HD23	1.86	0.41
1:D:204:GLU:HB3	1:D:208:ARG:HH12	1.84	0.41
1:D:312:ARG:NH1	1:D:327:GLU:OE1	2.53	0.41
1:D:612:ILE:HG12	1:D:667:VAL:HG22	2.02	0.41
1:E:44:ILE:HG22	1:E:46:LEU:HG	2.01	0.41
1:E:128:LEU:HD11	1:E:192:VAL:HG12	2.02	0.41
1:E:309:ASN:O	1:E:313:GLN:HG2	2.19	0.41
1:B:112:GLU:HA	1:B:183:THR:HB	2.03	0.41
1:B:431:TRP:O	1:B:432:ARG:HB2	2.20	0.41
1:C:395:ARG:CB	1:C:455:TYR:HA	2.51	0.41
1:C:617:VAL:HG21	1:C:664:HIS:HD2	1.84	0.41
1:D:319:HIS:NE2	1:D:367:SER:HB3	2.34	0.41
1:D:622:LYS:HB2	1:D:622:LYS:HE3	1.73	0.41
1:E:267:LEU:HA	1:E:270:LEU:HD12	2.02	0.41
1:E:348:ALA:H	1:E:484:ARG:HH21	1.67	0.41
1:A:281:PRO:O	1:A:285:VAL:HG12	2.20	0.41
1:A:600:LEU:N	1:A:702:MET:O	2.43	0.41
1:A:694:ARG:HD2	1:A:772:PRO:HG3	2.03	0.41
1:B:69:ALA:HA	1:B:88:ALA:HA	2.03	0.41
1:B:632:VAL:HA	1:B:635:GLU:CD	2.41	0.41
1:C:501:ILE:HG21	1:C:501:ILE:HD13	1.83	0.41
1:D:256:VAL:O	1:D:258:MET:HG3	2.20	0.41
1:D:633:MET:HE2	1:D:667:VAL:HG21	2.03	0.41
1:E:631:GLU:O	1:E:634:LYS:N	2.53	0.41
1:A:7:VAL:HG21	1:A:105:ALA:HB3	2.02	0.41
1:B:644:LEU:HD23	1:B:653:LEU:HD11	2.02	0.41
1:B:700:ILE:HG12	1:B:732:LYS:HB2	2.01	0.41
1:B:723:LEU:HA	1:B:723:LEU:HD23	1.82	0.41
1:C:369:ALA:HB1	1:C:374:ARG:O	2.21	0.41
1:C:537:GLU:CG	1:C:538:ALA:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:541:ARG:HG2	1:D:541:ARG:HH11	1.85	0.41
1:E:387:GLU:HG3	1:E:431:TRP:HB2	2.03	0.41
1:E:444:ASP:HA	1:E:484:ARG:HH12	1.86	0.41
1:E:507:TRP:HB3	1:E:508:PRO:HD3	2.02	0.41
1:E:683:MET:O	1:E:687:ILE:HG12	2.21	0.41
1:E:694:ARG:HD3	1:E:772:PRO:HG2	2.03	0.41
1:A:57:PRO:HD2	1:A:101:PRO:HB3	2.03	0.41
1:A:237:LEU:HD22	1:A:237:LEU:HA	1.79	0.41
1:B:225:TYR:O	1:B:229:GLN:HG2	2.20	0.41
1:B:552:ARG:HD2	1:C:335:VAL:HG21	2.02	0.41
1:C:119:ALA:O	1:C:122:ARG:HG2	2.21	0.41
1:C:233:ILE:HD11	1:D:226:LEU:CD2	2.50	0.41
1:D:270:LEU:O	1:D:273:LEU:HB2	2.20	0.41
1:D:536:ARG:NH2	1:D:584:ARG:O	2.54	0.41
1:A:207:LYS:O	1:A:211:GLN:OE1	2.38	0.41
1:A:316:ASP:HA	1:A:323:LYS:HZ2	1.85	0.41
1:B:598:GLN:O	1:B:701:ALA:HA	2.21	0.41
1:B:641:LEU:HD11	1:B:657:PHE:HE1	1.86	0.41
1:C:237:LEU:HD22	1:C:237:LEU:HA	1.94	0.41
1:C:385:ARG:HG2	1:C:428:SER:O	2.21	0.41
1:C:472:ASN:HB3	1:C:604:PRO:O	2.21	0.41
1:D:366:ARG:HG3	1:D:376:PHE:CD2	2.56	0.41
1:D:388:ALA:HB1	1:D:393:HIS:NE2	2.35	0.41
1:D:509:LYS:O	1:D:513:GLU:HG3	2.20	0.41
1:B:617:VAL:CG1	1:C:642:THR:HG23	2.51	0.41
1:B:694:ARG:HA	1:B:695:PRO:HD3	1.90	0.41
1:C:421:LEU:HD11	1:C:467:PHE:CD2	2.55	0.41
1:D:292:TRP:HH2	1:D:407:HIS:CD2	2.39	0.41
1:E:16:LEU:HB3	1:E:163:ASP:HB3	2.02	0.41
1:E:520:ILE:O	1:E:566:LEU:HD11	2.21	0.41
1:E:536:ARG:HH21	1:E:587:LYS:HD3	1.85	0.41
1:E:613:GLU:HG3	1:E:666:HIS:HB2	2.03	0.41
1:B:328:ARG:HB3	1:B:488:ILE:HD12	2.03	0.40
1:C:3:LEU:O	1:C:106:ARG:HA	2.21	0.40
1:C:225:TYR:HE2	1:C:229:GLN:HE21	1.69	0.40
1:C:537:GLU:HG2	1:C:538:ALA:H	1.86	0.40
1:D:230:MET:CE	1:D:274:GLU:HB3	2.51	0.40
1:D:507:TRP:HB3	1:D:508:PRO:HD3	2.02	0.40
1:E:495:ASN:ND2	1:E:531:ILE:HG23	2.37	0.40
1:E:569:ILE:HG23	1:E:577:TYR:HD2	1.85	0.40
1:E:632:VAL:HA	1:E:635:GLU:CD	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:TRP:CE2	1:A:511:VAL:HG21	2.56	0.40
1:B:574:ILE:O	1:B:578:LEU:N	2.43	0.40
1:B:613:GLU:HG3	1:C:708:LEU:HD13	2.03	0.40
1:C:258:MET:HG2	1:C:262:VAL:HB	2.04	0.40
1:C:418:VAL:HG13	1:C:466:PHE:HD1	1.86	0.40
1:E:90:ALA:HB3	1:E:110:PHE:CD1	2.56	0.40
1:E:425:ASP:OD1	1:E:425:ASP:N	2.51	0.40
1:E:698:MET:O	1:E:700:ILE:HG13	2.20	0.40
1:B:391:ARG:HH21	1:B:454:HIS:HD2	1.65	0.40
1:C:51:ASP:HB3	1:C:52:PRO:CD	2.48	0.40
1:C:346:ASN:HB3	1:C:348:ALA:HB3	2.03	0.40
1:C:602:TRP:HB2	1:C:720:GLU:HG2	2.03	0.40
1:D:392:GLY:O	1:D:454:HIS:HB2	2.22	0.40
1:E:51:ASP:HB3	1:E:52:PRO:CD	2.51	0.40
1:A:374:ARG:HD2	1:A:416:ASN:O	2.22	0.40
1:A:556:LYS:O	1:A:560:GLU:HG3	2.21	0.40
1:A:722:LEU:HD11	1:A:735:LEU:HD21	2.02	0.40
1:C:151:ALA:HB3	1:C:168:HIS:HE1	1.86	0.40
1:C:759:VAL:HG21	1:C:765:VAL:HG23	2.03	0.40
1:D:47:VAL:HB	1:D:62:LEU:HD22	2.03	0.40
1:D:227:ARG:HA	1:D:230:MET:CG	2.51	0.40
1:D:262:VAL:HG13	1:D:458:VAL:HG21	2.02	0.40
1:E:206:ASP:HA	1:E:209:VAL:HG12	2.04	0.40
1:A:212:ARG:HG3	1:C:232:ALA:HB1	2.03	0.40
1:B:11:ARG:NH2	1:B:24:ASP:HB2	2.37	0.40
1:D:385:ARG:HA	1:D:428:SER:O	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	A	771/793 (97%)	716 (93%)	55 (7%)	0	100	100
1	B	771/793 (97%)	704 (91%)	67 (9%)	0	100	100
1	C	771/793 (97%)	697 (90%)	74 (10%)	0	100	100
1	D	771/793 (97%)	705 (91%)	65 (8%)	1 (0%)	51	83
1	E	771/793 (97%)	714 (93%)	56 (7%)	1 (0%)	51	83
All	All	3855/3965 (97%)	3536 (92%)	317 (8%)	2 (0%)	54	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	320	TYR
1	E	52	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	649/665 (98%)	646 (100%)	3 (0%)	88	95
1	B	649/665 (98%)	646 (100%)	3 (0%)	88	95
1	C	649/665 (98%)	645 (99%)	4 (1%)	86	94
1	D	649/665 (98%)	644 (99%)	5 (1%)	81	91
1	E	649/665 (98%)	648 (100%)	1 (0%)	93	98
All	All	3245/3325 (98%)	3229 (100%)	16 (0%)	89	95

