Full wwPDB EM Validation Report ⓘ

May 18, 2025 – 09:07 AM EDT

PDB ID	:	8E6R / pdb_00008e6r
EMDB ID	:	EMD-27923
Title	:	Human TRPM2 ion channel in 1 mM dADPR
Authors	:	Wang, L.; Fu, T.M.; Xia, S.; Wu, H.
Deposited on	:	2022-08-23
Resolution	:	5.60 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:

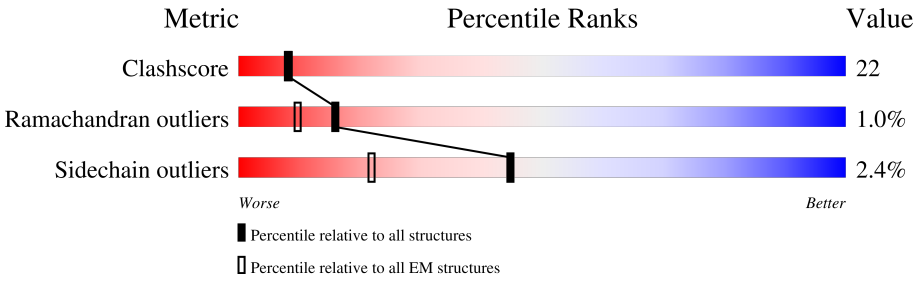
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 5.60 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	1503	36% 51% 35% • 12%
1	B	1503	37% 51% 35% • 12%
1	C	1503	36% 51% 35% • 12%
1	D	1503	38% 51% 35% • 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	AR6	A	1602	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	AR6	B	1602	X	-	-	-
3	AR6	C	1602	X	-	-	-
3	AR6	D	1602	X	-	-	-

2 Entry composition (i)

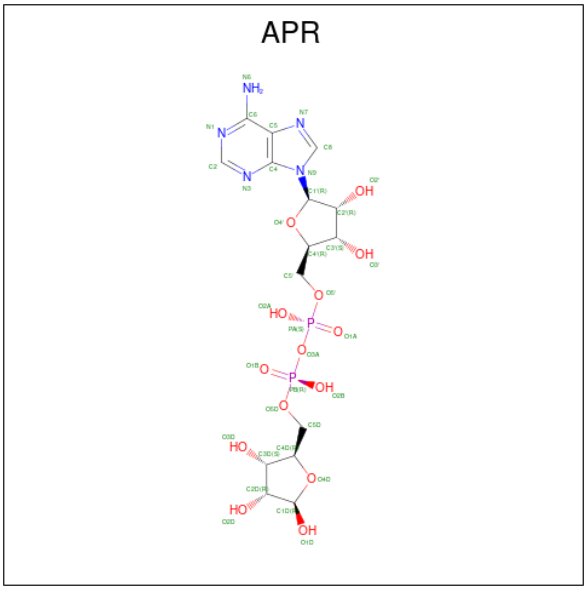
There are 3 unique types of molecules in this entry. The entry contains 42336 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Transient receptor potential cation channel subfamily M member 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1323	Total	C	N	O	S	0	0
			10523	6796	1829	1848	50		
1	B	1323	Total	C	N	O	S	0	0
			10523	6796	1829	1848	50		
1	C	1323	Total	C	N	O	S	0	0
			10523	6796	1829	1848	50		
1	D	1323	Total	C	N	O	S	0	0
			10523	6796	1829	1848	50		

- Molecule 2 is ADENOSINE-5-DIPHOSPHORIBOSE (CCD ID: APR) (formula: $C_{15}H_{23}N_5O_{14}P_2$).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			26	10	5	9	2	
2	B	1	Total	C	N	O	P	0
			26	10	5	9	2	

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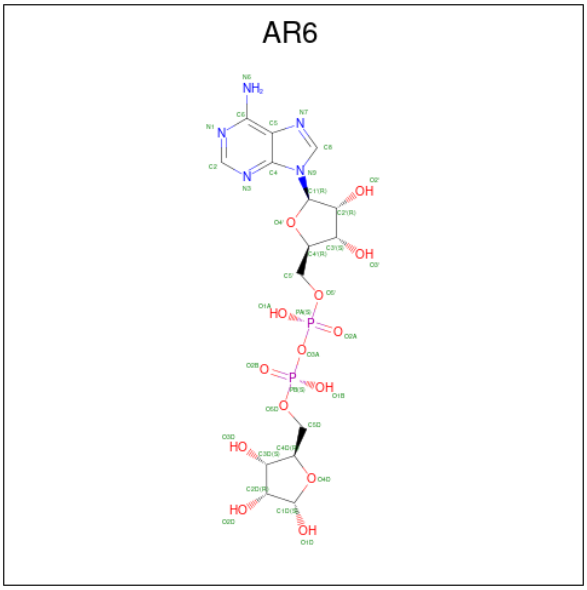
Mol	Chain	Residues	Atoms					AltConf
2	C	1	Total	C	N	O	P	0
			26	10	5	9	2	
2	D	1	Total	C	N	O	P	0
			26	10	5	9	2	

- Molecule 3 is [(2R,3S,4R,5R)-5-(6-AMINOPURIN-9-YL)-3,4-DIHYDROXY-OXOLAN-2-YL]METHYL[HYDROXY-[[(2R,3S,4R,5S)-3,4,5-TRIHYDROXYOXOLAN-2-YL]METHOXY]PHOSPHORYL] HYDROGEN PHOSPHATE (CCD ID: AR6) (formula: $C_{15}H_{23}N_5O_{14}P_2$).



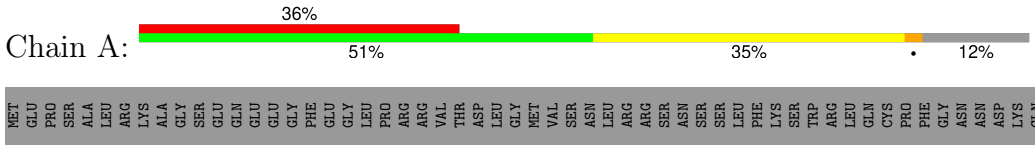
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			35	15	5	13	2	
3	B	1	Total	C	N	O	P	0
			35	15	5	13	2	
3	C	1	Total	C	N	O	P	0
			35	15	5	13	2	
3	D	1	Total	C	N	O	P	0
			35	15	5	13	2	

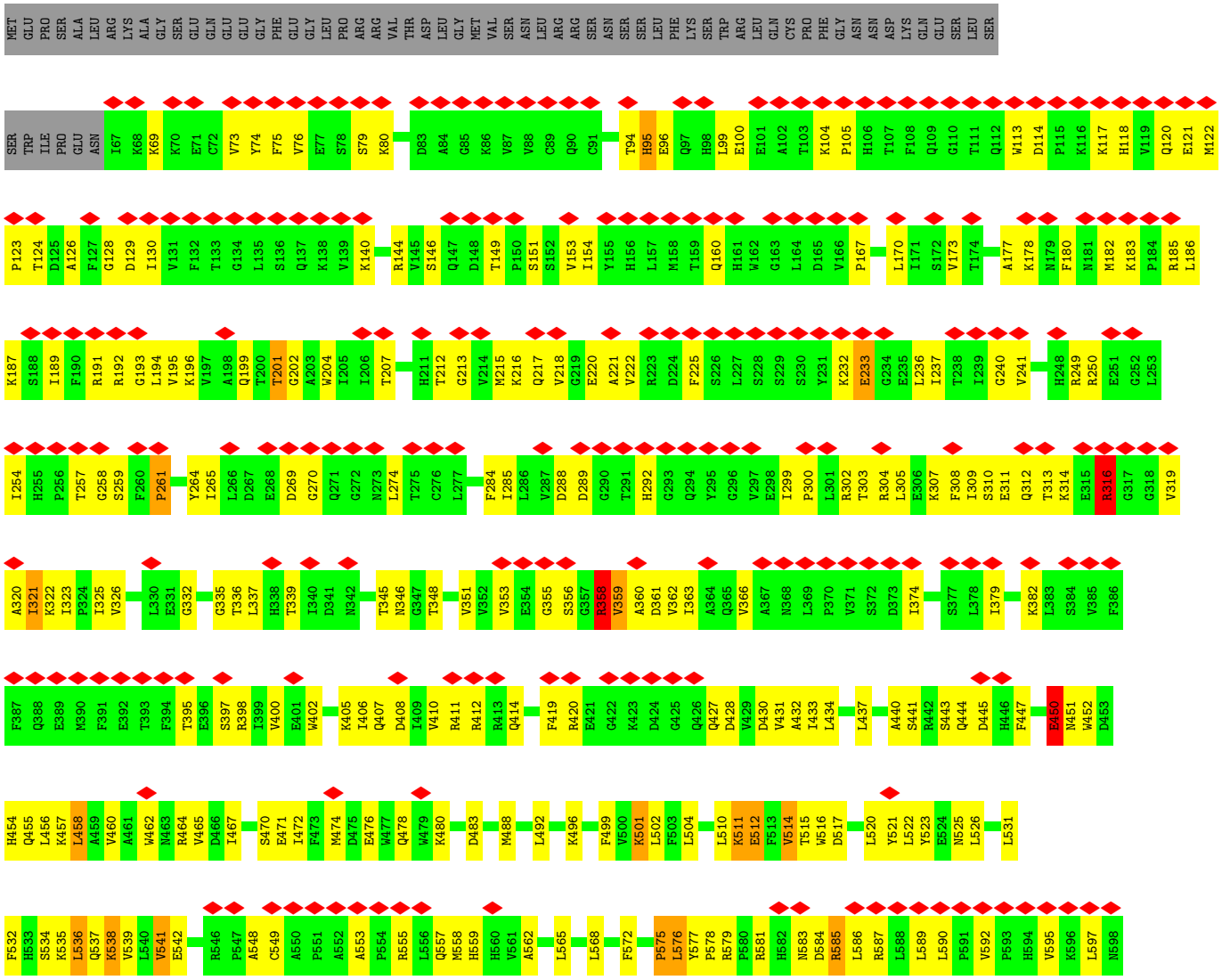
3 Residue-property plots (i)

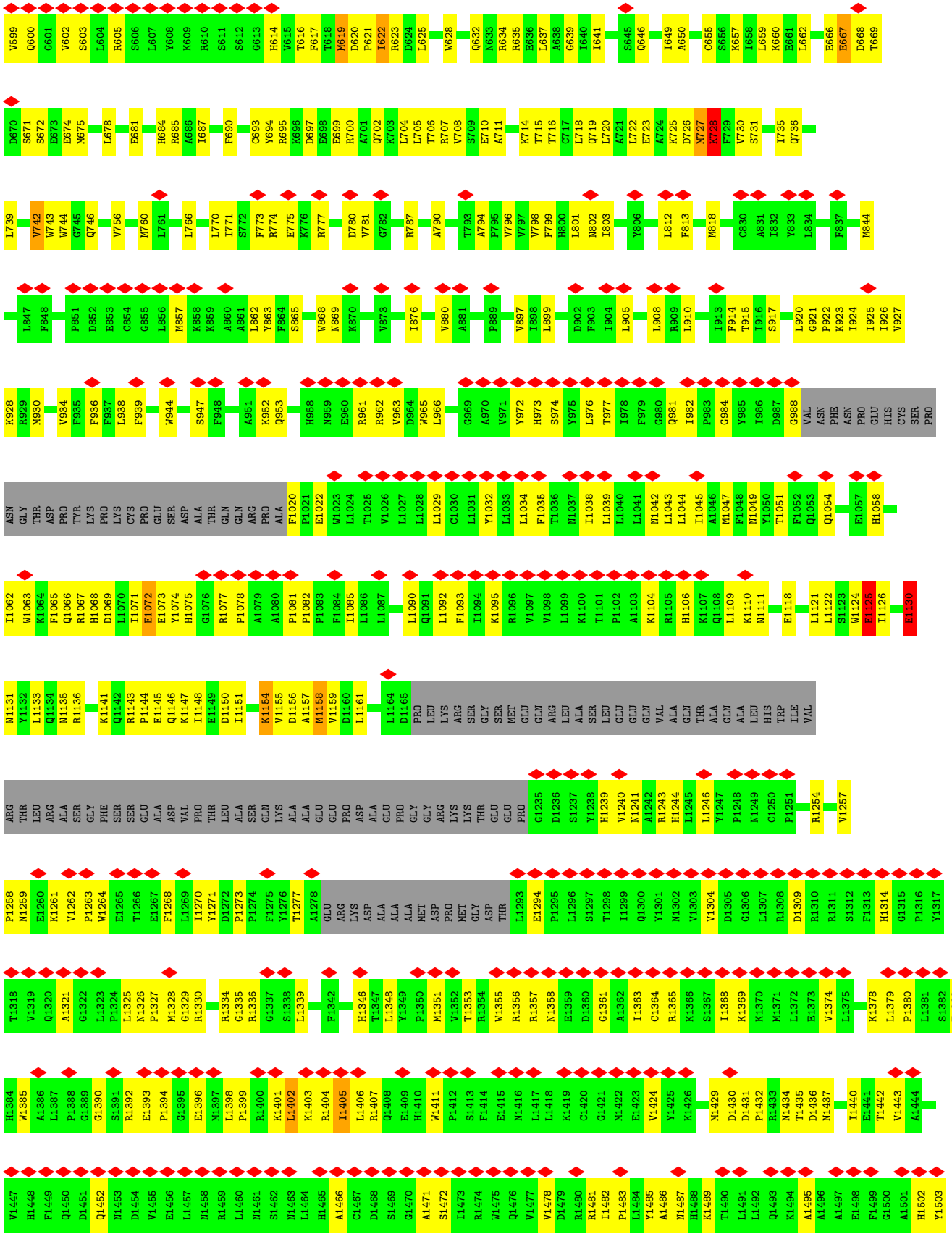
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Transient receptor potential cation channel subfamily M member 2

Chain A:

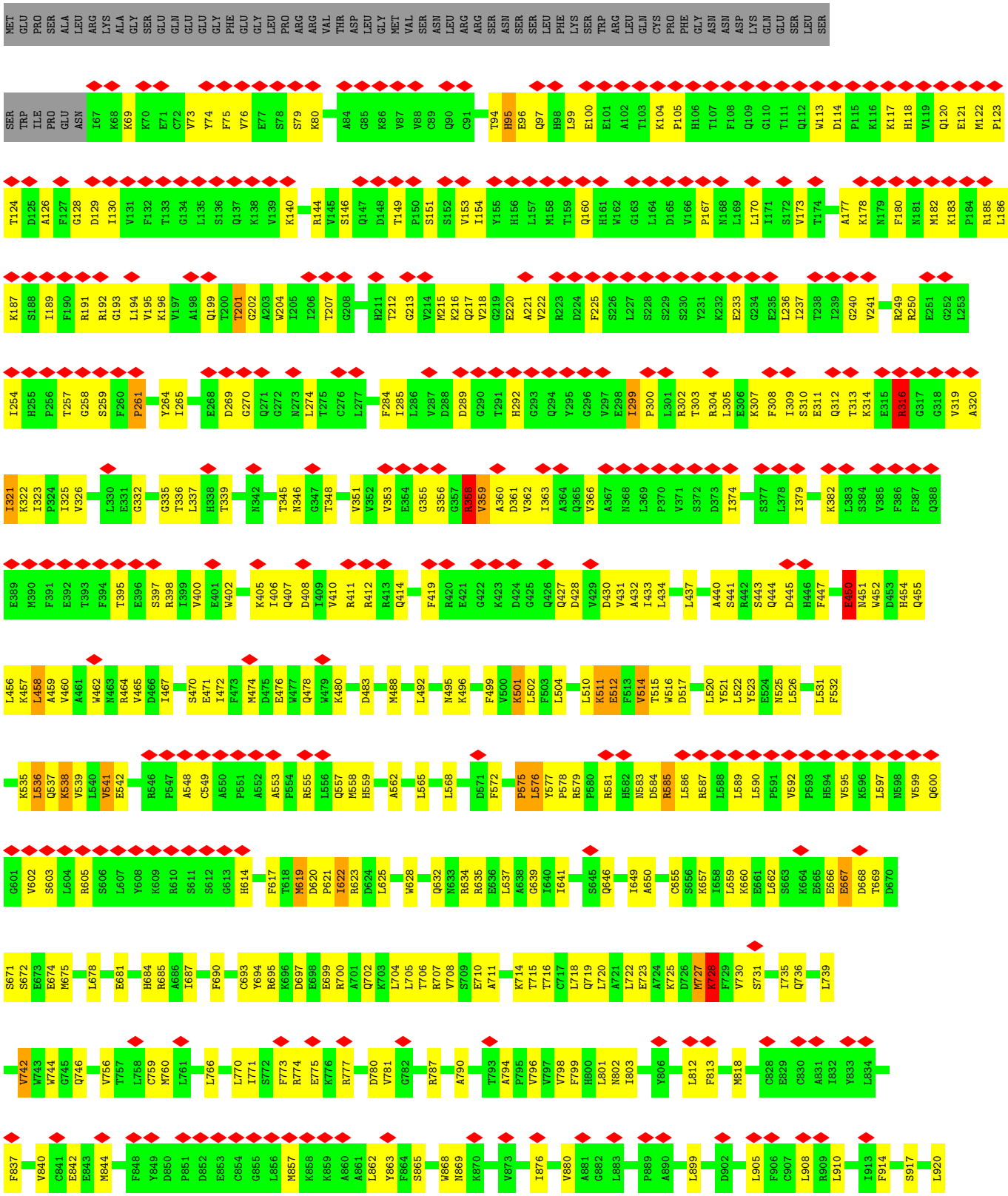


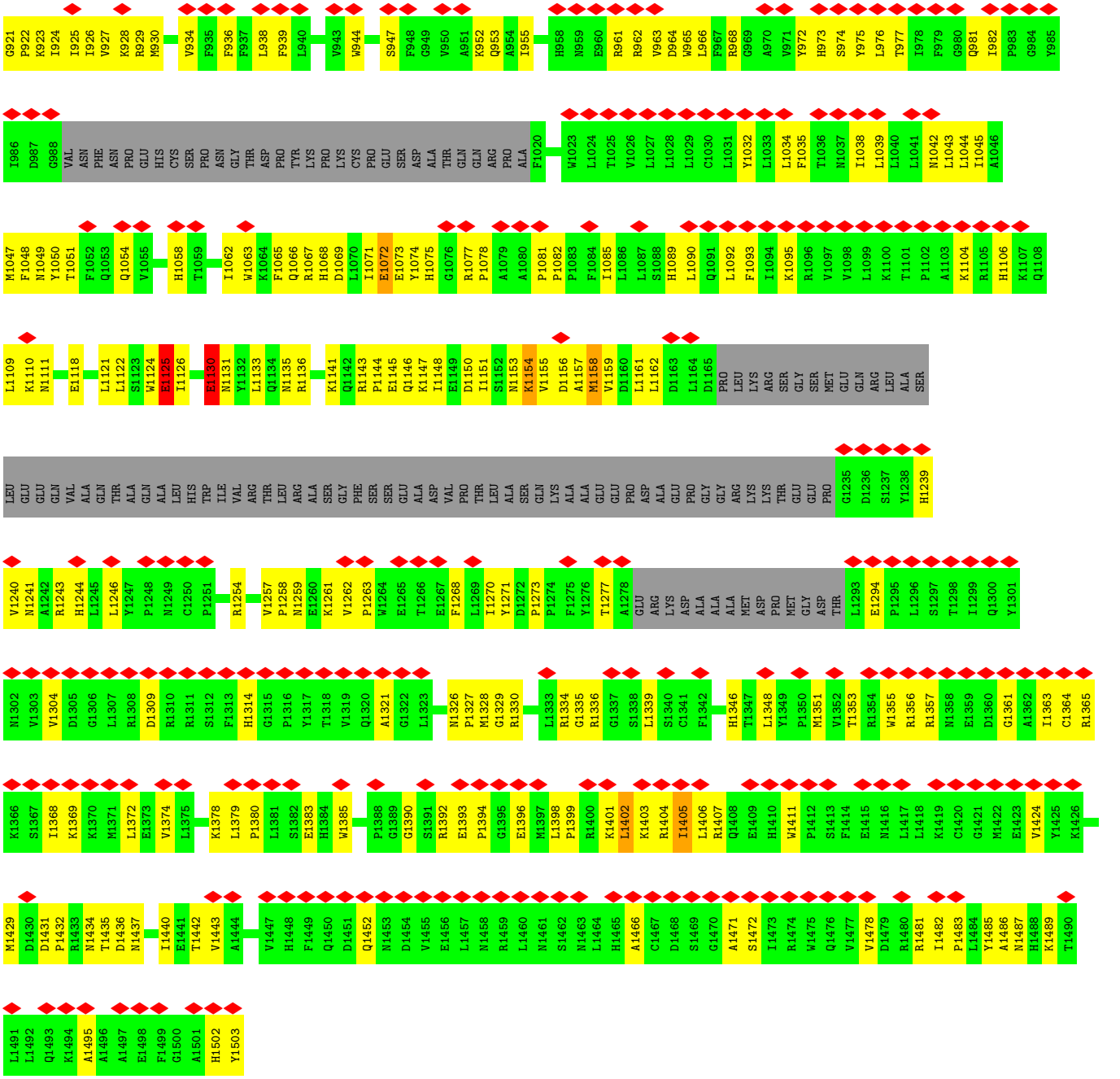




• Molecule 1: Transient receptor potential cation channel subfamily M member 2

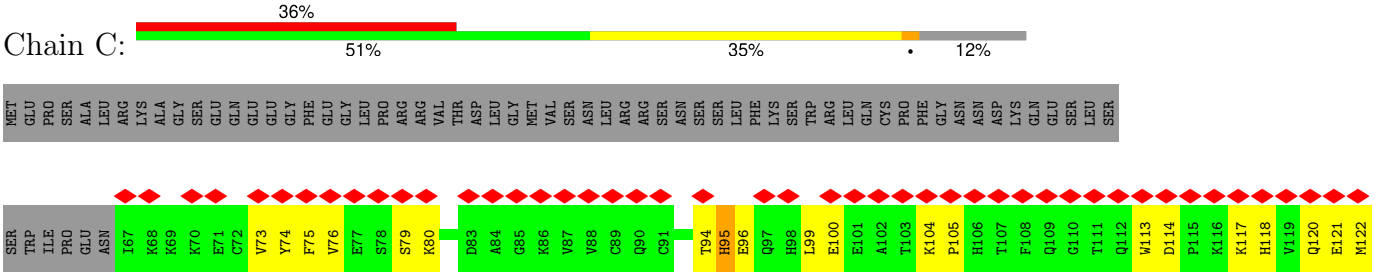
Chain B:

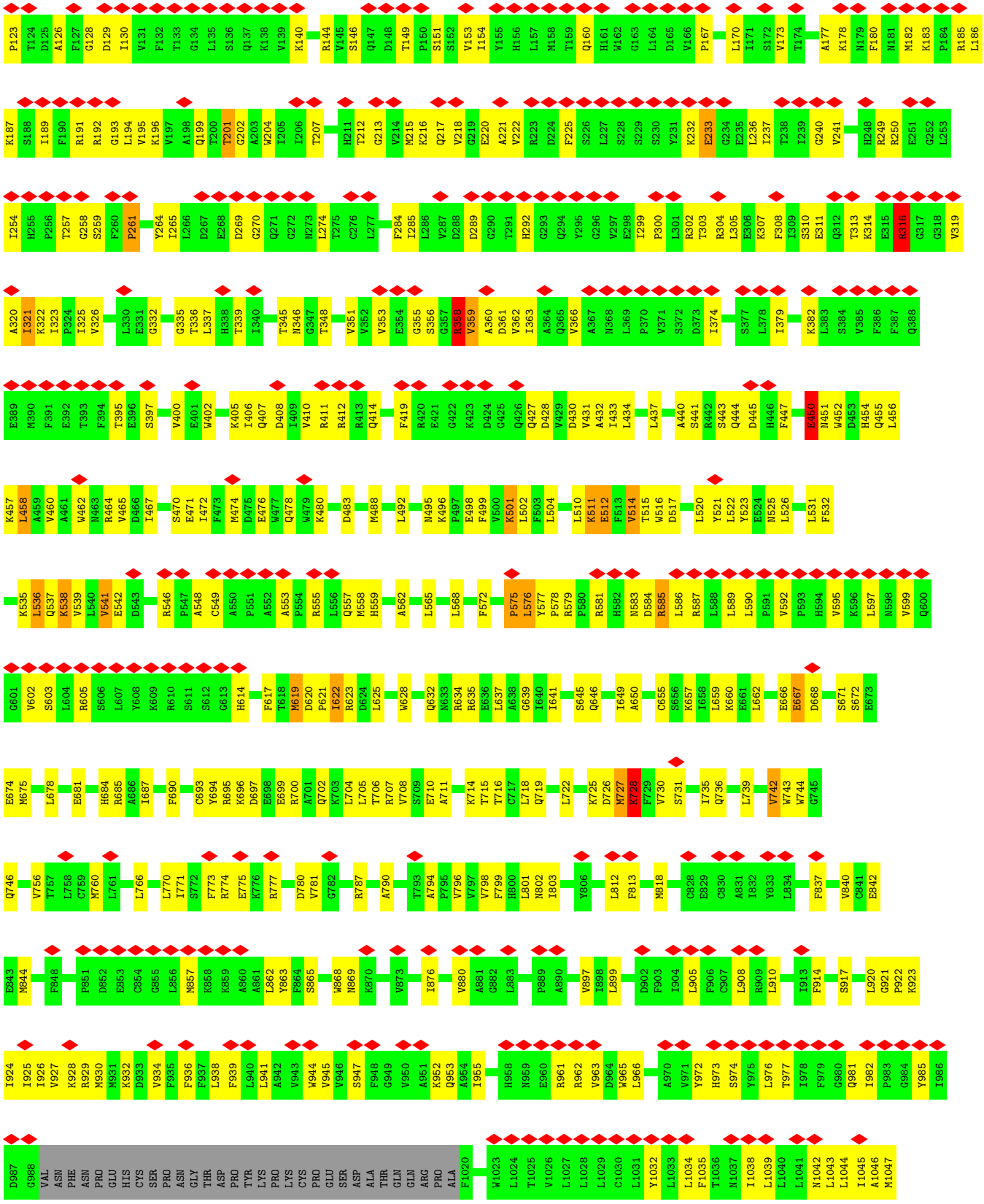




• Molecule 1: Transient receptor potential cation channel subfamily M member 2

Chain C:

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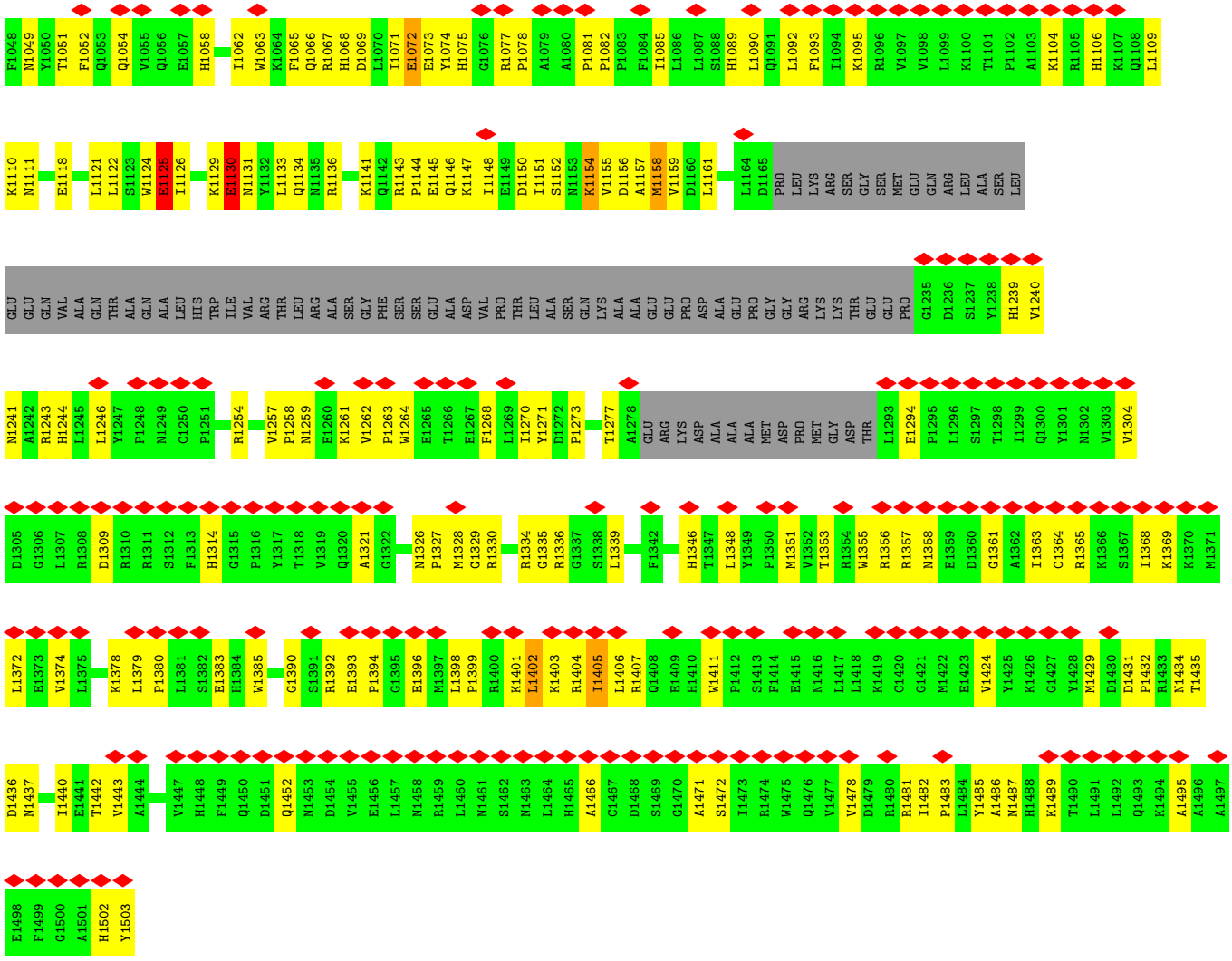
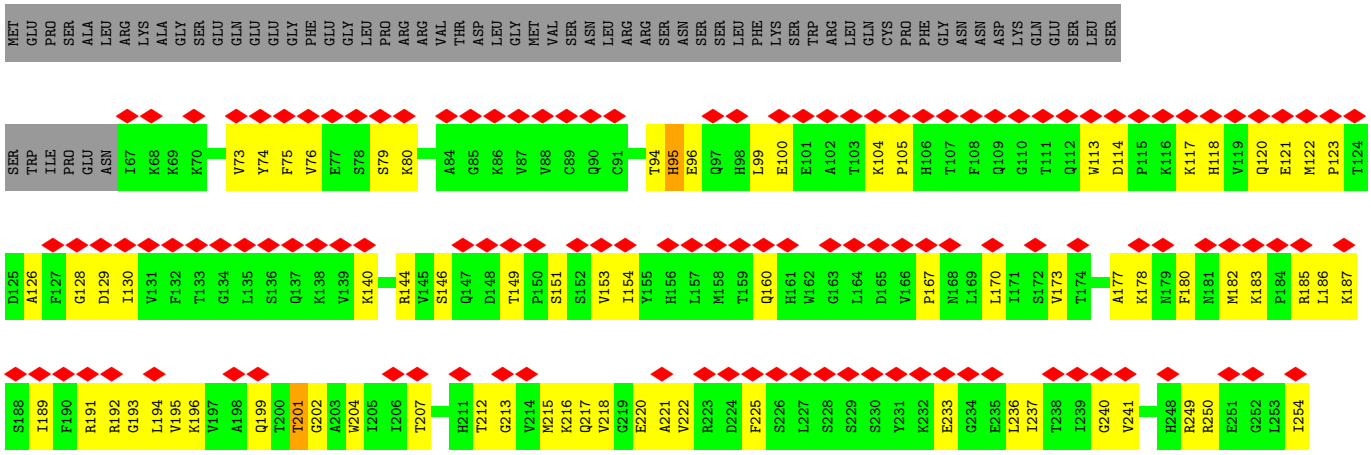
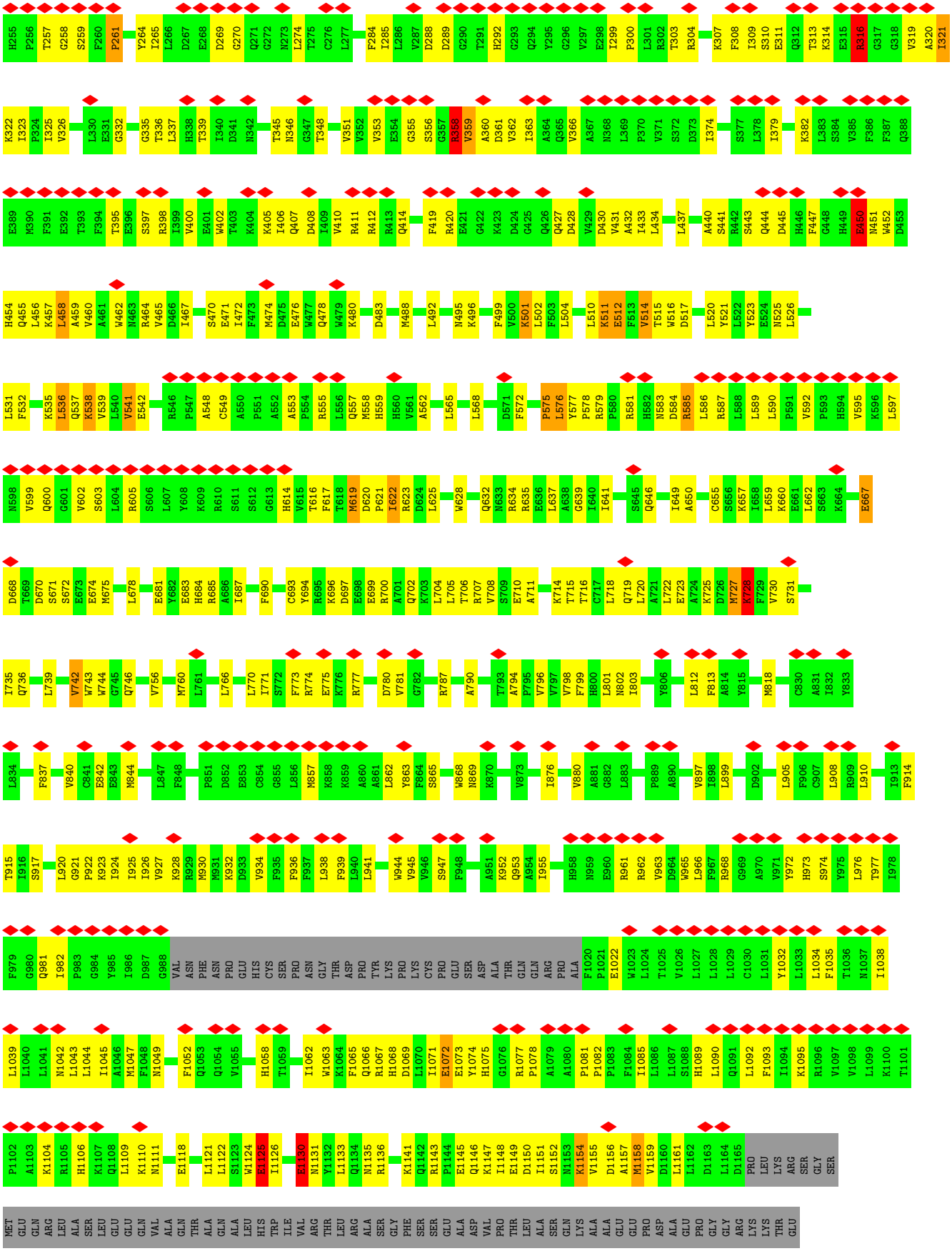
K187 S188 I189 F190 R191 R192 G193 L194 V195 K196 V197 A198 Q199 T200 T201 G202 A203 W204 I205 I206 T207 H211 T212 G213 V214 M215 K216 Q217 V218 G219 E220 A221 V222 R223 D224 F225 S226 L227 S228 S229 S230 Y231 K232 E233 G234 E235 L236 I237 T238 I239 G240 V241 H248 R249 R250 E251 G252 L253
I254 H255 P256 T257 G258 S259 F260 P261 Y264 I265 L266 D267 E268 D269 G270 Q271 G272 N273 L274 T275 C276 L277 F284 I285 L286 V287 D288 D289 G290 T291 H292 G293 Q294 Y295 G296 V297 E298 I299 P300 L301 R302 T303 R304 L305 E306 K307 F308 I309 S310 E311 Q312 T313 K314 E315 R316 G317 G318 V319
A320 I321 K322 I323 P324 I325 V326 L330 E331 G332 G335 T336 L337 H338 T339 I340 T345 N346 G347 T348 V351 V352 V353 E354 G355 S356 G357 R358 V359 A360 D361 V362 I363 A364 Q365 V366 A367 N368 L369 P370 V371 S372 D373 I374 S377 L378 I379 K382 L383 S384 V385 F386 F387 Q388
E389 M390 F391 E392 T393 F394 T395 E396 S397 V400 E401 W402 K405 I406 Q407 D408 I409 V410 R411 R412 R413 Q414 F419 R420 E421 G422 K423 D424 G425 Q426 Q427 D428 V429 D430 V431 A432 I433 L434 L437 A440 S441 R442 S443 Q444 D445 H446 F447 E450 N451 W452 D453 H454 Q455 L456
K457 L458 A459 V460 A461 W462 N463 R464 V465 D466 I467 S470 E471 I472 F473 M474 D475 E476 W477 Q478 W479 K480 D483 M488 L492 N495 K496 P497 E498 F499 V500 K501 L502 F503 L504 L510 K511 E512 F513 V514 T515 W516 D517 L520 Y521 L522 Y523 E524 N525 L526 L531 F532
K535 L536 Q537 K538 V539 L540 V541 E542 D543 R546 P547 A548 C549 A550 P551 A552 A553 P554 R555 L556 Q557 M558 H559 A562 L565 L568 F572 P575 L576 Y577 P578 R579 P580 R581 H582 N583 D584 R585 L586 R587 L588 L589 L590 P591 V592 P593 H594 V595 K596 L597 N598 V599 Q600
G601 V602 S603 L604 R605 S606 L607 Y608 K609 R610 S611 S612 G613 H614 F617 T618 M619 D620 P621 I622 R623 D624 L625 W628 Q632 W633 R634 R635 E636 L637 A638 G639 I640 I641 S645 Q646 I649 A650 C655 S656 K657 I658 L659 K660 E661 L662 E666 E667 D668 S671 S672 E673
E674 M675 L678 E681 H684 R685 A686 I687 F690 C693 Y694 R695 K696 D697 E698 E699 R700 A701 Q702 K703 L704 L705 T706 R707 V708 S709 E710 A711 K714 T715 T716 C717 L718 Q719 L722 K725 D726 M727 K728 F729 V730 S731 I735 Q736 L739 V742 W743 W744 G745
Q746 V756 T757 L758 C759 M760 L761 L766 L770 I771 S772 F773 R774 E775 K776 R777 D780 V781 G782 R787 A790 T793 A794 P795 V796 V797 V798 F799 H800 L801 N802 I803 Y806 L812 F813 M818 C828 E829 C830 A831 I832 Y833 L834 F837 V840 C841 E842
E843 M844 F848 P851 D852 E853 C854 G855 L856 M857 K858 K859 A860 A861 L862 Y863 F864 S865 W868 N869 K870 V873 I876 V880 A881 G882 L883 P889 A890 V897 I898 L899 D902 F903 I904 L905 F906 C907 L908 R909 L910 T913 F914 S917 L920 G921 P922 K923
I924 I925 I926 V927 K928 R929 M930 M931 K932 D933 V934 F935 F936 F937 L938 F939 L940 L941 A942 V943 W944 V945 V946 S947 F948 G949 V950 A951 K952 Q953 A954 I955 H958 N959 E960 R961 R962 V963 D964 W965 L966 A970 V971 Y972 H973 S974 Y975 L976 T977 I978 F979 G980 Q981 I982 P983 G984 Y985 I986
D987 G988 VAL ASN PHE ASN PRO GLU HIS CYS SER PRO ASN GLY THR ASP PRO TYR LYS PRO LYS CYS PRO GLU GLN SER ASP ALA THR GLN GLN ARG PRO ALA F1020 W1023 L1024 T1025 V1026 L1027 L1028 L1029 C1030 L1031 Y1032 L1033 L1034 F1035 T1036 N1037 I1038 L1039 L1040 L1041 N1042 L1043 L1044 I1045 A1046 M1047



