Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 07:50 PM EST

PDB ID	:	3IZ3
EMDB ID	:	EMD-5233
Title	:	CryoEM structure of cytoplasmic polyhedrosis virus
Authors	:	Cheng, L.; Sun, J.; Zhang, K.; Mou, Z.; Huang, X.; Ji, G.; Sun, F.; Zhang, J.; Zhu, P.
Deposited on	:	2010-09-14
Resolution	:	3.90 Å(reported)

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

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

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

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

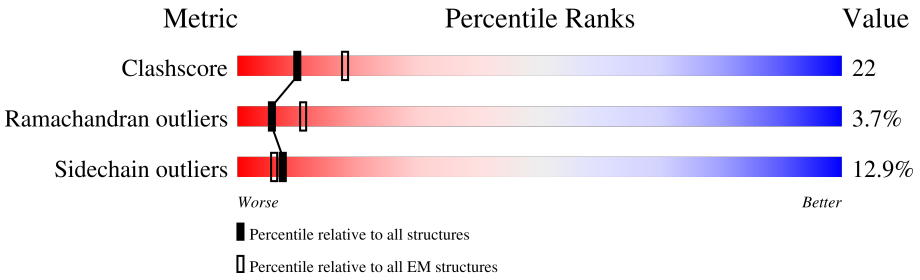
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.90 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	1058	93% 57% 34% 8%
2	B	1333	79% 59% 25% 11%
2	C	1333	80% 61% 27% 5% 7%
3	D	291	87% 48% 42% 9%
3	E	291	82% 46% 42% 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 32024 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 Structural protein VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1047	Total	C	N	O	S	0	0
			8349	5294	1439	1572	44		

- Molecule 2 is a protein called Structural protein VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1180	Total	C	N	O	S	0	0
			9317	5889	1621	1771	36		
2	C	1244	Total	C	N	O	S	0	0
			9806	6191	1704	1873	38		

- Molecule 3 is a protein called Viral structural protein 5.

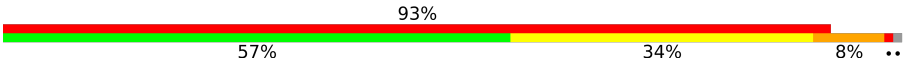
Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	291	Total	C	N	O	S	0	0
			2276	1446	398	424	8		
3	E	291	Total	C	N	O	S	0	0
			2276	1446	398	424	8		

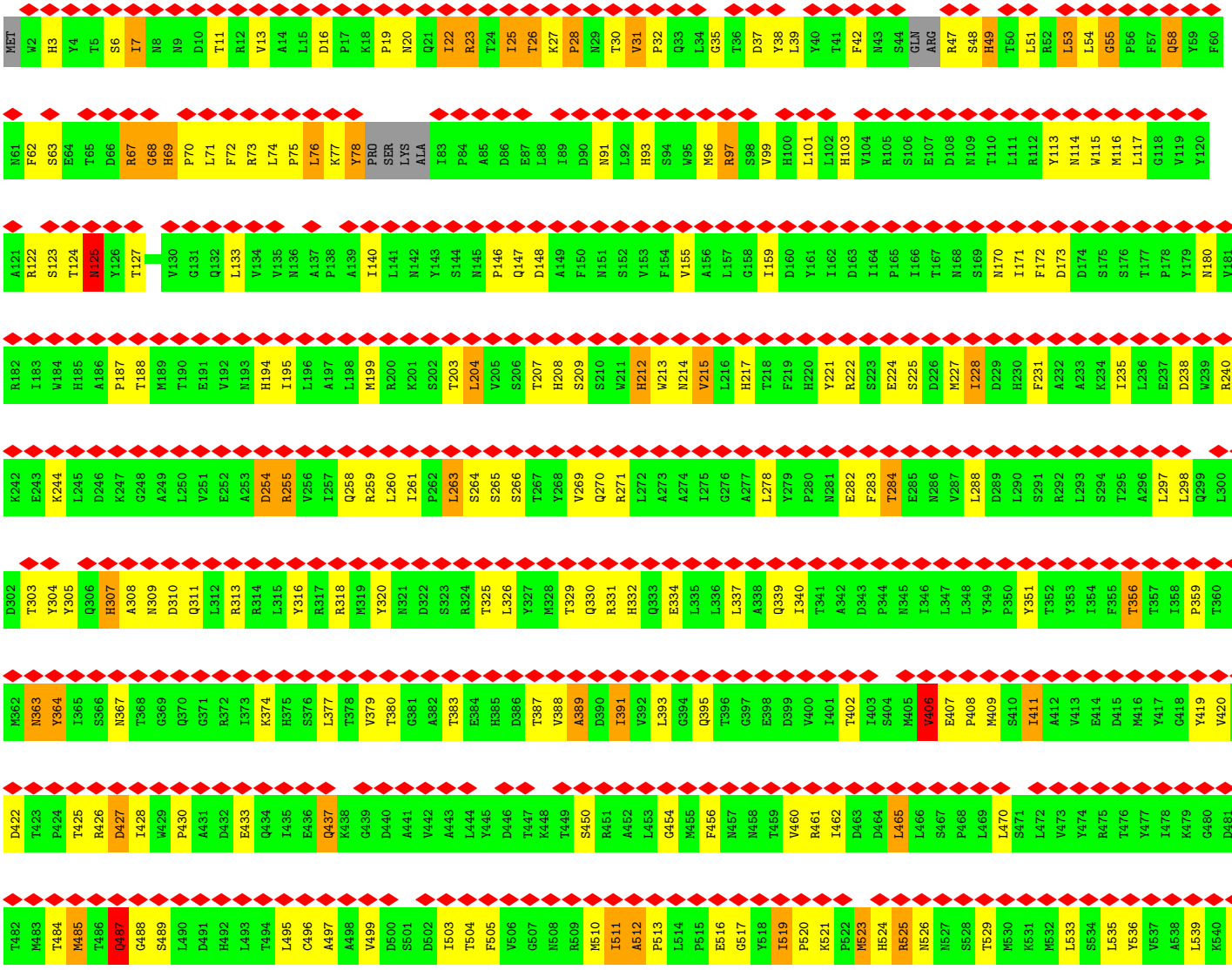
3 Residue-property plots (i)

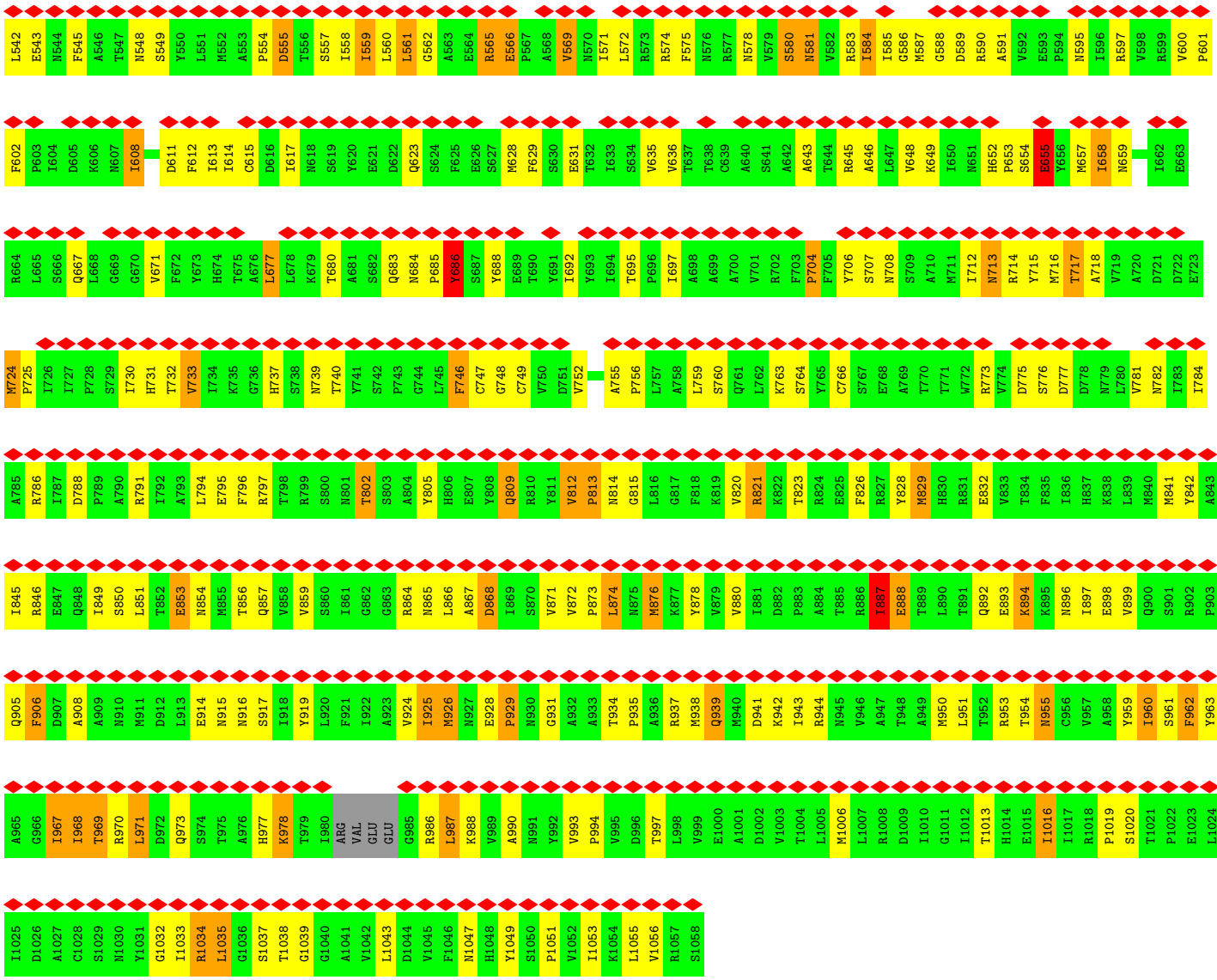
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Structural protein VP3

Chain A:

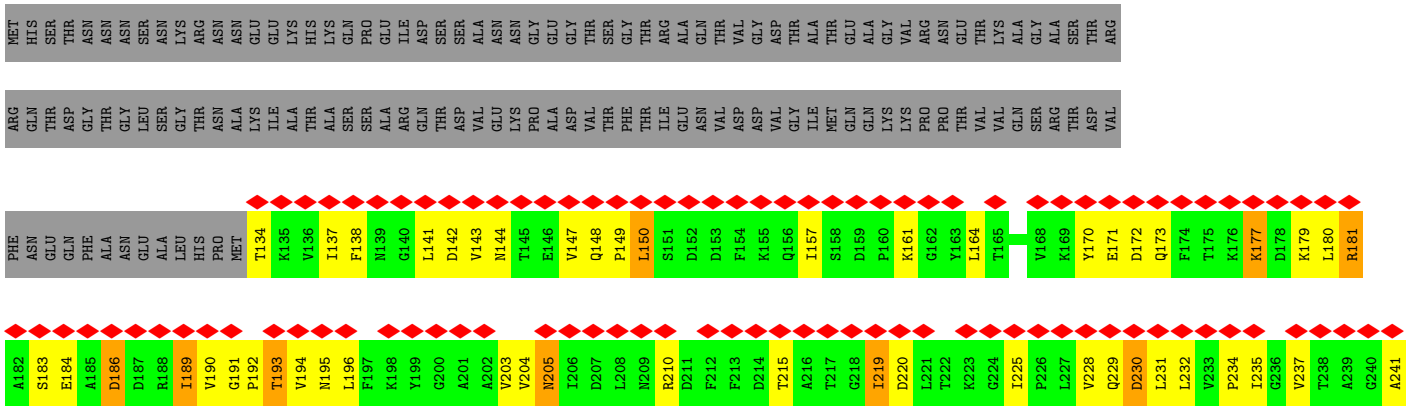


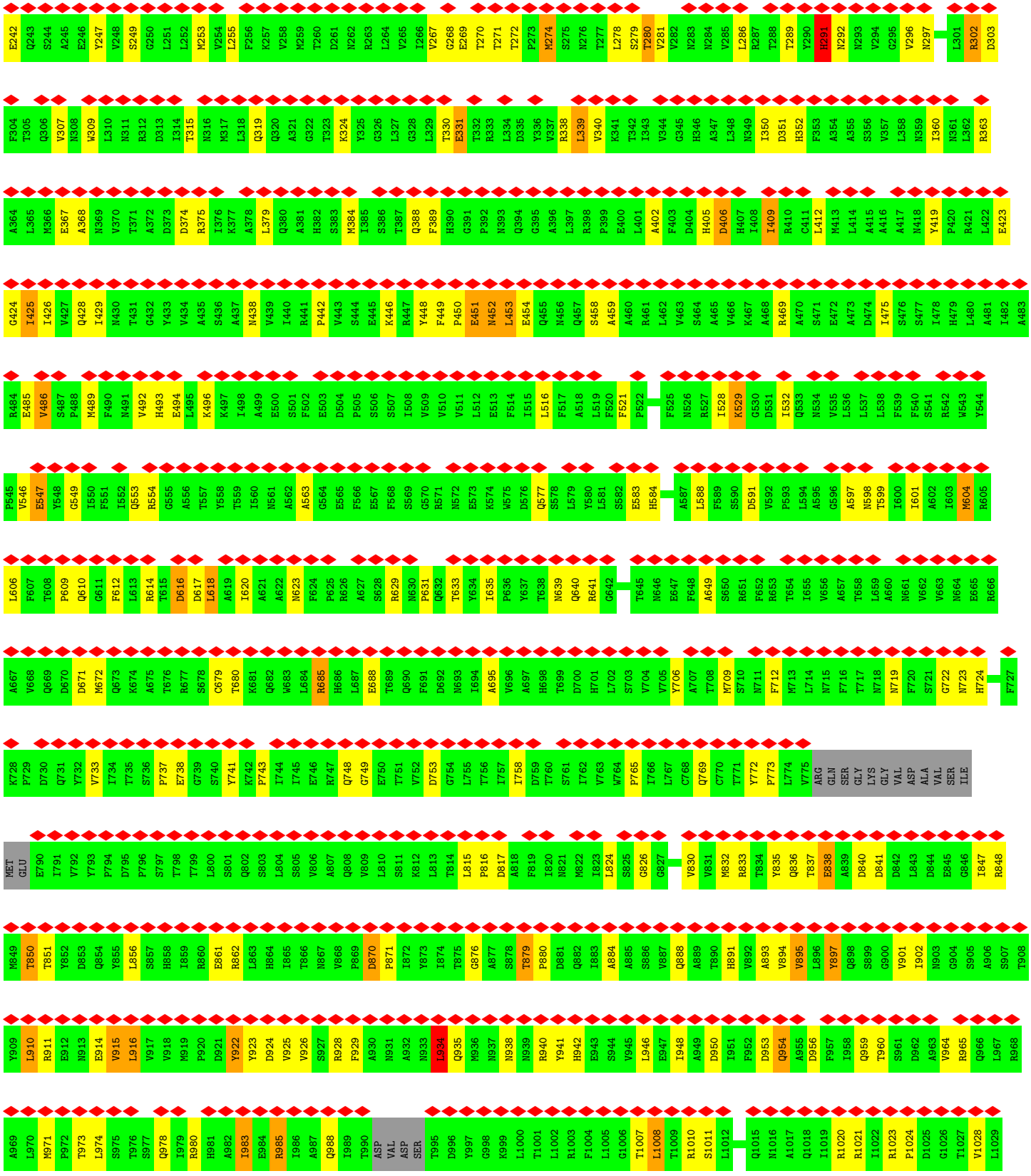


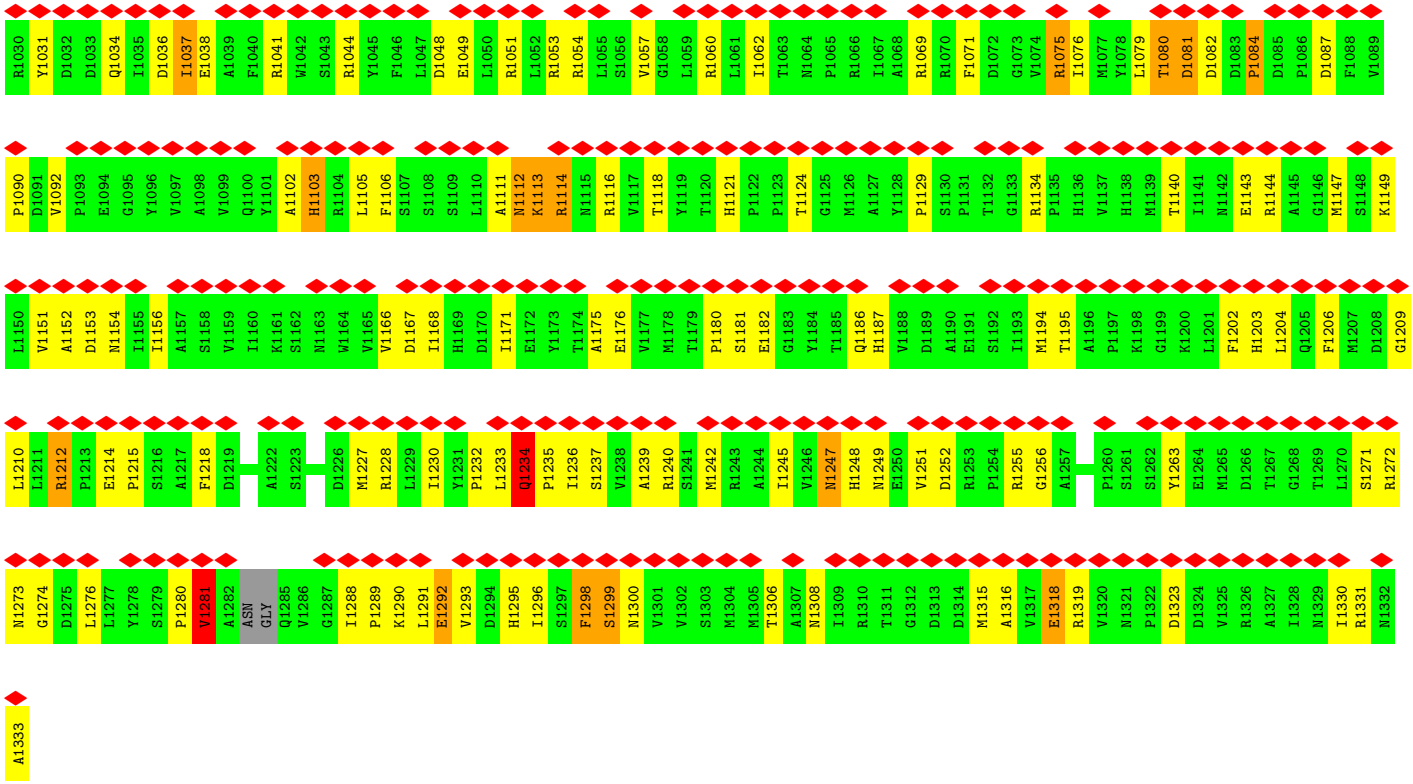


• Molecule 2: Structural protein VP1

Chain B:

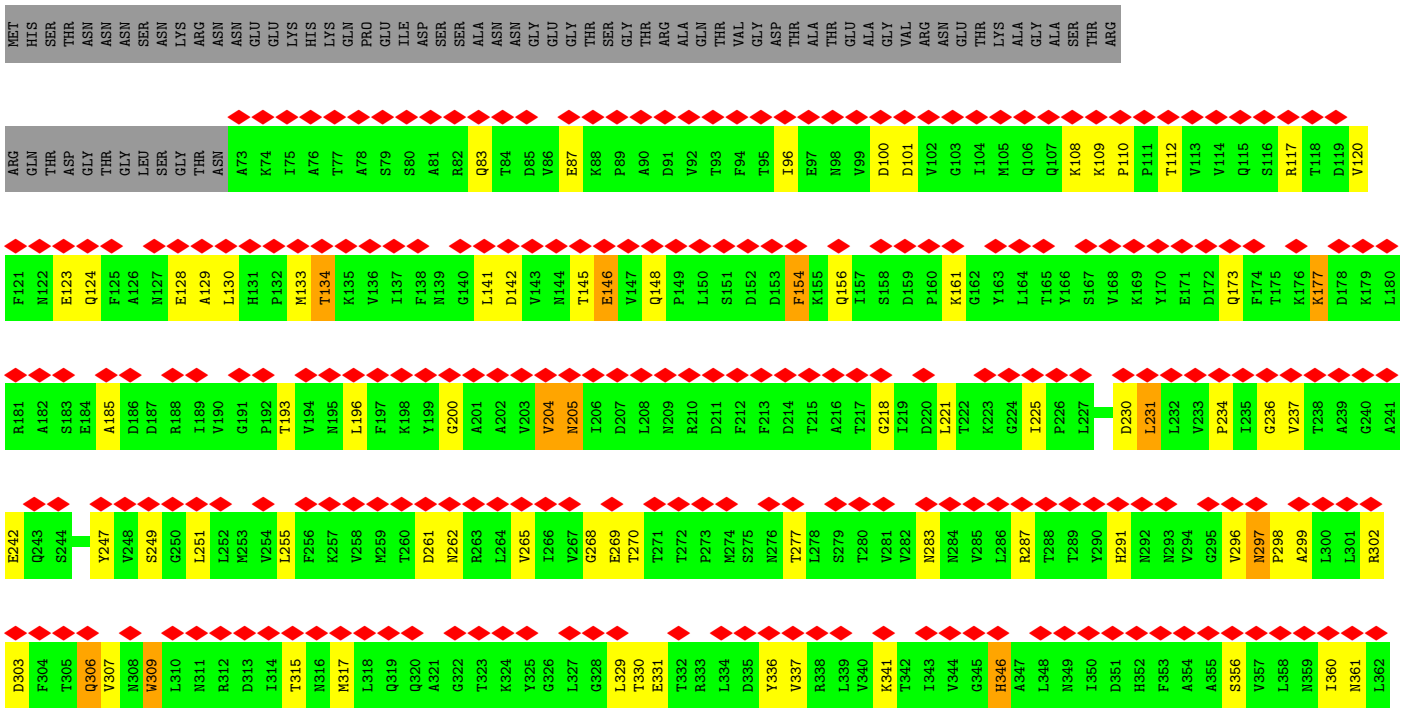


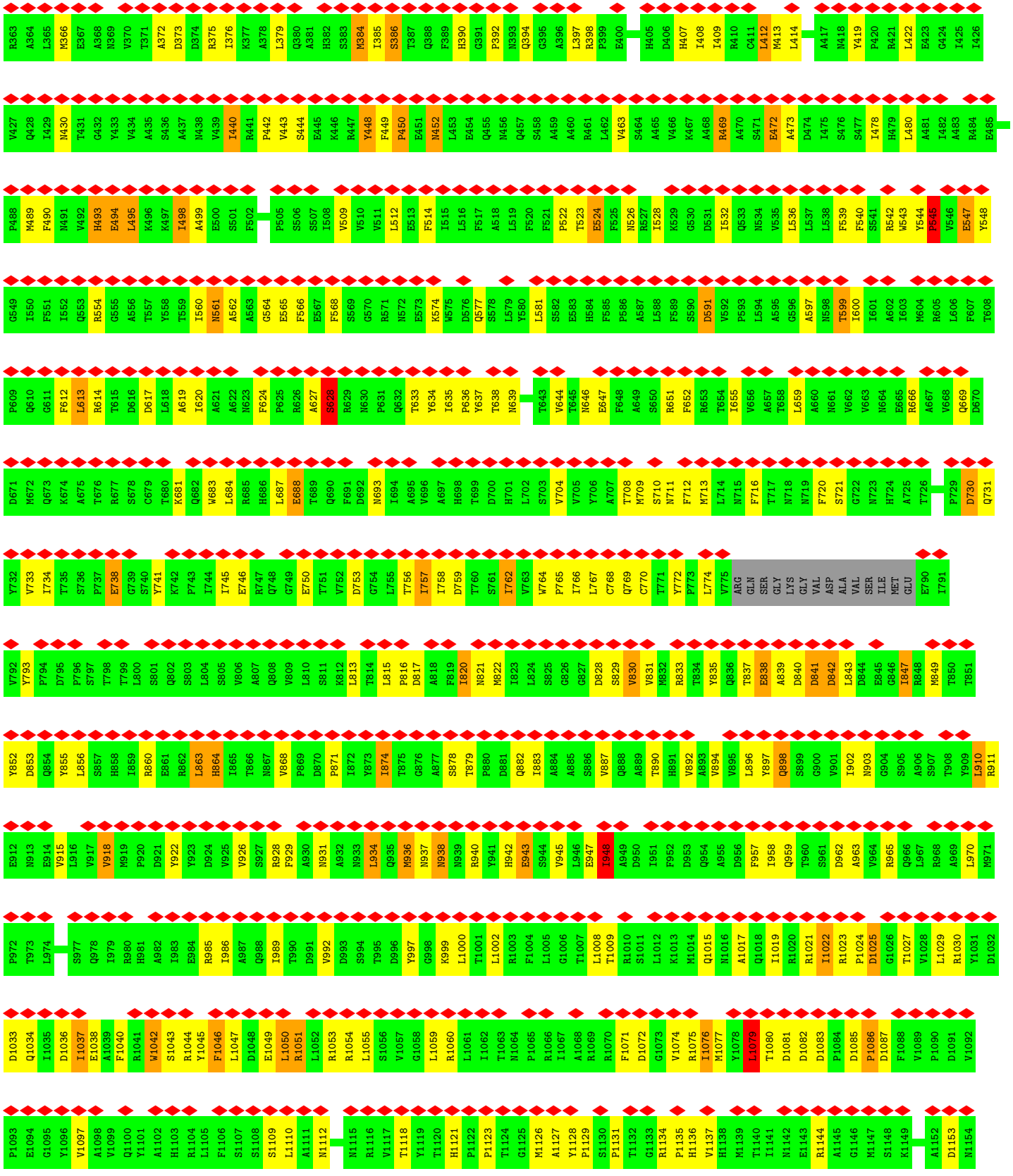

E242 Q243 S244 A245 E246 Y247 V248 S249 G250 L251 L252 M253 V254 L255 F256 K257 V258 M259 T260 D261 N262 R263 L264 V265 I266 V267 G268 E269 T270 T271 T272 P273 M274 S275 N276 T277 L278 S279 T280 V281 V282 N283 N284 V285 L286 R287 T288 T289 Y290 H291 N292 N293 V294 G295 V296 N297 L301 R302 D303
F304 T305 Q306 V307 N308 W309 L310 N311 R312 D313 I314 T315 N316 M317 L318 Q319 Q320 A321 G322 T323 K324 Y325 G326 L327 G328 L329 T330 E331 T332 R333 L334 D335 Y336 V337 R338 L339 V340 K341 T342 I343 V344 G345 H346 A347 L348 N349 I350 D351 H352 F353 A354 A355 S356 V357 L358 N359 I360 N361 L362 R363
A364 L365 M366 E367 A368 N369 V370 T371 A372 D373 D374 R375 I376 K377 A378 L379 Q380 A381 H382 S383 M384 I385 S386 T387 Q388 F389 H390 G391 P392 N393 Q394 G395 A396 L397 R398 P399 E400 L401 A402 F403 D404 H405 D406 H407 I408 I409 R410 C411 L412 M413 L414 A415 A416 A417 N418 Y419 P420 R421 L422 E423
G424 I425 I426 V427 Q428 I429 N430 T431 G432 Y433 V434 A435 S436 A437 N438 V439 I440 R441 P442 V443 S444 E445 K446 R447 Y448 F449 P450 E451 N452 L453 E454 Q455 N456 Q457 S458 A459 A460 R461 L462 V463 S464 A465 V466 K467 A468 R469 A470 S471 E472 A473 D474 I475 S476 S477 I478 H479 L480 A481 I482 A483
R484 E485 V486 S487 P488 M489 F490 N491 V492 H493 E494 L495 K496 K497 I498 A499 E500 S501 F502 E503 D504 P505 S506 S507 I508 V509 V510 V511 L512 E513 F514 I515 L516 F517 A518 L519 F520 F521 P522 F525 N526 R527 I528 K529 G530 D531 I532 Q533 N534 V535 L536 L537 L538 F539 F540 S541 R542 W543 Y544
P545 V546 E547 Y548 G549 I550 F551 I552 Q553 R554 G555 A556 T557 Y558 T559 I560 N561 A562 A563 G564 E565 F566 E567 F568 S569 G570 R571 N572 E573 K574 W575 D576 Q577 S578 L579 Y580 L581 S582 E583 H584 A587 L588 F589 S590 D591 V592 P593 L594 A595 G596 A597 N598 T599 I600 I601 A602 I603 M604 R605
L606 F607 T608 P609 Q610 G611 F612 L613 R614 T615 D616 D617 L618 A619 I620 A621 A622 N623 F624 P625 R626 A627 S628 R629 N630 P631 Q632 T633 Y634 I635 F636 Y637 T638 N639 Q640 R641 G642 T645 N646 E547 F648 A649 S650 R651 F652 R653 T654 I655 V656 A657 T658 L659 A660 N661 V662 V663 N664 E565 R666
A667 V668 Q669 D670 D671 M672 Q673 K674 A675 T676 R677 S678 C679 T680 K681 Q682 W683 L684 R685 H686 L687 E688 T689 Q690 F691 D692 N693 I694 A695 V696 A697 H698 T699 D700 H701 L702 S703 V704 V705 Y706 A707 T708 M709 S710 N711 F712 M713 L714 N715 F716 T717 N718 N719 F720 S721 G722 N723 H724 F727
K728 P729 D730 Q731 Y732 V733 I734 T735 S736 P737 E738 G739 S740 Y741 K742 P743 I744 I745 E746 R747 Q748 G749 E750 T751 V752 D753 G754 L755 T756 I757 I758 D759 T760 S761 I762 V763 W764 P765 I766 L767 C768 Q769 C770 T771 Y772 P773 L774 V775 ARG GLN SER GLY LYS GLY VAL ASP ALA VAL SER ILE
MET GLU E790 I791 V792 Y793 P794 D795 P796 S797 T798 T799 L800 S801 Q802 S803 L804 S805 V806 A807 Q808 V809 L810 S811 K812 L813 T814 L815 P816 D817 A818 F819 I820 N821 M822 I823 L824 S825 G826 G827 V830 V831 M832 R833 T834 Y835 Q836 T837 E838 A839 D840 D841 D842 L843 D844 E845 G846 I847 R848
M849 T850 T851 Y852 D853 Q854 Y855 L856 S857 H858 I859 R860 E861 R862 L863 H864 I865 T866 N867 V868 P869 D870 P871 I872 Y873 I874 T875 Q876 A877 S878 T879 P880 D881 Q882 I883 A884 A885 S886 V887 Q888 A889 T890 H891 V892 A893 V894 V895 L896 Y897 Q898 S899 G900 V901 I902 N903 G904 S905 A906 S907 T908
Y909 L910 R911 E912 N913 E914 V915 L916 V917 Y918 M919 P920 D921 Y922 Y923 D924 V925 V926 S927 R928 F929 A930 N931 A932 N933 L934 Q935 M936 N937 N938 N939 R940 Y941 H942 E943 S944 V945 L946 E947 I948 A949 D950 I951 F952 D953 Q954 A955 D956 F957 I958 Q959 T960 S961 D962 A963 V964 R965 Q966 L967 R968
A969 L970 M971 P972 T973 L974 S975 T976 S977 Q978 I979 R980 H981 A982 I983 E984 R985 T986 A987 Q988 I989 T990 ASP VAL ASP SER T995 D996 Y997 G998 K999 L1000 T1001 L1002 R1003 F1004 L1005 G1006 T1007 L1008 T1009 R1010 S1011 L1012 Q1015 N1016 A1017 Q1018 I1019 R1020 R1021 I1022 R1023 P1024 D1025 G1026 T1027 V1028 L1029

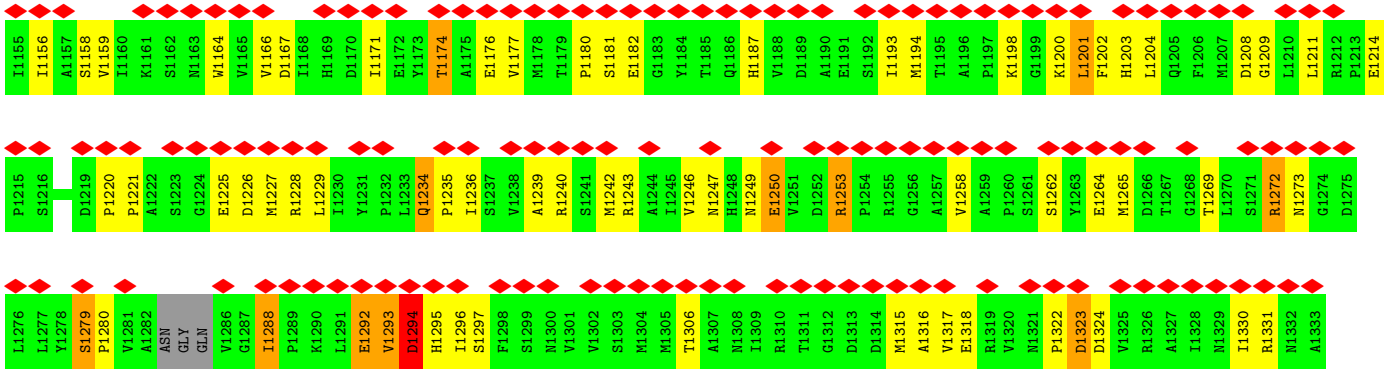


- Molecule 2: Structural protein VP1

Chain C:

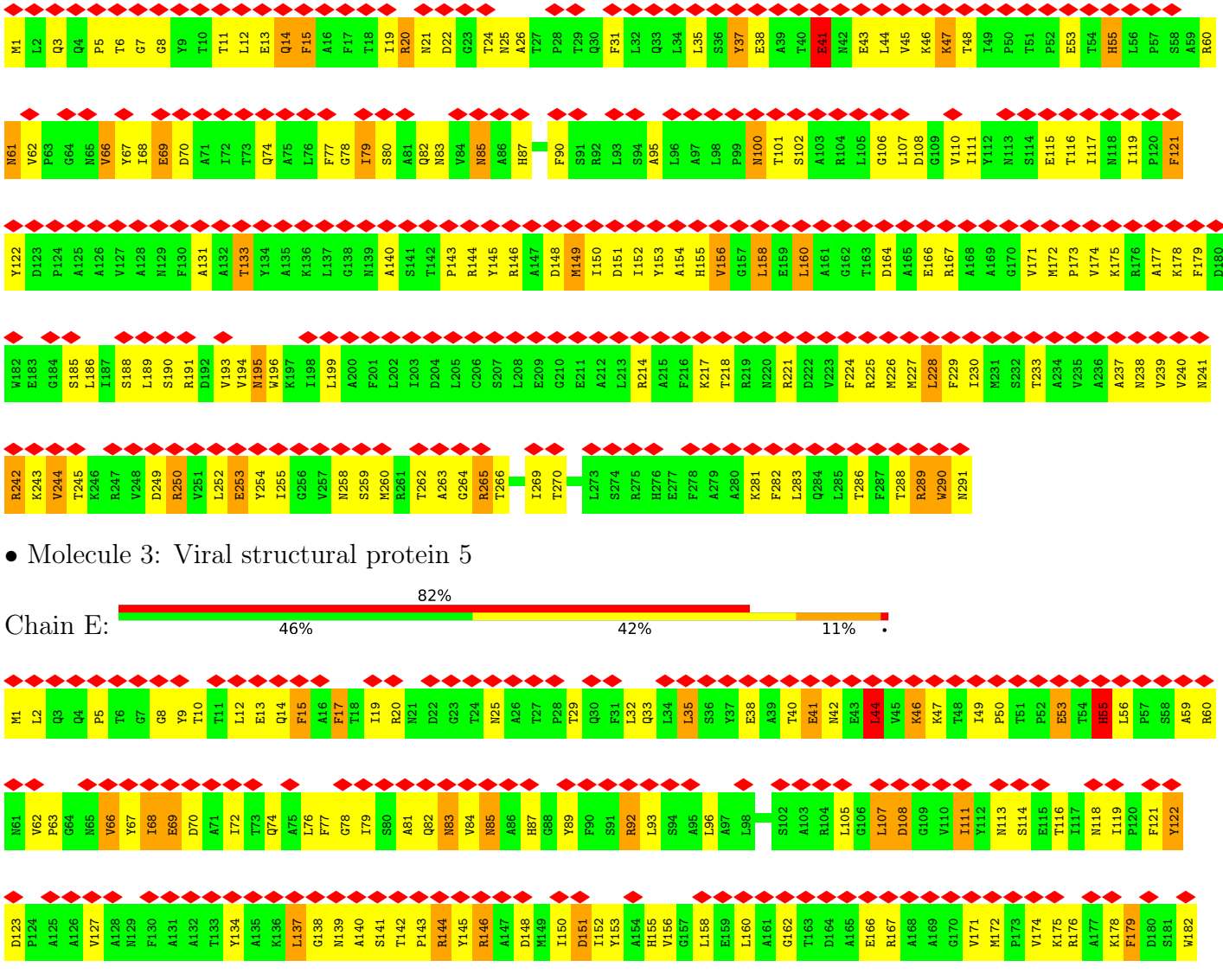



R363 A364 L365 M366 E367 A368 N369 V370 T371 A372 D373 D374 R375 I376 K377 A378 L379 Q380 A381 H382 S383 M384 I385 S386 T387 Q388 F389 H390 G391 P392 N393 Q394 G395 A396 L397 R398 P399 E400 H405 D406 H407 I408 I409 R410 C411 L412 M413 L414 A417 N418 Y419 P420 R421 L422 E423 G424 I425 I426
V427 Q428 I429 N430 T431 G432 Y433 V434 A435 S436 A437 N438 V439 I440 R441 P442 V443 S444 E445 K446 R447 Y448 F449 P450 E451 N452 L453 E454 Q455 N456 Q457 S458 A459 A460 R461 L462 V463 S464 A465 V466 K467 A468 R469 A470 S471 E472 A473 D474 I475 S476 S477 I478 H479 L480 A481 I482 A483 R484 E485
P488 M489 F490 N491 V492 H493 E494 L495 K496 K497 I498 A499 E500 S501 F502 P505 S506 S507 I508 V509 V510 V511 L512 E513 F514 I515 L516 F517 A518 L519 F520 F521 P522 T523 E524 F525 N526 R527 I528 K529 G530 D531 I532 Q533 N534 V535 L536 L537 L538 F539 F540 S541 R542 W543 Y544 P545 V546 E547 Y548
G549 I550 F551 I552 Q553 R554 G555 A556 T557 Y558 T559 I560 N561 A562 A563 G564 E565 F566 E567 F568 S569 G570 R571 N572 E573 K574 W575 D576 Q577 S578 L579 Y580 L581 S582 E583 H584 F585 P586 A587 L588 F589 S590 D591 V592 P593 L594 A595 G596 A597 N598 T599 I600 I601 A602 I603 M604 R605 L606 F607 T608
P609 Q610 G611 F612 L613 R614 T615 D616 D617 L618 A619 I620 A621 A622 N623 F624 P625 R626 A627 S628 R629 N630 P631 Q632 T633 Y634 I635 P636 Y637 T638 N639 T643 V644 T645 N646 E647 F648 A649 S650 R651 F652 R653 T654 I655 V656 A657 T658 L659 A660 N661 V662 V663 N664 E665 R666 A667 V668 Q669 D670
D671 M672 Q673 K674 A675 T676 R677 S678 C679 T680 K681 Q682 W683 L684 R685 H686 L687 E688 T689 Q690 F691 D692 N693 I694 A695 V696 A697 H698 T699 D700 H701 L702 S703 V704 V705 Y706 A707 T708 M709 S710 N711 F712 M713 L714 N715 F716 T717 N718 N719 F720 S721 G722 N723 H724 A725 T726 P729 D730 Q731
Y732 V733 T734 T735 S736 P737 E738 G739 S740 Y741 K742 P743 I744 I745 E746 R747 Q748 G749 E750 T751 V752 D753 G754 L755 T756 I757 I758 D759 T760 S761 T762 V763 W764 P765 I766 L767 C768 Q769 C770 T771 Y772 F773 L774 V775 ARG GLN SER GLY LYS GLY VAL ASP ALA VAL SER ILE MET GLU E790 I791
V792 Y793 P794 D795 P796 S797 T798 T799 L800 S801 Q802 S803 L804 S805 V806 A807 Q808 V809 L810 S811 K812 L813 T814 L815 P816 D817 A818 F819 I820 N821 M822 I823 L824 S825 G826 G827 D828 S829 V830 V831 M832 R833 T834 Y835 Q836 T837 E838 A839 D840 D841 D842 L843 D844 E845 G846 I847 R848 M849 T850 T851
Y852 D853 Q854 Y855 L856 S857 H858 I859 R860 E861 R862 L863 H864 I865 T866 N867 V868 P869 D870 P871 I872 Y873 I874 T875 G876 A877 S878 T879 P880 D881 Q882 I883 A884 A885 S886 V887 Q888 A889 T890 H891 V892 A893 V894 V895 L896 Y897 Q898 S899 G900 V901 I902 N903 G904 S905 A906 S907 T908 Y909 L910 R911
E912 N913 E914 V915 L916 V917 V918 M919 P920 D921 Y922 Y923 D924 V925 V926 S927 R928 F929 A930 N931 A932 N933 L934 Q935 M936 N937 N938 N939 R940 Y941 H942 E943 S944 V945 L946 E947 I948 A949 D950 I951 F952 D953 Q954 A955 D956 F957 I958 Q959 T960 S961 D962 A963 V964 R965 Q966 L967 R968 A969 L970 M971
P972 T973 L974 S977 Q978 I979 R980 H981 A982 I983 E984 R985 I986 A987 Q988 I989 T990 D991 V992 D993 S994 T995 D996 Y997 G998 K999 L1000 T1001 L1002 R1003 F1004 L1005 G1006 T1007 L1008 T1009 R1010 S1011 L1012 K1013 M1014 Q1015 N1016 A1017 Q1018 I1019 R1020 R1021 I1022 R1023 P1024 D1025 G1026 T1027 V1028 L1029 R1030 Y1031 D1032
D1033 Q1034 I1035 D1036 I1037 E1038 A1039 F1040 R1041 W1042 S1043 R1044 Y1045 F1046 L1047 D1048 E1049 L1050 R1051 L1052 R1053 R1054 L1055 S1056 V1057 G1058 L1059 R1060 L1061 I1062 T1063 N1064 P1065 R1066 I1067 A1068 R1069 R1070 F1071 D1072 G1073 V1074 R1075 I1076 M1077 Y1078 L1079 T1080 D1081 D1082 D1083 P1084 D1085 P1086 D1087 F1088 V1089 P1090 D1091 V1092
P1093 E1094 G1095 Y1096 V1097 A1098 V1099 Q1100 Y1101 A1102 H1103 R1104 L1105 F1106 S1107 S1108 S1109 L1110 A1111 N1112 N1115 R1116 V1117 T1118 Y1119 T1120 H1121 P1122 P1123 T1124 G1125 M1126 A1127 Y1128 P1129 S1130 P1131 T1132 G1133 R1134 P1135 H1136 V1137 H1138 M1139 T1140 I1141 N1142 E1143 R1144 A1145 G1146 M1147 S1148 K1149 A1152 D1153 N1154



• Molecule 3: Viral structural protein 5

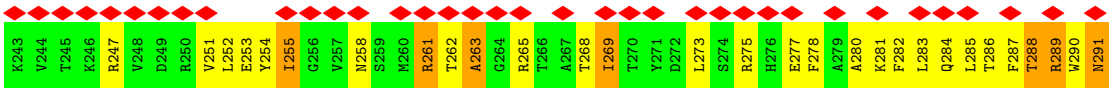
Chain D:



• Molecule 3: Viral structural protein 5

Chain E:


E183 G184 S185 L186 I187 S188 L189 S190 R191 D192 V193 V194 N195 W196 K197 I198 L199 A200 F201 L202 I203 D204 L205 C206 S207 L208 E209 G210 E211 A212 L213 R214 A215 F216 K217 T218 R219 N220 R221 D222 V223 F224 R225 M226 M227 L228 F229 I230 M231 S232 T233 A234 V235 A236 A237 N238 V239 V240 N241 R242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4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	29000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Each micrograph	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	0.8	Depositor
Maximum defocus (nm)	2.8	Depositor
Magnification	75000	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum map value	18.037	Depositor
Minimum map value	-16.951	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3.0	Depositor
Map size (Å)	761.60004, 761.60004, 595.0	wwPDB
Map dimensions	640, 640, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.19, 1.19, 1.19	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.36	0/8530	0.58	0/11613
2	B	0.34	0/9508	0.55	2/12941 (0.0%)
2	C	0.35	0/10006	0.56	4/13622 (0.0%)
3	D	0.37	0/2322	0.64	2/3156 (0.1%)
3	E	0.37	0/2322	0.74	5/3156 (0.2%)
All	All	0.35	0/32688	0.59	13/44488 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	2