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	220	ASN
1	A	237	LEU
1	A	243	LEU
1	B	27	ARG
1	B	143	ARG
1	B	243	LEU

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Mol	Chain	Res	Type
1	C	190	LYS
1	C	237	LEU
1	C	246	LEU
1	C	693	ARG
1	D	50	ARG
1	D	227	ARG
1	D	272	ARG
1	D	385	ARG
1	D	545	ARG
1	E	622	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	499	GLN
1	B	319	HIS
1	B	499	GLN
1	C	168	HIS
1	C	319	HIS
1	C	499	GLN
1	D	139	HIS
1	E	234	GLN
1	E	727	GLN

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

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ADP	A	801	-	24,29,29	0.96	1 (4%)	29,45,45	1.36	4 (13%)
2	ADP	C	801	-	24,29,29	0.91	1 (4%)	29,45,45	1.57	4 (13%)
2	ADP	D	801	-	24,29,29	0.91	1 (4%)	29,45,45	1.42	4 (13%)
2	ADP	B	801	-	24,29,29	0.92	1 (4%)	29,45,45	1.54	4 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	801	-	-	4/12/32/32	0/3/3/3
2	ADP	C	801	-	-	3/12/32/32	0/3/3/3
2	ADP	D	801	-	-	9/12/32/32	0/3/3/3
2	ADP	B	801	-	-	4/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	ADP	C5-C4	2.47	1.47	1.40
2	D	801	ADP	C5-C4	2.32	1.47	1.40
2	B	801	ADP	C5-C4	2.28	1.47	1.40
2	C	801	ADP	C5-C4	2.25	1.46	1.40

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	801	ADP	PA-O3A-PB	-4.45	117.55	132.83
2	C	801	ADP	PA-O3A-PB	-4.45	117.55	132.83
2	C	801	ADP	C3'-C2'-C1'	3.48	106.21	100.98
2	D	801	ADP	C3'-C2'-C1'	3.44	106.16	100.98
2	A	801	ADP	N3-C2-N1	-3.25	123.60	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	801	ADP	N3-C2-N1	-3.16	123.74	128.68
2	B	801	ADP	N3-C2-N1	-3.11	123.82	128.68
2	D	801	ADP	PA-O3A-PB	-2.97	122.62	132.83
2	C	801	ADP	N3-C2-N1	-2.95	124.07	128.68
2	A	801	ADP	PA-O3A-PB	-2.83	123.11	132.83
2	B	801	ADP	C3'-C2'-C1'	2.82	105.23	100.98
2	A	801	ADP	C3'-C2'-C1'	2.74	105.11	100.98
2	A	801	ADP	C4-C5-N7	-2.72	106.56	109.40
2	B	801	ADP	C4-C5-N7	-2.59	106.70	109.40
2	C	801	ADP	C4-C5-N7	-2.43	106.86	109.40
2	D	801	ADP	C4-C5-N7	-2.26	107.04	109.40

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	ADP	C5'-O5'-PA-O1A
2	B	801	ADP	C5'-O5'-PA-O3A
2	C	801	ADP	C5'-O5'-PA-O1A
2	C	801	ADP	C5'-O5'-PA-O3A
2	D	801	ADP	PA-O3A-PB-O2B
2	D	801	ADP	C5'-O5'-PA-O1A
2	D	801	ADP	C5'-O5'-PA-O2A
2	D	801	ADP	O4'-C4'-C5'-O5'
2	B	801	ADP	C3'-C4'-C5'-O5'
2	D	801	ADP	C3'-C4'-C5'-O5'
2	D	801	ADP	PB-O3A-PA-O5'
2	A	801	ADP	C5'-O5'-PA-O3A
2	D	801	ADP	C4'-C5'-O5'-PA
2	B	801	ADP	C5'-O5'-PA-O1A
2	B	801	ADP	O4'-C4'-C5'-O5'
2	D	801	ADP	PA-O3A-PB-O1B
2	A	801	ADP	O4'-C4'-C5'-O5'
2	D	801	ADP	C5'-O5'-PA-O3A
2	C	801	ADP	O4'-C4'-C5'-O5'
2	A	801	ADP	C5'-O5'-PA-O2A

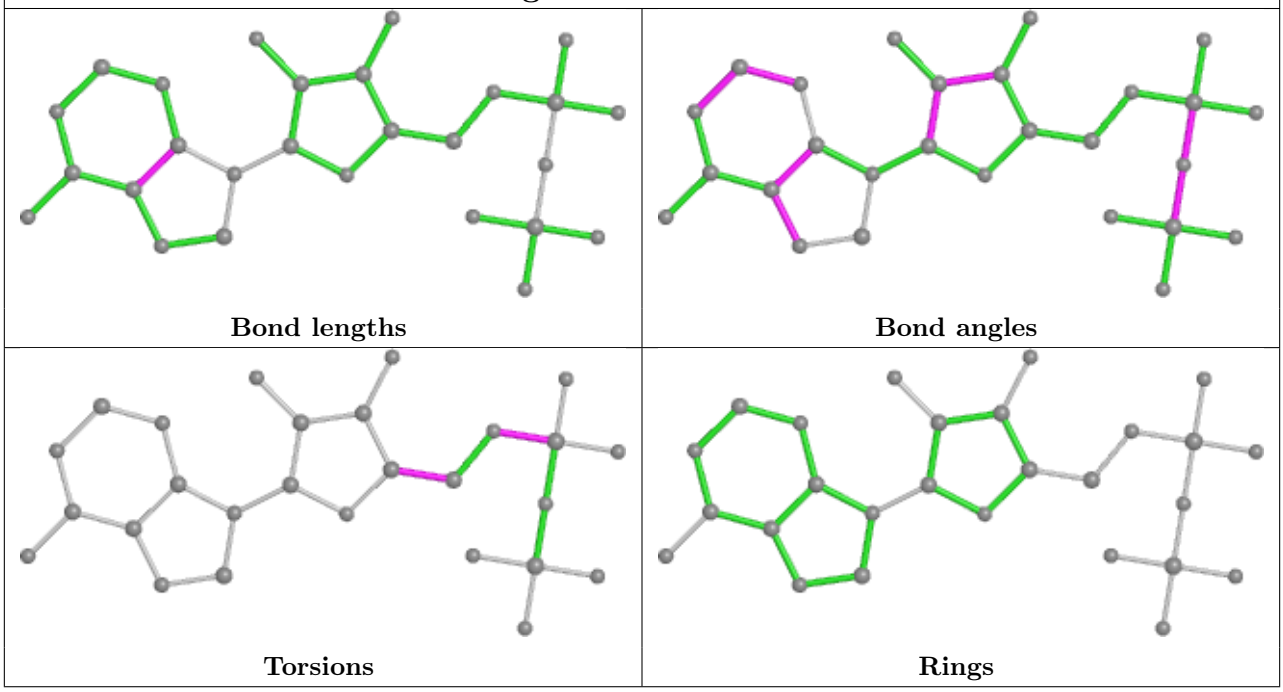
There are no ring outliers.