• Molecule 1: Transient receptor potential cation channel subfamily M member 2

Chain D:

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K322 I323 P324 I325 V326 L330 E331 G332 G335 T336 L337 H338 T339 I340 D341 N342 T345 N346 G347 T348 V351 V352 V353 E354 G355 S356 G357 R358 V359 A360 D361 V362 I363 A364 Q365 V366 A367 N368 L369 P370 V371 S372 D373 I374 S377 L378 I379 K382 L383 S384 V385 F386 F387 Q388
E389 M390 F391 E392 T393 P394 T395 E396 S397 R398 I399 V400 E401 W402 T403 K404 K405 I406 Q407 D408 I409 V410 R411 R412 R413 Q414 F419 R420 F421 G422 K423 D424 G425 Q426 Q427 D428 V429 D430 V431 A432 I433 L434 L437 A440 S441 R442 S443 Q444 D445 H446 F447 G448 H449 E450 N451 W452 D453
H454 Q455 L456 K457 L458 A459 V460 A461 W462 N463 R464 V465 D466 I467 S470 E471 I472 F473 M474 D475 E476 W477 Q478 W479 K480 D483 M488 L492 N495 K496 F499 V500 K501 L502 F503 L504 L510 K511 E512 F513 V514 T515 W516 D517 L520 Y521 L522 Y523 E524 N525 L526
L531 F532 K535 L536 Q537 K538 V539 L540 V541 E542 R546 P547 A548 C549 A550 P551 A552 A553 P554 R555 L556 Q557 M558 H559 H560 V561 A562 L565 L568 D571 F572 P575 L576 Y577 P578 R579 P580 R581 H582 N583 D584 R585 L586 R587 L588 L589 L590 P591 V592 P593 H594 V595 K596 L597
N598 V599 Q600 G601 V602 S603 L604 R605 S606 L607 Y608 K609 R610 S611 S612 G613 H614 V615 T616 F617 T618 M619 D620 P621 I622 R623 D624 L625 W628 Q632 N633 R634 R635 E636 L637 A638 G639 I640 I641 S645 Q646 I649 A650 C655 S656 K657 I658 L659 K660 E661 L662 S663 K664 E667
D668 T669 D670 S671 S672 E673 E674 H675 L678 E681 Y682 E683 H684 R685 A686 I687 F690 C693 Y694 R695 K696 D697 E698 E699 R700 A701 Q702 K703 L704 L705 T706 R707 V708 S709 E710 A711 K714 T715 T716 C717 L718 Q719 L720 A721 L722 E723 A724 K725 D726 M727 K728 F729 V730 S731
I735 Q736 L739 V742 W743 W744 G745 Q746 V756 M760 L761 L766 L770 I771 S772 F773 R774 E775 K776 R777 D780 V781 G782 R787 A790 T793 A794 F795 V796 V797 V798 F799 H800 L801 N802 I803 Y806 L812 F813 A814 Y815 M818 C830 A831 I832 Y833
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F979 G980 Q981 I982 P983 G984 Y985 I986 D987 G988 VAL ASN PHE ASN PRO GLU HIS CYS SER PRO ASN GLY THR ASP PRO PRO TYR LYS PRO LYS CYS PRO GLU SER ASP ALA THR GLN GLN ARG PRO ALA F1020 P1021 E1022 W1023 L1024 T1025 V1026 L1027 L1028 L1029 C1030 L1031 Y1032 L1033 L1034 F1035 T1036 N1037 I1038
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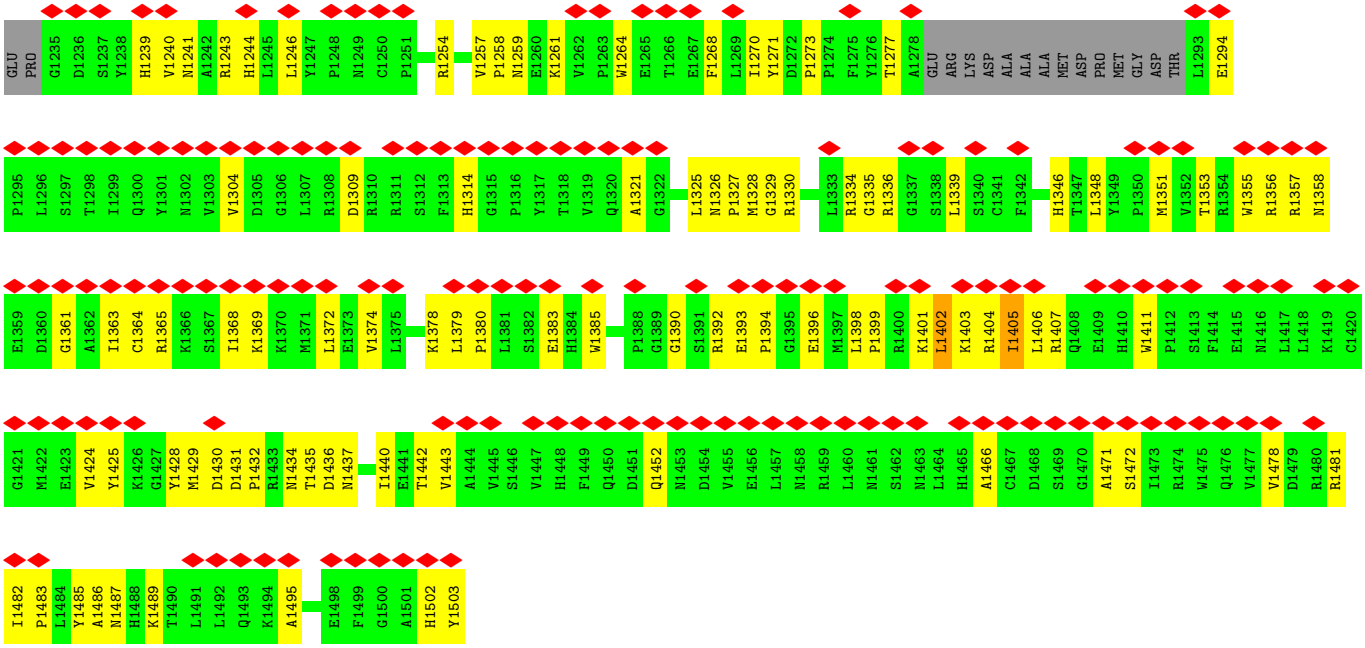
MET GLU GLN ARG LEU ALA SER LEU GLU GLU GLN VAL ALA GLN THR ALA GLN ALA LEU HIS TRP ILE VAL ARG THR LEU ARG ALA SER GLY PHE SER SER GLU ALA ASP VAL PRO THR LEU ALA SER GLN LYS ALA ALA GLU GLU PRO ASP ALA GLU PRO GLY GLY ARG LYS LYS THR GLU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P1295 L1296 S1297 T1298 I1299 Q1300 Y1301 N1302 V1303 V1304 D1305 G1306 L1307 R1308 D1309 R1310 R1311 S1312 F1313 H1314 G1315 P1316 Y1317 T1318 V1319 Q1320 A1321 G1322 L1325 N1326 P1327 M1328 G1329 R1330 L1333 R1334 G1335 R1336 G1337 S1338 L1339 S1340 C1341 F1342 H1346 T1347 L1348 Y1349 P1350 M1351 V1352 T1353 R1354 W1355 R1356 R1357 N1358
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G1421 M1422 E1423 V1424 Y1425 K1426 G1427 Y1428 M1429 D1430 D1431 P1432 R1433 N1434 T1435 D1436 N1437 I1440 E1441 T1442 V1443 A1444 V1445 S1446 V1447 H1448 F1449 Q1450 D1451 Q1452 N1453 D1454 V1455 E1456 L1457 N1458 R1459 L1460 N1461 S1462 N1463 L1464 H1465 A1466 C1467 D1468 S1469 G1470 A1471 S1472 I1473 R1474 W1475 Q1476 V1477 V1478 D1479 R1480 R1481
I1482 P1483 L1484 Y1485 A1486 N1487 H1488 K1489 T1490 L1491 L1492 Q1493 K1494 A1495 E1498 F1499 G1500 A1501 H1502 Y1503

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	86858	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 ($e^-/Å^2$)	42	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.070	Depositor
Minimum map value	-0.025	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0118	Depositor
Map size (Å)	324.0, 324.0, 324.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: APR, AR6

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	0.19	0/10789	0.62	11/14649 (0.1%)
1	B	0.19	0/10789	0.62	11/14649 (0.1%)
1	C	0.19	0/10789	0.62	11/14649 (0.1%)
1	D	0.19	0/10789	0.62	11/14649 (0.1%)
All	All	0.19	0/43156	0.62	44/58596 (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
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	8

There are no bond length outliers.

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	316	ARG	CA-CB-CG	7.37	128.84	114.10
1	B	316	ARG	CA-CB-CG	7.36	128.82	114.10
1	A	316	ARG	CA-CB-CG	7.35	128.80	114.10
1	D	316	ARG	CA-CB-CG	7.33	128.77	114.10
1	A	728	LYS	CB-CG-CD	6.43	126.10	111.30
1	B	728	LYS	CB-CG-CD	6.43	126.10	111.30
1	D	728	LYS	CB-CG-CD	6.43	126.10	111.30
1	C	728	LYS	CB-CG-CD	6.41	126.05	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	667	GLU	CA-C-N	6.41	133.78	121.54
1	D	667	GLU	C-N-CA	6.41	133.78	121.54
1	B	667	GLU	CA-C-N	6.39	133.74	121.54
1	B	667	GLU	C-N-CA	6.39	133.74	121.54
1	C	667	GLU	CA-C-N	6.38	133.73	121.54
1	C	667	GLU	C-N-CA	6.38	133.73	121.54
1	A	667	GLU	CA-C-N	6.37	133.71	121.54
1	A	667	GLU	C-N-CA	6.37	133.71	121.54
1	A	1402	LEU	N-CA-C	-6.34	105.30	113.16
1	B	1402	LEU	N-CA-C	-6.34	105.30	113.16
1	D	1402	LEU	N-CA-C	-6.33	105.31	113.16
1	C	1402	LEU	N-CA-C	-6.33	105.32	113.16
1	B	1125	GLU	CA-CB-CG	6.16	126.42	114.10
1	D	1125	GLU	CA-CB-CG	6.14	126.38	114.10
1	A	1125	GLU	CA-CB-CG	6.13	126.36	114.10
1	C	1125	GLU	CA-CB-CG	6.12	126.33	114.10
1	B	450	GLU	CA-CB-CG	5.55	125.20	114.10
1	A	450	GLU	CA-CB-CG	5.55	125.20	114.10
1	C	450	GLU	CA-CB-CG	5.54	125.19	114.10
1	D	450	GLU	CA-CB-CG	5.53	125.16	114.10
1	A	316	ARG	CB-CG-CD	5.52	123.99	111.30
1	D	316	ARG	CB-CG-CD	5.51	123.96	111.30
1	C	316	ARG	CB-CG-CD	5.50	123.94	111.30
1	B	316	ARG	CB-CG-CD	5.49	123.94	111.30
1	D	400	VAL	N-CA-C	-5.25	107.63	112.83
1	C	400	VAL	N-CA-C	-5.24	107.64	112.83
1	A	400	VAL	N-CA-C	-5.23	107.65	112.83
1	B	400	VAL	N-CA-C	-5.23	107.65	112.83
1	C	1130	GLU	CA-CB-CG	5.21	124.52	114.10
1	D	1130	GLU	CA-CB-CG	5.21	124.51	114.10
1	A	1130	GLU	CA-CB-CG	5.20	124.50	114.10
1	A	585	ARG	CG-CD-NE	-5.20	100.57	112.00
1	C	585	ARG	CG-CD-NE	-5.19	100.58	112.00
1	D	585	ARG	CG-CD-NE	-5.18	100.59	112.00
1	B	585	ARG	CG-CD-NE	-5.18	100.60	112.00
1	B	1130	GLU	CA-CB-CG	5.18	124.45	114.10

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	160	GLN	Peptide

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Mol	Chain	Res	Type	Group
1	A	358	ARG	Peptide
1	B	160	GLN	Peptide
1	B	358	ARG	Peptide
1	C	160	GLN	Peptide
1	C	358	ARG	Peptide
1	D	160	GLN	Peptide
1	D	358	ARG	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	10523	0	10458	475	0
1	B	10523	0	10458	467	0
1	C	10523	0	10458	467	0
1	D	10523	0	10458	468	0
2	A	26	0	10	1	0
2	B	26	0	10	1	0
2	C	26	0	10	1	0
2	D	26	0	10	1	0
3	A	35	0	19	1	0
3	B	35	0	19	1	0
3	C	35	0	19	0	0
3	D	35	0	19	0	0
All	All	42336	0	41948	1817	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 22.

