Full wwPDB EM Validation Report

Oct 1, 2024 – 03:17 pm BST

PDB ID	:	8RRW
EMDB ID	:	EMD-19467
Title	:	Structure of RyR1 in detergent in open state in complex with FKBP and Nb9657.
Authors	:	Li, C.; Efremov, R.G.
Deposited on	:	2024-01-23
Resolution	:	4.20 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:

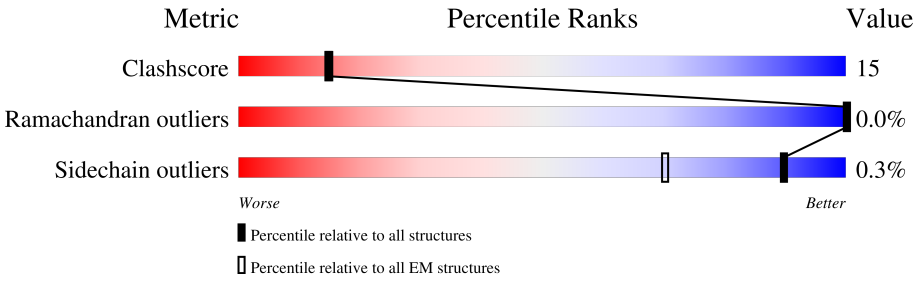
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 4.20 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	B	5027	57% 28% 14%
1	E	5027	57% 28% 14%
1	G	5027	58% 28% 14%
1	J	5027	58% 28% 14%
2	A	107	40% 78% 22%
2	D	107	41% 77% 23%
2	H	107	40% 77% 23%
2	I	107	40% 75% 25%

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Mol	Chain	Length	Quality of chain
3	C	137	5% 56% 36% 8%
3	F	137	5% 55% 36% 8%
3	K	137	5% 55% 36% 8%
3	M	137	5% 55% 36% 8%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 143744 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 Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	4319	Total	C	N	O	S	1	0
			34104	21737	5881	6261	225		
1	E	4319	Total	C	N	O	S	1	0
			34104	21737	5881	6261	225		
1	G	4319	Total	C	N	O	S	1	0
			34104	21737	5881	6261	225		
1	J	4319	Total	C	N	O	S	1	0
			34104	21737	5881	6261	225		

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	D	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	I	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ASP	GLY	conflict	UNP Q8HYX6
D	100	ASP	GLY	conflict	UNP Q8HYX6
H	100	ASP	GLY	conflict	UNP Q8HYX6
I	100	ASP	GLY	conflict	UNP Q8HYX6

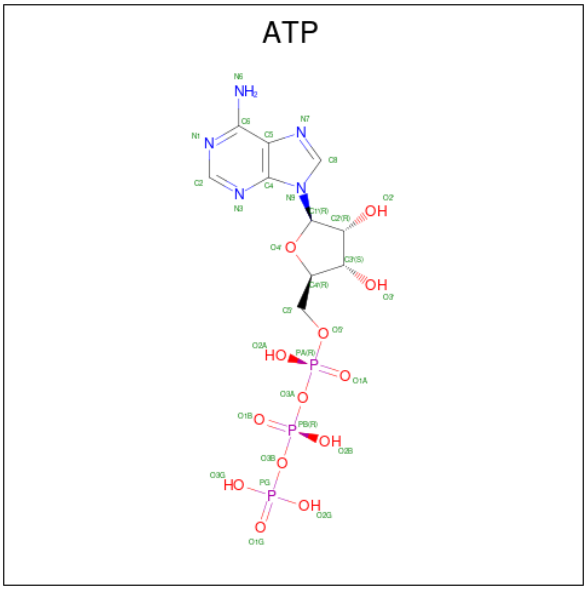
- Molecule 3 is a protein called Nanobody 9657.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	126	Total	C	N	O	S	0	0
			967	597	170	195	5		
3	F	126	Total	C	N	O	S	0	0
			967	597	170	195	5		
3	K	126	Total	C	N	O	S	0	0
			967	597	170	195	5		
3	M	126	Total	C	N	O	S	0	0
			967	597	170	195	5		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total	Zn	0
			1	1	
4	E	1	Total	Zn	0
			1	1	
4	G	1	Total	Zn	0
			1	1	
4	J	1	Total	Zn	0
			1	1	

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
5	B	1	Total	C	N	O	P	0
			31	10	5	13	3	

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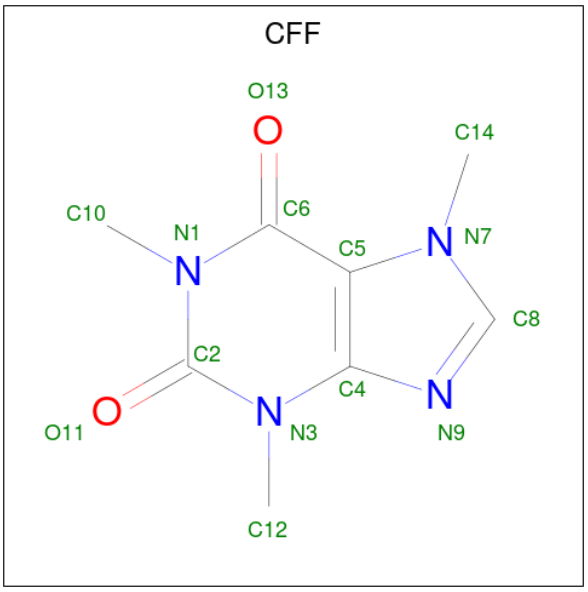
Mol	Chain	Residues	Atoms					AltConf
5	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	G	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	J	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 6 is CAFFEINE (three-letter code: CFF) (formula: $C_8H_{10}N_4O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total	C	N	O	0
			14	8	4	2	
6	E	1	Total	C	N	O	0
			14	8	4	2	
6	G	1	Total	C	N	O	0
			14	8	4	2	
6	J	1	Total	C	N	O	0
			14	8	4	2	

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
7	B	1	Total	Ca	0
			1	1	

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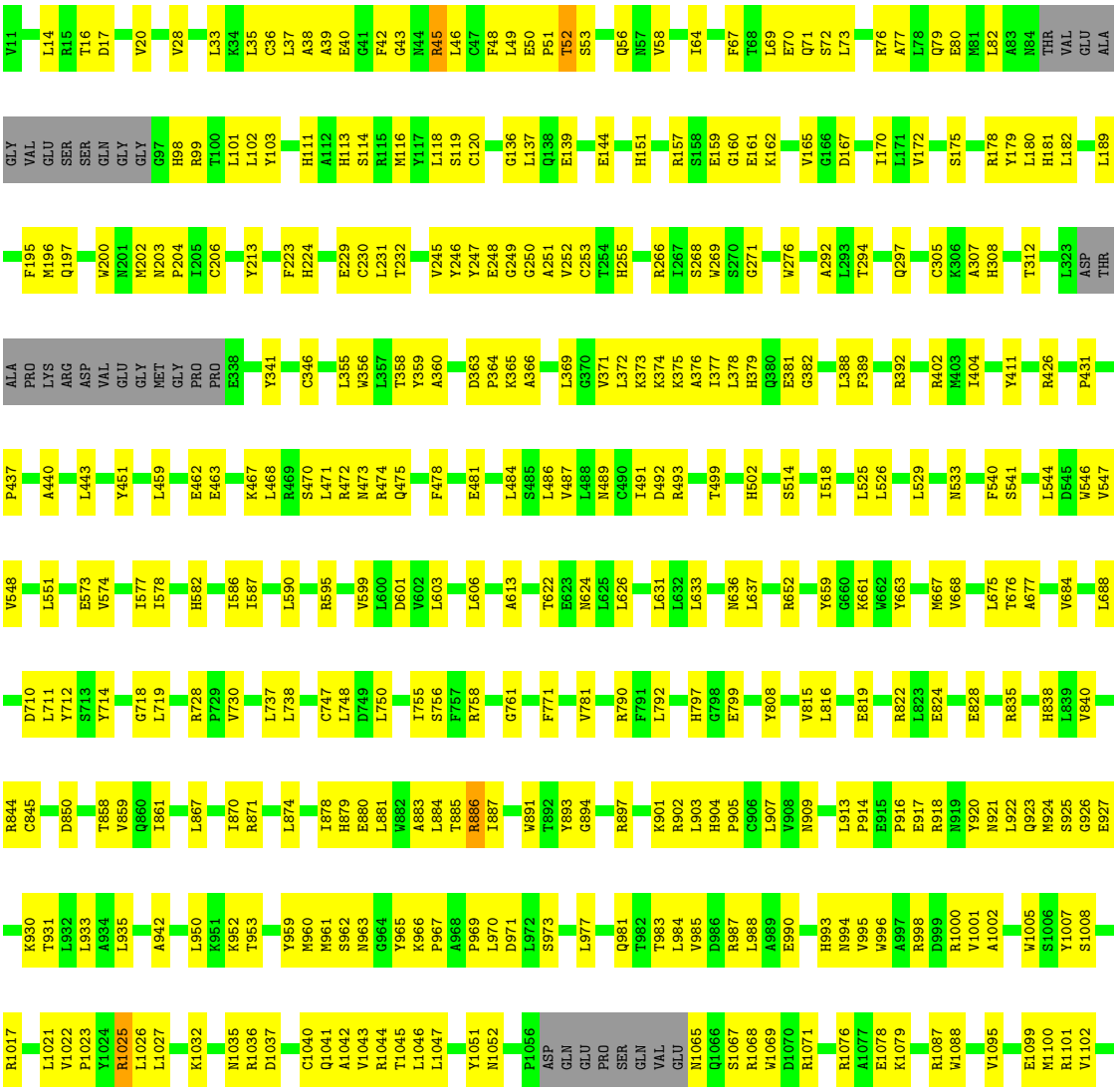
Mol	Chain	Residues	Atoms	AltConf
7	E	1	Total Ca 1 1	0
7	G	1	Total Ca 1 1	0
7	J	1	Total Ca 1 1	0

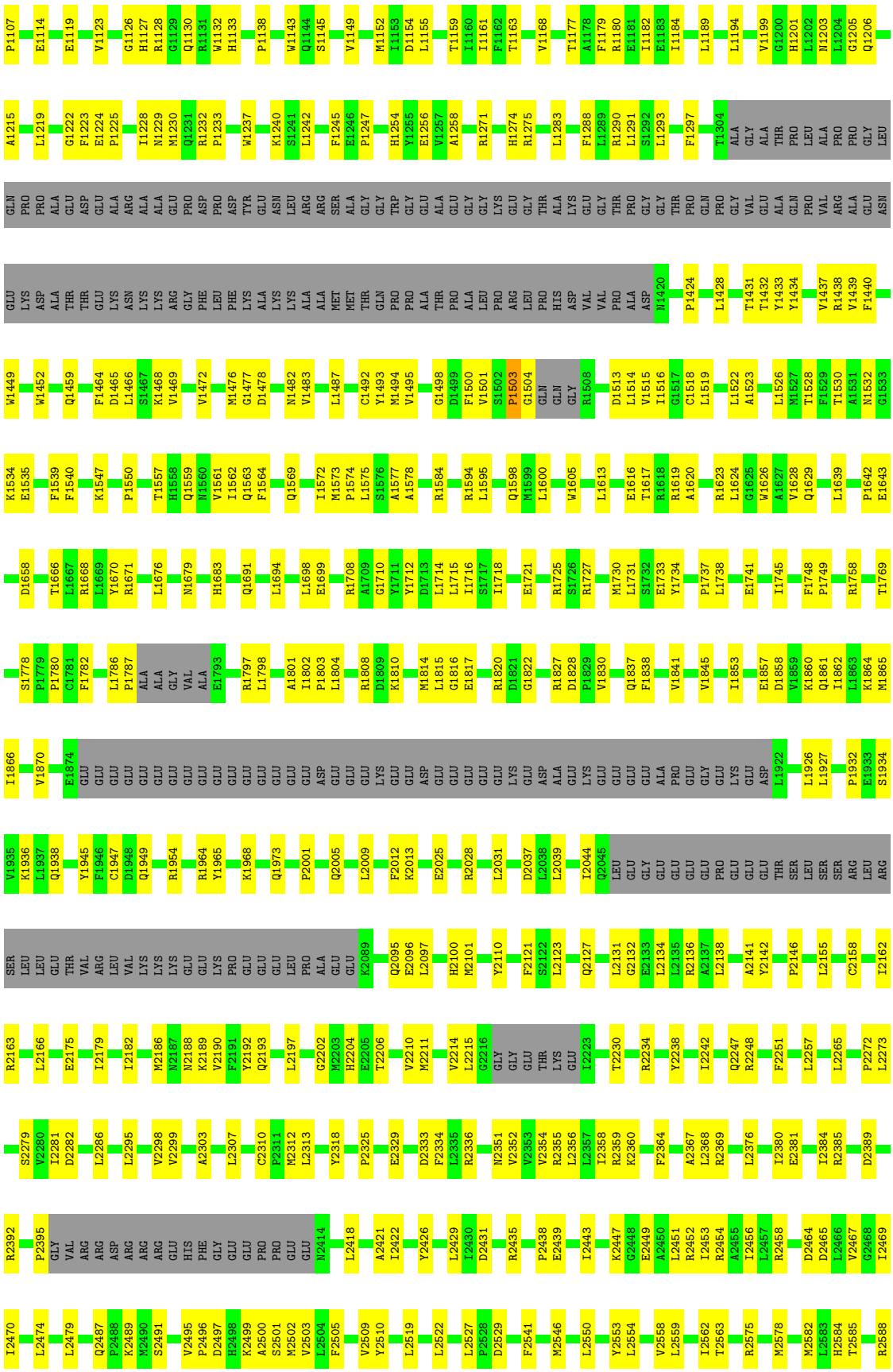
3 Residue-property plots (i)

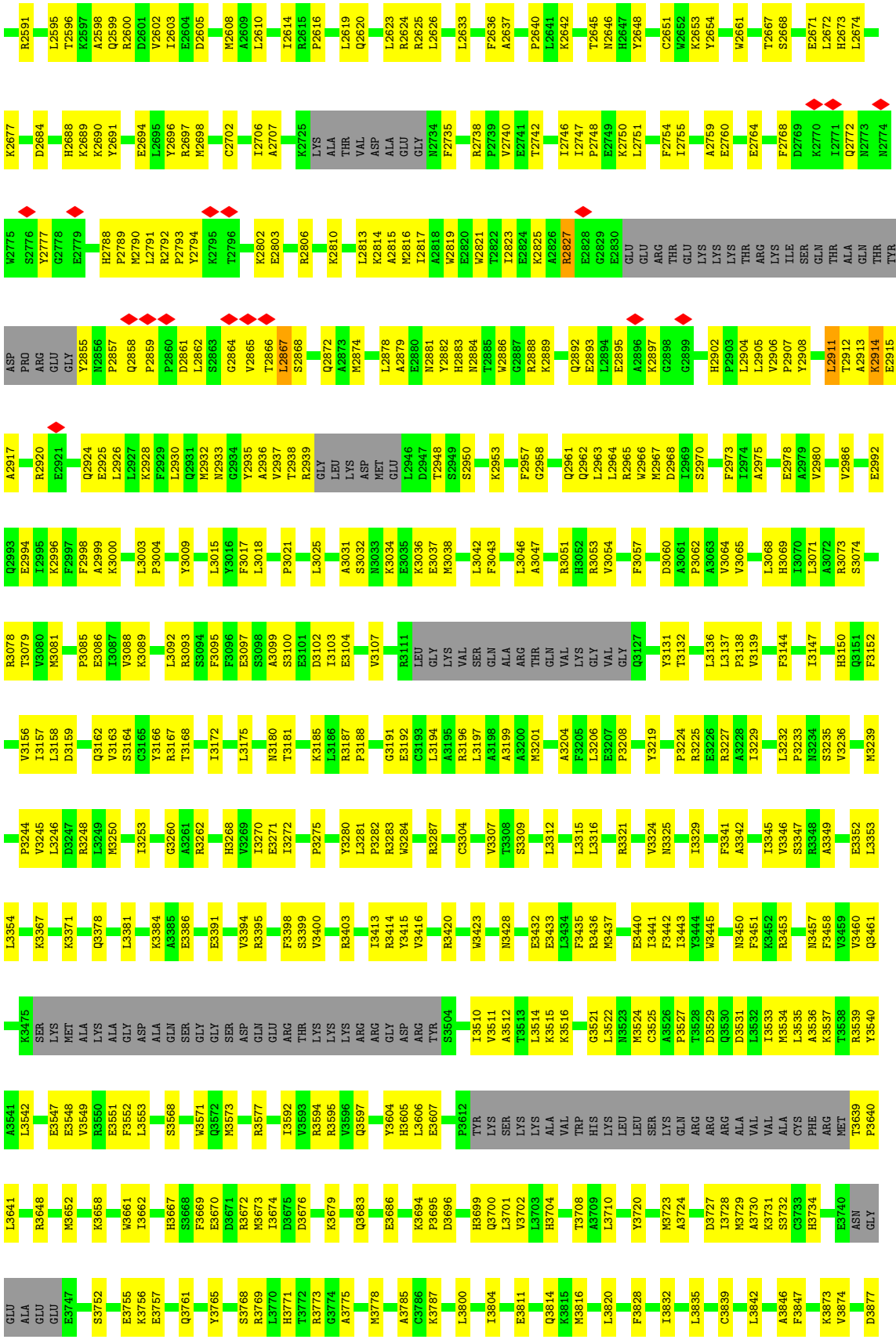
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

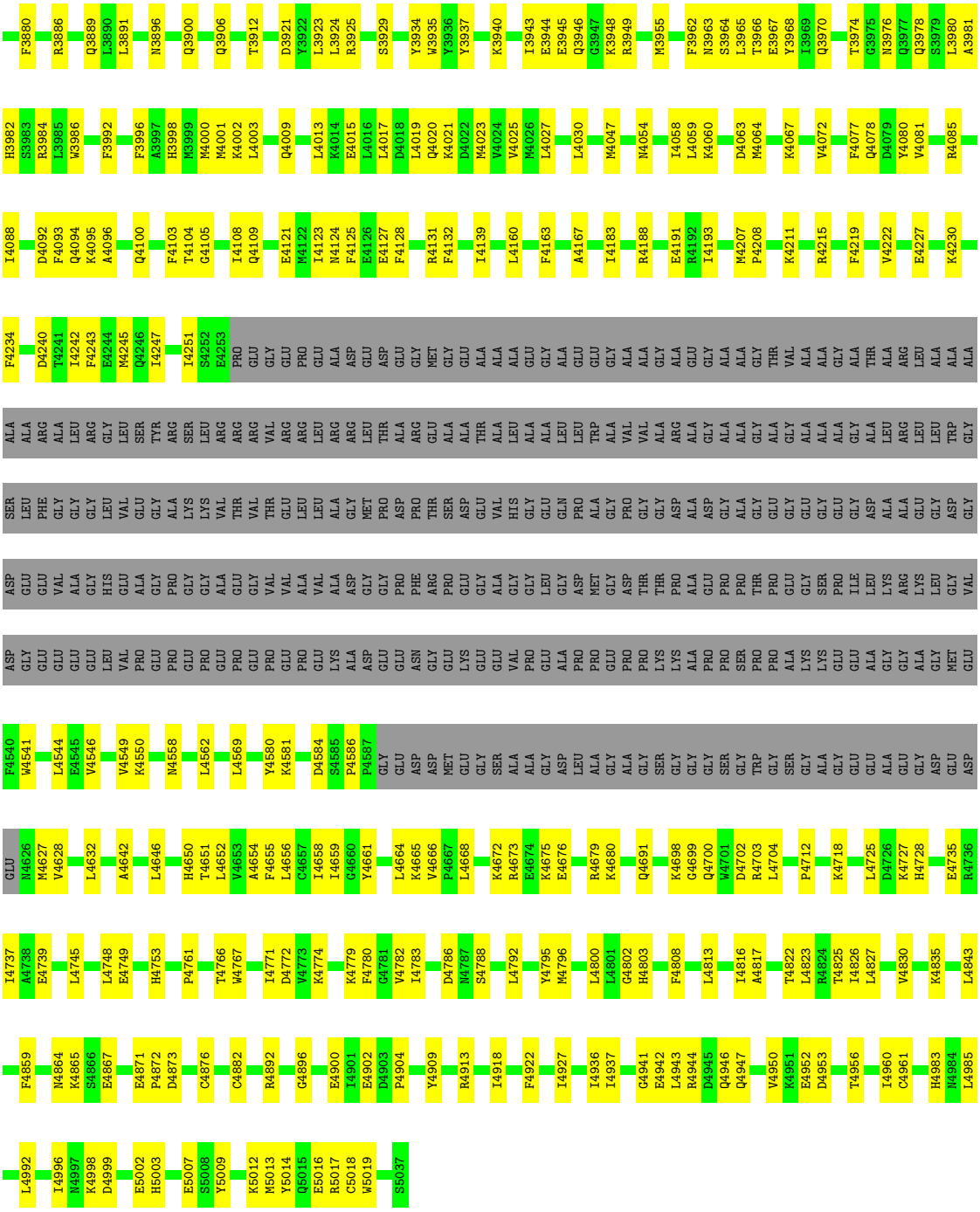
- Molecule 1: Ryanodine receptor 1

Chain B:



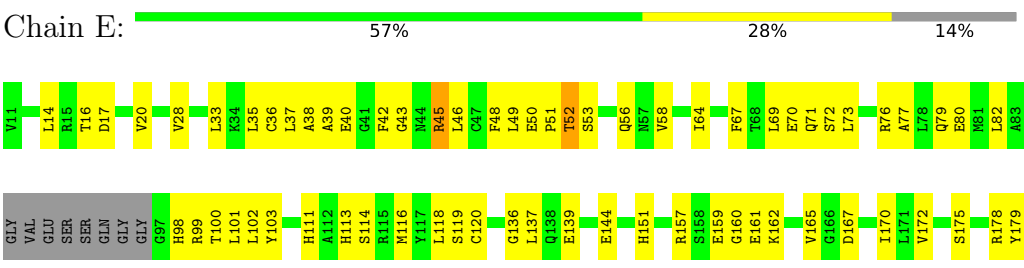


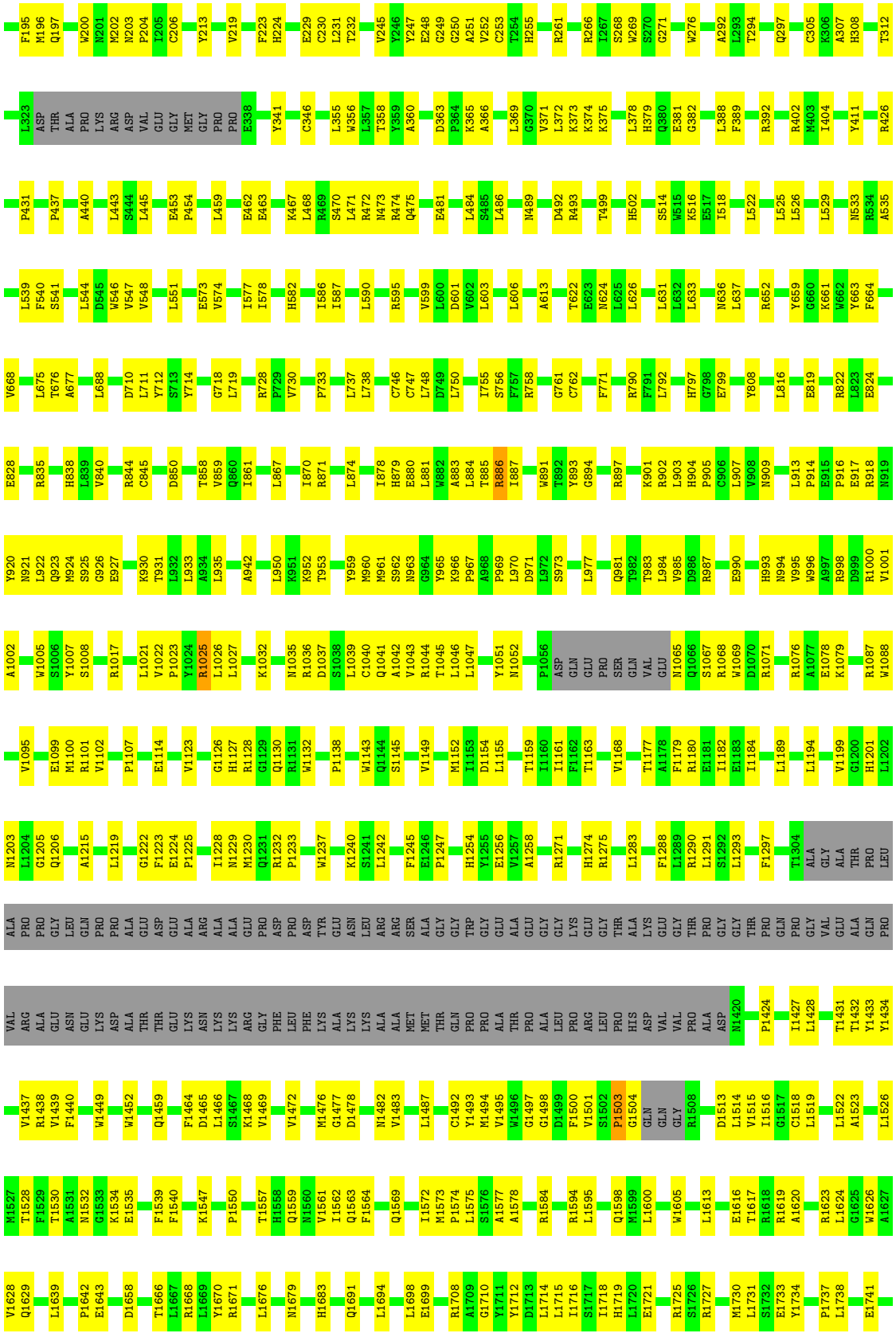


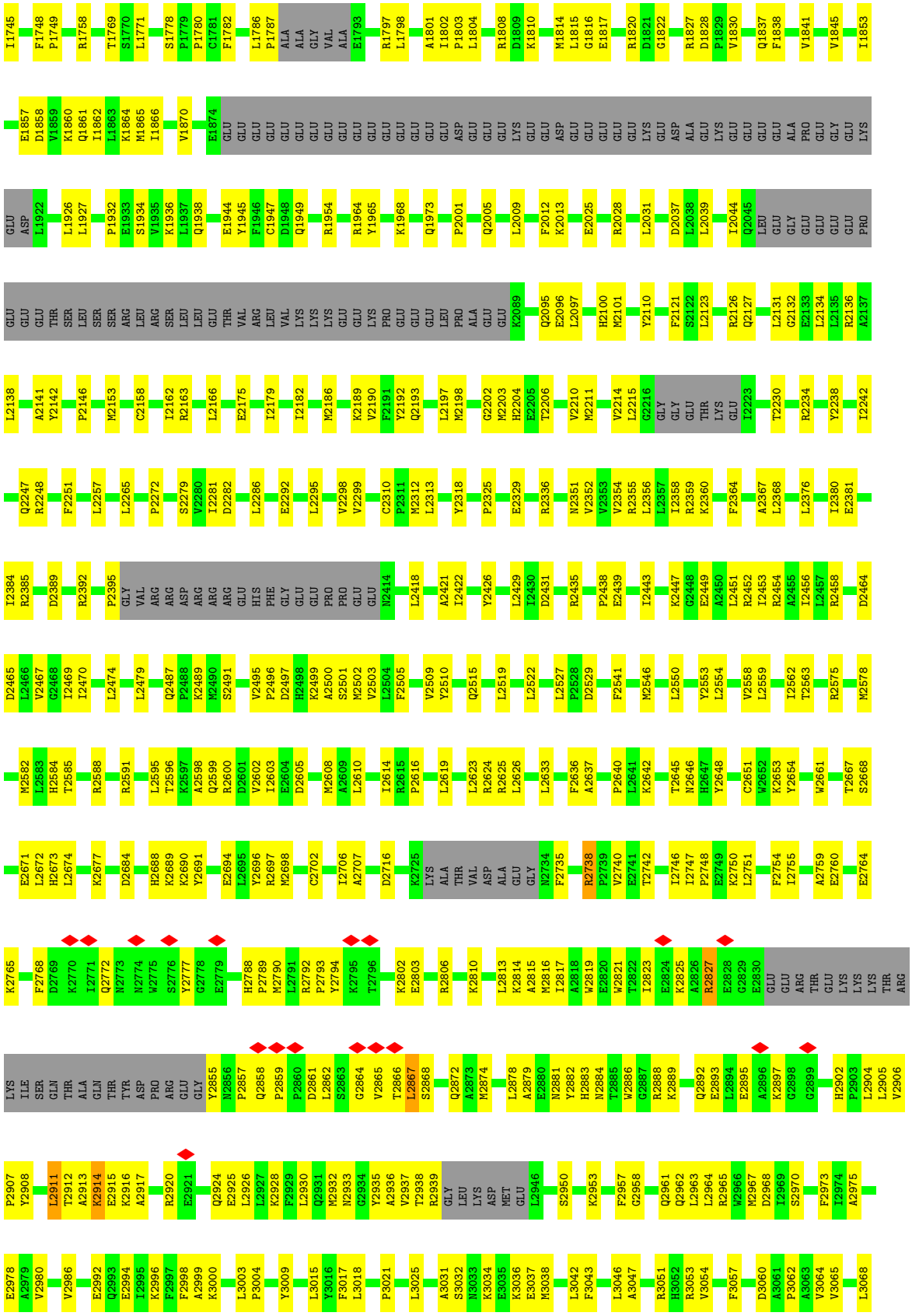


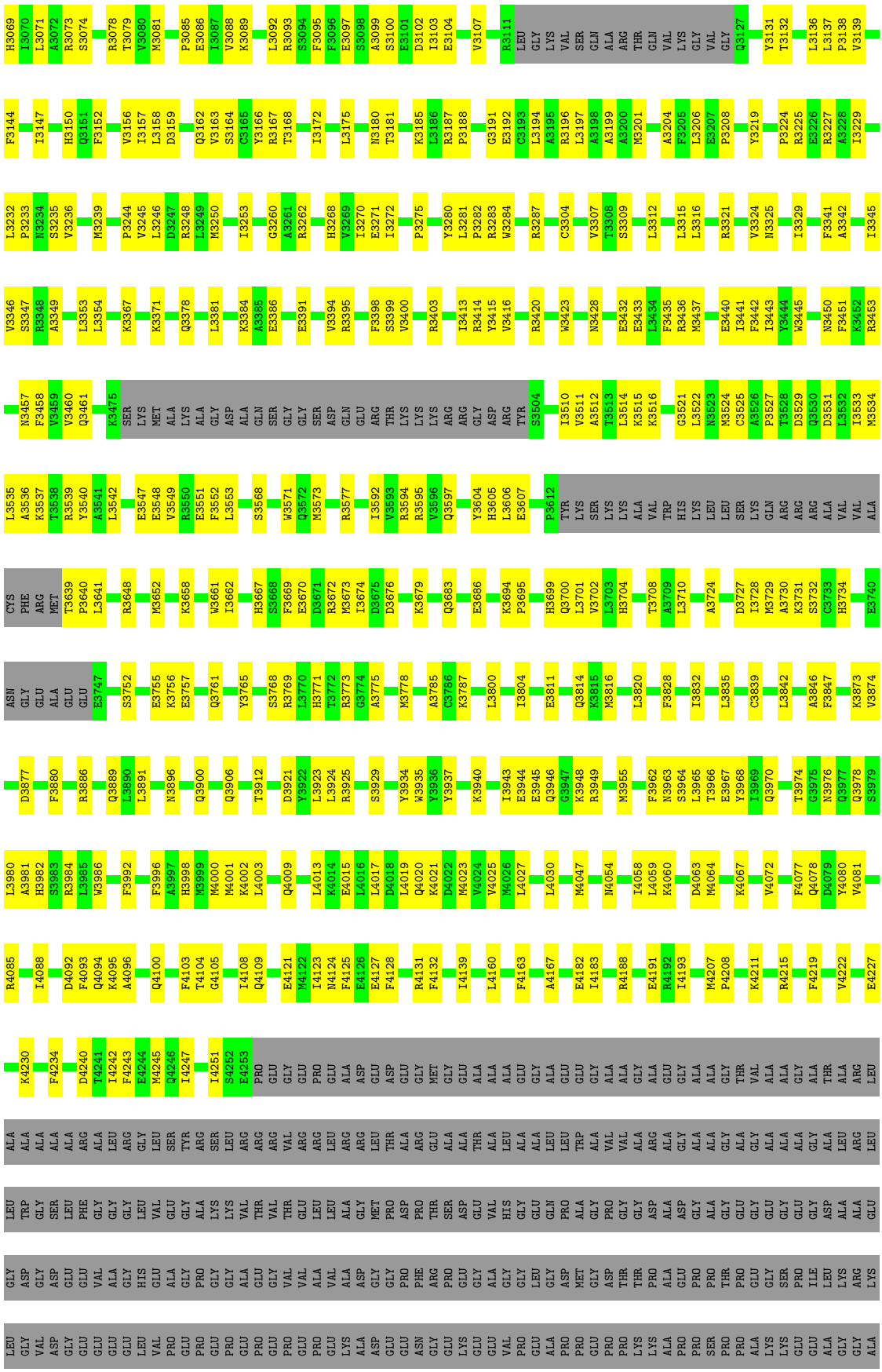
• Molecule 1: Ryanodine receptor 1

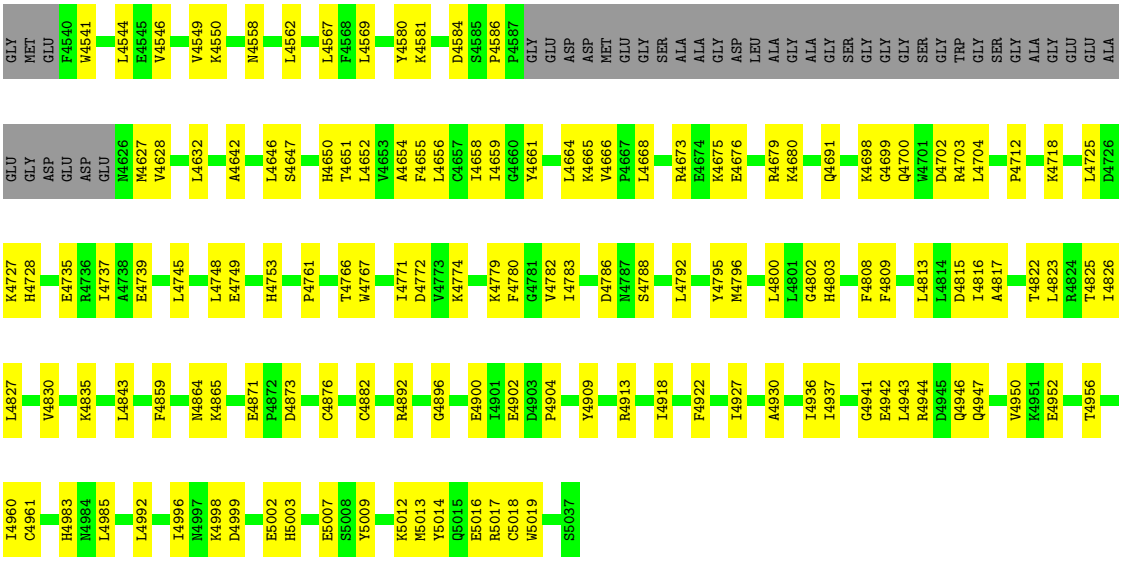
Chain E:




F195 M196 Q197 W200 N201 M202 N203 P204 I205 C206 Y213 V219 F223 H224 E229 C230 L231 T232 V245 Y246 Y247 E248 G249 G250 A251 V252 C253 T254 H255 R261 R266 I267 S268 W269 S270 G271 W276 A292 L293 T294 Q297 C305 K306 A307 H308 T312
L323 ASP THR ALA PRO LYS ARG ASP VAL GLU GLY MET GLY PRO PRO E338 Y341 C346 L355 W356 L357 T358 Y359 A360 D363 P364 K365 A366 L369 G370 V371 L372 K373 K374 K375 L378 H379 Q380 E381 G382 L388 F389 R392 R402 M403 I404 Y411 R426
P431 P437 A440 L443 S444 L445 E453 P454 L459 E462 E463 K467 L468 R469 S470 L471 R472 N473 R474 Q475 E481 L484 S485 L486 N489 D492 R493 T499 H502 S514 W515 K516 E517 I518 L522 L525 L526 L529 N533 R534 A535
L539 F540 S541 L544 D545 W546 V547 V548 L551 E573 V574 I577 I578 H582 I586 I587 L590 R595 V599 L600 D601 V602 L603 L606 A613 T622 E623 N624 L625 L626 L631 L632 L633 N636 L637 R652 Y659 G660 K661 W662 Y663 F664
V668 L675 T676 A677 L688 D710 L711 Y712 S713 Y714 G718 L719 R728 P729 V730 P733 I737 L738 C746 C747 L748 D749 L750 I755 S756 F757 R758 G761 C762 F771 R790 F791 L792 L797 G798 E799 Y808 L816 E819 R822 L823 E824
E828 R835 H838 L839 V840 R844 C845 D850 T858 V859 Q860 I861 L867 I870 R871 L874 I878 H879 E880 L881 W882 A883 L884 T885 R886 I887 W891 T892 Y893 G894 R897 K901 R902 L903 H904 P905 C906 L907 V908 N909 L913 P914 E915 P916 E917 R918 N919
Y920 N921 L922 Q923 M924 S925 G926 E927 K930 T931 L932 L933 A934 L935 A942 L950 K951 K952 T953 Y959 M960 M961 S962 N963 G964 Y965 K966 P967 A968 P969 L970 D971 L972 S973 L977 Q981 T982 T983 L984 V985 D986 R987 E990 N993 N994 V995 W996 A997 R998 D999 R1000 V1001
A1002 W1005 S1006 Y1007 S1008 R1017 L1021 V1022 P1023 Y1024 R1025 L1026 L1027 K1032 N1035 R1036 D1037 S1038 L1039 C1040 Q1041 A1042 V1043 R1044 T1045 L1046 L1047 Y1051 N1052 P1056 ASP GLN GLU PRO SER GLN VAL GLU N1065 Q1066 S1067 R1068 W1069 D1070 R1071 R1076 A1077 E1078 K1079 R1087 W1088
V1095 E1099 M1100 R1101 V1102 P1107 E1114 V1123 G1126 H1127 R1128 C1129 Q1130 R1131 W1132 P1138 W1143 Q1144 S1145 V1149 M1152 I1153 D1154 L1155 T1159 I1160 I1161 F1162 T1163 V1168 T1177 A1178 F1179 R1180 E1181 I1182 E1183 I1184 L1189 L1194 V1199 G1200 H1201 L1202
N1203 L1204 G1205 Q1206 A1215 L1219 G1222 F1223 E1224 P1225 I1228 N1229 M1230 Q1231 R1232 P1233 W1237 K1240 S1241 L1242 F1245 E1246 P1247 H1254 Y1255 E1256 V1257 A1258 R1271 H1274 R1275 L1283 F1288 L1289 R1290 L1291 S1292 L1293 F1297 T1304 ALA GLY ALA THR PRO LEU
ALA PRO PRO GLY LEU GLN PRO PRO ALA GLU ASP GLU ALA ARG ALA ALA ALA GLU PRO ASP PRO ASP TYR GLU ASN LEU ARG ARG SER ALA GLY GLY TRP GLY GLU ALA GLU GLY GLY LYS GLU GLY THR ALA LYS GLU GLY THR PRO GLY GLY GLY THR PRO GLN PRO GLY VAL GLU ALA GLN PRO
VAL ARG ALA GLU ASN GLU LYS ASP ALA THR THR GLU LYS ASN LYS LYS ARG GLY PHE LEU PHE LYS ALA LYS LYS ARG LEU PRO ARG LEU PRO HIS ASP VAL VAL PRO ALA ASP N1420 P1424 I1427 L1428 T1431 T1432 Y1433 Y1434
V1437 R1438 V1439 F1440 W1449 W1452 Q1459 F1464 D1465 L1466 S1467 K1468 V1469 V1472 M1476 G1477 D1478 N1482 V1483 L1487 C1492 Y1493 M1494 V1495 W1496 G1497 G1498 D1499 F1500 V1501 S1502 P1503 G1504 GLN GLN GLY R1508 D1513 L1514 V1515 I1516 G1517 C1518 L1519 L1522 A1523 L1526
M1527 T1528 F1529 T1530 A1531 N1532 G1533 K1534 E1535 F1539 F1540 K1547 P1550 T1557 H1558 Q1559 N1560 V1561 I1562 Q1563 F1564 Q1569 I1572 M1573 P1574 L1575 S1576 A1577 A1578 R1584 R1594 L1595 Q1598 M1599 L1600 W1605 L1613 E1616 T1617 R1618 R1619 A1620 R1623 L1624 G1625 W1626 A1627
V1628 Q1629 L1639 P1642 E1643 D1658 T1666 L1667 R1668 L1669 Y1670 R1671 L1676 N1679 H1683 Q1691 L1694 L1698 E1699 R1708 A1709 G1710 Y1711 Y1712 D1713 L1714 L1715 I1716 S1717 I1718 H1719 L1720 E1721 R1725 S1726 R1727 M1730 L1731 S1732 E1733 Y1734 P1737 L1738 E1741