4 monomers are involved in 8 short contacts:

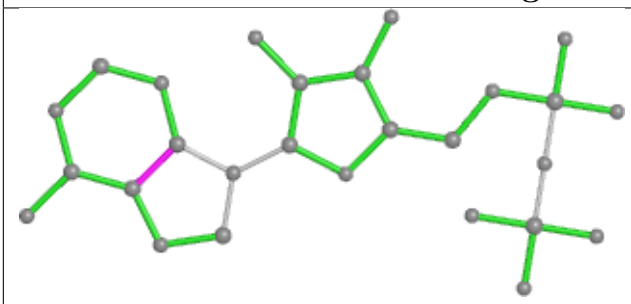
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	ADP	1	0
2	C	801	ADP	3	0
2	D	801	ADP	3	0
2	B	801	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

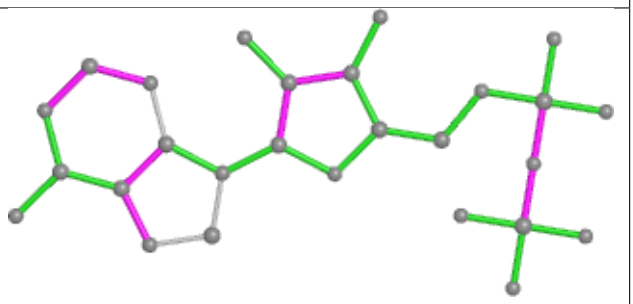
Ligand ADP A 801



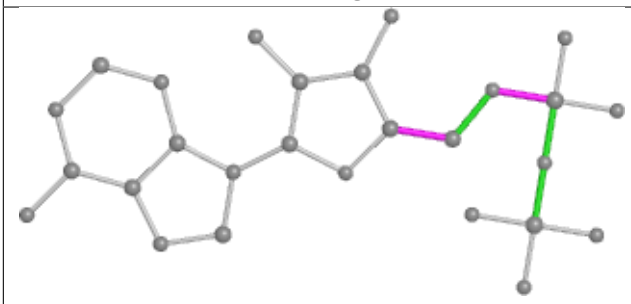
Ligand ADP C 801



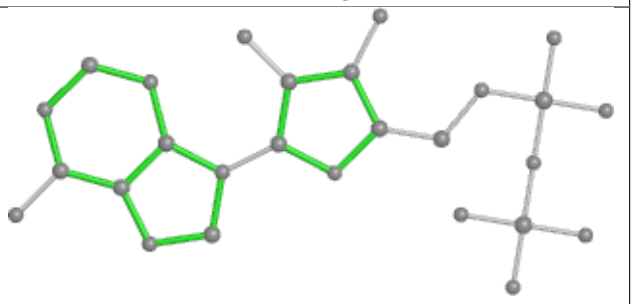
Bond lengths



Bond angles

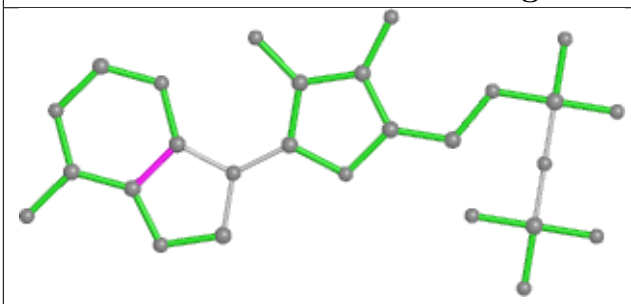


Torsions

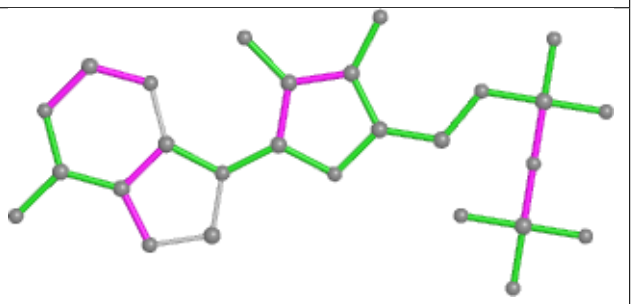


Rings

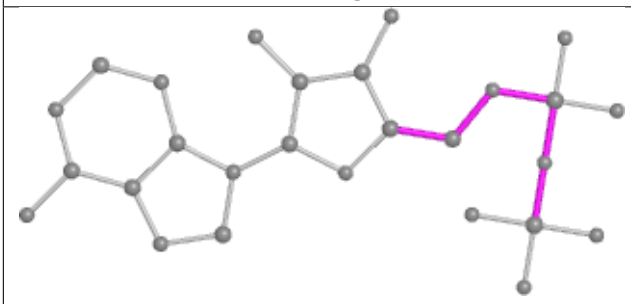
Ligand ADP D 801



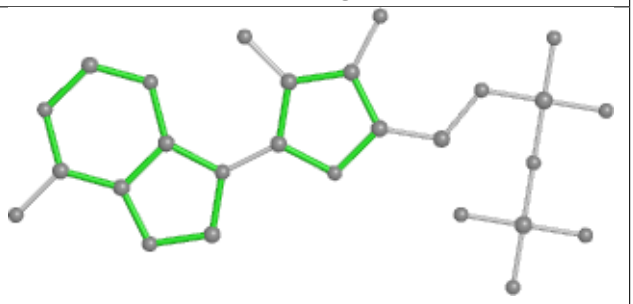
Bond lengths



Bond angles

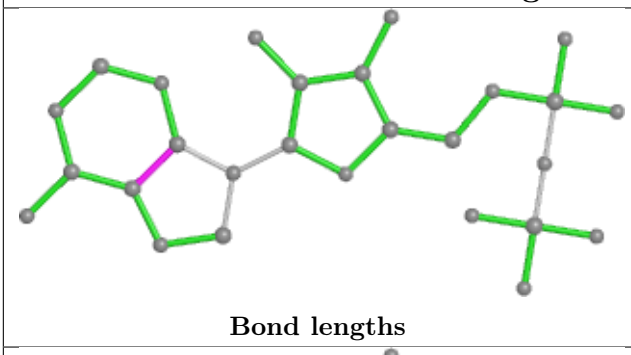


Torsions

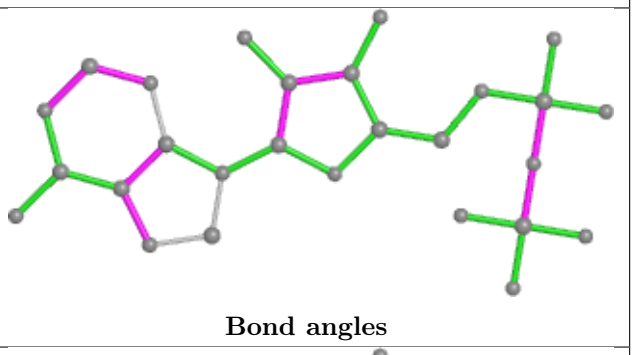


Rings

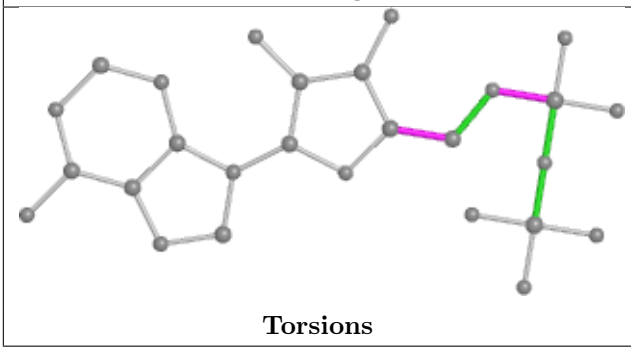
Ligand ADP B 801



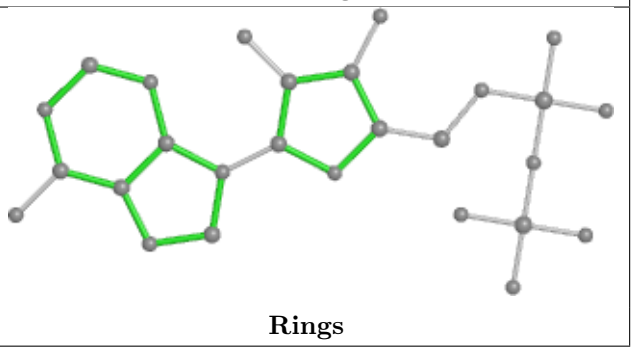
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