All (1817) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:727:MET:H	1:B:727:MET:HE2	1.20	1.06
1:A:727:MET:H	1:A:727:MET:HE2	1.20	1.06
1:C:727:MET:H	1:C:727:MET:HE2	1.20	1.05
1:D:727:MET:HE2	1:D:727:MET:H	1.20	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1429:MET:HB3	1:A:1487:ASN:HD21	1.37	0.89
1:D:1429:MET:HB3	1:D:1487:ASN:HD21	1.37	0.89
1:C:926:ILE:HG22	1:C:930:MET:HE1	1.55	0.89
1:B:926:ILE:HG22	1:B:930:MET:HE1	1.55	0.88
1:D:926:ILE:HG22	1:D:930:MET:HE1	1.55	0.88
1:C:1429:MET:HB3	1:C:1487:ASN:HD21	1.37	0.87
1:B:1429:MET:HB3	1:B:1487:ASN:HD21	1.37	0.87
1:A:926:ILE:HG22	1:A:930:MET:HE1	1.55	0.87
1:B:314:LYS:HE3	1:B:323:ILE:HG13	1.61	0.83
1:C:314:LYS:HE3	1:C:323:ILE:HG13	1.61	0.83
1:A:962:ARG:HG3	1:A:965:TRP:HB2	1.60	0.82
1:A:314:LYS:HE3	1:A:323:ILE:HG13	1.61	0.82
1:D:314:LYS:HE3	1:D:323:ILE:HG13	1.61	0.81
1:A:549:CYS:SG	1:A:587:ARG:NH1	2.54	0.81
1:D:549:CYS:SG	1:D:587:ARG:NH1	2.54	0.81
1:B:962:ARG:HG3	1:B:965:TRP:HB2	1.60	0.81
1:B:549:CYS:SG	1:B:587:ARG:NH1	2.54	0.81
1:C:549:CYS:SG	1:C:587:ARG:NH1	2.54	0.81
1:D:962:ARG:HG3	1:D:965:TRP:HB2	1.60	0.80
1:C:962:ARG:HG3	1:C:965:TRP:HB2	1.60	0.80
1:B:1365:ARG:NH1	1:B:1368:ILE:O	2.15	0.80
1:D:1357:ARG:NH1	1:D:1361:GLY:O	2.15	0.80
1:C:1365:ARG:NH1	1:C:1368:ILE:O	2.15	0.79
1:D:1365:ARG:NH1	1:D:1368:ILE:O	2.15	0.79
1:D:558:MET:HB2	1:D:585:ARG:HD2	1.64	0.79
1:B:558:MET:HB2	1:B:585:ARG:HD2	1.64	0.79
1:B:1357:ARG:NH1	1:B:1361:GLY:O	2.15	0.79
1:A:1357:ARG:NH1	1:A:1361:GLY:O	2.15	0.79
1:A:1365:ARG:NH1	1:A:1368:ILE:O	2.15	0.79
1:A:558:MET:HB2	1:A:585:ARG:HD2	1.64	0.78
1:B:930:MET:O	1:B:934:VAL:N	2.16	0.78
1:C:930:MET:O	1:C:934:VAL:N	2.16	0.78
1:C:558:MET:HB2	1:C:585:ARG:HD2	1.64	0.78
1:C:1357:ARG:NH1	1:C:1361:GLY:O	2.15	0.78
1:D:728:LYS:HA	1:D:728:LYS:HE3	1.65	0.78
1:B:1043:LEU:HD11	1:C:930:MET:HE3	1.65	0.77
1:D:217:GLN:NE2	1:D:220:GLU:OE1	2.18	0.77
1:A:728:LYS:HA	1:A:728:LYS:HE3	1.65	0.77
1:B:728:LYS:HA	1:B:728:LYS:HE3	1.66	0.77
1:C:781:VAL:HG11	1:C:787:ARG:HH11	1.50	0.77
1:B:1047:MET:SD	1:C:923:LYS:HG2	2.24	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:781:VAL:HG11	1:B:787:ARG:HH11	1.50	0.77
1:C:728:LYS:HE3	1:C:728:LYS:HA	1.65	0.77
1:A:781:VAL:HG11	1:A:787:ARG:HH11	1.50	0.77
1:C:1355:TRP:HB3	1:C:1363:ILE:HD13	1.67	0.77
1:C:217:GLN:NE2	1:C:220:GLU:OE1	2.18	0.76
1:A:217:GLN:NE2	1:A:220:GLU:OE1	2.18	0.76
1:D:1355:TRP:HB3	1:D:1363:ILE:HD13	1.67	0.76
1:D:471:GLU:HG3	1:D:472:ILE:HG12	1.68	0.76
1:B:217:GLN:NE2	1:B:220:GLU:OE1	2.18	0.76
1:D:930:MET:O	1:D:934:VAL:N	2.16	0.76
1:A:471:GLU:HG3	1:A:472:ILE:HG12	1.67	0.76
1:B:1355:TRP:HB3	1:B:1363:ILE:HD13	1.67	0.76
1:D:781:VAL:HG11	1:D:787:ARG:HH11	1.50	0.76
1:C:471:GLU:HG3	1:C:472:ILE:HG12	1.68	0.76
1:D:927:VAL:HA	1:D:930:MET:HE2	1.69	0.75
1:A:1355:TRP:HB3	1:A:1363:ILE:HD13	1.67	0.75
1:B:471:GLU:HG3	1:B:472:ILE:HG12	1.68	0.75
1:C:927:VAL:HA	1:C:930:MET:HE2	1.69	0.74
1:A:927:VAL:HA	1:A:930:MET:HE2	1.69	0.74
1:A:930:MET:O	1:A:934:VAL:N	2.16	0.74
1:A:982:ILE:HB	1:B:981:GLN:HB2	1.68	0.74
1:A:443:SER:HB2	1:A:1481:ARG:HH21	1.52	0.74
1:A:1065:PHE:O	1:A:1068:HIS:ND1	2.20	0.74
1:B:927:VAL:HA	1:B:930:MET:HE2	1.69	0.73
1:A:667:GLU:HB3	1:A:672:SER:HB3	1.71	0.73
1:C:443:SER:HB2	1:C:1481:ARG:HH21	1.52	0.73
1:D:443:SER:HB2	1:D:1481:ARG:HH21	1.52	0.73
1:B:1065:PHE:O	1:B:1068:HIS:ND1	2.20	0.73
1:C:1065:PHE:O	1:C:1068:HIS:ND1	2.20	0.73
1:B:667:GLU:HB3	1:B:672:SER:HB3	1.70	0.73
1:B:746:GLN:HB2	1:B:774:ARG:HH21	1.53	0.73
1:C:512:GLU:N	1:C:512:GLU:OE1	2.22	0.73
1:B:443:SER:HB2	1:B:1481:ARG:HH21	1.52	0.72
1:C:445:ASP:O	1:C:452:TRP:NE1	2.21	0.72
1:A:445:ASP:O	1:A:452:TRP:NE1	2.21	0.72
1:D:445:ASP:O	1:D:452:TRP:NE1	2.21	0.72
1:D:512:GLU:OE1	1:D:512:GLU:N	2.22	0.72
1:D:667:GLU:HB3	1:D:672:SER:HB3	1.71	0.72
1:A:982:ILE:O	1:B:981:GLN:NE2	2.18	0.72
1:B:512:GLU:OE1	1:B:512:GLU:N	2.22	0.72
1:C:667:GLU:HB3	1:C:672:SER:HB3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:746:GLN:HB2	1:A:774:ARG:HH21	1.53	0.71
1:B:445:ASP:O	1:B:452:TRP:NE1	2.21	0.71
1:C:746:GLN:HB2	1:C:774:ARG:HH21	1.53	0.71
1:D:746:GLN:HB2	1:D:774:ARG:HH21	1.54	0.71
1:A:379:ILE:HD11	1:A:402:TRP:HD1	1.56	0.71
1:C:379:ILE:HD11	1:C:402:TRP:HD1	1.56	0.71
1:D:727:MET:HG2	1:D:1062:ILE:HG22	1.72	0.71
1:B:379:ILE:HD11	1:B:402:TRP:HD1	1.56	0.71
1:D:379:ILE:HD11	1:D:402:TRP:HD1	1.56	0.71
1:C:727:MET:H	1:C:727:MET:CE	2.02	0.70
1:B:707:ARG:N	1:B:716:THR:OG1	2.24	0.70
1:A:938:LEU:HD23	1:D:1034:LEU:HD22	1.74	0.70
1:A:512:GLU:OE1	1:A:512:GLU:N	2.22	0.70
1:D:1065:PHE:O	1:D:1068:HIS:ND1	2.20	0.70
1:A:678:LEU:HA	1:A:681:GLU:HG3	1.74	0.70
1:A:944:TRP:O	1:A:1032:TYR:OH	2.09	0.70
1:B:727:MET:H	1:B:727:MET:CE	2.02	0.70
1:D:944:TRP:O	1:D:1032:TYR:OH	2.09	0.70
1:B:678:LEU:HA	1:B:681:GLU:HG3	1.74	0.70
1:C:212:THR:HA	1:C:216:LYS:HD2	1.74	0.70
1:D:212:THR:HA	1:D:216:LYS:HD2	1.74	0.70
1:C:944:TRP:O	1:C:1032:TYR:OH	2.09	0.69
1:D:678:LEU:HA	1:D:681:GLU:HG3	1.74	0.69
1:C:727:MET:HG2	1:C:1062:ILE:HG22	1.72	0.69
1:D:1150:ASP:O	1:D:1154:LYS:HE3	1.92	0.69
1:A:1049:ASN:OD1	1:D:1049:ASN:ND2	2.25	0.69
1:C:678:LEU:HA	1:C:681:GLU:HG3	1.74	0.69
1:C:1150:ASP:O	1:C:1154:LYS:HE3	1.92	0.69
1:B:700:ARG:HH21	1:B:1121:LEU:HD23	1.58	0.69
1:D:707:ARG:N	1:D:716:THR:OG1	2.24	0.69
1:B:944:TRP:O	1:B:1032:TYR:OH	2.09	0.69
1:C:977:THR:HG22	1:C:982:ILE:HA	1.75	0.69
1:A:700:ARG:HH21	1:A:1121:LEU:HD23	1.58	0.69
1:A:707:ARG:N	1:A:716:THR:OG1	2.24	0.69
1:A:727:MET:HG2	1:A:1062:ILE:HG22	1.73	0.69
1:B:977:THR:HG22	1:B:982:ILE:HA	1.75	0.69
1:B:1150:ASP:O	1:B:1154:LYS:HE3	1.92	0.69
1:C:555:ARG:HG2	1:C:589:LEU:HD11	1.75	0.69
1:D:727:MET:H	1:D:727:MET:CE	2.02	0.69
1:B:212:THR:HA	1:B:216:LYS:HD2	1.74	0.69
1:C:700:ARG:HH21	1:C:1121:LEU:HD23	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:555:ARG:HG2	1:D:589:LEU:HD11	1.75	0.69
1:D:700:ARG:HH21	1:D:1121:LEU:HD23	1.58	0.69
1:A:1150:ASP:O	1:A:1154:LYS:HE3	1.92	0.69
1:B:727:MET:HG2	1:B:1062:ILE:HG22	1.73	0.69
1:D:977:THR:HG22	1:D:982:ILE:HA	1.75	0.68
1:A:938:LEU:CD2	1:D:1034:LEU:HD22	2.23	0.68
1:C:707:ARG:N	1:C:716:THR:OG1	2.24	0.68
1:A:1020:PHE:HA	1:B:964:ASP:HB3	1.76	0.68
1:A:977:THR:HG22	1:A:982:ILE:HA	1.75	0.68
1:B:555:ARG:HG2	1:B:589:LEU:HD11	1.75	0.68
1:A:727:MET:H	1:A:727:MET:CE	2.03	0.68
1:A:75:PHE:HB2	1:A:146:SER:HB2	1.76	0.68
1:A:212:THR:HA	1:A:216:LYS:HD2	1.74	0.68
1:A:1034:LEU:HD12	1:A:1038:ILE:HG13	1.76	0.68
1:B:75:PHE:HB2	1:B:146:SER:HB2	1.76	0.68
1:C:1034:LEU:HD12	1:C:1038:ILE:HG13	1.76	0.68
1:A:183:LYS:NZ	1:A:356:SER:O	2.26	0.67
1:A:555:ARG:HG2	1:A:589:LEU:HD11	1.75	0.67
1:B:597:LEU:HB3	1:B:599:VAL:HG22	1.76	0.67
1:D:75:PHE:HB2	1:D:146:SER:HB2	1.76	0.67
1:A:464:ARG:HB3	1:A:467:ILE:HB	1.76	0.67
1:B:1034:LEU:HD12	1:B:1038:ILE:HG13	1.76	0.67
1:D:464:ARG:HB3	1:D:467:ILE:HB	1.76	0.67
1:A:746:GLN:NE2	1:A:790:ALA:O	2.28	0.67
1:D:1034:LEU:HD12	1:D:1038:ILE:HG13	1.76	0.67
1:C:75:PHE:HB2	1:C:146:SER:HB2	1.76	0.67
1:D:1118:GLU:HA	1:D:1121:LEU:HD12	1.77	0.67
1:C:1118:GLU:HA	1:C:1121:LEU:HD12	1.77	0.67
1:B:430:ASP:HB2	1:B:462:TRP:HE1	1.60	0.67
1:D:1356:ARG:NH1	1:D:1364:CYS:O	2.29	0.67
1:B:1356:ARG:NH1	1:B:1364:CYS:O	2.28	0.66
1:D:746:GLN:NE2	1:D:790:ALA:O	2.28	0.66
1:A:1042:ASN:OD1	1:B:1045:ILE:HG12	1.96	0.66
1:B:464:ARG:HB3	1:B:467:ILE:HB	1.76	0.66
1:B:746:GLN:NE2	1:B:790:ALA:O	2.28	0.66
1:D:430:ASP:HB2	1:D:462:TRP:HE1	1.61	0.66
1:D:476:GLU:O	1:D:478:GLN:NE2	2.29	0.66
1:A:988:GLY:HA3	1:B:968:ARG:HE	1.61	0.66
1:C:746:GLN:NE2	1:C:790:ALA:O	2.28	0.66
1:C:430:ASP:HB2	1:C:462:TRP:HE1	1.61	0.66
1:B:454:HIS:HA	1:B:457:LYS:HE2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:ARG:NH1	1:B:192:ARG:HG2	2.10	0.66
1:D:307:LYS:HD2	1:D:346:ASN:HB3	1.77	0.66
1:B:1118:GLU:HA	1:B:1121:LEU:HD12	1.77	0.66
1:C:454:HIS:HA	1:C:457:LYS:HE2	1.78	0.66
1:C:464:ARG:HB3	1:C:467:ILE:HB	1.76	0.66
1:D:454:HIS:HA	1:D:457:LYS:HE2	1.78	0.66
1:A:597:LEU:HB3	1:A:599:VAL:HG22	1.77	0.66
1:A:1118:GLU:HA	1:A:1121:LEU:HD12	1.77	0.66
1:A:191:ARG:NH1	1:A:192:ARG:HG2	2.11	0.66
1:B:770:LEU:HD23	1:B:771:ILE:HG23	1.78	0.66
1:B:476:GLU:O	1:B:478:GLN:NE2	2.29	0.65
1:C:191:ARG:NH1	1:C:192:ARG:HG2	2.10	0.65
1:C:770:LEU:HD23	1:C:771:ILE:HG23	1.78	0.65
1:D:597:LEU:HB3	1:D:599:VAL:HG22	1.77	0.65
1:D:770:LEU:HD23	1:D:771:ILE:HG23	1.78	0.65
1:A:307:LYS:HD2	1:A:346:ASN:HB3	1.77	0.65
1:A:454:HIS:HA	1:A:457:LYS:HE2	1.78	0.65
1:A:430:ASP:HB2	1:A:462:TRP:HE1	1.60	0.65
1:A:476:GLU:O	1:A:478:GLN:NE2	2.29	0.65
1:B:521:TYR:O	1:B:525:ASN:ND2	2.29	0.65
1:C:307:LYS:HD2	1:C:346:ASN:HB3	1.77	0.65
1:D:191:ARG:NH1	1:D:192:ARG:HG2	2.10	0.65
1:A:1356:ARG:NH1	1:A:1364:CYS:O	2.28	0.65
1:C:1356:ARG:NH1	1:C:1364:CYS:O	2.28	0.65
1:A:1043:LEU:HG	1:B:1048:PHE:CD2	2.31	0.65
1:B:183:LYS:NZ	1:B:356:SER:O	2.26	0.65
1:A:635:ARG:HD3	1:A:678:LEU:HD22	1.79	0.65
1:A:770:LEU:HD23	1:A:771:ILE:HG23	1.78	0.65
1:C:521:TYR:O	1:C:525:ASN:ND2	2.29	0.65
1:D:521:TYR:O	1:D:525:ASN:ND2	2.29	0.65
1:B:635:ARG:HD3	1:B:678:LEU:HD22	1.79	0.65
1:C:476:GLU:O	1:C:478:GLN:NE2	2.29	0.65
1:A:521:TYR:O	1:A:525:ASN:ND2	2.29	0.65
1:C:597:LEU:HB3	1:C:599:VAL:HG22	1.76	0.65
1:A:1045:ILE:HG23	1:D:1045:ILE:HG21	1.80	0.64
1:B:307:LYS:HD2	1:B:346:ASN:HB3	1.77	0.64
1:A:1431:ASP:OD1	1:A:1487:ASN:ND2	2.30	0.64
1:C:249:ARG:HH11	1:C:265:ILE:H	1.45	0.64
1:B:326:VAL:HG21	1:B:433:ILE:HB	1.80	0.64
1:C:1143:ARG:HE	1:C:1145:GLU:HB2	1.63	0.64
1:C:1049:ASN:ND2	1:D:1049:ASN:OD1	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:VAL:HG21	1:A:433:ILE:HB	1.80	0.64
1:B:1431:ASP:OD1	1:B:1487:ASN:ND2	2.30	0.64
1:C:1043:LEU:HD11	1:D:930:MET:HE3	1.80	0.64
1:D:249:ARG:HH11	1:D:265:ILE:H	1.45	0.64
1:B:1143:ARG:HE	1:B:1145:GLU:HB2	1.63	0.63
1:D:1143:ARG:HE	1:D:1145:GLU:HB2	1.63	0.63
1:C:635:ARG:HD3	1:C:678:LEU:HD22	1.79	0.63
1:A:441:SER:OG	1:A:455:GLN:NE2	2.29	0.63
1:D:714:LYS:HD2	1:D:715:THR:HG23	1.80	0.63
1:B:249:ARG:HH11	1:B:265:ILE:H	1.45	0.63
1:A:984:GLY:HA3	1:B:981:GLN:HG2	1.80	0.63
1:B:1398:LEU:HD23	1:B:1403:LYS:HG3	1.81	0.63
1:C:326:VAL:HG21	1:C:433:ILE:HB	1.80	0.63
1:D:326:VAL:HG21	1:D:433:ILE:HB	1.80	0.63
1:D:1398:LEU:HD23	1:D:1403:LYS:HG3	1.81	0.63
1:D:1258:PRO:HD2	1:D:1261:LYS:HE2	1.80	0.63
1:A:1398:LEU:HD23	1:A:1403:LYS:HG3	1.81	0.63
1:A:249:ARG:HH11	1:A:265:ILE:H	1.45	0.62
1:A:578:PRO:HG2	1:A:583:ASN:HD22	1.64	0.62
1:A:1143:ARG:HE	1:A:1145:GLU:HB2	1.63	0.62
1:D:944:TRP:CD1	1:D:1032:TYR:HH	2.17	0.62
1:A:1258:PRO:HD2	1:A:1261:LYS:HE2	1.80	0.62
1:C:183:LYS:NZ	1:C:356:SER:O	2.26	0.62
1:C:1258:PRO:HD2	1:C:1261:LYS:HE2	1.80	0.62
1:B:95:HIS:HB2	1:B:99:LEU:HD13	1.81	0.62
1:B:578:PRO:HG2	1:B:583:ASN:HD22	1.65	0.62
1:C:441:SER:OG	1:C:455:GLN:NE2	2.29	0.62
1:A:714:LYS:HD2	1:A:715:THR:HG23	1.80	0.62
1:A:1042:ASN:OD1	1:B:1045:ILE:HA	1.98	0.62
1:C:1043:LEU:CD1	1:D:930:MET:HE3	2.29	0.62
1:C:1398:LEU:HD23	1:C:1403:LYS:HG3	1.81	0.62
1:D:635:ARG:HD3	1:D:678:LEU:HD22	1.79	0.62
1:A:75:PHE:HD2	1:A:289:ASP:HA	1.65	0.62
1:A:95:HIS:HB2	1:A:99:LEU:HD13	1.81	0.62
1:B:1258:PRO:HD2	1:B:1261:LYS:HE2	1.80	0.62
1:A:79:SER:HB2	1:A:99:LEU:HD11	1.81	0.62
1:A:430:ASP:O	1:A:433:ILE:HG12	2.00	0.62
1:B:75:PHE:HD2	1:B:289:ASP:HA	1.65	0.62
1:B:430:ASP:O	1:B:433:ILE:HG12	2.00	0.62
1:C:95:HIS:HB2	1:C:99:LEU:HD13	1.81	0.62
1:C:395:THR:HG23	1:C:397:SER:H	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:578:PRO:HG2	1:D:583:ASN:HD22	1.64	0.62
1:C:578:PRO:HG2	1:C:583:ASN:HD22	1.64	0.62
1:C:75:PHE:HD2	1:C:289:ASP:HA	1.65	0.62
1:C:79:SER:HB2	1:C:99:LEU:HD11	1.82	0.62
1:C:1047:MET:SD	1:D:923:LYS:HG2	2.40	0.62
1:D:395:THR:HG23	1:D:397:SER:H	1.65	0.62
1:C:714:LYS:HD2	1:C:715:THR:HG23	1.80	0.61
1:C:1431:ASP:OD1	1:C:1487:ASN:ND2	2.30	0.61
1:D:1486:ALA:HA	1:D:1489:LYS:HD3	1.83	0.61
1:C:1159:VAL:HG12	1:D:1158:MET:HE3	1.82	0.61
1:A:395:THR:HG23	1:A:397:SER:H	1.65	0.61
1:A:1486:ALA:HA	1:A:1489:LYS:HD3	1.82	0.61
1:B:441:SER:OG	1:B:455:GLN:NE2	2.29	0.61
1:C:1130:GLU:HA	1:C:1133:LEU:HG	1.83	0.61
1:D:183:LYS:NZ	1:D:356:SER:O	2.26	0.61
1:A:1130:GLU:HA	1:A:1133:LEU:HG	1.83	0.61
1:B:79:SER:HB2	1:B:99:LEU:HD11	1.81	0.61
1:B:714:LYS:HD2	1:B:715:THR:HG23	1.80	0.61
1:C:1045:ILE:HG21	1:D:1045:ILE:HG23	1.82	0.61
1:D:730:VAL:HA	1:D:735:ILE:HG21	1.83	0.61
1:D:1073:GLU:OE2	1:D:1077:ARG:NH2	2.34	0.61
1:B:925:ILE:HG13	1:B:1063:TRP:HB2	1.82	0.61
1:B:1486:ALA:HA	1:B:1489:LYS:HD3	1.83	0.61
1:C:925:ILE:HG13	1:C:1063:TRP:HB2	1.82	0.61
1:A:730:VAL:HA	1:A:735:ILE:HG21	1.83	0.61
1:C:1073:GLU:OE2	1:C:1077:ARG:NH2	2.34	0.61
1:D:95:HIS:HB2	1:D:99:LEU:HD13	1.81	0.61
1:B:1034:LEU:CD2	1:C:934:VAL:HG13	2.31	0.61
1:B:1130:GLU:HA	1:B:1133:LEU:HG	1.83	0.61
1:C:182:MET:HE3	1:C:186:LEU:HB3	1.83	0.61
1:C:430:ASP:O	1:C:433:ILE:HG12	2.00	0.61
1:C:1429:MET:HB3	1:C:1487:ASN:ND2	2.14	0.61
1:C:1486:ALA:HA	1:C:1489:LYS:HD3	1.83	0.61
1:A:944:TRP:CD1	1:A:1032:TYR:HH	2.18	0.61
1:C:80:LYS:HA	1:C:105:PRO:HB3	1.83	0.61
1:C:730:VAL:HA	1:C:735:ILE:HG21	1.83	0.61
1:D:80:LYS:HA	1:D:105:PRO:HB3	1.83	0.61
1:B:730:VAL:HA	1:B:735:ILE:HG21	1.83	0.60
1:D:1095:LYS:HB3	1:D:1104:LYS:HZ2	1.66	0.60
1:D:1154:LYS:O	1:D:1158:MET:HE2	2.01	0.60
1:A:1045:ILE:O	1:A:1049:ASN:ND2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1073:GLU:OE2	1:B:1077:ARG:NH2	2.34	0.60
1:C:944:TRP:CD1	1:C:1032:TYR:HH	2.19	0.60
1:C:1154:LYS:O	1:C:1158:MET:HE2	2.01	0.60
1:D:1130:GLU:HA	1:D:1133:LEU:HG	1.83	0.60
1:D:1351:MET:HE2	1:D:1353:THR:HG21	1.84	0.60
1:A:182:MET:HE3	1:A:186:LEU:HB3	1.82	0.60
1:B:395:THR:HG23	1:B:397:SER:H	1.65	0.60
1:D:75:PHE:HD2	1:D:289:ASP:HA	1.65	0.60
1:A:925:ILE:HG13	1:A:1063:TRP:HB2	1.82	0.60
1:A:1073:GLU:OE2	1:A:1077:ARG:NH2	2.34	0.60
1:B:80:LYS:HA	1:B:105:PRO:HB3	1.83	0.60
1:D:1355:TRP:HB2	1:D:1357:ARG:HH21	1.66	0.60
1:A:532:PHE:HB2	1:A:662:LEU:HD11	1.84	0.60
1:A:1155:VAL:O	1:A:1159:VAL:HG13	2.02	0.60
1:A:1351:MET:HE2	1:A:1353:THR:HG21	1.83	0.60
1:B:532:PHE:HB2	1:B:662:LEU:HD11	1.84	0.60
1:B:1154:LYS:O	1:B:1158:MET:HE2	2.01	0.60
1:D:79:SER:HB2	1:D:99:LEU:HD11	1.81	0.60
1:D:441:SER:OG	1:D:455:GLN:NE2	2.29	0.60
1:D:1431:ASP:OD1	1:D:1487:ASN:ND2	2.30	0.60
1:A:1154:LYS:O	1:A:1158:MET:HE2	2.01	0.60
1:B:1045:ILE:HG22	1:B:1049:ASN:HD21	1.67	0.60
1:A:314:LYS:HB2	1:A:316:ARG:NH1	2.17	0.60
1:B:182:MET:HE3	1:B:186:LEU:HB3	1.83	0.60
1:C:311:GLU:OE1	1:C:322:LYS:NZ	2.35	0.60
1:D:182:MET:HE3	1:D:186:LEU:HB3	1.82	0.60
1:D:311:GLU:OE1	1:D:322:LYS:NZ	2.35	0.60
1:C:532:PHE:HB2	1:C:662:LEU:HD11	1.84	0.60
1:C:1355:TRP:HB2	1:C:1357:ARG:HH21	1.66	0.60
1:D:430:ASP:O	1:D:433:ILE:HG12	2.00	0.60
1:D:707:ARG:HG2	1:D:708:VAL:N	2.17	0.60
1:D:1155:VAL:O	1:D:1159:VAL:HG13	2.02	0.60
1:A:222:VAL:HG23	1:A:236:LEU:HD22	1.84	0.60
1:A:707:ARG:HG2	1:A:708:VAL:N	2.17	0.60
1:A:981:GLN:HB2	1:D:982:ILE:HB	1.83	0.60
1:C:427:GLN:NE2	1:C:431:VAL:HB	2.17	0.60
1:D:427:GLN:NE2	1:D:431:VAL:HB	2.17	0.60
1:D:697:ASP:HB3	1:D:700:ARG:HB2	1.83	0.60
1:D:1045:ILE:O	1:D:1049:ASN:ND2	2.34	0.60
1:A:577:TYR:HB3	1:A:585:ARG:HH22	1.67	0.60
1:B:314:LYS:HB2	1:B:316:ARG:NH1	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1045:ILE:O	1:C:1049:ASN:ND2	2.35	0.60
1:C:1090:LEU:HA	1:C:1093:PHE:HB2	1.84	0.60
1:D:532:PHE:HB2	1:D:662:LEU:HD11	1.84	0.60
1:D:1090:LEU:HA	1:D:1093:PHE:HB2	1.84	0.60
1:A:80:LYS:HA	1:A:105:PRO:HB3	1.83	0.59
1:B:311:GLU:OE1	1:B:322:LYS:NZ	2.35	0.59
1:B:671:SER:HA	1:B:674:GLU:HG3	1.84	0.59
1:B:1271:TYR:OH	1:B:1436:ASP:OD2	2.20	0.59
1:C:314:LYS:HB2	1:C:316:ARG:NH1	2.17	0.59
1:C:952:LYS:NZ	1:C:973:HIS:O	2.35	0.59
1:D:314:LYS:HB2	1:D:316:ARG:NH1	2.17	0.59
1:A:1355:TRP:HB2	1:A:1357:ARG:HH21	1.66	0.59
1:B:213:GLY:O	1:B:216:LYS:HG2	2.03	0.59
1:B:355:GLY:N	1:B:361:ASP:OD1	2.35	0.59
1:B:1045:ILE:O	1:B:1049:ASN:ND2	2.34	0.59
1:D:213:GLY:O	1:D:216:LYS:HG2	2.03	0.59
1:A:1038:ILE:HD12	1:B:1044:LEU:HD23	1.84	0.59
1:A:355:GLY:N	1:A:361:ASP:OD1	2.35	0.59
1:A:427:GLN:NE2	1:A:431:VAL:HB	2.17	0.59
1:C:575:PRO:O	1:C:577:TYR:N	2.36	0.59
1:C:1271:TYR:OH	1:C:1436:ASP:OD2	2.21	0.59
1:D:430:ASP:CB	1:D:462:TRP:HE1	2.16	0.59
1:D:925:ILE:HG13	1:D:1063:TRP:HB2	1.82	0.59
1:D:1045:ILE:HG22	1:D:1049:ASN:HD21	1.67	0.59
1:A:671:SER:HA	1:A:674:GLU:HG3	1.85	0.59
1:A:981:GLN:NE2	1:D:982:ILE:O	2.32	0.59
1:B:427:GLN:NE2	1:B:431:VAL:HB	2.17	0.59
1:B:1155:VAL:O	1:B:1159:VAL:HG13	2.02	0.59
1:B:1429:MET:HB3	1:B:1487:ASN:ND2	2.14	0.59
1:D:222:VAL:HG23	1:D:236:LEU:HD22	1.84	0.59
1:D:671:SER:HA	1:D:674:GLU:HG3	1.85	0.59
1:A:1271:TYR:OH	1:A:1436:ASP:OD2	2.21	0.59
1:B:1090:LEU:HA	1:B:1093:PHE:HB2	1.84	0.59
1:C:1045:ILE:HG22	1:C:1049:ASN:HD21	1.67	0.59
1:D:575:PRO:O	1:D:577:TYR:N	2.36	0.59
1:D:952:LYS:NZ	1:D:973:HIS:O	2.35	0.59
1:A:575:PRO:O	1:A:577:TYR:N	2.36	0.59
1:C:577:TYR:HB3	1:C:585:ARG:HH22	1.67	0.59
1:C:697:ASP:HB3	1:C:700:ARG:HB2	1.83	0.59
1:C:1351:MET:HE2	1:C:1353:THR:HG21	1.84	0.59
1:A:1045:ILE:HG22	1:A:1049:ASN:HD21	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:GLU:OE1	1:A:322:LYS:NZ	2.35	0.59
1:B:222:VAL:HG23	1:B:236:LEU:HD22	1.84	0.59
1:B:707:ARG:HG2	1:B:708:VAL:N	2.17	0.59
1:B:1355:TRP:HB2	1:B:1357:ARG:HH21	1.66	0.59
1:C:222:VAL:HG23	1:C:236:LEU:HD22	1.84	0.59
1:A:213:GLY:O	1:A:216:LYS:HG2	2.03	0.59
1:A:697:ASP:HB3	1:A:700:ARG:HB2	1.83	0.59
1:C:1155:VAL:O	1:C:1159:VAL:HG13	2.02	0.59
1:B:559:HIS:HB2	1:B:585:ARG:HB2	1.85	0.58
1:B:575:PRO:O	1:B:577:TYR:N	2.36	0.58
1:B:952:LYS:NZ	1:B:973:HIS:O	2.35	0.58
1:C:213:GLY:O	1:C:216:LYS:HG2	2.03	0.58
1:C:430:ASP:CB	1:C:462:TRP:HE1	2.16	0.58
1:C:707:ARG:HG2	1:C:708:VAL:N	2.17	0.58
1:D:577:TYR:HB3	1:D:585:ARG:HH22	1.67	0.58
1:A:314:LYS:HD2	1:A:321:ILE:HB	1.85	0.58
1:B:577:TYR:HB3	1:B:585:ARG:HH22	1.67	0.58
1:B:1351:MET:HE2	1:B:1353:THR:HG21	1.84	0.58
1:D:1271:TYR:OH	1:D:1436:ASP:OD2	2.20	0.58
1:A:191:ARG:HA	1:A:194:LEU:HG	1.85	0.58
1:A:430:ASP:CB	1:A:462:TRP:HE1	2.16	0.58
1:A:1090:LEU:HA	1:A:1093:PHE:HB2	1.84	0.58
1:B:191:ARG:HA	1:B:194:LEU:HG	1.85	0.58
1:B:430:ASP:CB	1:B:462:TRP:HE1	2.16	0.58
1:B:517:ASP:HA	1:B:520:LEU:HD12	1.84	0.58
1:D:314:LYS:HD2	1:D:321:ILE:HB	1.85	0.58
1:B:684:HIS:HA	1:B:687:ILE:HD12	1.86	0.58
1:C:355:GLY:N	1:C:361:ASP:OD1	2.35	0.58
1:A:559:HIS:HB2	1:A:585:ARG:HB2	1.85	0.58
1:C:1141:LYS:O	1:C:1147:LYS:NZ	2.36	0.58
1:D:515:THR:OG1	1:D:517:ASP:OD1	2.21	0.58
1:D:517:ASP:HA	1:D:520:LEU:HD12	1.84	0.58
1:D:559:HIS:HB2	1:D:585:ARG:HB2	1.85	0.58
1:B:515:THR:OG1	1:B:517:ASP:OD1	2.21	0.58
1:C:517:ASP:HA	1:C:520:LEU:HD12	1.84	0.58
1:C:671:SER:HA	1:C:674:GLU:HG3	1.85	0.58
1:B:697:ASP:HB3	1:B:700:ARG:HB2	1.83	0.58
1:D:1489:LYS:HB3	1:D:1503:TYR:OH	2.04	0.58
1:A:515:THR:OG1	1:A:517:ASP:OD1	2.21	0.58
1:A:684:HIS:HA	1:A:687:ILE:HD12	1.86	0.58
1:A:1141:LYS:O	1:A:1147:LYS:NZ	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:944:TRP:CD1	1:B:1032:TYR:HH	2.21	0.58
1:B:1141:LYS:O	1:B:1147:LYS:NZ	2.36	0.58
1:A:517:ASP:HA	1:A:520:LEU:HD12	1.84	0.58
1:A:921:GLY:HA3	1:A:1063:TRP:CE2	2.39	0.58
1:A:952:LYS:NZ	1:A:973:HIS:O	2.35	0.58
1:A:1368:ILE:H	1:A:1502:HIS:HE1	1.51	0.58
1:C:191:ARG:HA	1:C:194:LEU:HG	1.85	0.58
1:C:605:ARG:HE	1:C:614:HIS:HB3	1.69	0.58
1:B:1043:LEU:CD1	1:C:930:MET:HE3	2.33	0.58
1:C:684:HIS:HA	1:C:687:ILE:HD12	1.86	0.58
1:D:1368:ILE:H	1:D:1502:HIS:HE1	1.51	0.58
1:B:1489:LYS:HB3	1:B:1503:TYR:OH	2.04	0.57
1:C:705:LEU:HD12	1:C:718:LEU:HD21	1.86	0.57
1:D:605:ARG:HE	1:D:614:HIS:HB3	1.69	0.57
1:D:921:GLY:HA3	1:D:1063:TRP:CE2	2.39	0.57
1:A:1368:ILE:H	1:A:1502:HIS:CE1	2.23	0.57
1:A:1489:LYS:HB3	1:A:1503:TYR:OH	2.04	0.57
1:C:515:THR:OG1	1:C:517:ASP:OD1	2.21	0.57
1:C:559:HIS:HB2	1:C:585:ARG:HB2	1.85	0.57
1:C:921:GLY:HA3	1:C:1063:TRP:CE2	2.39	0.57
1:D:191:ARG:HA	1:D:194:LEU:HG	1.85	0.57
1:D:462:TRP:HB2	1:D:464:ARG:HG2	1.85	0.57
1:A:1429:MET:HB3	1:A:1487:ASN:ND2	2.14	0.57
1:A:1431:ASP:O	1:A:1434:ASN:ND2	2.37	0.57
1:B:454:HIS:O	1:B:458:LEU:HD22	2.05	0.57
1:D:454:HIS:O	1:D:458:LEU:HD22	2.05	0.57
1:D:1431:ASP:O	1:D:1434:ASN:ND2	2.37	0.57
1:A:462:TRP:HB2	1:A:464:ARG:HG2	1.85	0.57
1:B:462:TRP:HB2	1:B:464:ARG:HG2	1.85	0.57
1:B:605:ARG:HE	1:B:614:HIS:HB3	1.69	0.57
1:B:1431:ASP:O	1:B:1434:ASN:ND2	2.37	0.57
1:C:314:LYS:HD2	1:C:321:ILE:HB	1.85	0.57
1:C:1431:ASP:O	1:C:1434:ASN:ND2	2.37	0.57
1:C:1478:VAL:HA	1:C:1482:ILE:HD11	1.87	0.57
1:D:355:GLY:N	1:D:361:ASP:OD1	2.35	0.57
1:A:690:PHE:CE1	1:A:694:TYR:HB2	2.40	0.57
1:B:1478:VAL:HA	1:B:1482:ILE:HD11	1.87	0.57
1:D:358:ARG:O	1:D:360:ALA:N	2.38	0.57
1:D:684:HIS:HA	1:D:687:ILE:HD12	1.86	0.57
1:A:695:ARG:HH21	1:D:670:ASP:HA	1.69	0.57
1:A:936:PHE:HA	1:A:939:PHE:CE1	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1429:MET:HB3	1:D:1487:ASN:ND2	2.14	0.57
1:D:1478:VAL:HA	1:D:1482:ILE:HD11	1.87	0.57
1:A:605:ARG:HE	1:A:614:HIS:HB3	1.69	0.57
1:A:1081:PRO:O	1:A:1085:ILE:N	2.38	0.57
1:C:1489:LYS:HB3	1:C:1503:TYR:OH	2.04	0.57
1:D:1407:ARG:NH1	1:D:1411:TRP:HA	2.19	0.57
1:B:314:LYS:HD2	1:B:321:ILE:HB	1.85	0.57
1:B:358:ARG:O	1:B:360:ALA:N	2.38	0.57
1:B:1081:PRO:O	1:B:1085:ILE:N	2.38	0.57
1:B:1407:ARG:NH1	1:B:1411:TRP:HA	2.19	0.57
1:C:1407:ARG:NH1	1:C:1411:TRP:HA	2.19	0.57
1:A:1478:VAL:HA	1:A:1482:ILE:HD11	1.87	0.56
1:B:705:LEU:HD12	1:B:718:LEU:HD21	1.86	0.56
1:B:921:GLY:HA3	1:B:1063:TRP:CE2	2.39	0.56
1:B:1368:ILE:H	1:B:1502:HIS:CE1	2.23	0.56
1:C:454:HIS:O	1:C:458:LEU:HD22	2.05	0.56
1:A:516:TRP:HZ2	1:A:585:ARG:HD3	1.70	0.56
1:A:1022:GLU:HG3	1:B:968:ARG:HB2	1.88	0.56
1:A:1407:ARG:NH1	1:A:1411:TRP:HA	2.19	0.56
1:B:1368:ILE:H	1:B:1502:HIS:HE1	1.51	0.56
1:C:936:PHE:HA	1:C:939:PHE:CE1	2.40	0.56
1:D:73:VAL:HG21	1:D:121:GLU:OE1	2.06	0.56
1:A:1029:LEU:HG	1:B:975:TYR:HE2	1.71	0.56
1:A:1369:LYS:H	1:A:1502:HIS:CE1	2.23	0.56
1:B:130:ILE:N	1:B:140:LYS:O	2.36	0.56
1:B:936:PHE:HA	1:B:939:PHE:CE1	2.40	0.56
1:C:462:TRP:HB2	1:C:464:ARG:HG2	1.85	0.56
1:C:1326:ASN:ND2	1:C:1435:THR:O	2.38	0.56
1:C:1368:ILE:H	1:C:1502:HIS:HE1	1.51	0.56
1:D:408:ASP:O	1:D:411:ARG:NH1	2.39	0.56
1:D:705:LEU:HD12	1:D:718:LEU:HD21	1.86	0.56
1:D:1141:LYS:O	1:D:1147:LYS:NZ	2.36	0.56
1:D:1368:ILE:H	1:D:1502:HIS:CE1	2.23	0.56
1:A:408:ASP:O	1:A:411:ARG:NH1	2.39	0.56
1:A:1042:ASN:HA	1:A:1045:ILE:HD12	1.87	0.56
1:A:1424:VAL:HG21	1:A:1495:ALA:HA	1.88	0.56
1:B:73:VAL:HG21	1:B:121:GLU:OE1	2.06	0.56
1:D:719:GLN:HG3	1:D:722:LEU:HD12	1.88	0.56
1:A:73:VAL:HG21	1:A:121:GLU:OE1	2.06	0.56
1:A:358:ARG:O	1:A:360:ALA:N	2.38	0.56
1:A:445:ASP:OD1	1:A:455:GLN:NE2	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:516:TRP:HZ2	1:B:585:ARG:HD3	1.70	0.56
1:C:73:VAL:HG21	1:C:121:GLU:OE1	2.06	0.56
1:C:300:PRO:O	1:C:303:THR:OG1	2.24	0.56
1:C:1081:PRO:O	1:C:1085:ILE:N	2.38	0.56
1:B:690:PHE:CE1	1:B:694:TYR:HB2	2.40	0.56
1:B:1369:LYS:H	1:B:1502:HIS:CE1	2.23	0.56
1:C:358:ARG:O	1:C:360:ALA:N	2.38	0.56
1:D:1122:LEU:O	1:D:1126:ILE:HG13	2.06	0.56
1:A:510:LEU:O	1:A:514:VAL:HG23	2.06	0.56
1:A:1326:ASN:ND2	1:A:1435:THR:O	2.38	0.56
1:B:408:ASP:O	1:B:411:ARG:NH1	2.39	0.56
1:B:620:ASP:CB	1:B:623:ARG:HE	2.19	0.56
1:C:719:GLN:HG3	1:C:722:LEU:HD12	1.88	0.56
1:D:130:ILE:N	1:D:140:LYS:O	2.36	0.56
1:D:690:PHE:CE1	1:D:694:TYR:HB2	2.40	0.56
1:D:1122:LEU:HA	1:D:1125:GLU:OE2	2.06	0.56
1:A:359:VAL:HA	1:A:362:VAL:HG12	1.88	0.56
1:A:454:HIS:O	1:A:458:LEU:HD22	2.05	0.56
1:A:719:GLN:HG3	1:A:722:LEU:HD12	1.88	0.56
1:B:1326:ASN:ND2	1:B:1435:THR:O	2.38	0.56
1:C:620:ASP:CB	1:C:623:ARG:HE	2.19	0.56
1:C:690:PHE:CE1	1:C:694:TYR:HB2	2.40	0.56
1:D:516:TRP:HZ2	1:D:585:ARG:HD3	1.70	0.56
1:D:620:ASP:CB	1:D:623:ARG:HE	2.19	0.56
1:D:1398:LEU:HD11	1:D:1402:LEU:HD22	1.88	0.56
1:B:1122:LEU:HA	1:B:1125:GLU:OE2	2.06	0.56
1:B:1424:VAL:HG21	1:B:1495:ALA:HA	1.88	0.56
1:C:362:VAL:HA	1:C:382:LYS:HE2	1.88	0.56
1:C:408:ASP:O	1:C:411:ARG:NH1	2.39	0.56
1:C:1368:ILE:H	1:C:1502:HIS:CE1	2.23	0.56
1:C:1369:LYS:H	1:C:1502:HIS:CE1	2.23	0.56
1:D:936:PHE:HA	1:D:939:PHE:CE1	2.40	0.56
1:A:620:ASP:CB	1:A:623:ARG:HE	2.19	0.56
1:A:1122:LEU:O	1:A:1126:ILE:HG13	2.06	0.56
1:B:526:LEU:HA	1:B:632:GLN:HE21	1.71	0.56
1:B:1122:LEU:O	1:B:1126:ILE:HG13	2.06	0.56
1:B:1162:LEU:HD23	1:C:1161:LEU:HG	1.88	0.56
1:B:1398:LEU:HD11	1:B:1402:LEU:HD22	1.88	0.56
1:B:510:LEU:O	1:B:514:VAL:HG23	2.06	0.55
1:B:576:LEU:HD11	1:B:579:ARG:HH21	1.71	0.55
1:D:526:LEU:HA	1:D:632:GLN:HE21	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1081:PRO:O	1:D:1085:ILE:N	2.38	0.55
1:D:1336:ARG:HG2	1:D:1339:LEU:HB2	1.88	0.55
1:A:526:LEU:HA	1:A:632:GLN:HE21	1.72	0.55
1:A:1038:ILE:HG23	1:B:1044:LEU:HD21	1.88	0.55
1:B:465:VAL:HG13	1:B:502:LEU:HD11	1.88	0.55
1:B:1336:ARG:HG2	1:B:1339:LEU:HB2	1.89	0.55
1:C:1042:ASN:HA	1:C:1045:ILE:HD12	1.87	0.55
1:C:1122:LEU:O	1:C:1126:ILE:HG13	2.06	0.55
1:C:1355:TRP:HB2	1:C:1357:ARG:NH2	2.22	0.55
1:C:1398:LEU:HD11	1:C:1402:LEU:HD22	1.88	0.55
1:B:359:VAL:HA	1:B:362:VAL:HG12	1.88	0.55
1:D:359:VAL:HA	1:D:362:VAL:HG12	1.88	0.55
1:D:1042:ASN:HA	1:D:1045:ILE:HD12	1.87	0.55
1:A:130:ILE:N	1:A:140:LYS:O	2.36	0.55
1:A:705:LEU:HD12	1:A:718:LEU:HD21	1.86	0.55
1:A:1042:ASN:HD21	1:B:1045:ILE:N	2.04	0.55
1:A:1122:LEU:HA	1:A:1125:GLU:OE2	2.06	0.55
1:D:465:VAL:HG13	1:D:502:LEU:HD11	1.88	0.55
1:D:510:LEU:O	1:D:514:VAL:HG23	2.06	0.55
1:A:1336:ARG:HG2	1:A:1339:LEU:HB2	1.88	0.55
1:A:1355:TRP:HB2	1:A:1357:ARG:NH2	2.22	0.55
1:C:1122:LEU:HA	1:C:1125:GLU:OE2	2.06	0.55
1:C:1336:ARG:HG2	1:C:1339:LEU:HB2	1.89	0.55
1:D:100:GLU:HB3	1:D:105:PRO:HD3	1.88	0.55
1:C:1039:LEU:O	1:C:1043:LEU:HB2	2.07	0.55
1:A:300:PRO:O	1:A:303:THR:OG1	2.24	0.55
1:A:362:VAL:HA	1:A:382:LYS:HE2	1.88	0.55
1:A:465:VAL:HG13	1:A:502:LEU:HD11	1.88	0.55
1:C:379:ILE:HD11	1:C:402:TRP:CD1	2.41	0.55
1:C:910:LEU:O	1:C:914:PHE:N	2.37	0.55
1:A:1039:LEU:O	1:A:1043:LEU:HB2	2.06	0.55
1:A:1398:LEU:HD11	1:A:1402:LEU:HD22	1.88	0.55
1:B:719:GLN:HG3	1:B:722:LEU:HD12	1.88	0.55
1:B:1355:TRP:HB2	1:B:1357:ARG:NH2	2.22	0.55
1:A:1327:PRO:HB2	1:A:1328:MET:SD	2.47	0.55
1:B:74:TYR:N	1:B:122:MET:O	2.31	0.55
1:D:1369:LYS:H	1:D:1502:HIS:CE1	2.23	0.55
1:D:1424:VAL:HG21	1:D:1495:ALA:HA	1.88	0.55
1:B:727:MET:HE2	1:B:727:MET:N	2.05	0.55
1:B:1131:ASN:O	1:B:1135:ASN:ND2	2.40	0.55
1:C:359:VAL:HA	1:C:362:VAL:HG12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:576:LEU:HD11	1:A:579:ARG:HH21	1.71	0.54
1:B:1039:LEU:O	1:B:1043:LEU:HB2	2.06	0.54
1:B:1277:THR:HG23	1:B:1336:ARG:HB3	1.90	0.54
1:C:578:PRO:HB2	1:C:583:ASN:HB3	1.90	0.54
1:C:621:PRO:HB2	1:C:622:ILE:HD12	1.89	0.54
1:B:75:PHE:CD2	1:B:289:ASP:HA	2.43	0.54
1:B:151:SER:HB3	1:B:308:PHE:HD2	1.72	0.54
1:C:510:LEU:O	1:C:514:VAL:HG23	2.06	0.54
1:D:300:PRO:O	1:D:303:THR:OG1	2.24	0.54
1:D:362:VAL:HA	1:D:382:LYS:HE2	1.88	0.54
1:A:1131:ASN:O	1:A:1135:ASN:ND2	2.40	0.54
1:B:1042:ASN:HA	1:B:1045:ILE:HD12	1.87	0.54
1:C:576:LEU:HD11	1:C:579:ARG:HH21	1.71	0.54
1:C:1424:VAL:HG21	1:C:1495:ALA:HA	1.88	0.54
1:D:974:SER:O	1:D:977:THR:OG1	2.26	0.54
1:C:100:GLU:HB3	1:C:105:PRO:HD3	1.88	0.54
1:C:516:TRP:HZ2	1:C:585:ARG:HD3	1.71	0.54
1:C:1277:THR:HG23	1:C:1336:ARG:HB3	1.90	0.54
1:D:1277:THR:HG23	1:D:1336:ARG:HB3	1.90	0.54
1:D:1327:PRO:HB2	1:D:1328:MET:SD	2.47	0.54
1:D:1355:TRP:HB2	1:D:1357:ARG:NH2	2.22	0.54
1:A:897:VAL:HG12	1:D:955:ILE:HG12	1.90	0.54
1:A:1038:ILE:CG2	1:B:1044:LEU:HD21	2.37	0.54
1:C:465:VAL:HG13	1:C:502:LEU:HD11	1.88	0.54
1:D:621:PRO:HB2	1:D:622:ILE:HD12	1.89	0.54