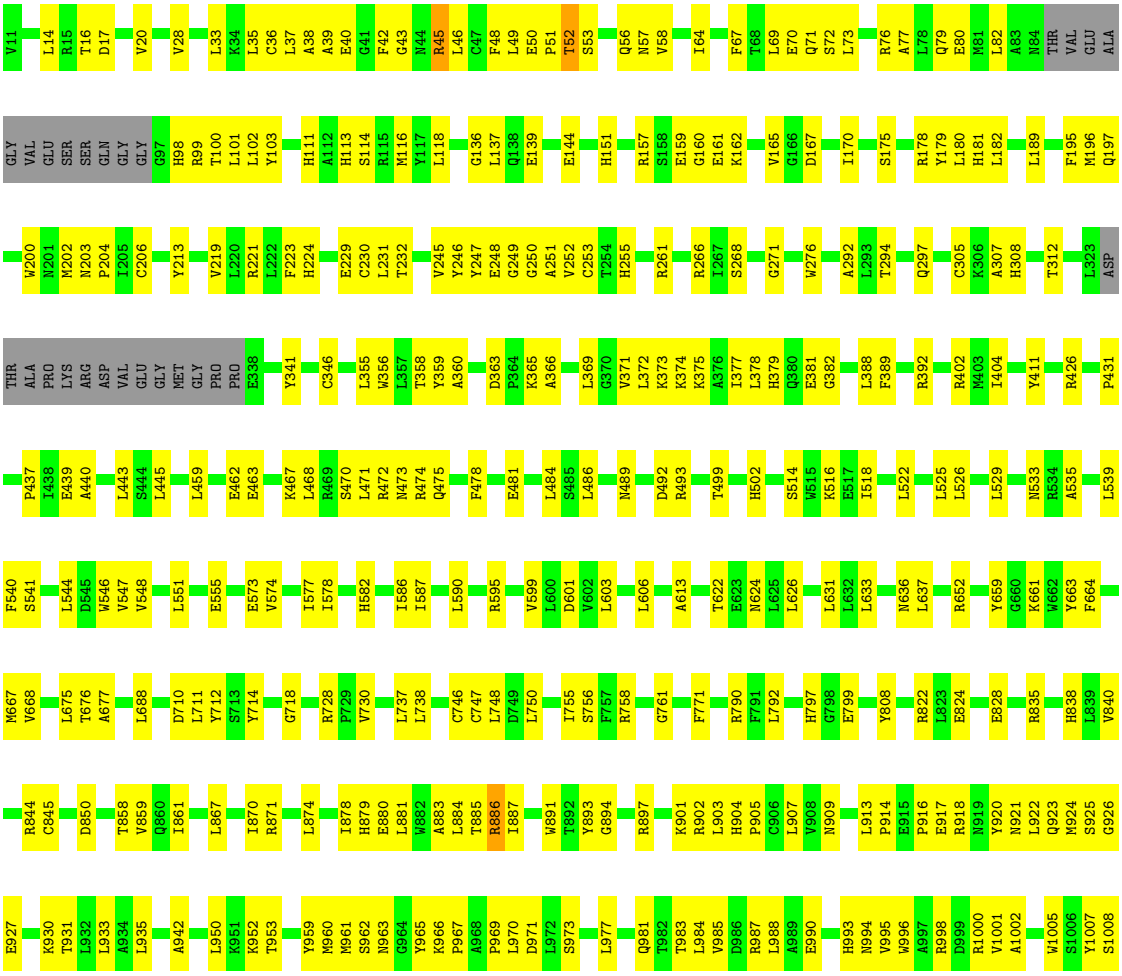


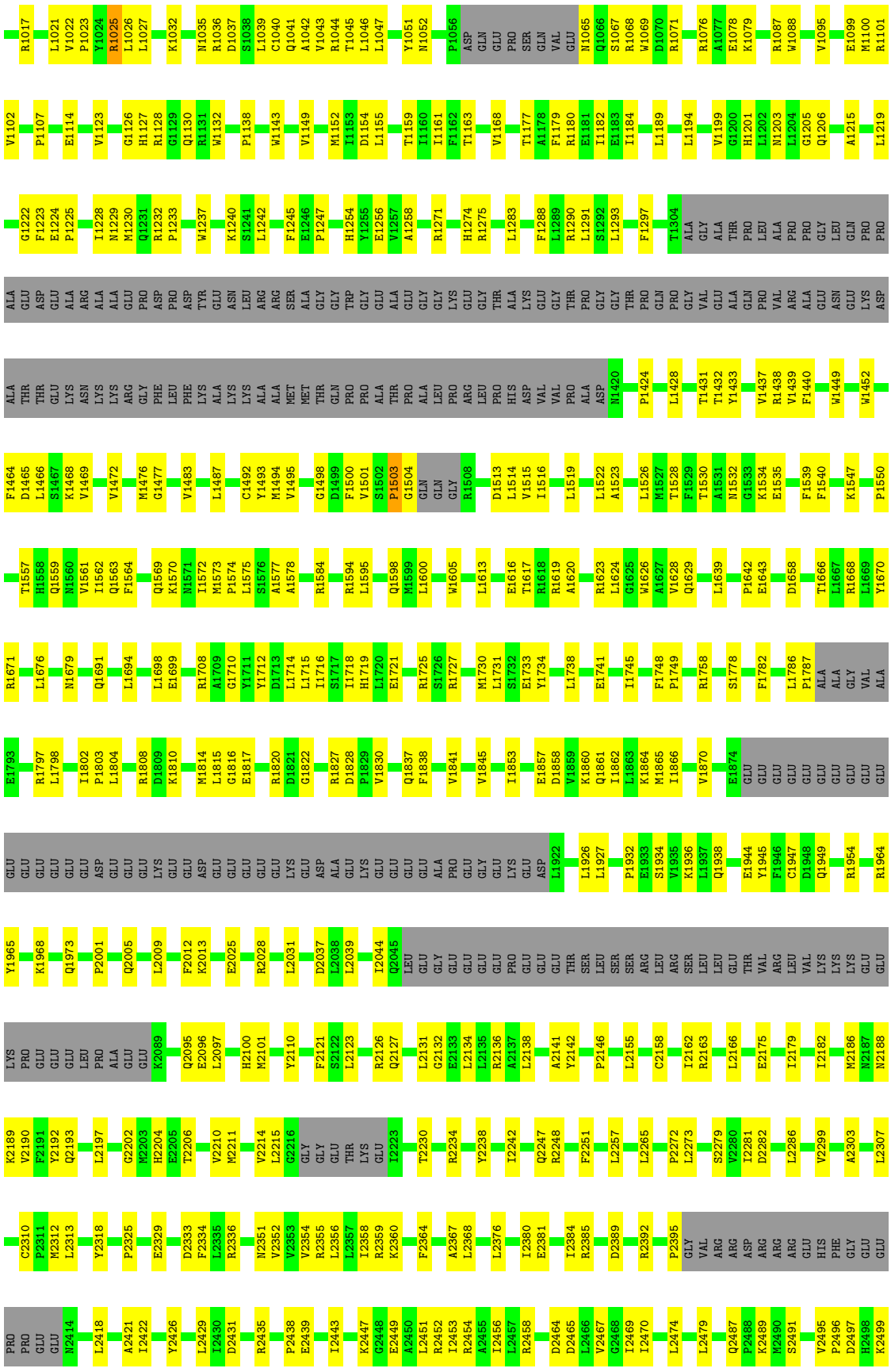


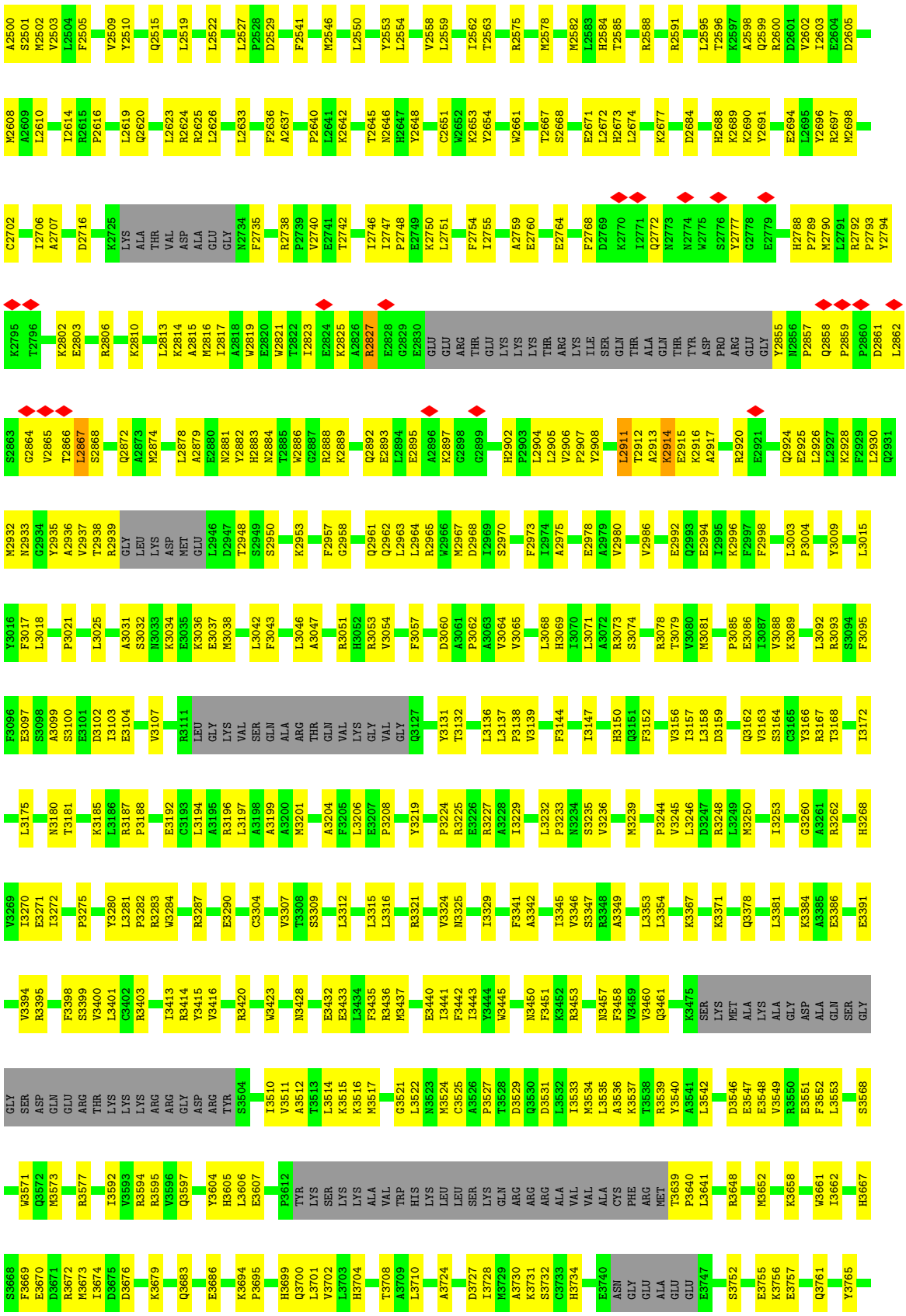


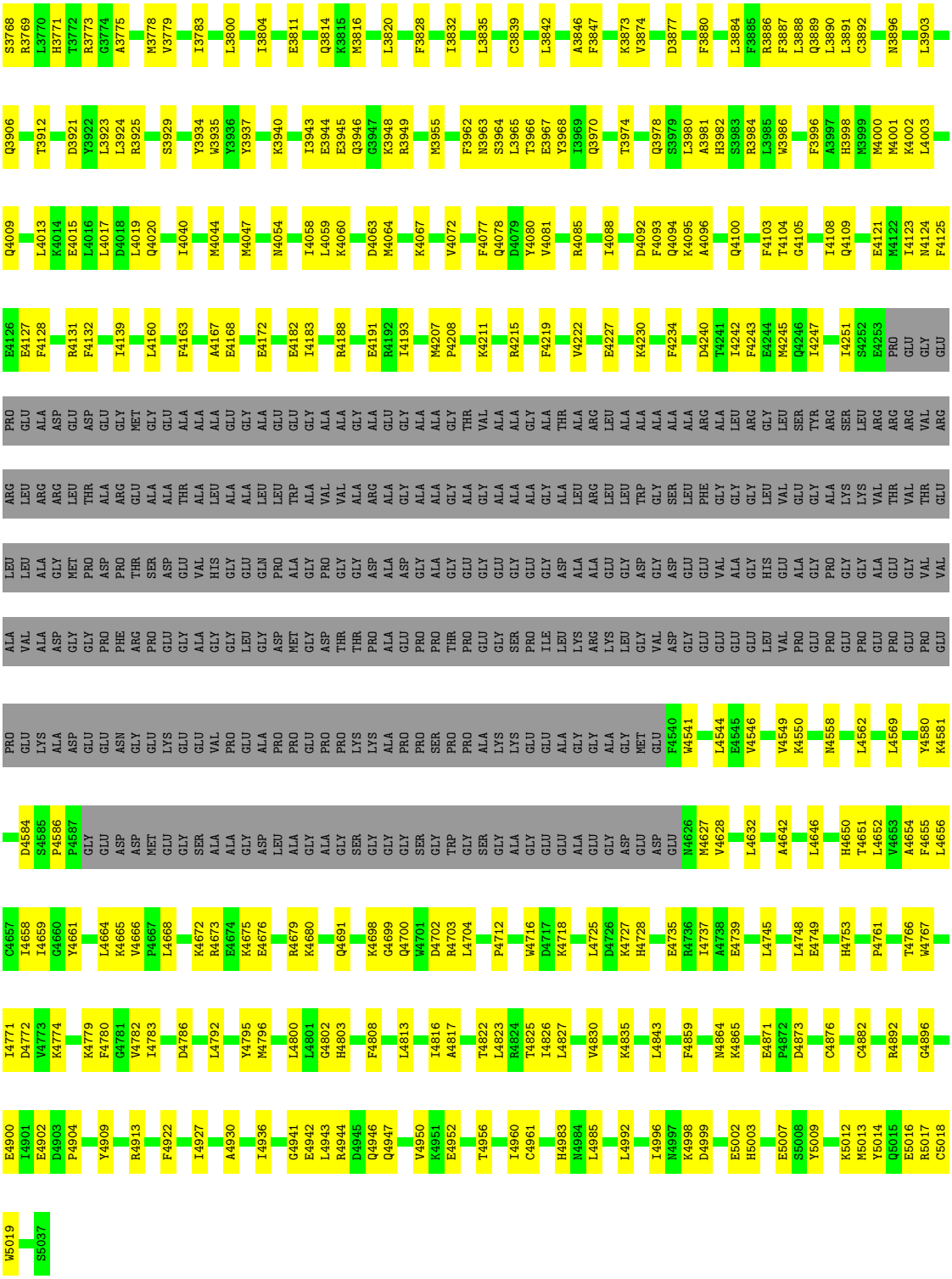
• Molecule 1: Ryanodine receptor 1

Chain G:



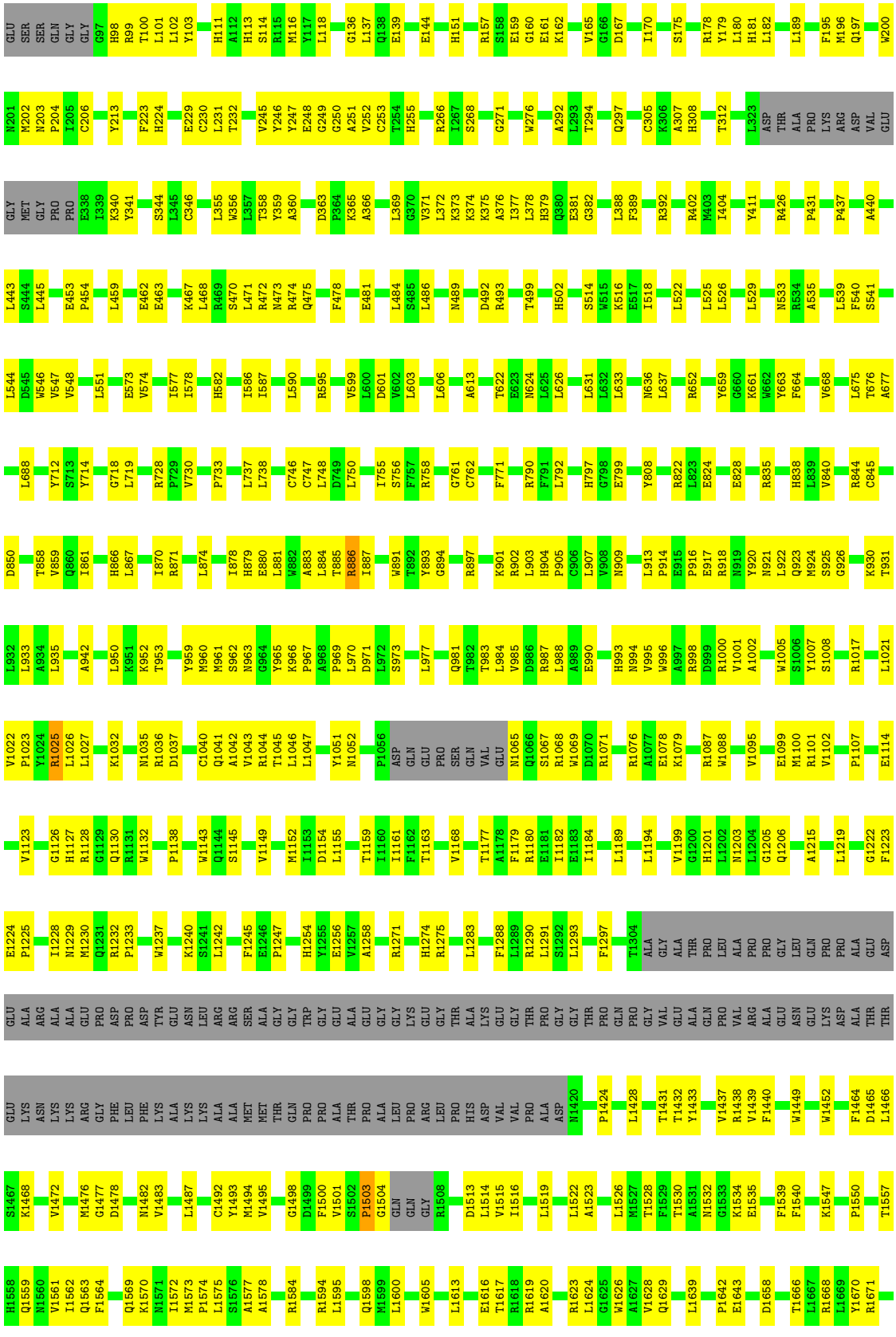


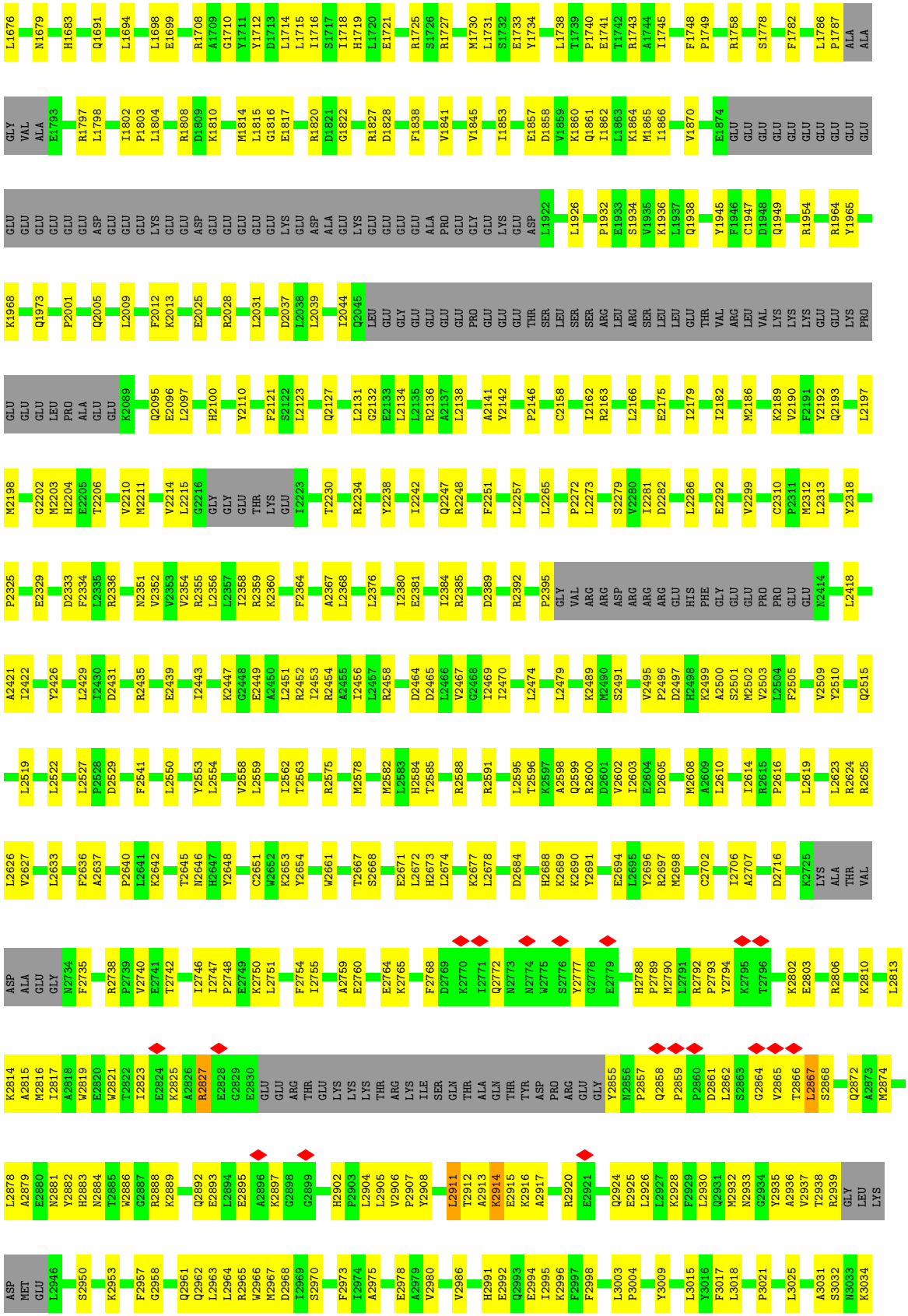




• Molecule 1: Ryanodine receptor 1

Chain J:





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R3111 LEU GLY LYS VAL SER GLN ALA ARG THR GLN VAL LYS GLY VAL GLY Q3127 Y3131 T3132 L3136 L3137 P3138 V3139 F3144 I3147 H3150 Q3151 F3152 V3156 I3157 L3158 D3159 Q3162 V3163 S3164 C3165 Y3166 R3167 T3168 I3172 L3175 N3180 T3181 K3185 L3186 R3187 P3188 E3192

C3193 L3194 A3195 R3196 L3197 A3198 A3199 A3200 M3201 A3204 F3205 L3206 E3207 P3208 Y3219 P3224 R3225 E3226 R3227 A3228 I3229 L3232 P3233 N3234 S3235 V3236 M3239 V3245 L3246 D3247 R3248 L3249 M3250 I3253 G3260 A3261 R3262 H3268 V3269 I3270 E3271 I3272 P3275 Y3280 L3281 P3282 R3283 W3284

R3287 E3290 C3304 V3307 T3308 S3309 L3312 L3315 L3316 R3321 V3324 N3325 I3329 F3341 A3342 I3345 V3346 S3347 R3348 A3349 E3352 L3353 L3354 K3367 K3371 Q3378 L3381 K3384 A3385 E3386 E3391 V3394 R3395 F3398 S3399 V3400 L3401 C3402 R3403 I3413

R3414 Y3415 V3416 R3420 W3423 N3428 E3432 E3433 L3434 F3435 R3436 M3437 E3440 I3441 F3442 I3443 Y3444 W3445 N3450 F3451 K3452 R3453 N3457 F3458 V3459 V3460 Q3461 K3475 SER LYS MET ALA LYS ALA GLY ASP ALA GLN SER GLY GLY SER ASP GLN GLU ARG THR LYS LYS ARG ARG

GLY ASP ARG TYR S3504 I3510 V3511 A3512 T3513 L3514 K3515 K3516 M3517 G3521 M3524 P3527 T3528 D3529 Q3530 D3531 L3532 I3533 M3534 L3535 A3536 K3537 T3538 R3539 Y3540 A3541 L3542 E3547 E3548 V3549 R3550 E3551 F3552 L3553 S3568 W3571 Q3572 M3573 R3577 I3592 V3593 R3594 R3595 V3596 Q3597 Y3604

H3605 L3606 E3607 P3612 TYR LYS SER LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG ARG ARG ALA VAL VAL ALA CYS PHE ARG MET T3639 P3640 L3641 R3648 M3652 K3658 W3661 I3662 H3667 S3668 F3669 E3670 D3671 R3672 M3673 I3674 D3675 D3676 K3679 Q3683 E3686

K3694 P3695 H3699 Q3700 L3701 V3702 L3703 H3704 T3708 A3709 L3710 A3724 Y3725 A3726 D3727 I3728 M3729 A3730 K3731 S3732 C3733 H3734 E3740 ASN GLY GLU ALA GLU GLU E3747 S3752 E3755 K3756 E3757 Q3761 Y3765 S3768 R3769 L3770 H3771 T3772 R3773 G3774 A3775 M3778 V3779 I3783 S3784

A3785 C3786 K3787 L3800 I3804 E3811 Q3814 K3815 M3816 L3820 F3828 I3832 L3835 C3839 L3842 A3846 F3847 K3873 V3874 D3877 F3880 R3886 Q3889 L3890 L3891 N3896 Q3900 Q3906 T3912 D3921 Y3922 L3923 L3924 R3925 S3929 Y3934 W3935

Y3936 Y3937 K3940 I3943 E3944 E3945 Q3946 G3947 K3948 R3949 M3955 F3962 N3963 S3964 L3965 T3966 E3967 Y3968 I3969 Q3970 T3974 G3975 N3976 Q3977 Q3978 S3979 L3980 A3981 H3982 S3983 R3984 L3985 W3986 F3996 A3997 H3998 M3999 M4000 M4001 K4002 L4003 Q4009 L4013 K4014 E4015 L4016 L4017 D4018 L4019 Q4020 K4021 D4022

M4023 V4024 V4025 M4026 L4027 L4030 I4040 M4044 M4047 N4054 I4058 L4059 K4060 D4063 M4064 K4067 V4072 F4077 Q4078 D4079 Y4080 V4081 R4085 I4088 D4092 F4093 Q4094 K4095 A4096 Q4100 F4103 T4104 G4105 I4108 Q4109 E4121 M4122 I4123 N4124 F4125 E4126 E4127 F4128

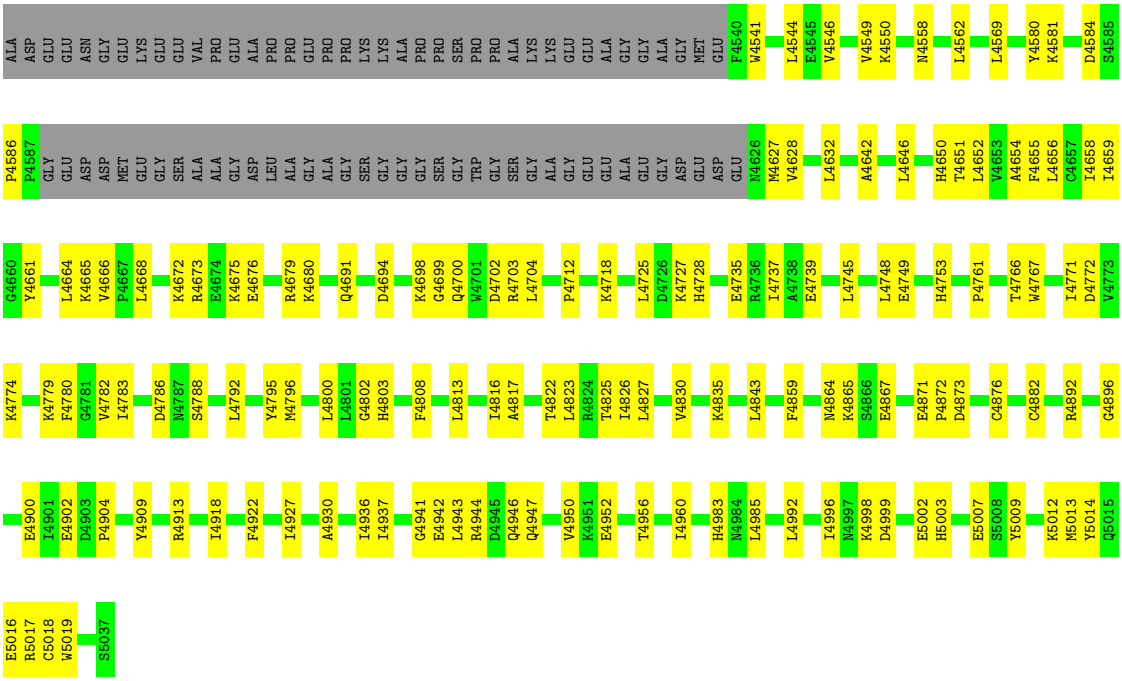
R4131 F4132 I4139 L4160 F4163 A4167 E4168 E4172 E4182 I4183 R4188 E4191 R4192 I4193 M4207 P4208 K4211 R4215 F4219 V4222 E4227 K4230 F4234 D4240 T4241 I4242 F4243 E4244 M4245 Q4246 I4247 I4251 S4252 E4253 PRO GLU GLY GLU PRO GLU ALA

ASP GLU ASP GLU GLY MET GLY GLU ALA ALA ALA GLU GLY ALA GLU GLU GLY ALA ALA GLY ALA GLU GLY ALA ALA GLY THR VAL ALA ALA GLY ALA THR ALA ARG LEU ALA ALA ALA ALA ALA ARG ALA LEU ARG GLY LEU SER TYR ARG SER LEU ARG ARG ARG VAL ARG ARG LEU ARG

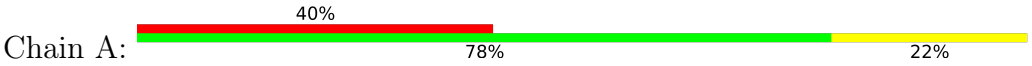
ARG LEU THR ALA ARG GLU ALA ALA THR ALA LEU ALA ALA LEU LEU TRP ALA VAL VAL ALA ARG ALA GLY ALA ALA GLY ALA GLY ALA ALA ALA GLY ALA LEU ARG LEU LEU TRP GLY SER LEU PHE GLY GLY GLY LEU VAL GLU GLY ALA LYS LYS VAL THR VAL THR GLU LEU ALA

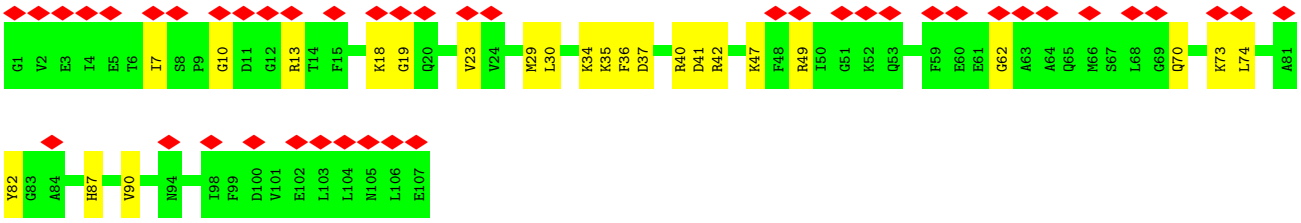
GLY MET PRO ASP PRO THR SER ASP GLU VAL HIS GLY GLU GLN PRO ALA GLY PRO GLY GLY ASP ALA ASP GLY ALA GLY GLU GLY GLU GLY GLU GLY ASP ALA ALA GLU GLY ASP GLY ASP GLU VAL ALA GLY HIS GLU ALA GLY PRO GLY GLY ALA GLU GLY VAL VAL ALA VAL ALA

ASP GLY GLY PRO PHE ARG PRO GLU GLY ALA GLY GLY LEU GLY ASP MET GLY ASP THR THR PRO ALA GLU PRO PRO THR PRO GLU GLY GLY SER PRO ILE LEU LYS ARG LYS LEU GLY VAL ASP GLY GLU GLU GLU GLU LEU VAL PRO GLU PRO GLU PRO GLU PRO GLU PRO GLU LYS

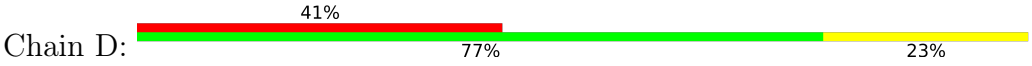


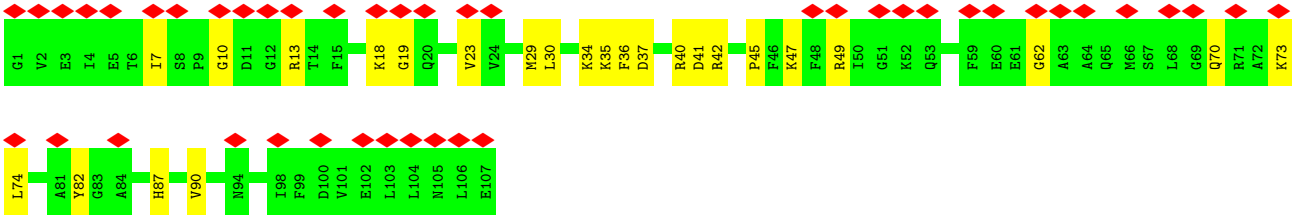
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



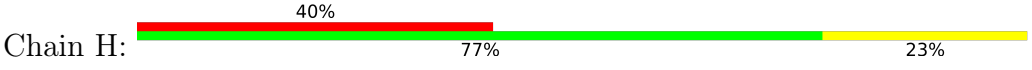


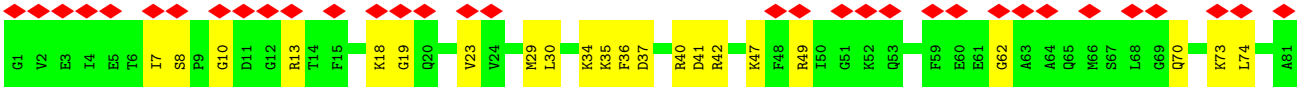
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