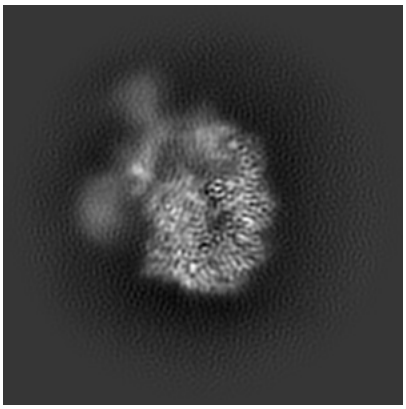
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-34113. These allow visual inspection of the internal detail of the map and identification of artifacts.

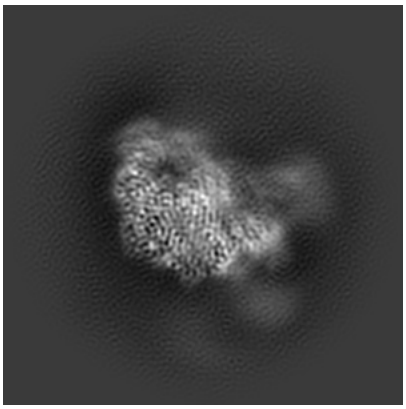
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

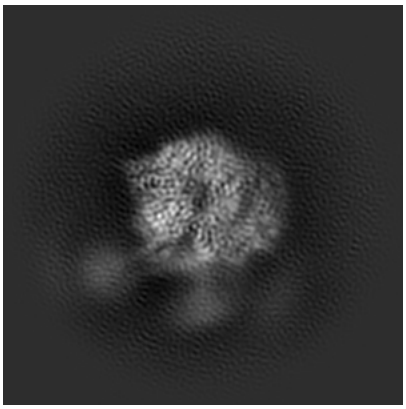
6.1.1 Primary map



X

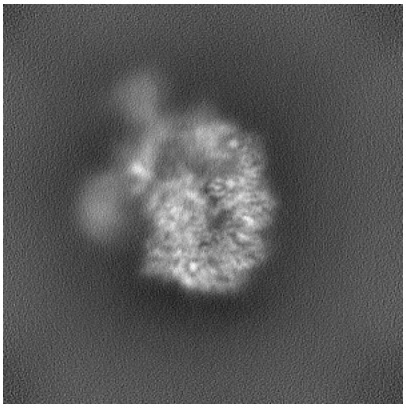


Y

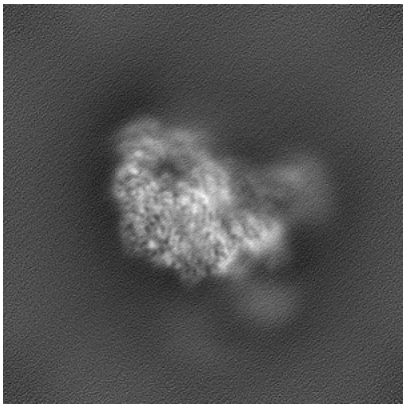


Z

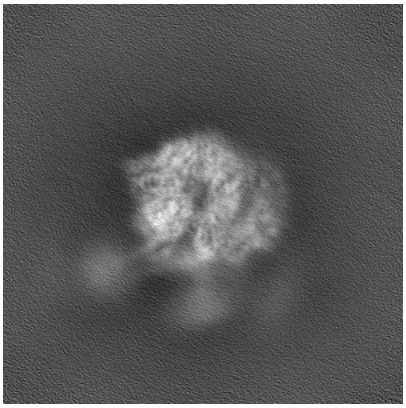
6.1.2 Raw map



X



Y

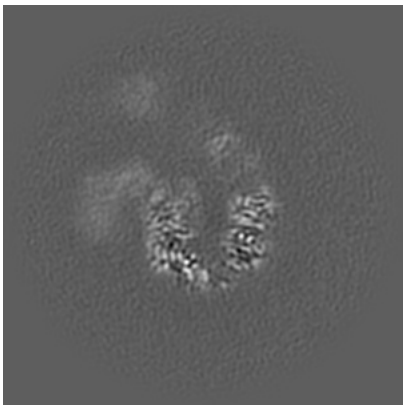


Z

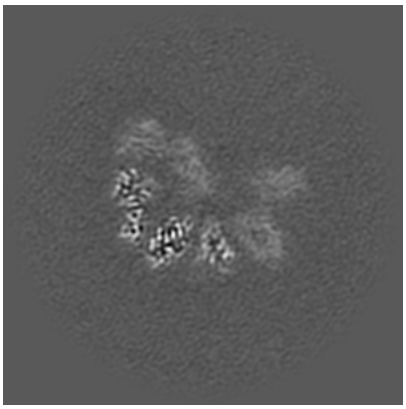
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