1:D:1039:LEU:O	1:D:1043:LEU:HB2	2.07	0.54
1:D:1131:ASN:O	1:D:1135:ASN:ND2	2.40	0.54
1:A:335:GLY:O	1:A:339:THR:OG1	2.20	0.54
1:B:100:GLU:HB3	1:B:105:PRO:HD3	1.88	0.54
1:B:362:VAL:HA	1:B:382:LYS:HE2	1.88	0.54
1:C:562:ALA:HB1	1:C:579:ARG:HE	1.73	0.54
1:D:576:LEU:HD11	1:D:579:ARG:HH21	1.71	0.54
1:A:75:PHE:CD2	1:A:289:ASP:HA	2.43	0.54
1:A:319:VAL:HG13	1:A:320:ALA:H	1.73	0.54
1:A:411:ARG:NH1	1:A:412:ARG:HG3	2.23	0.54
1:C:75:PHE:CD2	1:C:289:ASP:HA	2.43	0.54
1:C:577:TYR:HB3	1:C:585:ARG:NH2	2.23	0.54
1:C:974:SER:O	1:C:977:THR:OG1	2.26	0.54
1:D:536:LEU:HA	1:D:539:VAL:HG12	1.90	0.54
1:D:578:PRO:HB2	1:D:583:ASN:HB3	1.90	0.54
1:A:1277:THR:HG23	1:A:1336:ARG:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:577:TYR:HB3	1:B:585:ARG:NH2	2.23	0.54
1:C:151:SER:HB3	1:C:308:PHE:HD2	1.73	0.54
1:C:304:ARG:HH21	1:C:308:PHE:HE2	1.55	0.54
1:D:319:VAL:HG13	1:D:320:ALA:H	1.73	0.54
1:B:182:MET:HB3	1:B:187:LYS:HZ3	1.73	0.54
1:B:578:PRO:HB2	1:B:583:ASN:HB3	1.90	0.54
1:C:445:ASP:OD1	1:C:455:GLN:NE2	2.34	0.54
1:A:460:VAL:HG11	1:A:496:LYS:HE2	1.90	0.54
1:A:562:ALA:HB1	1:A:579:ARG:HE	1.73	0.54
1:A:727:MET:HE2	1:A:727:MET:N	2.05	0.54
1:A:1392:ARG:HH22	1:A:1443:VAL:HB	1.73	0.54
1:B:1327:PRO:HB2	1:B:1328:MET:SD	2.47	0.54
1:A:577:TYR:HB3	1:A:585:ARG:NH2	2.23	0.53
1:A:649:ILE:HG13	1:A:650:ALA:H	1.73	0.53
1:A:1240:VAL:O	1:A:1244:HIS:NE2	2.42	0.53
1:B:304:ARG:HH21	1:B:308:PHE:HE2	1.55	0.53
1:C:526:LEU:HA	1:C:632:GLN:HE21	1.71	0.53
1:C:536:LEU:HA	1:C:539:VAL:HG12	1.90	0.53
1:B:319:VAL:HG13	1:B:320:ALA:H	1.73	0.53
1:C:411:ARG:NH1	1:C:412:ARG:HG3	2.23	0.53
1:C:620:ASP:HB3	1:C:623:ARG:HE	1.74	0.53
1:C:1327:PRO:HB2	1:C:1328:MET:SD	2.47	0.53
1:D:182:MET:HB3	1:D:187:LYS:HZ3	1.72	0.53
1:D:562:ALA:HB1	1:D:579:ARG:HE	1.73	0.53
1:D:577:TYR:HB3	1:D:585:ARG:NH2	2.23	0.53
1:B:562:ALA:HB1	1:B:579:ARG:HE	1.73	0.53
1:B:621:PRO:HB2	1:B:622:ILE:HD12	1.89	0.53
1:C:130:ILE:N	1:C:140:LYS:O	2.36	0.53
1:D:445:ASP:OD1	1:D:455:GLN:NE2	2.34	0.53
1:D:736:GLN:HA	1:D:739:LEU:HB3	1.91	0.53
1:A:100:GLU:HB3	1:A:105:PRO:HD3	1.88	0.53
1:B:1240:VAL:O	1:B:1244:HIS:NE2	2.42	0.53
1:C:80:LYS:HG2	1:C:105:PRO:HB2	1.91	0.53
1:C:1034:LEU:HD23	1:D:934:VAL:HG13	1.90	0.53
1:D:304:ARG:HH21	1:D:308:PHE:HE2	1.55	0.53
1:D:411:ARG:NH1	1:D:412:ARG:HG3	2.23	0.53
1:D:639:GLY:HA2	1:D:685:ARG:HH22	1.74	0.53
1:D:1326:ASN:ND2	1:D:1435:THR:O	2.38	0.53
1:A:578:PRO:HB2	1:A:583:ASN:HB3	1.90	0.53
1:A:639:GLY:HA2	1:A:685:ARG:HH22	1.74	0.53
1:A:775:GLU:O	1:A:780:ASP:N	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:955:ILE:HG12	1:D:897:VAL:HG12	1.89	0.53
1:D:335:GLY:O	1:D:339:THR:OG1	2.20	0.53
1:D:537:GLN:O	1:D:541:VAL:HG13	2.08	0.53
1:D:605:ARG:NE	1:D:614:HIS:HB3	2.24	0.53
1:B:445:ASP:OD1	1:B:455:GLN:NE2	2.34	0.53
1:C:649:ILE:HG13	1:C:650:ALA:H	1.73	0.53
1:C:1240:VAL:O	1:C:1244:HIS:NE2	2.42	0.53
1:D:80:LYS:HG2	1:D:105:PRO:HB2	1.91	0.53
1:A:868:TRP:HE1	1:A:928:LYS:HE3	1.74	0.53
1:D:1392:ARG:HH22	1:D:1443:VAL:HB	1.73	0.53
1:A:151:SER:HB3	1:A:308:PHE:HD2	1.73	0.53
1:A:621:PRO:HB2	1:A:622:ILE:HD12	1.89	0.53
1:B:80:LYS:HG2	1:B:105:PRO:HB2	1.91	0.53
1:B:411:ARG:NH1	1:B:412:ARG:HG3	2.23	0.53
1:C:74:TYR:N	1:C:122:MET:O	2.31	0.53
1:D:151:SER:HB3	1:D:308:PHE:HD2	1.72	0.53
1:D:460:VAL:HG11	1:D:496:LYS:HE2	1.90	0.53
1:D:620:ASP:HB3	1:D:623:ARG:HE	1.74	0.53
1:D:910:LEU:O	1:D:914:PHE:N	2.37	0.53
1:D:1240:VAL:O	1:D:1244:HIS:NE2	2.42	0.53
1:A:74:TYR:N	1:A:122:MET:O	2.31	0.53
1:A:470:SER:HA	1:A:474:MET:HE2	1.90	0.53
1:B:470:SER:HA	1:B:474:MET:HE2	1.90	0.53
1:B:868:TRP:HE1	1:B:928:LYS:HE3	1.74	0.53
1:B:1039:LEU:HA	1:B:1043:LEU:HD12	1.91	0.53
1:C:470:SER:HA	1:C:474:MET:HE2	1.90	0.53
1:C:537:GLN:O	1:C:541:VAL:HG13	2.08	0.53
1:C:1039:LEU:HA	1:C:1043:LEU:HD12	1.91	0.53
1:B:195:VAL:O	1:B:199:GLN:HG3	2.09	0.53
1:C:460:VAL:HG11	1:C:496:LYS:HE2	1.90	0.53
1:A:974:SER:O	1:A:977:THR:OG1	2.26	0.52
1:B:736:GLN:HA	1:B:739:LEU:HB3	1.91	0.52
1:B:1392:ARG:HH22	1:B:1443:VAL:HB	1.73	0.52
1:C:736:GLN:HA	1:C:739:LEU:HB3	1.91	0.52
1:A:332:GLY:O	1:A:358:ARG:NE	2.42	0.52
1:A:736:GLN:HA	1:A:739:LEU:HB3	1.91	0.52
1:B:620:ASP:HB3	1:B:623:ARG:HE	1.74	0.52
1:C:319:VAL:HG13	1:C:320:ALA:H	1.73	0.52
1:D:195:VAL:O	1:D:199:GLN:HG3	2.09	0.52
1:D:649:ILE:HG13	1:D:650:ALA:H	1.73	0.52
1:D:868:TRP:HE1	1:D:928:LYS:HE3	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:GLN:O	1:A:541:VAL:HG13	2.08	0.52
1:C:639:GLY:HA2	1:C:685:ARG:HH22	1.74	0.52
1:A:379:ILE:HD11	1:A:402:TRP:CD1	2.41	0.52
1:C:195:VAL:O	1:C:199:GLN:HG3	2.09	0.52
1:C:605:ARG:NE	1:C:614:HIS:HB3	2.24	0.52
1:D:129:ASP:HB3	1:D:261:PRO:HD3	1.92	0.52
1:A:605:ARG:NE	1:A:614:HIS:HB3	2.24	0.52
1:B:536:LEU:HA	1:B:539:VAL:HG12	1.90	0.52
1:B:639:GLY:HA2	1:B:685:ARG:HH22	1.74	0.52
1:C:177:ALA:O	1:C:178:LYS:HG3	2.10	0.52
1:C:727:MET:HE2	1:C:727:MET:N	2.05	0.52
1:B:177:ALA:O	1:B:178:LYS:HG3	2.10	0.52
1:B:537:GLN:O	1:B:541:VAL:HG13	2.08	0.52
1:B:605:ARG:NE	1:B:614:HIS:HB3	2.24	0.52
1:C:572:PHE:CD2	1:C:715:THR:HG21	2.45	0.52
1:C:917:SER:O	1:C:921:GLY:N	2.27	0.52
1:D:177:ALA:O	1:D:178:LYS:HG3	2.10	0.52
1:D:470:SER:HA	1:D:474:MET:HE2	1.90	0.52
1:A:80:LYS:HG2	1:A:105:PRO:HB2	1.91	0.52
1:A:536:LEU:HA	1:A:539:VAL:HG12	1.90	0.52
1:A:586:LEU:HB2	1:A:587:ARG:HD2	1.92	0.52
1:A:620:ASP:HB3	1:A:623:ARG:HE	1.74	0.52
1:B:170:LEU:HD22	1:B:310:SER:HB2	1.92	0.52
1:B:572:PHE:CD2	1:B:715:THR:HG21	2.45	0.52
1:C:1392:ARG:HH22	1:C:1443:VAL:HB	1.73	0.52
1:D:75:PHE:CD2	1:D:289:ASP:HA	2.43	0.52
1:D:1149:GLU:O	1:D:1152:SER:OG	2.26	0.52
1:A:304:ARG:HH21	1:A:308:PHE:HE2	1.55	0.52
1:A:1121:LEU:O	1:A:1124:TRP:N	2.42	0.52
1:A:1151:ILE:HD12	1:A:1151:ILE:H	1.75	0.52
1:C:1152:SER:HB3	1:D:1151:ILE:HD11	1.91	0.52
1:A:129:ASP:HB3	1:A:261:PRO:HD3	1.92	0.52
1:B:460:VAL:HG11	1:B:496:LYS:HE2	1.90	0.52
1:B:575:PRO:C	1:B:577:TYR:H	2.18	0.52
1:B:586:LEU:HB2	1:B:587:ARG:HD2	1.92	0.52
1:B:974:SER:O	1:B:977:THR:OG1	2.26	0.52
1:C:170:LEU:HD22	1:C:310:SER:HB2	1.92	0.52
1:D:1039:LEU:HA	1:D:1043:LEU:HD12	1.91	0.52
1:A:910:LEU:O	1:A:914:PHE:N	2.37	0.51
1:B:129:ASP:HB3	1:B:261:PRO:HD3	1.92	0.51
1:B:649:ILE:HG13	1:B:650:ALA:H	1.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1121:LEU:O	1:B:1124:TRP:N	2.42	0.51
1:B:1151:ILE:H	1:B:1151:ILE:HD12	1.75	0.51
1:C:332:GLY:O	1:C:358:ARG:NE	2.42	0.51
1:C:868:TRP:HE1	1:C:928:LYS:HE3	1.74	0.51
1:D:379:ILE:HD11	1:D:402:TRP:CD1	2.41	0.51
1:D:575:PRO:C	1:D:577:TYR:H	2.18	0.51
1:A:195:VAL:O	1:A:199:GLN:HG3	2.09	0.51
1:A:1039:LEU:HA	1:A:1043:LEU:HD12	1.91	0.51
1:B:300:PRO:O	1:B:303:THR:OG1	2.24	0.51
1:D:170:LEU:HD22	1:D:310:SER:HB2	1.92	0.51
1:D:1151:ILE:H	1:D:1151:ILE:HD12	1.75	0.51
1:A:177:ALA:O	1:A:178:LYS:HG3	2.10	0.51
1:C:575:PRO:C	1:C:577:TYR:H	2.18	0.51
1:D:74:TYR:N	1:D:122:MET:O	2.31	0.51
1:D:118:HIS:CE1	1:D:120:GLN:HB2	2.45	0.51
1:A:118:HIS:CE1	1:A:120:GLN:HB2	2.45	0.51
1:A:499:PHE:HA	1:A:502:LEU:HD12	1.93	0.51
1:A:572:PHE:CD2	1:A:715:THR:HG21	2.45	0.51
1:A:575:PRO:C	1:A:577:TYR:H	2.18	0.51
1:D:799:PHE:O	1:D:803:ILE:HG12	2.11	0.51
1:C:129:ASP:HB3	1:C:261:PRO:HD3	1.92	0.51
1:D:572:PHE:CD2	1:D:715:THR:HG21	2.45	0.51
1:A:799:PHE:O	1:A:803:ILE:HG12	2.11	0.51
1:A:917:SER:O	1:A:921:GLY:N	2.27	0.51
1:A:1353:THR:HG22	1:A:1374:VAL:HG12	1.92	0.51
1:D:922:PRO:O	1:D:926:ILE:HG13	2.11	0.51
1:A:586:LEU:HB3	1:A:587:ARG:HH11	1.76	0.51
1:B:118:HIS:CE1	1:B:120:GLN:HB2	2.45	0.51
1:C:1151:ILE:H	1:C:1151:ILE:HD12	1.75	0.51
1:B:193:GLY:HA2	1:B:428:ASP:HB3	1.93	0.51
1:B:669:THR:OG1	1:C:695:ARG:HB3	2.10	0.51
1:B:1385:TRP:CD1	1:B:1483:PRO:HG2	2.46	0.51
1:C:118:HIS:CE1	1:C:120:GLN:HB2	2.45	0.51
1:C:922:PRO:O	1:C:926:ILE:HG13	2.11	0.51
1:D:1121:LEU:O	1:D:1124:TRP:N	2.42	0.51
1:B:586:LEU:HB3	1:B:587:ARG:HH11	1.76	0.51
1:B:756:VAL:HG22	1:B:760:MET:HE3	1.93	0.51
1:C:193:GLY:HA2	1:C:428:ASP:HB3	1.93	0.51
1:D:499:PHE:HA	1:D:502:LEU:HD12	1.93	0.51
1:A:170:LEU:HD22	1:A:310:SER:HB2	1.92	0.51
1:A:1385:TRP:CD1	1:A:1483:PRO:HG2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:SER:OG	1:D:149:THR:HG23	2.11	0.51
1:D:1154:LYS:O	1:D:1157:ALA:N	2.44	0.51
1:A:922:PRO:O	1:A:926:ILE:HG13	2.11	0.50
1:B:922:PRO:O	1:B:926:ILE:HG13	2.11	0.50
1:C:586:LEU:HB2	1:C:587:ARG:HD2	1.92	0.50
1:C:1353:THR:HG22	1:C:1374:VAL:HG12	1.92	0.50
1:A:982:ILE:HG21	1:B:976:LEU:HD12	1.93	0.50
1:B:194:LEU:HD11	1:B:221:ALA:HB3	1.94	0.50
1:B:310:SER:HA	1:B:323:ILE:HB	1.92	0.50
1:C:310:SER:HA	1:C:323:ILE:HB	1.92	0.50
1:A:756:VAL:HG22	1:A:760:MET:HE3	1.93	0.50
1:C:586:LEU:HB3	1:C:587:ARG:HH11	1.76	0.50
1:C:799:PHE:O	1:C:803:ILE:HG12	2.11	0.50
1:C:1121:LEU:O	1:C:1124:TRP:N	2.42	0.50
1:C:194:LEU:HD11	1:C:221:ALA:HB3	1.94	0.50
1:D:193:GLY:HA2	1:D:428:ASP:HB3	1.93	0.50
1:D:586:LEU:HB2	1:D:587:ARG:HD2	1.92	0.50
1:D:586:LEU:HB3	1:D:587:ARG:HH11	1.76	0.50
1:A:146:SER:OG	1:A:149:THR:HG23	2.11	0.50
1:B:332:GLY:O	1:B:358:ARG:NE	2.42	0.50
1:B:335:GLY:O	1:B:339:THR:OG1	2.20	0.50
1:C:182:MET:HB3	1:C:187:LYS:HZ3	1.77	0.50
1:D:562:ALA:HB1	1:D:579:ARG:NE	2.27	0.50
1:D:1353:THR:HG22	1:D:1374:VAL:HG12	1.93	0.50
1:B:411:ARG:HH21	1:B:1244:HIS:CE1	2.30	0.50
1:B:910:LEU:O	1:B:914:PHE:N	2.37	0.50
1:C:775:GLU:O	1:C:780:ASP:N	2.34	0.50
1:C:1065:PHE:HB3	1:C:1066:GLN:OE1	2.12	0.50
1:D:728:LYS:HA	1:D:728:LYS:CE	2.39	0.50
1:A:310:SER:HA	1:A:323:ILE:HB	1.92	0.50
1:B:799:PHE:O	1:B:803:ILE:HG12	2.10	0.50
1:C:411:ARG:HH21	1:C:1244:HIS:CE1	2.30	0.50
1:C:562:ALA:HB1	1:C:579:ARG:NE	2.27	0.50
1:D:310:SER:HA	1:D:323:ILE:HB	1.92	0.50
1:A:199:GLN:HG2	1:A:225:PHE:CE1	2.47	0.50
1:B:146:SER:OG	1:B:149:THR:HG23	2.11	0.50
1:B:379:ILE:HD11	1:B:402:TRP:CD1	2.41	0.50
1:B:499:PHE:HA	1:B:502:LEU:HD12	1.93	0.50
1:B:1353:THR:HG22	1:B:1374:VAL:HG12	1.93	0.50
1:C:249:ARG:HG3	1:C:249:ARG:O	2.12	0.50
1:C:756:VAL:HG22	1:C:760:MET:HE3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:199:GLN:HG2	1:D:225:PHE:CE1	2.47	0.50
1:D:411:ARG:HH21	1:D:1244:HIS:CE1	2.30	0.50
1:A:562:ALA:HB1	1:A:579:ARG:NE	2.27	0.50
1:B:562:ALA:HB1	1:B:579:ARG:NE	2.27	0.50
1:B:955:ILE:HG12	1:C:897:VAL:HG12	1.92	0.50
1:C:335:GLY:O	1:C:339:THR:OG1	2.20	0.50
1:D:766:LEU:O	1:D:787:ARG:NH2	2.45	0.50
1:A:1065:PHE:HB3	1:A:1066:GLN:OE1	2.12	0.49
1:B:669:THR:HB	1:C:695:ARG:O	2.12	0.49
1:B:914:PHE:CE2	1:B:920:LEU:HD13	2.47	0.49
1:B:1065:PHE:HB3	1:B:1066:GLN:OE1	2.12	0.49
1:C:499:PHE:HA	1:C:502:LEU:HD12	1.93	0.49
1:D:1385:TRP:CD1	1:D:1483:PRO:HG2	2.46	0.49
1:A:182:MET:HB3	1:A:187:LYS:HZ3	1.76	0.49
1:A:669:THR:OG1	1:B:695:ARG:HB3	2.11	0.49
1:B:241:VAL:HG22	1:B:285:ILE:HB	1.95	0.49
1:C:766:LEU:O	1:C:787:ARG:NH2	2.45	0.49
1:A:193:GLY:HA2	1:A:428:ASP:HB3	1.93	0.49
1:A:194:LEU:HD11	1:A:221:ALA:HB3	1.94	0.49
1:A:241:VAL:HG22	1:A:285:ILE:HB	1.95	0.49
1:B:249:ARG:HG3	1:B:249:ARG:O	2.12	0.49
1:B:1239:HIS:NE2	1:B:1330:ARG:O	2.25	0.49
1:C:146:SER:OG	1:C:149:THR:HG23	2.11	0.49
1:C:1154:LYS:O	1:C:1157:ALA:N	2.44	0.49
1:D:700:ARG:O	1:D:704:LEU:HG	2.13	0.49
1:D:1065:PHE:HB3	1:D:1066:GLN:OE1	2.12	0.49
1:D:194:LEU:HD11	1:D:221:ALA:HB3	1.94	0.49
1:D:714:LYS:O	1:D:715:THR:OG1	2.24	0.49
1:A:319:VAL:HG13	1:A:320:ALA:N	2.28	0.49
1:C:1485:TYR:O	1:C:1489:LYS:HG3	2.13	0.49
1:D:241:VAL:HG22	1:D:285:ILE:HB	1.95	0.49
1:D:374:ILE:O	1:D:407:GLN:NE2	2.45	0.49
1:D:917:SER:O	1:D:921:GLY:N	2.27	0.49
1:D:1402:LEU:HA	1:D:1406:LEU:HD22	1.95	0.49
1:A:914:PHE:CE2	1:A:920:LEU:HD13	2.47	0.49
1:A:1151:ILE:HD11	1:D:1152:SER:HB3	1.93	0.49
1:A:1402:LEU:HA	1:A:1406:LEU:HD22	1.95	0.49
1:B:700:ARG:O	1:B:704:LEU:HG	2.13	0.49
1:B:1485:TYR:O	1:B:1489:LYS:HG3	2.13	0.49
1:A:249:ARG:HG3	1:A:249:ARG:O	2.12	0.49
1:A:411:ARG:HH21	1:A:1244:HIS:CE1	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:700:ARG:O	1:A:704:LEU:HG	2.13	0.49
1:D:319:VAL:HG13	1:D:320:ALA:N	2.28	0.49
1:B:199:GLN:HG2	1:B:225:PHE:CE1	2.47	0.49
1:B:501:LYS:O	1:B:504:LEU:HG	2.13	0.49
1:C:199:GLN:HG2	1:C:225:PHE:CE1	2.47	0.49
1:C:319:VAL:HG13	1:C:320:ALA:N	2.28	0.49
1:C:374:ILE:O	1:C:407:GLN:NE2	2.45	0.49
1:C:511:LYS:HG3	1:C:512:GLU:CD	2.38	0.49
1:C:862:LEU:O	1:C:865:SER:OG	2.30	0.49
1:C:1401:LYS:O	1:C:1406:LEU:HD13	2.13	0.49
1:C:1402:LEU:HA	1:C:1406:LEU:HD22	1.95	0.49
1:D:501:LYS:O	1:D:504:LEU:HG	2.13	0.49
1:D:756:VAL:HG22	1:D:760:MET:HE3	1.93	0.49
1:D:775:GLU:O	1:D:780:ASP:N	2.34	0.49
1:D:1401:LYS:O	1:D:1406:LEU:HD13	2.13	0.49
1:A:553:ALA:HA	1:A:589:LEU:HD12	1.95	0.49
1:A:1404:ARG:HG2	1:A:1405:ILE:HG13	1.95	0.49
1:B:319:VAL:HG13	1:B:320:ALA:N	2.28	0.49
1:C:1385:TRP:CD1	1:C:1483:PRO:HG2	2.46	0.49
1:B:1402:LEU:HA	1:B:1406:LEU:HD22	1.95	0.49
1:C:914:PHE:CE2	1:C:920:LEU:HD13	2.47	0.49
1:D:249:ARG:O	1:D:249:ARG:HG3	2.12	0.49
1:B:207:THR:HG21	1:B:218:VAL:HG11	1.95	0.48
1:B:766:LEU:O	1:B:787:ARG:NH2	2.45	0.48
1:D:617:PHE:HD2	1:D:620:ASP:N	2.11	0.48
1:A:501:LYS:O	1:A:504:LEU:HG	2.13	0.48
1:C:207:THR:HG21	1:C:218:VAL:HG11	1.95	0.48
1:C:700:ARG:O	1:C:704:LEU:HG	2.13	0.48
1:C:1390:GLY:H	1:C:1399:PRO:HB2	1.79	0.48
1:D:434:LEU:HA	1:D:437:LEU:HB2	1.95	0.48
1:D:1407:ARG:NH1	1:D:1411:TRP:HD1	2.12	0.48
1:A:96:GLU:O	1:A:99:LEU:N	2.42	0.48
1:A:207:THR:HG21	1:A:218:VAL:HG11	1.95	0.48
1:A:617:PHE:HD2	1:A:620:ASP:N	2.11	0.48
1:A:746:GLN:OE1	1:A:746:GLN:N	2.46	0.48
1:A:766:LEU:O	1:A:787:ARG:NH2	2.45	0.48
1:A:1407:ARG:NH1	1:A:1411:TRP:HD1	2.12	0.48
1:A:1485:TYR:O	1:A:1489:LYS:HG3	2.13	0.48
1:B:1383:GLU:OE1	1:B:1383:GLU:N	2.47	0.48
1:C:241:VAL:HG22	1:C:285:ILE:HB	1.95	0.48
1:C:1034:LEU:O	1:C:1038:ILE:HB	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:PRO:HB3	1:D:204:TRP:CD1	2.48	0.48
1:D:207:THR:HG21	1:D:218:VAL:HG11	1.95	0.48
1:D:862:LEU:O	1:D:865:SER:OG	2.30	0.48
1:D:1485:TYR:O	1:D:1489:LYS:HG3	2.13	0.48
1:B:511:LYS:HG3	1:B:512:GLU:CD	2.38	0.48
1:B:1154:LYS:O	1:B:1157:ALA:N	2.44	0.48
1:C:553:ALA:HA	1:C:589:LEU:HD12	1.95	0.48
1:C:617:PHE:HD2	1:C:620:ASP:N	2.11	0.48
1:C:1383:GLU:N	1:C:1383:GLU:OE1	2.47	0.48
1:D:523:TYR:CD1	1:D:628:TRP:HD1	2.32	0.48
1:A:1034:LEU:O	1:A:1038:ILE:HB	2.14	0.48
1:B:632:GLN:HB2	1:B:634:ARG:HG3	1.96	0.48
1:B:1034:LEU:O	1:B:1038:ILE:HB	2.14	0.48
1:D:914:PHE:CE2	1:D:920:LEU:HD13	2.47	0.48
1:A:632:GLN:HB2	1:A:634:ARG:HG3	1.96	0.48
1:B:746:GLN:N	1:B:746:GLN:OE1	2.46	0.48
1:B:775:GLU:O	1:B:780:ASP:N	2.34	0.48
1:B:1407:ARG:NH1	1:B:1411:TRP:HD1	2.12	0.48
1:C:728:LYS:HA	1:C:728:LYS:CE	2.39	0.48
1:D:511:LYS:HG3	1:D:512:GLU:CD	2.38	0.48
1:D:727:MET:HE2	1:D:727:MET:N	2.05	0.48
1:D:923:LYS:HG3	1:D:926:ILE:HD12	1.96	0.48
1:D:1383:GLU:OE1	1:D:1383:GLU:N	2.46	0.48
1:D:1385:TRP:HD1	1:D:1483:PRO:HG2	1.78	0.48
1:A:511:LYS:HG3	1:A:512:GLU:CD	2.38	0.48
1:A:1069:ASP:HA	1:A:1072:GLU:OE2	2.14	0.48
1:A:1106:HIS:O	1:A:1110:LYS:HD3	2.14	0.48
1:A:1390:GLY:H	1:A:1399:PRO:HB2	1.79	0.48
1:B:167:PRO:HB3	1:B:204:TRP:CD1	2.48	0.48
1:B:434:LEU:HA	1:B:437:LEU:HB2	1.95	0.48
1:B:523:TYR:CD1	1:B:628:TRP:HD1	2.32	0.48
1:B:617:PHE:HD2	1:B:620:ASP:N	2.12	0.48
1:B:1385:TRP:HD1	1:B:1483:PRO:HG2	1.78	0.48
1:B:1404:ARG:HG2	1:B:1405:ILE:HG13	1.95	0.48
1:C:522:LEU:O	1:C:628:TRP:NE1	2.36	0.48
1:D:96:GLU:O	1:D:99:LEU:N	2.42	0.48
1:D:100:GLU:HB2	1:D:104:LYS:HA	1.95	0.48
1:D:620:ASP:OD2	1:D:623:ARG:HG3	2.14	0.48
1:D:1404:ARG:HG2	1:D:1405:ILE:HG13	1.95	0.48
1:A:167:PRO:HB3	1:A:204:TRP:CD1	2.48	0.48
1:A:728:LYS:HA	1:A:728:LYS:CE	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:923:LYS:HG3	1:A:926:ILE:HD12	1.96	0.48
1:B:923:LYS:HG3	1:B:926:ILE:HD12	1.96	0.48
1:B:962:ARG:HD2	1:B:963:VAL:N	2.29	0.48
1:B:1069:ASP:HA	1:B:1072:GLU:OE2	2.14	0.48
1:B:1390:GLY:H	1:B:1399:PRO:HB2	1.79	0.48
1:C:501:LYS:O	1:C:504:LEU:HG	2.13	0.48
1:C:632:GLN:HB2	1:C:634:ARG:HG3	1.96	0.48
1:C:746:GLN:OE1	1:C:746:GLN:N	2.46	0.48
1:C:962:ARG:HD2	1:C:963:VAL:N	2.29	0.48
1:C:985:TYR:HD1	1:D:968:ARG:HH22	1.62	0.48
1:D:660:LYS:HE3	1:D:725:LYS:HE2	1.96	0.48
1:D:746:GLN:OE1	1:D:746:GLN:N	2.46	0.48
1:D:1034:LEU:O	1:D:1038:ILE:HB	2.14	0.48
1:A:930:MET:HE3	1:D:1043:LEU:CD1	2.44	0.48
1:A:1383:GLU:OE1	1:A:1383:GLU:N	2.46	0.48
1:C:201:THR:OG1	1:C:202:GLY:N	2.47	0.48
1:C:523:TYR:CD1	1:C:628:TRP:HD1	2.32	0.48
1:C:1407:ARG:NH1	1:C:1411:TRP:HD1	2.12	0.48
1:D:332:GLY:O	1:D:358:ARG:NE	2.42	0.48
1:D:553:ALA:HA	1:D:589:LEU:HD12	1.95	0.48
1:A:620:ASP:OD2	1:A:623:ARG:HG3	2.14	0.48
1:A:862:LEU:O	1:A:865:SER:OG	2.30	0.48
1:A:1385:TRP:HD1	1:A:1483:PRO:HG2	1.78	0.48
1:B:254:ILE:HG13	1:B:254:ILE:O	2.14	0.48
1:C:153:VAL:HG13	1:C:154:ILE:HG23	1.96	0.48
1:C:167:PRO:HB3	1:C:204:TRP:CD1	2.48	0.48
1:C:620:ASP:OD2	1:C:623:ARG:HG3	2.14	0.48
1:D:632:GLN:HB2	1:D:634:ARG:HG3	1.96	0.48
1:D:1390:GLY:H	1:D:1399:PRO:HB2	1.79	0.48
1:A:153:VAL:HG13	1:A:154:ILE:HG23	1.96	0.47
1:B:100:GLU:HB2	1:B:104:LYS:HA	1.95	0.47
1:C:1404:ARG:HG2	1:C:1405:ILE:HG13	1.95	0.47
1:D:183:LYS:HB2	1:D:186:LEU:HD12	1.96	0.47
1:D:1069:ASP:HA	1:D:1072:GLU:OE2	2.14	0.47
1:A:183:LYS:HB2	1:A:186:LEU:HD12	1.96	0.47
1:A:1401:LYS:O	1:A:1406:LEU:HD13	2.13	0.47
1:B:947:SER:HB3	1:B:1032:TYR:OH	2.15	0.47
1:B:1401:LYS:O	1:B:1406:LEU:HD13	2.13	0.47
1:C:434:LEU:HA	1:C:437:LEU:HB2	1.95	0.47
1:C:1075:HIS:O	1:C:1075:HIS:ND1	2.47	0.47
1:C:1385:TRP:HD1	1:C:1483:PRO:HG2	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:947:SER:HB3	1:D:1032:TYR:OH	2.14	0.47
1:A:254:ILE:O	1:A:254:ILE:HG13	2.14	0.47
1:A:523:TYR:CD1	1:A:628:TRP:HD1	2.32	0.47
1:A:531:LEU:O	1:A:535:LYS:HG2	2.15	0.47
1:A:660:LYS:HE3	1:A:725:LYS:HE2	1.96	0.47
1:B:309:ILE:O	1:B:313:THR:OG1	2.29	0.47
1:B:620:ASP:OD2	1:B:623:ARG:HG3	2.14	0.47
1:A:434:LEU:HA	1:A:437:LEU:HB2	1.95	0.47
1:A:714:LYS:O	1:A:715:THR:OG1	2.24	0.47
1:A:962:ARG:HD2	1:A:963:VAL:N	2.29	0.47
1:B:201:THR:OG1	1:B:202:GLY:N	2.47	0.47
1:B:441:SER:HA	1:B:444:GLN:HB2	1.97	0.47
1:B:917:SER:O	1:B:921:GLY:N	2.27	0.47
1:C:1405:ILE:O	1:C:1406:LEU:HD12	2.15	0.47
1:D:531:LEU:O	1:D:535:LYS:HG2	2.15	0.47
1:D:1106:HIS:O	1:D:1110:LYS:HD3	2.14	0.47
1:D:1405:ILE:O	1:D:1406:LEU:HD12	2.15	0.47
1:B:153:VAL:HG13	1:B:154:ILE:HG23	1.96	0.47
1:C:254:ILE:HG13	1:C:254:ILE:O	2.14	0.47
1:C:923:LYS:HG3	1:C:926:ILE:HD12	1.96	0.47
1:C:1141:LYS:HA	1:C:1146:GLN:OE1	2.15	0.47
1:D:774:ARG:HG3	1:D:777:ARG:HE	1.80	0.47
1:A:73:VAL:HA	1:A:123:PRO:HA	1.97	0.47
1:A:308:PHE:O	1:A:313:THR:HG23	2.15	0.47
1:A:351:VAL:HG21	1:A:432:ALA:HB1	1.97	0.47
1:B:308:PHE:O	1:B:313:THR:HG23	2.15	0.47
1:B:553:ALA:HA	1:B:589:LEU:HD12	1.95	0.47
1:B:1106:HIS:O	1:B:1110:LYS:HD3	2.14	0.47
1:B:1141:LYS:HA	1:B:1146:GLN:OE1	2.15	0.47
1:C:531:LEU:O	1:C:535:LYS:HG2	2.15	0.47
1:D:153:VAL:HG13	1:D:154:ILE:HG23	1.96	0.47
1:A:430:ASP:OD1	1:A:431:VAL:N	2.48	0.47
1:A:947:SER:HB3	1:A:1032:TYR:OH	2.15	0.47
1:A:1130:GLU:OE1	1:A:1131:ASN:N	2.48	0.47
1:A:1145:GLU:HA	1:A:1148:ILE:HD12	1.97	0.47
1:A:1154:LYS:O	1:A:1157:ALA:N	2.44	0.47
1:A:1405:ILE:O	1:A:1406:LEU:HD12	2.15	0.47
1:B:73:VAL:HA	1:B:123:PRO:HA	1.97	0.47
1:B:183:LYS:HB2	1:B:186:LEU:HD12	1.96	0.47
1:B:495:ASN:OD1	1:B:496:LYS:N	2.44	0.47
1:B:531:LEU:O	1:B:535:LYS:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1405:ILE:O	1:B:1406:LEU:HD12	2.15	0.47
1:C:100:GLU:HB2	1:C:104:LYS:HA	1.95	0.47
1:C:430:ASP:OD1	1:C:431:VAL:N	2.48	0.47
1:C:660:LYS:HE3	1:C:725:LYS:HE2	1.96	0.47
1:C:947:SER:HB3	1:C:1032:TYR:OH	2.15	0.47
1:C:1106:HIS:O	1:C:1110:LYS:HD3	2.14	0.47
1:D:254:ILE:O	1:D:254:ILE:HG13	2.14	0.47
1:D:430:ASP:OD1	1:D:431:VAL:N	2.48	0.47
1:D:962:ARG:HD2	1:D:963:VAL:N	2.29	0.47
1:D:1145:GLU:HA	1:D:1148:ILE:HD12	1.97	0.47
1:A:1145:GLU:HG3	1:A:1148:ILE:HD12	1.97	0.47
1:C:1034:LEU:HD22	1:D:938:LEU:HD23	1.97	0.47
1:C:1145:GLU:HA	1:C:1148:ILE:HD12	1.97	0.47
1:A:100:GLU:HB2	1:A:104:LYS:HA	1.95	0.47
1:A:441:SER:HA	1:A:444:GLN:HB2	1.97	0.47
1:A:930:MET:HE3	1:D:1043:LEU:HD11	1.97	0.47
1:B:1145:GLU:HG3	1:B:1148:ILE:HD12	1.97	0.47
1:C:565:LEU:HD23	1:C:568:LEU:HD12	1.96	0.47
1:C:1069:ASP:HA	1:C:1072:GLU:OE2	2.14	0.47
1:D:659:LEU:HD13	1:D:678:LEU:HD12	1.97	0.47
1:D:727:MET:O	1:D:731:SER:OG	2.24	0.47
1:A:451:ASN:HA	1:A:454:HIS:CD2	2.50	0.47
1:B:660:LYS:HE3	1:B:725:LYS:HE2	1.96	0.46
1:B:727:MET:O	1:B:731:SER:OG	2.24	0.46
1:B:1130:GLU:OE1	1:B:1131:ASN:N	2.48	0.46
1:C:451:ASN:HA	1:C:454:HIS:CD2	2.50	0.46
1:D:538:LYS:O	1:D:542:GLU:HG2	2.15	0.46
1:D:1130:GLU:OE1	1:D:1131:ASN:N	2.48	0.46
1:D:1145:GLU:HG3	1:D:1148:ILE:HD12	1.97	0.46
1:B:565:LEU:HD23	1:B:568:LEU:HD12	1.96	0.46
1:D:308:PHE:O	1:D:313:THR:HG23	2.15	0.46
1:D:451:ASN:HA	1:D:454:HIS:CD2	2.50	0.46
1:D:1239:HIS:NE2	1:D:1330:ARG:O	2.25	0.46
1:A:249:ARG:NH1	1:A:265:ILE:HG12	2.31	0.46
1:A:374:ILE:O	1:A:407:GLN:NE2	2.46	0.46
1:A:590:LEU:O	1:A:592:VAL:N	2.48	0.46
1:B:96:GLU:O	1:B:99:LEU:N	2.42	0.46
1:B:1067:ARG:O	1:B:1071:ILE:HG12	2.16	0.46
1:C:183:LYS:HB2	1:C:186:LEU:HD12	1.96	0.46
1:C:249:ARG:NH1	1:C:265:ILE:HG12	2.31	0.46
1:C:308:PHE:O	1:C:313:THR:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:590:LEU:O	1:C:592:VAL:N	2.48	0.46
1:C:1145:GLU:HG3	1:C:1148:ILE:HD12	1.97	0.46
1:A:427:GLN:HG2	1:A:428:ASP:N	2.31	0.46
1:A:1043:LEU:HD23	1:B:1048:PHE:HB3	1.97	0.46
1:B:351:VAL:HG21	1:B:432:ALA:HB1	1.97	0.46
1:B:671:SER:O	1:B:675:MET:HG2	2.16	0.46
1:C:441:SER:HA	1:C:444:GLN:HB2	1.97	0.46
1:C:495:ASN:OD1	1:C:496:LYS:N	2.44	0.46
1:C:659:LEU:HD13	1:C:678:LEU:HD12	1.97	0.46
1:C:1067:ARG:O	1:C:1071:ILE:HG12	2.16	0.46
1:D:73:VAL:HA	1:D:123:PRO:HA	1.97	0.46
1:D:427:GLN:HG2	1:D:428:ASP:N	2.31	0.46
1:A:565:LEU:HD23	1:A:568:LEU:HD12	1.96	0.46
1:A:1141:LYS:HA	1:A:1146:GLN:OE1	2.15	0.46
1:B:451:ASN:HA	1:B:454:HIS:CD2	2.50	0.46
1:B:728:LYS:HA	1:B:728:LYS:CE	2.39	0.46
1:C:774:ARG:HG3	1:C:777:ARG:HE	1.80	0.46
1:A:617:PHE:C	1:A:619:MET:H	2.24	0.46
1:A:1239:HIS:NE2	1:A:1330:ARG:O	2.25	0.46
1:B:249:ARG:NH1	1:B:265:ILE:HG12	2.31	0.46
1:B:430:ASP:OD1	1:B:431:VAL:N	2.48	0.46
1:C:96:GLU:O	1:C:99:LEU:N	2.42	0.46
1:D:706:THR:HG22	1:D:1109:LEU:HD11	1.97	0.46
1:A:727:MET:O	1:A:731:SER:OG	2.24	0.46
1:A:1358:ASN:OD1	1:A:1358:ASN:N	2.48	0.46
1:B:862:LEU:O	1:B:865:SER:OG	2.30	0.46
1:B:1034:LEU:HD23	1:C:934:VAL:HG13	1.97	0.46
1:B:1145:GLU:HA	1:B:1148:ILE:HD12	1.97	0.46
1:C:538:LYS:O	1:C:542:GLU:HG2	2.16	0.46
1:C:1130:GLU:OE1	1:C:1131:ASN:N	2.48	0.46
1:D:249:ARG:NH1	1:D:265:ILE:HG12	2.31	0.46
1:D:685:ARG:HG2	1:D:1136:ARG:NH1	2.31	0.46
1:D:690:PHE:HA	1:D:693:CYS:SG	2.56	0.46
1:D:1141:LYS:HA	1:D:1146:GLN:OE1	2.15	0.46
1:B:581:ARG:HE	1:B:584:ASP:CG	2.24	0.46
1:B:1273:PRO:HG2	1:B:1334:ARG:HE	1.81	0.46
1:A:581:ARG:HE	1:A:584:ASP:CG	2.24	0.46
1:A:646:GLN:HE22	1:A:1126:ILE:HD11	1.81	0.46
1:A:690:PHE:HA	1:A:693:CYS:SG	2.56	0.46
1:B:525:ASN:O	1:B:632:GLN:NE2	2.49	0.46
1:B:538:LYS:O	1:B:542:GLU:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:623:ARG:HH22	1:B:711:ALA:HB1	1.81	0.46
1:C:351:VAL:HG21	1:C:432:ALA:HB1	1.97	0.46
1:C:646:GLN:HE22	1:C:1126:ILE:HD11	1.81	0.46
1:D:441:SER:HA	1:D:444:GLN:HB2	1.97	0.46
1:A:79:SER:HA	1:A:113:TRP:CH2	2.51	0.46
1:A:538:LYS:O	1:A:542:GLU:HG2	2.15	0.46
1:A:659:LEU:HD13	1:A:678:LEU:HD12	1.97	0.46
1:B:374:ILE:O	1:B:407:GLN:NE2	2.46	0.46
1:B:492:LEU:HB3	1:B:628:TRP:CH2	2.51	0.46
1:B:602:VAL:HG23	1:B:602:VAL:O	2.16	0.46
1:B:690:PHE:HA	1:B:693:CYS:SG	2.56	0.46
1:B:706:THR:HG22	1:B:1109:LEU:HD11	1.97	0.46
1:B:1151:ILE:HG22	1:C:1151:ILE:HG12	1.97	0.46
1:C:73:VAL:HA	1:C:123:PRO:HA	1.97	0.46
1:C:250:ARG:HH21	1:C:274:LEU:HD21	1.81	0.46
1:C:427:GLN:HG2	1:C:428:ASP:N	2.31	0.46
1:C:492:LEU:HB3	1:C:628:TRP:CH2	2.51	0.46
1:D:671:SER:O	1:D:675:MET:HG2	2.16	0.46
1:A:623:ARG:HH22	1:A:711:ALA:HB1	1.81	0.45
1:A:774:ARG:HG3	1:A:777:ARG:HE	1.80	0.45
1:A:818:MET:HE2	1:A:818:MET:HA	1.98	0.45
1:B:522:LEU:O	1:B:628:TRP:NE1	2.36	0.45
1:C:195:VAL:HG23	1:C:196:LYS:HD2	1.99	0.45
1:C:706:THR:HG22	1:C:1109:LEU:HD11	1.97	0.45
1:C:1034:LEU:HD22	1:D:938:LEU:CD2	2.46	0.45
1:D:250:ARG:HH21	1:D:274:LEU:HD21	1.81	0.45
1:D:351:VAL:HG21	1:D:432:ALA:HB1	1.97	0.45
1:D:617:PHE:C	1:D:619:MET:H	2.24	0.45
1:D:1314:HIS:NE2	1:D:1328:MET:SD	2.89	0.45
1:A:144:ARG:NH2	1:A:288:ASP:OD2	2.41	0.45
1:A:706:THR:HG22	1:A:1109:LEU:HD11	1.97	0.45
1:B:191:ARG:HH11	1:B:192:ARG:HG2	1.81	0.45
1:B:427:GLN:HG2	1:B:428:ASP:N	2.31	0.45
1:B:774:ARG:HG3	1:B:777:ARG:HE	1.80	0.45
1:C:685:ARG:HG2	1:C:1136:ARG:NH1	2.31	0.45
1:D:79:SER:HA	1:D:113:TRP:CH2	2.51	0.45
1:D:126:ALA:HB3	1:D:144:ARG:HB2	1.98	0.45
1:D:565:LEU:HD23	1:D:568:LEU:HD12	1.96	0.45
1:D:623:ARG:HH22	1:D:711:ALA:HB1	1.81	0.45
1:A:492:LEU:HB3	1:A:628:TRP:CH2	2.51	0.45
1:A:671:SER:O	1:A:675:MET:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1067:ARG:O	1:A:1071:ILE:HG12	2.16	0.45
1:A:1273:PRO:HG2	1:A:1334:ARG:HE	1.81	0.45
1:B:126:ALA:HB3	1:B:144:ARG:HB2	1.98	0.45
1:B:250:ARG:HH21	1:B:274:LEU:HD21	1.81	0.45
1:B:1158:MET:HA	1:B:1161:LEU:HB2	1.98	0.45
1:C:581:ARG:HE	1:C:584:ASP:CG	2.24	0.45
1:C:602:VAL:HG23	1:C:602:VAL:O	2.16	0.45
1:C:617:PHE:C	1:C:619:MET:H	2.24	0.45
1:C:690:PHE:HA	1:C:693:CYS:SG	2.56	0.45
1:D:559:HIS:ND1	1:D:562:ALA:HB3	2.32	0.45
1:D:602:VAL:O	1:D:602:VAL:HG23	2.16	0.45
1:B:659:LEU:HD13	1:B:678:LEU:HD12	1.97	0.45
1:C:353:VAL:HA	1:C:419:PHE:HB3	1.99	0.45
1:C:456:LEU:O	1:C:460:VAL:HG13	2.17	0.45
1:C:623:ARG:HH22	1:C:711:ALA:HB1	1.81	0.45
1:D:581:ARG:HE	1:D:584:ASP:CG	2.24	0.45
1:D:1326:ASN:N	1:D:1436:ASP:O	2.47	0.45
1:A:602:VAL:HG23	1:A:602:VAL:O	2.16	0.45
1:A:1075:HIS:O	1:A:1075:HIS:ND1	2.47	0.45
1:A:1314:HIS:NE2	1:A:1328:MET:SD	2.89	0.45
1:C:559:HIS:ND1	1:C:562:ALA:HB3	2.32	0.45
1:C:1239:HIS:NE2	1:C:1330:ARG:O	2.25	0.45
1:D:249:ARG:HH11	1:D:265:ILE:HG12	1.82	0.45
1:A:456:LEU:O	1:A:460:VAL:HG13	2.16	0.45
1:A:637:LEU:O	1:A:641:ILE:HG12	2.17	0.45
1:A:667:GLU:O	1:A:668:ASP:OD1	2.35	0.45
1:B:195:VAL:HG23	1:B:196:LYS:HD2	1.98	0.45
1:B:249:ARG:HH11	1:B:265:ILE:HG12	1.82	0.45
1:B:249:ARG:HD3	1:B:265:ILE:H	1.82	0.45
1:B:353:VAL:HA	1:B:419:PHE:HB3	1.99	0.45
1:B:637:LEU:O	1:B:641:ILE:HG12	2.17	0.45
1:C:79:SER:HA	1:C:113:TRP:CH2	2.51	0.45
1:C:802:ASN:HD22	1:C:1082:PRO:HG3	1.82	0.45
1:C:1314:HIS:NE2	1:C:1328:MET:SD	2.89	0.45
1:D:195:VAL:HG23	1:D:196:LYS:HD2	1.98	0.45
1:D:353:VAL:HA	1:D:419:PHE:HB3	1.99	0.45
1:D:444:GLN:HA	1:D:447:PHE:CE1	2.52	0.45
1:D:480:LYS:HD2	1:D:480:LYS:HA	1.70	0.45
1:D:1067:ARG:O	1:D:1071:ILE:HG12	2.16	0.45
1:D:1158:MET:HA	1:D:1161:LEU:HB2	1.98	0.45
1:A:965:TRP:CD1	1:D:1022:GLU:HG3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:444:GLN:HA	1:C:447:PHE:CE1	2.52	0.45
1:C:667:GLU:O	1:C:668:ASP:OD1	2.35	0.45
1:D:525:ASN:O	1:D:632:GLN:NE2	2.49	0.45
1:D:1273:PRO:HG2	1:D:1334:ARG:HE	1.81	0.45
1:A:185:ARG:O	1:A:189:ILE:HD12	2.17	0.45
1:A:525:ASN:O	1:A:632:GLN:NE2	2.49	0.45
1:A:1082:PRO:HA	1:A:1085:ILE:HB	1.99	0.45
1:B:185:ARG:O	1:B:189:ILE:HD12	2.17	0.45
1:B:646:GLN:HE22	1:B:1126:ILE:HD11	1.81	0.45
1:C:191:ARG:HH11	1:C:192:ARG:HG2	1.81	0.45
1:C:671:SER:O	1:C:675:MET:HG2	2.16	0.45
1:D:646:GLN:HE22	1:D:1126:ILE:HD11	1.81	0.45
1:B:79:SER:HA	1:B:113:TRP:CH2	2.51	0.45
1:B:1125:GLU:OE1	1:B:1125:GLU:N	2.50	0.45
1:B:1243:ARG:NH2	1:B:1259:ASN:OD1	2.48	0.45
1:C:363:ILE:HA	1:C:366:VAL:HG12	1.99	0.45
1:C:637:LEU:O	1:C:641:ILE:HG12	2.17	0.45
1:C:818:MET:HA	1:C:818:MET:HE2	1.98	0.45
1:C:1158:MET:HA	1:C:1161:LEU:HB2	1.98	0.45
1:D:185:ARG:O	1:D:189:ILE:HD12	2.17	0.45
1:D:456:LEU:O	1:D:460:VAL:HG13	2.16	0.45
1:D:492:LEU:HB3	1:D:628:TRP:CH2	2.51	0.45