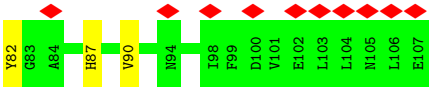




• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

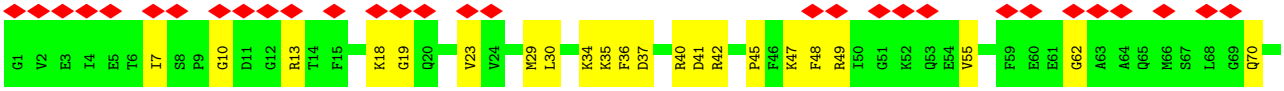


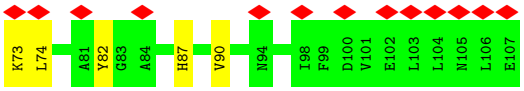




• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

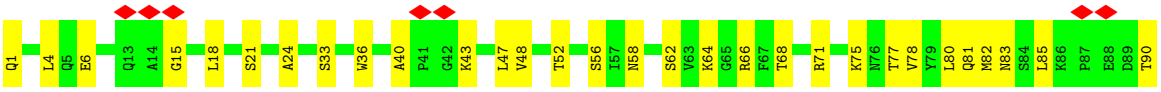
Chain I:





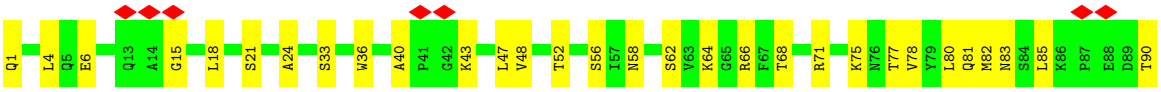
• Molecule 3: Nanobody 9657

Chain C:



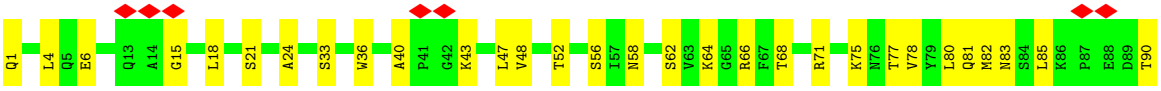
• Molecule 3: Nanobody 9657

Chain F:



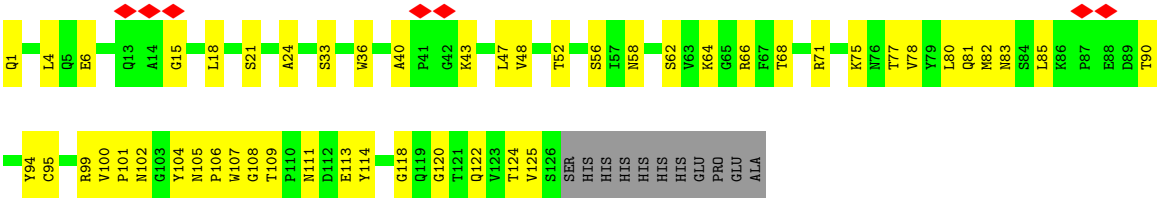
• Molecule 3: Nanobody 9657

Chain K:



• Molecule 3: Nanobody 9657

Chain M:


Q1
L4
Q5
E6
Q13
A14
G15
L18
S21
A24
S33
W36
A40
P41
G42
K43
L47
V48
T52
S56
I57
N58
S62
V63
K64
G65
R66
F67
T68
R71
K75
N76
T77
V78
Y79
L80
Q81
M82
N83
S84
L85
K86
P87
E88
D89
T90
Y94
C95
R99
V100
P101
N102
G103
Y104
N105
P106
W107
G108
T109
P110
N111
D112
E113
Y114
G118
Q119
G120
T121
Q122
V123
T124
V125
S126
SER
HIS
HIS
HIS
HIS
HIS
HIS
GLU
PRO
GLU
ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	29246	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.150	Depositor
Minimum map value	-0.183	Depositor
Average map value	0.061	Depositor
Map value standard deviation	0.123	Depositor
Recommended contour level	0.28	Depositor
Map size (Å)	500.64, 500.64, 500.64	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.49, 1.49, 1.49	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CFF, ATP, CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	B	0.25	0/34879	0.51	3/47278 (0.0%)
1	E	0.25	0/34879	0.51	3/47278 (0.0%)
1	G	0.25	0/34879	0.51	3/47278 (0.0%)
1	J	0.25	0/34879	0.51	3/47278 (0.0%)
2	A	0.25	0/834	0.54	0/1123
2	D	0.25	0/834	0.54	0/1123
2	H	0.25	0/834	0.54	0/1123
2	I	0.25	0/834	0.54	0/1123
3	C	0.26	0/987	0.51	0/1340
3	F	0.26	0/987	0.51	0/1340
3	K	0.26	0/987	0.51	0/1340
3	M	0.26	0/987	0.51	0/1340
All	All	0.25	0/146800	0.51	12/198964 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	961	MET	CG-SD-CE	7.22	111.75	100.20
1	G	961	MET	CG-SD-CE	7.22	111.75	100.20
1	J	961	MET	CG-SD-CE	7.22	111.75	100.20
1	B	961	MET	CG-SD-CE	7.21	111.74	100.20
1	B	2911	LEU	CB-CG-CD2	-5.96	100.86	111.00
1	E	2911	LEU	CB-CG-CD2	-5.94	100.91	111.00
1	J	2911	LEU	CB-CG-CD2	-5.93	100.91	111.00
1	G	2911	LEU	CB-CG-CD2	-5.92	100.94	111.00
1	B	1503	PRO	N-CA-CB	5.63	110.06	103.30
1	E	1503	PRO	N-CA-CB	5.63	110.06	103.30
1	G	1503	PRO	N-CA-CB	5.63	110.06	103.30
1	J	1503	PRO	N-CA-CB	5.63	110.06	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	34104	0	33492	1033	0
1	E	34104	0	33492	1027	0
1	G	34104	0	33492	1024	0
1	J	34104	0	33492	1018	0
2	A	818	0	824	19	0
2	D	818	0	824	21	0
2	H	818	0	824	21	0
2	I	818	0	824	20	0
3	C	967	0	916	44	0
3	F	967	0	916	46	0
3	K	967	0	916	44	0
3	M	967	0	916	46	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	J	1	0	0	0	0
5	B	31	0	12	1	0
5	E	31	0	12	1	0
5	G	31	0	12	1	0
5	J	31	0	12	1	0
6	B	14	0	10	1	0
6	E	14	0	10	1	0
6	G	14	0	10	4	0
6	J	14	0	10	1	0
7	B	1	0	0	0	0
7	E	1	0	0	0	0
7	G	1	0	0	0	0
7	J	1	0	0	0	0
All	All	143744	0	141016	4248	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (4248) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2911:LEU:HD13	1:E:2915:GLU:HG3	1.53	0.90
1:G:3197:LEU:O	1:G:3201:MET:HB2	1.71	0.90
1:J:3197:LEU:O	1:J:3201:MET:HB2	1.71	0.90
1:J:2911:LEU:HD13	1:J:2915:GLU:HG3	1.53	0.90
1:G:2911:LEU:HD13	1:G:2915:GLU:HG3	1.53	0.90
1:B:2911:LEU:HD13	1:B:2915:GLU:HG3	1.53	0.89
1:B:3967:GLU:HA	1:B:3970:GLN:HG2	1.55	0.89
1:E:3197:LEU:O	1:E:3201:MET:HB2	1.71	0.89
1:E:3967:GLU:HA	1:E:3970:GLN:HG2	1.54	0.88
1:B:3197:LEU:O	1:B:3201:MET:HB2	1.71	0.88
1:J:3967:GLU:HA	1:J:3970:GLN:HG2	1.55	0.88
1:G:4961:CYS:SG	1:G:4983:HIS:CE1	2.67	0.88
1:E:4961:CYS:SG	1:E:4983:HIS:CE1	2.67	0.86
1:B:4961:CYS:SG	1:B:4983:HIS:CE1	2.67	0.86
1:G:3967:GLU:HA	1:G:3970:GLN:HG2	1.57	0.85
1:E:3889:GLN:HB2	1:E:3967:GLU:HG3	1.59	0.84
1:G:1947:CYS:SG	1:G:2127:GLN:NE2	2.51	0.84
1:E:1947:CYS:SG	1:E:2127:GLN:NE2	2.51	0.84
1:J:1947:CYS:SG	1:J:2127:GLN:NE2	2.51	0.83
1:B:3889:GLN:HB2	1:B:3967:GLU:HG3	1.59	0.83
1:B:1947:CYS:SG	1:B:2127:GLN:NE2	2.51	0.82
1:G:2793:PRO:HA	1:G:2855:TYR:HB2	1.62	0.82
1:J:3889:GLN:HB2	1:J:3967:GLU:HG3	1.59	0.82
1:G:3889:GLN:HB2	1:G:3967:GLU:HG3	1.61	0.81
1:G:4999:ASP:HB2	1:G:5002:GLU:HG2	1.61	0.80
1:J:2793:PRO:HA	1:J:2855:TYR:HB2	1.62	0.80
1:E:2793:PRO:HA	1:E:2855:TYR:HB2	1.62	0.80
1:G:3670:GLU:HB2	1:G:3728:ILE:HG23	1.63	0.80
1:B:3315:LEU:HD22	1:B:3345:ILE:HG12	1.64	0.80
1:B:2793:PRO:HA	1:B:2855:TYR:HB2	1.62	0.80
1:J:3670:GLU:HB2	1:J:3728:ILE:HG23	1.63	0.80
1:B:3670:GLU:HB2	1:B:3728:ILE:HG23	1.63	0.79
3:K:4:LEU:HD21	3:K:95:CYS:HB3	1.65	0.79
1:J:3315:LEU:HD22	1:J:3345:ILE:HG12	1.64	0.78
1:E:3670:GLU:HB2	1:E:3728:ILE:HG23	1.63	0.78
1:E:2755:ILE:HD12	1:E:2813:LEU:HG	1.66	0.78
1:B:3054:VAL:HG11	1:B:3131:TYR:HB2	1.65	0.78
3:C:66:ARG:HD2	3:C:83:ASN:HB2	1.66	0.78
1:E:3054:VAL:HG11	1:E:3131:TYR:HB2	1.65	0.78
3:F:66:ARG:HD2	3:F:83:ASN:HB2	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3315:LEU:HD22	1:G:3345:ILE:HG12	1.64	0.78
3:M:4:LEU:HD21	3:M:95:CYS:HB3	1.65	0.78
1:J:2755:ILE:HD12	1:J:2813:LEU:HG	1.66	0.78
3:C:4:LEU:HD21	3:C:95:CYS:HB3	1.65	0.78
3:K:66:ARG:HD2	3:K:83:ASN:HB2	1.66	0.78
1:E:3315:LEU:HD22	1:E:3345:ILE:HG12	1.64	0.77
1:E:633:LEU:HB3	1:E:1639:LEU:HD11	1.66	0.77
1:J:2595:LEU:HB2	1:J:2600:ARG:HE	1.50	0.77
1:J:3054:VAL:HG11	1:J:3131:TYR:HB2	1.65	0.77
3:M:66:ARG:HD2	3:M:83:ASN:HB2	1.66	0.77
1:B:2595:LEU:HB2	1:B:2600:ARG:HE	1.50	0.77
1:B:2867:LEU:HG	1:B:2868:SER:H	1.50	0.77
3:F:4:LEU:HD21	3:F:95:CYS:HB3	1.65	0.77
1:G:633:LEU:HB3	1:G:1639:LEU:HD11	1.66	0.77
1:B:633:LEU:HB3	1:B:1639:LEU:HD11	1.66	0.77
1:G:2755:ILE:HD12	1:G:2813:LEU:HG	1.65	0.77
1:E:2867:LEU:HG	1:E:2868:SER:H	1.50	0.76
1:E:2882:TYR:HB3	1:E:2886:TRP:HZ3	1.51	0.76
1:B:2755:ILE:HD12	1:B:2813:LEU:HG	1.65	0.76
1:E:2595:LEU:HB2	1:E:2600:ARG:HE	1.50	0.76
1:G:3054:VAL:HG11	1:G:3131:TYR:HB2	1.65	0.76
1:G:2595:LEU:HB2	1:G:2600:ARG:HE	1.50	0.76
1:J:633:LEU:HB3	1:J:1639:LEU:HD11	1.66	0.76
1:B:1152:MET:HB2	1:B:1161:ILE:O	1.86	0.76
1:J:2882:TYR:HB3	1:J:2886:TRP:HZ3	1.51	0.76
1:B:2882:TYR:HB3	1:B:2886:TRP:HZ3	1.51	0.76
1:G:2975:ALA:HA	1:G:3053:ARG:HH12	1.52	0.76
1:G:1152:MET:HB2	1:G:1161:ILE:O	1.86	0.75
1:E:1152:MET:HB2	1:E:1161:ILE:O	1.86	0.75
1:E:2975:ALA:HA	1:E:3053:ARG:HH12	1.52	0.75
1:G:2882:TYR:HB3	1:G:2886:TRP:HZ3	1.51	0.75
1:J:2975:ALA:HA	1:J:3053:ARG:HH12	1.52	0.75
1:E:730:VAL:HA	1:E:1476:MET:HE1	1.69	0.75
1:J:1152:MET:HB2	1:J:1161:ILE:O	1.86	0.75
1:J:2867:LEU:HG	1:J:2868:SER:H	1.50	0.75
1:B:2975:ALA:HA	1:B:3053:ARG:HH12	1.52	0.74
1:B:3986:TRP:HB3	1:B:4047:MET:HE3	1.69	0.74
1:G:2867:LEU:HG	1:G:2868:SER:H	1.50	0.74
1:E:371:VAL:HG12	1:E:373:LYS:H	1.53	0.74
1:J:3986:TRP:HB3	1:J:4047:MET:HE3	1.69	0.74
3:F:105:ASN:ND2	3:F:111:ASN:HB2	2.03	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:105:ASN:ND2	3:K:111:ASN:HB2	2.03	0.74
3:M:105:ASN:ND2	3:M:111:ASN:HB2	2.03	0.74
1:G:3842:LEU:HB2	1:G:3929:SER:HB2	1.70	0.74
1:B:3842:LEU:HB2	1:B:3929:SER:HB2	1.70	0.74
1:G:144:GLU:HG3	1:G:175:SER:HB2	1.70	0.74
1:J:3842:LEU:HB2	1:J:3929:SER:HB2	1.70	0.73
2:H:23:VAL:HG12	2:H:47:LYS:HG2	1.70	0.73
1:B:835:ARG:HH21	1:B:1203:ASN:HD22	1.36	0.73
1:J:223:PHE:HA	1:J:230:CYS:HA	1.70	0.73
1:B:622:THR:HA	1:B:626:LEU:HD13	1.70	0.73
1:E:3842:LEU:HB2	1:E:3929:SER:HB2	1.70	0.73
1:G:730:VAL:HA	1:G:1476:MET:HE1	1.69	0.73
2:I:23:VAL:HG12	2:I:47:LYS:HG2	1.70	0.73
3:C:105:ASN:ND2	3:C:111:ASN:HB2	2.02	0.73
1:E:622:THR:HA	1:E:626:LEU:HD13	1.70	0.73
1:E:835:ARG:HH21	1:E:1203:ASN:HD22	1.36	0.73
2:D:23:VAL:HG12	2:D:47:LYS:HG2	1.70	0.73
3:C:68:THR:HB	3:C:81:GLN:HB3	1.71	0.73
1:G:247:TYR:HB2	1:G:374:LYS:HB2	1.69	0.73
1:J:144:GLU:HG3	1:J:175:SER:HB2	1.70	0.73
1:J:973:SER:HA	1:J:1044:ARG:HH21	1.54	0.73
1:J:835:ARG:HH21	1:J:1203:ASN:HD22	1.37	0.73
1:E:3986:TRP:HB3	1:E:4047:MET:HE3	1.70	0.72
1:G:835:ARG:HH21	1:G:1203:ASN:HD22	1.36	0.72
1:B:223:PHE:HA	1:B:230:CYS:HA	1.70	0.72
2:D:13:ARG:NH1	2:D:13:ARG:O	2.22	0.72
3:K:68:THR:HB	3:K:81:GLN:HB3	1.71	0.72
1:B:144:GLU:HG3	1:B:175:SER:HB2	1.70	0.72
1:B:990:GLU:OE2	1:B:994:ASN:ND2	2.23	0.72
1:G:990:GLU:OE2	1:G:994:ASN:ND2	2.23	0.72
1:G:3730:ALA:O	1:G:3734:HIS:ND1	2.22	0.72
1:G:2496:PRO:HG3	1:G:2550:LEU:HD23	1.72	0.72
3:F:68:THR:HB	3:F:81:GLN:HB3	1.71	0.72
1:E:3730:ALA:O	1:E:3734:HIS:ND1	2.22	0.72
1:J:730:VAL:HA	1:J:1476:MET:HE1	1.72	0.72
1:J:3730:ALA:O	1:J:3734:HIS:ND1	2.23	0.72
2:A:23:VAL:HG12	2:A:47:LYS:HG2	1.70	0.72
1:E:223:PHE:HA	1:E:230:CYS:HA	1.70	0.72
1:E:973:SER:HA	1:E:1044:ARG:HH21	1.54	0.72
1:G:248:GLU:HB2	1:G:373:LYS:HD3	1.71	0.72
1:J:799:GLU:HB2	1:J:1623:ARG:HH12	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:13:ARG:O	2:H:13:ARG:NH1	2.22	0.72
1:B:3730:ALA:O	1:B:3734:HIS:ND1	2.23	0.72
1:G:223:PHE:HA	1:G:230:CYS:HA	1.70	0.72
1:E:859:VAL:HA	1:E:930:LYS:HD3	1.72	0.71
1:G:622:THR:HA	1:G:626:LEU:HD13	1.70	0.71
1:J:990:GLU:OE2	1:J:994:ASN:ND2	2.23	0.71
1:B:973:SER:HA	1:B:1044:ARG:HH21	1.54	0.71
1:E:4651:THR:HG1	1:E:4803:HIS:HE2	1.37	0.71
1:G:1616:GLU:HG3	1:G:1629:GLN:HG3	1.72	0.71
1:B:1616:GLU:HG3	1:B:1629:GLN:HG3	1.72	0.71
1:B:2496:PRO:HG3	1:B:2550:LEU:HD23	1.72	0.71
1:B:4902:GLU:O	1:B:4913:ARG:NH2	2.23	0.71
1:E:4902:GLU:O	1:E:4913:ARG:NH2	2.23	0.71
1:J:38:ALA:HB1	1:J:64:ILE:HG13	1.73	0.71
1:J:4651:THR:HG1	1:J:4803:HIS:HE2	1.37	0.71
3:M:68:THR:HB	3:M:81:GLN:HB3	1.71	0.71
1:J:622:THR:HA	1:J:626:LEU:HD13	1.70	0.71
1:J:2496:PRO:HG3	1:J:2550:LEU:HD23	1.72	0.71
1:B:38:ALA:HB1	1:B:64:ILE:HG13	1.73	0.71
1:G:371:VAL:HG12	1:G:373:LYS:H	1.56	0.71
1:E:144:GLU:HG3	1:E:175:SER:HB2	1.70	0.71
1:J:4902:GLU:O	1:J:4913:ARG:NH2	2.23	0.71
1:B:799:GLU:HB2	1:B:1623:ARG:HH12	1.55	0.70
1:E:248:GLU:HB2	1:E:373:LYS:HD3	1.72	0.70
1:G:38:ALA:HB1	1:G:64:ILE:HG13	1.73	0.70
1:B:3081:MET:HG3	1:B:3156:VAL:HA	1.74	0.70
1:E:990:GLU:OE2	1:E:994:ASN:ND2	2.23	0.70
1:G:3986:TRP:HB3	1:G:4047:MET:HE3	1.73	0.70
1:J:247:TYR:HB2	1:J:374:LYS:HD2	1.73	0.70
1:E:38:ALA:HB1	1:E:64:ILE:HG13	1.73	0.70
1:G:799:GLU:HB2	1:G:1623:ARG:HH12	1.55	0.70
1:G:859:VAL:HA	1:G:930:LYS:HD3	1.72	0.70
1:B:859:VAL:HA	1:B:930:LYS:HD3	1.72	0.70
1:G:3081:MET:HG3	1:G:3156:VAL:HA	1.74	0.70
1:E:1616:GLU:HG3	1:E:1629:GLN:HG3	1.72	0.70
1:E:2496:PRO:HG3	1:E:2550:LEU:HD23	1.72	0.70
1:G:973:SER:HA	1:G:1044:ARG:HH21	1.54	0.70
1:B:247:TYR:HB2	1:B:374:LYS:HD2	1.73	0.70
1:E:953:THR:HB	1:E:969:PRO:HG2	1.73	0.70
1:J:1256:GLU:HB2	1:J:1275:ARG:HE	1.57	0.70
1:E:1256:GLU:HB2	1:E:1275:ARG:HE	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3081:MET:HG3	1:E:3156:VAL:HA	1.74	0.70
1:G:953:THR:HB	1:G:969:PRO:HG2	1.73	0.70
1:G:1256:GLU:HB2	1:G:1275:ARG:HE	1.57	0.70
2:A:13:ARG:NH1	2:A:13:ARG:O	2.22	0.70
1:J:2874:MET:HE1	1:J:2939:ARG:HG3	1.73	0.70
1:E:4127:GLU:OE1	1:E:4131:ARG:NH2	2.25	0.70
1:E:4865:LYS:NZ	1:E:4900:GLU:O	2.25	0.70
1:G:4902:GLU:O	1:G:4913:ARG:NH2	2.23	0.70
1:J:4127:GLU:OE1	1:J:4131:ARG:NH2	2.25	0.69
1:J:859:VAL:HA	1:J:930:LYS:HD3	1.72	0.69
1:J:1616:GLU:HG3	1:J:1629:GLN:HG3	1.72	0.69
1:J:3081:MET:HG3	1:J:3156:VAL:HA	1.74	0.69
1:B:4865:LYS:NZ	1:B:4900:GLU:O	2.25	0.69
1:E:2970:SER:HA	1:E:2973:PHE:CE2	2.28	0.69
1:E:2865:VAL:HG23	1:E:2928:LYS:HE3	1.75	0.69
1:G:3147:ILE:HG23	1:G:3152:PHE:HB2	1.75	0.69
1:J:886:ARG:HB3	1:J:891:TRP:HB3	1.75	0.69
1:J:2865:VAL:HG23	1:J:2928:LYS:HE3	1.75	0.69
1:J:953:THR:HB	1:J:969:PRO:HG2	1.73	0.69
1:J:2970:SER:HA	1:J:2973:PHE:CE2	2.28	0.69
1:B:371:VAL:HG12	1:B:373:LYS:H	1.57	0.69
1:B:886:ARG:HB3	1:B:891:TRP:HB3	1.75	0.69
1:B:3147:ILE:HG23	1:B:3152:PHE:HB2	1.75	0.69
1:E:799:GLU:HB2	1:E:1623:ARG:HH12	1.55	0.69
1:G:2865:VAL:HG23	1:G:2928:LYS:HE3	1.75	0.69
1:B:953:THR:HB	1:B:969:PRO:HG2	1.73	0.69
1:B:1870:VAL:HG11	1:B:2097:LEU:HD22	1.75	0.69
1:E:886:ARG:HB3	1:E:891:TRP:HB3	1.75	0.69
1:G:1870:VAL:HG11	1:G:2097:LEU:HD22	1.75	0.69
1:G:2519:LEU:HA	1:G:2522:LEU:HD12	1.74	0.69
1:J:372:LEU:O	1:J:374:LYS:HG3	1.93	0.69
1:J:4865:LYS:NZ	1:J:4900:GLU:O	2.25	0.69
1:B:950:LEU:HD13	1:B:970:LEU:HD21	1.75	0.69
1:B:1256:GLU:HB2	1:B:1275:ARG:HE	1.57	0.69
1:B:4127:GLU:OE1	1:B:4131:ARG:NH2	2.25	0.69
1:J:2616:PRO:HA	1:J:2619:LEU:HB3	1.75	0.69
1:B:2519:LEU:HA	1:B:2522:LEU:HD12	1.74	0.69
1:B:2865:VAL:HG23	1:B:2928:LYS:HE3	1.75	0.69
1:G:223:PHE:HB2	1:G:389:PHE:HB3	1.75	0.69
1:G:886:ARG:HB3	1:G:891:TRP:HB3	1.75	0.69
1:G:2970:SER:HA	1:G:2973:PHE:CE2	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4127:GLU:OE1	1:G:4131:ARG:NH2	2.25	0.69
2:I:13:ARG:O	2:I:13:ARG:NH1	2.22	0.69
1:B:2616:PRO:HA	1:B:2619:LEU:HB3	1.75	0.68
1:B:2970:SER:HA	1:B:2973:PHE:CE2	2.28	0.68
1:G:4865:LYS:NZ	1:G:4900:GLU:O	2.25	0.68
1:B:223:PHE:HB2	1:B:389:PHE:HB3	1.75	0.68
1:E:1671:ARG:HH21	1:E:1710:GLY:HA2	1.59	0.68
1:B:2913:ALA:O	1:B:2917:ALA:N	2.24	0.68
1:J:1870:VAL:HG11	1:J:2097:LEU:HD22	1.75	0.68
1:J:3147:ILE:HG23	1:J:3152:PHE:HB2	1.75	0.68
1:B:248:GLU:HB2	1:B:373:LYS:HD3	1.75	0.68
1:E:180:LEU:O	1:E:200:TRP:NE1	2.24	0.68
1:E:3147:ILE:HG23	1:E:3152:PHE:HB2	1.75	0.68
1:G:950:LEU:HD13	1:G:970:LEU:HD21	1.75	0.68
1:B:1671:ARG:HH21	1:B:1710:GLY:HA2	1.59	0.68
1:G:2616:PRO:HA	1:G:2619:LEU:HB3	1.75	0.68
1:E:223:PHE:HB2	1:E:389:PHE:HB3	1.75	0.68
1:E:2874:MET:HE1	1:E:2939:ARG:HG3	1.74	0.68
1:J:248:GLU:HB2	1:J:373:LYS:HD3	1.75	0.68
1:B:372:LEU:O	1:B:374:LYS:HG3	1.93	0.68
1:G:1671:ARG:HH21	1:G:1710:GLY:HA2	1.59	0.68
1:J:371:VAL:HG12	1:J:373:LYS:H	1.57	0.68
1:E:1870:VAL:HG11	1:E:2097:LEU:HD22	1.75	0.68
1:G:2913:ALA:O	1:G:2917:ALA:N	2.24	0.68
1:J:223:PHE:HB2	1:J:389:PHE:HB3	1.75	0.68
1:J:180:LEU:O	1:J:200:TRP:NE1	2.24	0.68
1:J:247:TYR:HB2	1:J:374:LYS:HB2	1.76	0.68
1:B:1008:SER:HB2	1:B:1017:ARG:HE	1.59	0.67
1:E:2519:LEU:HA	1:E:2522:LEU:HD12	1.74	0.67
1:E:2616:PRO:HA	1:E:2619:LEU:HB3	1.75	0.67
1:J:1671:ARG:HH21	1:J:1710:GLY:HA2	1.59	0.67
1:B:195:PHE:HE2	1:G:2359:ARG:HA	1.59	0.67
1:J:1008:SER:HB2	1:J:1017:ARG:HE	1.59	0.67
1:J:2519:LEU:HA	1:J:2522:LEU:HD12	1.74	0.67
1:J:3965:LEU:HA	1:J:3968:TYR:CD2	2.30	0.67
1:B:3224:PRO:HA	1:B:3227:ARG:HD2	1.77	0.67
1:J:950:LEU:HD13	1:J:970:LEU:HD21	1.75	0.67
1:B:3965:LEU:HA	1:B:3968:TYR:CD2	2.30	0.67
1:E:2913:ALA:O	1:E:2917:ALA:N	2.24	0.67
1:G:3224:PRO:HA	1:G:3227:ARG:HD2	1.77	0.67
1:E:1008:SER:HB2	1:E:1017:ARG:HE	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:797:HIS:CE1	1:E:1626:TRP:HD1	2.12	0.67
1:E:3224:PRO:HA	1:E:3227:ARG:HD2	1.77	0.67
1:G:1008:SER:HB2	1:G:1017:ARG:HE	1.59	0.67
1:J:3224:PRO:HA	1:J:3227:ARG:HD2	1.77	0.67
1:B:636:ASN:HD22	2:A:35:LYS:HE3	1.60	0.67
1:B:2359:ARG:HA	1:E:195:PHE:HE2	1.60	0.67
1:E:950:LEU:HD13	1:E:970:LEU:HD21	1.75	0.67
1:E:3100:SER:HB3	1:E:3167:ARG:HD3	1.76	0.67
1:G:636:ASN:HD22	2:H:35:LYS:HE3	1.60	0.67
1:J:3021:PRO:HD3	1:J:3036:LYS:HZ3	1.58	0.67
1:E:372:LEU:O	1:E:374:LYS:HG3	1.95	0.67
1:J:636:ASN:HD22	2:I:35:LYS:HE3	1.60	0.67
1:E:2359:ARG:HA	1:J:195:PHE:HE2	1.59	0.66
1:G:3100:SER:HB3	1:G:3167:ARG:HD3	1.76	0.66
1:G:3965:LEU:HA	1:G:3968:TYR:CD2	2.31	0.66
1:B:247:TYR:HB2	1:B:374:LYS:HB2	1.76	0.66
1:B:730:VAL:HA	1:B:1476:MET:HE1	1.78	0.66
1:B:797:HIS:CE1	1:B:1626:TRP:HD1	2.12	0.66
1:J:797:HIS:CE1	1:J:1626:TRP:HD1	2.13	0.66
1:E:3965:LEU:HA	1:E:3968:TYR:CD2	2.30	0.66
1:G:3886:ARG:HD2	1:G:3889:GLN:HE21	1.60	0.66
1:B:1179:PHE:HB2	1:B:1182:ILE:HD11	1.78	0.66
1:E:247:TYR:HB2	1:E:374:LYS:HB2	1.76	0.66
1:E:636:ASN:HD22	2:D:35:LYS:HE3	1.61	0.66
1:E:2902:HIS:CE1	1:E:2904:LEU:HB2	2.31	0.66
1:B:3695:PRO:HG2	1:B:3700:GLN:HG2	1.78	0.66
1:E:3695:PRO:HG2	1:E:3700:GLN:HG2	1.78	0.66
1:G:178:ARG:HA	1:G:195:PHE:HD1	1.61	0.66
1:G:797:HIS:CE1	1:G:1626:TRP:HD1	2.13	0.66
1:G:2902:HIS:CE1	1:G:2904:LEU:HB2	2.31	0.66
1:J:3695:PRO:HG2	1:J:3700:GLN:HG2	1.78	0.66
1:G:180:LEU:O	1:G:200:TRP:NE1	2.24	0.66
1:G:195:PHE:HE2	1:J:2359:ARG:HA	1.59	0.66
1:G:3695:PRO:HG2	1:G:3700:GLN:HG2	1.78	0.66
1:G:4242:ILE:HG21	6:G:5103:CFF:H81	1.77	0.66
1:E:103:TYR:HB2	1:E:159:GLU:HA	1.78	0.66
1:G:1179:PHE:HB2	1:G:1182:ILE:HD11	1.78	0.66
1:J:3100:SER:HB3	1:J:3167:ARG:HD3	1.76	0.66
1:G:2637:ALA:HA	1:G:2640:PRO:HG2	1.78	0.66
1:J:1179:PHE:HB2	1:J:1182:ILE:HD11	1.78	0.66
1:B:2637:ALA:HA	1:B:2640:PRO:HG2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1179:PHE:HB2	1:E:1182:ILE:HD11	1.78	0.65
1:E:2637:ALA:HA	1:E:2640:PRO:HG2	1.78	0.65
1:J:178:ARG:HA	1:J:195:PHE:HD1	1.61	0.65
1:G:2813:LEU:HA	1:G:2816:MET:HG3	1.78	0.65
1:E:3031:ALA:O	1:E:3036:LYS:NZ	2.27	0.65
1:E:4546:VAL:HG22	1:E:4550:LYS:HE3	1.79	0.65
1:J:758:ARG:HH11	1:J:761:GLY:HA2	1.62	0.65
1:B:4183:ILE:HD12	1:B:4188:ARG:HH21	1.61	0.65
1:B:4546:VAL:HG22	1:B:4550:LYS:HE3	1.79	0.65
1:E:2768:PHE:HB2	1:E:2857:PRO:HD2	1.77	0.65
1:J:2637:ALA:HA	1:J:2640:PRO:HG2	1.78	0.65
1:B:3100:SER:HB3	1:B:3167:ARG:HD3	1.77	0.65
1:E:1101:ARG:HH12	1:E:1114:GLU:HB3	1.62	0.65
1:G:2980:VAL:HB	1:G:2986:VAL:HB	1.79	0.65