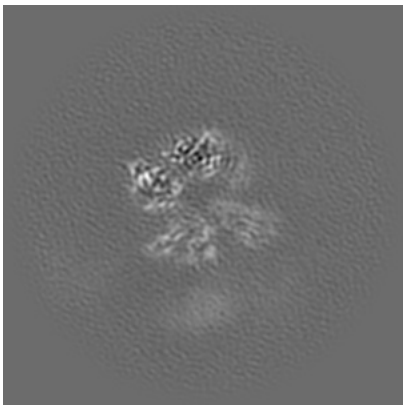
6.2.1 Primary map



X Index: 168

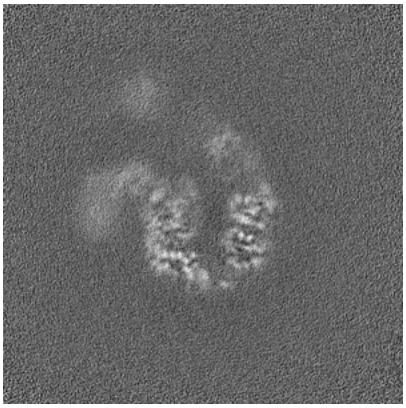


Y Index: 168

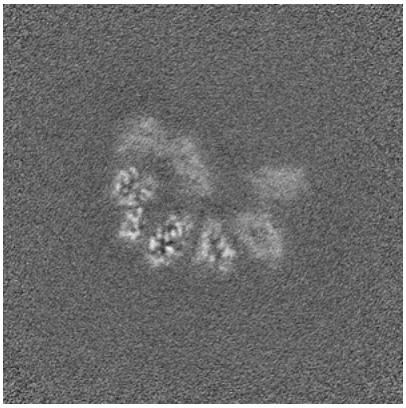


Z Index: 168

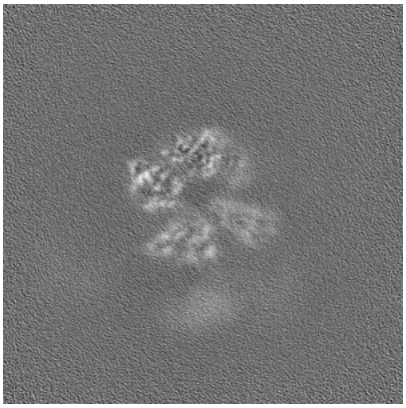
6.2.2 Raw map



X Index: 168



Y Index: 168

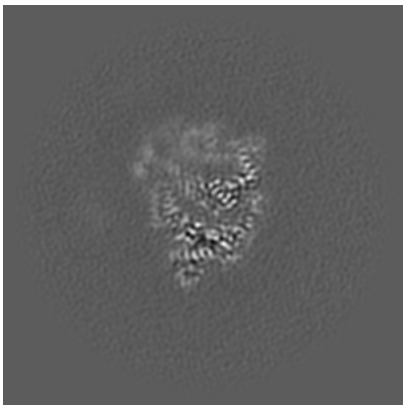


Z Index: 168

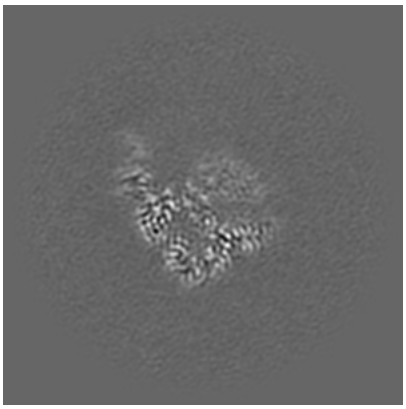
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



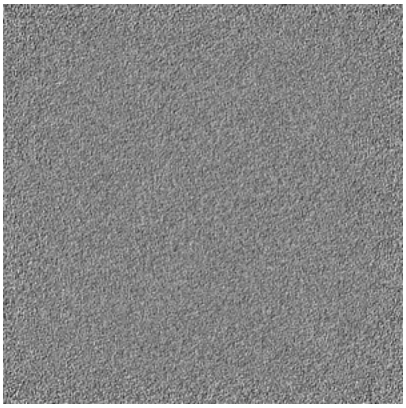
X Index: 134



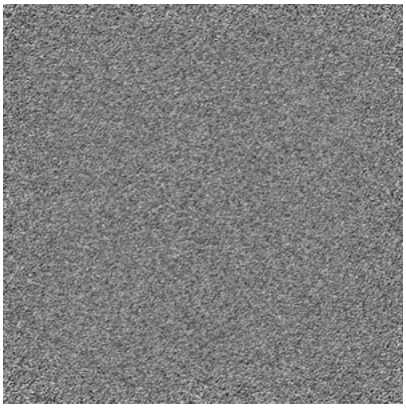
Y Index: 200

Z Index: 116

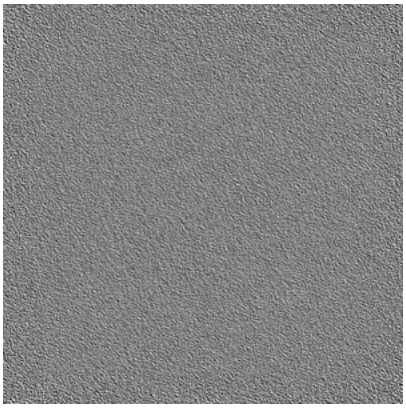
6.3.2 Raw map



X Index: 0



Y Index: 0

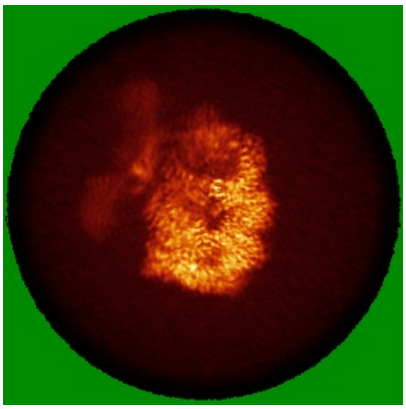


Z Index: 0

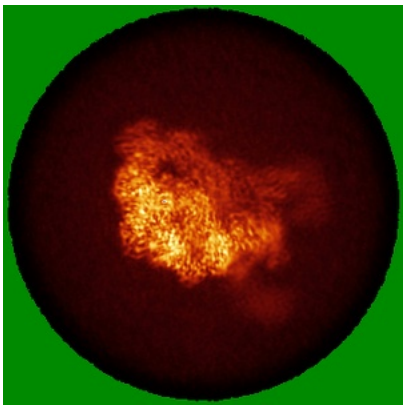
The images above show the largest variance slices of the map in three orthogonal directions.

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

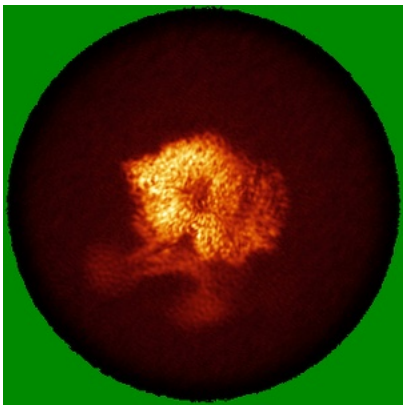
6.4.1 Primary map



X

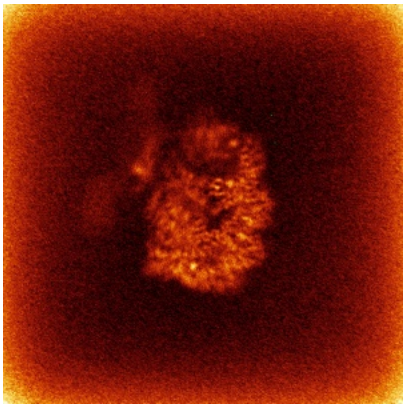


Y

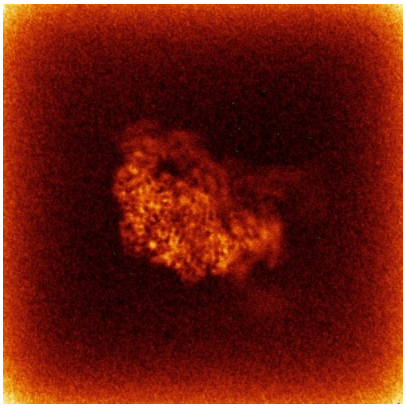


Z

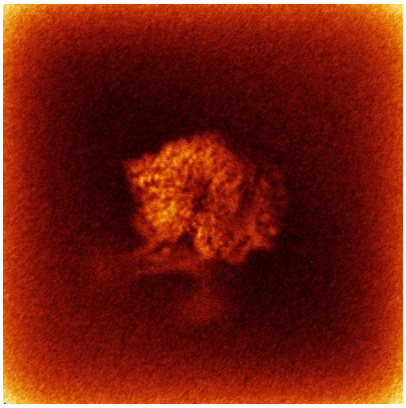
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.17. 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.