1:D:495:ASN:OD1	1:D:496:LYS:N	2.44	0.45
1:A:250:ARG:HH21	1:A:274:LEU:HD21	1.81	0.45
1:A:522:LEU:O	1:A:628:TRP:NE1	2.36	0.45
1:A:924:ILE:O	1:A:927:VAL:HG12	2.17	0.45
1:B:414:GLN:O	1:B:440:ALA:HA	2.17	0.45
1:B:685:ARG:HG2	1:B:1136:ARG:NH1	2.31	0.45
1:C:185:ARG:O	1:C:189:ILE:HD12	2.17	0.45
1:C:249:ARG:HH11	1:C:265:ILE:HG12	1.82	0.45
1:D:575:PRO:C	1:D:577:TYR:N	2.75	0.45
1:A:685:ARG:HG2	1:A:1136:ARG:NH1	2.31	0.44
1:A:802:ASN:HD22	1:A:1082:PRO:HG3	1.82	0.44
1:A:863:TYR:CZ	1:A:869:ASN:HB3	2.53	0.44
1:B:444:GLN:HA	1:B:447:PHE:CE1	2.52	0.44
1:C:126:ALA:HB3	1:C:144:ARG:HB2	1.98	0.44
1:C:742:VAL:HG23	1:C:1075:HIS:HD2	1.82	0.44
1:C:1082:PRO:HA	1:C:1085:ILE:HB	1.99	0.44
1:C:1273:PRO:HG2	1:C:1334:ARG:HE	1.81	0.44
1:D:249:ARG:HD3	1:D:265:ILE:H	1.82	0.44
1:D:1243:ARG:NH2	1:D:1259:ASN:OD1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:ARG:HH11	1:A:265:ILE:HG12	1.82	0.44
1:A:444:GLN:HA	1:A:447:PHE:CE1	2.52	0.44
1:A:559:HIS:ND1	1:A:562:ALA:HB3	2.32	0.44
1:A:1058:HIS:O	1:A:1062:ILE:HG12	2.18	0.44
1:A:1125:GLU:OE1	1:A:1125:GLU:N	2.51	0.44
1:A:1243:ARG:NH2	1:A:1259:ASN:OD1	2.48	0.44
1:B:303:THR:HB	1:B:346:ASN:ND2	2.33	0.44
1:C:575:PRO:C	1:C:577:TYR:N	2.75	0.44
1:C:863:TYR:CZ	1:C:869:ASN:HB3	2.53	0.44
1:A:269:ASP:OD1	1:A:270:GLY:N	2.51	0.44
1:A:708:VAL:HG23	1:A:710:GLU:HG2	1.99	0.44
1:A:1348:LEU:HB3	1:A:1399:PRO:HG3	2.00	0.44
1:A:1357:ARG:HD2	1:A:1452:GLN:CB	2.48	0.44
1:B:617:PHE:C	1:B:619:MET:H	2.24	0.44
1:B:667:GLU:O	1:B:668:ASP:OD1	2.35	0.44
1:B:924:ILE:O	1:B:927:VAL:HG12	2.17	0.44
1:C:760:MET:HE2	1:C:760:MET:N	2.33	0.44
1:D:1357:ARG:HD2	1:D:1452:GLN:CB	2.48	0.44
1:B:1314:HIS:NE2	1:B:1328:MET:SD	2.89	0.44
1:C:430:ASP:HB2	1:C:462:TRP:NE1	2.32	0.44
1:C:434:LEU:O	1:C:434:LEU:HD23	2.18	0.44
1:C:645:SER:O	1:C:1129:LYS:NZ	2.43	0.44
1:C:1058:HIS:O	1:C:1062:ILE:HG12	2.17	0.44
1:D:742:VAL:HG23	1:D:1075:HIS:HD2	1.82	0.44
1:D:863:TYR:CZ	1:D:869:ASN:HB3	2.52	0.44
1:A:801:LEU:HD12	1:A:1081:PRO:HB3	2.00	0.44
1:A:934:VAL:O	1:A:938:LEU:HG	2.17	0.44
1:B:456:LEU:O	1:B:460:VAL:HG13	2.16	0.44
1:B:863:TYR:CZ	1:B:869:ASN:HB3	2.53	0.44
1:B:1058:HIS:O	1:B:1062:ILE:HG12	2.17	0.44
1:B:1393:GLU:OE1	1:B:1394:PRO:HD2	2.18	0.44
1:C:303:THR:HB	1:C:346:ASN:ND2	2.33	0.44
1:C:480:LYS:HD2	1:C:480:LYS:HA	1.70	0.44
1:C:1348:LEU:HB3	1:C:1399:PRO:HG3	2.00	0.44
1:C:1357:ARG:HD2	1:C:1452:GLN:CB	2.48	0.44
1:D:590:LEU:O	1:D:592:VAL:N	2.48	0.44
1:D:1268:PHE:CZ	1:D:1270:ILE:HB	2.53	0.44
1:D:1348:LEU:HB3	1:D:1399:PRO:HG3	2.00	0.44
1:A:923:LYS:HG2	1:D:1047:MET:SD	2.57	0.44
1:A:1268:PHE:CZ	1:A:1270:ILE:HB	2.53	0.44
1:B:1357:ARG:HD2	1:B:1452:GLN:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1151:ILE:O	1:C:1155:VAL:HG13	2.18	0.44
1:C:1268:PHE:CZ	1:C:1270:ILE:HB	2.53	0.44
1:D:191:ARG:HH11	1:D:192:ARG:HG2	1.81	0.44
1:D:345:THR:OG1	1:D:412:ARG:NH1	2.51	0.44
1:D:414:GLN:O	1:D:440:ALA:HA	2.17	0.44
1:D:818:MET:HE2	1:D:818:MET:HA	1.98	0.44
1:D:924:ILE:O	1:D:927:VAL:HG12	2.17	0.44
1:A:201:THR:OG1	1:A:202:GLY:N	2.46	0.44
1:A:303:THR:HB	1:A:346:ASN:ND2	2.33	0.44
1:A:760:MET:HE2	1:A:760:MET:N	2.33	0.44
1:B:575:PRO:C	1:B:577:TYR:N	2.75	0.44
1:B:760:MET:N	1:B:760:MET:HE2	2.33	0.44
1:B:802:ASN:HD22	1:B:1082:PRO:HG3	1.82	0.44
1:C:269:ASP:OD1	1:C:270:GLY:N	2.51	0.44
1:C:345:THR:OG1	1:C:412:ARG:NH1	2.51	0.44
1:C:525:ASN:O	1:C:632:GLN:NE2	2.49	0.44
1:D:363:ILE:HA	1:D:366:VAL:HG12	1.99	0.44
1:D:708:VAL:HG23	1:D:710:GLU:HG2	1.99	0.44
1:D:1082:PRO:HA	1:D:1085:ILE:HB	1.99	0.44
1:A:345:THR:OG1	1:A:412:ARG:NH1	2.51	0.44
1:A:568:LEU:O	1:A:657:LYS:NZ	2.51	0.44
1:A:1393:GLU:OE1	1:A:1394:PRO:HD2	2.18	0.44
1:B:345:THR:OG1	1:B:412:ARG:NH1	2.51	0.44
1:B:444:GLN:HA	1:B:447:PHE:HE1	1.83	0.44
1:B:818:MET:HE2	1:B:818:MET:HA	1.98	0.44
1:B:934:VAL:O	1:B:938:LEU:HG	2.17	0.44
1:B:1348:LEU:HB3	1:B:1399:PRO:HG3	2.00	0.44
1:C:516:TRP:CZ2	1:C:585:ARG:HD3	2.52	0.44
1:C:568:LEU:O	1:C:657:LYS:NZ	2.51	0.44
1:C:801:LEU:HD12	1:C:1081:PRO:HB3	2.00	0.44
1:C:934:VAL:O	1:C:938:LEU:HG	2.18	0.44
1:C:982:ILE:HB	1:D:981:GLN:HB2	2.00	0.44
1:C:1042:ASN:O	1:C:1045:ILE:HB	2.18	0.44
1:C:1143:ARG:HA	1:C:1144:PRO:HD3	1.92	0.44
1:C:1393:GLU:OE1	1:C:1394:PRO:HD2	2.18	0.44
1:D:434:LEU:HD23	1:D:434:LEU:O	2.18	0.44
1:D:667:GLU:O	1:D:668:ASP:OD1	2.35	0.44
1:D:934:VAL:O	1:D:938:LEU:HG	2.17	0.44
1:A:195:VAL:HG23	1:A:196:LYS:HD2	1.98	0.44
1:A:353:VAL:HA	1:A:419:PHE:HB3	1.99	0.44
1:A:363:ILE:HA	1:A:366:VAL:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:707:ARG:HG2	1:A:708:VAL:H	1.83	0.44
1:B:568:LEU:O	1:B:657:LYS:NZ	2.51	0.44
1:B:801:LEU:HD12	1:B:1081:PRO:HB3	2.00	0.44
1:C:414:GLN:O	1:C:440:ALA:HA	2.17	0.44
1:D:144:ARG:NH2	1:D:288:ASP:OD2	2.41	0.44
1:D:269:ASP:OD1	1:D:270:GLY:N	2.51	0.44
1:D:420:ARG:HD3	1:D:420:ARG:HA	1.79	0.44
1:D:637:LEU:O	1:D:641:ILE:HG12	2.17	0.44
1:D:707:ARG:HG2	1:D:708:VAL:H	1.83	0.44
1:D:760:MET:HE2	1:D:760:MET:N	2.33	0.44
1:D:1393:GLU:OE1	1:D:1394:PRO:HD2	2.18	0.44
1:A:1151:ILE:O	1:A:1155:VAL:HG13	2.18	0.43
1:A:1158:MET:HA	1:A:1161:LEU:HB2	1.98	0.43
1:B:269:ASP:OD1	1:B:270:GLY:N	2.51	0.43
1:B:559:HIS:ND1	1:B:562:ALA:HB3	2.32	0.43
1:C:1125:GLU:OE1	1:C:1125:GLU:N	2.51	0.43
1:D:303:THR:HB	1:D:346:ASN:ND2	2.33	0.43
1:D:801:LEU:HD12	1:D:1081:PRO:HB3	2.00	0.43
1:D:802:ASN:HD22	1:D:1082:PRO:HG3	1.82	0.43
1:D:1042:ASN:O	1:D:1045:ILE:HB	2.18	0.43
1:A:249:ARG:HD3	1:A:265:ILE:H	1.82	0.43
1:B:430:ASP:HB2	1:B:462:TRP:NE1	2.32	0.43
1:B:1042:ASN:O	1:B:1045:ILE:HB	2.18	0.43
1:C:444:GLN:HA	1:C:447:PHE:HE1	1.83	0.43
1:C:744:TRP:H	1:C:796:VAL:HG13	1.83	0.43
1:C:924:ILE:O	1:C:927:VAL:HG12	2.18	0.43
1:D:568:LEU:O	1:D:657:LYS:NZ	2.51	0.43
1:B:1268:PHE:CZ	1:B:1270:ILE:HB	2.53	0.43
1:C:708:VAL:HG23	1:C:710:GLU:HG2	1.99	0.43
1:C:714:LYS:O	1:C:715:THR:OG1	2.24	0.43
1:C:715:THR:HG22	1:C:719:GLN:OE1	2.19	0.43
1:D:1125:GLU:OE1	1:D:1125:GLU:N	2.50	0.43
1:D:1151:ILE:O	1:D:1155:VAL:HG13	2.18	0.43
1:A:126:ALA:HB3	1:A:144:ARG:HB2	1.98	0.43
1:A:398:ARG:HD2	1:A:398:ARG:HA	1.86	0.43
1:A:414:GLN:O	1:A:440:ALA:HA	2.17	0.43
1:A:420:ARG:HD3	1:A:420:ARG:HA	1.79	0.43
1:B:363:ILE:HA	1:B:366:VAL:HG12	1.99	0.43
1:B:590:LEU:O	1:B:592:VAL:N	2.48	0.43
1:B:715:THR:HG22	1:B:719:GLN:OE1	2.18	0.43
1:C:249:ARG:HD3	1:C:265:ILE:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:201:THR:OG1	1:D:202:GLY:N	2.46	0.43
1:D:577:TYR:CB	1:D:585:ARG:HH22	2.31	0.43
1:D:744:TRP:H	1:D:796:VAL:HG13	1.83	0.43
1:D:1425:TYR:OH	1:D:1428:TYR:O	2.28	0.43
1:A:434:LEU:HD23	1:A:434:LEU:O	2.18	0.43
1:A:744:TRP:H	1:A:796:VAL:HG13	1.83	0.43
1:A:1143:ARG:HA	1:A:1144:PRO:HD3	1.92	0.43
1:B:742:VAL:HG23	1:B:1075:HIS:HD2	1.83	0.43
1:C:130:ILE:HD11	1:C:264:TYR:HB2	2.01	0.43
1:C:1390:GLY:HA3	1:C:1401:LYS:NZ	2.34	0.43
1:D:1058:HIS:O	1:D:1062:ILE:HG12	2.18	0.43
1:D:1264:TRP:NE1	1:D:1326:ASN:O	2.48	0.43
1:D:1346:HIS:O	1:D:1392:ARG:HG2	2.19	0.43
1:D:1390:GLY:HA3	1:D:1401:LYS:HZ3	1.83	0.43
1:A:1042:ASN:O	1:A:1045:ILE:HB	2.18	0.43
1:A:1130:GLU:OE1	1:A:1130:GLU:C	2.62	0.43
1:C:696:LYS:HE2	1:C:696:LYS:HB2	1.87	0.43
1:C:1034:LEU:CD2	1:D:934:VAL:HG13	2.48	0.43
1:D:1390:GLY:HA3	1:D:1401:LYS:NZ	2.34	0.43
1:A:406:ILE:O	1:A:410:VAL:HG23	2.18	0.43
1:A:577:TYR:CB	1:A:585:ARG:HH22	2.31	0.43
1:A:1489:LYS:HE2	1:A:1503:TYR:OH	2.19	0.43
1:B:708:VAL:HG23	1:B:710:GLU:HG2	1.99	0.43
1:B:924:ILE:HA	1:B:927:VAL:HG12	2.00	0.43
1:B:1082:PRO:HA	1:B:1085:ILE:HB	1.99	0.43
1:A:130:ILE:HD11	1:A:264:TYR:HB2	2.01	0.43
1:A:430:ASP:HB2	1:A:462:TRP:NE1	2.32	0.43
1:A:699:GLU:O	1:A:702:GLN:HG2	2.19	0.43
1:A:1047:MET:SD	1:B:923:LYS:HG2	2.59	0.43
1:A:1339:LEU:HD21	1:A:1440:ILE:HD11	2.01	0.43
1:B:744:TRP:H	1:B:796:VAL:HG13	1.83	0.43
1:B:1390:GLY:HA3	1:B:1401:LYS:NZ	2.34	0.43
1:C:727:MET:O	1:C:731:SER:OG	2.24	0.43
1:C:1243:ARG:NH2	1:C:1259:ASN:OD1	2.48	0.43
1:C:1358:ASN:OD1	1:C:1358:ASN:N	2.48	0.43
1:D:450:GLU:OE1	1:D:450:GLU:C	2.62	0.43
1:D:952:LYS:HE3	1:D:953:GLN:HE21	1.84	0.43
1:D:1109:LEU:HD23	1:D:1111:ASN:H	1.84	0.43
1:B:699:GLU:O	1:B:702:GLN:HG2	2.19	0.43
1:C:1109:LEU:HD23	1:C:1111:ASN:H	1.84	0.43
1:C:1304:VAL:HA	1:C:1309:ASP:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:130:ILE:HD11	1:D:264:TYR:HB2	2.01	0.43
1:D:444:GLN:HA	1:D:447:PHE:HE1	1.83	0.43
1:D:715:THR:HG22	1:D:719:GLN:OE1	2.18	0.43
1:A:742:VAL:HG23	1:A:1075:HIS:HD2	1.83	0.43
1:A:794:ALA:O	1:A:798:VAL:HG23	2.19	0.43
1:A:813:PHE:CZ	1:A:899:LEU:HD12	2.54	0.43
1:B:406:ILE:O	1:B:410:VAL:HG23	2.18	0.43
1:B:450:GLU:C	1:B:450:GLU:OE1	2.62	0.43
1:D:427:GLN:NE2	1:D:428:ASP:O	2.52	0.43
1:D:1339:LEU:HD21	1:D:1440:ILE:HD11	2.01	0.43
1:D:1378:LYS:HB3	1:D:1472:SER:HB3	2.01	0.43
1:A:548:ALA:O	1:A:587:ARG:NH2	2.52	0.42
1:A:1325:LEU:HD23	1:A:1325:LEU:HA	1.86	0.42
1:B:130:ILE:HD11	1:B:264:TYR:HB2	2.01	0.42
1:B:434:LEU:O	1:B:434:LEU:HD23	2.18	0.42
1:B:548:ALA:O	1:B:587:ARG:NH2	2.52	0.42
1:B:1075:HIS:O	1:B:1075:HIS:ND1	2.47	0.42
1:B:1151:ILE:O	1:B:1155:VAL:HG13	2.18	0.42
1:B:1304:VAL:HA	1:B:1309:ASP:HA	2.01	0.42
1:C:406:ILE:O	1:C:410:VAL:HG23	2.18	0.42
1:C:623:ARG:NH2	1:C:711:ALA:HB1	2.34	0.42
1:D:794:ALA:O	1:D:798:VAL:HG23	2.19	0.42
1:D:924:ILE:HA	1:D:927:VAL:HG12	2.00	0.42
1:A:444:GLN:HA	1:A:447:PHE:HE1	1.83	0.42
1:A:773:PHE:O	1:A:777:ARG:N	2.53	0.42
1:A:924:ILE:HA	1:A:927:VAL:HG12	2.00	0.42
1:A:952:LYS:HE3	1:A:953:GLN:HE21	1.84	0.42
1:A:1346:HIS:O	1:A:1392:ARG:HG2	2.19	0.42
1:A:1380:PRO:HG3	1:A:1471:ALA:HB2	2.01	0.42
1:B:398:ARG:HD2	1:B:398:ARG:HA	1.86	0.42
1:B:595:VAL:HG23	1:B:603:SER:HB2	2.01	0.42
1:B:813:PHE:CZ	1:B:899:LEU:HD12	2.54	0.42
1:B:952:LYS:HE3	1:B:953:GLN:HE21	1.84	0.42
1:B:1339:LEU:HD21	1:B:1440:ILE:HD11	2.01	0.42
1:C:1043:LEU:HD13	1:D:930:MET:HE3	2.00	0.42
1:C:1378:LYS:HB3	1:C:1472:SER:HB3	2.01	0.42
1:C:1398:LEU:HA	1:C:1399:PRO:HD3	1.91	0.42
1:D:406:ILE:O	1:D:410:VAL:HG23	2.18	0.42
1:A:336:THR:O	1:A:339:THR:HB	2.19	0.42
1:A:773:PHE:CD2	1:A:787:ARG:HD2	2.54	0.42
1:A:1109:LEU:HD23	1:A:1111:ASN:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1243:ARG:NH1	1:A:1257:VAL:O	2.52	0.42
1:B:623:ARG:NH2	1:B:711:ALA:HB1	2.34	0.42
1:B:1254:ARG:NH2	1:B:1432:PRO:O	2.53	0.42
1:C:314:LYS:CE	1:C:323:ILE:HG13	2.42	0.42
1:C:336:THR:O	1:C:339:THR:HB	2.19	0.42
1:C:548:ALA:O	1:C:587:ARG:NH2	2.52	0.42
1:D:623:ARG:NH2	1:D:711:ALA:HB1	2.34	0.42
1:D:813:PHE:CZ	1:D:899:LEU:HD12	2.54	0.42
1:A:427:GLN:NE2	1:A:428:ASP:O	2.52	0.42
1:B:516:TRP:CZ2	1:B:585:ARG:HD3	2.52	0.42
1:B:558:MET:HB3	1:B:585:ARG:NH1	2.35	0.42
1:B:1243:ARG:NH1	1:B:1257:VAL:O	2.52	0.42
1:B:1429:MET:CE	1:B:1442:THR:HG23	2.50	0.42
1:C:558:MET:HB3	1:C:585:ARG:NH1	2.35	0.42
1:C:655:CYS:O	1:C:659:LEU:HG	2.20	0.42
1:C:794:ALA:O	1:C:798:VAL:HG23	2.19	0.42
1:C:924:ILE:HA	1:C:927:VAL:HG12	2.00	0.42
1:C:1489:LYS:HE2	1:C:1503:TYR:OH	2.19	0.42
1:D:558:MET:HB3	1:D:585:ARG:NH1	2.35	0.42
1:D:1130:GLU:OE1	1:D:1130:GLU:C	2.62	0.42
1:D:1489:LYS:HE2	1:D:1503:TYR:OH	2.19	0.42
1:A:480:LYS:HB3	1:A:483:ASP:HB2	2.01	0.42
1:A:905:LEU:O	1:A:908:LEU:HG	2.20	0.42
1:A:1254:ARG:NH2	1:A:1432:PRO:O	2.53	0.42
1:C:450:GLU:C	1:C:450:GLU:OE1	2.62	0.42
1:C:511:LYS:HG3	1:C:512:GLU:OE1	2.20	0.42
1:C:699:GLU:O	1:C:702:GLN:HG2	2.19	0.42
1:C:773:PHE:CD2	1:C:787:ARG:HD2	2.54	0.42
1:D:336:THR:O	1:D:339:THR:HB	2.19	0.42
1:D:622:ILE:O	1:D:625:LEU:HB2	2.20	0.42
1:D:1335:GLY:O	1:D:1437:ASN:HB2	2.19	0.42
1:A:575:PRO:C	1:A:577:TYR:N	2.75	0.42
1:B:427:GLN:NE2	1:B:428:ASP:O	2.52	0.42
1:B:488:MET:HE3	1:B:492:LEU:HD21	2.02	0.42
1:B:655:CYS:O	1:B:659:LEU:HG	2.20	0.42
1:B:773:PHE:CD2	1:B:787:ARG:HD2	2.54	0.42
1:B:794:ALA:O	1:B:798:VAL:HG23	2.19	0.42
1:B:1109:LEU:HD23	1:B:1111:ASN:H	1.84	0.42
1:B:1489:LYS:HE2	1:B:1503:TYR:OH	2.19	0.42
1:C:303:THR:O	1:C:346:ASN:ND2	2.53	0.42
1:C:488:MET:HE3	1:C:492:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1254:ARG:NH2	1:C:1432:PRO:O	2.53	0.42
1:C:1335:GLY:O	1:C:1437:ASN:HB2	2.19	0.42
1:D:558:MET:HE2	1:D:577:TYR:CE1	2.55	0.42
1:A:180:PHE:CE2	1:A:182:MET:HB2	2.55	0.42
1:A:215:MET:HA	1:A:218:VAL:HG12	2.01	0.42
1:A:450:GLU:C	1:A:450:GLU:OE1	2.62	0.42
1:A:511:LYS:HG3	1:A:512:GLU:OE1	2.20	0.42
1:A:1304:VAL:HA	1:A:1309:ASP:HA	2.00	0.42
1:A:1390:GLY:HA3	1:A:1401:LYS:NZ	2.34	0.42
1:B:183:LYS:HB2	1:B:186:LEU:HB2	2.01	0.42
1:B:511:LYS:HG3	1:B:512:GLU:OE1	2.20	0.42
1:B:1154:LYS:HE3	1:B:1154:LYS:H	1.85	0.42
1:B:1346:HIS:O	1:B:1392:ARG:HG2	2.19	0.42
1:C:501:LYS:HA	1:C:504:LEU:HG	2.02	0.42
1:C:532:PHE:O	1:C:536:LEU:HD23	2.20	0.42
1:C:595:VAL:HG23	1:C:603:SER:HB2	2.01	0.42
1:C:622:ILE:O	1:C:625:LEU:HB2	2.20	0.42
1:C:799:PHE:HD1	1:C:1074:TYR:CE2	2.38	0.42
1:C:1346:HIS:O	1:C:1392:ARG:HG2	2.19	0.42
1:D:303:THR:O	1:D:346:ASN:ND2	2.53	0.42
1:D:773:PHE:CD2	1:D:787:ARG:HD2	2.54	0.42
1:D:1304:VAL:HA	1:D:1309:ASP:HA	2.01	0.42
1:D:1429:MET:CE	1:D:1442:THR:HG23	2.50	0.42
1:A:715:THR:HG22	1:A:719:GLN:OE1	2.18	0.42
1:A:1044:LEU:HA	1:A:1047:MET:HE3	2.02	0.42
1:A:1335:GLY:O	1:A:1437:ASN:HB2	2.19	0.42
1:B:114:ASP:HB3	1:B:117:LYS:HG2	2.02	0.42
1:B:532:PHE:O	1:B:536:LEU:HD23	2.20	0.42
1:B:577:TYR:CB	1:B:585:ARG:HH22	2.31	0.42
1:B:622:ILE:O	1:B:625:LEU:HB2	2.19	0.42
1:B:905:LEU:O	1:B:908:LEU:HG	2.20	0.42
1:B:1257:VAL:HG13	1:B:1261:LYS:HG3	2.02	0.42
1:C:114:ASP:HB3	1:C:117:LYS:HG2	2.02	0.42
1:C:183:LYS:HB2	1:C:186:LEU:HB2	2.01	0.42
1:C:215:MET:HA	1:C:218:VAL:HG12	2.01	0.42
1:C:558:MET:HE2	1:C:577:TYR:CE1	2.55	0.42
1:C:952:LYS:HE3	1:C:953:GLN:HE21	1.84	0.42
1:C:1429:MET:CE	1:C:1442:THR:HG23	2.50	0.42
1:D:180:PHE:CE2	1:D:182:MET:HB2	2.55	0.42
1:D:511:LYS:HG3	1:D:512:GLU:OE1	2.20	0.42
1:D:516:TRP:CZ2	1:D:585:ARG:HD3	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:699:GLU:O	1:D:702:GLN:HG2	2.19	0.42
1:D:1154:LYS:HE3	1:D:1154:LYS:H	1.85	0.42
1:D:1325:LEU:HD23	1:D:1325:LEU:HA	1.86	0.42
1:A:303:THR:O	1:A:346:ASN:ND2	2.53	0.42
1:A:558:MET:HE2	1:A:577:TYR:CE1	2.55	0.42
1:A:1264:TRP:NE1	1:A:1326:ASN:O	2.48	0.42
1:A:1429:MET:CE	1:A:1442:THR:HG23	2.50	0.42
1:B:74:TYR:HB3	1:B:76:VAL:HB	2.02	0.42
1:B:501:LYS:HA	1:B:504:LEU:HG	2.02	0.42
1:B:558:MET:HE2	1:B:577:TYR:CE1	2.55	0.42
1:B:1130:GLU:OE1	1:B:1130:GLU:C	2.62	0.42
1:C:1154:LYS:HE3	1:C:1154:LYS:H	1.85	0.42
1:D:114:ASP:HB3	1:D:117:LYS:HG2	2.02	0.42
1:D:548:ALA:O	1:D:587:ARG:NH2	2.52	0.42
1:D:583:ASN:O	1:D:585:ARG:HG3	2.20	0.42
1:D:905:LEU:O	1:D:908:LEU:HG	2.20	0.42
1:D:1075:HIS:O	1:D:1075:HIS:ND1	2.47	0.42
1:A:114:ASP:HB3	1:A:117:LYS:HG2	2.02	0.42
1:A:655:CYS:O	1:A:659:LEU:HG	2.20	0.42
1:A:1326:ASN:N	1:A:1436:ASP:O	2.48	0.42
1:A:1378:LYS:HB3	1:A:1472:SER:HB3	2.01	0.42
1:B:94:THR:HB	1:B:292:HIS:HB3	2.02	0.42
1:B:180:PHE:CE2	1:B:182:MET:HB2	2.55	0.42
1:B:257:THR:HG22	1:B:258:GLY:N	2.35	0.42
1:B:773:PHE:O	1:B:777:ARG:N	2.53	0.42
1:B:961:ARG:HB2	1:B:966:LEU:HB2	2.02	0.42
1:B:1143:ARG:NE	1:B:1145:GLU:HB2	2.34	0.42
1:B:1335:GLY:O	1:B:1437:ASN:HB2	2.19	0.42
1:C:74:TYR:HB3	1:C:76:VAL:HB	2.02	0.42
1:C:813:PHE:CZ	1:C:899:LEU:HD12	2.54	0.42
1:D:532:PHE:O	1:D:536:LEU:HD23	2.20	0.42
1:D:655:CYS:O	1:D:659:LEU:HG	2.20	0.42
1:D:799:PHE:HD1	1:D:1074:TYR:CE2	2.38	0.42
1:D:932:LYS:HA	1:D:932:LYS:HD2	1.85	0.42
1:A:257:THR:HG22	1:A:258:GLY:N	2.35	0.41
1:A:309:ILE:O	1:A:313:THR:OG1	2.29	0.41
1:A:622:ILE:O	1:A:625:LEU:HB2	2.20	0.41
1:B:1378:LYS:HB3	1:B:1472:SER:HB3	2.01	0.41
1:B:1406:LEU:HA	1:B:1466:ALA:HA	2.02	0.41
1:C:173:VAL:HB	1:C:207:THR:HG22	2.02	0.41
1:C:337:LEU:HD23	1:C:405:LYS:HE3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:427:GLN:NE2	1:C:428:ASP:O	2.52	0.41
1:C:1380:PRO:HG3	1:C:1471:ALA:HB2	2.01	0.41
1:D:309:ILE:O	1:D:313:THR:OG1	2.29	0.41
1:D:480:LYS:HB3	1:D:483:ASP:HB2	2.01	0.41
1:D:1380:PRO:HG3	1:D:1471:ALA:HB2	2.01	0.41
1:A:314:LYS:CE	1:A:323:ILE:HG13	2.42	0.41
1:A:595:VAL:HG23	1:A:603:SER:HB2	2.01	0.41
1:A:972:TYR:O	1:A:976:LEU:HD23	2.20	0.41
1:A:1405:ILE:O	1:A:1405:ILE:HG22	2.21	0.41
1:A:1429:MET:N	1:A:1429:MET:SD	2.93	0.41
1:B:173:VAL:HB	1:B:207:THR:HG22	2.02	0.41
1:B:480:LYS:HB3	1:B:483:ASP:HB2	2.01	0.41
1:B:707:ARG:HG2	1:B:708:VAL:H	1.83	0.41
1:B:1077:ARG:HG3	1:B:1078:PRO:HD2	2.03	0.41
1:C:876:ILE:O	1:C:880:VAL:HG23	2.21	0.41
1:C:1044:LEU:HA	1:C:1047:MET:HE3	2.01	0.41
1:C:1130:GLU:OE1	1:C:1130:GLU:C	2.62	0.41
1:D:337:LEU:HD23	1:D:405:LYS:HE3	2.02	0.41
1:D:1405:ILE:O	1:D:1405:ILE:HG22	2.20	0.41
1:A:173:VAL:HB	1:A:207:THR:HG22	2.02	0.41
1:A:250:ARG:HH22	1:A:292:HIS:CD2	2.38	0.41
1:A:501:LYS:HA	1:A:504:LEU:HG	2.01	0.41
1:A:799:PHE:HD1	1:A:1074:TYR:CE2	2.38	0.41
1:A:1257:VAL:HG13	1:A:1261:LYS:HG3	2.02	0.41
1:B:250:ARG:HH22	1:B:292:HIS:CD2	2.38	0.41
1:B:336:THR:O	1:B:339:THR:HB	2.19	0.41
1:B:1143:ARG:HA	1:B:1144:PRO:HD3	1.92	0.41
1:B:1429:MET:N	1:B:1429:MET:SD	2.93	0.41
1:C:257:THR:HG22	1:C:258:GLY:N	2.35	0.41
1:C:583:ASN:O	1:C:585:ARG:HG3	2.20	0.41
1:C:1339:LEU:HD21	1:C:1440:ILE:HD11	2.01	0.41
1:D:240:GLY:O	1:D:284:PHE:HA	2.21	0.41
1:D:649:ILE:HG13	1:D:650:ALA:N	2.36	0.41
1:D:773:PHE:O	1:D:777:ARG:N	2.52	0.41
1:D:876:ILE:O	1:D:880:VAL:HG23	2.20	0.41
1:A:128:GLY:HA3	1:A:259:SER:OG	2.21	0.41
1:A:558:MET:HB3	1:A:585:ARG:NH1	2.35	0.41
1:A:1406:LEU:HA	1:A:1466:ALA:HA	2.02	0.41
1:B:240:GLY:O	1:B:284:PHE:HA	2.21	0.41
1:B:303:THR:O	1:B:346:ASN:ND2	2.53	0.41
1:B:799:PHE:HD1	1:B:1074:TYR:CE2	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1044:LEU:HA	1:B:1047:MET:HE3	2.02	0.41
1:B:1380:PRO:HG3	1:B:1471:ALA:HB2	2.01	0.41
1:C:302:ARG:HA	1:C:305:LEU:HB3	2.03	0.41
1:C:707:ARG:HG2	1:C:708:VAL:H	1.83	0.41
1:C:773:PHE:O	1:C:777:ARG:N	2.52	0.41
1:C:1257:VAL:HG13	1:C:1261:LYS:HG3	2.02	0.41
1:C:1406:LEU:HA	1:C:1466:ALA:HA	2.02	0.41
1:C:1429:MET:N	1:C:1429:MET:SD	2.93	0.41
1:D:595:VAL:HG23	1:D:603:SER:HB2	2.01	0.41
1:D:961:ARG:HB2	1:D:966:LEU:HB2	2.02	0.41
1:A:191:ARG:HH11	1:A:192:ARG:HG2	1.81	0.41
1:A:240:GLY:O	1:A:284:PHE:HA	2.21	0.41
1:A:583:ASN:O	1:A:585:ARG:HG3	2.20	0.41
1:A:623:ARG:NH2	1:A:711:ALA:HB1	2.34	0.41
1:A:1158:MET:SD	1:A:1161:LEU:HD22	2.61	0.41
1:A:1239:HIS:CE1	1:A:1329:GLY:HA3	2.56	0.41
1:B:128:GLY:HA3	1:B:259:SER:OG	2.21	0.41
1:B:583:ASN:O	1:B:585:ARG:HG3	2.20	0.41
1:B:1035:PHE:O	1:B:1039:LEU:HB2	2.21	0.41
1:C:180:PHE:CE2	1:C:182:MET:HB2	2.55	0.41
1:C:232:LYS:O	1:C:233:GLU:C	2.64	0.41
1:C:240:GLY:O	1:C:284:PHE:HA	2.21	0.41
1:C:480:LYS:HB3	1:C:483:ASP:HB2	2.01	0.41
1:C:905:LEU:O	1:C:908:LEU:HG	2.19	0.41
1:C:1355:TRP:CZ3	1:C:1372:LEU:HB3	2.56	0.41
1:C:1405:ILE:O	1:C:1405:ILE:HG22	2.20	0.41
1:D:173:VAL:HB	1:D:207:THR:HG22	2.02	0.41
1:D:215:MET:HA	1:D:218:VAL:HG12	2.01	0.41
1:D:257:THR:HG22	1:D:258:GLY:N	2.35	0.41
1:D:972:TYR:O	1:D:976:LEU:HD23	2.20	0.41
1:A:1077:ARG:HG3	1:A:1078:PRO:HD2	2.03	0.41
1:A:1396:GLU:C	1:A:1398:LEU:H	2.29	0.41
1:B:1158:MET:SD	1:B:1161:LEU:HD22	2.61	0.41
1:B:1355:TRP:CZ3	1:B:1372:LEU:HB3	2.56	0.41
1:B:1390:GLY:HA3	1:B:1401:LYS:HZ3	1.85	0.41
1:C:128:GLY:HA3	1:C:259:SER:OG	2.21	0.41
1:C:182:MET:HB3	1:C:187:LYS:NZ	2.35	0.41
1:C:1035:PHE:O	1:C:1039:LEU:HB2	2.21	0.41
1:C:1264:TRP:NE1	1:C:1326:ASN:O	2.48	0.41
1:C:1273:PRO:HG2	1:C:1334:ARG:HG3	2.03	0.41
1:D:398:ARG:HD2	1:D:398:ARG:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:915:THR:HG23	1:D:924:ILE:HB	2.03	0.41
1:D:1035:PHE:O	1:D:1039:LEU:HB2	2.21	0.41
1:D:1044:LEU:HA	1:D:1047:MET:HE3	2.02	0.41
1:D:1406:LEU:HA	1:D:1466:ALA:HA	2.02	0.41
1:D:1429:MET:N	1:D:1429:MET:SD	2.93	0.41
1:A:182:MET:HB3	1:A:187:LYS:NZ	2.35	0.41
1:A:961:ARG:HB2	1:A:966:LEU:HB2	2.02	0.41
1:A:1273:PRO:HG2	1:A:1334:ARG:HG3	2.03	0.41
1:B:842:GLU:HG2	1:B:1089:HIS:HE1	1.85	0.41
1:B:1051:THR:HA	1:B:1054:GLN:HG2	2.03	0.41
1:B:1257:VAL:HA	1:B:1261:LYS:HE2	2.03	0.41
1:C:250:ARG:HH22	1:C:292:HIS:CD2	2.38	0.41
1:C:1077:ARG:HG3	1:C:1078:PRO:HD2	2.03	0.41
1:C:1243:ARG:NH1	1:C:1257:VAL:O	2.52	0.41
1:D:488:MET:HE3	1:D:492:LEU:HD21	2.02	0.41
1:D:799:PHE:HA	1:D:1074:TYR:CZ	2.55	0.41
1:D:837:PHE:HA	1:D:840:VAL:HG22	2.02	0.41
1:D:1156:ASP:O	1:D:1159:VAL:HG22	2.20	0.41
1:D:1254:ARG:NH2	1:D:1432:PRO:O	2.53	0.41
1:A:69:LYS:NZ	1:A:124:THR:OG1	2.52	0.41
1:A:232:LYS:O	1:A:233:GLU:C	2.64	0.41
1:A:325:ILE:HG12	1:A:348:THR:HG23	2.03	0.41
1:A:337:LEU:HD23	1:A:405:LYS:HE3	2.02	0.41
1:A:478:GLN:C	1:A:480:LYS:H	2.28	0.41
1:A:516:TRP:CZ2	1:A:585:ARG:HD3	2.52	0.41
1:A:799:PHE:HA	1:A:1074:TYR:CZ	2.55	0.41
1:A:1095:LYS:HB3	1:A:1104:LYS:NZ	2.36	0.41
1:A:1154:LYS:HE3	1:A:1154:LYS:H	1.85	0.41
1:A:1487:ASN:HB3	2:A:1601:APR:H61	1.86	0.41
1:B:837:PHE:HA	1:B:840:VAL:HG22	2.02	0.41
1:B:876:ILE:O	1:B:880:VAL:HG23	2.21	0.41
1:B:972:TYR:O	1:B:976:LEU:HD23	2.20	0.41
1:B:1396:GLU:C	1:B:1398:LEU:H	2.29	0.41
1:C:1095:LYS:HB3	1:C:1104:LYS:NZ	2.36	0.41
1:C:1158:MET:SD	1:C:1161:LEU:HD22	2.61	0.41
1:D:94:THR:HB	1:D:292:HIS:HB3	2.02	0.41
1:D:842:GLU:HG2	1:D:1089:HIS:HE1	1.85	0.41
1:D:1396:GLU:C	1:D:1398:LEU:H	2.29	0.41
1:A:183:LYS:HB2	1:A:186:LEU:HB2	2.02	0.41
1:A:619:MET:HE2	1:A:710:GLU:O	2.21	0.41
1:A:915:THR:HG23	1:A:924:ILE:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1038:ILE:HD12	1:B:1044:LEU:CD2	2.50	0.41
1:A:1092:LEU:HA	1:A:1095:LYS:HB2	2.03	0.41
1:B:182:MET:HB3	1:B:187:LYS:NZ	2.35	0.41
1:B:478:GLN:C	1:B:480:LYS:H	2.28	0.41
1:B:600:GLN:O	1:B:602:VAL:HG13	2.21	0.41
1:B:1239:HIS:CE1	1:B:1329:GLY:HA3	2.56	0.41
1:B:1273:PRO:HG2	1:B:1334:ARG:HG3	2.03	0.41
1:C:325:ILE:HG12	1:C:348:THR:HG23	2.03	0.41
1:C:478:GLN:C	1:C:480:LYS:H	2.28	0.41
1:C:941:LEU:O	1:C:945:VAL:HG23	2.21	0.41
1:C:961:ARG:HB2	1:C:966:LEU:HB2	2.02	0.41
1:C:1051:THR:HA	1:C:1054:GLN:HG2	2.03	0.41
1:C:1092:LEU:HA	1:C:1095:LYS:HB2	2.03	0.41
1:C:1241:ASN:HA	1:C:1244:HIS:CD2	2.56	0.41
1:C:1396:GLU:C	1:C:1398:LEU:H	2.29	0.41
1:D:74:TYR:HB3	1:D:76:VAL:HB	2.02	0.41
1:D:182:MET:HB3	1:D:187:LYS:NZ	2.35	0.41
1:D:250:ARG:HH22	1:D:292:HIS:CD2	2.38	0.41
1:D:325:ILE:HG12	1:D:348:THR:HG23	2.03	0.41
1:D:619:MET:HE2	1:D:710:GLU:O	2.21	0.41
1:D:743:TRP:HB2	1:D:1071:ILE:HD12	2.03	0.41
1:D:743:TRP:NE1	1:D:796:VAL:HG12	2.36	0.41
1:D:1158:MET:SD	1:D:1161:LEU:HD22	2.61	0.41
1:D:1161:LEU:HD12	1:D:1161:LEU:HA	1.92	0.41
1:D:1241:ASN:HB2	1:D:1430:ASP:HB3	2.03	0.41
1:D:1355:TRP:CZ3	1:D:1372:LEU:HB3	2.56	0.41
1:D:1358:ASN:OD1	1:D:1358:ASN:N	2.48	0.41
1:A:74:TYR:HB3	1:A:76:VAL:HB	2.02	0.41
1:A:452:TRP:CZ3	1:A:472:ILE:HD12	2.56	0.41
1:A:516:TRP:HE3	1:A:616:THR:HA	1.86	0.41
1:A:532:PHE:O	1:A:536:LEU:HD23	2.20	0.41
1:A:917:SER:HB3	1:A:920:LEU:HD12	2.03	0.41
1:A:1035:PHE:O	1:A:1039:LEU:HB2	2.21	0.41
1:A:1051:THR:HA	1:A:1054:GLN:HG2	2.03	0.41
1:A:1156:ASP:O	1:A:1159:VAL:HG22	2.20	0.41
1:B:215:MET:HA	1:B:218:VAL:HG12	2.02	0.41
1:B:325:ILE:HG12	1:B:348:THR:HG23	2.03	0.41
1:B:799:PHE:HA	1:B:1074:TYR:CZ	2.55	0.41
1:B:1262:VAL:N	1:B:1263:PRO:HD2	2.36	0.41
1:C:799:PHE:HA	1:C:1074:TYR:CZ	2.56	0.41
1:C:932:LYS:HA	1:C:932:LYS:HD2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:972:TYR:O	1:C:976:LEU:HD23	2.20	0.41
1:C:1262:VAL:N	1:C:1263:PRO:HD2	2.36	0.41
1:D:183:LYS:HB2	1:D:186:LEU:HB2	2.01	0.41
1:D:501:LYS:HA	1:D:504:LEU:HG	2.02	0.41
1:D:1077:ARG:HG3	1:D:1078:PRO:HD2	2.03	0.41
1:D:1239:HIS:HE1	1:D:1329:GLY:HA3	1.86	0.41
1:A:94:THR:HB	1:A:292:HIS:HB3	2.02	0.40
1:A:302:ARG:HA	1:A:305:LEU:HB3	2.03	0.40
1:A:488:MET:HE3	1:A:492:LEU:HD21	2.02	0.40
1:A:600:GLN:O	1:A:602:VAL:HG13	2.21	0.40
1:A:876:ILE:O	1:A:880:VAL:HG23	2.20	0.40
1:B:337:LEU:HD23	1:B:405:LYS:HE3	2.02	0.40
1:B:917:SER:HB3	1:B:920:LEU:HD12	2.03	0.40
1:C:726:ASP:O	1:C:730:VAL:HG22	2.22	0.40
1:C:1156:ASP:O	1:C:1159:VAL:HG22	2.20	0.40
1:C:1239:HIS:CE1	1:C:1329:GLY:HA3	2.56	0.40
1:C:1487:ASN:HB3	2:C:1601:APR:H61	1.86	0.40
1:D:456:LEU:HA	1:D:459:ALA:HB3	2.03	0.40
1:D:696:LYS:HE2	1:D:696:LYS:HB2	1.87	0.40
1:D:1092:LEU:HA	1:D:1095:LYS:HB2	2.03	0.40
1:D:1239:HIS:CE1	1:D:1329:GLY:HA3	2.56	0.40
1:D:1273:PRO:HG2	1:D:1334:ARG:HG3	2.03	0.40
1:A:666:GLU:OE2	1:A:668:ASP:HB3	2.22	0.40
1:A:743:TRP:HB2	1:A:1071:ILE:HD12	2.03	0.40
1:A:938:LEU:HD21	1:D:1034:LEU:HD22	2.02	0.40
1:A:1241:ASN:HB2	1:A:1430:ASP:HB3	2.03	0.40
1:B:666:GLU:OE2	1:B:668:ASP:HB3	2.22	0.40
1:B:1156:ASP:O	1:B:1159:VAL:HG22	2.20	0.40
1:C:649:ILE:HG13	1:C:650:ALA:N	2.36	0.40
1:C:842:GLU:HG2	1:C:1089:HIS:HE1	1.85	0.40
1:C:1143:ARG:NE	1:C:1145:GLU:HB2	2.34	0.40
1:C:1257:VAL:HA	1:C:1261:LYS:HE2	2.03	0.40
1:D:516:TRP:HE3	1:D:616:THR:HA	1.86	0.40
1:D:600:GLN:O	1:D:602:VAL:HG13	2.21	0.40
1:D:720:LEU:HA	1:D:723:GLU:OE2	2.21	0.40
1:D:941:LEU:O	1:D:945:VAL:HG23	2.21	0.40
1:D:1429:MET:HE2	1:D:1429:MET:HB2	1.94	0.40
1:A:151:SER:HB3	1:A:308:PHE:CD2	2.55	0.40
1:A:531:LEU:O	1:A:534:SER:OG	2.36	0.40
1:A:720:LEU:HA	1:A:723:GLU:OE2	2.21	0.40
1:A:1068:HIS:O	1:A:1072:GLU:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1257:VAL:HA	1:A:1261:LYS:HE2	2.03	0.40
1:A:1262:VAL:N	1:A:1263:PRO:HD2	2.36	0.40
1:B:69:LYS:NZ	1:B:124:THR:OG1	2.52	0.40
1:B:96:GLU:HB3	1:B:97:GLN:H	1.78	0.40
1:B:308:PHE:HA	1:B:312:GLN:OE1	2.21	0.40
1:B:549:CYS:HB3	1:B:587:ARG:HG3	2.04	0.40
1:B:720:LEU:HA	1:B:723:GLU:OE2	2.21	0.40
1:B:1092:LEU:HA	1:B:1095:LYS:HB2	2.03	0.40
1:B:1241:ASN:HA	1:B:1244:HIS:CD2	2.56	0.40
1:B:1378:LYS:HB2	1:B:1385:TRP:CE3	2.56	0.40
1:B:1405:ILE:O	1:B:1405:ILE:HG22	2.20	0.40
1:C:546:ARG:HA	1:C:546:ARG:HD3	1.94	0.40
1:C:549:CYS:HB3	1:C:587:ARG:HG3	2.03	0.40
1:C:743:TRP:HB2	1:C:1071:ILE:HD12	2.03	0.40
1:C:743:TRP:NE1	1:C:796:VAL:HG12	2.36	0.40
1:D:549:CYS:HB3	1:D:587:ARG:HG3	2.03	0.40
1:D:683:GLU:O	1:D:687:ILE:HG13	2.22	0.40
1:D:917:SER:HB3	1:D:920:LEU:HD12	2.03	0.40
1:A:308:PHE:HA	1:A:312:GLN:OE1	2.21	0.40
1:A:1143:ARG:NE	1:A:1145:GLU:HB2	2.34	0.40
1:B:299:ILE:HB	1:B:300:PRO:HD3	2.04	0.40
1:B:1050:TYR:HB3	1:C:1052:PHE:HE2	1.87	0.40
1:B:1095:LYS:HB3	1:B:1104:LYS:NZ	2.36	0.40
1:B:1487:ASN:HB3	2:B:1601:APR:H61	1.86	0.40
1:C:94:THR:HB	1:C:292:HIS:HB3	2.02	0.40
1:C:452:TRP:CZ3	1:C:472:ILE:HD12	2.56	0.40
1:C:837:PHE:HA	1:C:840:VAL:HG22	2.02	0.40
1:C:917:SER:HB3	1:C:920:LEU:HD12	2.03	0.40
1:C:929:ARG:CZ	1:C:930:MET:SD	3.10	0.40
1:C:1046:ALA:HB1	1:D:1052:PHE:CB	2.52	0.40
1:D:128:GLY:HA3	1:D:259:SER:OG	2.21	0.40
1:D:1487:ASN:HB3	2:D:1601:APR:H61	1.86	0.40
1:A:335:GLY:H	3:A:1602:AR6:PB	2.44	0.40
1:A:549:CYS:HB3	1:A:587:ARG:HG3	2.03	0.40
1:A:726:ASP:O	1:A:730:VAL:HG22	2.22	0.40
1:A:1374:VAL:HG22	1:A:1478:VAL:HG22	2.03	0.40
1:B:302:ARG:HA	1:B:305:LEU:HB3	2.03	0.40
1:B:335:GLY:H	3:B:1602:AR6:PB	2.44	0.40
1:B:452:TRP:CZ3	1:B:472:ILE:HD12	2.57	0.40
1:B:456:LEU:HA	1:B:459:ALA:HB3	2.03	0.40
1:B:756:VAL:O	1:B:759:CYS:N	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:929:ARG:CZ	1:B:930:MET:SD	3.10	0.40
1:B:1068:HIS:O	1:B:1072:GLU:HG3	2.22	0.40
1:B:1153:ASN:HB2	1:B:1154:LYS:HE3	2.03	0.40
1:C:151:SER:HB3	1:C:308:PHE:CD2	2.55	0.40
1:C:498:GLU:OE1	1:C:501:LYS:HG2	2.22	0.40
1:C:666:GLU:OE2	1:C:668:ASP:HB3	2.22	0.40
1:C:976:LEU:HB3	1:C:981:GLN:HB3	2.03	0.40
1:C:1378:LYS:HB2	1:C:1385:TRP:CE3	2.56	0.40
1:D:1257:VAL:HG13	1:D:1261:LYS:HG3	2.02	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	1313/1503 (87%)	1140 (87%)	160 (12%)	13 (1%)	13	49
1	B	1313/1503 (87%)	1140 (87%)	160 (12%)	13 (1%)	13	49
1	C	1313/1503 (87%)	1140 (87%)	160 (12%)	13 (1%)	13	49
1	D	1313/1503 (87%)	1140 (87%)	160 (12%)	13 (1%)	13	49
All	All	5252/6012 (87%)	4560 (87%)	640 (12%)	52 (1%)	16	49