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	59	ALA	CB-CA-C	-11.46	92.90	110.10
3	E	60	ARG	N-CA-CB	-7.76	96.63	110.60
3	D	7	GLY	N-CA-C	-6.59	96.62	113.10
3	E	263	ALA	N-CA-C	-5.95	94.94	111.00
2	C	1201	LEU	CA-CB-CG	5.67	128.34	115.30
2	B	618	LEU	CA-CB-CG	5.56	128.08	115.30
3	E	44	LEU	CA-CB-CG	5.40	127.72	115.30
2	C	495	LEU	CA-CB-CG	5.40	127.72	115.30
3	D	41	GLU	N-CA-C	5.38	125.52	111.00
2	C	1079	LEU	CA-CB-CG	5.34	127.58	115.30
3	E	60	ARG	N-CA-C	5.17	124.97	111.00
2	C	613	LEU	CA-CB-CG	5.06	126.93	115.30
2	B	934	LEU	CA-CB-CG	5.04	126.90	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	1225	GLU	Peptide
2	C	628	SER	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	8349	0	8304	321	0
2	B	9317	0	9236	358	0
2	C	9806	0	9713	369	0
3	D	2276	0	2273	286	0
3	E	2276	0	2277	257	0
All	All	32024	0	31803	1395	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 (1395) 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)
2:B:271:THR:CG2	2:C:237:VAL:HG23	1.18	1.64
2:B:274:MET:CG	2:C:234:PRO:HD3	1.35	1.51
3:E:46:LYS:HD3	3:E:155:HIS:CE1	1.49	1.45
2:B:1273:ASN:OD1	3:D:79:ILE:CG2	1.68	1.40
2:B:1273:ASN:ND2	3:D:191:ARG:HA	1.38	1.39
2:B:363:ARG:CZ	3:D:80:SER:OG	1.71	1.39
2:B:271:THR:HG21	2:C:237:VAL:CG2	1.52	1.38
3:E:53:GLU:HG2	3:E:145:TYR:CD1	1.57	1.37
2:B:274:MET:HG3	2:C:234:PRO:CD	1.54	1.36
3:E:46:LYS:CD	3:E:155:HIS:HE1	1.41	1.31
3:D:253:GLU:OE1	3:D:254:TYR:CE2	1.83	1.30
3:D:253:GLU:HG3	3:D:254:TYR:CD2	1.68	1.29
2:B:891:HIS:CD2	3:D:240:VAL:CG2	2.17	1.28
3:D:8:GLY:O	3:D:11:THR:HG22	1.34	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:337:VAL:HG22	3:E:187:ILE:CD1	1.66	1.25
2:B:271:THR:CG2	2:C:237:VAL:CG2	2.09	1.25
3:D:253:GLU:OE1	3:D:254:TYR:HE2	1.03	1.25
3:E:32:LEU:O	3:E:35:LEU:CD1	1.84	1.24
2:B:954:GLN:CD	3:D:240:VAL:HG12	1.59	1.23
1:A:159:ILE:HD11	2:B:1333:ALA:O	1.32	1.23
2:B:954:GLN:CD	3:D:240:VAL:CG1	2.09	1.21
3:E:68:ILE:C	3:E:68:ILE:HD13	1.56	1.21
2:B:950:ASP:HA	3:D:243:LYS:NZ	1.56	1.20
3:D:5:PRO:O	3:D:6:THR:CG2	1.90	1.20
3:E:289:ARG:HD2	3:E:289:ARG:O	1.40	1.19
3:E:182:TRP:O	3:E:183:GLU:HG2	1.08	1.18
3:D:5:PRO:O	3:D:6:THR:HG22	1.01	1.17
3:E:55:HIS:HD2	3:E:145:TYR:CE2	1.63	1.17
2:B:950:ASP:C	3:D:243:LYS:HZ2	1.45	1.16
3:D:45:VAL:HG13	3:D:171:VAL:HG22	1.19	1.16
2:B:1273:ASN:OD1	3:D:79:ILE:HG22	1.39	1.15
3:E:107:LEU:HA	3:E:122:TYR:HE1	1.06	1.15
2:B:1044:ARG:NH2	3:D:266:THR:HG22	1.59	1.15
2:B:891:HIS:CD2	3:D:240:VAL:HG23	1.82	1.15
2:B:1044:ARG:HH21	3:D:266:THR:HG22	1.01	1.15
3:D:149:MET:HE3	3:D:260:MET:HE1	1.14	1.14
2:B:338:ARG:HH21	2:C:1002:LEU:HD22	0.98	1.14
3:E:158:LEU:O	3:E:162:GLY:HA3	1.48	1.13
1:A:159:ILE:CD1	2:B:1333:ALA:O	1.96	1.12
3:D:217:LYS:HD3	3:D:290:TRP:CH2	1.82	1.12
1:A:512:ALA:HB3	1:A:513:PRO:HA	1.27	1.11
3:E:205:LEU:HD13	3:E:205:LEU:O	1.49	1.11
3:E:175:LYS:HB2	3:E:255:ILE:CD1	1.80	1.11
1:A:188:THR:HG21	3:D:144:ARG:HG2	1.34	1.10
2:B:891:HIS:NE2	3:D:240:VAL:HG23	1.67	1.10
2:C:1080:THR:HG21	2:C:1227:MET:SD	1.91	1.10
3:E:137:LEU:HD23	3:E:137:LEU:C	1.72	1.09
2:B:134:THR:HG21	2:C:472:GLU:OE2	1.52	1.09
2:B:271:THR:HG23	2:C:237:VAL:HG23	1.13	1.09
2:B:279:SER:CB	2:C:1198:LYS:HE2	1.83	1.09
2:C:1025:ASP:OD2	3:D:95:ALA:HB2	1.53	1.09
3:E:49:ILE:HG23	3:E:50:PRO:HD2	1.35	1.09
2:C:100:ASP:OD1	3:E:82:GLN:NE2	1.84	1.08
2:C:1273:ASN:O	3:E:183:GLU:OE1	1.70	1.08
2:C:878:SER:HB3	2:C:903:ASN:HB2	1.34	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:950:ASP:CA	3:D:243:LYS:NZ	2.16	1.08
2:B:891:HIS:CD2	3:D:240:VAL:HG21	1.84	1.07
1:A:554:PRO:HB3	1:A:580:SER:OG	1.52	1.07
3:E:182:TRP:O	3:E:183:GLU:CG	2.01	1.07
3:D:217:LYS:HD3	3:D:290:TRP:CZ3	1.88	1.07
2:B:388:GLN:OE1	2:C:499:ALA:HB1	1.53	1.06
2:C:1273:ASN:HA	3:E:183:GLU:OE1	1.53	1.05
3:E:191:ARG:HG3	3:E:191:ARG:NH1	1.60	1.05
1:A:904:PHE:HE2	1:A:906:PHE:HB3	1.16	1.04
2:B:950:ASP:O	3:D:243:LYS:NZ	1.90	1.04
3:E:32:LEU:O	3:E:35:LEU:HD12	1.57	1.04
3:E:175:LYS:CB	3:E:255:ILE:HD11	1.86	1.04
1:A:159:ILE:CD1	2:B:1333:ALA:C	2.27	1.03
3:E:107:LEU:HA	3:E:122:TYR:CE1	1.93	1.03
2:C:337:VAL:HG22	3:E:187:ILE:HD12	1.06	1.03
2:B:338:ARG:NH2	2:C:1002:LEU:HD22	1.73	1.02
2:B:950:ASP:HA	3:D:243:LYS:HZ1	1.21	1.02
3:D:149:MET:HE3	3:D:260:MET:CE	1.90	1.01
3:E:53:GLU:CG	3:E:145:TYR:HD1	1.73	1.01
3:E:191:ARG:HH11	3:E:191:ARG:CG	1.72	1.01
3:E:32:LEU:O	3:E:35:LEU:HD11	1.57	1.01
2:B:137:ILE:HD11	2:C:759:ASP:CG	1.81	1.01
2:C:1051:ARG:HH11	2:C:1051:ARG:HG2	1.24	1.00
3:E:262:THR:HG22	3:E:263:ALA:O	1.61	1.00
1:A:194:HIS:CE1	3:D:146:ARG:NH1	2.30	1.00
2:C:864:HIS:NE2	2:C:1030:ARG:NH2	2.10	0.99
2:C:1050:LEU:HD12	2:C:1054:ARG:HH21	1.23	0.99
3:E:46:LYS:CD	3:E:155:HIS:CE1	2.25	0.99
2:B:1044:ARG:HE	3:D:266:THR:CG2	1.74	0.99
3:E:1:MET:HE1	3:E:121:PHE:CE2	1.96	0.99
2:B:442:PRO:HG3	2:B:475:ILE:HB	1.40	0.99
2:B:338:ARG:HH21	2:C:1002:LEU:CD2	1.75	0.99
2:B:1044:ARG:NE	3:D:266:THR:CG2	2.26	0.98
3:E:127:VAL:HG12	3:E:203:ILE:HD11	1.44	0.98
3:E:158:LEU:O	3:E:162:GLY:CA	2.10	0.98
3:D:253:GLU:CG	3:D:254:TYR:CD2	2.46	0.98
3:D:153:TYR:HA	3:D:156:VAL:HG12	1.42	0.98
1:A:49:HIS:HE2	1:A:172:PHE:HD1	1.01	0.98
2:B:954:GLN:CG	3:D:240:VAL:HG12	1.93	0.98
3:E:68:ILE:C	3:E:68:ILE:CD1	2.30	0.98
3:E:68:ILE:HD13	3:E:68:ILE:O	1.62	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:261:ARG:HH12	3:E:265:ARG:NH2	1.62	0.97
2:B:1273:ASN:OD1	3:D:79:ILE:HG23	1.64	0.97
2:C:1037:ILE:HG22	2:C:1038:GLU:H	1.27	0.96
2:B:870:ASP:HB3	2:B:871:PRO:HA	1.47	0.96
1:A:194:HIS:NE2	3:D:146:ARG:NH1	2.14	0.96
3:E:55:HIS:CD2	3:E:145:TYR:CE2	2.53	0.96
3:D:149:MET:CE	3:D:260:MET:HE1	1.95	0.96
3:E:53:GLU:CG	3:E:145:TYR:CD1	2.47	0.96
1:A:426:ARG:HB2	1:A:707:SER:HB2	1.47	0.96
3:E:261:ARG:HH12	3:E:265:ARG:HH21	1.11	0.96
2:B:134:THR:CG2	2:C:472:GLU:OE2	2.13	0.96
2:C:146:GLU:HB2	2:C:1317:VAL:O	1.63	0.96
3:D:262:THR:HG21	3:D:270:THR:HA	1.47	0.95
2:C:528:ILE:HD11	2:C:758:ILE:HD12	1.47	0.95
2:B:338:ARG:NH2	2:C:1002:LEU:CD2	2.29	0.95
3:E:53:GLU:HG2	3:E:145:TYR:HD1	0.80	0.95
3:E:68:ILE:HD11	3:E:72:ILE:CD1	1.96	0.95
1:A:986:ARG:HB3	1:A:994:PRO:HB3	1.44	0.95
2:B:956:ASP:OD1	3:D:266:THR:OG1	1.83	0.95
3:E:107:LEU:HD23	3:E:122:TYR:CE1	2.02	0.95
3:D:153:TYR:HA	3:D:156:VAL:CG1	1.96	0.94
3:E:191:ARG:HG3	3:E:191:ARG:HH11	0.79	0.94
2:B:954:GLN:OE1	3:D:240:VAL:HG12	1.67	0.94
2:B:368:ALA:O	3:D:83:ASN:HB2	1.69	0.93
3:E:200:ALA:O	3:E:204:ASP:OD2	1.85	0.93
1:A:225:SER:OG	2:B:563:ALA:HA	1.69	0.93
2:B:891:HIS:NE2	3:D:240:VAL:CG2	2.26	0.93
3:D:253:GLU:CD	3:D:254:TYR:CE2	2.41	0.93
3:E:1:MET:CE	3:E:121:PHE:CE2	2.53	0.92
2:C:1273:ASN:CA	3:E:183:GLU:OE1	2.18	0.91
3:D:214:ARG:O	3:D:218:THR:HG23	1.69	0.91
2:B:271:THR:HG21	2:C:237:VAL:HG23	1.01	0.91
2:C:878:SER:HB3	2:C:903:ASN:CB	1.99	0.91
2:C:1025:ASP:OD2	3:D:95:ALA:CB	2.18	0.91
1:A:967:ILE:HG13	1:A:978:LYS:HB2	1.52	0.91
1:A:27:LYS:HB3	1:A:28:PRO:HD3	1.53	0.91
2:B:350:ILE:HG22	2:B:351:ASP:H	1.35	0.91
2:B:279:SER:HB2	2:C:1198:LYS:HE2	1.52	0.90
3:E:289:ARG:HD2	3:E:289:ARG:C	1.87	0.90
3:D:44:LEU:HD11	3:D:154:ALA:HA	1.50	0.90
2:C:565:GLU:HG2	2:C:566:PHE:N	1.86	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1050:LEU:HD12	2:C:1054:ARG:NH2	1.86	0.90
3:D:253:GLU:HG3	3:D:254:TYR:HD2	1.10	0.90
2:B:1273:ASN:HD22	3:D:191:ARG:HA	1.09	0.89
2:B:1273:ASN:HD21	3:D:191:ARG:HA	1.34	0.89
2:B:1288:ILE:HD12	3:D:20:ARG:NH2	1.88	0.89
1:A:406:VAL:CB	1:A:407:GLU:HA	2.03	0.89
1:A:194:HIS:CE1	3:D:146:ARG:HH11	1.88	0.89
2:B:183:SER:HB3	2:B:186:ASP:HB2	1.54	0.89
2:B:1044:ARG:HE	3:D:266:THR:HG21	1.37	0.89
3:D:156:VAL:HG23	3:D:228:LEU:CD2	2.02	0.89
1:A:406:VAL:HB	1:A:407:GLU:CA	2.03	0.88
2:B:368:ALA:HA	3:D:83:ASN:ND2	1.88	0.88
2:B:231:LEU:HB2	2:B:249:SER:HB2	1.54	0.88
2:B:340:VAL:HG21	2:C:1008:LEU:HD23	1.56	0.88
2:B:279:SER:OG	2:C:1198:LYS:HE2	1.73	0.88
2:C:397:LEU:HD11	3:E:265:ARG:HB3	1.56	0.88
2:B:274:MET:CG	2:C:234:PRO:CD	2.29	0.88
3:E:160:LEU:HD11	3:E:229:PHE:HB2	1.55	0.88
3:D:8:GLY:O	3:D:11:THR:CG2	2.20	0.87
2:B:888:GLN:NE2	3:D:38:GLU:OE1	2.06	0.87
2:C:337:VAL:CG2	3:E:187:ILE:HD12	1.99	0.87
1:A:406:VAL:HB	1:A:407:GLU:HA	1.57	0.87
3:D:149:MET:CE	3:D:260:MET:CE	2.50	0.87
3:E:12:LEU:HG	3:E:14:GLN:HE21	1.38	0.87
3:E:68:ILE:HD11	3:E:72:ILE:HD12	1.57	0.87
2:B:1023:ARG:HB2	2:B:1024:PRO:HD2	1.55	0.87
1:A:970:ARG:HH22	1:A:977:HIS:HA	1.38	0.87
2:B:1248:HIS:ND1	2:B:1251:VAL:HG22	1.90	0.87
2:B:891:HIS:HD2	3:D:240:VAL:CG2	1.85	0.87
2:C:638:THR:HB	2:C:1331:ARG:HH21	1.41	0.86
1:A:868:ASP:O	1:A:871:VAL:HG23	1.75	0.86
3:D:153:TYR:O	3:D:156:VAL:HG13	1.74	0.86
1:A:194:HIS:CD2	3:D:146:ARG:NH1	2.44	0.86
1:A:512:ALA:CB	1:A:513:PRO:HA	2.06	0.86
3:E:49:ILE:CG2	3:E:50:PRO:HD2	2.06	0.86
2:B:1273:ASN:ND2	3:D:191:ARG:CA	2.33	0.85
2:C:1023:ARG:HG2	2:C:1024:PRO:HD2	1.56	0.85
2:B:950:ASP:CA	3:D:243:LYS:HZ2	1.80	0.85
3:E:160:LEU:CD1	3:E:229:PHE:HB2	2.05	0.85
1:A:31:VAL:HG23	1:A:32:PRO:HD3	1.59	0.85
2:B:186:ASP:HA	2:B:189:ILE:HG22	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:69:GLU:C	3:E:69:GLU:CD	2.35	0.85
3:D:172:MET:HE3	3:D:175:LYS:HG3	1.57	0.84
3:E:175:LYS:HB2	3:E:255:ILE:HD11	0.90	0.84
2:B:956:ASP:CG	3:D:266:THR:OG1	2.15	0.84
2:C:1071:PHE:HB3	2:C:1234:GLN:HG3	1.58	0.84
3:E:146:ARG:CZ	3:E:277:GLU:OE2	2.26	0.84
2:B:274:MET:HG2	2:C:234:PRO:HD3	1.54	0.84
3:E:55:HIS:CG	3:E:55:HIS:O	2.30	0.84
1:A:49:HIS:NE2	1:A:172:PHE:HD1	1.76	0.83
1:A:76:LEU:O	1:A:78:TYR:N	2.10	0.83
2:C:619:ALA:HB2	2:C:711:ASN:HB2	1.60	0.83
3:D:5:PRO:C	3:D:6:THR:HG22	1.98	0.83
2:C:1050:LEU:CD1	2:C:1054:ARG:HH21	1.92	0.83
1:A:904:PHE:CE2	1:A:906:PHE:HB3	2.08	0.83
1:A:159:ILE:HD13	2:B:1333:ALA:C	1.98	0.82
2:B:870:ASP:HB3	2:B:871:PRO:CA	2.09	0.82
3:D:181:SER:HB3	3:D:250:ARG:HG2	1.62	0.82
3:E:69:GLU:HG2	3:E:199:LEU:HB2	1.61	0.82
2:B:1273:ASN:CG	3:D:79:ILE:HG22	1.98	0.82
1:A:406:VAL:HG21	1:A:408:PRO:HD3	1.59	0.82
2:B:954:GLN:CD	3:D:240:VAL:HG13	1.97	0.82
2:C:449:PHE:N	2:C:450:PRO:HD3	1.95	0.82
1:A:427:ASP:HA	1:A:704:PRO:HD2	1.61	0.82
2:B:363:ARG:NE	3:D:80:SER:OG	2.13	0.82
2:B:954:GLN:OE1	3:D:240:VAL:CG1	2.24	0.82
3:E:79:ILE:HA	3:E:269:ILE:HD13	1.62	0.82
1:A:188:THR:HG21	3:D:144:ARG:CG	2.09	0.82
3:D:100:ASN:H	3:D:100:ASN:HD22	1.24	0.82
3:E:166:GLU:OE2	3:E:171:VAL:O	1.97	0.82
3:D:258:ASN:OD1	3:D:259:SER:O	1.98	0.82
1:A:978:LYS:HG2	1:A:987:LEU:HD13	1.62	0.81
1:A:124:THR:O	1:A:125:ASN:HB2	1.79	0.81
2:B:954:GLN:HG2	3:D:240:VAL:HG12	1.61	0.81
2:C:1273:ASN:C	3:E:183:GLU:OE1	2.19	0.81
3:E:85:ASN:ND2	3:E:141:SER:HB3	1.95	0.81
2:B:1044:ARG:NH2	3:D:266:THR:CG2	2.43	0.81
2:B:1273:ASN:CG	3:D:79:ILE:CG2	2.47	0.81
2:B:219:ILE:HG22	2:B:220:ASP:H	1.45	0.81
1:A:597:ARG:HH11	1:A:597:ARG:HG3	1.45	0.80
3:D:41:GLU:OE1	3:D:41:GLU:HA	1.79	0.80
2:C:443:VAL:HG22	2:C:444:SER:H	1.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:864:ARG:HG3	1:A:866:LEU:H	1.46	0.80
2:B:1263:TYR:CG	2:B:1295:HIS:HD2	1.99	0.80
3:D:264:GLY:O	3:D:266:THR:N	2.14	0.80
2:B:442:PRO:HD3	2:B:475:ILE:HD12	1.62	0.80
2:C:1051:ARG:HG2	2:C:1051:ARG:NH1	1.88	0.80
2:C:154:PHE:HB3	2:C:262:ASN:HB2	1.62	0.80
3:D:153:TYR:O	3:D:156:VAL:CG1	2.30	0.80
1:A:27:LYS:O	1:A:30:THR:HG23	1.82	0.80
3:D:253:GLU:CG	3:D:254:TYR:HD2	1.89	0.79
3:E:55:HIS:HD2	3:E:145:TYR:CZ	2.00	0.79
2:B:733:VAL:HG21	2:B:741:TYR:CD1	2.18	0.79
1:A:406:VAL:CG2	1:A:407:GLU:HA	2.13	0.79
2:B:1234:GLN:HE21	2:B:1234:GLN:HA	1.47	0.79
2:B:950:ASP:C	3:D:243:LYS:NZ	2.28	0.79
2:B:1274:GLY:CA	3:D:191:ARG:HG3	2.12	0.79
2:C:864:HIS:CE1	2:C:1030:ARG:NH2	2.50	0.79
3:E:137:LEU:HD23	3:E:137:LEU:O	1.82	0.79
1:A:55:GLY:H	1:A:58:GLN:HG2	1.47	0.79
2:B:1044:ARG:CZ	3:D:266:THR:CG2	2.60	0.79
3:D:41:GLU:OE1	3:D:41:GLU:CA	2.30	0.79
2:B:368:ALA:O	3:D:83:ASN:CB	2.31	0.79
2:C:1042:TRP:CG	2:C:1043:SER:HA	2.18	0.79
3:E:40:THR:CG2	3:E:41:GLU:OE2	2.30	0.79
1:A:648:VAL:HG22	1:A:649:LYS:N	1.99	0.78
3:D:153:TYR:CA	3:D:156:VAL:HG12	2.12	0.78
3:E:40:THR:HG23	3:E:41:GLU:OE2	1.83	0.78
2:C:750:GLU:HB3	2:C:757:ILE:HD13	1.63	0.78
2:B:1037:ILE:HG12	2:B:1038:GLU:H	1.48	0.78
2:C:291:HIS:HD2	2:C:346:HIS:CD2	2.01	0.78
2:C:385:ILE:HG13	2:C:708:THR:HG22	1.65	0.78
3:E:158:LEU:O	3:E:162:GLY:N	2.16	0.78
1:A:48:SER:O	1:A:49:HIS:HB3	1.83	0.78
2:C:565:GLU:HG2	2:C:566:PHE:H	1.45	0.78
3:E:56:LEU:HD23	3:E:56:LEU:H	1.49	0.77
1:A:730:ILE:HG22	1:A:731:HIS:H	1.48	0.77
2:B:363:ARG:NH2	3:D:80:SER:OG	2.16	0.77
1:A:717:THR:HG21	1:A:1020:SER:HB2	1.67	0.77
2:C:450:PRO:C	2:C:452:ASN:H	1.86	0.77
2:C:141:LEU:HG	2:C:142:ASP:H	1.50	0.77
3:D:217:LYS:CD	3:D:290:TRP:CZ3	2.67	0.77
3:D:107:LEU:O	3:D:108:ASP:CG	2.23	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:45:VAL:HG13	3:D:171:VAL:CG2	2.10	0.76
3:E:68:ILE:HD11	3:E:72:ILE:HD11	1.64	0.76
2:C:1051:ARG:HH11	2:C:1051:ARG:CG	1.98	0.76
3:E:262:THR:CG2	3:E:263:ALA:O	2.33	0.76
1:A:228:ILE:HD12	2:B:563:ALA:HB1	1.67	0.76
3:E:42:ASN:HB2	3:E:174:VAL:HB	1.68	0.76
3:E:107:LEU:HD23	3:E:122:TYR:CZ	2.20	0.76
2:C:638:THR:HB	2:C:1331:ARG:NH2	2.00	0.75
3:E:68:ILE:HD13	3:E:69:GLU:N	2.00	0.75
2:C:838:GLU:HB3	2:C:934:LEU:HB2	1.68	0.75
1:A:560:LEU:HD12	1:A:569:VAL:HG23	1.67	0.75
2:B:137:ILE:CD1	2:C:759:ASP:OD1	2.34	0.75
3:E:69:GLU:CG	3:E:199:LEU:HB2	2.17	0.75
2:B:271:THR:HA	2:C:236:GLY:HA3	1.67	0.75
3:E:235:VAL:HG13	3:E:258:ASN:HD22	1.51	0.75
1:A:194:HIS:CG	3:D:146:ARG:HH11	2.05	0.75
2:B:620:ILE:HG21	2:B:631:PRO:HG3	1.69	0.75
2:B:1044:ARG:NE	3:D:266:THR:HG23	2.02	0.74
2:B:1044:ARG:CZ	3:D:266:THR:HG22	2.16	0.74
2:B:1156:ILE:HD11	2:B:1194:MET:HG3	1.68	0.74
2:C:390:HIS:HB2	2:C:1318:GLU:OE2	1.87	0.74
3:D:238:ASN:HB2	3:D:253:GLU:HB2	1.68	0.74
2:C:963:ALA:HB3	2:C:1059:LEU:CD2	2.18	0.74
3:E:156:VAL:HG13	3:E:228:LEU:HD12	1.68	0.74
2:B:956:ASP:OD2	3:D:266:THR:OG1	2.06	0.74
2:C:841:ASP:O	2:C:842:ASP:HB2	1.87	0.74
3:E:137:LEU:C	3:E:137:LEU:CD2	2.49	0.74
2:B:177:LYS:HE3	2:B:177:LYS:H	1.51	0.73
2:C:639:ASN:H	2:C:1331:ARG:NH2	1.85	0.73
3:D:108:ASP:OD1	3:D:110:VAL:HG23	1.88	0.73
2:B:1273:ASN:HB2	3:D:194:VAL:HG11	1.69	0.73
2:B:960:THR:HG23	2:B:965:ARG:HH12	1.52	0.73
3:E:182:TRP:C	3:E:183:GLU:HG2	2.04	0.73
2:B:234:PRO:HD2	2:B:242:GLU:HB3	1.70	0.73
2:B:363:ARG:NH1	3:D:80:SER:OG	2.20	0.73
3:E:150:ILE:HG22	3:E:150:ILE:O	1.87	0.73
3:D:172:MET:HG3	3:D:173:PRO:HD2	1.69	0.72
3:E:137:LEU:HD11	3:E:278:PHE:CZ	2.23	0.72
3:E:214:ARG:O	3:E:218:THR:HG23	1.89	0.72
1:A:406:VAL:HG23	1:A:407:GLU:HA	1.71	0.72
2:B:891:HIS:HA	3:D:242:ARG:HD2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1121:HIS:HD2	2:B:1124:THR:HG22	1.55	0.72
1:A:97:ARG:HH11	1:A:97:ARG:HB2	1.54	0.72
2:B:836:GLN:O	2:B:935:GLN:HB3	1.89	0.72
3:E:53:GLU:HG2	3:E:145:TYR:CE1	2.24	0.72
3:E:253:GLU:OE2	3:E:254:TYR:CZ	2.43	0.72
3:D:282:PHE:O	3:D:286:THR:HG22	1.90	0.72
2:B:1263:TYR:CG	2:B:1295:HIS:CD2	2.78	0.71
2:B:137:ILE:CD1	2:C:759:ASP:CG	2.59	0.71
3:D:265:ARG:HA	3:D:265:ARG:NE	2.05	0.71
1:A:406:VAL:CG2	1:A:408:PRO:HD3	2.21	0.71
3:D:156:VAL:HG23	3:D:228:LEU:HD21	1.71	0.71
2:C:440:ILE:HD12	2:C:478:ILE:HG21	1.72	0.71
2:B:137:ILE:HD11	2:C:759:ASP:OD1	1.91	0.71
2:C:628:SER:O	2:C:1037:ILE:HD11	1.90	0.71
1:A:420:VAL:HG12	1:A:970:ARG:HG3	1.71	0.71
2:C:449:PHE:HB2	2:C:683:TRP:CD1	2.26	0.71
2:B:1272:ARG:HH12	3:D:69:GLU:CD	1.93	0.70
2:C:898:GLN:OE1	3:D:3:GLN:NE2	2.24	0.70
2:C:841:ASP:CG	2:C:842:ASP:H	1.94	0.70
3:E:192:ASP:OD1	3:E:192:ASP:C	2.30	0.70
1:A:648:VAL:HG22	1:A:649:LYS:H	1.57	0.70
2:B:954:GLN:CG	3:D:240:VAL:CG1	2.63	0.70
3:E:13:GLU:CD	3:E:13:GLU:O	2.30	0.70
3:D:47:LYS:HG3	3:D:48:THR:H	1.57	0.69
1:A:963:TYR:HE2	1:A:978:LYS:HB3	1.57	0.69
1:A:764:SER:HA	1:A:795:GLU:HG3	1.74	0.69
1:A:887:ILE:HG22	1:A:888:GLU:H	1.56	0.69
2:C:270:THR:HG22	2:C:291:HIS:HA	1.74	0.69
3:E:13:GLU:OE1	3:E:13:GLU:C	2.30	0.69
2:C:528:ILE:O	2:C:528:ILE:HG22	1.90	0.69
1:A:925:ILE:HD13	1:A:937:ARG:HH12	1.56	0.69
1:A:928:GLU:HG3	1:A:929:PRO:HD2	1.73	0.69
2:C:376:ILE:HD11	2:C:1317:VAL:HG21	1.75	0.69
2:C:963:ALA:HB3	2:C:1059:LEU:HD21	1.75	0.69
3:D:61:ASN:OD1	3:D:61:ASN:C	2.30	0.69
3:E:46:LYS:HD3	3:E:155:HIS:HE1	0.56	0.69
3:E:253:GLU:HG3	3:E:254:TYR:CD2	2.28	0.69
1:A:19:PRO:O	1:A:22:ILE:HG22	1.93	0.69
2:B:1271:SER:OG	3:D:195:ASN:OD1	2.11	0.69
1:A:842:TYR:HA	1:A:845:ILE:HG22	1.74	0.69
3:E:69:GLU:CD	3:E:69:GLU:O	2.31	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:244:VAL:HG12	3:D:245:THR:H	1.57	0.68
2:C:1166:VAL:HG12	2:C:1167:ASP:H	1.57	0.68
3:E:35:LEU:HB3	3:E:179:PHE:HB3	1.75	0.68
1:A:23:ARG:O	1:A:28:PRO:HD2	1.93	0.68
1:A:658:ILE:HD11	1:A:692:ILE:HD11	1.75	0.68
2:B:1272:ARG:NH1	3:D:69:GLU:OE1	2.27	0.68
1:A:713:ASN:HA	1:A:716:MET:HB2	1.74	0.68
2:B:368:ALA:CA	3:D:83:ASN:HD22	2.06	0.68
2:B:737:PRO:HA	2:B:861:GLU:HG2	1.75	0.68
2:B:1306:THR:HG23	2:B:1308:ASN:H	1.59	0.68
2:B:486:VAL:HG21	2:B:709:MET:HB3	1.76	0.68
2:C:146:GLU:O	2:C:1316:ALA:HA	1.93	0.68
1:A:926:MET:HG3	1:A:928:GLU:H	1.57	0.68
1:A:1034:ARG:HA	1:A:1034:ARG:NE	2.09	0.68
2:C:540:PHE:HB3	2:C:600:ILE:HD11	1.75	0.68
1:A:73:ARG:O	1:A:75:PRO:HD3	1.94	0.67
1:A:377:LEU:HD12	1:A:377:LEU:H	1.59	0.67
1:A:659:ASN:HD21	1:A:706:TYR:H	1.40	0.67
2:C:853:ASP:HB2	3:D:117:ILE:CD1	2.24	0.67
2:B:733:VAL:HG21	2:B:741:TYR:HD1	1.59	0.67
2:B:1051:ARG:HG2	2:B:1054:ARG:HH12	1.58	0.67
3:D:78:GLY:O	3:D:269:ILE:HD11	1.95	0.67
3:E:56:LEU:H	3:E:56:LEU:CD2	2.08	0.67
3:E:153:TYR:HD1	3:E:156:VAL:HG21	1.59	0.67
3:E:162:GLY:HA2	3:E:172:MET:CE	2.24	0.67
3:E:139:ASN:C	3:E:139:ASN:OD1	2.33	0.67
2:C:1072:ASP:O	2:C:1234:GLN:NE2	2.28	0.67
2:C:1042:TRP:CD1	2:C:1043:SER:HA	2.30	0.67
3:E:68:ILE:CD1	3:E:72:ILE:HD12	2.24	0.67
2:B:1289:PRO:HD2	3:D:20:ARG:CD	2.25	0.67
2:C:841:ASP:N	2:C:940:ARG:HH12	1.93	0.67
1:A:238:ASP:OD2	1:A:259:ARG:HG3	1.95	0.66
1:A:962:PHE:CG	1:A:963:TYR:N	2.64	0.66
2:C:1076:ILE:HG23	2:C:1166:VAL:HB	1.77	0.66
3:E:261:ARG:NH1	3:E:265:ARG:NH2	2.39	0.66
1:A:523:MET:HG3	1:A:524:HIS:H	1.59	0.66
1:A:203:THR:H	2:B:629:ARG:HG2	1.61	0.66
2:C:853:ASP:HB2	3:D:117:ILE:HG13	1.78	0.66
2:C:879:THR:O	2:C:883:ILE:HG12	1.94	0.66
3:D:239:VAL:HG12	3:D:250:ARG:HH12	1.61	0.66
2:B:954:GLN:NE2	3:D:240:VAL:HG13	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:178:LYS:O	3:D:178:LYS:HG3	1.96	0.66
2:C:414:LEU:HB2	2:C:1045:TYR:HE2	1.61	0.66
2:C:910:LEU:HD13	2:C:915:VAL:HG23	1.77	0.65
3:D:100:ASN:H	3:D:100:ASN:ND2	1.94	0.65
3:E:221:ARG:HH11	3:E:225:ARG:HD2	1.60	0.65
1:A:512:ALA:HB3	1:A:513:PRO:CA	2.16	0.65
2:C:902:ILE:HB	2:C:929:PHE:HB3	1.78	0.65
1:A:1039:GLY:O	1:A:1043:LEU:HB2	1.96	0.65
2:B:368:ALA:HA	3:D:83:ASN:HD22	1.61	0.65
3:E:247:ARG:HE	3:E:247:ARG:HA	1.62	0.65
3:E:69:GLU:OE1	3:E:70:ASP:N	2.30	0.65
3:E:12:LEU:O	3:E:14:GLN:NE2	2.30	0.65
3:E:56:LEU:HD23	3:E:56:LEU:N	2.11	0.65
2:B:956:ASP:OD2	3:D:266:THR:CG2	2.44	0.65
1:A:484:THR:HB	1:A:511:ILE:HG21	1.76	0.65
2:C:837:THR:HA	2:C:936:MET:HG3	1.77	0.65
3:D:85:ASN:C	3:D:85:ASN:HD22	2.00	0.65
2:B:1060:ARG:HH12	2:B:1292:GLU:HA	1.61	0.65
3:E:134:TYR:OH	3:E:286:THR:HG22	1.97	0.65
3:E:53:GLU:N	3:E:53:GLU:OE2	2.30	0.65
2:B:956:ASP:OD2	3:D:266:THR:HG23	1.96	0.64
2:C:309:TRP:CD1	2:C:1253:ARG:HB3	2.32	0.64
3:D:153:TYR:CA	3:D:156:VAL:CG1	2.72	0.64
2:C:523:THR:O	2:C:524:GLU:HB3	1.95	0.64
3:E:195:ASN:OD1	3:E:195:ASN:N	2.30	0.64
1:A:93:HIS:HE1	1:A:97:ARG:HH12	1.45	0.64
1:A:555:ASP:HA	1:A:583:ARG:HH22	1.61	0.64
3:D:144:ARG:HD2	3:D:144:ARG:O	1.98	0.64
3:E:69:GLU:C	3:E:69:GLU:OE1	2.35	0.64
1:A:559:ILE:HG22	1:A:613:ILE:HG12	1.79	0.64
1:A:963:TYR:HE2	1:A:978:LYS:CB	2.10	0.64
2:C:373:ASP:HB2	2:C:394:GLN:HG3	1.79	0.64
3:E:284:GLN:O	3:E:288:THR:HG22	1.96	0.64
2:B:269:GLU:HB3	2:B:292:ASN:HD22	1.61	0.64
2:B:274:MET:HG3	2:C:234:PRO:HD3	0.66	0.64
3:E:68:ILE:CD1	3:E:69:GLU:N	2.59	0.64
2:B:1106:PHE:HB3	2:B:1151:VAL:HG21	1.79	0.64
2:C:291:HIS:CD2	2:C:346:HIS:CD2	2.86	0.64
3:D:143:PRO:O	3:D:144:ARG:HB3	1.96	0.64
3:D:22:ASP:C	3:D:22:ASP:OD1	2.36	0.64
3:E:1:MET:HE1	3:E:121:PHE:HE2	1.56	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:VAL:HB	1:A:407:GLU:C	2.17	0.64
2:C:449:PHE:N	2:C:450:PRO:CD	2.61	0.64
3:D:82:GLN:HA	3:D:82:GLN:OE1	1.98	0.64
2:B:1273:ASN:OD1	3:D:79:ILE:HG21	1.89	0.64
2:B:271:THR:HG21	2:C:237:VAL:HG21	1.72	0.63
2:C:1042:TRP:HB3	2:C:1043:SER:HB2	1.79	0.63
3:E:137:LEU:HD23	3:E:138:GLY:N	2.13	0.63
1:A:470:LEU:HB3	1:A:497:ALA:HB1	1.81	0.63
2:C:440:ILE:HD11	2:C:770:CYS:HB2	1.80	0.63
2:C:878:SER:CB	2:C:903:ASN:CB	2.76	0.63
2:C:931:ASN:ND2	2:C:934:LEU:O	2.29	0.63
3:E:55:HIS:CD2	3:E:145:TYR:HE2	2.15	0.63
3:E:55:HIS:O	3:E:55:HIS:ND1	2.30	0.63
1:A:426:ARG:HG3	1:A:428:ILE:H	1.62	0.63
2:B:271:THR:HG23	2:C:237:VAL:CG2	2.01	0.63
2:B:279:SER:OG	2:C:1198:LYS:CE	2.46	0.63
2:B:924:ASP:HA	2:B:938:ASN:ND2	2.14	0.63
3:D:55:HIS:ND1	3:D:55:HIS:C	2.50	0.63
3:D:100:ASN:HD22	3:D:100:ASN:N	1.92	0.63
2:B:147:VAL:HG22	2:B:1315:MET:H	1.62	0.63
2:C:856:LEU:HD11	3:D:117:ILE:HD12	1.81	0.63
1:A:926:MET:HB3	1:A:931:GLY:H	1.64	0.63
2:C:528:ILE:CD1	2:C:758:ILE:HD12	2.25	0.63
3:D:41:GLU:OE1	3:D:41:GLU:N	2.30	0.63
2:B:954:GLN:NE2	3:D:240:VAL:CG1	2.61	0.63
2:B:1273:ASN:CB	3:D:194:VAL:HG11	2.28	0.63
3:D:242:ARG:HH11	3:D:242:ARG:CG	2.11	0.63
1:A:194:HIS:CD2	3:D:146:ARG:HH11	2.13	0.63