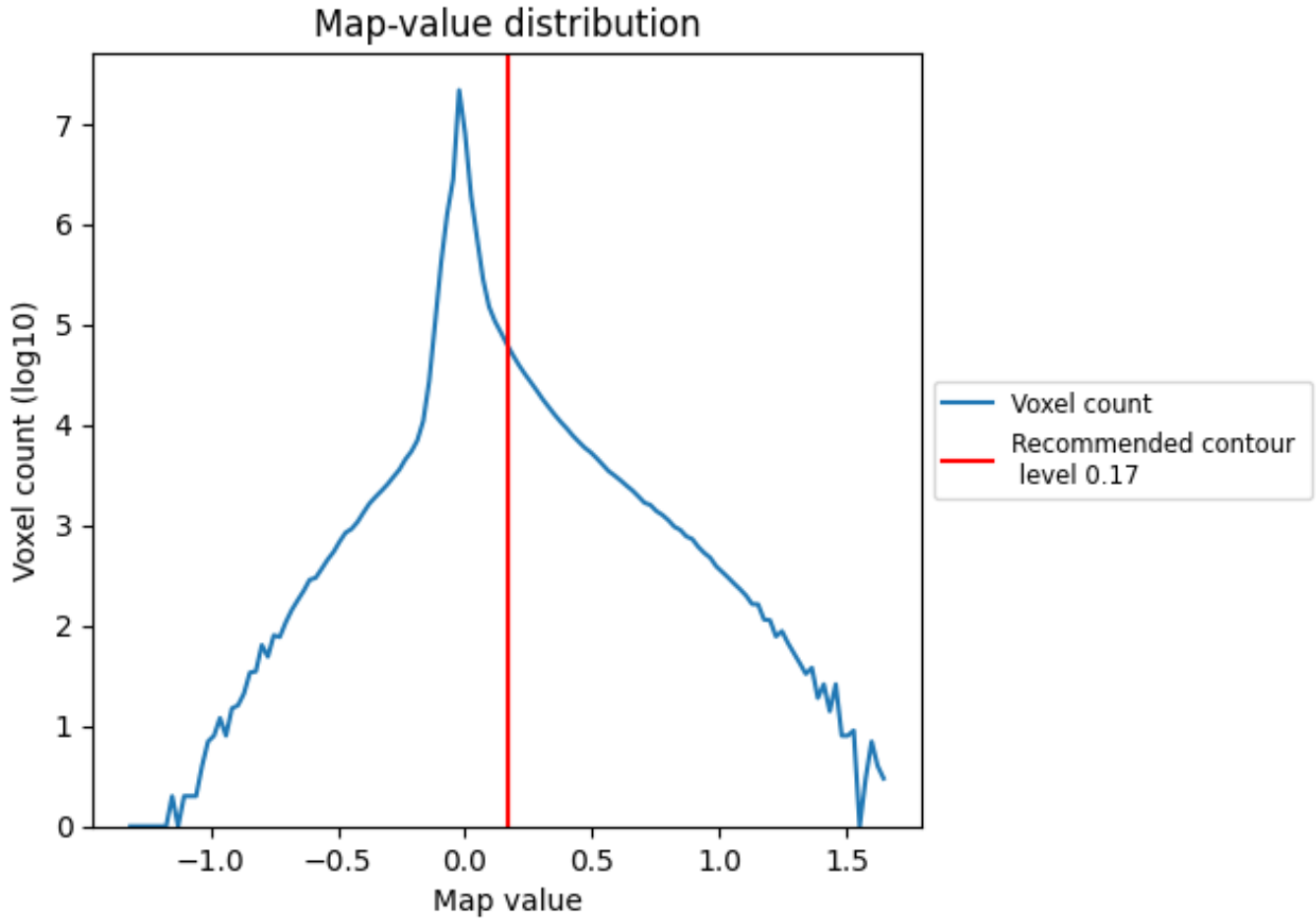
6.6 Mask visualisation (i)

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

7 Map analysis

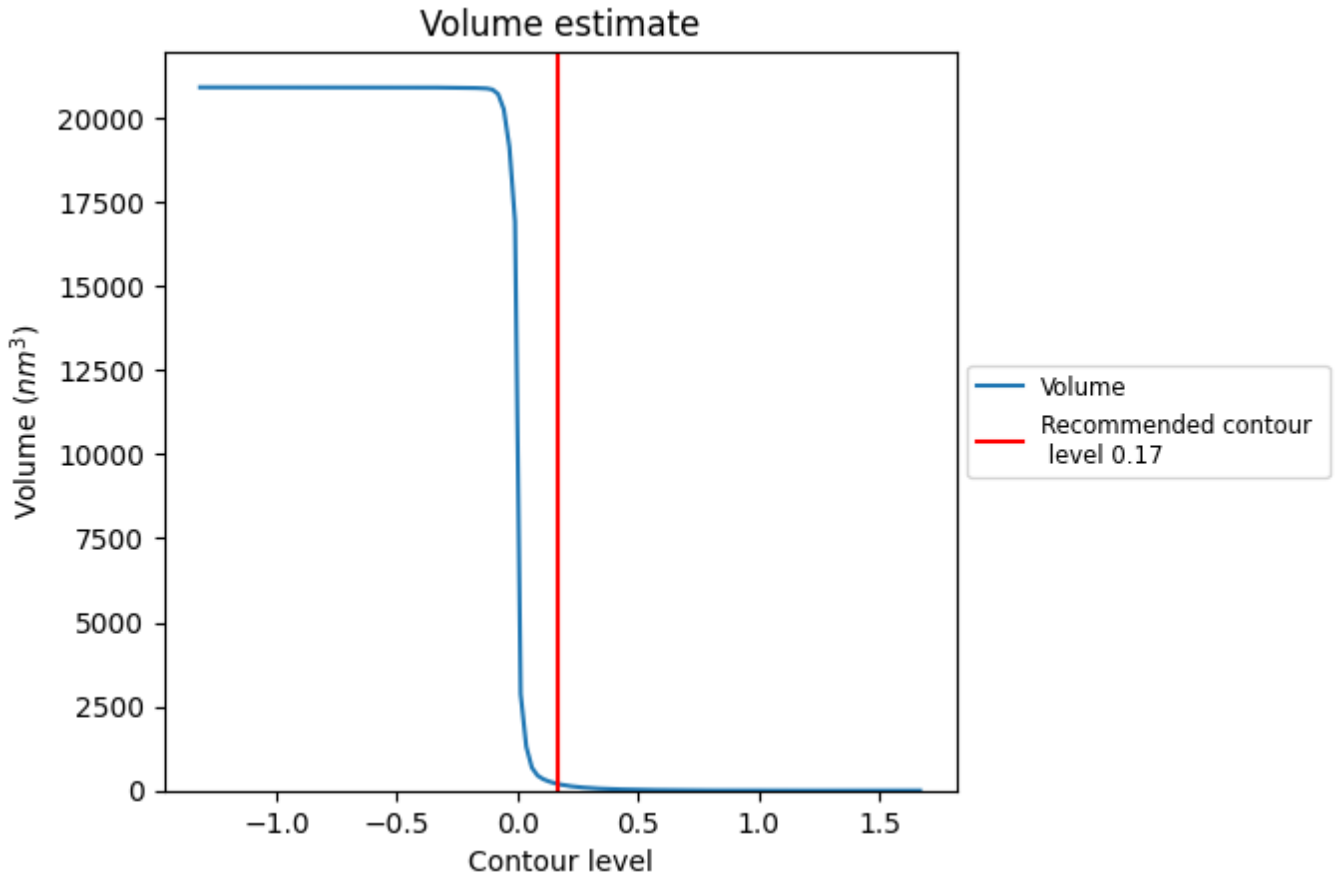
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