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95	HIS
1	A	261	PRO
1	A	1294	GLU
1	A	1321	ALA
1	B	95	HIS
1	B	261	PRO

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Mol	Chain	Res	Type
1	B	1294	GLU
1	B	1321	ALA
1	C	95	HIS
1	C	261	PRO
1	C	1294	GLU
1	C	1321	ALA
1	D	95	HIS
1	D	261	PRO
1	D	1294	GLU
1	D	1321	ALA
1	A	233	GLU
1	A	576	LEU
1	B	233	GLU
1	B	576	LEU
1	C	233	GLU
1	C	576	LEU
1	D	233	GLU
1	D	576	LEU
1	A	299	ILE
1	A	575	PRO
1	B	299	ILE
1	B	575	PRO
1	C	299	ILE
1	C	575	PRO
1	D	299	ILE
1	D	575	PRO
1	A	201	THR
1	A	358	ARG
1	B	201	THR
1	B	358	ARG
1	C	201	THR
1	C	358	ARG
1	D	201	THR
1	D	358	ARG
1	A	237	ILE
1	A	1405	ILE
1	B	237	ILE
1	B	1405	ILE
1	C	237	ILE
1	C	1405	ILE
1	D	237	ILE
1	D	1405	ILE

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Mol	Chain	Res	Type
1	A	359	VAL
1	B	359	VAL
1	C	359	VAL
1	D	359	VAL

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	1116/1318 (85%)	1089 (98%)	27 (2%)	44	62
1	B	1116/1318 (85%)	1089 (98%)	27 (2%)	44	62
1	C	1116/1318 (85%)	1088 (98%)	28 (2%)	42	61
1	D	1116/1318 (85%)	1089 (98%)	27 (2%)	44	62
All	All	4464/5272 (85%)	4355 (98%)	109 (2%)	45	62

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	316	ARG
1	A	321	ILE
1	A	450	GLU
1	A	458	LEU
1	A	501	LYS
1	A	511	LYS
1	A	512	GLU
1	A	514	VAL
1	A	536	LEU
1	A	538	LYS
1	A	541	VAL
1	A	557	GLN
1	A	619	MET
1	A	622	ILE
1	A	727	MET
1	A	728	LYS
1	A	742	VAL