2:C:1153:ASP:HA	2:C:1156:ILE:HG22	1.81	0.63
3:E:234:ALA:O	3:E:263:ALA:HB2	1.98	0.63
1:A:76:LEU:C	1:A:78:TYR:H	2.00	0.62
3:E:12:LEU:O	3:E:13:GLU:HB3	1.98	0.62
2:B:368:ALA:CA	3:D:83:ASN:ND2	2.61	0.62
2:B:635:ILE:HG22	2:B:706:TYR:HB3	1.81	0.62
3:D:35:LEU:HD23	3:D:179:PHE:HB3	1.81	0.62
3:E:77:PHE:CE1	3:E:227:MET:HB2	2.34	0.62
1:A:846:ARG:HA	1:A:849:ILE:HD11	1.80	0.62
2:B:950:ASP:O	3:D:243:LYS:CE	2.46	0.62
2:C:148:GLN:HE21	2:C:379:LEU:HD11	1.63	0.62
1:A:904:PHE:HE2	1:A:906:PHE:CB	2.02	0.62
3:D:237:ALA:HB3	3:D:253:GLU:HG2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:845:ILE:O	1:A:849:ILE:HG12	1.99	0.62
2:B:838:GLU:O	2:B:935:GLN:HG3	2.00	0.62
2:C:853:ASP:HB2	3:D:117:ILE:HD11	1.80	0.62
2:B:388:GLN:OE1	2:C:499:ALA:CB	2.41	0.62
2:C:231:LEU:CB	2:C:249:SER:HB2	2.30	0.62
2:C:864:HIS:NE2	2:C:1030:ARG:CZ	2.62	0.62
2:B:271:THR:HG23	2:C:237:VAL:N	2.14	0.62
2:C:450:PRO:C	2:C:452:ASN:N	2.53	0.62
2:B:148:GLN:O	2:B:375:ARG:HD3	2.00	0.62
2:C:1037:ILE:HG22	2:C:1038:GLU:N	2.09	0.62
3:E:209:GLU:O	3:E:213:LEU:HB2	2.00	0.62
1:A:155:VAL:O	2:C:548:TYR:HE1	1.83	0.61
3:E:235:VAL:HG13	3:E:258:ASN:ND2	2.14	0.61
3:E:1:MET:O	3:E:2:LEU:HB2	2.00	0.61
3:E:42:ASN:CB	3:E:174:VAL:HB	2.29	0.61
1:A:648:VAL:CG2	1:A:649:LYS:H	2.13	0.61
2:C:112:THR:HG22	2:C:134:THR:HB	1.82	0.61
2:C:1042:TRP:CB	2:C:1043:SER:HA	2.30	0.61
1:A:460:VAL:HG11	1:A:1034:ARG:HD2	1.83	0.61
3:D:107:LEU:O	3:D:108:ASP:OD2	2.17	0.61
3:E:66:VAL:HG23	3:E:89:TYR:CD2	2.36	0.61
3:E:85:ASN:HD22	3:E:141:SER:HB3	1.65	0.61
2:C:1240:ARG:HD3	2:C:1258:VAL:HG21	1.81	0.61
3:D:21:ASN:O	3:D:22:ASP:CG	2.39	0.61
1:A:731:HIS:HB2	1:A:746:PHE:HB3	1.82	0.61
2:C:539:PHE:O	2:C:543:TRP:HB3	2.00	0.61
2:B:629:ARG:HD2	2:B:1034:GLN:O	2.01	0.61
2:C:853:ASP:HB2	3:D:117:ILE:CG1	2.31	0.61
2:B:935:GLN:HG2	2:B:940:ARG:NE	2.16	0.61
2:C:494:GLU:O	2:C:757:ILE:HA	2.00	0.61
3:D:148:ASP:N	3:D:148:ASP:OD1	2.34	0.61
3:E:40:THR:CG2	3:E:41:GLU:N	2.63	0.61
3:E:46:LYS:HD2	3:E:155:HIS:CE1	2.34	0.61
1:A:648:VAL:CG2	1:A:649:LYS:N	2.63	0.60
1:A:866:LEU:O	1:A:867:ALA:HB3	2.01	0.60
3:E:55:HIS:CD2	3:E:145:TYR:CZ	2.84	0.60
2:C:302:ARG:HG3	2:C:303:ASP:OD1	2.01	0.60
3:E:1:MET:HE3	3:E:121:PHE:CD2	2.36	0.60
3:E:40:THR:HG22	3:E:41:GLU:N	2.15	0.60
2:B:1288:ILE:HD12	3:D:20:ARG:HH22	1.66	0.60
2:C:853:ASP:O	3:D:117:ILE:HD11	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:659:ASN:ND2	1:A:706:TYR:H	1.97	0.60
2:C:540:PHE:O	2:C:548:TYR:HB2	2.00	0.60
2:B:1181:SER:O	2:B:1182:GLU:HB3	2.00	0.60
2:C:1288:ILE:HG13	2:C:1293:VAL:HG21	1.83	0.60
3:D:217:LYS:CE	3:D:290:TRP:CE3	2.85	0.60
2:C:397:LEU:CD1	3:E:265:ARG:HB3	2.31	0.60
3:D:37:TYR:HD1	3:D:177:ALA:HB2	1.66	0.60
3:E:85:ASN:ND2	3:E:141:SER:CB	2.63	0.60
1:A:379:VAL:HG13	1:A:791:ARG:HH21	1.67	0.60
1:A:393:LEU:HD13	1:A:748:GLY:HA3	1.83	0.60
1:A:561:LEU:HD22	1:A:587:MET:HB2	1.83	0.60
1:A:749:CYS:HA	1:A:782:ASN:HA	1.84	0.60
2:B:1214:GLU:HB2	2:B:1215:PRO:HD2	1.84	0.60
2:B:1273:ASN:HD21	3:D:79:ILE:HG21	1.67	0.60
3:E:85:ASN:HD21	3:E:141:SER:CB	2.14	0.60
2:B:1274:GLY:HA2	3:D:191:ARG:HG3	1.83	0.60
3:E:209:GLU:HG3	3:E:210:GLY:H	1.66	0.60
1:A:717:THR:HG21	1:A:1020:SER:CB	2.31	0.60
2:C:112:THR:HG22	2:C:134:THR:CB	2.32	0.60
3:D:242:ARG:HH11	3:D:242:ARG:HG2	1.66	0.60
2:B:614:ARG:O	2:B:633:THR:HG22	2.02	0.59
1:A:49:HIS:HB3	1:A:76:LEU:HD11	1.83	0.59
1:A:796:PHE:O	1:A:874:LEU:HD12	2.01	0.59
2:B:1273:ASN:HD22	3:D:191:ARG:CA	2.01	0.59
2:C:230:ASP:HB3	2:C:985:ARG:HE	1.67	0.59
2:C:522:PRO:HG3	2:C:636:PRO:HB2	1.84	0.59
1:A:566:GLU:OE2	1:A:569:VAL:HG12	2.01	0.59
1:A:597:ARG:HG3	1:A:597:ARG:NH1	2.17	0.59
2:B:1273:ASN:HD21	3:D:191:ARG:CA	2.08	0.59
3:D:224:PHE:O	3:D:228:LEU:HB2	2.02	0.59
1:A:42:PHE:HA	1:A:49:HIS:HA	1.85	0.59
1:A:96:MET:O	1:A:99:VAL:HG12	2.03	0.59
2:B:547:GLU:HB2	2:B:597:ALA:HB2	1.83	0.59
2:C:1042:TRP:HB3	2:C:1043:SER:CA	2.32	0.59
2:B:1079:LEU:HD12	2:B:1090:PRO:HB3	1.83	0.59
3:D:5:PRO:O	3:D:6:THR:CB	2.50	0.59
3:D:47:LYS:HG3	3:D:48:THR:N	2.18	0.59
1:A:880:VAL:HB	1:A:899:VAL:HG12	1.83	0.59
2:C:448:TYR:HA	2:C:768:CYS:SG	2.43	0.59
1:A:560:LEU:HD23	1:A:614:ILE:HB	1.85	0.59
2:B:954:GLN:HG2	3:D:240:VAL:CG1	2.29	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:838:GLU:CB	2:C:934:LEU:HB2	2.33	0.59
3:E:67:TYR:HB3	3:E:70:ASP:HB3	1.85	0.59
3:E:262:THR:O	3:E:263:ALA:C	2.41	0.59
1:A:35:GLY:H	1:A:38:TYR:HE1	1.51	0.59
2:C:1045:TYR:O	2:C:1046:PHE:CD1	2.56	0.59
3:D:153:TYR:C	3:D:156:VAL:HG12	2.22	0.59
1:A:159:ILE:CD1	2:B:1333:ALA:OXT	2.51	0.59
2:B:338:ARG:NH2	2:C:1002:LEU:HD21	2.18	0.59
2:C:449:PHE:H	2:C:450:PRO:HD3	1.68	0.58
2:C:1054:ARG:HG2	2:C:1054:ARG:HH11	1.68	0.58
3:E:1:MET:CE	3:E:121:PHE:CD2	2.85	0.58
3:E:153:TYR:CD1	3:E:156:VAL:HG21	2.37	0.58
3:E:68:ILE:CD1	3:E:72:ILE:CD1	2.77	0.58
3:E:85:ASN:CG	3:E:85:ASN:O	2.41	0.58
1:A:569:VAL:HG22	1:A:584:ILE:HG22	1.85	0.58
2:B:459:ALA:HB2	2:B:679:CYS:HB3	1.85	0.58
3:D:217:LYS:HE2	3:D:290:TRP:CE3	2.38	0.58
1:A:70:PRO:HA	1:A:73:ARG:HB3	1.85	0.58
3:D:77:PHE:CZ	3:D:227:MET:HB2	2.39	0.58
1:A:820:VAL:HG12	1:A:821:ARG:H	1.69	0.58
2:B:191:GLY:HA2	2:B:193:THR:N	2.19	0.58
1:A:49:HIS:NE2	1:A:172:PHE:CD1	2.63	0.58
1:A:407:GLU:OE1	1:A:1034:ARG:HB3	2.04	0.58
2:B:205:ASN:HB2	2:B:1239:ALA:HB1	1.85	0.58
2:C:469:ARG:HH12	2:C:498:ILE:HD13	1.69	0.58
3:E:113:ASN:O	3:E:114:SER:OG	2.16	0.58
1:A:730:ILE:HG22	1:A:731:HIS:N	2.18	0.58
2:C:356:SER:O	2:C:360:ILE:HG12	2.04	0.58
3:D:217:LYS:CE	3:D:290:TRP:CZ3	2.87	0.58
1:A:934:THR:HG23	1:A:935:PRO:HD3	1.86	0.58
2:B:179:LYS:HG3	2:B:181:ARG:HE	1.68	0.58
2:B:835:TYR:CZ	2:B:925:VAL:HG21	2.39	0.58
1:A:228:ILE:CD1	2:B:563:ALA:HB1	2.32	0.57
2:B:924:ASP:HA	2:B:938:ASN:HD21	1.68	0.57
3:E:205:LEU:O	3:E:205:LEU:CD1	2.39	0.57
1:A:27:LYS:HB3	1:A:28:PRO:CD	2.31	0.57
2:B:817:ASP:HA	2:B:983:ILE:HG21	1.86	0.57
2:B:935:GLN:HG2	2:B:940:ARG:CZ	2.34	0.57
2:C:297:ASN:HD22	2:C:298:PRO:HD2	1.68	0.57
3:D:85:ASN:C	3:D:85:ASN:ND2	2.55	0.57
2:C:878:SER:CB	2:C:903:ASN:HB2	2.23	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1072:ASP:H	2:C:1234:GLN:NE2	2.02	0.57
2:B:1274:GLY:HA3	3:D:191:ARG:HG3	1.87	0.57
2:C:741:TYR:OH	2:C:1022:ILE:HD11	2.05	0.57
2:C:1272:ARG:HD2	3:E:247:ARG:HH22	1.69	0.57
2:B:1242:MET:HG3	2:B:1245:ILE:HD11	1.87	0.57
2:B:143:VAL:HG12	2:B:1316:ALA:HB1	1.86	0.57
2:C:874:ILE:HG21	2:C:897:TYR:HD1	1.70	0.57
3:D:144:ARG:O	3:D:144:ARG:CD	2.52	0.57
2:C:543:TRP:HD1	2:C:544:TYR:HD1	1.53	0.57
2:B:137:ILE:HD12	2:C:759:ASP:OD1	2.04	0.56
2:C:129:ALA:O	2:C:130:LEU:HB2	2.03	0.56
2:C:385:ILE:O	2:C:386:SER:HB3	2.04	0.56
2:C:565:GLU:CG	2:C:566:PHE:N	2.66	0.56
2:C:1079:LEU:HD23	2:C:1081:ASP:OD2	2.05	0.56
2:B:817:ASP:HA	2:B:983:ILE:CG2	2.35	0.56
2:B:956:ASP:OD1	3:D:266:THR:CB	2.52	0.56
2:B:1288:ILE:CD1	3:D:20:ARG:NH2	2.66	0.56
2:B:148:GLN:O	2:B:150:LEU:N	2.39	0.56
2:B:902:ILE:HD11	2:B:929:PHE:HE1	1.70	0.56
2:B:956:ASP:CG	3:D:266:THR:CG2	2.73	0.56
2:B:1263:TYR:CD1	2:B:1295:HIS:CD2	2.93	0.56
2:C:841:ASP:CG	2:C:842:ASP:N	2.59	0.56
2:C:1033:ASP:O	2:C:1034:GLN:HB2	2.06	0.56
2:C:1322:PRO:O	2:C:1323:ASP:CB	2.53	0.56
2:B:350:ILE:HG22	2:B:351:ASP:N	2.14	0.56
2:C:1072:ASP:N	2:C:1234:GLN:NE2	2.53	0.56
3:E:53:GLU:HB2	3:E:145:TYR:HE1	1.69	0.56
2:B:1273:ASN:ND2	3:D:79:ILE:HG21	2.21	0.56
2:C:1042:TRP:HB3	2:C:1043:SER:CB	2.35	0.56
2:C:141:LEU:HD23	2:C:141:LEU:H	1.71	0.56
2:C:1250:GLU:OE1	2:C:1250:GLU:HA	2.05	0.56
3:D:239:VAL:HG23	3:D:263:ALA:HB1	1.87	0.56
3:E:44:LEU:HD13	3:E:172:MET:O	2.05	0.56
1:A:238:ASP:HB2	1:A:258:GLN:HB2	1.88	0.56
3:E:108:ASP:OD2	3:E:108:ASP:N	2.30	0.56
3:E:235:VAL:CG1	3:E:258:ASN:HA	2.35	0.56
1:A:554:PRO:HB3	1:A:580:SER:HG	1.68	0.56
1:A:686:TYR:HD2	1:A:686:TYR:O	1.89	0.56
2:B:1289:PRO:CD	3:D:20:ARG:HD2	2.36	0.56
2:C:261:ASP:O	2:C:1054:ARG:NH1	2.39	0.56
2:C:291:HIS:HD2	2:C:346:HIS:HD2	1.49	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:142:THR:HG23	3:E:143:PRO:HD2	1.87	0.56
1:A:484:THR:O	1:A:485:MET:HG3	2.05	0.56
1:A:986:ARG:HB3	1:A:994:PRO:CB	2.29	0.56
2:B:709:MET:HA	2:B:712:PHE:HD2	1.70	0.56
2:C:407:HIS:CD2	2:C:1047:LEU:HA	2.40	0.56
2:C:833:ARG:HB2	2:C:942:HIS:HB2	1.88	0.56
2:C:1288:ILE:HD13	2:C:1288:ILE:H	1.69	0.56
2:C:1323:ASP:CG	2:C:1324:ASP:H	2.08	0.56
1:A:22:ILE:HG12	1:A:25:ILE:HD11	1.86	0.56
1:A:407:GLU:HG3	1:A:829:MET:O	2.05	0.55
1:A:919:TYR:HB2	1:A:955:ASN:HB3	1.86	0.55
2:B:494:GLU:HG2	2:B:577:GLN:HG3	1.87	0.55
3:E:150:ILE:O	3:E:150:ILE:CG2	2.54	0.55
3:E:81:ALA:H	3:E:275:ARG:HH21	1.54	0.55
2:B:148:GLN:C	2:B:150:LEU:H	2.09	0.55
2:B:709:MET:HA	2:B:712:PHE:CD2	2.42	0.55
3:E:49:ILE:CG2	3:E:50:PRO:CD	2.84	0.55
3:E:85:ASN:C	3:E:85:ASN:OD1	2.44	0.55
1:A:892:GLN:C	1:A:894:LYS:H	2.09	0.55
2:B:895:VAL:HG22	2:B:915:VAL:HG22	1.88	0.55
2:C:185:ALA:HB3	2:C:277:THR:O	2.07	0.55
3:E:209:GLU:O	3:E:213:LEU:CB	2.55	0.55
3:E:284:GLN:O	3:E:288:THR:CG2	2.54	0.55
2:C:337:VAL:CG2	3:E:187:ILE:CD1	2.62	0.55
2:C:734:ILE:HG23	2:C:1017:ALA:HB1	1.88	0.55
2:C:864:HIS:CE1	2:C:1030:ARG:HH21	2.18	0.55
2:B:1274:GLY:HA3	3:D:191:ARG:CG	2.36	0.55
1:A:849:ILE:HD12	1:A:872:VAL:HG12	1.89	0.55
2:B:1048:ASP:HB3	2:B:1051:ARG:HB2	1.87	0.55
2:B:144:ASN:HB2	2:B:1318:GLU:HA	1.88	0.55
2:B:926:VAL:HG12	2:B:926:VAL:O	2.07	0.55
1:A:63:SER:HB3	1:A:123:SER:HA	1.87	0.55
2:B:612:PHE:CZ	2:B:1331:ARG:HD2	2.42	0.55
2:C:1074:VAL:HG12	2:C:1171:ILE:HG21	1.88	0.55
3:E:1:MET:O	3:E:121:PHE:O	2.24	0.55
1:A:967:ILE:HG23	1:A:968:ILE:H	1.72	0.54
2:B:604:MET:C	2:B:606:LEU:H	2.10	0.54
2:B:960:THR:HG23	2:B:965:ARG:NH1	2.19	0.54
2:B:147:VAL:HG12	2:B:379:LEU:HD22	1.89	0.54
3:E:107:LEU:HD23	3:E:122:TYR:HE1	1.70	0.54
2:C:407:HIS:CE1	2:C:1047:LEU:HD12	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:1:MET:O	3:E:2:LEU:CB	2.55	0.54
3:E:285:LEU:O	3:E:288:THR:HG23	2.08	0.54
1:A:484:THR:CB	1:A:511:ILE:HG21	2.37	0.54
2:C:390:HIS:O	2:C:1317:VAL:HG23	2.08	0.54
1:A:146:PRO:O	1:A:147:GLN:HB3	2.06	0.54
1:A:755:ALA:N	1:A:756:PRO:HD2	2.22	0.54
1:A:963:TYR:CE2	1:A:978:LYS:HB3	2.41	0.54
2:C:1181:SER:O	2:C:1182:GLU:HB3	2.07	0.54
2:C:1234:GLN:HB2	2:C:1235:PRO:C	2.28	0.54
3:D:253:GLU:CD	3:D:254:TYR:CD2	2.76	0.54
3:D:290:TRP:HE3	3:D:290:TRP:C	2.11	0.54
3:E:253:GLU:O	3:E:254:TYR:CD1	2.61	0.54
1:A:409:MET:HG2	1:A:465:LEU:HD22	1.90	0.54
2:B:255:LEU:HD12	2:B:1062:ILE:HG21	1.89	0.54
2:B:862:ARG:HH12	2:B:948:ILE:HD13	1.73	0.54
3:E:238:ASN:O	3:E:253:GLU:HB2	2.06	0.54
2:C:793:TYR:OH	2:C:1323:ASP:O	2.15	0.54
3:D:25:ASN:C	3:D:25:ASN:OD1	2.45	0.54
3:E:229:PHE:CE1	3:E:252:LEU:CD1	2.90	0.54
1:A:383:THR:HG21	1:A:805:TYR:HB3	1.88	0.54
1:A:194:HIS:CD2	3:D:146:ARG:HH12	2.19	0.54
1:A:600:VAL:HG12	1:A:601:PRO:HA	1.88	0.54
2:B:1111:ALA:HB3	2:B:1116:ARG:HD2	1.90	0.54
3:E:14:GLN:N	3:E:14:GLN:CD	2.61	0.54
3:E:262:THR:HG22	3:E:263:ALA:N	2.22	0.54
1:A:69:HIS:CD2	1:A:71:LEU:H	2.27	0.53
1:A:208:HIS:HB3	1:A:260:LEU:HD23	1.90	0.53
2:B:833:ARG:HG2	2:B:922:TYR:OH	2.07	0.53
2:C:372:ALA:HA	2:C:398:ARG:HD3	1.90	0.53
2:C:1037:ILE:HD13	2:C:1040:PHE:HE1	1.73	0.53
2:C:1126:MET:HG3	2:C:1127:ALA:H	1.73	0.53
1:A:1034:ARG:NH2	1:A:1035:LEU:HB2	2.23	0.53
2:C:547:GLU:HG3	2:C:597:ALA:HA	1.91	0.53
2:C:838:GLU:HA	2:C:940:ARG:CZ	2.38	0.53
2:C:892:VAL:HG13	2:C:894:VAL:H	1.73	0.53
2:B:639:ASN:HB3	2:B:641:ARG:HG3	1.89	0.53
2:B:953:ASP:O	3:D:241:ASN:OD1	2.26	0.53
2:B:1076:ILE:HB	2:B:1166:VAL:HG23	1.91	0.53
3:E:142:THR:HG22	3:E:144:ARG:H	1.73	0.53
1:A:495:LEU:HA	1:A:503:ILE:HD13	1.91	0.53
2:C:469:ARG:HE	2:C:469:ARG:HA	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:178:LYS:O	3:D:178:LYS:CG	2.56	0.53
3:D:239:VAL:HG23	3:D:263:ALA:CB	2.38	0.53
3:E:76:LEU:HD12	3:E:76:LEU:H	1.73	0.53
2:C:148:GLN:NE2	2:C:379:LEU:HD11	2.24	0.53
1:A:38:TYR:HA	1:A:53:LEU:HA	1.89	0.53
1:A:406:VAL:HG21	1:A:826:PHE:CD1	2.44	0.53
1:A:636:VAL:HG22	1:A:648:VAL:HG21	1.90	0.53
2:C:1180:PRO:HB3	2:C:1209:GLY:HA2	1.89	0.53
1:A:78:TYR:N	1:A:78:TYR:CD2	2.76	0.53
2:B:884:ALA:O	2:B:888:GLN:HG2	2.08	0.53
2:C:384:MET:HA	2:C:708:THR:HG21	1.91	0.53
2:C:822:MET:HG3	2:C:1044:ARG:HD2	1.90	0.53
3:D:115:GLU:OE2	3:D:115:GLU:N	2.30	0.53
3:E:214:ARG:O	3:E:218:THR:CG2	2.57	0.53
1:A:195:ILE:O	1:A:199:MET:HB2	2.08	0.53
2:C:385:ILE:O	2:C:386:SER:CB	2.57	0.53
1:A:23:ARG:HH21	1:A:27:LYS:HB3	1.73	0.53
1:A:228:ILE:HD12	2:B:563:ALA:CB	2.38	0.53
2:B:234:PRO:HD2	2:B:242:GLU:CB	2.39	0.53
2:B:1289:PRO:CD	3:D:20:ARG:CD	2.87	0.53
2:C:565:GLU:CG	2:C:566:PHE:H	2.18	0.53
2:B:232:LEU:HD22	2:B:974:LEU:HD21	1.91	0.53
2:B:1044:ARG:CZ	3:D:266:THR:HG23	2.37	0.53
3:D:111:ILE:O	3:D:111:ILE:HG23	2.07	0.53
3:D:189:LEU:HB3	3:D:230:ILE:HD11	1.91	0.53
3:D:242:ARG:HG2	3:D:242:ARG:NH1	2.23	0.53
3:E:229:PHE:HE1	3:E:252:LEU:HD12	1.73	0.53
1:A:28:PRO:C	1:A:30:THR:H	2.11	0.52
1:A:282:GLU:HB2	1:A:363:ASN:HB2	1.90	0.52
1:A:894:LYS:C	1:A:896:ASN:H	2.12	0.52
2:B:180:LEU:HB3	2:B:195:ASN:HD21	1.74	0.52
2:C:1042:TRP:CB	2:C:1043:SER:CA	2.87	0.52
1:A:204:LEU:HA	1:A:264:SER:O	2.09	0.52
2:B:1103:HIS:H	2:B:1103:HIS:CD2	2.26	0.52
2:B:1118:THR:HG22	2:B:1129:PRO:HA	1.90	0.52
2:C:1293:VAL:O	2:C:1294:ASP:HB2	2.08	0.52
1:A:213:TRP:O	1:A:215:VAL:N	2.41	0.52
2:B:142:ASP:HB3	2:B:1318:GLU:HG2	1.91	0.52
2:C:154:PHE:HA	2:C:262:ASN:HD22	1.74	0.52
2:C:524:GLU:OE1	2:C:758:ILE:HG21	2.09	0.52
2:C:1027:THR:HG22	3:D:102:SER:OG	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:980:ARG:HH22	2:B:1011:SER:HA	1.74	0.52
2:C:828:ASP:O	2:C:948:ILE:HA	2.09	0.52
3:D:172:MET:CE	3:D:175:LYS:HG3	2.33	0.52
1:A:55:GLY:N	1:A:58:GLN:HG2	2.20	0.52
2:B:281:VAL:CG1	2:B:302:ARG:HD2	2.40	0.52
2:C:1264:GLU:HA	2:C:1297:SER:HA	1.91	0.52
1:A:406:VAL:CG2	1:A:826:PHE:CD1	2.92	0.52
2:C:306:GLN:HE21	2:C:306:GLN:N	2.08	0.52
2:C:1273:ASN:O	3:E:183:GLU:CD	2.45	0.52
3:D:156:VAL:HG23	3:D:228:LEU:HD23	1.88	0.52
1:A:450:SER:H	1:A:718:ALA:HB1	1.74	0.52
1:A:766:CYS:HB3	1:A:786:ARG:O	2.10	0.52
2:B:546:VAL:HG13	2:B:547:GLU:HG3	1.92	0.52
2:B:1175:ALA:HB2	2:B:1204:LEU:HB2	1.91	0.52
2:C:112:THR:HG22	2:C:134:THR:OG1	2.10	0.52
3:E:74:GLN:O	3:E:78:GLY:HA3	2.10	0.52
1:A:261:ILE:HD11	1:A:326:LEU:HB3	1.91	0.52
1:A:856:THR:H	1:A:916:ASN:HB3	1.74	0.52
2:B:837:THR:O	2:B:838:GLU:HB2	2.09	0.52
3:E:240:VAL:O	3:E:251:VAL:HG22	2.09	0.52
2:B:1087:ASP:OD2	2:B:1235:PRO:HB2	2.09	0.52
3:D:217:LYS:HE2	3:D:290:TRP:CZ3	2.45	0.52
3:E:107:LEU:HD23	3:E:122:TYR:OH	2.09	0.52
1:A:613:ILE:HG13	1:A:643:ALA:HB2	1.93	0.51
1:A:963:TYR:CE2	1:A:967:ILE:HG21	2.45	0.51
2:B:405:HIS:CD2	2:B:623:ASN:HD21	2.27	0.51
3:E:290:TRP:HD1	3:E:291:ASN:HB3	1.75	0.51
1:A:26:THR:HG23	1:A:27:LYS:H	1.76	0.51
1:A:388:VAL:HG22	1:A:389:ALA:H	1.75	0.51
1:A:495:LEU:HD13	1:A:575:PHE:HA	1.90	0.51
2:B:891:HIS:HD2	3:D:240:VAL:CB	2.22	0.51
2:B:1273:ASN:ND2	3:D:79:ILE:CG2	2.73	0.51
2:C:1077:MET:SD	2:C:1079:LEU:HD12	2.50	0.51
1:A:27:LYS:CB	1:A:28:PRO:HD3	2.34	0.51
1:A:756:PRO:HB3	1:A:809:GLN:HA	1.92	0.51
1:A:954:THR:HB	1:A:1056:VAL:HG23	1.92	0.51
2:C:1042:TRP:HA	2:C:1042:TRP:CE3	2.45	0.51
2:C:1081:ASP:O	2:C:1082:ASP:HB2	2.11	0.51
2:C:443:VAL:HG22	2:C:444:SER:N	2.20	0.51
3:D:44:LEU:HD11	3:D:154:ALA:CA	2.31	0.51
3:E:53:GLU:HB2	3:E:145:TYR:CE1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:925:ILE:HA	1:A:937:ARG:HH22	1.75	0.51
1:A:962:PHE:HB3	1:A:1049:TYR:CD2	2.44	0.51
1:A:986:ARG:CB	1:A:994:PRO:HB3	2.30	0.51
2:B:442:PRO:HG3	2:B:475:ILE:CB	2.29	0.51
2:B:528:ILE:HG12	2:B:758:ILE:HG21	1.91	0.51
2:B:649:ALA:HB2	2:B:695:ALA:HB2	1.91	0.51
3:E:1:MET:HE2	3:E:123:ASP:HA	1.92	0.51
2:B:685:ARG:HH11	2:B:685:ARG:HA	1.75	0.51
2:C:414:LEU:HB2	2:C:1045:TYR:CE2	2.42	0.51
2:C:1085:ASP:HB3	2:C:1243:ARG:HH22	1.76	0.51
2:C:1322:PRO:O	2:C:1323:ASP:CG	2.48	0.51
3:E:82:GLN:HG2	3:E:83:ASN:OD1	2.10	0.51
3:E:283:LEU:O	3:E:287:PHE:HB2	2.11	0.51
3:E:290:TRP:CD1	3:E:290:TRP:C	2.84	0.51
1:A:1034:ARG:HA	1:A:1034:ARG:HE	1.74	0.51
3:D:214:ARG:O	3:D:218:THR:CG2	2.51	0.51
1:A:62:PHE:HZ	1:A:171:ILE:HD12	1.76	0.51
1:A:422:ASP:HB3	1:A:677:LEU:HD12	1.91	0.51
2:C:815:LEU:N	2:C:816:PRO:HD2	2.26	0.51
2:C:838:GLU:O	2:C:940:ARG:NH1	2.44	0.51
3:E:262:THR:O	3:E:263:ALA:HB3	2.11	0.51
3:E:289:ARG:O	3:E:289:ARG:CD	2.35	0.51
3:E:83:ASN:OD1	3:E:83:ASN:N	2.43	0.51
1:A:925:ILE:HA	1:A:937:ARG:NH2	2.26	0.51
1:A:955:ASN:HD21	1:A:1055:LEU:HB3	1.75	0.51
2:B:847:ILE:HD11	2:B:911:ARG:HE	1.76	0.51
2:C:1131:PRO:HA	2:C:1134:ARG:NH1	2.26	0.51
3:E:12:LEU:HD23	3:E:15:PHE:CZ	2.46	0.51
1:A:561:LEU:HB3	1:A:615:CYS:HA	1.92	0.50
2:C:840:ASP:O	2:C:841:ASP:OD1	2.28	0.50
2:C:855:TYR:HB2	2:C:918:VAL:HG11	1.92	0.50
3:D:21:ASN:O	3:D:24:THR:O	2.29	0.50
3:D:153:TYR:C	3:D:156:VAL:CG1	2.79	0.50
3:D:290:TRP:CE3	3:D:290:TRP:C	2.85	0.50
3:E:236:ALA:O	3:E:263:ALA:HA	2.10	0.50
1:A:69:HIS:HD2	1:A:71:LEU:H	1.59	0.50
1:A:560:LEU:O	1:A:586:GLY:HA2	2.11	0.50
2:B:1023:ARG:HB2	2:B:1024:PRO:CD	2.35	0.50
3:D:289:ARG:HA	3:D:289:ARG:NE	2.24	0.50
2:B:910:LEU:HD23	2:B:915:VAL:HG13	1.92	0.50
2:C:408:ILE:O	2:C:412:LEU:HB2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:250:ARG:HB3	3:D:250:ARG:HH11	1.76	0.50
3:E:62:VAL:HG23	3:E:63:PRO:HD2	1.93	0.50
3:E:191:ARG:NH1	3:E:191:ARG:CG	2.42	0.50
1:A:13:VAL:HG22	1:A:213:TRP:CD1	2.47	0.50
2:B:272:THR:HG22	2:B:289:THR:HB	1.93	0.50
2:B:956:ASP:OD1	3:D:266:THR:HG21	2.11	0.50
2:C:841:ASP:H	2:C:940:ARG:HH12	1.58	0.50
3:E:160:LEU:HD11	3:E:229:PHE:CB	2.36	0.50
1:A:643:ALA:HB3	1:A:646:ALA:HB2	1.93	0.50
2:B:134:THR:CG2	2:C:472:GLU:CD	2.79	0.50
2:B:959:GLN:HG3	2:B:964:VAL:HG11	1.94	0.50
1:A:180:ASN:CG	1:A:222:ARG:HH22	2.15	0.50
1:A:437:GLN:HG3	1:A:655:GLU:OE1	2.12	0.50
3:D:107:LEU:HD23	3:D:122:TYR:CE1	2.47	0.50
3:E:41:GLU:O	3:E:41:GLU:OE1	2.30	0.50
1:A:68:GLY:O	1:A:69:HIS:O	2.30	0.50
1:A:265:SER:HB2	1:A:269:VAL:HG21	1.93	0.50
1:A:536:TYR:CG	1:A:572:LEU:HD11	2.46	0.50
2:C:931:ASN:HB2	2:C:936:MET:SD	2.52	0.50
2:C:1174:THR:HG23	2:C:1203:HIS:HB3	1.93	0.50
3:D:291:ASN:OD1	3:D:291:ASN:C	2.50	0.50
3:E:10:THR:HG23	3:E:17:PHE:HZ	1.77	0.50
1:A:308:ALA:HB1	1:A:313:ARG:N	2.26	0.50
1:A:959:TYR:HB2	1:A:1051:PRO:HD2	1.93	0.50
2:B:280:THR:HG23	2:B:281:VAL:H	1.76	0.50
2:B:871:PRO:HG3	2:B:894:VAL:HG13	1.93	0.50
2:C:1121:HIS:CD2	2:C:1135:PRO:HD2	2.47	0.50
3:D:15:PHE:N	3:D:15:PHE:CD1	2.80	0.50
3:E:69:GLU:O	3:E:69:GLU:OE2	2.30	0.50
1:A:304:TYR:HD1	1:A:364:TYR:HE2	1.60	0.49
1:A:487:GLN:HG3	1:A:488:GLY:N	2.27	0.49
1:A:505:PHE:CE1	1:A:511:ILE:HG22	2.47	0.49
2:B:772:TYR:HB3	2:B:773:PRO:HD2	1.95	0.49
2:C:204:VAL:CG2	2:C:1242:MET:HG3	2.42	0.49
2:B:1080:THR:HA	2:B:1228:ARG:H	1.77	0.49
3:D:153:TYR:HA	3:D:156:VAL:HG11	1.86	0.49
3:D:153:TYR:CE2	3:D:258:ASN:ND2	2.80	0.49
3:E:13:GLU:CD	3:E:13:GLU:C	2.71	0.49
1:A:967:ILE:HG23	1:A:968:ILE:N	2.26	0.49
1:A:512:ALA:CB	1:A:513:PRO:CA	2.80	0.49
2:B:360:ILE:HD11	2:B:1057:VAL:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:363:ARG:CZ	3:D:80:SER:CB	2.84	0.49
2:B:935:GLN:HA	2:B:940:ARG:HD3	1.93	0.49
2:C:528:ILE:O	2:C:528:ILE:CG2	2.60	0.49
3:D:172:MET:HG3	3:D:173:PRO:CD	2.42	0.49
3:E:20:ARG:HD2	3:E:25:ASN:HB3	1.94	0.49
1:A:318:ARG:CZ	3:D:43:GLU:HG2	2.43	0.49
2:B:1149:LYS:HG3	2:B:1195:THR:HG21	1.95	0.49
2:C:926:VAL:CG2	2:C:938:ASN:HB2	2.42	0.49
2:B:193:THR:HG23	2:B:297:ASN:H	1.76	0.49
2:C:1272:ARG:HD2	3:E:247:ARG:NH2	2.28	0.49
3:E:84:VAL:HG23	3:E:85:ASN:N	2.28	0.49
3:E:85:ASN:O	3:E:85:ASN:OD1	2.30	0.49
3:D:21:ASN:O	3:D:22:ASP:OD1	2.31	0.49
3:D:181:SER:HB2	3:D:185:SER:OG	2.13	0.49
2:C:200:GLY:HA2	2:C:1246:VAL:HG22	1.94	0.49
3:E:53:GLU:OE2	3:E:53:GLU:O	2.30	0.49
3:E:92:ARG:O	3:E:92:ARG:HD3	2.12	0.49
2:C:838:GLU:HA	2:C:940:ARG:NE	2.28	0.49
3:D:164:ASP:HA	3:D:167:ARG:HG2	1.94	0.49
3:E:66:VAL:HG13	3:E:111:ILE:CG2	2.42	0.49
1:A:204:LEU:HD13	1:A:221:TYR:HB2	1.95	0.49
1:A:516:GLU:OE1	1:A:516:GLU:HA	2.12	0.49
2:B:389:PHE:CE1	2:B:1319:ARG:HG2	2.48	0.49
2:B:529:LYS:HA	2:B:532:ILE:HG22	1.94	0.49
3:E:12:LEU:HG	3:E:14:GLN:HG2	1.95	0.49
2:B:424:GLY:O	2:B:428:GLN:HB2	2.13	0.48
2:C:231:LEU:HB3	2:C:249:SER:HB2	1.93	0.48
2:C:302:ARG:HD2	2:C:315:THR:HG22	1.95	0.48
3:D:255:ILE:O	3:D:255:ILE:HG13	2.13	0.48
3:E:72:ILE:O	3:E:76:LEU:CD1	2.61	0.48
3:E:139:ASN:OD1	3:E:139:ASN:O	2.30	0.48
1:A:857:GLN:HE22	1:A:917:SER:HA	1.78	0.48
2:B:235:ILE:HG23	2:B:978:GLN:HG2	1.93	0.48
2:C:449:PHE:HE2	2:C:463:VAL:HG22	1.78	0.48
3:E:13:GLU:O	3:E:13:GLU:OE1	2.30	0.48
3:E:38:GLU:HB3	3:E:176:ARG:HB3	1.95	0.48
1:A:724:MET:SD	1:A:725:PRO:HD3	2.53	0.48
1:A:1037:SER:O	1:A:1039:GLY:N	2.46	0.48
2:B:1206:PHE:HE1	2:B:1232:PRO:HG3	1.79	0.48
2:C:841:ASP:O	2:C:842:ASP:CB	2.61	0.48
2:C:1027:THR:CG2	3:D:102:SER:OG	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:121:PHE:N	3:D:121:PHE:CD1	2.82	0.48
3:D:185:SER:O	3:D:188:SER:N	2.43	0.48
1:A:271:ARG:HG3	1:A:316:TYR:OH	2.12	0.48
2:B:837:THR:O	2:B:838:GLU:CB	2.61	0.48
2:C:268:GLY:O	2:C:269:GLU:HB2	2.11	0.48
1:A:562:GLY:O	1:A:588:GLY:HA3	2.14	0.48
1:A:797:ARG:HH12	1:A:871:VAL:HG11	1.77	0.48
2:B:368:ALA:C	3:D:83:ASN:HB2	2.33	0.48
3:D:149:MET:CE	3:D:260:MET:HE2	2.39	0.48
1:A:159:ILE:HD12	2:B:1333:ALA:OXT	2.14	0.48
2:B:147:VAL:HG22	2:B:1315:MET:N	2.28	0.48