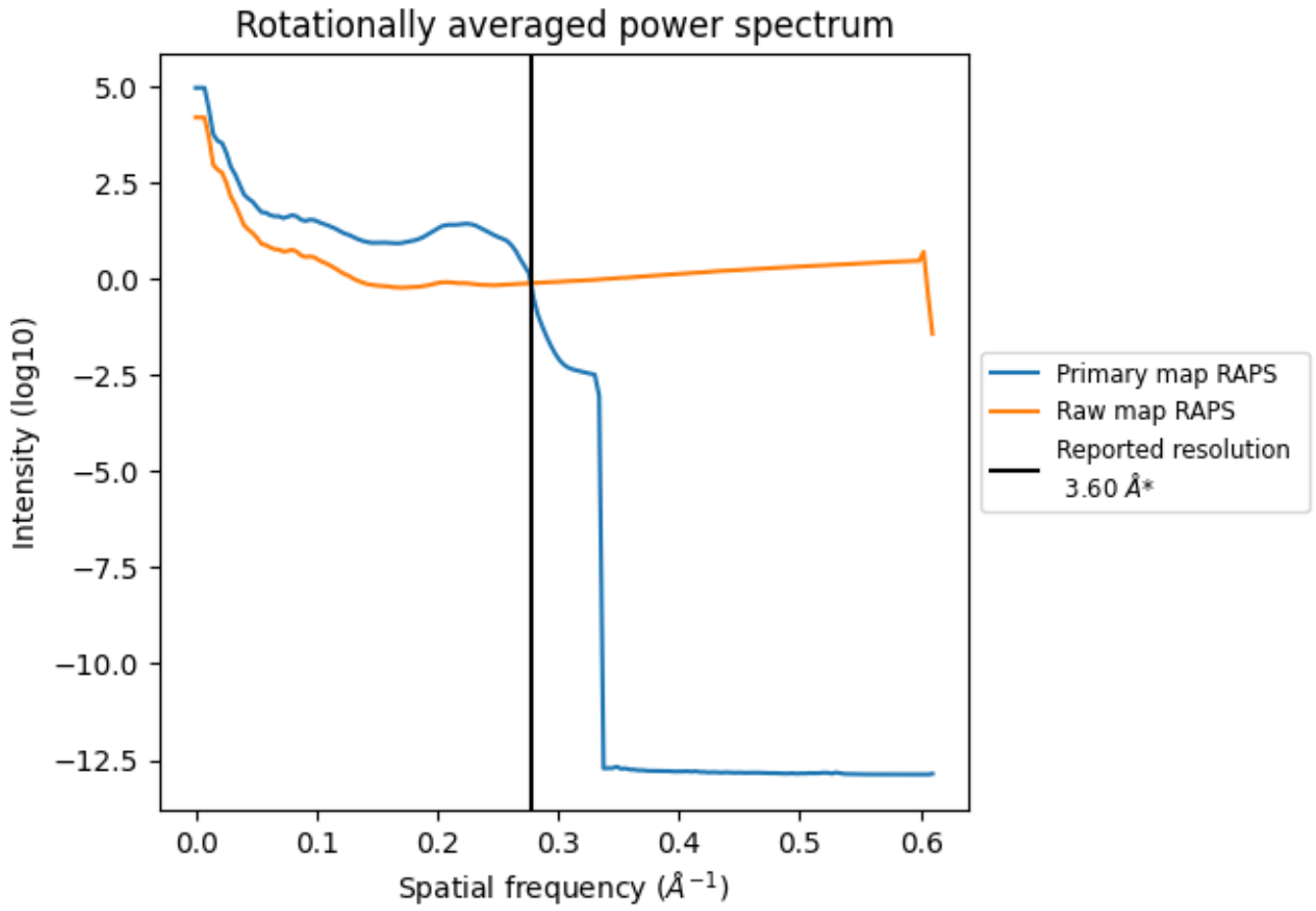
7.2 Volume estimate



The volume at the recommended contour level is 193 nm^3; this corresponds to an approximate mass of 174 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)

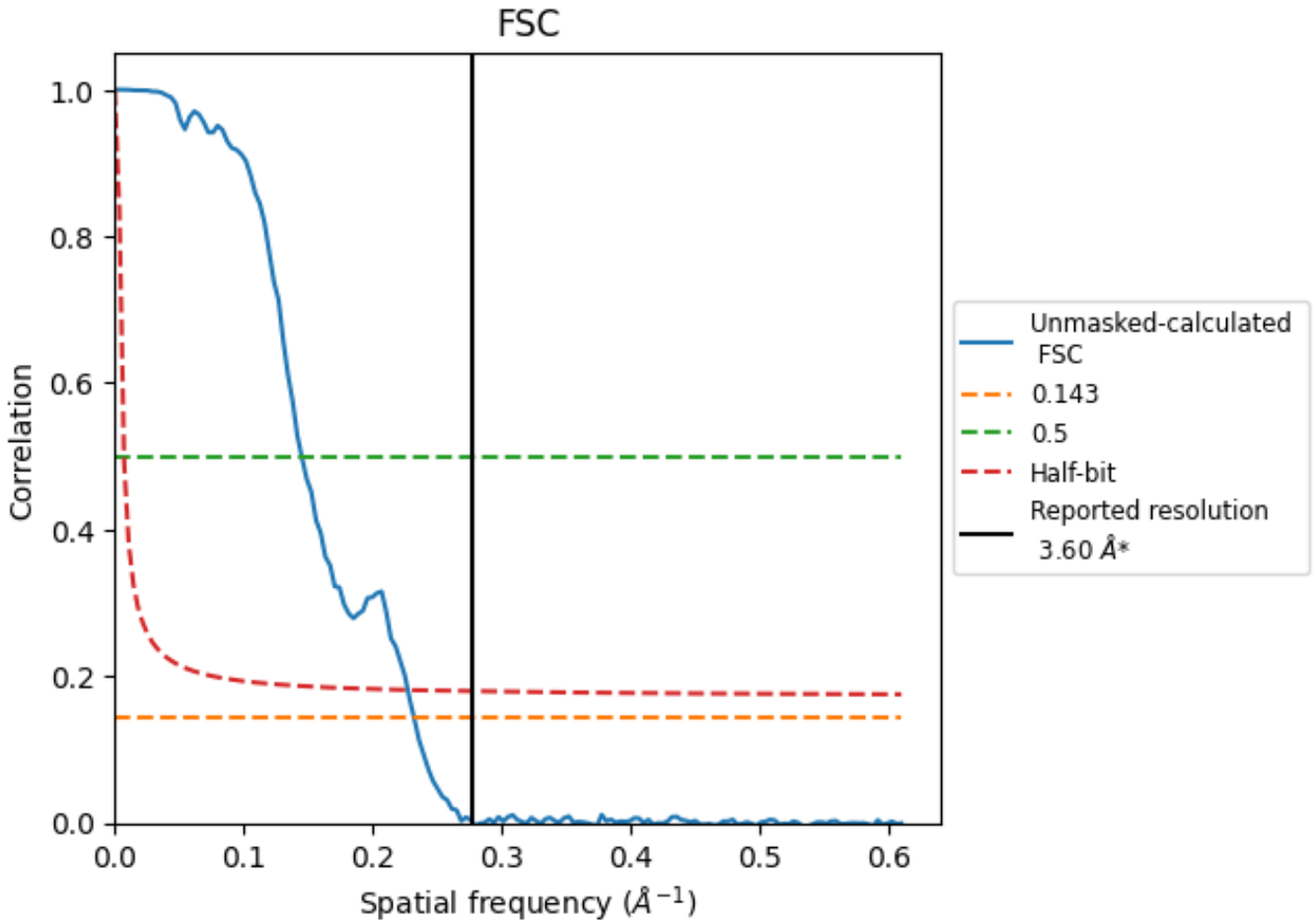


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

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 0.278 Å^{-1}

8.2 Resolution estimates (i)

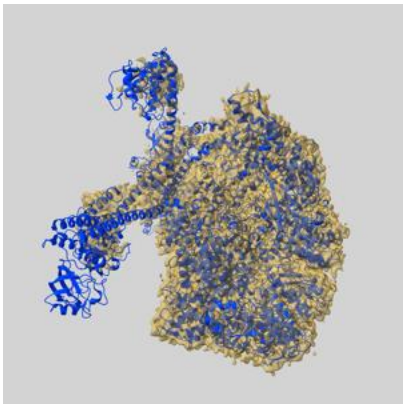
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.31	6.90	4.40

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.31 differs from the reported value 3.6 by more than 10 %

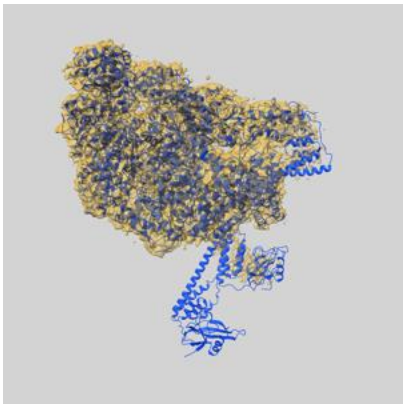
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-34113 and PDB model 7YUW. Per-residue inclusion information can be found in section 3 on page 5.