1:J:2454:ARG:HD2	1:J:2458:ARG:HH21	1.61	0.65
1:B:180:LEU:O	1:B:200:TRP:NE1	2.24	0.65
1:B:1101:ARG:HH12	1:B:1114:GLU:HB3	1.62	0.65
1:J:2902:HIS:CE1	1:J:2904:LEU:HB2	2.31	0.65
1:J:2980:VAL:HB	1:J:2986:VAL:HB	1.79	0.65
1:B:924:MET:HE2	3:C:107:TRP:HB2	1.78	0.65
1:B:2902:HIS:CE1	1:B:2904:LEU:HB2	2.31	0.65
1:G:2454:ARG:HD2	1:G:2458:ARG:HH21	1.61	0.65
1:J:103:TYR:HB2	1:J:159:GLU:HA	1.78	0.65
1:E:4183:ILE:HD12	1:E:4188:ARG:HH21	1.61	0.65
1:B:758:ARG:HH11	1:B:761:GLY:HA2	1.62	0.65
1:B:3187:ARG:HG3	1:B:3188:PRO:HD3	1.79	0.65
1:G:758:ARG:HH11	1:G:761:GLY:HA2	1.62	0.65
1:G:887:ILE:HD13	1:G:959:TYR:HB3	1.79	0.65
1:B:2980:VAL:HB	1:B:2986:VAL:HB	1.79	0.65
1:G:728:ARG:HE	1:G:1487:LEU:HD12	1.61	0.65
1:G:2768:PHE:HB2	1:G:2857:PRO:HD2	1.78	0.65
1:E:758:ARG:HH11	1:E:761:GLY:HA2	1.61	0.64
1:B:103:TYR:HB2	1:B:159:GLU:HA	1.78	0.64
1:B:178:ARG:HA	1:B:195:PHE:HD1	1.61	0.64
1:B:1519:LEU:HD11	1:B:1572:ILE:HD13	1.80	0.64
1:B:2454:ARG:HD2	1:B:2458:ARG:HH21	1.61	0.64
1:E:2980:VAL:HB	1:E:2986:VAL:HB	1.79	0.64
1:G:4546:VAL:HG22	1:G:4550:LYS:HE3	1.79	0.64
1:J:1101:ARG:HH12	1:J:1114:GLU:HB3	1.62	0.64
1:B:2813:LEU:HA	1:B:2816:MET:HG3	1.79	0.64
1:E:247:TYR:HB2	1:E:374:LYS:HD2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2454:ARG:HD2	1:E:2458:ARG:HH21	1.61	0.64
1:G:103:TYR:HB2	1:G:159:GLU:HA	1.78	0.64
1:J:2768:PHE:HB2	1:J:2857:PRO:HD2	1.77	0.64
1:J:3433:GLU:HA	1:J:3436:ARG:HD2	1.80	0.64
1:G:372:LEU:O	1:G:374:LYS:HG3	1.97	0.64
1:G:1101:ARG:HH12	1:G:1114:GLU:HB3	1.62	0.64
1:J:887:ILE:HD13	1:J:959:TYR:HB3	1.79	0.64
1:B:728:ARG:HE	1:B:1487:LEU:HD12	1.61	0.64
1:B:1291:LEU:HD12	1:B:1550:PRO:HG2	1.80	0.64
1:B:2768:PHE:HB2	1:B:2857:PRO:HD2	1.78	0.64
1:J:4183:ILE:HD12	1:J:4188:ARG:HH21	1.61	0.64
1:B:197:GLN:OE1	1:B:197:GLN:N	2.31	0.64
1:B:887:ILE:HD13	1:B:959:TYR:HB3	1.79	0.64
1:B:1815:LEU:HD22	1:B:1845:VAL:HG21	1.79	0.64
1:B:2214:VAL:HG13	1:B:2215:LEU:HD12	1.79	0.64
1:E:2431:ASP:HB2	1:E:2501:SER:HB2	1.80	0.64
1:E:3187:ARG:HG3	1:E:3188:PRO:HD3	1.79	0.64
1:E:3433:GLU:HA	1:E:3436:ARG:HD2	1.80	0.64
1:G:718:GLY:HA3	1:G:737:LEU:HA	1.80	0.64
1:G:3196:ARG:HH12	1:G:3341:PHE:HZ	1.46	0.64
1:J:622:THR:HG23	1:J:626:LEU:HD22	1.79	0.64
1:J:3187:ARG:HG3	1:J:3188:PRO:HD3	1.79	0.64
1:J:4546:VAL:HG22	1:J:4550:LYS:HE3	1.79	0.64
1:B:3433:GLU:HA	1:B:3436:ARG:HD2	1.80	0.64
1:G:197:GLN:OE1	1:G:197:GLN:N	2.30	0.64
1:G:4183:ILE:HD12	1:G:4188:ARG:HH21	1.61	0.64
1:J:197:GLN:OE1	1:J:197:GLN:N	2.30	0.64
1:J:2813:LEU:HA	1:J:2816:MET:HG3	1.79	0.64
1:J:3031:ALA:O	1:J:3036:LYS:NZ	2.27	0.64
1:B:3196:ARG:HH12	1:B:3341:PHE:HZ	1.46	0.64
1:E:601:ASP:OD1	1:E:1668:ARG:NH2	2.31	0.64
1:E:1291:LEU:HD12	1:E:1550:PRO:HG2	1.80	0.64
1:G:622:THR:HG23	1:G:626:LEU:HD22	1.79	0.64
1:G:1291:LEU:HD12	1:G:1550:PRO:HG2	1.80	0.64
1:G:2138:LEU:HB3	1:G:3658:LYS:HE2	1.80	0.64
1:J:728:ARG:HE	1:J:1487:LEU:HD12	1.61	0.64
1:J:3986:TRP:HB3	1:J:4047:MET:CE	2.28	0.64
1:B:622:THR:HG23	1:B:626:LEU:HD22	1.79	0.64
1:B:3031:ALA:O	1:B:3036:LYS:NZ	2.27	0.64
1:B:3078:ARG:HG3	1:B:3152:PHE:HD1	1.63	0.64
1:E:178:ARG:HA	1:E:195:PHE:HD1	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:728:ARG:HE	1:E:1487:LEU:HD12	1.61	0.64
1:G:601:ASP:OD1	1:G:1668:ARG:NH2	2.31	0.64
1:G:2214:VAL:HG13	1:G:2215:LEU:HD12	1.79	0.64
1:G:3021:PRO:HD3	1:G:3036:LYS:HZ3	1.62	0.64
1:J:1815:LEU:HD22	1:J:1845:VAL:HG21	1.79	0.64
1:J:2431:ASP:HB2	1:J:2501:SER:HB2	1.80	0.64
1:E:668:VAL:HG21	1:E:738:LEU:HD12	1.80	0.63
1:G:1815:LEU:HD22	1:G:1845:VAL:HG21	1.79	0.63
1:J:601:ASP:OD1	1:J:1668:ARG:NH2	2.31	0.63
1:B:668:VAL:HG21	1:B:738:LEU:HD12	1.80	0.63
1:E:165:VAL:O	1:E:203:ASN:ND2	2.31	0.63
1:E:365:LYS:HE2	1:E:369:LEU:HD21	1.79	0.63
1:E:1738:LEU:HB2	1:E:2146:PRO:HD3	1.79	0.63
1:G:913:LEU:HB3	1:G:917:GLU:HB2	1.80	0.63
1:G:3986:TRP:HB3	1:G:4047:MET:CE	2.28	0.63
1:J:1738:LEU:HB2	1:J:2146:PRO:HD3	1.79	0.63
1:J:2138:LEU:HB3	1:J:3658:LYS:HE2	1.80	0.63
1:B:82:LEU:HD11	1:B:144:GLU:HB3	1.79	0.63
1:G:663:TYR:OH	1:G:758:ARG:NH2	2.32	0.63
1:G:4712:PRO:HB2	1:G:4718:LYS:HA	1.80	0.63
1:J:913:LEU:HB3	1:J:917:GLU:HB2	1.80	0.63
1:J:1528:THR:HG23	1:J:1539:PHE:HE1	1.63	0.63
1:B:601:ASP:OD1	1:B:1668:ARG:NH2	2.31	0.63
1:E:197:GLN:OE1	1:E:197:GLN:N	2.30	0.63
1:E:622:THR:HG23	1:E:626:LEU:HD22	1.79	0.63
1:E:663:TYR:OH	1:E:758:ARG:NH2	2.32	0.63
1:E:2214:VAL:HG13	1:E:2215:LEU:HD12	1.79	0.63
1:J:718:GLY:HA3	1:J:737:LEU:HA	1.80	0.63
1:J:2684:ASP:O	1:J:2688:HIS:ND1	2.32	0.63
1:B:913:LEU:HB3	1:B:917:GLU:HB2	1.80	0.63
1:B:1738:LEU:HB2	1:B:2146:PRO:HD3	1.79	0.63
1:E:1519:LEU:HD11	1:E:1572:ILE:HD13	1.80	0.63
1:E:2813:LEU:HA	1:E:2816:MET:HG3	1.79	0.63
1:G:3187:ARG:HG3	1:G:3188:PRO:HD3	1.79	0.63
1:J:1291:LEU:HD12	1:J:1550:PRO:HG2	1.80	0.63
1:J:3078:ARG:HG3	1:J:3152:PHE:HD1	1.63	0.63
1:E:718:GLY:HA3	1:E:737:LEU:HA	1.80	0.63
1:G:1738:LEU:HB2	1:G:2146:PRO:HD3	1.79	0.63
1:G:3078:ARG:HG3	1:G:3152:PHE:HD1	1.63	0.63
1:B:663:TYR:OH	1:B:758:ARG:NH2	2.32	0.63
1:B:1099:GLU:HA	1:B:1127:HIS:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2431:ASP:HB2	1:B:2501:SER:HB2	1.80	0.63
1:B:2599:GLN:O	1:B:2603:ILE:HG12	1.99	0.63
1:E:1815:LEU:HD22	1:E:1845:VAL:HG21	1.79	0.63
1:G:3433:GLU:HA	1:G:3436:ARG:HD2	1.80	0.63
1:J:82:LEU:HD11	1:J:144:GLU:HB3	1.79	0.63
1:J:1519:LEU:HD11	1:J:1572:ILE:HD13	1.80	0.63
1:E:2138:LEU:HB3	1:E:3658:LYS:HE2	1.80	0.63
1:E:2684:ASP:O	1:E:2688:HIS:ND1	2.32	0.63
1:G:82:LEU:HD11	1:G:144:GLU:HB3	1.79	0.63
1:G:1519:LEU:HD11	1:G:1572:ILE:HD13	1.80	0.63
1:B:165:VAL:O	1:B:203:ASN:ND2	2.32	0.63
1:B:2684:ASP:O	1:B:2688:HIS:ND1	2.32	0.63
1:E:887:ILE:HD13	1:E:959:TYR:HB3	1.80	0.63
1:E:3078:ARG:HG3	1:E:3152:PHE:HD1	1.63	0.63
1:J:365:LYS:HE2	1:J:369:LEU:HD21	1.80	0.63
1:J:4712:PRO:HB2	1:J:4718:LYS:HA	1.80	0.63
1:E:3986:TRP:HB3	1:E:4047:MET:CE	2.28	0.62
1:E:5013:MET:HE3	1:E:5018:CYS:HB3	1.80	0.62
1:G:2866:THR:O	1:G:2928:LYS:NZ	2.22	0.62
1:J:165:VAL:O	1:J:203:ASN:ND2	2.31	0.62
1:J:663:TYR:OH	1:J:758:ARG:NH2	2.32	0.62
1:B:917:GLU:HB3	3:C:104:TYR:HH	1.65	0.62
1:E:2582:MET:HA	1:E:2585:THR:HG22	1.81	0.62
1:G:165:VAL:O	1:G:203:ASN:ND2	2.32	0.62
1:G:2684:ASP:O	1:G:2688:HIS:ND1	2.32	0.62
1:J:2214:VAL:HG13	1:J:2215:LEU:HD12	1.79	0.62
1:B:2418:LEU:O	1:B:2422:ILE:HG12	2.00	0.62
1:G:2454:ARG:HG2	1:G:2458:ARG:HE	1.64	0.62
1:G:2582:MET:HA	1:G:2585:THR:HG22	1.82	0.62
1:B:2138:LEU:HB3	1:B:3658:LYS:HE2	1.80	0.62
1:B:2454:ARG:HG2	1:B:2458:ARG:HE	1.64	0.62
1:G:2431:ASP:HB2	1:G:2501:SER:HB2	1.80	0.62
1:J:2582:MET:HA	1:J:2585:THR:HG22	1.81	0.62
1:B:3986:TRP:HB3	1:B:4047:MET:CE	2.28	0.62
1:E:82:LEU:HD11	1:E:144:GLU:HB3	1.79	0.62
1:E:861:ILE:HG21	1:E:933:LEU:HD22	1.81	0.62
1:E:1099:GLU:HA	1:E:1127:HIS:HB2	1.80	0.62
1:E:2599:GLN:O	1:E:2603:ILE:HG12	1.99	0.62
1:G:1099:GLU:HA	1:G:1127:HIS:HB2	1.80	0.62
1:G:1528:THR:HG23	1:G:1539:PHE:HE1	1.63	0.62
1:G:2599:GLN:O	1:G:2603:ILE:HG12	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3962:PHE:CE2	1:G:4019:LEU:HD11	2.35	0.62
1:J:668:VAL:HG21	1:J:738:LEU:HD12	1.80	0.62
1:J:2599:GLN:O	1:J:2603:ILE:HG12	1.99	0.62
1:G:668:VAL:HG21	1:G:738:LEU:HD12	1.80	0.62
1:G:2902:HIS:HE1	1:G:2904:LEU:HB2	1.65	0.62
1:G:3981:ALA:HA	1:G:3986:TRP:HZ2	1.64	0.62
1:J:1099:GLU:HA	1:J:1127:HIS:HB2	1.80	0.62
1:B:718:GLY:HA3	1:B:737:LEU:HA	1.79	0.62
1:B:5013:MET:HE3	1:B:5018:CYS:HB3	1.82	0.62
1:E:913:LEU:HB3	1:E:917:GLU:HB2	1.80	0.62
1:E:2454:ARG:HG2	1:E:2458:ARG:HE	1.64	0.62
1:E:3592:ILE:HG12	1:E:3595:ARG:HH21	1.65	0.62
1:E:4712:PRO:HB2	1:E:4718:LYS:HA	1.80	0.62
1:G:3262:ARG:HG2	1:G:3329:ILE:HG21	1.82	0.62
1:J:3592:ILE:HG12	1:J:3595:ARG:HH21	1.65	0.62
1:B:365:LYS:HE2	1:B:369:LEU:HD21	1.80	0.62
1:G:861:ILE:HG21	1:G:933:LEU:HD22	1.81	0.62
1:G:2310:CYS:HB3	1:G:2313:LEU:HD23	1.82	0.62
1:G:2418:LEU:O	1:G:2422:ILE:HG12	2.00	0.62
1:B:2310:CYS:HB3	1:B:2313:LEU:HD23	1.82	0.62
1:B:2866:THR:O	1:B:2928:LYS:NZ	2.22	0.62
1:B:3962:PHE:HA	1:B:3965:LEU:HD12	1.82	0.62
1:B:3980:LEU:HD12	1:B:4030:LEU:HD21	1.82	0.62
1:B:3981:ALA:HA	1:B:3986:TRP:HZ2	1.65	0.62
1:B:4712:PRO:HB2	1:B:4718:LYS:HA	1.80	0.62
1:E:2418:LEU:O	1:E:2422:ILE:HG12	2.00	0.62
1:E:3196:ARG:HH12	1:E:3341:PHE:HZ	1.46	0.62
1:G:3594:ARG:NH2	1:G:3597:GLN:OE1	2.33	0.62
1:J:2310:CYS:HB3	1:J:2313:LEU:HD23	1.82	0.62
1:B:3021:PRO:HD3	1:B:3036:LYS:HZ3	1.65	0.62
1:E:985:VAL:HG22	1:E:1043:VAL:HG21	1.82	0.62
1:J:985:VAL:HG22	1:J:1043:VAL:HG21	1.82	0.62
1:J:1291:LEU:HD13	1:J:1595:LEU:HD11	1.81	0.62
1:J:2866:THR:O	1:J:2928:LYS:NZ	2.22	0.62
1:J:3980:LEU:HD12	1:J:4030:LEU:HD21	1.81	0.62
1:J:3981:ALA:HA	1:J:3986:TRP:HZ2	1.65	0.62
1:E:20:VAL:HG11	1:E:202:MET:SD	2.40	0.61
1:E:1528:THR:HG23	1:E:1539:PHE:HE1	1.63	0.61
1:G:1291:LEU:HD13	1:G:1595:LEU:HD11	1.81	0.61
1:J:2913:ALA:O	1:J:2917:ALA:N	2.24	0.61
1:B:1291:LEU:HD13	1:B:1595:LEU:HD11	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1694:LEU:HD11	1:B:1718:ILE:HD11	1.82	0.61
1:E:1694:LEU:HD11	1:E:1718:ILE:HD11	1.82	0.61
1:J:5013:MET:HE3	1:J:5018:CYS:HB3	1.82	0.61
1:B:2582:MET:HA	1:B:2585:THR:HG22	1.81	0.61
1:B:2764:GLU:HG2	1:B:2857:PRO:HD3	1.82	0.61
1:E:3980:LEU:HD12	1:E:4030:LEU:HD21	1.81	0.61
1:G:1547:LYS:NZ	1:G:1642:PRO:O	2.34	0.61
1:J:861:ILE:HG21	1:J:933:LEU:HD22	1.81	0.61
1:B:3262:ARG:HG2	1:B:3329:ILE:HG21	1.82	0.61
1:B:4892:ARG:HH11	1:E:4896:GLY:HA3	1.65	0.61
1:E:1291:LEU:HD13	1:E:1595:LEU:HD11	1.81	0.61
1:E:2764:GLU:HG2	1:E:2857:PRO:HD3	1.82	0.61
1:J:2265:LEU:HD21	1:J:2272:PRO:HG2	1.82	0.61
1:J:3196:ARG:HH12	1:J:3341:PHE:HZ	1.46	0.61
1:J:4072:VAL:O	1:J:4078:GLN:NE2	2.34	0.61
1:E:3282:PRO:HG3	1:E:3345:ILE:HD13	1.83	0.61
1:B:3594:ARG:NH2	1:B:3597:GLN:OE1	2.33	0.61
1:B:4072:VAL:O	1:B:4078:GLN:NE2	2.34	0.61
1:E:1547:LYS:NZ	1:E:1642:PRO:O	2.34	0.61
1:E:2902:HIS:HE1	1:E:2904:LEU:HB2	1.65	0.61
1:E:4072:VAL:O	1:E:4078:GLN:NE2	2.34	0.61
1:G:247:TYR:HE2	1:G:359:TYR:HA	1.66	0.61
1:J:20:VAL:HG11	1:J:202:MET:SD	2.40	0.61
1:J:3262:ARG:HG2	1:J:3329:ILE:HG21	1.82	0.61
1:E:3962:PHE:HA	1:E:3965:LEU:HD12	1.82	0.61
1:B:1547:LYS:NZ	1:B:1642:PRO:O	2.34	0.61
1:B:2902:HIS:HE1	1:B:2904:LEU:HB2	1.65	0.61
1:B:3592:ILE:HG12	1:B:3595:ARG:HH21	1.65	0.61
1:E:4864:ASN:ND2	1:E:4871:GLU:OE2	2.33	0.61
1:G:2764:GLU:HG2	1:G:2857:PRO:HD3	1.82	0.61
1:G:4072:VAL:O	1:G:4078:GLN:NE2	2.34	0.61
1:G:4864:ASN:ND2	1:G:4871:GLU:OE2	2.33	0.61
2:A:87:HIS:HB2	2:A:90:VAL:HG22	1.83	0.61
1:B:3967:GLU:HA	1:B:3970:GLN:CG	2.30	0.61
1:E:2746:ILE:HA	1:E:2814:LYS:HE3	1.82	0.61
1:G:985:VAL:HG22	1:G:1043:VAL:HG21	1.82	0.61
1:G:4896:GLY:HA3	1:J:4892:ARG:HH11	1.65	0.61
1:J:3962:PHE:HA	1:J:3965:LEU:HD12	1.82	0.61
1:J:4864:ASN:ND2	1:J:4871:GLU:OE2	2.33	0.61
1:B:985:VAL:HG22	1:B:1043:VAL:HG21	1.82	0.61
1:B:1528:THR:HG23	1:B:1539:PHE:HE1	1.63	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2746:ILE:HA	1:B:2814:LYS:HE3	1.82	0.61
1:G:20:VAL:HG11	1:G:202:MET:SD	2.40	0.61
2:H:87:HIS:HB2	2:H:90:VAL:HG22	1.83	0.61
1:B:2299:VAL:HG12	1:B:2360:LYS:HD2	1.83	0.60
1:E:2310:CYS:HB3	1:E:2313:LEU:HD23	1.82	0.60
1:G:917:GLU:HB3	3:M:104:TYR:HH	1.65	0.60
1:G:3592:ILE:HG12	1:G:3595:ARG:HH21	1.65	0.60
1:B:20:VAL:HG11	1:B:202:MET:SD	2.40	0.60
1:E:3262:ARG:HG2	1:E:3329:ILE:HG21	1.82	0.60
1:J:1547:LYS:NZ	1:J:1642:PRO:O	2.34	0.60
1:J:2764:GLU:HG2	1:J:2857:PRO:HD3	1.82	0.60
2:I:87:HIS:HB2	2:I:90:VAL:HG22	1.83	0.60
1:B:840:VAL:HG12	1:B:1199:VAL:HG12	1.84	0.60
1:B:4864:ASN:ND2	1:B:4871:GLU:OE2	2.33	0.60
1:J:3282:PRO:HG3	1:J:3345:ILE:HD13	1.83	0.60
2:D:87:HIS:HB2	2:D:90:VAL:HG22	1.83	0.60
1:E:4892:ARG:HH11	1:J:4896:GLY:HA3	1.67	0.60
1:G:1694:LEU:HD11	1:G:1718:ILE:HD11	1.82	0.60
1:G:2265:LEU:HD21	1:G:2272:PRO:HG2	1.82	0.60
1:G:2746:ILE:HA	1:G:2814:LYS:HE3	1.82	0.60
1:J:2454:ARG:HG2	1:J:2458:ARG:HE	1.64	0.60
1:J:2746:ILE:HA	1:J:2814:LYS:HE3	1.82	0.60
1:B:2265:LEU:HD21	1:B:2272:PRO:HG2	1.82	0.60
1:E:2265:LEU:HD21	1:E:2272:PRO:HG2	1.82	0.60
1:J:840:VAL:HG12	1:J:1199:VAL:HG12	1.84	0.60
1:J:4876:CYS:HA	1:J:4882:CYS:HB2	1.83	0.60
1:B:861:ILE:HG21	1:B:933:LEU:HD22	1.81	0.60
1:G:3031:ALA:O	1:G:3036:LYS:NZ	2.27	0.60
1:G:3282:PRO:HG3	1:G:3345:ILE:HD13	1.82	0.60
1:J:1694:LEU:HD11	1:J:1718:ILE:HD11	1.82	0.60
1:B:952:LYS:HA	1:B:970:LEU:HA	1.84	0.60
1:B:3282:PRO:HG3	1:B:3345:ILE:HD13	1.82	0.60
1:E:840:VAL:HG12	1:E:1199:VAL:HG12	1.84	0.60
1:E:952:LYS:HA	1:E:970:LEU:HA	1.84	0.60
1:E:4876:CYS:HA	1:E:4882:CYS:HB2	1.83	0.60
1:G:2299:VAL:HG12	1:G:2360:LYS:HD2	1.83	0.60
1:J:2418:LEU:O	1:J:2422:ILE:HG12	2.00	0.60
1:E:3981:ALA:HA	1:E:3986:TRP:HZ2	1.65	0.60
1:J:2902:HIS:HE1	1:J:2904:LEU:HB2	1.65	0.60
1:B:4983:HIS:O	5:B:5102:ATP:N6	2.35	0.60
1:E:2299:VAL:HG12	1:E:2360:LYS:HD2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3967:GLU:HA	1:G:3970:GLN:CG	2.30	0.60
1:B:3391:GLU:O	1:B:3395:ARG:HG3	2.02	0.60
1:E:2470:ILE:HB	1:E:2502:MET:HE3	1.84	0.60
1:G:2882:TYR:HB3	1:G:2886:TRP:CZ3	2.36	0.60
1:J:595:ARG:NH1	1:J:1643:GLU:OE2	2.35	0.60
1:B:4876:CYS:HA	1:B:4882:CYS:HB2	1.83	0.59
1:E:3594:ARG:NH2	1:E:3597:GLN:OE1	2.33	0.59
1:G:4983:HIS:O	5:G:5102:ATP:N6	2.35	0.59
1:J:35:LEU:HG	1:J:51:PRO:HA	1.84	0.59
2:I:10:GLY:HA3	2:I:70:GLN:HB2	1.84	0.59
3:F:122:GLN:NE2	3:F:124:THR:OG1	2.34	0.59
1:E:3208:PRO:HB3	1:E:3236:VAL:HB	1.84	0.59
1:E:3391:GLU:O	1:E:3395:ARG:HG3	2.02	0.59
1:E:3669:PHE:CE1	1:E:3672:ARG:HB3	2.38	0.59
1:G:840:VAL:HG12	1:G:1199:VAL:HG12	1.84	0.59
1:G:3346:VAL:HG13	1:G:3414:ARG:HG2	1.85	0.59
1:G:3531:ASP:HA	1:G:3534:MET:SD	2.42	0.59
2:D:10:GLY:HA3	2:D:70:GLN:HB2	1.84	0.59
1:B:2882:TYR:HB3	1:B:2886:TRP:CZ3	2.36	0.59
1:B:3346:VAL:HG13	1:B:3414:ARG:HG2	1.85	0.59
1:E:35:LEU:HG	1:E:51:PRO:HA	1.84	0.59
1:G:247:TYR:HB2	1:G:374:LYS:HD2	1.83	0.59
1:J:917:GLU:HB3	3:K:104:TYR:HH	1.67	0.59
1:J:3669:PHE:CE1	1:J:3672:ARG:HB3	2.38	0.59
1:B:2495:VAL:HG22	1:B:2497:ASP:H	1.68	0.59
1:E:2866:THR:O	1:E:2928:LYS:NZ	2.22	0.59
1:E:3539:ARG:HD3	1:E:3542:LEU:HD12	1.85	0.59
1:E:3757:GLU:O	1:E:3761:GLN:HG2	2.02	0.59
1:G:3208:PRO:HB3	1:G:3236:VAL:HB	1.84	0.59
1:J:2642:LYS:HE3	1:J:2646:ASN:HD21	1.68	0.59
1:J:2882:TYR:HB3	1:J:2886:TRP:CZ3	2.36	0.59
1:B:246:TYR:CD1	1:B:375:LYS:HA	2.37	0.59
1:B:3531:ASP:HA	1:B:3534:MET:SD	2.42	0.59
1:J:870:ILE:O	1:J:874:LEU:HG	2.02	0.59
1:J:952:LYS:HA	1:J:970:LEU:HA	1.84	0.59
2:H:10:GLY:HA3	2:H:70:GLN:HB2	1.84	0.59
1:E:3346:VAL:HG13	1:E:3414:ARG:HG2	1.84	0.59
1:G:870:ILE:O	1:G:874:LEU:HG	2.02	0.59
1:G:3669:PHE:CE1	1:G:3672:ARG:HB3	2.38	0.59
1:J:3594:ARG:NH2	1:J:3597:GLN:OE1	2.33	0.59
1:B:870:ILE:O	1:B:874:LEU:HG	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3981:ALA:HA	1:B:3986:TRP:CZ2	2.37	0.59
1:B:4896:GLY:HA3	1:G:4892:ARG:HH11	1.67	0.59
1:E:870:ILE:O	1:E:874:LEU:HG	2.02	0.59
1:E:917:GLU:HB3	3:F:104:TYR:HH	1.67	0.59
1:E:3457:ASN:HA	1:E:3460:VAL:HG12	1.84	0.59
1:G:3457:ASN:HA	1:G:3460:VAL:HG12	1.84	0.59
1:J:3531:ASP:HA	1:J:3534:MET:SD	2.42	0.59
1:B:35:LEU:HG	1:B:51:PRO:HA	1.84	0.59
1:B:1465:ASP:OD1	1:B:1466:LEU:N	2.36	0.59
1:B:2624:ARG:HH22	1:B:2912:THR:HG22	1.68	0.59
1:E:3981:ALA:HA	1:E:3986:TRP:CZ2	2.37	0.59
1:E:4817:ALA:HB1	1:E:4827:LEU:HD11	1.85	0.59
1:E:4983:HIS:O	5:E:5102:ATP:N6	2.35	0.59
1:G:4876:CYS:HA	1:G:4882:CYS:HB2	1.83	0.59
1:B:2642:LYS:HE3	1:B:2646:ASN:HD21	1.68	0.59
1:B:3208:PRO:HB3	1:B:3236:VAL:HB	1.84	0.59
1:B:4817:ALA:HB1	1:B:4827:LEU:HD11	1.85	0.59
1:E:942:ALA:HB2	1:E:1052:ASN:HB3	1.85	0.59
1:G:952:LYS:HA	1:G:970:LEU:HA	1.84	0.59
1:J:2299:VAL:HG12	1:J:2360:LYS:HD2	1.83	0.59
1:J:3346:VAL:HG13	1:J:3414:ARG:HG2	1.84	0.59
1:B:3539:ARG:HD3	1:B:3542:LEU:HD12	1.85	0.59
1:E:2624:ARG:HH22	1:E:2912:THR:HG22	1.68	0.59
1:G:35:LEU:HG	1:G:51:PRO:HA	1.84	0.59
1:G:595:ARG:NH1	1:G:1643:GLU:OE2	2.35	0.59
1:J:246:TYR:CD1	1:J:375:LYS:HA	2.37	0.59
1:E:2642:LYS:HE3	1:E:2646:ASN:HD21	1.68	0.58
1:G:58:VAL:HG12	1:G:305:CYS:HA	1.85	0.58
1:G:2202:GLY:HA2	1:G:2204:HIS:CE1	2.38	0.58
1:G:3416:VAL:O	1:G:3420:ARG:HB2	2.03	0.58
1:G:3962:PHE:HE2	1:G:4019:LEU:HD11	1.68	0.58
1:G:3981:ALA:HA	1:G:3986:TRP:CZ2	2.37	0.58
1:J:3539:ARG:HD3	1:J:3542:LEU:HD12	1.85	0.58
1:J:3981:ALA:HA	1:J:3986:TRP:CZ2	2.37	0.58
1:J:4817:ALA:HB1	1:J:4827:LEU:HD11	1.85	0.58
1:J:4983:HIS:O	5:J:5102:ATP:N6	2.35	0.58
1:B:631:LEU:HD22	1:B:1594:ARG:HH12	1.68	0.58
1:B:942:ALA:HB2	1:B:1052:ASN:HB3	1.85	0.58
1:B:3669:PHE:CE1	1:B:3672:ARG:HB3	2.38	0.58
1:G:1032:LYS:HB3	1:G:1036:ARG:HH22	1.68	0.58