2:B:204:VAL:CG2	2:B:1242:MET:HG2	2.44	0.48
2:B:1273:ASN:CG	3:D:79:ILE:HG21	2.32	0.48
2:C:860:ARG:O	2:C:864:HIS:HB2	2.14	0.48
2:C:1037:ILE:CG2	2:C:1038:GLU:H	2.09	0.48
3:E:122:TYR:N	3:E:122:TYR:CD1	2.82	0.48
2:C:1144:ARG:HD2	2:C:1194:MET:HA	1.96	0.48
3:D:166:GLU:OE2	3:D:166:GLU:HA	2.13	0.48
3:E:12:LEU:HG	3:E:14:GLN:NE2	2.18	0.48
3:E:33:GLN:C	3:E:35:LEU:H	2.17	0.48
3:E:196:TRP:HH2	3:E:226:MET:HG2	1.79	0.48
1:A:51:LEU:O	1:A:171:ILE:HG12	2.13	0.48
2:B:1247:ASN:HD22	2:B:1247:ASN:H	1.61	0.48
3:D:60:ARG:O	3:D:62:VAL:HG23	2.14	0.48
3:E:1:MET:SD	3:E:121:PHE:CZ	3.06	0.48
3:E:5:PRO:HB2	3:E:8:GLY:O	2.14	0.48
3:E:191:ARG:HD2	3:E:191:ARG:HA	1.60	0.48
1:A:28:PRO:C	1:A:30:THR:N	2.67	0.48
1:A:133:LEU:HD21	2:C:545:PRO:HG3	1.96	0.48
1:A:853:GLU:CD	1:A:854:ASN:H	2.17	0.48
1:A:866:LEU:O	1:A:867:ALA:CB	2.62	0.48
3:D:190:SER:O	3:D:194:VAL:HG23	2.14	0.47
3:E:192:ASP:OD1	3:E:192:ASP:O	2.31	0.47
1:A:254:ASP:O	1:A:255:ARG:HB2	2.13	0.47
2:C:109:LYS:HZ2	2:C:109:LYS:HB3	1.78	0.47
2:C:242:GLU:O	2:C:1200:LYS:HG2	2.14	0.47
2:C:1046:PHE:HE2	2:C:1055:LEU:HD22	1.78	0.47
2:C:1159:VAL:HG23	2:C:1164:TRP:O	2.14	0.47
3:D:152:ILE:O	3:D:155:HIS:HB2	2.14	0.47
3:D:221:ARG:NH1	3:D:225:ARG:HH21	2.12	0.47
1:A:124:THR:O	1:A:125:ASN:CB	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:ILE:HA	1:A:465:LEU:HB2	1.96	0.47
2:C:871:PRO:HB2	2:C:896:LEU:HD23	1.96	0.47
3:D:77:PHE:HE1	3:D:227:MET:O	1.96	0.47
1:A:133:LEU:HD21	2:C:545:PRO:CG	2.45	0.47
1:A:1019:PRO:HB2	1:A:1047:ASN:HD21	1.79	0.47
2:B:419:TYR:CE1	2:B:1007:THR:HA	2.49	0.47
1:A:377:LEU:HD23	1:A:759:LEU:O	2.15	0.47
1:A:496:CYS:SG	1:A:497:ALA:N	2.87	0.47
2:B:612:PHE:CE1	2:B:1331:ARG:HD2	2.48	0.47
2:B:893:ALA:HB1	2:B:915:VAL:HA	1.96	0.47
3:D:143:PRO:O	3:D:144:ARG:CB	2.63	0.47
3:E:166:GLU:CD	3:E:171:VAL:O	2.53	0.47
1:A:93:HIS:HE1	1:A:97:ARG:NH1	2.12	0.47
2:C:1087:ASP:HB3	2:C:1236:ILE:HG13	1.97	0.47
3:D:244:VAL:HG12	3:D:245:THR:N	2.28	0.47
1:A:337:LEU:HA	1:A:340:ILE:HG22	1.97	0.47
1:A:959:TYR:O	1:A:960:ILE:HG13	2.14	0.47
2:B:956:ASP:OD1	3:D:266:THR:CG2	2.63	0.47
2:C:1087:ASP:HB2	2:C:1235:PRO:HB2	1.97	0.47
3:D:242:ARG:HH11	3:D:242:ARG:CB	2.27	0.47
1:A:212:HIS:HD2	1:A:217:HIS:NE2	2.13	0.47
2:B:815:LEU:HB3	2:B:816:PRO:HD3	1.96	0.47
2:B:1134:ARG:NH2	2:B:1154:ASN:OD1	2.48	0.47
2:C:1071:PHE:HB3	2:C:1234:GLN:CG	2.40	0.47
3:D:37:TYR:HD1	3:D:177:ALA:CB	2.28	0.47
2:C:948:ILE:HG12	2:C:962:ASP:HB2	1.96	0.47
3:D:44:LEU:HB2	3:D:174:VAL:HG23	1.97	0.47
3:E:148:ASP:OD1	3:E:151:ASP:HB2	2.15	0.47
3:E:288:THR:HG23	3:E:289:ARG:H	1.80	0.47
2:B:891:HIS:HD2	3:D:240:VAL:HB	1.80	0.47
2:C:372:ALA:HB1	2:C:1315:MET:HE3	1.96	0.47
3:E:105:LEU:O	3:E:121:PHE:HB2	2.15	0.47
1:A:487:GLN:HE22	1:A:548:ASN:HA	1.79	0.46
1:A:600:VAL:CG1	1:A:601:PRO:HA	2.45	0.46
2:B:340:VAL:HG21	2:C:1008:LEU:CD2	2.37	0.46
2:B:956:ASP:CG	3:D:266:THR:HG21	2.35	0.46
2:C:109:LYS:HZ2	2:C:110:PRO:HD2	1.80	0.46
3:E:49:ILE:HG23	3:E:50:PRO:CD	2.24	0.46
1:A:97:ARG:HB2	1:A:97:ARG:NH1	2.26	0.46
1:A:955:ASN:ND2	1:A:1055:LEU:HB3	2.31	0.46
2:B:230:ASP:O	2:B:985:ARG:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:950:ASP:OD2	3:D:243:LYS:NZ	2.37	0.46
2:C:193:THR:HA	2:C:296:VAL:HG12	1.97	0.46
2:C:360:ILE:HD12	2:C:1053:ARG:NH2	2.31	0.46
2:C:764:TRP:N	2:C:765:PRO:CD	2.78	0.46
3:E:53:GLU:OE1	3:E:145:TYR:CD1	2.69	0.46
2:B:1276:LEU:HB3	2:B:1290:LYS:HG2	1.96	0.46
1:A:93:HIS:CE1	1:A:97:ARG:HH12	2.28	0.46
1:A:411:ILE:HD13	1:A:411:ILE:N	2.31	0.46
1:A:510:MET:O	1:A:511:ILE:HG13	2.16	0.46
1:A:929:PRO:O	1:A:993:VAL:HG12	2.15	0.46
2:B:274:MET:HG2	2:C:234:PRO:CD	2.27	0.46
3:D:53:GLU:HG2	3:D:145:TYR:HE1	1.81	0.46
3:D:67:TYR:CD1	3:D:110:VAL:HG22	2.50	0.46
3:E:33:GLN:C	3:E:35:LEU:N	2.69	0.46
1:A:747:CYS:HB3	1:A:784:ILE:HD13	1.97	0.46
2:C:306:GLN:HE21	2:C:306:GLN:H	1.62	0.46
2:C:337:VAL:HA	3:E:187:ILE:HD13	1.97	0.46
2:C:177:LYS:H	2:C:177:LYS:HD3	1.80	0.46
2:C:330:THR:HG22	2:C:331:GLU:N	2.30	0.46
3:D:217:LYS:O	3:D:221:ARG:HB3	2.15	0.46
3:E:162:GLY:HA2	3:E:172:MET:HE2	1.95	0.46
1:A:62:PHE:CZ	1:A:171:ILE:HG23	2.50	0.46
2:B:824:LEU:C	2:B:826:GLY:H	2.19	0.46
2:B:1037:ILE:HG12	2:B:1038:GLU:N	2.24	0.46
2:C:87:GLU:OE2	2:C:161:LYS:HB2	2.16	0.46
2:C:341:LYS:HG3	2:C:1306:THR:HB	1.98	0.46
2:C:561:ASN:O	2:C:562:ALA:HB3	2.15	0.46
3:E:1:MET:SD	3:E:121:PHE:CE2	3.09	0.46
1:A:591:ALA:HB1	1:A:595:ASN:HB2	1.97	0.46
2:B:649:ALA:HB2	2:B:695:ALA:CB	2.46	0.46
2:C:329:LEU:HD23	2:C:346:HIS:CE1	2.51	0.46
3:D:233:THR:HG22	3:D:252:LEU:HD13	1.97	0.46
1:A:653:PRO:O	1:A:712:ILE:HG23	2.15	0.46
2:C:96:ILE:HD11	2:C:101:ASP:HB3	1.98	0.46
2:C:829:SER:CB	2:C:965:ARG:HD2	2.46	0.46
2:C:856:LEU:HA	2:C:860:ARG:HB2	1.98	0.46
2:C:1080:THR:HB	2:C:1226:ASP:O	2.16	0.46
3:D:66:VAL:O	3:D:111:ILE:HG22	2.16	0.46
3:D:140:ALA:HA	3:D:281:LYS:HG3	1.97	0.46
3:E:53:GLU:O	3:E:53:GLU:CD	2.55	0.46
1:A:557:SER:HB3	1:A:583:ARG:HE	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:134:THR:HG22	2:C:472:GLU:CD	2.36	0.45
2:B:489:MET:HE1	2:B:492:VAL:HA	1.96	0.45
2:B:1080:THR:HG22	2:B:1227:MET:HB3	1.98	0.45
2:B:1276:LEU:HB3	2:B:1290:LYS:CG	2.46	0.45
2:C:883:ILE:O	2:C:887:VAL:HB	2.15	0.45
3:D:185:SER:HB3	3:D:186:LEU:H	1.50	0.45
2:C:443:VAL:HG12	2:C:769:GLN:HA	1.98	0.45
2:C:1279:SER:HB3	2:C:1280:PRO:C	2.36	0.45
1:A:631:GLU:O	1:A:635:VAL:HG23	2.17	0.45
2:B:228:VAL:HG21	2:B:253:MET:HG3	1.98	0.45
2:B:1075:ARG:HG3	2:B:1075:ARG:O	2.17	0.45
2:B:1168:ILE:HG21	2:B:1171:ILE:HD12	1.97	0.45
3:E:53:GLU:CG	3:E:145:TYR:CE1	2.93	0.45
1:A:284:THR:HG23	1:A:367:ASN:HB3	1.97	0.45
1:A:496:CYS:HB2	1:A:571:ILE:HG23	1.97	0.45
2:B:765:PRO:HA	2:B:769:GLN:HB2	1.97	0.45
2:B:1008:LEU:HD13	2:B:1008:LEU:H	1.81	0.45
2:C:141:LEU:HG	2:C:142:ASP:N	2.27	0.45
2:C:413:MET:HG2	2:C:1019:ILE:HD13	1.98	0.45
2:C:514:PHE:CD2	2:C:532:ILE:HD11	2.51	0.45
1:A:38:TYR:O	1:A:38:TYR:CG	2.70	0.45
3:D:19:ILE:HD11	3:D:31:PHE:HB2	1.97	0.45
1:A:938:MET:O	1:A:942:LYS:HB2	2.16	0.45
2:B:330:THR:HG23	2:B:331:GLU:HG3	1.98	0.45
2:C:231:LEU:HB2	2:C:249:SER:HB2	1.98	0.45
2:C:841:ASP:CA	2:C:940:ARG:HH12	2.30	0.45
2:C:1036:ASP:C	2:C:1037:ILE:HD12	2.37	0.45
2:C:1137:VAL:HG22	2:C:1164:TRP:CE2	2.52	0.45
3:D:106:GLY:HA2	3:D:121:PHE:HB3	1.98	0.45
3:E:166:GLU:HG3	3:E:172:MET:SD	2.57	0.45
3:E:229:PHE:HE1	3:E:252:LEU:CD1	2.29	0.45
1:A:559:ILE:CG2	1:A:613:ILE:HG12	2.46	0.45
3:E:70:ASP:O	3:E:70:ASP:OD2	2.35	0.45
3:E:148:ASP:O	3:E:280:ALA:HB1	2.16	0.45
1:A:6:SER:O	1:A:7:ILE:HB	2.16	0.45
1:A:565:ARG:O	1:A:566:GLU:HB3	2.17	0.45
2:C:523:THR:O	2:C:524:GLU:CB	2.63	0.45
3:D:110:VAL:HG12	3:D:111:ILE:N	2.32	0.45
3:D:131:ALA:C	3:D:133:THR:H	2.19	0.45
3:D:144:ARG:CG	3:D:144:ARG:O	2.64	0.45
1:A:908:ALA:HB2	1:A:943:ILE:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:291:HIS:HB3	2:B:292:ASN:H	1.54	0.45
2:C:330:THR:HG22	2:C:331:GLU:H	1.81	0.45
2:C:614:ARG:HB3	2:C:635:ILE:HD11	1.98	0.45
2:C:772:TYR:C	2:C:774:LEU:H	2.19	0.45
2:C:635:ILE:H	2:C:636:PRO:HA	1.82	0.45
2:C:986:ILE:O	2:C:989:ILE:HG22	2.17	0.45
2:C:999:LYS:HB3	2:C:1009:THR:HG22	1.98	0.45
1:A:617:ILE:HD11	1:A:635:VAL:HG11	1.98	0.44
2:B:204:VAL:HG22	2:B:1242:MET:HG2	1.98	0.44
2:B:1084:PRO:HG3	2:B:1212:ARG:HH11	1.82	0.44
2:C:413:MET:HG2	2:C:1019:ILE:CD1	2.47	0.44
2:C:442:PRO:HB3	2:C:473:ALA:HB1	1.99	0.44
3:D:221:ARG:HH12	3:D:225:ARG:HH21	1.63	0.44
3:E:116:THR:HG21	3:E:119:ILE:HD12	1.99	0.44
1:A:16:ASP:HB3	1:A:113:TYR:O	2.17	0.44
1:A:303:THR:HG21	1:A:813:PRO:HD3	1.99	0.44
1:A:525:ARG:H	1:A:525:ARG:HD3	1.82	0.44
1:A:775:ASP:O	1:A:777:ASP:N	2.50	0.44
2:B:916:LEU:H	2:B:916:LEU:HD23	1.83	0.44
2:B:924:ASP:O	2:B:928:ARG:NH2	2.46	0.44
2:B:1147:MET:HB3	2:B:1152:ALA:HB2	1.97	0.44
2:C:1060:ARG:HH22	2:C:1292:GLU:HA	1.81	0.44
2:C:1134:ARG:H	2:C:1135:PRO:HA	1.81	0.44
3:D:100:ASN:ND2	3:D:100:ASN:N	2.61	0.44
2:B:451:GLU:C	2:B:453:LEU:H	2.19	0.44
2:C:1220:PRO:HA	2:C:1221:PRO:HD3	1.80	0.44
3:D:255:ILE:O	3:D:255:ILE:CG1	2.65	0.44
2:B:350:ILE:CG2	2:B:351:ASP:H	2.17	0.44
2:B:950:ASP:CG	3:D:243:LYS:HZ3	2.20	0.44
2:B:1112:ASN:ND2	2:B:1113:LYS:H	2.16	0.44
2:B:1121:HIS:CD2	2:B:1124:THR:HG22	2.43	0.44
2:C:770:CYS:O	2:C:770:CYS:SG	2.75	0.44
2:C:957:PHE:O	2:C:958:ILE:HG12	2.18	0.44
2:C:1042:TRP:HB3	2:C:1043:SER:HA	1.95	0.44
3:D:178:LYS:HD2	3:D:249:ASP:HB3	1.99	0.44
2:B:172:ASP:O	2:B:173:GLN:HB3	2.17	0.44
2:B:367:GLU:HG3	3:D:82:GLN:HA	2.00	0.44
2:B:923:TYR:CE1	2:B:924:ASP:HB3	2.53	0.44
3:D:14:GLN:NE2	3:D:107:LEU:HD13	2.32	0.44
3:E:186:LEU:HD13	3:E:186:LEU:HA	1.60	0.44
2:B:425:ILE:HD13	2:B:425:ILE:H	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1079:LEU:O	2:B:1081:ASP:N	2.50	0.44
2:C:298:PRO:O	2:C:299:ALA:HB3	2.17	0.44
3:D:160:LEU:HD23	3:D:229:PHE:HA	1.99	0.44
1:A:766:CYS:CB	1:A:786:ARG:O	2.65	0.44
1:A:1034:ARG:CZ	1:A:1035:LEU:H	2.31	0.44
2:B:1289:PRO:HD2	3:D:20:ARG:NE	2.33	0.44
2:C:652:PHE:HE1	2:C:688:GLU:HA	1.82	0.44
3:D:181:SER:CB	3:D:250:ARG:HG2	2.41	0.44
3:E:2:LEU:HD11	3:E:107:LEU:CD1	2.48	0.44
3:E:68:ILE:HD13	3:E:69:GLU:CA	2.47	0.44
1:A:539:LEU:HD11	1:A:612:PHE:HB3	2.00	0.44
1:A:562:GLY:O	1:A:588:GLY:CA	2.66	0.44
1:A:864:ARG:HG3	1:A:865:ASN:N	2.33	0.44
1:A:914:GLU:HA	1:A:950:MET:HB3	2.00	0.44
2:B:1280:PRO:O	2:B:1281:VAL:HG12	2.18	0.44
2:B:1298:PHE:O	2:B:1299:SER:HB3	2.18	0.44
3:E:33:GLN:O	3:E:35:LEU:N	2.51	0.44
3:E:42:ASN:HB3	3:E:174:VAL:CG2	2.48	0.44
3:E:286:THR:O	3:E:290:TRP:CB	2.65	0.44
1:A:732:THR:O	1:A:733:VAL:HB	2.17	0.44
1:A:971:LEU:HD23	1:A:971:LEU:O	2.18	0.44
2:C:1118:THR:HG22	2:C:1129:PRO:HA	2.00	0.44
3:D:25:ASN:OD1	3:D:26:ALA:N	2.51	0.44
3:D:116:THR:OG1	3:D:119:ILE:HD12	2.18	0.44
3:D:150:ILE:HG22	3:D:151:ASP:N	2.33	0.44
3:D:238:ASN:H	3:D:253:GLU:HB3	1.82	0.44
3:E:46:LYS:CG	3:E:155:HIS:CE1	3.00	0.44
1:A:1034:ARG:NH1	1:A:1035:LEU:HD23	2.32	0.43
2:B:1255:ARG:HB3	2:B:1256:GLY:H	1.57	0.43
2:C:544:TYR:HA	2:C:545:PRO:HD3	1.74	0.43
1:A:504:THR:O	1:A:512:ALA:HA	2.18	0.43
1:A:654:SER:HB3	1:A:715:TYR:HE2	1.83	0.43
2:B:138:PHE:O	2:C:759:ASP:OD1	2.35	0.43
2:B:870:ASP:CB	2:B:871:PRO:CA	2.90	0.43
2:C:317:MET:SD	2:C:1262:SER:HB3	2.58	0.43
2:C:709:MET:HA	2:C:712:PHE:CE1	2.54	0.43
1:A:203:THR:HG23	1:A:204:LEU:H	1.82	0.43
1:A:224:GLU:O	1:A:227:MET:HB3	2.17	0.43
1:A:680:THR:O	1:A:683:GLN:HG3	2.19	0.43
2:B:225:ILE:HG23	2:B:247:TYR:CD2	2.52	0.43
3:E:32:LEU:O	3:E:35:LEU:CG	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:93:LEU:O	3:E:96:LEU:HB2	2.18	0.43
1:A:629:PHE:CD2	1:A:657:MET:HE1	2.52	0.43
1:A:959:TYR:HB3	1:A:960:ILE:H	1.70	0.43
2:B:210:ARG:HH21	2:B:215:THR:HG21	1.83	0.43
2:B:449:PHE:HA	2:B:450:PRO:HD2	1.83	0.43
2:C:526:ASN:HB2	2:C:721:SER:HB2	1.99	0.43
1:A:30:THR:HG22	1:A:97:ARG:HD3	2.00	0.43
1:A:580:SER:HB2	1:A:581:ASN:H	1.67	0.43
2:B:241:ALA:O	2:B:242:GLU:HG3	2.19	0.43
2:B:1103:HIS:CD2	2:B:1103:HIS:N	2.85	0.43
2:C:855:TYR:CZ	2:C:896:LEU:HD21	2.53	0.43
2:C:1322:PRO:O	2:C:1323:ASP:HB3	2.17	0.43
3:E:152:ILE:H	3:E:152:ILE:HD12	1.83	0.43
3:E:122:TYR:CE2	3:E:203:ILE:HG21	2.53	0.43
1:A:535:LEU:HD12	1:A:614:ILE:HG12	2.00	0.43
2:C:392:PRO:HG2	2:C:1315:MET:HG3	2.00	0.43
2:C:449:PHE:HB2	2:C:683:TRP:HD1	1.78	0.43
2:C:509:VAL:HG12	2:C:509:VAL:O	2.19	0.43
2:C:617:ASP:HA	2:C:620:ILE:HG22	2.00	0.43
3:D:46:LYS:HE3	3:D:158:LEU:HD22	2.00	0.43
3:E:253:GLU:HG3	3:E:254:TYR:CE2	2.54	0.43
3:E:282:PHE:CZ	3:E:286:THR:HG21	2.53	0.43
1:A:941:ASP:HA	1:A:944:ARG:HB3	2.00	0.43
2:B:1289:PRO:HD2	3:D:20:ARG:HD2	1.97	0.43
2:C:816:PRO:O	2:C:820:ILE:HG22	2.19	0.43
2:C:837:THR:HA	2:C:936:MET:HB2	2.01	0.43
2:C:874:ILE:HG21	2:C:897:TYR:CD1	2.53	0.43
3:D:66:VAL:HG23	3:D:67:TYR:N	2.33	0.43
3:D:241:ASN:HB3	3:D:250:ARG:HD2	2.01	0.43
3:E:162:GLY:O	3:E:167:ARG:NH1	2.48	0.43
1:A:67:ARG:O	1:A:72:PHE:HD1	2.02	0.43
1:A:263:LEU:HB3	1:A:264:SER:H	1.68	0.43
1:A:685:PRO:O	1:A:686:TYR:CD2	2.72	0.43
1:A:437:GLN:HE21	1:A:437:GLN:CA	2.32	0.43
1:A:730:ILE:CG2	1:A:731:HIS:H	2.26	0.43
1:A:873:PRO:HD2	1:A:876:MET:HB2	1.99	0.43
2:C:1072:ASP:H	2:C:1234:GLN:HE22	1.66	0.43
3:D:14:GLN:HE22	3:D:107:LEU:HD13	1.84	0.43
2:B:280:THR:HG23	2:B:281:VAL:HG23	2.01	0.42
2:B:406:ASP:HA	2:B:409:ILE:HG22	1.99	0.42
2:C:733:VAL:HG11	2:C:1022:ILE:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1121:HIS:ND1	2:C:1123:PRO:HD2	2.34	0.42
3:D:217:LYS:HE2	3:D:290:TRP:O	2.18	0.42
1:A:437:GLN:HE21	1:A:437:GLN:N	2.16	0.42
1:A:526:ASN:OD1	1:A:529:THR:HG23	2.20	0.42
2:B:141:LEU:HG	2:B:142:ASP:H	1.83	0.42
2:C:837:THR:HG22	2:C:934:LEU:HD21	2.00	0.42
3:E:210:GLY:O	3:E:214:ARG:HG3	2.18	0.42
1:A:454:GLY:C	1:A:456:PHE:H	2.23	0.42
1:A:496:CYS:SG	1:A:533:LEU:HD11	2.59	0.42
1:A:961:SER:HA	1:A:997:THR:OG1	2.20	0.42
2:C:627:ALA:H	2:C:716:PHE:HB2	1.84	0.42
3:D:74:GLN:OE1	3:D:74:GLN:HA	2.19	0.42
3:E:1:MET:CE	3:E:123:ASP:HA	2.49	0.42
1:A:76:LEU:C	1:A:78:TYR:N	2.66	0.42
1:A:114:ASN:HD21	1:A:117:LEU:HB3	1.85	0.42
1:A:305:TYR:CE1	1:A:313:ARG:HG3	2.54	0.42
1:A:590:ARG:HA	1:A:597:ARG:HH12	1.84	0.42
1:A:850:SER:HB3	1:A:872:VAL:HG21	2.01	0.42
2:B:267:VAL:HG12	2:B:1306:THR:HA	2.01	0.42
2:B:452:ASN:C	2:B:454:GLU:H	2.22	0.42
2:B:983:ILE:HG22	2:B:983:ILE:O	2.19	0.42
2:C:543:TRP:CD1	2:C:544:TYR:HD1	2.33	0.42
2:C:738:GLU:HB3	2:C:1015:GLN:HG3	2.02	0.42
2:C:817:ASP:O	2:C:821:ASN:HB3	2.19	0.42
3:D:53:GLU:CG	3:D:145:TYR:HE1	2.31	0.42
3:D:153:TYR:O	3:D:156:VAL:HG12	2.11	0.42
1:A:752:VAL:HG12	1:A:812:VAL:HG23	2.01	0.42
1:A:828:TYR:HA	1:A:1032:GLY:O	2.20	0.42
2:B:193:THR:O	2:B:193:THR:HG22	2.20	0.42
2:B:935:GLN:OE1	2:B:940:ARG:HB3	2.19	0.42
2:C:341:LYS:CG	2:C:1306:THR:HB	2.50	0.42
2:C:852:TYR:CE2	2:C:856:LEU:HD23	2.55	0.42
2:C:1134:ARG:NH1	2:C:1158:SER:OG	2.52	0.42
1:A:555:ASP:OD1	1:A:555:ASP:N	2.53	0.42
1:A:967:ILE:C	1:A:969:THR:H	2.23	0.42
2:B:426:ILE:HA	2:B:429:ILE:HG22	2.02	0.42
2:C:863:LEU:HD11	2:C:871:PRO:HD3	2.02	0.42
1:A:93:HIS:CE1	1:A:97:ARG:NH1	2.87	0.42
1:A:311:GLN:NE2	1:A:359:PRO:HG3	2.34	0.42
1:A:519:ILE:HA	1:A:520:PRO:HD2	1.96	0.42
2:B:402:ALA:HB2	3:D:83:ASN:ND2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:635:ILE:HD12	2:B:635:ILE:O	2.18	0.42
2:B:733:VAL:HG22	2:B:741:TYR:HB2	2.01	0.42
2:B:956:ASP:OD2	3:D:266:THR:CB	2.67	0.42
2:B:1080:THR:HA	2:B:1227:MET:HA	2.02	0.42
2:C:336:TYR:CE1	3:E:191:ARG:HG2	2.54	0.42
2:C:554:ARG:HD3	2:C:568:PHE:CD1	2.55	0.42
2:C:564:GLY:O	2:C:565:GLU:HB3	2.20	0.42
2:C:843:LEU:HD11	2:C:943:GLU:HB3	2.02	0.42
2:C:1136:HIS:HA	2:C:1164:TRP:CD1	2.54	0.42
3:E:69:GLU:HG3	3:E:199:LEU:HB2	1.98	0.42
3:E:247:ARG:HA	3:E:247:ARG:NE	2.30	0.42
1:A:377:LEU:H	1:A:377:LEU:CD1	2.30	0.42
2:B:302:ARG:HD3	2:B:315:THR:HG22	2.01	0.42
2:B:598:ASN:HA	2:B:601:ILE:HG22	2.02	0.42
2:C:1023:ARG:HG2	2:C:1024:PRO:CD	2.40	0.42
3:E:32:LEU:HD13	3:E:225:ARG:NH1	2.35	0.42
3:E:158:LEU:CD2	3:E:172:MET:HB3	2.49	0.42
3:E:268:THR:OG1	3:E:269:ILE:N	2.48	0.42
2:B:862:ARG:NH1	2:B:948:ILE:HD13	2.35	0.42
2:C:526:ASN:HB2	2:C:721:SER:CB	2.50	0.42
2:C:822:MET:CG	2:C:1044:ARG:HD2	2.50	0.42
2:C:1126:MET:HB3	2:C:1128:TYR:CE2	2.54	0.42
3:D:239:VAL:CG1	3:D:250:ARG:HH12	2.30	0.42
2:B:549:GLY:O	2:B:553:GLN:HB2	2.19	0.42
2:B:836:GLN:HG2	2:B:941:TYR:HA	2.02	0.42
2:C:931:ASN:OD1	2:C:934:LEU:HD22	2.19	0.42
2:C:1208:ASP:CG	2:C:1209:GLY:H	2.23	0.42
1:A:127:THR:CG2	2:B:639:ASN:HB2	2.49	0.41
1:A:496:CYS:HB2	1:A:571:ILE:CG2	2.50	0.41
2:B:493:HIS:CG	2:B:758:ILE:HD13	2.55	0.41
2:B:1071:PHE:HB3	2:B:1234:GLN:HG3	2.01	0.41
2:B:1112:ASN:CG	2:B:1113:LYS:H	2.23	0.41
2:B:1140:THR:HA	2:B:1167:ASP:HB2	2.02	0.41
2:B:1236:ILE:CG1	2:B:1237:SER:H	2.33	0.41
2:B:1249:ASN:O	2:C:1109:SER:HA	2.19	0.41
2:C:633:THR:HG21	2:C:710:SER:OG	2.20	0.41
2:C:835:TYR:HB2	2:C:847:ILE:HD11	2.03	0.41
3:D:152:ILE:HG21	3:D:283:LEU:HB3	2.01	0.41
3:E:2:LEU:HD11	3:E:107:LEU:HD11	2.02	0.41
3:E:32:LEU:CD1	3:E:225:ARG:NE	2.83	0.41
3:E:72:ILE:O	3:E:76:LEU:HD12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:686:TYR:HE1	1:A:1034:ARG:NH1	2.18	0.41
2:B:1263:TYR:CD1	2:B:1295:HIS:HD2	2.32	0.41
2:C:375:ARG:HG2	2:C:398:ARG:HH21	1.86	0.41
2:C:443:VAL:CG2	2:C:444:SER:H	2.26	0.41
3:E:140:ALA:HB1	3:E:281:LYS:HG3	2.02	0.41
1:A:828:TYR:O	1:A:1033:ILE:HA	2.19	0.41
1:A:1016:ILE:HD13	1:A:1016:ILE:H	1.84	0.41
2:B:722:GLY:O	2:B:723:ASN:HB3	2.20	0.41
2:C:772:TYR:C	2:C:774:LEU:N	2.74	0.41
2:C:898:GLN:OE1	3:D:3:GLN:OE1	2.39	0.41
3:D:193:VAL:HG11	3:D:230:ILE:HD12	2.02	0.41
1:A:240:ARG:HH21	1:A:288:LEU:HD23	1.84	0.41
1:A:525:ARG:HD3	1:A:525:ARG:N	2.35	0.41
3:D:12:LEU:HD23	3:D:14:GLN:HB2	2.01	0.41
3:D:69:GLU:HB2	3:D:199:LEU:HD11	2.02	0.41
3:E:205:LEU:CD1	3:E:289:ARG:HG3	2.50	0.41
1:A:38:TYR:HD2	1:A:51:LEU:HD11	1.85	0.41
1:A:541:LYS:HG2	1:A:971:LEU:HD22	2.02	0.41
1:A:968:ILE:H	1:A:968:ILE:HG13	1.69	0.41
2:B:196:LEU:HD22	2:B:296:VAL:HG11	2.02	0.41
3:D:69:GLU:HG3	3:D:199:LEU:HG	2.02	0.41
2:B:164:LEU:HD22	2:B:1296:ILE:HD13	2.02	0.41
2:B:609:PRO:HD3	2:B:724:HIS:NE2	2.35	0.41
2:B:1292:GLU:OE1	2:B:1293:VAL:HG13	2.20	0.41
2:C:478:ILE:HD12	2:C:766:ILE:HG23	2.02	0.41
2:C:704:VAL:HG22	2:C:1330:ILE:HD11	2.03	0.41
2:C:1236:ILE:HG13	2:C:1236:ILE:H	1.76	0.41
3:E:76:LEU:HD21	3:E:282:PHE:CD2	2.55	0.41
1:A:170:ASN:HB3	1:A:173:ASP:HB2	2.02	0.41
1:A:496:CYS:SG	1:A:533:LEU:CD1	3.09	0.41
1:A:543:GLU:HA	1:A:645:ARG:HH22	1.84	0.41
1:A:559:ILE:HG12	1:A:585:ILE:HB	2.03	0.41
1:A:797:ARG:HH22	1:A:878:TYR:HB2	1.86	0.41
2:B:485:GLU:OE1	2:B:521:PHE:HB3	2.21	0.41
2:B:583:GLU:O	2:B:584:HIS:HB2	2.21	0.41
2:B:879:THR:HA	2:B:880:PRO:HD3	1.95	0.41
2:C:299:ALA:HB2	2:C:1265:MET:SD	2.61	0.41
2:C:612:PHE:O	2:C:635:ILE:HD13	2.19	0.41
2:C:958:ILE:O	2:C:958:ILE:HG13	2.20	0.41
2:C:1087:ASP:HB2	2:C:1235:PRO:CB	2.51	0.41
1:A:155:VAL:HG12	2:C:548:TYR:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:850:THR:HG22	2:B:851:THR:H	1.86	0.41
2:B:1102:ALA:O	2:B:1105:LEU:HG	2.21	0.41
2:B:1263:TYR:CD2	2:B:1295:HIS:CD2	3.09	0.41
2:C:651:ARG:O	2:C:655:ILE:HG12	2.21	0.41
2:C:868:VAL:HB	2:C:890:THR:HA	2.02	0.41
2:C:898:GLN:OE1	3:D:3:GLN:CD	2.59	0.41
2:C:1029:LEU:HB3	2:C:1030:ARG:H	1.63	0.41
3:E:182:TRP:CD1	3:E:185:SER:HB3	2.55	0.41
1:A:325:THR:HG22	1:A:351:TYR:HB3	2.03	0.41
1:A:383:THR:HG21	1:A:805:TYR:CB	2.51	0.41
1:A:411:ILE:HD13	1:A:411:ILE:H	1.86	0.41
1:A:686:TYR:O	1:A:686:TYR:CD2	2.71	0.41
2:B:219:ILE:HG22	2:B:220:ASP:N	2.24	0.41
2:B:876:GLY:HA2	2:B:902:ILE:CG2	2.50	0.41
2:B:1031:TYR:CE2	2:B:1041:ARG:HD3	2.56	0.41
2:C:218:GLY:HA3	2:C:989:ILE:HD11	2.03	0.41
2:C:547:GLU:HG2	2:C:599:THR:HG23	2.02	0.41
2:C:624:PHE:CD2	2:C:713:MET:HA	2.56	0.41
2:C:887:VAL:HA	2:C:890:THR:HG22	2.02	0.41
2:C:926:VAL:HG22	2:C:938:ASN:HB2	2.03	0.41
3:D:258:ASN:OD1	3:D:259:SER:N	2.53	0.41
3:E:66:VAL:HG13	3:E:111:ILE:HG21	2.03	0.41
3:E:140:ALA:CB	3:E:281:LYS:HG3	2.51	0.41
1:A:309:ASN:O	1:A:311:GLN:N	2.53	0.41
2:B:268:GLY:O	2:B:269:GLU:HB2	2.21	0.41
2:B:363:ARG:NE	3:D:80:SER:CB	2.83	0.41
2:C:524:GLU:OE2	2:C:758:ILE:HD13	2.21	0.41
2:C:547:GLU:HB3	2:C:600:ILE:HD12	2.01	0.41
2:C:687:LEU:HD11	2:C:764:TRP:HZ3	1.86	0.41
2:C:730:ASP:O	2:C:730:ASP:CG	2.59	0.41
2:C:878:SER:HB3	2:C:903:ASN:CG	2.40	0.41
1:A:329:THR:O	1:A:331:ARG:N	2.54	0.40
1:A:731:HIS:HB2	1:A:746:PHE:HD2	1.86	0.40
2:B:980:ARG:NH2	2:B:1010:ARG:O	2.53	0.40
2:B:1084:PRO:HB2	2:B:1209:GLY:HA3	2.02	0.40
2:B:1114:ARG:HG3	2:B:1116:ARG:HH21	1.85	0.40
2:C:205:ASN:HB2	2:C:1239:ALA:HB1	2.02	0.40
2:C:225:ILE:HG23	2:C:247:TYR:HD2	1.86	0.40
2:C:1323:ASP:CG	2:C:1324:ASP:N	2.73	0.40
3:D:239:VAL:HG12	3:D:250:ARG:NH1	2.33	0.40
1:A:75:PRO:HD2	1:A:76:LEU:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:THR:CG2	3:D:144:ARG:CG	2.91	0.40
1:A:872:VAL:HA	1:A:873:PRO:HA	1.84	0.40
1:A:967:ILE:HB	1:A:978:LYS:HD3	2.03	0.40
2:B:1298:PHE:O	2:B:1299:SER:CB	2.68	0.40
1:A:407:GLU:CG	1:A:829:MET:O	2.69	0.40
1:A:430:PRO:HB2	1:A:433:GLU:HG3	2.03	0.40
1:A:484:THR:N	1:A:511:ILE:HG21	2.36	0.40
1:A:939:GLN:O	1:A:943:ILE:HG12	2.22	0.40
1:A:1013:THR:O	1:A:1055:LEU:HD12	2.21	0.40
2:B:934:LEU:O	2:B:935:GLN:HB2	2.21	0.40
2:B:1236:ILE:HG12	2:B:1237:SER:H	1.85	0.40
2:C:838:GLU:HG3	2:C:839:ALA:N	2.36	0.40
2:C:1076:ILE:HD13	2:C:1159:VAL:HG21	2.02	0.40
2:C:1097:VAL:HG13	2:C:1137:VAL:HG12	2.03	0.40
3:E:70:ASP:OD2	3:E:70:ASP:C	2.60	0.40
3:E:140:ALA:O	3:E:146:ARG:HA	2.22	0.40
2:B:281:VAL:HG11	2:B:302:ARG:HD2	2.03	0.40
2:C:493:HIS:HB3	2:C:756:THR:HA	2.02	0.40
2:C:1086:PRO:HG3	2:C:1177:VAL:HG12	2.03	0.40
1:A:419:TYR:HB3	1:A:680:THR:HG23	2.03	0.40
2:B:172:ASP:O	2:B:173:GLN:CB	2.70	0.40
2:B:184:GLU:C	2:B:186:ASP:H	2.24	0.40
2:B:733:VAL:HA	2:B:743:PRO:HA	2.04	0.40
2:C:490:PHE:HA	2:C:745:ILE:HG22	2.04	0.40
2:C:997:TYR:C	2:C:999:LYS:H	2.25	0.40
2:C:1049:GLU:CD	2:C:1053:ARG:HG3	2.42	0.40
3:E:53:GLU:CB	3:E:145:TYR:CE1	3.05	0.40
3:E:261:ARG:O	3:E:262:THR:HB	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1039/1058 (98%)	775 (75%)	180 (17%)	84 (8%)	1 14
2	B	1172/1333 (88%)	915 (78%)	219 (19%)	38 (3%)	4 32
2	C	1238/1333 (93%)	974 (79%)	240 (19%)	24 (2%)	8 41
3	D	289/291 (99%)	253 (88%)	33 (11%)	3 (1%)	15 52
3	E	289/291 (99%)	254 (88%)	34 (12%)	1 (0%)	41 75
All	All	4027/4306 (94%)	3171 (79%)	706 (18%)	150 (4%)	6 29