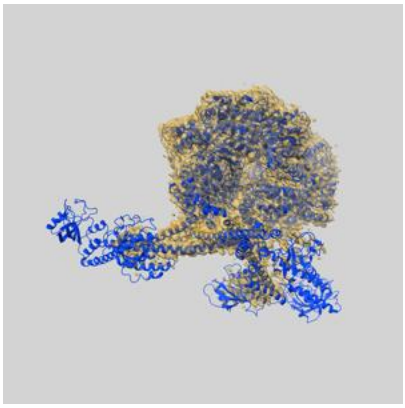
9.1 Map-model overlay



X



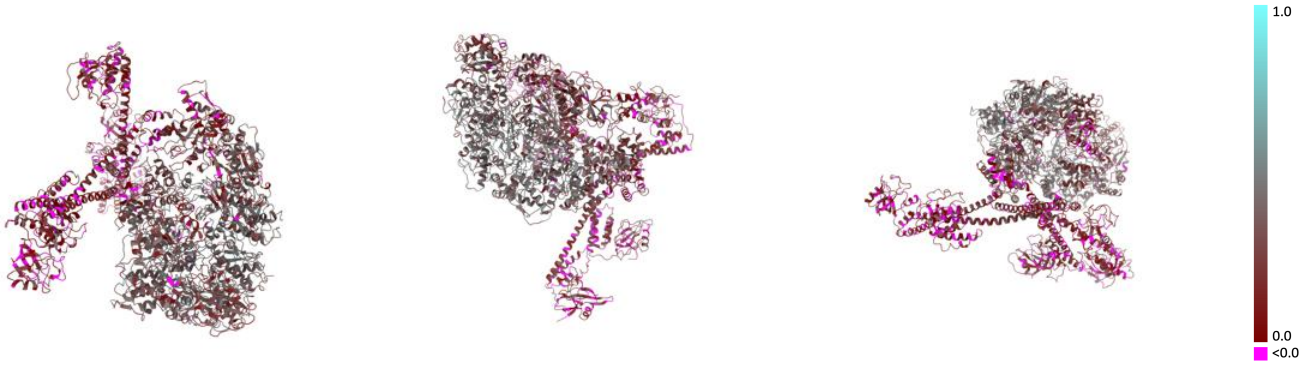
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.17 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

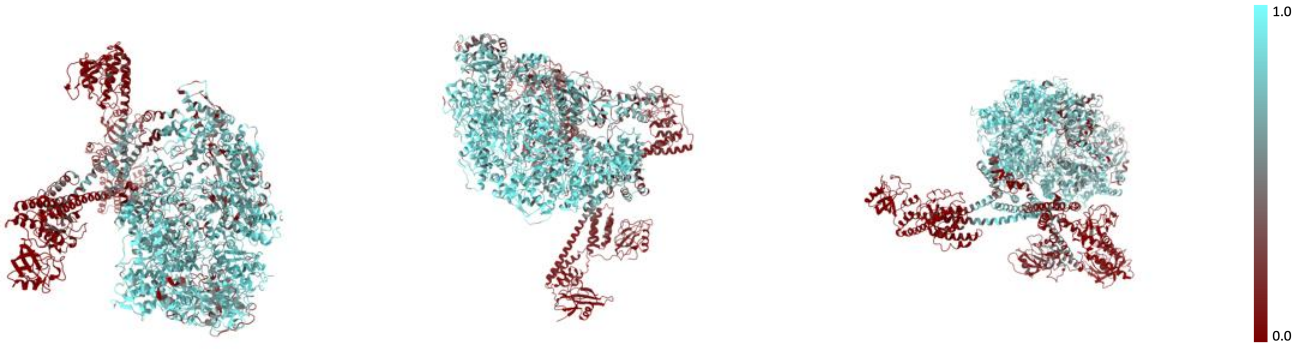
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

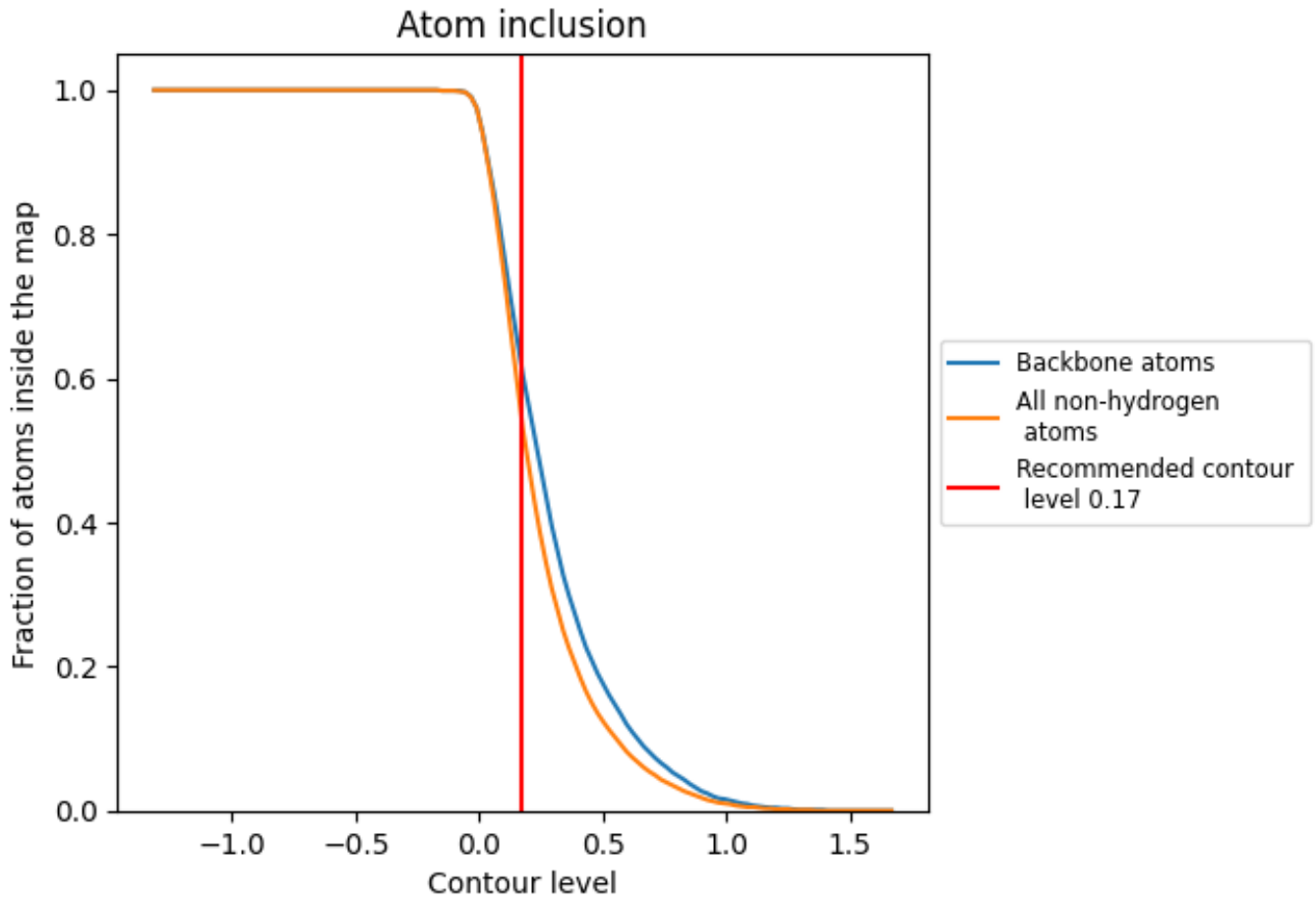
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.17).

9.4 Atom inclusion (i)



At the recommended contour level, 62% of all backbone atoms, 55% 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 (0.17) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5470	0.2830
A	0.4960	0.2490
B	0.5700	0.3150
C	0.6160	0.3280
D	0.5890	0.3130
E	0.4630	0.2070