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Mol	Chain	Res	Type
1	A	812	LEU
1	A	844	MET
1	A	857	MET
1	A	1072	GLU
1	A	1125	GLU
1	A	1130	GLU
1	A	1154	LYS
1	A	1158	MET
1	A	1246	LEU
1	A	1379	LEU
1	B	316	ARG
1	B	321	ILE
1	B	450	GLU
1	B	458	LEU
1	B	501	LYS
1	B	511	LYS
1	B	512	GLU
1	B	514	VAL
1	B	536	LEU
1	B	538	LYS
1	B	541	VAL
1	B	557	GLN
1	B	619	MET
1	B	622	ILE
1	B	727	MET
1	B	728	LYS
1	B	742	VAL
1	B	812	LEU
1	B	844	MET
1	B	857	MET
1	B	1072	GLU
1	B	1125	GLU
1	B	1130	GLU
1	B	1154	LYS
1	B	1158	MET
1	B	1246	LEU
1	B	1379	LEU
1	C	316	ARG
1	C	321	ILE
1	C	450	GLU
1	C	458	LEU
1	C	501	LYS

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Mol	Chain	Res	Type
1	C	511	LYS
1	C	512	GLU
1	C	514	VAL
1	C	536	LEU
1	C	538	LYS
1	C	541	VAL
1	C	557	GLN
1	C	619	MET
1	C	622	ILE
1	C	727	MET
1	C	728	LYS
1	C	742	VAL
1	C	812	LEU
1	C	844	MET
1	C	857	MET
1	C	1072	GLU
1	C	1125	GLU
1	C	1130	GLU
1	C	1134	GLN
1	C	1154	LYS
1	C	1158	MET
1	C	1246	LEU
1	C	1379	LEU
1	D	316	ARG
1	D	321	ILE
1	D	450	GLU
1	D	458	LEU
1	D	501	LYS
1	D	511	LYS
1	D	512	GLU
1	D	514	VAL
1	D	536	LEU
1	D	538	LYS
1	D	541	VAL
1	D	557	GLN
1	D	619	MET
1	D	622	ILE
1	D	727	MET
1	D	728	LYS
1	D	742	VAL
1	D	812	LEU
1	D	844	MET

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Mol	Chain	Res	Type
1	D	857	MET
1	D	1072	GLU
1	D	1125	GLU
1	D	1130	GLU
1	D	1154	LYS
1	D	1158	MET
1	D	1246	LEU
1	D	1379	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	HIS
1	A	118	HIS
1	A	217	GLN
1	A	248	HIS
1	A	255	HIS
1	A	346	ASN
1	A	449	HIS
1	A	454	HIS
1	A	525	ASN
1	A	537	GLN
1	A	1037	ASN
1	A	1054	GLN
1	A	1116	ASN
1	A	1131	ASN
1	A	1134	GLN
1	A	1135	ASN
1	A	1140	GLN
1	A	1302	ASN
1	A	1434	ASN
1	B	106	HIS
1	B	118	HIS
1	B	217	GLN
1	B	248	HIS
1	B	255	HIS
1	B	346	ASN
1	B	388	GLN
1	B	449	HIS
1	B	478	GLN
1	B	525	ASN
1	B	1037	ASN

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Mol	Chain	Res	Type
1	B	1049	ASN
1	B	1116	ASN
1	B	1131	ASN
1	B	1134	GLN
1	B	1135	ASN
1	B	1302	ASN
1	B	1434	ASN
1	C	106	HIS
1	C	118	HIS
1	C	217	GLN
1	C	248	HIS
1	C	255	HIS
1	C	342	ASN
1	C	346	ASN
1	C	449	HIS
1	C	454	HIS
1	C	455	GLN
1	C	478	GLN
1	C	525	ASN
1	C	1037	ASN
1	C	1049	ASN
1	C	1054	GLN
1	C	1116	ASN
1	C	1131	ASN
1	C	1302	ASN
1	C	1434	ASN
1	D	106	HIS
1	D	118	HIS
1	D	217	GLN
1	D	248	HIS
1	D	255	HIS
1	D	346	ASN
1	D	388	GLN
1	D	449	HIS
1	D	454	HIS
1	D	478	GLN
1	D	525	ASN
1	D	802	ASN
1	D	1116	ASN
1	D	1131	ASN
1	D	1134	GLN
1	D	1135	ASN

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Mol	Chain	Res	Type
1	D	1302	ASN
1	D	1434	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	APR	D	1601	-	24,28,39	1.00	1 (4%)	30,43,60	0.97	2 (6%)
2	APR	C	1601	-	24,28,39	1.01	1 (4%)	30,43,60	0.98	2 (6%)
3	AR6	B	1602	-	35,38,39	0.67	0	43,58,60	0.78	2 (4%)
2	APR	A	1601	-	24,28,39	1.01	1 (4%)	30,43,60	0.98	2 (6%)
3	AR6	A	1602	-	35,38,39	0.66	0	43,58,60	0.78	2 (4%)
3	AR6	D	1602	-	35,38,39	0.66	0	43,58,60	0.78	2 (4%)
3	AR6	C	1602	-	35,38,39	0.67	0	43,58,60	0.78	1 (2%)
2	APR	B	1601	-	24,28,39	1.01	1 (4%)	30,43,60	0.97	2 (6%)

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
3	AR6	B	1602	-	1/1/9/10	5/18/50/54	0/4/4/4
2	APR	C	1601	-	-	3/12/28/54	0/3/3/4
2	APR	D	1601	-	-	3/12/28/54	0/3/3/4
2	APR	A	1601	-	-	3/12/28/54	0/3/3/4
3	AR6	A	1602	-	1/1/9/10	5/18/50/54	0/4/4/4
3	AR6	D	1602	-	1/1/9/10	5/18/50/54	0/4/4/4
3	AR6	C	1602	-	1/1/9/10	5/18/50/54	0/4/4/4
2	APR	B	1601	-	-	3/12/28/54	0/3/3/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1601	APR	PB-O1B	3.34	1.60	1.50
2	B	1601	APR	PB-O1B	3.32	1.60	1.50
2	A	1601	APR	PB-O1B	3.32	1.60	1.50
2	D	1601	APR	PB-O1B	3.32	1.60	1.50

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1601	APR	O5D-PB-O2B	2.78	118.22	107.80
2	D	1601	APR	O5D-PB-O2B	2.77	118.19	107.80
2	B	1601	APR	O5D-PB-O2B	2.77	118.18	107.80
2	A	1601	APR	O5D-PB-O2B	2.76	118.17	107.80
3	D	1602	AR6	C5-C6-N6	2.32	123.85	120.31
3	C	1602	AR6	C5-C6-N6	2.32	123.84	120.31
3	B	1602	AR6	C5-C6-N6	2.29	123.79	120.31
3	A	1602	AR6	C5-C6-N6	2.28	123.78	120.31
2	C	1601	APR	C5-C6-N6	2.27	123.76	120.31
2	A	1601	APR	C5-C6-N6	2.26	123.75	120.31
2	D	1601	APR	C5-C6-N6	2.25	123.74	120.31
2	B	1601	APR	C5-C6-N6	2.24	123.72	120.31
3	A	1602	AR6	O4D-C1D-C2D	-2.02	101.88	104.67
3	D	1602	AR6	O4D-C1D-C2D	-2.02	101.88	104.67
3	B	1602	AR6	O4D-C1D-C2D	-2.01	101.89	104.67

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1602	AR6	C1'
3	B	1602	AR6	C1'
3	C	1602	AR6	C1'
3	D	1602	AR6	C1'

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1602	AR6	C5'-O5'-PA-O3A
3	A	1602	AR6	C3'-C4'-C5'-O5'
3	A	1602	AR6	O4'-C4'-C5'-O5'
3	B	1602	AR6	C5'-O5'-PA-O3A
3	B	1602	AR6	C3'-C4'-C5'-O5'
3	B	1602	AR6	O4'-C4'-C5'-O5'
3	C	1602	AR6	C5'-O5'-PA-O3A
3	C	1602	AR6	C3'-C4'-C5'-O5'
3	C	1602	AR6	O4'-C4'-C5'-O5'
3	D	1602	AR6	C5'-O5'-PA-O3A
3	D	1602	AR6	C3'-C4'-C5'-O5'
3	D	1602	AR6	O4'-C4'-C5'-O5'
3	A	1602	AR6	C4'-C5'-O5'-PA
3	B	1602	AR6	C4'-C5'-O5'-PA
3	C	1602	AR6	C4'-C5'-O5'-PA
3	D	1602	AR6	C4'-C5'-O5'-PA
2	A	1601	APR	C4'-C5'-O5'-PA
2	B	1601	APR	C4'-C5'-O5'-PA
2	C	1601	APR	C4'-C5'-O5'-PA
2	D	1601	APR	C4'-C5'-O5'-PA
3	A	1602	AR6	C5'-O5'-PA-O2A
3	B	1602	AR6	C5'-O5'-PA-O2A
3	C	1602	AR6	C5'-O5'-PA-O2A
3	D	1602	AR6	C5'-O5'-PA-O2A
2	A	1601	APR	C3'-C4'-C5'-O5'
2	B	1601	APR	C3'-C4'-C5'-O5'
2	C	1601	APR	C3'-C4'-C5'-O5'
2	D	1601	APR	C3'-C4'-C5'-O5'
2	A	1601	APR	O4'-C4'-C5'-O5'
2	B	1601	APR	O4'-C4'-C5'-O5'
2	C	1601	APR	O4'-C4'-C5'-O5'
2	D	1601	APR	O4'-C4'-C5'-O5'

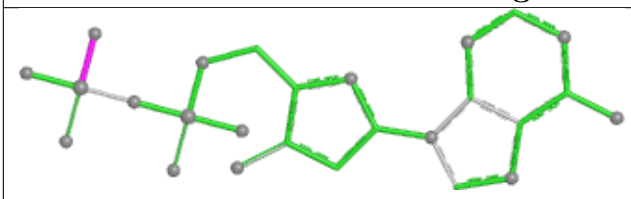
There are no ring outliers.

6 monomers are involved in 6 short contacts:

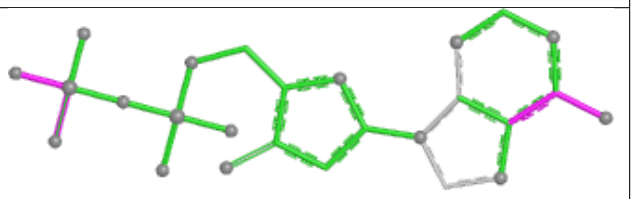
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1601	APR	1	0
2	C	1601	APR	1	0
3	B	1602	AR6	1	0
2	A	1601	APR	1	0
3	A	1602	AR6	1	0
2	B	1601	APR	1	0

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.

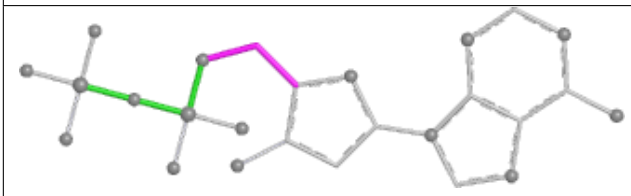
Ligand APR D 1601



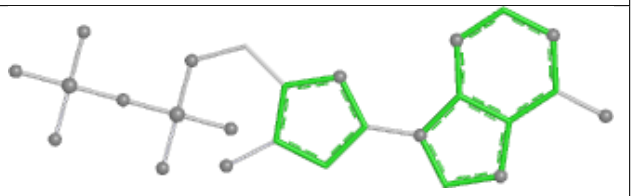
Bond lengths



Bond angles

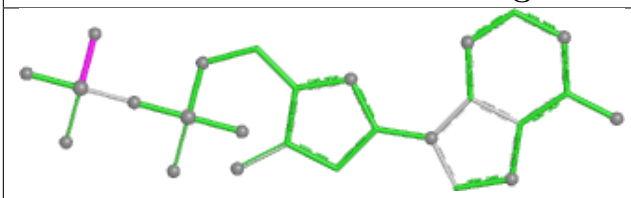


Torsions

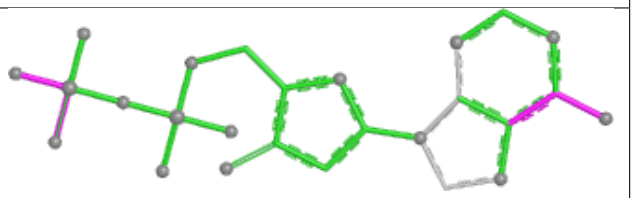


Rings

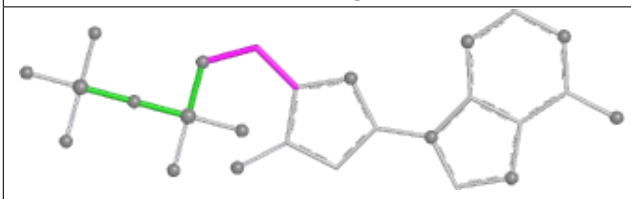
Ligand APR C 1601



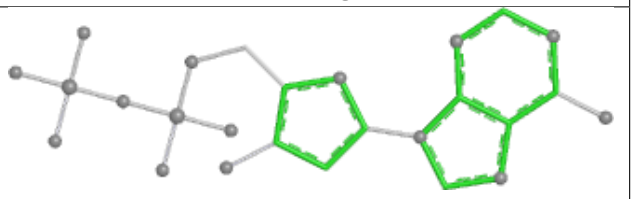
Bond lengths



Bond angles

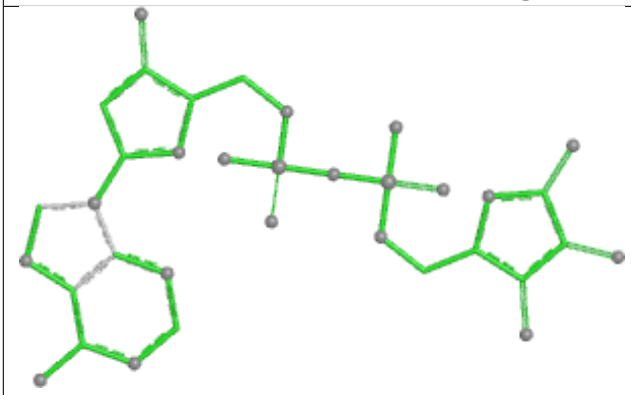


Torsions

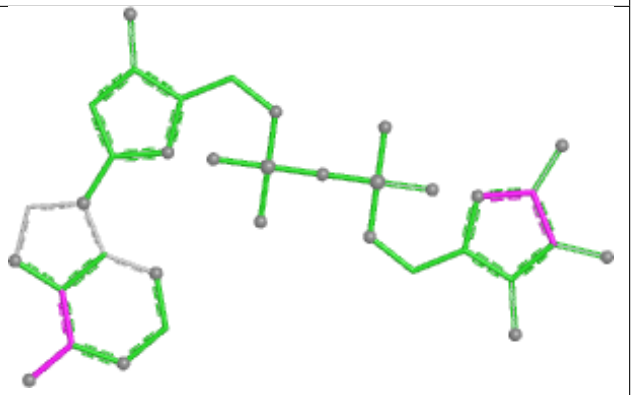


Rings

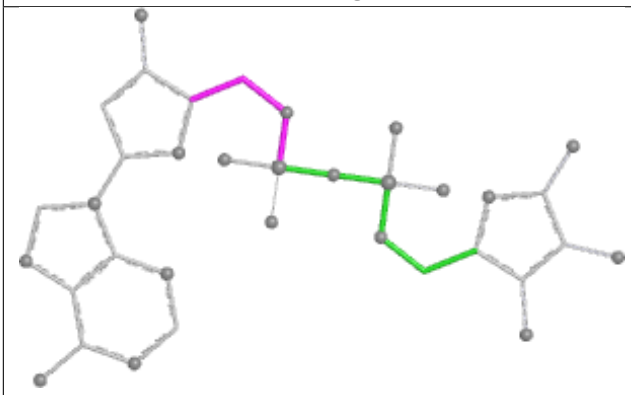
Ligand AR6 B 1602



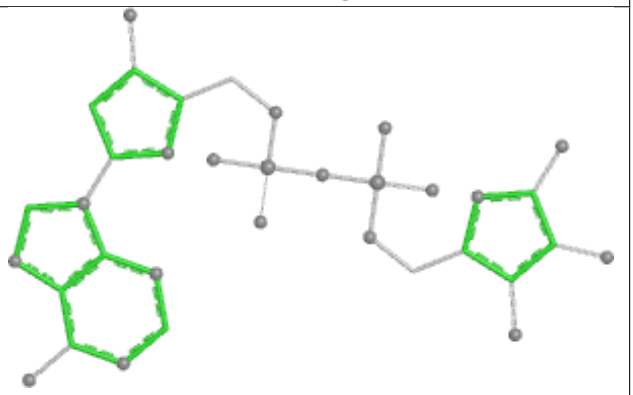
Bond lengths



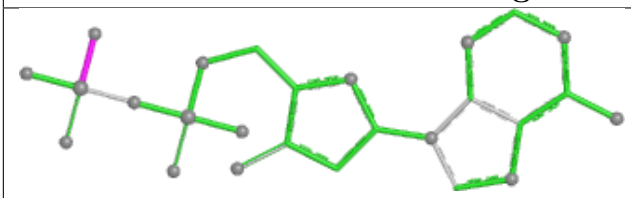
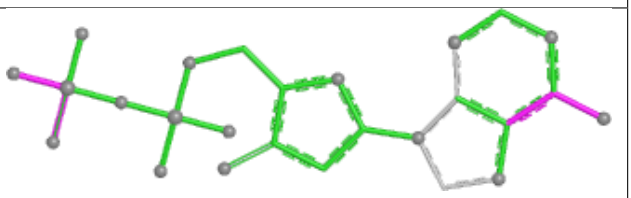
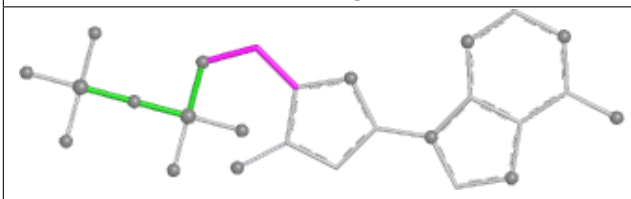
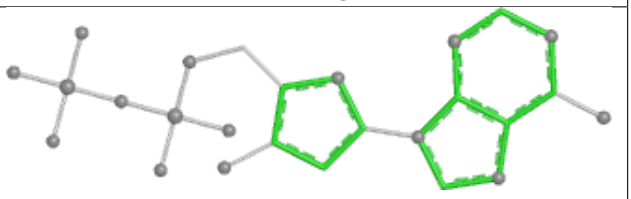
Bond angles

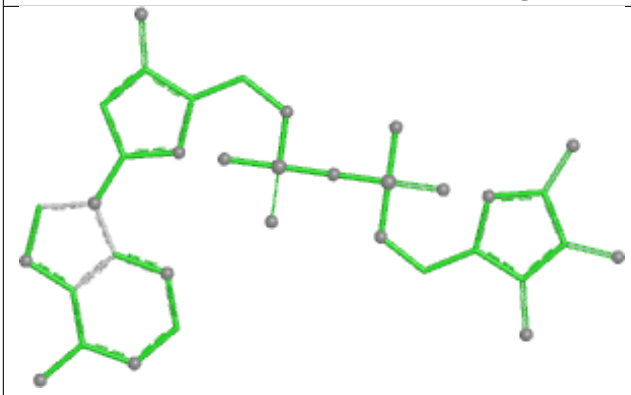
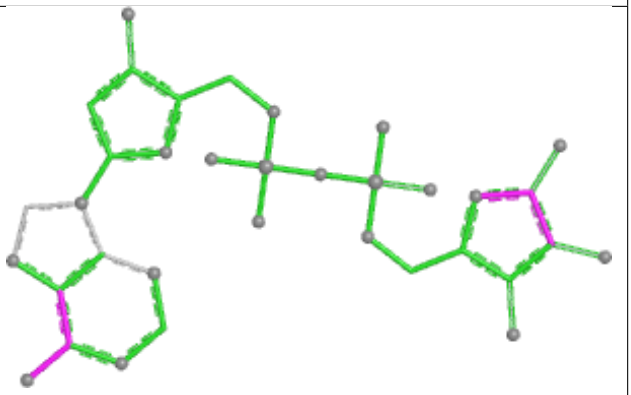
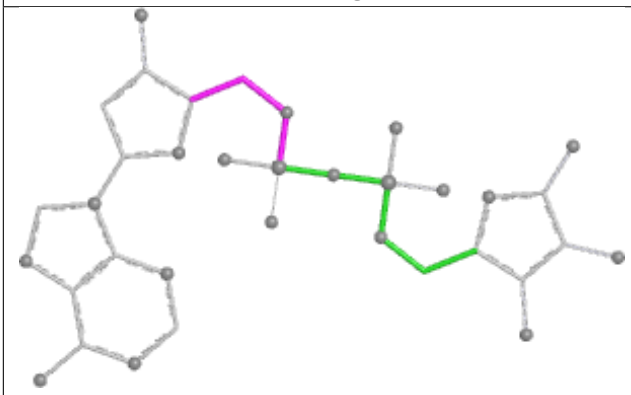
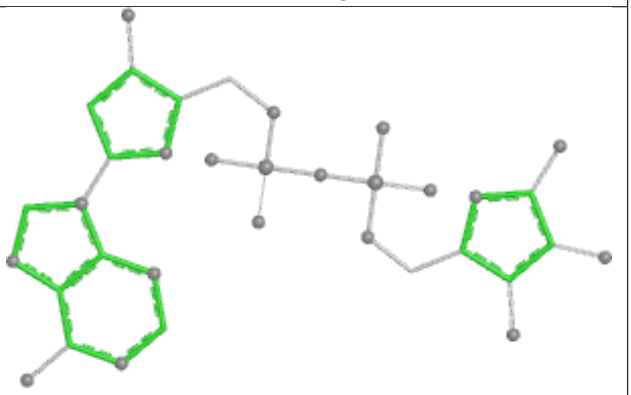


Torsions

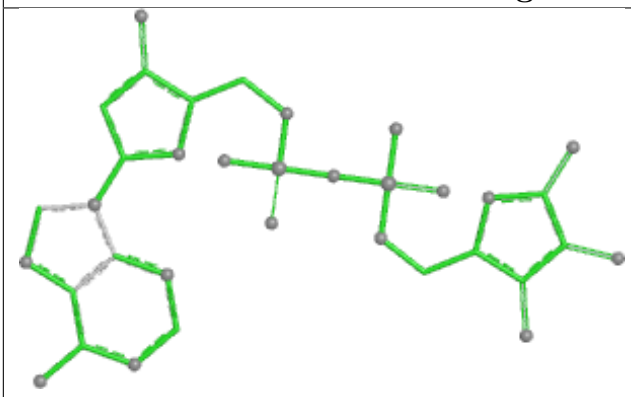


Rings

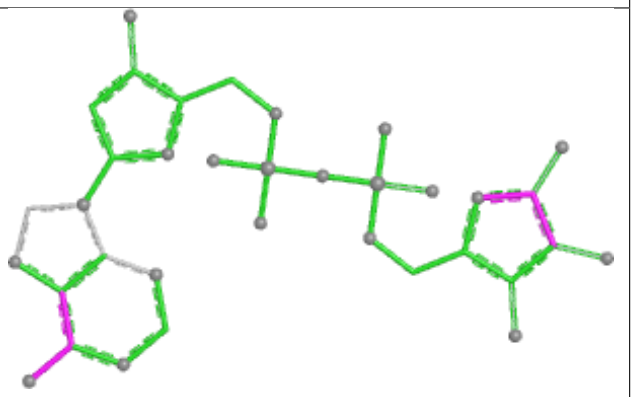
Ligand APR A 1601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand AR6 A 1602	
 Bond lengths	 Bond angles
 Torsions	 Rings

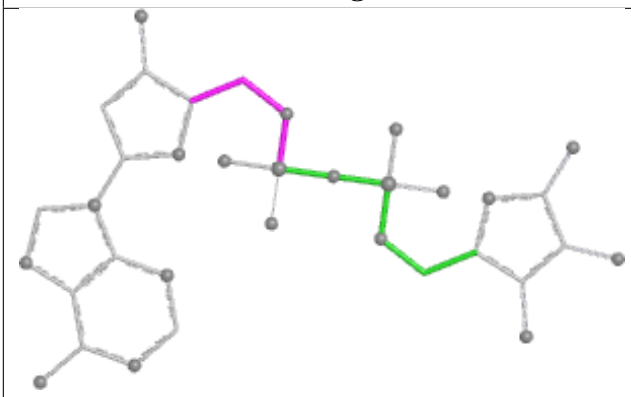
Ligand AR6 D 1602



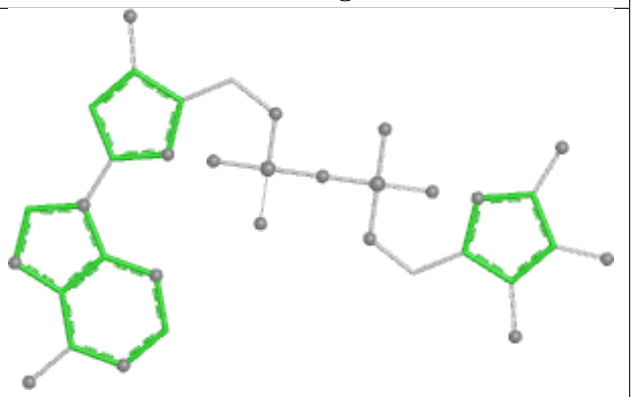
Bond lengths



Bond angles

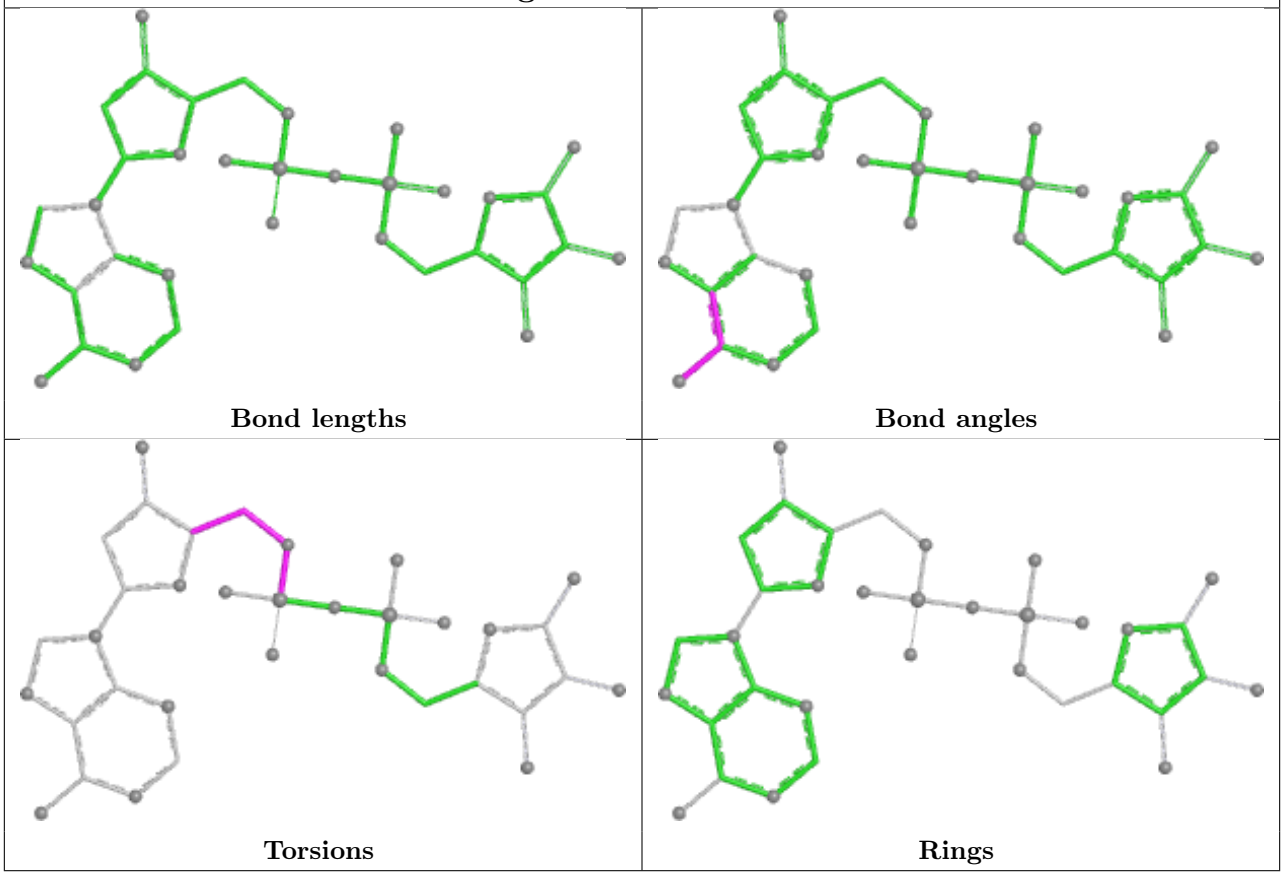


Torsions

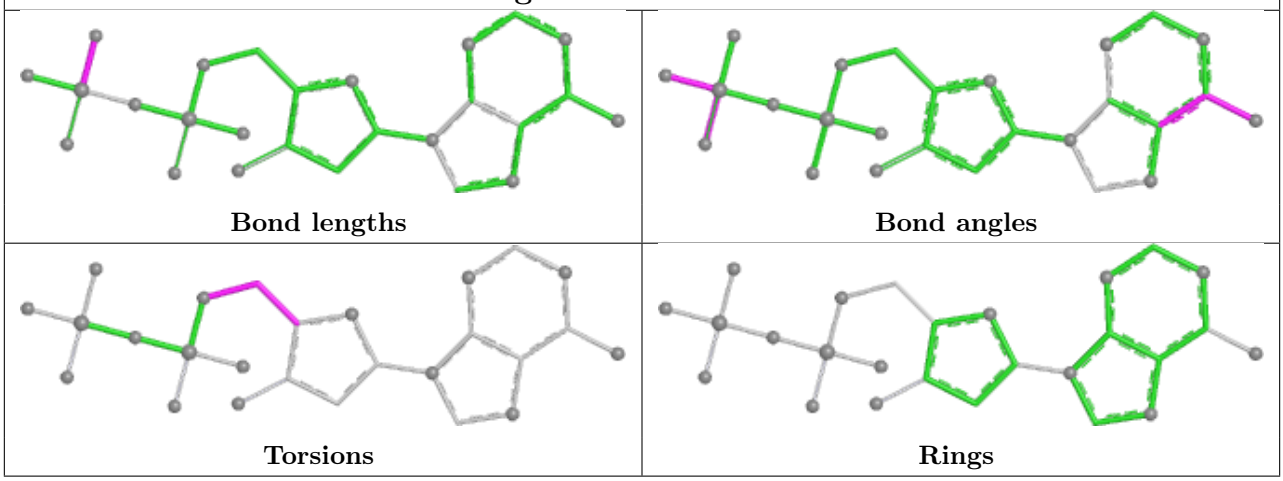


Rings

Ligand AR6 C 1602



Ligand APR B 1601



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	B	1
1	C	1
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	462:TRP	C	463:ASN	N	3.00
1	B	462:TRP	C	463:ASN	N	3.00
1	C	462:TRP	C	463:ASN	N	3.00
1	D	462:TRP	C	463:ASN	N	3.00

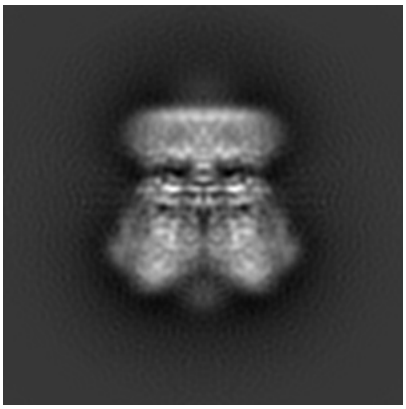
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-27923. These allow visual inspection of the internal detail of the map and identification of artifacts.