All (150) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	ILE
1	A	25	ILE
1	A	49	HIS
1	A	55	GLY
1	A	69	HIS
1	A	76	LEU
1	A	77	LYS
1	A	125	ASN
1	A	255	ARG
1	A	330	GLN
1	A	364	TYR
1	A	391	ILE
1	A	485	MET
1	A	487	GLN
1	A	511	ILE
1	A	549	SER
1	A	580	SER
1	A	608	ILE
1	A	776	SER
1	A	813	PRO
1	A	853	GLU
1	A	924	VAL
1	A	962	PHE
1	A	964	GLU
1	A	1035	LEU
1	A	1038	THR
2	B	280	THR
2	B	616	ASP
2	B	838	GLU
2	B	870	ASP
2	B	1080	THR

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Mol	Chain	Res	Type
2	B	1281	VAL
2	B	1299	SER
2	C	628	SER
2	C	842	ASP
2	C	1037	ILE
2	C	1323	ASP
1	A	3	HIS
1	A	116	MET
1	A	187	PRO
1	A	212	HIS
1	A	263	LEU
1	A	284	THR
1	A	395	GLN
1	A	499	VAL
1	A	512	ALA
1	A	671	VAL
1	A	688	TYR
1	A	697	ILE
1	A	733	VAL
1	A	851	LEU
1	A	915	ASN
1	A	926	MET
1	A	990	ALA
2	B	149	PRO
2	B	150	LEU
2	B	671	ASP
2	B	897	TYR
2	B	901	VAL
2	B	914	GLU
2	C	1294	ASP
3	D	244	VAL
1	A	209	SER
1	A	214	ASN
1	A	266	SER
1	A	387	THR
1	A	389	ALA
1	A	519	ILE
1	A	655	GLU
1	A	686	TYR
1	A	829	MET
1	A	888	GLU
2	B	229	GLN