1:G:1786:LEU:HD12	1:G:1787:PRO:HD2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:58:VAL:HG12	1:J:305:CYS:HA	1.85	0.58
1:B:3846:ALA:HB1	1:B:3873:LYS:HG2	1.86	0.58
1:E:3531:ASP:HA	1:E:3534:MET:SD	2.42	0.58
1:J:1465:ASP:OD1	1:J:1466:LEU:N	2.36	0.58
1:J:3457:ASN:HA	1:J:3460:VAL:HG12	1.84	0.58
1:B:58:VAL:HG12	1:B:305:CYS:HA	1.85	0.58
1:B:2651:CYS:HB3	1:B:2654:TYR:HB3	1.85	0.58
1:E:2651:CYS:HB3	1:E:2654:TYR:HB3	1.85	0.58
1:G:924:MET:HE2	3:M:107:TRP:HB2	1.85	0.58
1:G:2642:LYS:HE3	1:G:2646:ASN:HD21	1.68	0.58
1:J:2961:GLN:HA	1:J:2964:LEU:HD12	1.86	0.58
1:B:675:LEU:HG	1:B:676:THR:HG23	1.86	0.58
1:B:3416:VAL:O	1:B:3420:ARG:HB2	2.04	0.58
1:E:3227:ARG:HB3	1:E:3232:LEU:HB2	1.86	0.58
1:G:360:ALA:HB3	1:G:375:LYS:HB3	1.85	0.58
1:G:2495:VAL:HG22	1:G:2497:ASP:H	1.68	0.58
1:J:1032:LYS:HB3	1:J:1036:ARG:HH22	1.68	0.58
1:J:2495:VAL:HG22	1:J:2497:ASP:H	1.68	0.58
1:J:2624:ARG:HH22	1:J:2912:THR:HG22	1.68	0.58
3:K:105:ASN:HD21	3:K:111:ASN:HB2	1.68	0.58
1:B:1862:ILE:O	1:B:1866:ILE:HG13	2.04	0.58
1:B:2961:GLN:HA	1:B:2964:LEU:HD12	1.86	0.58
1:B:3757:GLU:O	1:B:3761:GLN:HG2	2.02	0.58
1:E:1465:ASP:OD1	1:E:1466:LEU:N	2.36	0.58
1:E:2961:GLN:HA	1:E:2964:LEU:HD12	1.86	0.58
1:G:748:LEU:HD13	1:G:755:ILE:HG12	1.86	0.58
1:G:3757:GLU:O	1:G:3761:GLN:HG2	2.03	0.58
1:J:631:LEU:HD22	1:J:1594:ARG:HH12	1.68	0.58
1:J:3227:ARG:HB3	1:J:3232:LEU:HB2	1.86	0.58
1:B:1786:LEU:HD12	1:B:1787:PRO:HD2	1.85	0.58
1:B:3227:ARG:HB3	1:B:3232:LEU:HB2	1.86	0.58
1:E:1032:LYS:HB3	1:E:1036:ARG:HH22	1.68	0.58
1:E:3967:GLU:HA	1:E:3970:GLN:CG	2.30	0.58
1:G:574:VAL:HA	1:G:577:ILE:HG22	1.85	0.58
1:G:1503:PRO:O	1:G:1534:LYS:NZ	2.36	0.58
1:G:1721:GLU:OE2	1:G:1725:ARG:NH2	2.36	0.58
1:G:3227:ARG:HB3	1:G:3232:LEU:HB2	1.86	0.58
1:J:3416:VAL:O	1:J:3420:ARG:HB2	2.03	0.58
2:A:10:GLY:HA3	2:A:70:GLN:HB2	1.84	0.58
1:B:1032:LYS:HB3	1:B:1036:ARG:HH22	1.68	0.58
1:B:2202:GLY:HA2	1:B:2204:HIS:CE1	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:58:VAL:HG12	1:E:305:CYS:HA	1.85	0.58
1:E:574:VAL:HA	1:E:577:ILE:HG22	1.85	0.58
1:E:1503:PRO:O	1:E:1534:LYS:NZ	2.36	0.58
1:E:2257:LEU:HD22	1:E:2272:PRO:HB3	1.86	0.58
1:E:3846:ALA:HB1	1:E:3873:LYS:HG2	1.86	0.58
1:E:3900:GLN:HB3	1:E:3976:ASN:HD21	1.69	0.58
1:G:631:LEU:HD22	1:G:1594:ARG:HH12	1.68	0.58
1:G:2874:MET:HE1	1:G:2939:ARG:HG3	1.86	0.58
1:G:3391:GLU:O	1:G:3395:ARG:HG3	2.03	0.58
1:G:3539:ARG:HD3	1:G:3542:LEU:HD12	1.85	0.58
1:J:3391:GLU:O	1:J:3395:ARG:HG3	2.02	0.58
2:A:30:LEU:HB2	2:A:34:LYS:HB2	1.86	0.58
2:H:30:LEU:HB2	2:H:34:LYS:HB2	1.86	0.58
1:B:904:HIS:HD2	1:B:907:LEU:H	1.51	0.58
1:B:2325:PRO:O	1:B:2329:GLU:HG2	2.04	0.58
1:B:3457:ASN:HA	1:B:3460:VAL:HG12	1.84	0.58
1:E:3416:VAL:O	1:E:3420:ARG:HB2	2.03	0.58
1:G:2624:ARG:HH22	1:G:2912:THR:HG22	1.68	0.58
1:G:3846:ALA:HB1	1:G:3873:LYS:HG2	1.86	0.58
1:G:5013:MET:HE3	1:G:5018:CYS:HB3	1.86	0.58
1:J:1862:ILE:O	1:J:1866:ILE:HG13	2.03	0.58
1:J:3208:PRO:HB3	1:J:3236:VAL:HB	1.84	0.58
2:I:30:LEU:HB2	2:I:34:LYS:HB2	1.86	0.58
3:K:122:GLN:NE2	3:K:124:THR:OG1	2.34	0.58
1:B:294:THR:HG23	1:B:297:GLN:H	1.69	0.58
1:E:631:LEU:HD22	1:E:1594:ARG:HH12	1.68	0.58
1:J:1503:PRO:O	1:J:1534:LYS:NZ	2.36	0.58
1:J:2202:GLY:HA2	1:J:2204:HIS:CE1	2.39	0.58
1:J:2325:PRO:O	1:J:2329:GLU:HG2	2.04	0.58
2:D:30:LEU:HB2	2:D:34:LYS:HB2	1.86	0.58
1:B:544:LEU:HD12	1:B:574:VAL:HB	1.86	0.57
1:B:2257:LEU:HD22	1:B:2272:PRO:HB3	1.86	0.57
1:B:2881:ASN:HA	1:B:2884:ASN:ND2	2.20	0.57
1:G:1973:GLN:HE22	1:G:3641:LEU:H	1.52	0.57
1:G:4817:ALA:HB1	1:G:4827:LEU:HD11	1.85	0.57
1:J:748:LEU:HD13	1:J:755:ILE:HG12	1.86	0.57
1:B:574:VAL:HA	1:B:577:ILE:HG22	1.85	0.57
1:B:3900:GLN:HB3	1:B:3976:ASN:HD21	1.69	0.57
1:E:2881:ASN:HA	1:E:2884:ASN:ND2	2.19	0.57
1:G:942:ALA:HB2	1:G:1052:ASN:HB3	1.85	0.57
1:G:2325:PRO:O	1:G:2329:GLU:HG2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4952:GLU:O	1:G:4956:THR:HG23	2.05	0.57
1:J:942:ALA:HB2	1:J:1052:ASN:HB3	1.85	0.57
1:J:981:GLN:O	1:J:985:VAL:HG23	2.04	0.57
1:J:1973:GLN:HE22	1:J:3641:LEU:H	1.52	0.57
1:B:3835:LEU:HD22	1:B:3880:PHE:HZ	1.70	0.57
1:E:544:LEU:HD12	1:E:574:VAL:HB	1.86	0.57
1:E:2202:GLY:HA2	1:E:2204:HIS:CE1	2.39	0.57
1:E:2882:TYR:HB3	1:E:2886:TRP:CZ3	2.36	0.57
1:E:1862:ILE:O	1:E:1866:ILE:HG13	2.03	0.57
1:G:1465:ASP:OD1	1:G:1466:LEU:N	2.36	0.57
1:G:2881:ASN:HA	1:G:2884:ASN:ND2	2.19	0.57
1:G:3835:LEU:HD22	1:G:3880:PHE:HZ	1.70	0.57
1:J:1786:LEU:HD12	1:J:1787:PRO:HD2	1.85	0.57
1:J:2881:ASN:HA	1:J:2884:ASN:ND2	2.19	0.57
1:E:294:THR:HG23	1:E:297:GLN:H	1.69	0.57
1:G:365:LYS:HE2	1:G:369:LEU:HD21	1.86	0.57
1:G:2961:GLN:HA	1:G:2964:LEU:HD12	1.86	0.57
1:J:904:HIS:HD2	1:J:907:LEU:H	1.51	0.57
1:J:3900:GLN:HB3	1:J:3976:ASN:HD21	1.69	0.57
1:B:595:ARG:NH1	1:B:1643:GLU:OE2	2.35	0.57
1:B:981:GLN:O	1:B:985:VAL:HG23	2.04	0.57
1:B:1973:GLN:HE22	1:B:3641:LEU:H	1.52	0.57
1:B:2768:PHE:O	1:B:2772:GLN:HG2	2.05	0.57
1:E:983:THR:HB	1:E:987:ARG:HH12	1.70	0.57
1:G:981:GLN:O	1:G:985:VAL:HG23	2.04	0.57
1:G:1449:TRP:HB3	1:G:1494:MET:HG3	1.87	0.57
1:J:2651:CYS:HB3	1:J:2654:TYR:HB3	1.85	0.57
1:J:3757:GLU:O	1:J:3761:GLN:HG2	2.03	0.57
1:J:3967:GLU:HA	1:J:3970:GLN:CG	2.30	0.57
1:B:4952:GLU:O	1:B:4956:THR:HG23	2.05	0.57
1:E:595:ARG:NH1	1:E:1643:GLU:OE2	2.35	0.57
1:E:675:LEU:HG	1:E:676:THR:HG23	1.86	0.57
1:E:2768:PHE:O	1:E:2772:GLN:HG2	2.05	0.57
1:J:574:VAL:HA	1:J:577:ILE:HG22	1.85	0.57
1:J:3846:ALA:HB1	1:J:3873:LYS:HG2	1.86	0.57
1:E:1973:GLN:HE22	1:E:3641:LEU:H	1.52	0.57
1:G:1862:ILE:O	1:G:1866:ILE:HG13	2.04	0.57
1:J:1232:ARG:NH2	1:J:1828:ASP:O	2.37	0.57
1:J:2768:PHE:O	1:J:2772:GLN:HG2	2.05	0.57
1:J:3270:ILE:H	1:J:3270:ILE:HD12	1.70	0.57
1:J:3835:LEU:HD22	1:J:3880:PHE:HZ	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:4676:GLU:O	1:J:4680:LYS:HG2	2.05	0.57
3:F:105:ASN:HD21	3:F:111:ASN:HB2	1.68	0.57
3:M:105:ASN:HD21	3:M:111:ASN:HB2	1.68	0.57
1:B:3018:LEU:HB2	1:B:3074:SER:HA	1.87	0.57
1:E:2495:VAL:HG22	1:E:2497:ASP:H	1.68	0.57
1:G:675:LEU:HG	1:G:676:THR:HG23	1.86	0.57
1:J:3695:PRO:HB2	1:J:3699:HIS:HB3	1.87	0.57
1:B:1102:VAL:HG11	1:B:1149:VAL:HG11	1.87	0.57
1:E:1206:GLN:HE22	1:E:1233:PRO:HA	1.70	0.57
1:G:294:THR:HG23	1:G:297:GLN:H	1.69	0.57
1:G:983:THR:HB	1:G:987:ARG:HH12	1.69	0.57
1:G:2651:CYS:HB3	1:G:2654:TYR:HB3	1.85	0.57
1:G:2768:PHE:O	1:G:2772:GLN:HG2	2.05	0.57
1:G:3695:PRO:HB2	1:G:3699:HIS:HB3	1.87	0.57
1:B:748:LEU:HD13	1:B:755:ILE:HG12	1.86	0.56
1:B:2751:LEU:O	1:B:2755:ILE:HG12	2.05	0.56
1:E:16:THR:HB	1:E:98:HIS:HA	1.87	0.56
1:E:981:GLN:O	1:E:985:VAL:HG23	2.04	0.56
1:E:1679:ASN:ND2	1:E:1797:ARG:O	2.37	0.56
1:G:3043:PHE:HA	1:G:3071:LEU:HD13	1.87	0.56
1:J:3413:ILE:HG23	1:J:3516:LYS:HE2	1.87	0.56
1:B:16:THR:HB	1:B:98:HIS:HA	1.87	0.56
1:B:1449:TRP:HB3	1:B:1494:MET:HG3	1.87	0.56
1:E:748:LEU:HD13	1:E:755:ILE:HG12	1.86	0.56
1:E:904:HIS:HD2	1:E:907:LEU:H	1.51	0.56
1:E:3158:LEU:O	1:E:3162:GLN:NE2	2.38	0.56
1:E:3413:ILE:HG23	1:E:3516:LYS:HE2	1.87	0.56
1:E:3835:LEU:HD22	1:E:3880:PHE:HZ	1.70	0.56
1:G:1023:PRO:HD2	1:G:1026:LEU:HD22	1.88	0.56
1:G:3312:LEU:HB2	1:G:3345:ILE:HD11	1.87	0.56
1:G:5009:TYR:HA	1:G:5012:LYS:HE3	1.87	0.56
1:J:294:THR:HG23	1:J:297:GLN:H	1.69	0.56
1:J:675:LEU:HG	1:J:676:THR:HG23	1.86	0.56
1:J:1023:PRO:HD2	1:J:1026:LEU:HD22	1.87	0.56
1:J:3158:LEU:O	1:J:3162:GLN:NE2	2.38	0.56
1:B:1206:GLN:HE22	1:B:1233:PRO:HA	1.70	0.56
1:B:3312:LEU:HB2	1:B:3345:ILE:HD11	1.87	0.56
1:B:4676:GLU:O	1:B:4680:LYS:HG2	2.05	0.56
1:E:1786:LEU:HD12	1:E:1787:PRO:HD2	1.85	0.56
1:E:2131:LEU:HD11	1:E:3662:ILE:HG12	1.88	0.56
1:E:2325:PRO:O	1:E:2329:GLU:HG2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2751:LEU:O	1:E:2755:ILE:HG12	2.05	0.56
1:E:3270:ILE:H	1:E:3270:ILE:HD12	1.70	0.56
1:E:3312:LEU:HB2	1:E:3345:ILE:HD11	1.88	0.56
1:E:4952:GLU:O	1:E:4956:THR:HG23	2.05	0.56
1:G:544:LEU:HD12	1:G:574:VAL:HB	1.86	0.56
1:J:544:LEU:HD12	1:J:574:VAL:HB	1.86	0.56
1:J:1206:GLN:HE22	1:J:1233:PRO:HA	1.70	0.56
1:J:1721:GLU:OE2	1:J:1725:ARG:NH2	2.36	0.56
1:J:2257:LEU:HD22	1:J:2272:PRO:HB3	1.86	0.56
1:J:4952:GLU:O	1:J:4956:THR:HG23	2.05	0.56
1:J:5009:TYR:HA	1:J:5012:LYS:HE3	1.87	0.56
3:M:122:GLN:NE2	3:M:124:THR:OG1	2.34	0.56
1:B:365:LYS:O	1:B:369:LEU:HG	2.06	0.56
1:B:2131:LEU:HD11	1:B:3662:ILE:HG12	1.88	0.56
1:E:2527:LEU:HD11	1:E:2582:MET:HB3	1.88	0.56
1:E:3065:VAL:O	1:E:3069:HIS:ND1	2.38	0.56
1:G:2257:LEU:HD22	1:G:2272:PRO:HB3	1.86	0.56
1:G:3270:ILE:H	1:G:3270:ILE:HD12	1.70	0.56
1:B:2449:GLU:O	1:B:2453:ILE:HG12	2.06	0.56
1:B:3065:VAL:O	1:B:3069:HIS:ND1	2.39	0.56
1:B:3219:TYR:OH	1:B:3235:SER:N	2.39	0.56
1:B:3695:PRO:HB2	1:B:3699:HIS:HB3	1.87	0.56
1:B:3768:SER:HA	1:B:3771:HIS:CD2	2.41	0.56
1:E:3018:LEU:HB2	1:E:3074:SER:HA	1.87	0.56
1:E:3800:LEU:O	1:E:3804:ILE:HG12	2.06	0.56
1:G:883:ALA:HA	1:G:886:ARG:HE	1.70	0.56
1:G:3158:LEU:O	1:G:3162:GLN:NE2	2.38	0.56
1:J:883:ALA:HA	1:J:886:ARG:HE	1.70	0.56
3:C:105:ASN:HD21	3:C:111:ASN:HB2	1.70	0.56
1:B:2364:PHE:HD1	1:B:2429:LEU:HD21	1.71	0.56
1:B:3158:LEU:O	1:B:3162:GLN:NE2	2.38	0.56
1:E:844:ARG:HE	1:E:845:CYS:H	1.54	0.56
1:G:2123:LEU:O	1:G:2127:GLN:HG2	2.06	0.56
1:G:3065:VAL:O	1:G:3069:HIS:ND1	2.38	0.56
1:J:3312:LEU:HB2	1:J:3345:ILE:HD11	1.87	0.56
3:C:122:GLN:NE2	3:C:124:THR:OG1	2.34	0.56
1:B:1240:LYS:HE3	1:B:1242:LEU:HB3	1.87	0.56
1:B:1503:PRO:O	1:B:1534:LYS:NZ	2.36	0.56
1:B:3270:ILE:H	1:B:3270:ILE:HD12	1.70	0.56
1:B:3800:LEU:O	1:B:3804:ILE:HG12	2.06	0.56
1:E:1102:VAL:HG11	1:E:1149:VAL:HG11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3695:PRO:HB2	1:E:3699:HIS:HB3	1.87	0.56
1:E:3768:SER:HA	1:E:3771:HIS:CD2	2.41	0.56
1:G:904:HIS:HD2	1:G:907:LEU:H	1.51	0.56
1:G:1206:GLN:HE22	1:G:1233:PRO:HA	1.70	0.56
1:G:2449:GLU:O	1:G:2453:ILE:HG12	2.06	0.56
1:G:3018:LEU:HB2	1:G:3074:SER:HA	1.87	0.56
1:J:2131:LEU:HD11	1:J:3662:ILE:HG12	1.88	0.56
1:J:3065:VAL:O	1:J:3069:HIS:ND1	2.38	0.56
1:J:3940:LYS:O	1:J:4002:LYS:NZ	2.36	0.56
1:B:983:THR:HB	1:B:987:ARG:HH12	1.70	0.56
1:B:3413:ILE:HG23	1:B:3516:LYS:HE2	1.87	0.56
1:E:3043:PHE:HA	1:E:3071:LEU:HD13	1.87	0.56
1:E:4676:GLU:O	1:E:4680:LYS:HG2	2.05	0.56
1:G:2527:LEU:HD11	1:G:2582:MET:HB3	1.88	0.56
1:J:16:THR:HB	1:J:98:HIS:HA	1.87	0.56
1:J:3219:TYR:OH	1:J:3235:SER:N	2.39	0.56
1:B:2527:LEU:HD11	1:B:2582:MET:HB3	1.88	0.56
1:E:1023:PRO:HD2	1:E:1026:LEU:HD22	1.87	0.56
1:E:1721:GLU:OE2	1:E:1725:ARG:NH2	2.36	0.56
1:E:2123:LEU:O	1:E:2127:GLN:HG2	2.06	0.56
1:G:499:THR:HG23	1:G:502:HIS:H	1.71	0.56
1:G:2364:PHE:HD1	1:G:2429:LEU:HD21	1.71	0.56
1:G:3413:ILE:HG23	1:G:3516:LYS:HE2	1.87	0.56
1:J:1240:LYS:HE3	1:J:1242:LEU:HB3	1.87	0.56
1:J:3768:SER:HA	1:J:3771:HIS:CD2	2.41	0.56
1:B:844:ARG:HE	1:B:845:CYS:H	1.54	0.56
1:B:1155:LEU:HD22	1:B:1184:ILE:HG12	1.88	0.56
1:E:1449:TRP:HB3	1:E:1494:MET:HG3	1.87	0.56
1:E:2238:TYR:O	1:E:2242:ILE:HG12	2.06	0.56
1:G:1782:PHE:O	2:H:82:TYR:OH	2.22	0.56
1:G:3800:LEU:O	1:G:3804:ILE:HG12	2.06	0.56
1:G:4673:ARG:NH2	1:G:4702:ASP:OD1	2.39	0.56
1:G:4676:GLU:O	1:G:4680:LYS:HG2	2.05	0.56
1:J:2449:GLU:O	1:J:2453:ILE:HG12	2.06	0.56
1:J:2751:LEU:O	1:J:2755:ILE:HG12	2.05	0.56
1:B:1023:PRO:HD2	1:B:1026:LEU:HD22	1.88	0.55
1:B:2626:LEU:HG	1:B:2640:PRO:HB3	1.88	0.55
1:B:3043:PHE:HA	1:B:3071:LEU:HD13	1.87	0.55
1:E:2449:GLU:O	1:E:2453:ILE:HG12	2.06	0.55
1:E:4673:ARG:NH2	1:E:4702:ASP:OD1	2.39	0.55
1:G:2238:TYR:O	1:G:2242:ILE:HG12	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2751:LEU:O	1:G:2755:ILE:HG12	2.05	0.55
1:J:499:THR:HG23	1:J:502:HIS:H	1.71	0.55
1:J:983:THR:HB	1:J:987:ARG:HH12	1.69	0.55
1:J:1449:TRP:HB3	1:J:1494:MET:HG3	1.87	0.55
1:J:2123:LEU:O	1:J:2127:GLN:HG2	2.06	0.55
1:B:2238:TYR:O	1:B:2242:ILE:HG12	2.06	0.55
1:B:3847:PHE:HB2	1:B:3874:VAL:HG12	1.87	0.55
1:E:3021:PRO:HD3	1:E:3036:LYS:HZ3	1.71	0.55
1:G:844:ARG:HE	1:G:845:CYS:H	1.54	0.55
1:G:1102:VAL:HG11	1:G:1149:VAL:HG11	1.87	0.55
1:J:365:LYS:O	1:J:369:LEU:HG	2.06	0.55
1:J:844:ARG:HE	1:J:845:CYS:H	1.54	0.55
1:J:1155:LEU:HD22	1:J:1184:ILE:HG12	1.88	0.55
1:J:3043:PHE:HA	1:J:3071:LEU:HD13	1.87	0.55
1:J:3206:LEU:HB2	1:J:3246:LEU:HD23	1.88	0.55
1:J:3800:LEU:O	1:J:3804:ILE:HG12	2.06	0.55
1:B:499:THR:HG23	1:B:502:HIS:H	1.71	0.55
1:B:1232:ARG:NH2	1:B:1828:ASP:O	2.36	0.55
1:E:3219:TYR:OH	1:E:3235:SER:N	2.39	0.55
1:G:1232:ARG:NH2	1:G:1828:ASP:O	2.37	0.55
1:G:2131:LEU:HD11	1:G:3662:ILE:HG12	1.88	0.55
1:G:3847:PHE:HB2	1:G:3874:VAL:HG12	1.87	0.55
1:J:4749:GLU:HG3	1:J:4753:HIS:NE2	2.21	0.55
1:B:3967:GLU:CA	1:B:3970:GLN:HG2	2.34	0.55
1:B:4673:ARG:NH2	1:B:4702:ASP:OD1	2.39	0.55
1:E:883:ALA:HA	1:E:886:ARG:HE	1.70	0.55
1:G:16:THR:HB	1:G:98:HIS:HA	1.86	0.55
1:G:2131:LEU:HB3	1:G:3667:HIS:CE1	2.42	0.55
1:G:3884:LEU:O	1:G:3888:LEU:HG	2.06	0.55
1:G:4735:GLU:O	1:G:4739:GLU:HG2	2.07	0.55
1:J:355:LEU:HB3	1:J:378:LEU:HB3	1.88	0.55
1:B:2131:LEU:HB3	1:B:3667:HIS:CE1	2.42	0.55
1:B:2464:ASP:OD1	1:B:2465:ASP:N	2.40	0.55
1:E:3847:PHE:HB2	1:E:3874:VAL:HG12	1.87	0.55
1:G:3219:TYR:OH	1:G:3235:SER:N	2.39	0.55
1:B:248:GLU:HB2	1:B:373:LYS:HA	1.88	0.55
1:B:355:LEU:HB3	1:B:378:LEU:HB3	1.88	0.55
1:B:2039:LEU:HB3	1:B:2044:ILE:HB	1.89	0.55
1:B:3206:LEU:HB2	1:B:3246:LEU:HD23	1.88	0.55
1:E:2364:PHE:HD1	1:E:2429:LEU:HD21	1.71	0.55
1:E:2626:LEU:HG	1:E:2640:PRO:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1240:LYS:HE3	1:G:1242:LEU:HB3	1.87	0.55
1:G:1504:GLY:O	1:G:1532:ASN:ND2	2.40	0.55
1:G:3768:SER:HA	1:G:3771:HIS:CD2	2.41	0.55
1:J:3018:LEU:HB2	1:J:3074:SER:HA	1.87	0.55
1:J:3847:PHE:HB2	1:J:3874:VAL:HG12	1.88	0.55
1:J:4735:GLU:O	1:J:4739:GLU:HG2	2.07	0.55
1:B:1721:GLU:OE2	1:B:1725:ARG:NH2	2.36	0.55
1:B:2123:LEU:O	1:B:2127:GLN:HG2	2.06	0.55
1:B:5009:TYR:HA	1:B:5012:LYS:HE3	1.87	0.55
1:E:499:THR:HG23	1:E:502:HIS:H	1.71	0.55
1:E:2978:GLU:HB2	1:E:3053:ARG:HH11	1.72	0.55
1:E:4749:GLU:HG3	1:E:4753:HIS:NE2	2.21	0.55
1:G:897:ARG:HD3	1:G:905:PRO:HD3	1.89	0.55
1:G:2039:LEU:HB3	1:G:2044:ILE:HB	1.89	0.55
1:J:2527:LEU:HD11	1:J:2582:MET:HB3	1.88	0.55
1:J:5012:LYS:O	1:J:5016:GLU:HG2	2.07	0.55
1:B:157:ARG:NH2	1:B:162:LYS:O	2.37	0.55
1:B:232:THR:HG21	1:B:252:VAL:HG11	1.88	0.55
1:B:2978:GLU:HB2	1:B:3053:ARG:HH11	1.72	0.55
1:B:4735:GLU:O	1:B:4739:GLU:HG2	2.07	0.55
1:E:2747:ILE:HD12	1:E:2817:ILE:HD13	1.89	0.55
1:E:4999:ASP:HB2	1:E:5002:GLU:HG2	1.89	0.55
1:G:4749:GLU:HG3	1:G:4753:HIS:NE2	2.21	0.55
1:J:897:ARG:HD3	1:J:905:PRO:HD3	1.89	0.55
1:J:1041:GLN:O	1:J:1045:THR:HG23	2.07	0.55
1:J:4584:ASP:HA	1:J:4627:MET:HA	1.89	0.55
1:J:4673:ARG:NH2	1:J:4702:ASP:OD1	2.39	0.55
1:B:489:ASN:OD1	1:B:493:ARG:NH1	2.40	0.55
1:B:4999:ASP:HB2	1:B:5002:GLU:HG2	1.89	0.55
1:E:5009:TYR:HA	1:E:5012:LYS:HE3	1.87	0.55
1:G:4584:ASP:HA	1:G:4627:MET:HA	1.89	0.55
1:J:2238:TYR:O	1:J:2242:ILE:HG12	2.06	0.55
2:A:29:MET:HA	2:A:35:LYS:HA	1.89	0.55
2:H:29:MET:HA	2:H:35:LYS:HA	1.89	0.55
1:B:4584:ASP:HA	1:B:4627:MET:HA	1.89	0.55
1:E:1041:GLN:O	1:E:1045:THR:HG23	2.07	0.55
1:E:1240:LYS:HE3	1:E:1242:LEU:HB3	1.87	0.55
1:J:247:TYR:HE2	1:J:359:TYR:HA	1.72	0.55
1:J:1102:VAL:HG11	1:J:1149:VAL:HG11	1.87	0.55
1:J:2364:PHE:HD1	1:J:2429:LEU:HD21	1.71	0.55
1:B:897:ARG:HD3	1:B:905:PRO:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:355:LEU:HB3	1:E:378:LEU:HB3	1.88	0.54
1:E:1155:LEU:HD22	1:E:1184:ILE:HG12	1.88	0.54
1:E:1504:GLY:O	1:E:1532:ASN:ND2	2.40	0.54
1:E:4584:ASP:HA	1:E:4627:MET:HA	1.89	0.54
1:G:952:LYS:HA	1:G:971:ASP:H	1.72	0.54
1:G:2978:GLU:HB2	1:G:3053:ARG:HH11	1.72	0.54
1:J:952:LYS:HA	1:J:971:ASP:H	1.72	0.54
1:J:1504:GLY:O	1:J:1532:ASN:ND2	2.40	0.54
1:J:2039:LEU:HB3	1:J:2044:ILE:HB	1.89	0.54
1:J:2464:ASP:OD1	1:J:2465:ASP:N	2.40	0.54
1:B:730:VAL:HA	1:B:1476:MET:CE	2.38	0.54
1:B:4749:GLU:HG3	1:B:4753:HIS:NE2	2.21	0.54
1:B:5012:LYS:O	1:B:5016:GLU:HG2	2.07	0.54
1:E:37:LEU:HA	1:E:49:LEU:HD23	1.90	0.54
1:E:103:TYR:OH	1:E:167:ASP:OD2	2.26	0.54
1:E:924:MET:HE2	3:F:107:TRP:HB2	1.90	0.54
1:E:4077:PHE:O	1:E:4081:VAL:HG23	2.08	0.54
1:E:5012:LYS:O	1:E:5016:GLU:HG2	2.07	0.54
1:G:1041:GLN:O	1:G:1045:THR:HG23	2.07	0.54
1:B:883:ALA:HA	1:B:886:ARG:HE	1.70	0.54
1:B:1041:GLN:O	1:B:1045:THR:HG23	2.07	0.54
1:E:489:ASN:OD1	1:E:493:ARG:NH1	2.40	0.54
1:E:797:HIS:CE1	1:E:1626:TRP:CD1	2.95	0.54
1:E:3206:LEU:HB2	1:E:3246:LEU:HD23	1.88	0.54
1:G:355:LEU:HB3	1:G:378:LEU:HB3	1.88	0.54
1:G:489:ASN:OD1	1:G:493:ARG:NH1	2.40	0.54
1:G:2883:HIS:HE1	1:G:2907:PRO:HA	1.73	0.54
1:G:5012:LYS:O	1:G:5016:GLU:HG2	2.07	0.54