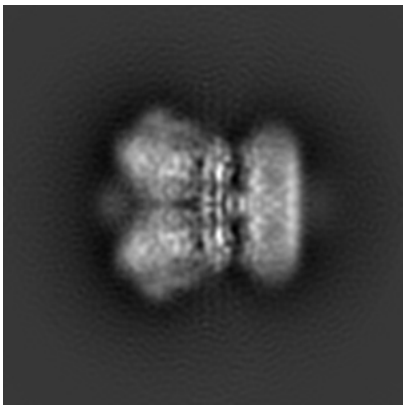
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

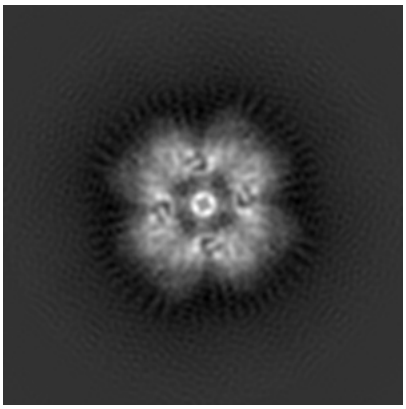
6.1.1 Primary map



X

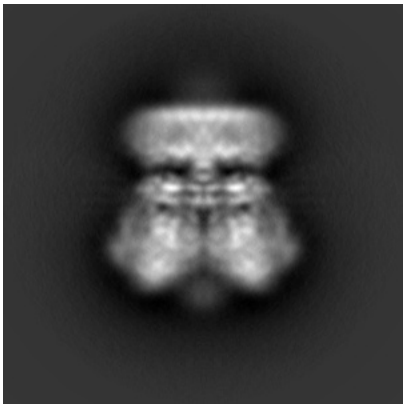


Y

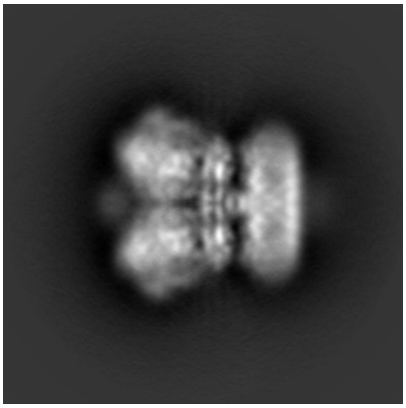


Z

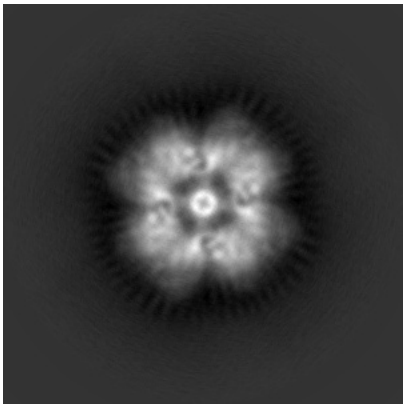
6.1.2 Raw map



X



Y



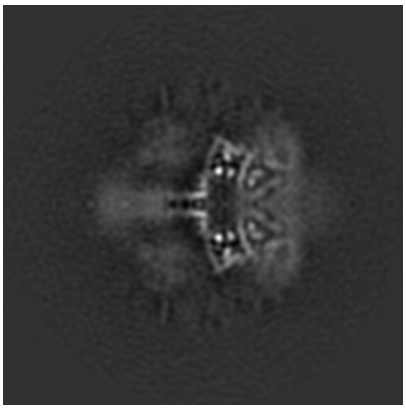
Z

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

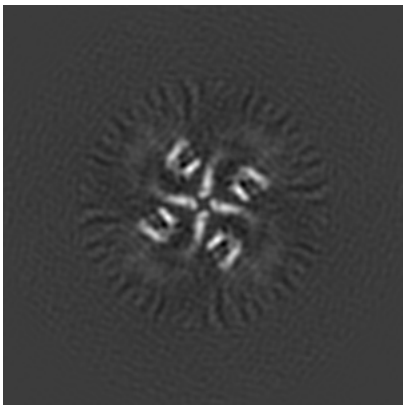
6.2 Central slices (i)

6.2.1 Primary map

X Index: 150

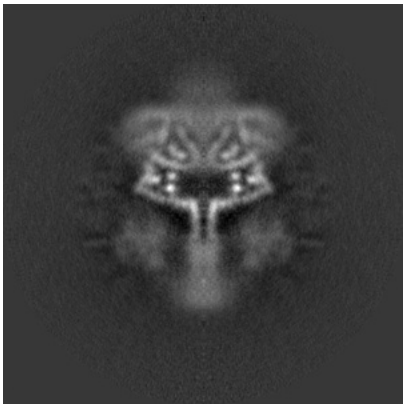


Y Index: 150

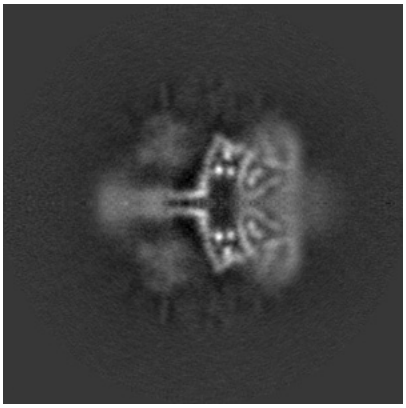


Z Index: 150

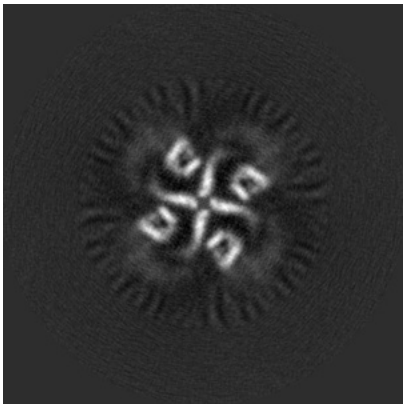
6.2.2 Raw map



X Index: 150



Y Index: 150



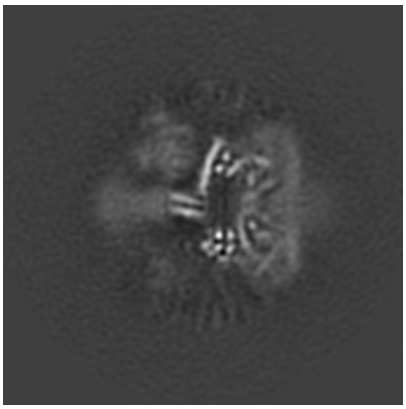
Z Index: 150

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

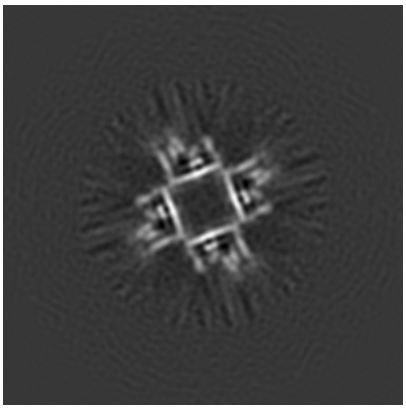
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 154

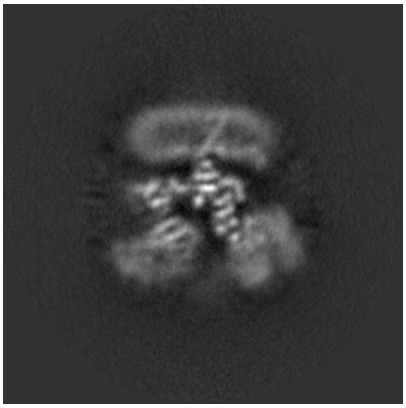


Y Index: 146

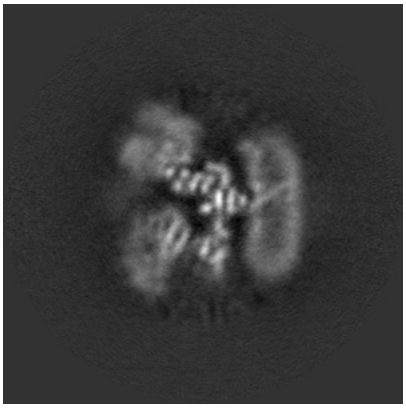


Z Index: 161

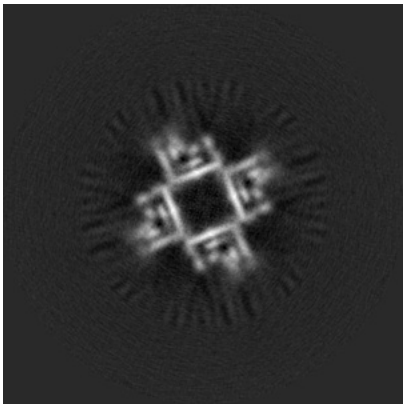
6.3.2 Raw map



X Index: 174



Y Index: 126

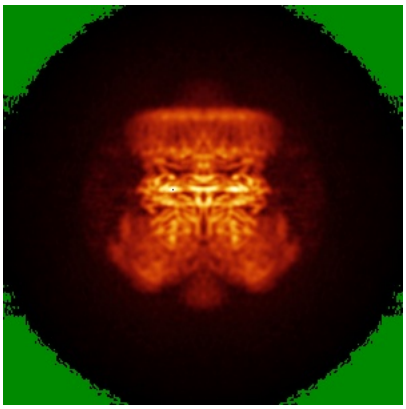


Z Index: 162

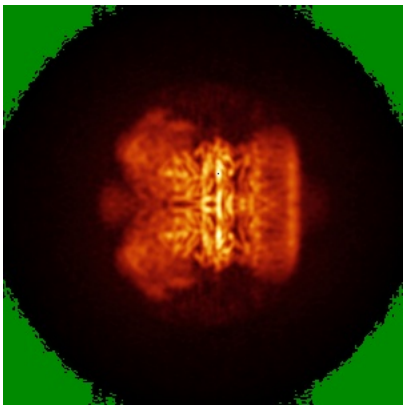
The images above show the largest variance slices of the map in three orthogonal directions.

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

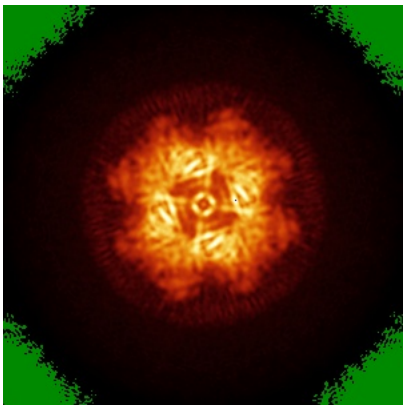
6.4.1 Primary map



X

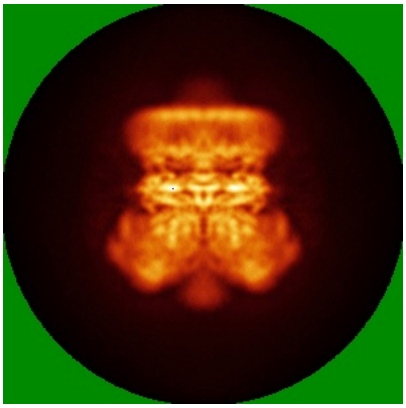


Y

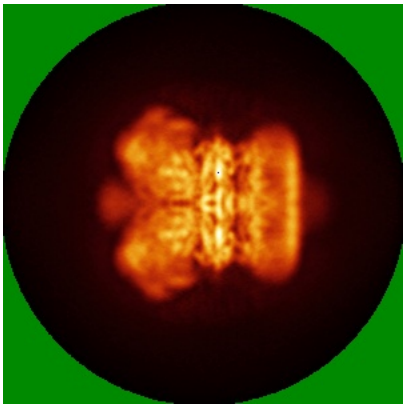


Z

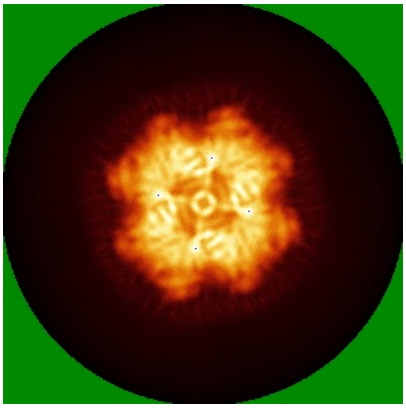
6.4.2 Raw map



X



Y

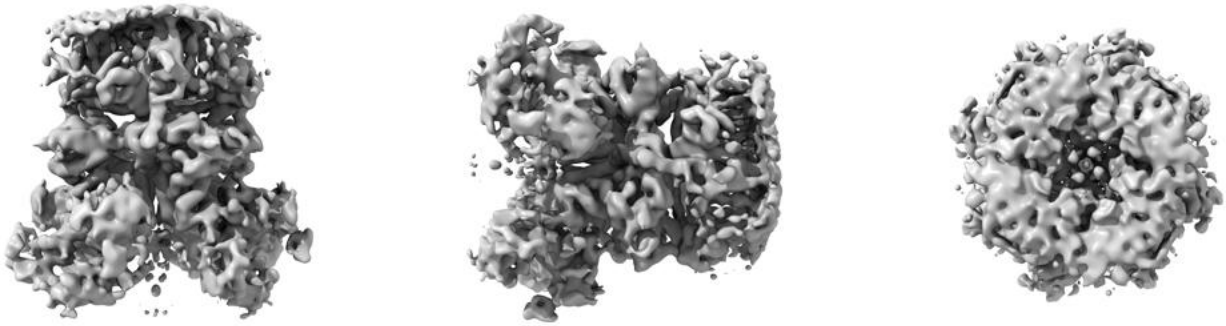


Z

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 0.0118. 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.

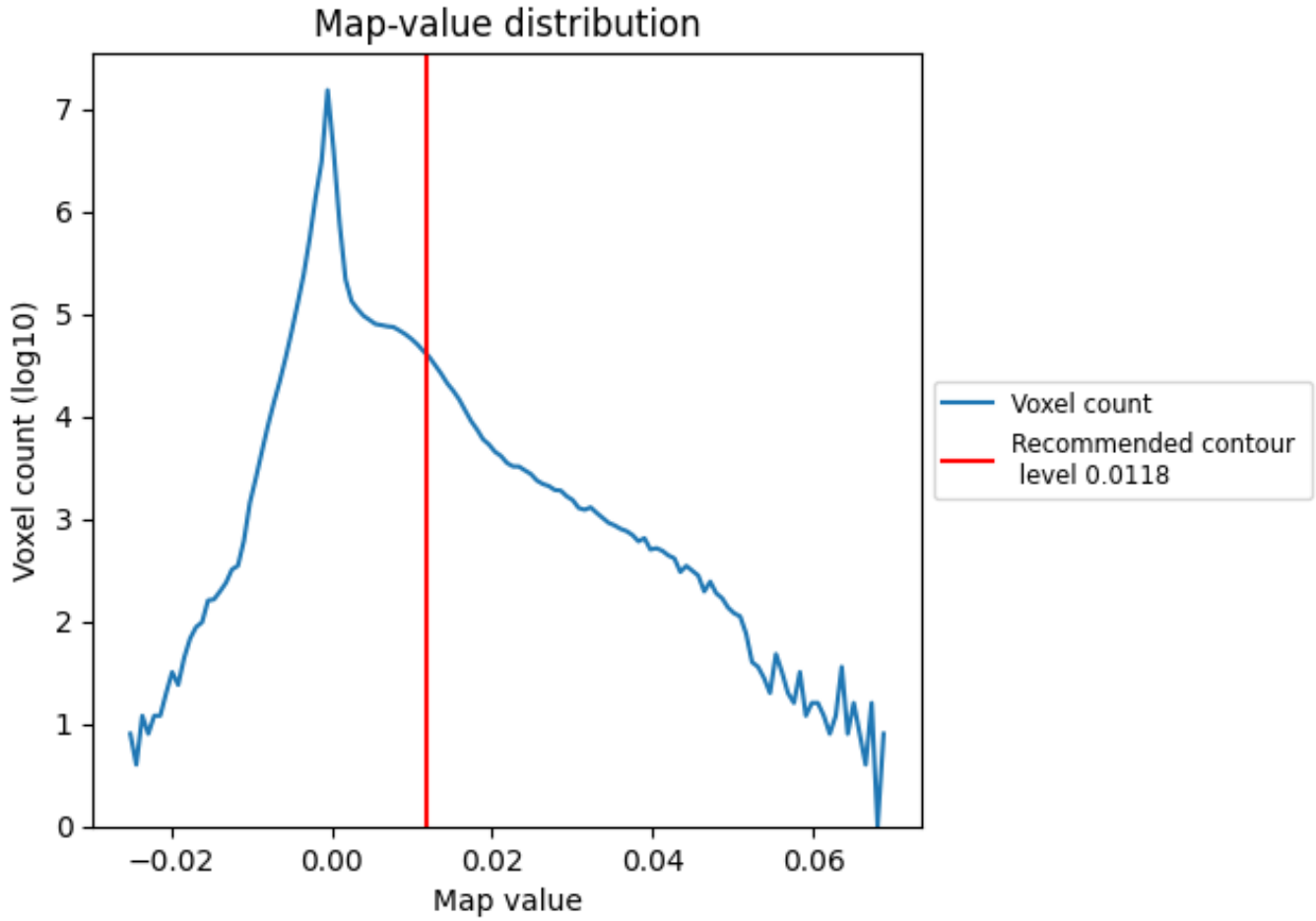
6.6 Mask visualisation (i)

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

7 Map analysis

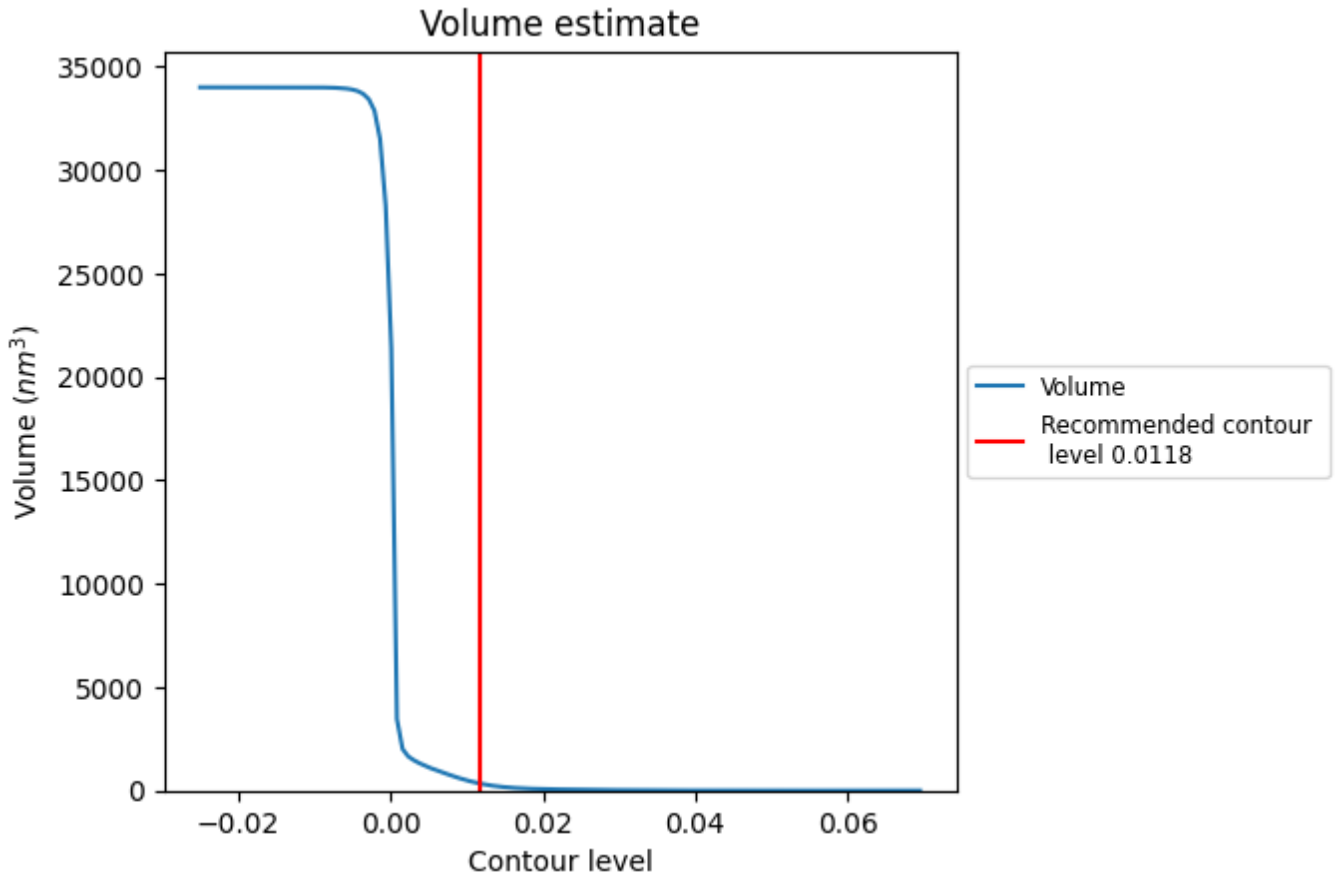
This section contains the results of statistical analysis of the map.

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.

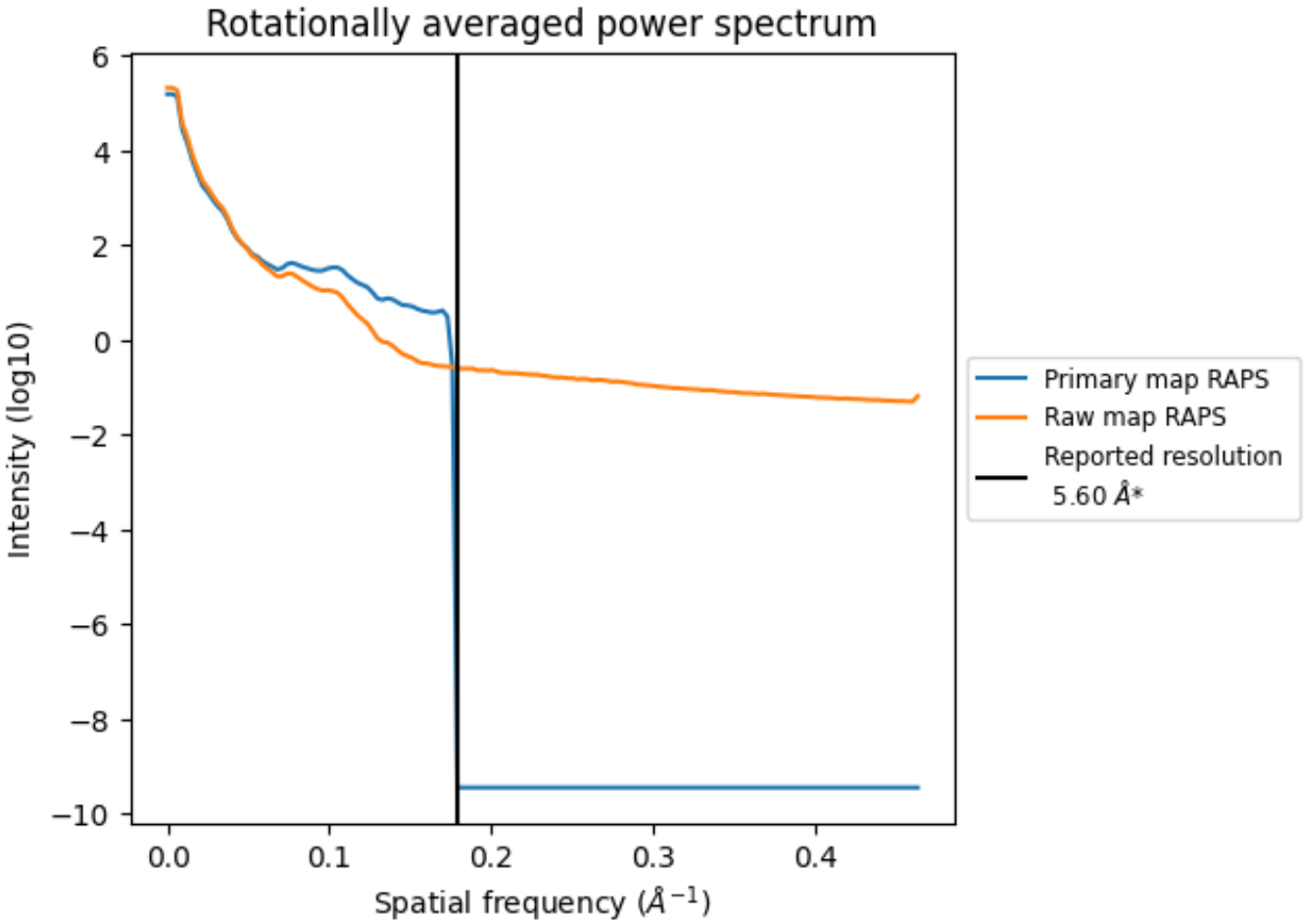
7.2 Volume estimate



The volume at the recommended contour level is 334 nm^3; this corresponds to an approximate mass of 302 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)

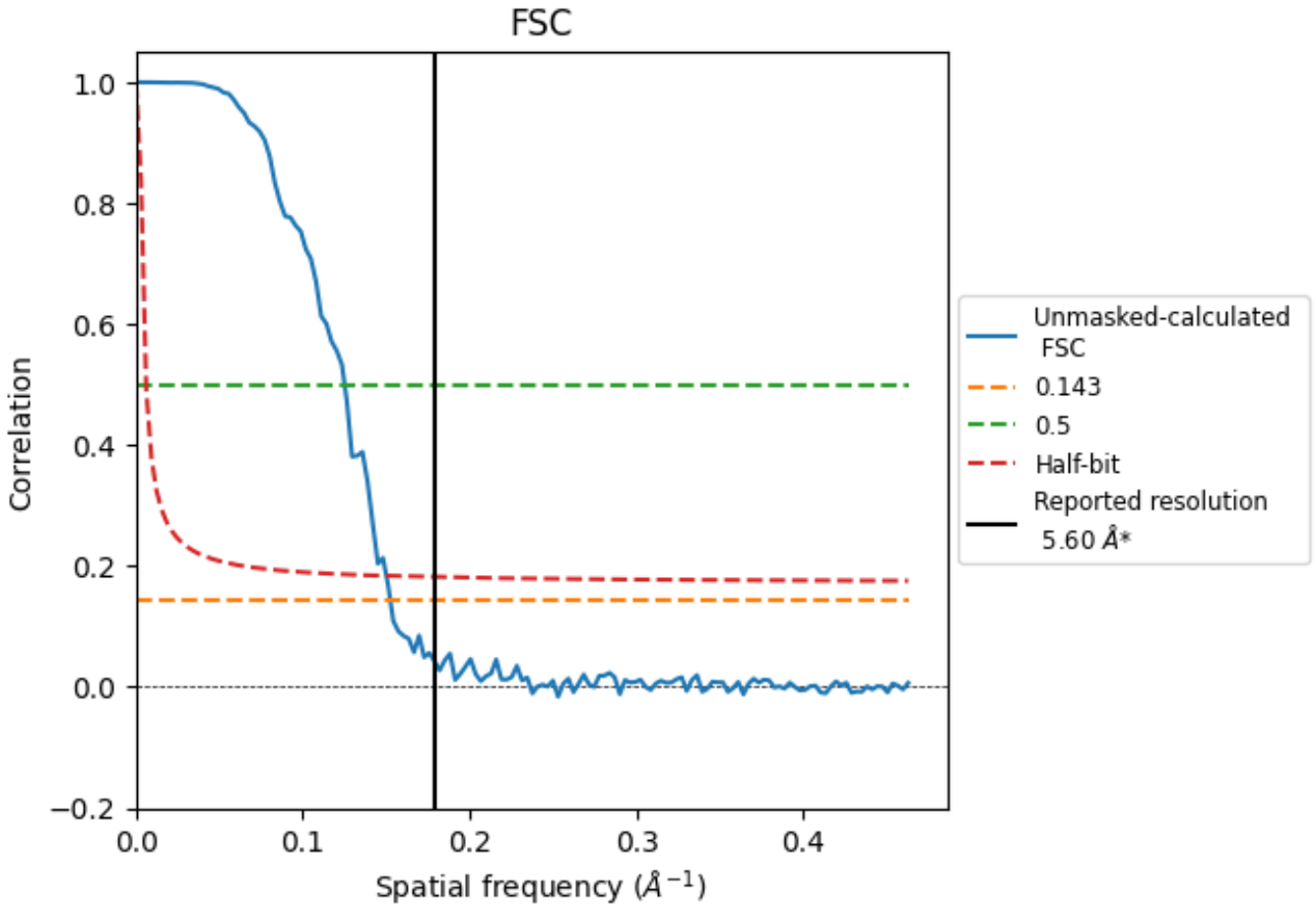


*Reported resolution corresponds to spatial frequency of 0.179 Å^{-1}

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 0.179 Å^{-1}

8.2 Resolution estimates (i)

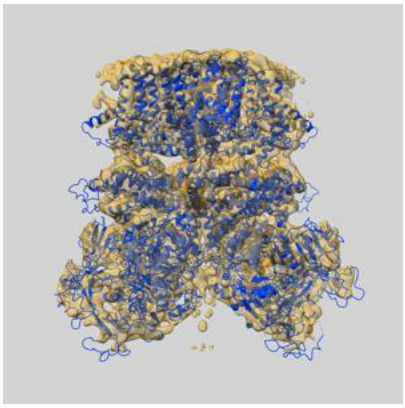
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.55	7.99	6.66

*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 6.55 differs from the reported value 5.6 by more than 10 %

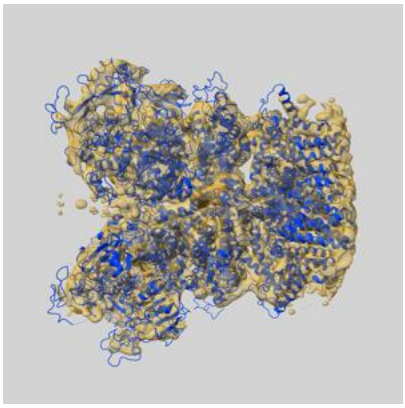
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-27923 and PDB model 8E6R. Per-residue inclusion information can be found in section 3 on page 6.

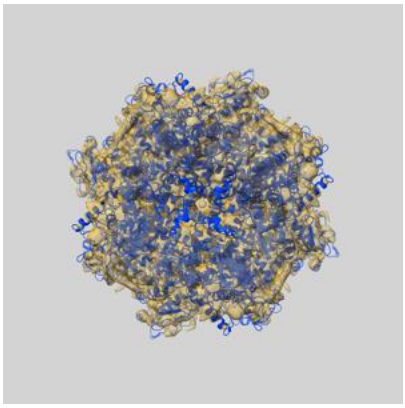
9.1 Map-model overlay



X



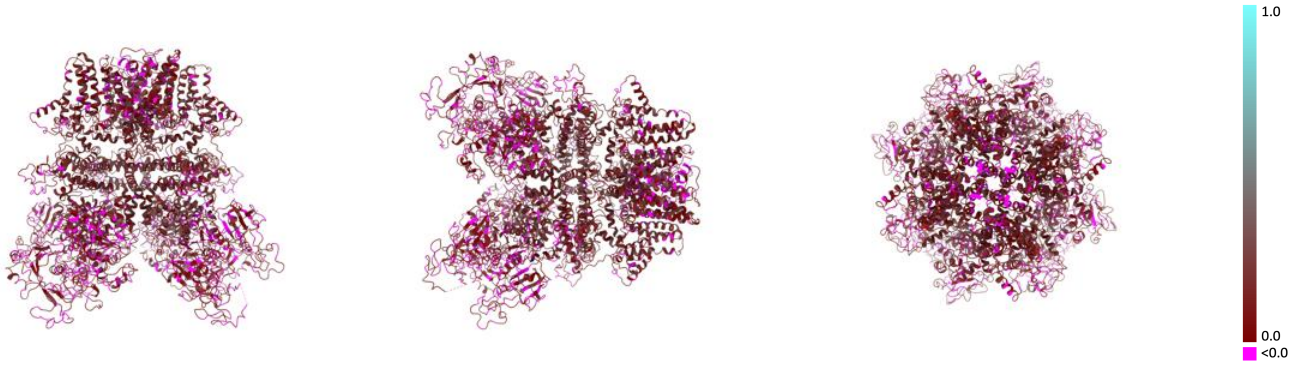
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0118 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.

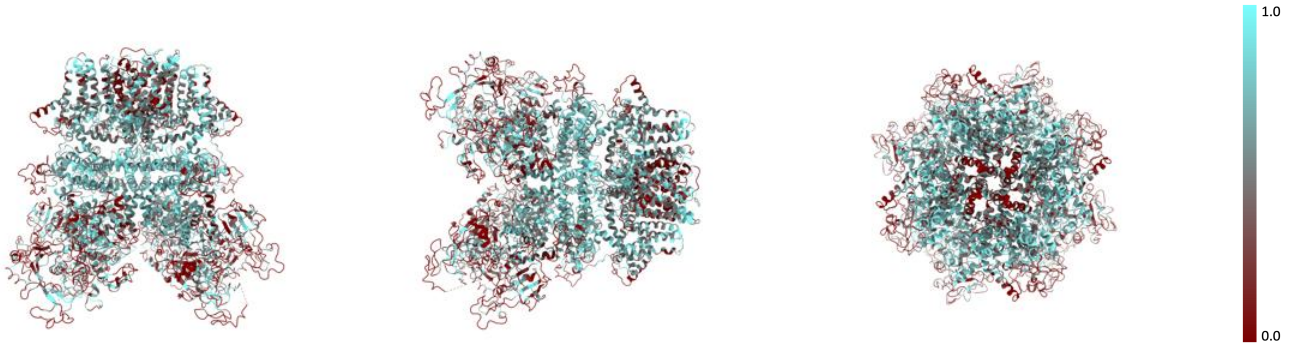
9.2 Q-score mapped to coordinate model (i)



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.

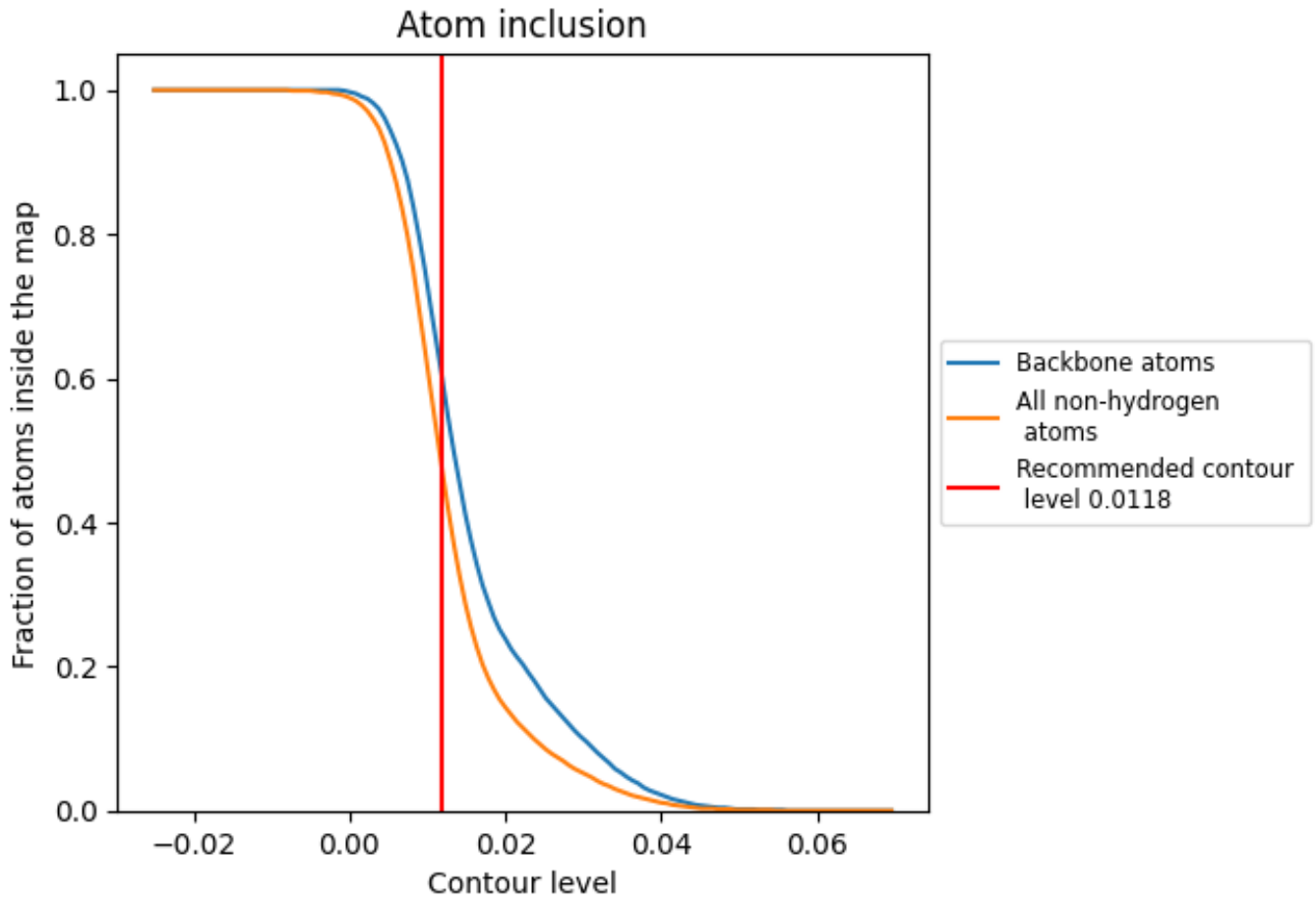
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0118).

9.4 Atom inclusion (i)



At the recommended contour level, 61% of all backbone atoms, 48% 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 (0.0118) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4790	0.1230
A	0.4810	0.1250
B	0.4770	0.1220
C	0.4820	0.1240
D	0.4770	0.1210