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Mol	Chain	Res	Type
2	B	291	HIS
2	B	339	LEU
2	B	753	ASP
2	B	973	THR
2	C	386	SER
2	C	450	PRO
2	C	992	VAL
2	C	1234	GLN
3	D	253	GLU
1	A	37	ASP
1	A	380	THR
1	A	406	VAL
1	A	566	GLU
1	A	684	ASN
1	A	740	THR
1	A	893	GLU
1	A	894	LYS
1	A	960	ILE
2	B	193	THR
2	B	451	GLU
2	B	1112	ASN
2	B	1234	GLN
2	C	666	ARG
2	C	1249	ASN
3	D	265	ARG
1	A	115	TRP
1	A	307	HIS
1	A	310	ASP
1	A	363	ASN
1	A	523	MET
1	A	623	GLN
1	A	760	SER
1	A	821	ARG
1	A	968	ILE
2	B	190	VAL
2	B	307	VAL
2	B	438	ASN
2	B	452	ASN
2	C	545	PRO
2	C	591	ASP
2	C	831	VAL
2	C	948	ILE

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Mol	Chain	Res	Type
1	A	28	PRO
1	A	74	LEU
1	A	356	THR
1	A	489	SER
1	A	517	GLY
1	A	802	THR
1	A	815	GLY
2	B	840	ASP
2	B	915	VAL
2	C	757	ILE
2	C	830	VAL
2	C	838	GLU
2	C	938	ASN
3	E	55	HIS
1	A	68	GLY
1	A	929	PRO
2	B	983	ILE
2	C	762	ILE
2	C	1279	SER
2	B	749	GLY
2	B	830	VAL
2	C	1086	PRO
1	A	602	PHE
1	A	704	PRO
2	B	157	ILE
2	B	219	ILE
2	B	1037	ILE
1	A	887	ILE
2	B	194	VAL
1	A	925	ILE
2	B	1084	PRO
2	B	1180	PRO
2	C	307	VAL
2	C	644	VAL
2	B	192	PRO

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	933/943 (99%)	813 (87%)	120 (13%)	4	23
2	B	1029/1155 (89%)	913 (89%)	116 (11%)	6	27
2	C	1085/1155 (94%)	944 (87%)	141 (13%)	4	23
3	D	240/240 (100%)	205 (85%)	35 (15%)	3	19
3	E	240/240 (100%)	198 (82%)	42 (18%)	2	13
All	All	3527/3733 (94%)	3073 (87%)	454 (13%)	7	23

All (454) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	THR
1	A	20	ASN
1	A	22	ILE
1	A	23	ARG
1	A	26	THR
1	A	31	VAL
1	A	39	LEU
1	A	47	ARG
1	A	53	LEU
1	A	54	LEU
1	A	58	GLN
1	A	67	ARG
1	A	78	TYR
1	A	91	ASN
1	A	97	ARG
1	A	101	LEU
1	A	103	HIS
1	A	122	ARG
1	A	125	ASN
1	A	140	ILE
1	A	148	ASP
1	A	204	LEU
1	A	207	THR
1	A	215	VAL
1	A	228	ILE
1	A	231	PHE
1	A	235	ILE
1	A	244	LYS
1	A	254	ASP

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Mol	Chain	Res	Type
1	A	270	GLN
1	A	278	LEU
1	A	283	PHE
1	A	297	LEU
1	A	298	LEU
1	A	307	HIS
1	A	320	TYR
1	A	332	HIS
1	A	334	GLU
1	A	339	GLN
1	A	356	THR
1	A	374	LYS
1	A	391	ILE
1	A	402	THR
1	A	406	VAL
1	A	411	ILE
1	A	425	THR
1	A	427	ASP
1	A	437	GLN
1	A	461	ARG
1	A	465	LEU
1	A	487	GLN
1	A	521	LYS
1	A	525	ARG
1	A	542	LEU
1	A	545	PHE
1	A	555	ASP
1	A	558	ILE
1	A	559	ILE
1	A	561	LEU
1	A	565	ARG
1	A	569	VAL
1	A	574	ARG
1	A	578	ASN
1	A	581	ASN
1	A	584	ILE
1	A	589	ASP
1	A	608	ILE
1	A	611	ASP
1	A	628	MET
1	A	652	HIS
1	A	655	GLU

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Mol	Chain	Res	Type
1	A	658	ILE
1	A	667	GLN
1	A	677	LEU
1	A	686	TYR
1	A	695	THR
1	A	708	ASN
1	A	713	ASN
1	A	714	ARG
1	A	717	THR
1	A	724	MET
1	A	737	HIS
1	A	739	ASN
1	A	746	PHE
1	A	763	LYS
1	A	773	ARG
1	A	781	VAL
1	A	788	ASP
1	A	794	LEU
1	A	802	THR
1	A	809	GLN
1	A	812	VAL
1	A	814	ASN
1	A	823	THR
1	A	832	GLU
1	A	841	MET
1	A	859	VAL
1	A	868	ASP
1	A	874	LEU
1	A	876	MET
1	A	887	ILE
1	A	897	ILE
1	A	898	GLU
1	A	905	GLN
1	A	906	PHE
1	A	939	GLN
1	A	951	LEU
1	A	953	ARG
1	A	955	ASN
1	A	967	ILE
1	A	969	THR
1	A	971	LEU
1	A	973	GLN

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Mol	Chain	Res	Type
1	A	978	LYS
1	A	987	LEU
1	A	988	LYS
1	A	1006	MET
1	A	1016	ILE
1	A	1034	ARG
1	A	1053	ILE
2	B	161	LYS
2	B	170	TYR
2	B	171	GLU
2	B	177	LYS
2	B	181	ARG
2	B	186	ASP
2	B	189	ILE
2	B	203	VAL
2	B	205	ASN
2	B	230	ASP
2	B	237	VAL
2	B	270	THR
2	B	274	MET
2	B	278	LEU
2	B	286	LEU
2	B	291	HIS
2	B	302	ARG
2	B	303	ASP
2	B	309	TRP
2	B	319	GLN
2	B	324	LYS
2	B	331	GLU
2	B	339	LEU
2	B	352	HIS
2	B	374	ASP
2	B	384	MET
2	B	406	ASP
2	B	409	ILE
2	B	412	LEU
2	B	423	GLU
2	B	425	ILE
2	B	446	LYS
2	B	448	TYR
2	B	453	LEU
2	B	458	SER

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Mol	Chain	Res	Type
2	B	469	ARG
2	B	486	VAL
2	B	496	LYS
2	B	516	LEU
2	B	529	LYS
2	B	547	GLU
2	B	554	ARG
2	B	588	LEU
2	B	591	ASP
2	B	599	THR
2	B	604	MET
2	B	610	GLN
2	B	616	ASP
2	B	617	ASP
2	B	618	LEU
2	B	640	GLN
2	B	672	MET
2	B	680	THR
2	B	685	ARG
2	B	688	GLU
2	B	719	ASN
2	B	738	GLU
2	B	748	GLN
2	B	832	MET
2	B	841	ASP
2	B	848	ARG
2	B	850	THR
2	B	856	LEU
2	B	879	THR
2	B	895	VAL
2	B	897	TYR
2	B	910	LEU
2	B	916	LEU
2	B	922	TYR
2	B	934	LEU
2	B	942	HIS
2	B	946	LEU
2	B	954	GLN
2	B	971	MET
2	B	985	ARG
2	B	988	GLN
2	B	1008	LEU

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Mol	Chain	Res	Type
2	B	1020	ARG
2	B	1021	ARG
2	B	1028	VAL
2	B	1036	ASP
2	B	1049	GLU
2	B	1053	ARG
2	B	1069	ARG
2	B	1075	ARG
2	B	1081	ASP
2	B	1082	ASP
2	B	1092	VAL
2	B	1103	HIS
2	B	1113	LYS
2	B	1114	ARG
2	B	1143	GLU
2	B	1144	ARG
2	B	1153	ASP
2	B	1176	GLU
2	B	1186	GLN
2	B	1187	HIS
2	B	1202	PHE
2	B	1203	HIS
2	B	1210	LEU
2	B	1212	ARG
2	B	1218	PHE
2	B	1230	ILE
2	B	1233	LEU
2	B	1234	GLN
2	B	1240	ARG
2	B	1247	ASN
2	B	1252	ASP
2	B	1281	VAL
2	B	1291	LEU
2	B	1292	GLU
2	B	1298	PHE
2	B	1300	ASN
2	B	1318	GLU
2	B	1323	ASP
2	B	1330	ILE
2	C	83	GLN
2	C	108	LYS
2	C	117	ARG

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Mol	Chain	Res	Type
2	C	120	VAL
2	C	123	GLU
2	C	124	GLN
2	C	128	GLU
2	C	133	MET
2	C	134	THR
2	C	145	THR
2	C	146	GLU
2	C	154	PHE
2	C	156	GLN
2	C	173	GLN
2	C	177	LYS
2	C	196	LEU
2	C	204	VAL
2	C	205	ASN
2	C	221	LEU
2	C	231	LEU
2	C	251	LEU
2	C	255	LEU
2	C	265	VAL
2	C	283	ASN
2	C	287	ARG
2	C	297	ASN
2	C	306	GLN
2	C	309	TRP
2	C	346	HIS
2	C	361	ASN
2	C	366	MET
2	C	384	MET
2	C	409	ILE
2	C	412	LEU
2	C	419	TYR
2	C	422	LEU
2	C	430	ASN
2	C	440	ILE
2	C	448	TYR
2	C	452	ASN
2	C	469	ARG
2	C	472	GLU
2	C	480	LEU
2	C	489	MET
2	C	493	HIS

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Mol	Chain	Res	Type
2	C	494	GLU
2	C	495	LEU
2	C	498	ILE
2	C	512	LEU
2	C	524	GLU
2	C	536	LEU
2	C	542	ARG
2	C	545	PRO
2	C	547	GLU
2	C	560	ILE
2	C	561	ASN
2	C	574	LYS
2	C	577	GLN
2	C	581	LEU
2	C	591	ASP
2	C	599	THR
2	C	613	LEU
2	C	634	TYR
2	C	637	TYR
2	C	646	ASN
2	C	647	GLU
2	C	659	LEU
2	C	669	GLN
2	C	681	LYS
2	C	684	LEU
2	C	688	GLU
2	C	693	ASN
2	C	720	PHE
2	C	730	ASP
2	C	731	GLN
2	C	738	GLU
2	C	746	GLU
2	C	753	ASP
2	C	762	ILE
2	C	767	LEU
2	C	813	LEU
2	C	820	ILE
2	C	830	VAL
2	C	841	ASP
2	C	847	ILE
2	C	849	MET
2	C	863	LEU

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Mol	Chain	Res	Type
2	C	864	HIS
2	C	874	ILE
2	C	882	GLN
2	C	898	GLN
2	C	910	LEU
2	C	911	ARG
2	C	918	VAL
2	C	922	TYR
2	C	928	ARG
2	C	934	LEU
2	C	936	MET
2	C	937	ASN
2	C	943	GLU
2	C	945	VAL
2	C	947	GLU
2	C	948	ILE
2	C	959	GLN
2	C	970	LEU
2	C	1000	LEU
2	C	1021	ARG
2	C	1022	ILE
2	C	1025	ASP
2	C	1042	TRP
2	C	1046	PHE
2	C	1050	LEU
2	C	1051	ARG
2	C	1075	ARG
2	C	1076	ILE
2	C	1079	LEU
2	C	1083	ASP
2	C	1110	LEU
2	C	1112	ASN
2	C	1174	THR
2	C	1176	GLU
2	C	1187	HIS
2	C	1193	ILE
2	C	1201	LEU
2	C	1202	PHE
2	C	1204	LEU
2	C	1211	LEU
2	C	1214	GLU
2	C	1228	ARG

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Mol	Chain	Res	Type
2	C	1229	LEU
2	C	1247	ASN
2	C	1250	GLU
2	C	1253	ARG
2	C	1269	THR
2	C	1272	ARG
2	C	1288	ILE
2	C	1292	GLU
2	C	1293	VAL
2	C	1294	ASP
2	C	1295	HIS
2	C	1296	ILE
3	D	1	MET
3	D	13	GLU
3	D	14	GLN
3	D	15	PHE
3	D	20	ARG
3	D	37	TYR
3	D	41	GLU
3	D	47	LYS
3	D	55	HIS
3	D	61	ASN
3	D	66	VAL
3	D	68	ILE
3	D	69	GLU
3	D	70	ASP
3	D	79	ILE
3	D	85	ASN
3	D	87	HIS
3	D	90	PHE
3	D	100	ASN
3	D	101	THR
3	D	121	PHE
3	D	133	THR
3	D	149	MET
3	D	156	VAL
3	D	158	LEU
3	D	160	LEU
3	D	195	ASN
3	D	196	TRP
3	D	226	MET
3	D	228	LEU

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Mol	Chain	Res	Type
3	D	242	ARG
3	D	250	ARG
3	D	288	THR
3	D	289	ARG
3	D	290	TRP
3	E	9	TYR
3	E	15	PHE
3	E	17	PHE
3	E	19	ILE
3	E	29	THR
3	E	35	LEU
3	E	41	GLU
3	E	44	LEU
3	E	46	LYS
3	E	47	LYS
3	E	53	GLU
3	E	55	HIS
3	E	66	VAL
3	E	68	ILE
3	E	69	GLU
3	E	83	ASN
3	E	85	ASN
3	E	87	HIS
3	E	92	ARG
3	E	107	LEU
3	E	108	ASP
3	E	111	ILE
3	E	118	ASN
3	E	122	TYR
3	E	137	LEU
3	E	144	ARG
3	E	146	ARG
3	E	151	ASP
3	E	178	LYS
3	E	179	PHE
3	E	186	LEU
3	E	191	ARG
3	E	195	ASN
3	E	221	ARG
3	E	228	LEU
3	E	255	ILE
3	E	261	ARG

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Mol	Chain	Res	Type
3	E	269	ILE
3	E	273	LEU
3	E	288	THR
3	E	289	ARG
3	E	291	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (111) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	20	ASN
1	A	29	ASN
1	A	43	ASN
1	A	69	HIS
1	A	91	ASN
1	A	93	HIS
1	A	114	ASN
1	A	125	ASN
1	A	132	GLN
1	A	136	ASN
1	A	151	ASN
1	A	212	HIS
1	A	309	ASN
1	A	311	GLN
1	A	434	GLN
1	A	437	GLN
1	A	487	GLN
1	A	544	ASN
1	A	548	ASN
1	A	578	ASN
1	A	581	ASN
1	A	651	ASN
1	A	659	ASN
1	A	674	HIS
1	A	737	HIS
1	A	739	ASN
1	A	857	GLN
1	A	905	GLN
1	A	915	ASN
1	A	916	ASN
1	A	930	ASN
1	A	939	GLN

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Mol	Chain	Res	Type
1	A	955	ASN
1	A	973	GLN
1	A	991	ASN
1	A	1047	ASN
1	A	1048	HIS
2	B	195	ASN
2	B	205	ASN
2	B	292	ASN
2	B	293	ASN
2	B	346	HIS
2	B	369	ASN
2	B	430	ASN
2	B	561	ASN
2	B	610	GLN
2	B	623	ASN
2	B	632	GLN
2	B	646	ASN
2	B	693	ASN
2	B	701	HIS
2	B	731	GLN
2	B	748	GLN
2	B	769	GLN
2	B	821	ASN
2	B	836	GLN
2	B	858	HIS
2	B	891	HIS
2	B	931	ASN
2	B	933	ASN
2	B	938	ASN
2	B	978	GLN
2	B	1015	GLN
2	B	1103	HIS
2	B	1121	HIS
2	B	1203	HIS
2	B	1205	GLN
2	B	1247	ASN
2	B	1308	ASN
2	B	1332	ASN
2	C	115	GLN
2	C	122	ASN
2	C	173	GLN
2	C	195	ASN

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Mol	Chain	Res	Type
2	C	205	ASN
2	C	209	ASN
2	C	291	HIS
2	C	297	ASN
2	C	306	GLN
2	C	320	GLN
2	C	346	HIS
2	C	349	ASN
2	C	394	GLN
2	C	430	ASN
2	C	577	GLN
2	C	646	ASN
2	C	693	ASN
2	C	711	ASN
2	C	731	GLN
2	C	769	GLN
2	C	836	GLN
2	C	854	GLN
2	C	867	ASN
2	C	882	GLN
2	C	959	GLN
2	C	988	GLN
2	C	1112	ASN
2	C	1205	GLN
2	C	1234	GLN
2	C	1247	ASN
3	D	14	GLN
3	D	83	ASN
3	D	100	ASN
3	D	139	ASN
3	E	14	GLN
3	E	55	HIS
3	E	85	ASN
3	E	155	HIS
3	E	258	ASN
3	E	291	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

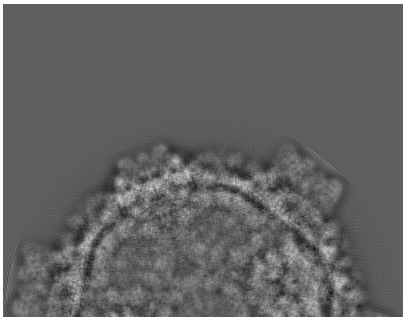
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-5233. These allow visual inspection of the internal detail of the map and identification of artifacts.

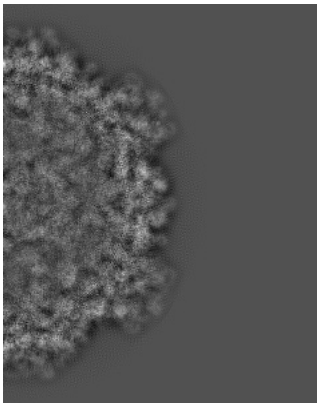
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

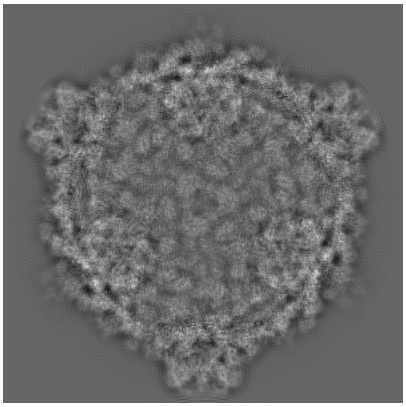
6.1.1 Primary map



X



Y

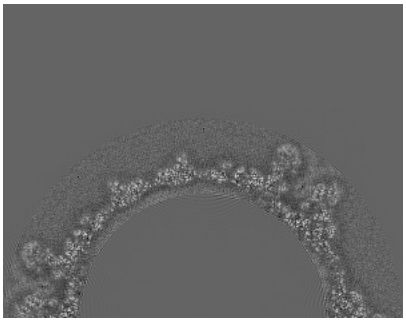


Z

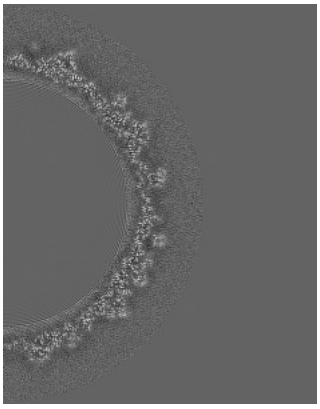
The images above show the map projected in three orthogonal directions.

6.2 Central slices

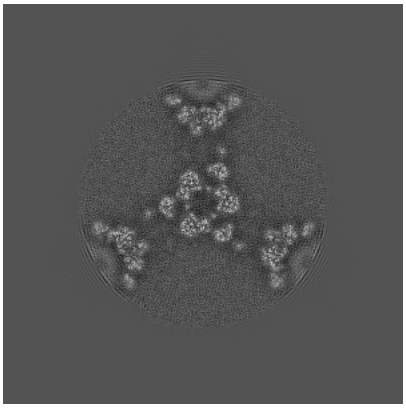
6.2.1 Primary map



X Index: 320



Y Index: 320

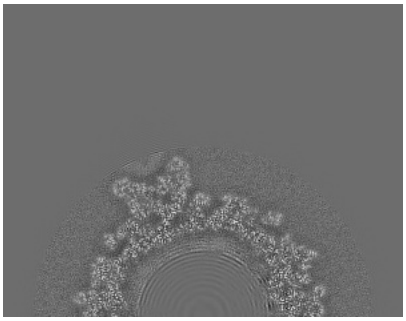


Z Index: 250

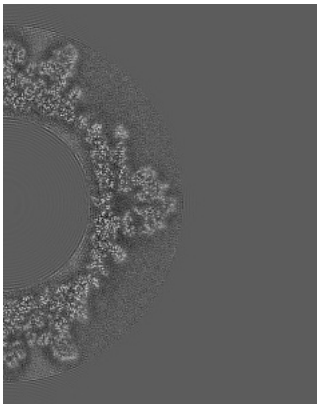
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

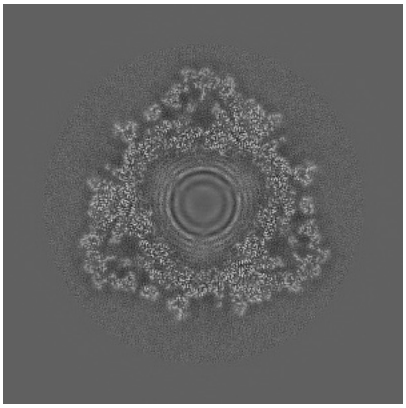
6.3.1 Primary map



X Index: 486



Y Index: 460



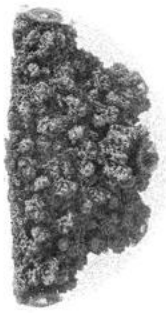
Z Index: 189

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

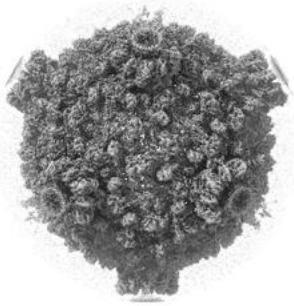
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

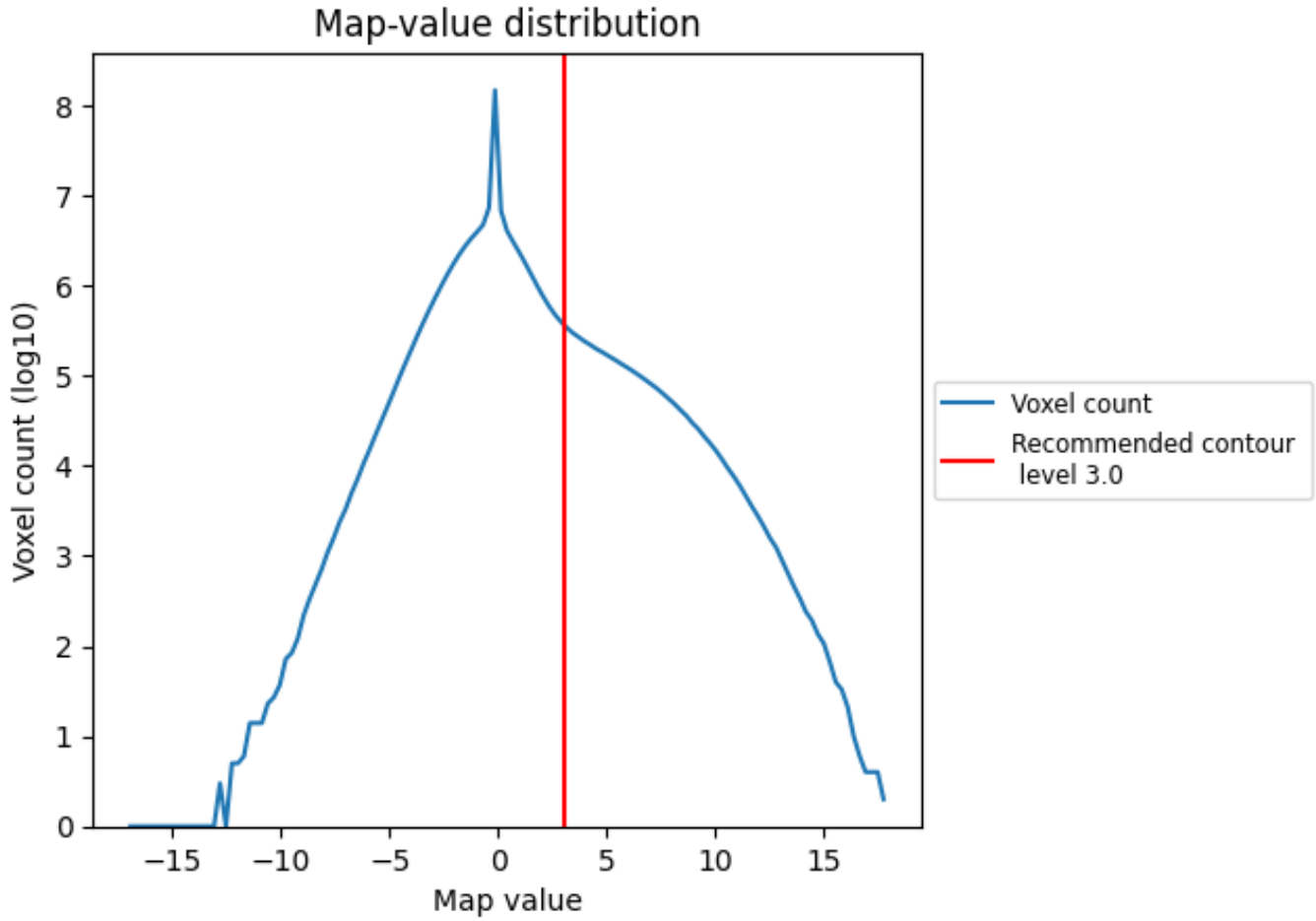
6.5 Mask visualisation (i)

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

7 Map analysis

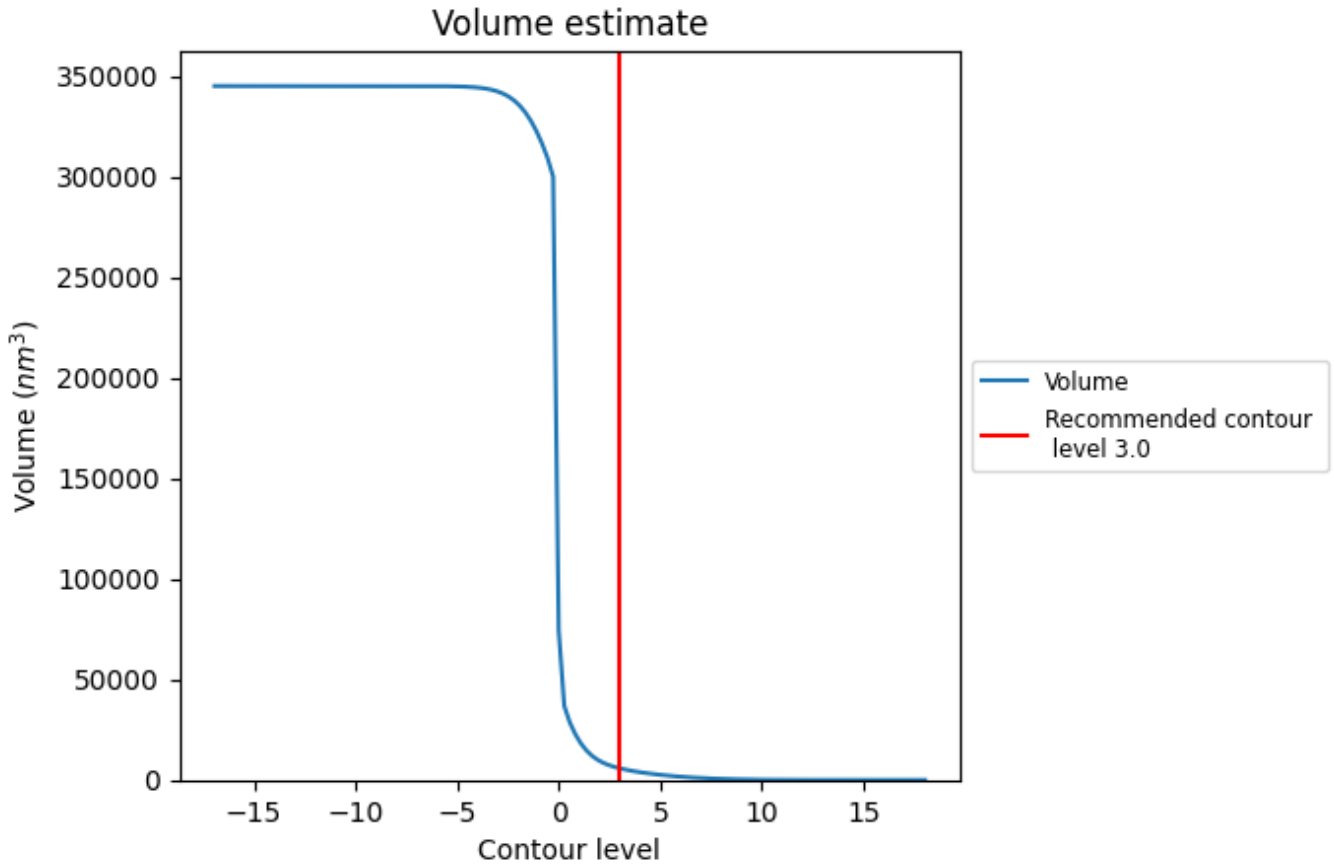
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

7.2 Volume estimate (i)



The volume at the recommended contour level is 5776 nm^3; this corresponds to an approximate mass of 5218 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)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation (i)

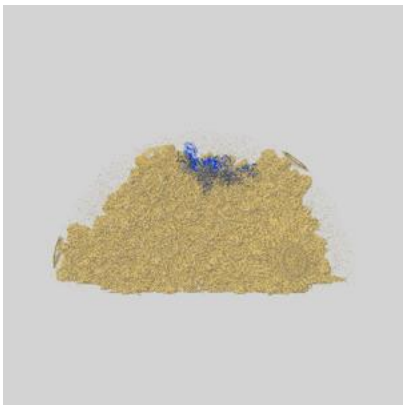
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

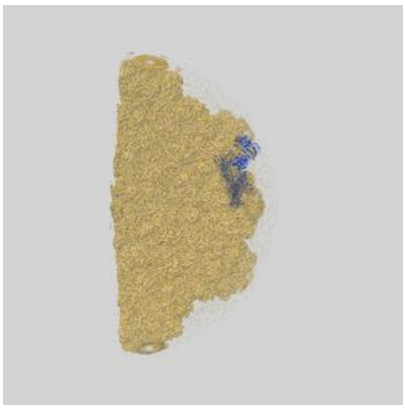
This section contains information regarding the fit between EMDB map EMD-5233 and PDB model 3IZ3. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlays

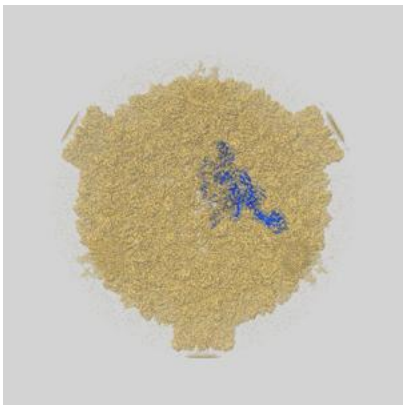
9.1.1 Map-model overlay



X

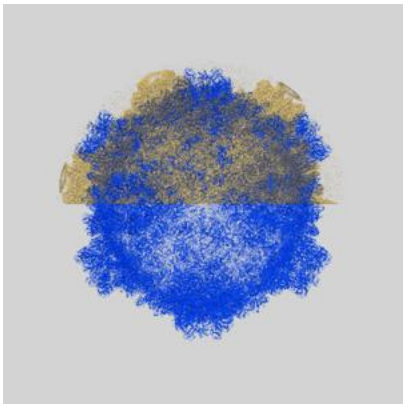


Y

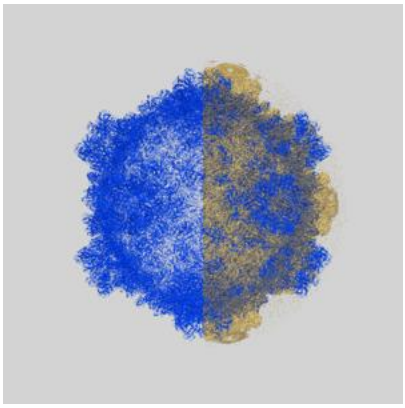


Z

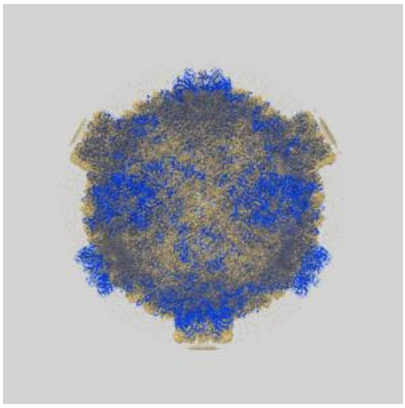
9.1.2 Map-model assembly overlay



X



Y



Z

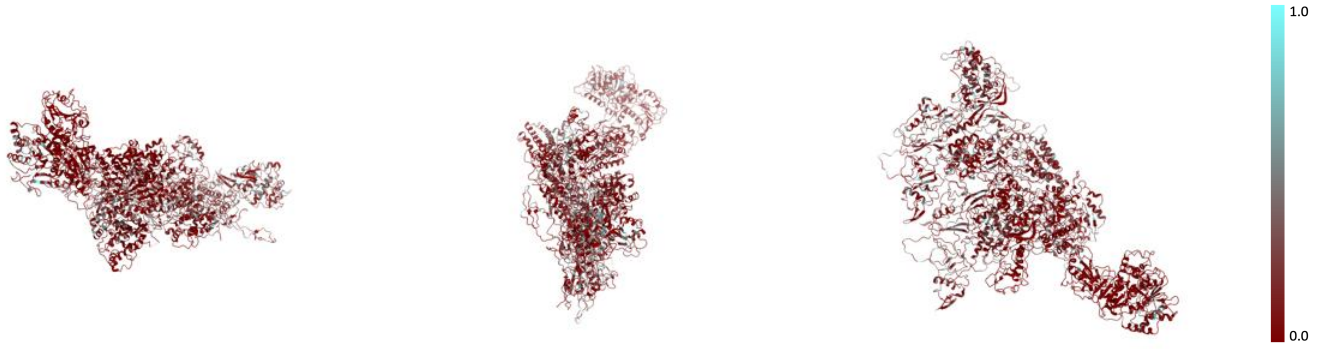
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model

X Y Z

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

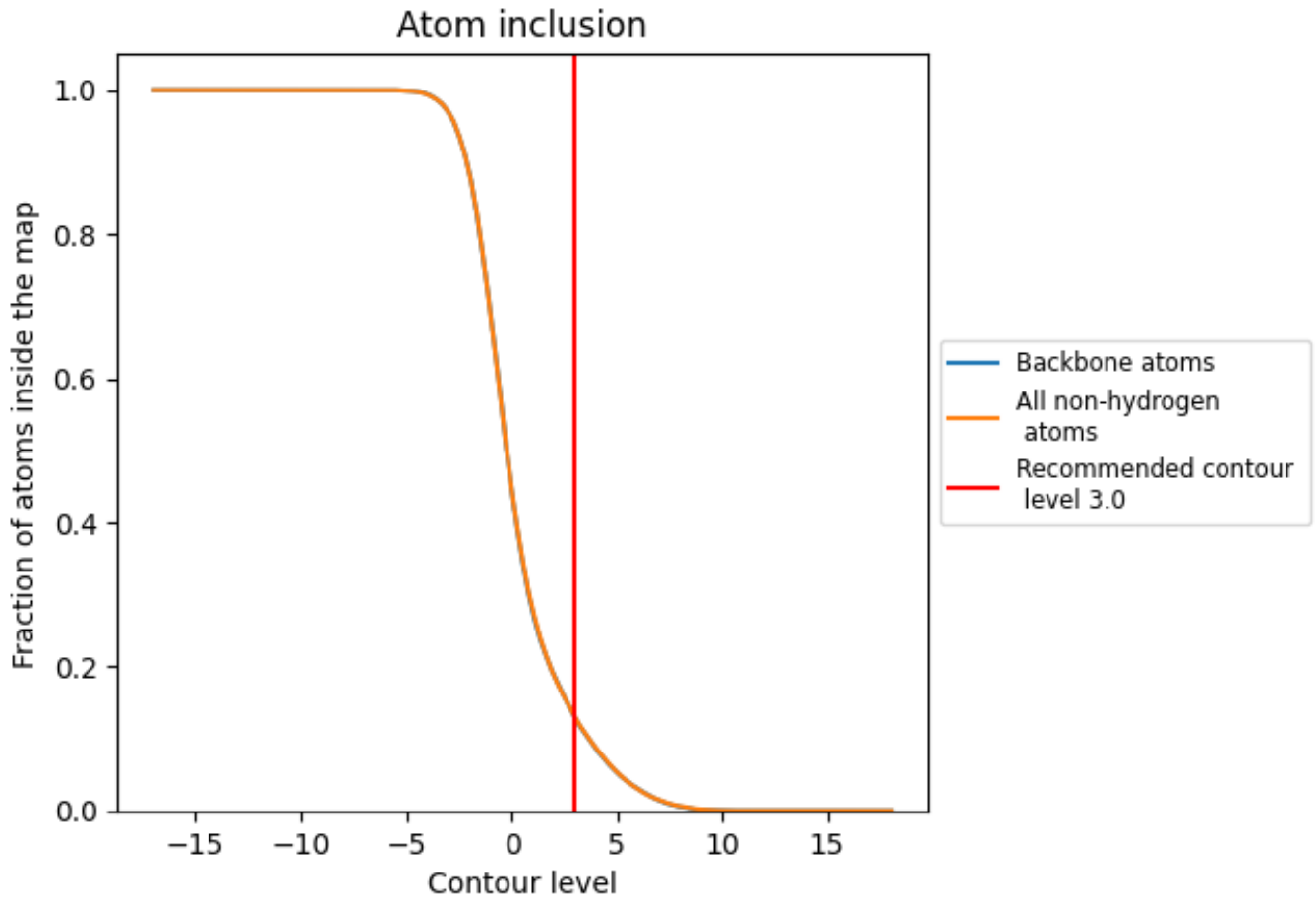
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.0).

9.4 Atom inclusion (i)



At the recommended contour level, 13% of all backbone atoms, 13% 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 (3.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.1310	-0.0110
A	0.0692	0.0000
B	0.1388	-0.0140
C	0.1647	-0.0200
D	0.1161	-0.0100
E	0.1944	-0.0040