1:J:797:HIS:CE1	1:J:1626:TRP:CD1	2.95	0.54
1:J:2747:ILE:HD12	1:J:2817:ILE:HD13	1.89	0.54
1:J:2978:GLU:HB2	1:J:3053:ARG:HH11	1.72	0.54
1:B:37:LEU:HA	1:B:49:LEU:HD23	1.90	0.54
1:B:103:TYR:OH	1:B:167:ASP:OD2	2.26	0.54
1:B:2883:HIS:HE1	1:B:2907:PRO:HA	1.73	0.54
1:E:2131:LEU:HB3	1:E:3667:HIS:CE1	2.42	0.54
1:E:4735:GLU:O	1:E:4739:GLU:HG2	2.07	0.54
1:G:3206:LEU:HB2	1:G:3246:LEU:HD23	1.88	0.54
1:G:4077:PHE:O	1:G:4081:VAL:HG23	2.08	0.54
1:G:103:TYR:OH	1:G:167:ASP:OD2	2.26	0.54
1:G:1155:LEU:HD22	1:G:1184:ILE:HG12	1.88	0.54
1:G:2626:LEU:HG	1:G:2640:PRO:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:37:LEU:HA	1:J:49:LEU:HD23	1.89	0.54
1:J:4131:ARG:HG3	1:J:4132:PHE:CD1	2.43	0.54
1:E:4826:ILE:O	1:E:4830:VAL:HG23	2.08	0.54
1:J:232:THR:HG21	1:J:252:VAL:HG11	1.88	0.54
1:J:2131:LEU:HB3	1:J:3667:HIS:CE1	2.42	0.54
1:B:247:TYR:HE2	1:B:359:TYR:HA	1.72	0.54
1:B:2806:ARG:HG3	1:B:2810:LYS:HZ3	1.73	0.54
1:E:69:LEU:HD21	1:E:101:LEU:HD11	1.90	0.54
1:E:2883:HIS:HE1	1:E:2907:PRO:HA	1.73	0.54
1:E:4085:ARG:NH1	1:E:4121:GLU:OE1	2.41	0.54
1:G:232:THR:HG21	1:G:252:VAL:HG11	1.88	0.54
1:G:4826:ILE:O	1:G:4830:VAL:HG23	2.08	0.54
1:J:248:GLU:HB2	1:J:373:LYS:HA	1.89	0.54
1:J:613:ALA:HB2	1:J:1676:LEU:HD12	1.90	0.54
1:J:3974:THR:O	1:J:3978:GLN:HG2	2.08	0.54
2:I:29:MET:HA	2:I:35:LYS:HA	1.89	0.54
3:F:90:THR:HG23	3:F:124:THR:HA	1.90	0.54
1:B:459:LEU:HB3	1:B:463:GLU:HG3	1.90	0.54
1:E:232:THR:HG21	1:E:252:VAL:HG11	1.89	0.54
1:E:2806:ARG:HG3	1:E:2810:LYS:HZ3	1.73	0.54
1:E:3967:GLU:CA	1:E:3970:GLN:HG2	2.34	0.54
1:G:2992:GLU:O	1:G:2996:LYS:HG2	2.08	0.54
1:J:879:HIS:CE1	1:J:921:ASN:HD22	2.26	0.54
1:J:2883:HIS:HE1	1:J:2907:PRO:HA	1.73	0.54
1:J:2992:GLU:O	1:J:2996:LYS:HG2	2.08	0.54
1:J:4999:ASP:HB2	1:J:5002:GLU:HG2	1.89	0.54
3:C:90:THR:HG23	3:C:124:THR:HA	1.90	0.54
1:B:69:LEU:HD21	1:B:101:LEU:HD11	1.90	0.54
1:B:797:HIS:CE1	1:B:1626:TRP:CD1	2.95	0.54
1:B:4767:TRP:O	1:B:4771:ILE:HG12	2.08	0.54
1:E:897:ARG:HD3	1:E:905:PRO:HD3	1.89	0.54
1:E:3923:LEU:HD21	1:E:3962:PHE:CE1	2.43	0.54
1:G:179:TYR:H	1:G:195:PHE:HA	1.73	0.54
1:G:3399:SER:O	1:G:3403:ARG:HG3	2.08	0.54
1:G:4085:ARG:NH1	1:G:4121:GLU:OE1	2.41	0.54
1:J:69:LEU:HD21	1:J:101:LEU:HD11	1.90	0.54
1:J:103:TYR:OH	1:J:167:ASP:OD2	2.26	0.54
1:J:179:TYR:H	1:J:195:PHE:HA	1.73	0.54
1:B:2747:ILE:HD12	1:B:2817:ILE:HD13	1.89	0.54
1:B:4843:LEU:HD22	1:G:4823:LEU:HD22	1.90	0.54
1:E:179:TYR:H	1:E:195:PHE:HA	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1232:ARG:NH2	1:E:1828:ASP:O	2.36	0.54
1:E:3974:THR:O	1:E:3978:GLN:HG2	2.08	0.54
1:E:4675:LYS:O	1:E:4679:ARG:HG2	2.08	0.54
1:E:4767:TRP:O	1:E:4771:ILE:HG12	2.08	0.54
1:G:365:LYS:O	1:G:369:LEU:HG	2.08	0.54
1:J:4077:PHE:O	1:J:4081:VAL:HG23	2.08	0.54
1:B:248:GLU:HA	1:B:372:LEU:O	2.08	0.53
1:B:4077:PHE:O	1:B:4081:VAL:HG23	2.08	0.53
1:E:70:GLU:HG2	1:E:71:GLN:HG3	1.90	0.53
1:E:365:LYS:O	1:E:369:LEU:HG	2.07	0.53
1:E:2827:ARG:NE	1:E:2935:TYR:OH	2.27	0.53
1:E:3940:LYS:O	1:E:4002:LYS:NZ	2.36	0.53
1:G:157:ARG:NH2	1:G:162:LYS:O	2.37	0.53
1:G:613:ALA:HB2	1:G:1676:LEU:HD12	1.90	0.53
1:J:960:MET:HB3	1:J:966:LYS:HB2	1.90	0.53
1:B:1095:VAL:HB	1:B:1199:VAL:HG23	1.90	0.53
1:B:1679:ASN:ND2	1:B:1797:ARG:O	2.37	0.53
1:B:2924:GLN:O	1:B:2928:LYS:HG2	2.08	0.53
1:B:3399:SER:O	1:B:3403:ARG:HG3	2.08	0.53
1:E:2039:LEU:HB3	1:E:2044:ILE:HB	1.89	0.53
1:E:2924:GLN:O	1:E:2928:LYS:HG2	2.09	0.53
1:G:3974:THR:O	1:G:3978:GLN:HG2	2.08	0.53
1:J:489:ASN:OD1	1:J:493:ARG:NH1	2.40	0.53
1:J:917:GLU:CD	3:K:101:PRO:HB2	2.29	0.53
1:J:2626:LEU:HG	1:J:2640:PRO:HB3	1.88	0.53
2:D:29:MET:HA	2:D:35:LYS:HA	1.89	0.53
1:B:960:MET:HB3	1:B:966:LYS:HB2	1.90	0.53
1:B:4131:ARG:HG3	1:B:4132:PHE:CD1	2.43	0.53
1:E:459:LEU:HB3	1:E:463:GLU:HG3	1.90	0.53
1:E:2464:ASP:OD1	1:E:2465:ASP:N	2.40	0.53
1:E:3085:PRO:HG2	1:E:3088:VAL:HB	1.91	0.53
1:G:37:LEU:HA	1:G:49:LEU:HD23	1.90	0.53
1:G:69:LEU:HD21	1:G:101:LEU:HD11	1.90	0.53
1:J:2505:PHE:O	1:J:2509:VAL:HG22	2.08	0.53
1:J:2806:ARG:HG3	1:J:2810:LYS:HZ3	1.73	0.53
1:J:2924:GLN:O	1:J:2928:LYS:HG2	2.08	0.53
1:J:3399:SER:O	1:J:3403:ARG:HG3	2.08	0.53
1:J:4767:TRP:O	1:J:4771:ILE:HG12	2.08	0.53
1:J:4942:GLU:O	1:J:4946:GLN:HG3	2.09	0.53
3:M:90:THR:HG23	3:M:124:THR:HA	1.90	0.53
1:B:1504:GLY:O	1:B:1532:ASN:ND2	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2248:ARG:HG3	1:B:2286:LEU:HD21	1.90	0.53
1:B:2505:PHE:O	1:B:2509:VAL:HG22	2.08	0.53
1:B:4823:LEU:HD22	1:E:4843:LEU:HD22	1.91	0.53
1:E:151:HIS:HB2	1:E:170:ILE:HB	1.90	0.53
1:E:4131:ARG:HG3	1:E:4132:PHE:CD1	2.43	0.53
1:G:1002:ALA:HB1	3:M:1:GLN:HE21	1.74	0.53
1:G:1095:VAL:HB	1:G:1199:VAL:HG23	1.90	0.53
1:G:2464:ASP:OD1	1:G:2465:ASP:N	2.40	0.53
1:G:2747:ILE:HD12	1:G:2817:ILE:HD13	1.89	0.53
1:G:3887:PHE:O	1:G:3891:LEU:HG	2.07	0.53
1:G:4131:ARG:HG3	1:G:4132:PHE:CD1	2.43	0.53
1:J:1804:LEU:HD12	1:J:1853:ILE:HG13	1.91	0.53
1:J:3967:GLU:CA	1:J:3970:GLN:HG2	2.34	0.53
3:K:90:THR:HG23	3:K:124:THR:HA	1.90	0.53
1:B:952:LYS:HA	1:B:971:ASP:H	1.72	0.53
1:G:247:TYR:CE2	1:G:359:TYR:HA	2.44	0.53
1:G:2806:ARG:HG3	1:G:2810:LYS:HZ3	1.74	0.53
1:J:4085:ARG:NH1	1:J:4121:GLU:OE1	2.41	0.53
1:B:3974:THR:O	1:B:3978:GLN:HG2	2.08	0.53
1:B:4675:LYS:O	1:B:4679:ARG:HG2	2.08	0.53
1:E:613:ALA:HB2	1:E:1676:LEU:HD12	1.90	0.53
1:E:960:MET:HB3	1:E:966:LYS:HB2	1.90	0.53
1:E:2992:GLU:O	1:E:2996:LYS:HG2	2.08	0.53
1:E:4243:PHE:O	1:E:4247:ILE:HG13	2.09	0.53
1:G:2505:PHE:O	1:G:2509:VAL:HG22	2.08	0.53
1:G:3037:GLU:HB2	1:G:3085:PRO:HG3	1.91	0.53
1:J:1079:LYS:HA	1:J:1189:LEU:HD11	1.91	0.53
1:B:909:ASN:HA	1:B:965:TYR:HA	1.91	0.53
1:B:1433:TYR:HE2	1:B:1577:ALA:HB3	1.74	0.53
1:B:2110:TYR:HB2	1:B:3695:PRO:HD2	1.91	0.53
1:B:4243:PHE:CE2	1:B:4247:ILE:HD11	2.44	0.53
1:B:4826:ILE:O	1:B:4830:VAL:HG23	2.08	0.53
1:E:1530:THR:HA	1:E:1535:GLU:HA	1.91	0.53
1:G:80:GLU:OE1	1:J:3935:TRP:NE1	2.33	0.53
1:G:1297:PHE:CD2	1:G:1522:LEU:HA	2.44	0.53
1:G:4243:PHE:CE2	1:G:4247:ILE:HD11	2.44	0.53
1:G:4943:LEU:O	1:G:4947:GLN:HG2	2.09	0.53
1:J:248:GLU:HA	1:J:372:LEU:O	2.08	0.53
1:J:1297:PHE:CD2	1:J:1522:LEU:HA	2.44	0.53
1:J:1530:THR:HA	1:J:1535:GLU:HA	1.91	0.53
1:J:4675:LYS:O	1:J:4679:ARG:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2992:GLU:O	1:B:2996:LYS:HG2	2.08	0.53
1:B:3037:GLU:HB2	1:B:3085:PRO:HG3	1.91	0.53
1:B:3923:LEU:HD21	1:B:3962:PHE:CE1	2.44	0.53
1:E:1437:VAL:HB	1:E:1516:ILE:HB	1.91	0.53
1:G:4675:LYS:O	1:G:4679:ARG:HG2	2.08	0.53
1:B:613:ALA:HB2	1:B:1676:LEU:HD12	1.90	0.53
1:B:1079:LYS:HA	1:B:1189:LEU:HD11	1.91	0.53
1:B:3085:PRO:HG2	1:B:3088:VAL:HB	1.91	0.53
1:B:4085:ARG:NH1	1:B:4121:GLU:OE1	2.41	0.53
1:E:1297:PHE:CD2	1:E:1522:LEU:HA	2.44	0.53
1:E:3900:GLN:HB3	1:E:3976:ASN:ND2	2.24	0.53
1:E:4942:GLU:O	1:E:4946:GLN:HG3	2.09	0.53
1:G:960:MET:HB3	1:G:966:LYS:HB2	1.90	0.53
1:G:1079:LYS:HA	1:G:1189:LEU:HD11	1.91	0.53
1:G:4104:THR:O	1:G:4108:ILE:HG12	2.09	0.53
1:J:1437:VAL:HB	1:J:1516:ILE:HB	1.91	0.53
1:J:3923:LEU:HD21	1:J:3962:PHE:CE1	2.44	0.53
1:J:4240:ASP:OD1	1:J:4675:LYS:NZ	2.40	0.53
1:B:179:TYR:H	1:B:195:PHE:HA	1.73	0.53
1:B:4943:LEU:O	1:B:4947:GLN:HG2	2.09	0.53
1:E:1079:LYS:HA	1:E:1189:LEU:HD11	1.91	0.53
1:E:2248:ARG:HG3	1:E:2286:LEU:HD21	1.90	0.53
1:E:4240:ASP:OD1	1:E:4675:LYS:NZ	2.40	0.53
1:G:909:ASN:HA	1:G:965:TYR:HA	1.91	0.53
1:G:1804:LEU:HD12	1:G:1853:ILE:HG13	1.91	0.53
1:J:4243:PHE:CE2	1:J:4247:ILE:HD11	2.44	0.53
1:J:4826:ILE:O	1:J:4830:VAL:HG23	2.08	0.53
1:B:80:GLU:OE1	1:G:3935:TRP:NE1	2.33	0.52
1:B:879:HIS:CE1	1:B:921:ASN:HD22	2.27	0.52
1:B:3547:GLU:O	1:B:3551:GLU:HG2	2.10	0.52
1:B:3980:LEU:O	1:B:3986:TRP:NE1	2.43	0.52
1:B:4240:ASP:OD1	1:B:4675:LYS:NZ	2.40	0.52
1:E:870:ILE:HD12	1:E:1051:TYR:CZ	2.45	0.52
1:E:2505:PHE:O	1:E:2509:VAL:HG22	2.08	0.52
1:G:459:LEU:HB3	1:G:463:GLU:HG3	1.90	0.52
1:G:1433:TYR:HB3	1:G:1575:LEU:HD23	1.91	0.52
1:G:1679:ASN:ND2	1:G:1797:ARG:O	2.37	0.52
1:G:2110:TYR:HB2	1:G:3695:PRO:HD2	1.91	0.52
1:G:2861:ASP:HB2	1:G:2925:GLU:HG2	1.91	0.52
1:G:2924:GLN:O	1:G:2928:LYS:HG2	2.08	0.52
1:G:3085:PRO:HG2	1:G:3088:VAL:HB	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3547:GLU:O	1:G:3551:GLU:HG2	2.10	0.52
1:G:4843:LEU:HD22	1:J:4823:LEU:HD22	1.90	0.52
1:J:459:LEU:HB3	1:J:463:GLU:HG3	1.90	0.52
1:J:2861:ASP:HB2	1:J:2925:GLU:HG2	1.91	0.52
1:B:56:GLN:O	1:B:308:HIS:HA	2.10	0.52
1:B:151:HIS:HB2	1:B:170:ILE:HB	1.90	0.52
1:B:3900:GLN:HB3	1:B:3976:ASN:ND2	2.24	0.52
1:E:952:LYS:HA	1:E:971:ASP:H	1.72	0.52
1:E:1573:MET:SD	1:E:1574:PRO:HD2	2.50	0.52
1:E:3399:SER:O	1:E:3403:ARG:HG3	2.08	0.52
1:G:917:GLU:CD	3:M:101:PRO:HB2	2.30	0.52
1:G:4767:TRP:O	1:G:4771:ILE:HG12	2.08	0.52
1:J:730:VAL:HA	1:J:1476:MET:CE	2.37	0.52
1:J:993:HIS:NE2	1:J:1022:VAL:O	2.41	0.52
1:J:3900:GLN:HB3	1:J:3976:ASN:ND2	2.24	0.52
1:J:4243:PHE:O	1:J:4247:ILE:HG13	2.09	0.52
1:B:3078:ARG:HG3	1:B:3152:PHE:CD1	2.44	0.52
1:E:102:LEU:HD12	1:E:160:GLY:HA2	1.92	0.52
1:E:1433:TYR:HE2	1:E:1577:ALA:HB3	1.74	0.52
1:E:1808:ARG:HD3	1:E:1853:ILE:HG22	1.92	0.52
1:E:4943:LEU:O	1:E:4947:GLN:HG2	2.09	0.52
1:J:102:LEU:HD12	1:J:160:GLY:HA2	1.92	0.52
1:J:870:ILE:HD12	1:J:1051:TYR:CZ	2.45	0.52
1:J:2893:GLU:O	1:J:2897:LYS:HG2	2.10	0.52
1:B:601:ASP:HA	1:B:1668:ARG:HH22	1.75	0.52
1:B:1297:PHE:CD2	1:B:1522:LEU:HA	2.44	0.52
1:B:4243:PHE:O	1:B:4247:ILE:HG13	2.09	0.52
1:E:157:ARG:NH2	1:E:162:LYS:O	2.37	0.52
1:E:1002:ALA:HB1	3:F:1:GLN:HE21	1.74	0.52
1:E:1095:VAL:HB	1:E:1199:VAL:HG23	1.90	0.52
1:E:3078:ARG:HG3	1:E:3152:PHE:CD1	2.44	0.52
1:E:3440:GLU:HA	1:E:3443:ILE:HG12	1.91	0.52
1:G:56:GLN:O	1:G:308:HIS:HA	2.10	0.52
1:G:2248:ARG:HG3	1:G:2286:LEU:HD21	1.90	0.52
1:J:56:GLN:O	1:J:308:HIS:HA	2.10	0.52
1:J:4104:THR:O	1:J:4108:ILE:HG12	2.09	0.52
1:B:70:GLU:HG2	1:B:71:GLN:HG3	1.90	0.52
1:E:1432:THR:HG23	1:E:1572:ILE:HG23	1.92	0.52
1:E:2380:ILE:HG21	1:E:2469:ILE:HD11	1.92	0.52
1:E:3037:GLU:HB2	1:E:3085:PRO:HG3	1.91	0.52
1:E:4092:ASP:HA	1:E:4095:LYS:HG2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:797:HIS:CE1	1:G:1626:TRP:CD1	2.95	0.52
1:G:1433:TYR:HE2	1:G:1577:ALA:HB3	1.74	0.52
1:G:4243:PHE:O	1:G:4247:ILE:HG13	2.09	0.52
1:G:4761:PRO:HB2	1:G:4766:THR:HG21	1.91	0.52
1:J:70:GLU:HG2	1:J:71:GLN:HG3	1.90	0.52
1:J:4092:ASP:HA	1:J:4095:LYS:HG2	1.92	0.52
1:B:4942:GLU:O	1:B:4946:GLN:HG3	2.09	0.52
1:E:56:GLN:O	1:E:308:HIS:HA	2.10	0.52
1:E:1804:LEU:HD12	1:E:1853:ILE:HG13	1.91	0.52
1:E:3891:LEU:O	1:E:3896:ASN:ND2	2.36	0.52
1:E:4823:LEU:HD22	1:J:4843:LEU:HD22	1.90	0.52
1:G:730:VAL:HA	1:G:1476:MET:CE	2.37	0.52
1:G:3051:ARG:HA	1:G:3131:TYR:CZ	2.45	0.52
1:J:1433:TYR:HB3	1:J:1575:LEU:HD23	1.91	0.52
1:J:2110:TYR:HB2	1:J:3695:PRO:HD2	1.91	0.52
1:J:3037:GLU:HB2	1:J:3085:PRO:HG3	1.91	0.52
1:J:3980:LEU:O	1:J:3986:TRP:NE1	2.43	0.52
3:C:105:ASN:HD21	3:C:107:TRP:HB3	1.75	0.52
1:B:102:LEU:HD12	1:B:160:GLY:HA2	1.92	0.52
1:B:2380:ILE:HG21	1:B:2469:ILE:HD11	1.92	0.52
1:B:3440:GLU:HA	1:B:3443:ILE:HG12	1.91	0.52
1:B:3940:LYS:O	1:B:4002:LYS:NZ	2.36	0.52
1:E:601:ASP:HA	1:E:1668:ARG:HH22	1.75	0.52
1:E:730:VAL:HA	1:E:1476:MET:CE	2.37	0.52
1:E:3384:LYS:NZ	1:E:3386:GLU:OE1	2.43	0.52
1:G:879:HIS:CE1	1:G:921:ASN:HD22	2.28	0.52
1:J:151:HIS:HB2	1:J:170:ILE:HB	1.90	0.52
1:J:1679:ASN:ND2	1:J:1797:ARG:O	2.37	0.52
1:J:1860:LYS:O	1:J:1864:LYS:HG2	2.10	0.52
2:I:13:ARG:HH11	2:I:13:ARG:C	2.12	0.52
1:B:1808:ARG:HD3	1:B:1853:ILE:HG22	1.92	0.52
1:E:28:VAL:HB	1:E:33:LEU:HD23	1.92	0.52
1:E:2893:GLU:O	1:E:2897:LYS:HG2	2.10	0.52
1:E:3674:ILE:HG13	1:E:3732:SER:CB	2.40	0.52
1:G:1573:MET:SD	1:G:1574:PRO:HD2	2.49	0.52
1:J:1432:THR:HG23	1:J:1572:ILE:HG23	1.92	0.52
1:J:2095:GLN:HA	1:J:2127:GLN:OE1	2.10	0.52
1:J:3132:THR:HA	1:J:3136:LEU:HB2	1.92	0.52
1:J:3194:LEU:HA	1:J:3197:LEU:HG	1.92	0.52
1:J:3891:LEU:O	1:J:3896:ASN:ND2	2.36	0.52
1:B:28:VAL:HB	1:B:33:LEU:HD23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1433:TYR:HB3	1:B:1575:LEU:HD23	1.91	0.52
1:B:1437:VAL:HB	1:B:1516:ILE:HB	1.91	0.52
1:B:1573:MET:SD	1:B:1574:PRO:HD2	2.50	0.52
1:B:2559:LEU:O	1:B:2563:THR:HG23	2.10	0.52
1:B:3674:ILE:HG13	1:B:3732:SER:CB	2.40	0.52
1:E:1758:ARG:HH12	1:E:2037:ASP:HA	1.75	0.52
1:E:1860:LYS:O	1:E:1864:LYS:HG2	2.10	0.52
1:E:2110:TYR:HB2	1:E:3695:PRO:HD2	1.91	0.52
1:E:3036:LYS:HD2	1:E:3079:THR:HG21	1.92	0.52
1:E:4104:THR:O	1:E:4108:ILE:HG12	2.09	0.52
1:E:4761:PRO:HB2	1:E:4766:THR:HG21	1.91	0.52
1:G:601:ASP:HA	1:G:1668:ARG:HH22	1.75	0.52
1:G:1437:VAL:HB	1:G:1516:ILE:HB	1.91	0.52
1:G:4942:GLU:O	1:G:4946:GLN:HG3	2.09	0.52
1:J:601:ASP:HA	1:J:1668:ARG:HH22	1.75	0.52
1:J:659:TYR:HB2	1:J:1017:ARG:HH12	1.75	0.52
1:J:858:THR:HG21	1:J:931:THR:HG22	1.92	0.52
1:J:3085:PRO:HG2	1:J:3088:VAL:HB	1.91	0.52
1:J:3674:ILE:HG13	1:J:3732:SER:CB	2.40	0.52
1:J:4092:ASP:OD1	1:J:4093:PHE:N	2.43	0.52
1:B:858:THR:HG21	1:B:931:THR:HG22	1.92	0.52
1:B:870:ILE:HD12	1:B:1051:TYR:CZ	2.45	0.52
1:B:1758:ARG:HH12	1:B:2037:ASP:HA	1.75	0.52
1:B:2861:ASP:HB2	1:B:2925:GLU:HG2	1.91	0.52
1:B:4761:PRO:HB2	1:B:4766:THR:HG21	1.91	0.52
1:E:917:GLU:CD	3:F:101:PRO:HB2	2.30	0.52
1:E:1694:LEU:HB3	1:E:1715:LEU:HD12	1.92	0.52
1:E:3051:ARG:HA	1:E:3131:TYR:CZ	2.45	0.52
1:E:4092:ASP:OD1	1:E:4093:PHE:N	2.43	0.52
1:E:4243:PHE:CE2	1:E:4247:ILE:HD11	2.44	0.52
1:E:5014:TYR:O	1:E:5017:ARG:NH2	2.43	0.52
1:G:1758:ARG:HH12	1:G:2037:ASP:HA	1.75	0.52
1:G:2893:GLU:O	1:G:2897:LYS:HG2	2.10	0.52
1:J:76:ARG:O	1:J:79:GLN:HG3	2.10	0.52
1:J:1573:MET:SD	1:J:1574:PRO:HD2	2.50	0.52
1:J:1758:ARG:HH12	1:J:2037:ASP:HA	1.75	0.52
1:J:4943:LEU:O	1:J:4947:GLN:HG2	2.09	0.52
1:J:5014:TYR:HD1	1:J:5019:TRP:HE1	1.58	0.52
1:B:72:SER:O	1:B:99:ARG:NH1	2.43	0.51
1:B:904:HIS:CD2	1:B:907:LEU:H	2.27	0.51
1:B:917:GLU:CD	3:C:101:PRO:HB2	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1464:PHE:HA	1:B:1468:LYS:HD2	1.92	0.51
1:B:4104:THR:O	1:B:4108:ILE:HG12	2.09	0.51
1:E:248:GLU:HA	1:E:372:LEU:O	2.11	0.51
1:E:2806:ARG:HH11	1:E:2810:LYS:HG3	1.76	0.51
1:E:3683:GLN:HA	1:E:3686:GLU:HG2	1.92	0.51
1:G:2380:ILE:HG21	1:G:2469:ILE:HD11	1.92	0.51
1:G:3036:LYS:HD2	1:G:3079:THR:HG21	1.92	0.51
1:G:3163:VAL:HA	1:G:3166:TYR:HD2	1.75	0.51
1:J:1095:VAL:HB	1:J:1199:VAL:HG23	1.90	0.51
1:J:2248:ARG:HG3	1:J:2286:LEU:HD21	1.90	0.51
1:J:3051:ARG:HA	1:J:3131:TYR:CZ	2.45	0.51
1:B:76:ARG:O	1:B:79:GLN:HG3	2.11	0.51
1:B:1860:LYS:O	1:B:1864:LYS:HG2	2.10	0.51
1:E:72:SER:O	1:E:99:ARG:NH1	2.43	0.51
1:G:714:TYR:HE1	1:G:1472:VAL:HG11	1.75	0.51
1:G:3674:ILE:HG13	1:G:3732:SER:CB	2.40	0.51
1:G:4092:ASP:HA	1:G:4095:LYS:HG2	1.92	0.51
1:J:526:LEU:HD11	1:J:540:PHE:HZ	1.75	0.51
1:J:663:TYR:HD1	1:J:747:CYS:HB3	1.75	0.51
1:J:747:CYS:HB2	1:J:808:TYR:CE2	2.46	0.51
1:J:1464:PHE:HA	1:J:1468:LYS:HD2	1.92	0.51
1:J:1808:ARG:HD3	1:J:1853:ILE:HG22	1.92	0.51
1:J:3078:ARG:HG3	1:J:3152:PHE:CD1	2.44	0.51
1:B:1087:ARG:HB3	1:B:1223:PHE:CD1	2.46	0.51
1:B:1804:LEU:HD12	1:B:1853:ILE:HG13	1.91	0.51
1:B:4092:ASP:HA	1:B:4095:LYS:HG2	1.92	0.51
1:E:2861:ASP:HB2	1:E:2925:GLU:HG2	1.91	0.51
1:G:72:SER:O	1:G:99:ARG:NH1	2.43	0.51
1:G:102:LEU:HD12	1:G:160:GLY:HA2	1.92	0.51
1:G:2470:ILE:HB	1:G:2502:MET:HE3	1.91	0.51
1:G:2806:ARG:HH11	1:G:2810:LYS:HG3	1.76	0.51
1:G:2963:LEU:O	1:G:2967:MET:HG2	2.11	0.51
1:G:4092:ASP:OD1	1:G:4093:PHE:N	2.43	0.51
1:J:904:HIS:CD2	1:J:907:LEU:H	2.27	0.51
1:J:1433:TYR:HE2	1:J:1577:ALA:HB3	1.74	0.51
1:J:3440:GLU:HA	1:J:3443:ILE:HG12	1.91	0.51
1:J:4655:PHE:O	1:J:4659:ILE:HG12	2.11	0.51
1:J:4761:PRO:HB2	1:J:4766:THR:HG21	1.91	0.51
1:J:4795:TYR:HD1	1:J:4796:MET:HE2	1.75	0.51
1:J:5014:TYR:O	1:J:5017:ARG:NH2	2.42	0.51
3:M:68:THR:O	3:M:80:LEU:HD12	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:993:HIS:NE2	1:B:1022:VAL:O	2.41	0.51
1:E:1492:CYS:SG	1:E:1493:TYR:N	2.84	0.51
1:E:3547:GLU:O	1:E:3551:GLU:HG2	2.10	0.51
1:E:4822:THR:O	1:E:4825:THR:OG1	2.23	0.51
1:G:70:GLU:HG2	1:G:71:GLN:HG3	1.90	0.51
1:G:663:TYR:HD1	1:G:747:CYS:HB3	1.75	0.51
1:G:920:TYR:HE1	3:M:99:ARG:HE	1.58	0.51
1:G:1530:THR:HA	1:G:1535:GLU:HA	1.91	0.51
1:G:3440:GLU:HA	1:G:3443:ILE:HG12	1.91	0.51
1:G:3887:PHE:CE2	1:G:3891:LEU:HD11	2.45	0.51
1:G:3967:GLU:CA	1:G:3970:GLN:HG2	2.36	0.51
1:J:2380:ILE:HG21	1:J:2469:ILE:HD11	1.92	0.51
1:J:3384:LYS:NZ	1:J:3386:GLU:OE1	2.43	0.51
1:J:4941:GLY:HA2	1:J:4944:ARG:HE	1.76	0.51
3:F:68:THR:O	3:F:80:LEU:HD12	2.10	0.51
1:B:1530:THR:HA	1:B:1535:GLU:HA	1.91	0.51
1:B:3051:ARG:HA	1:B:3131:TYR:CZ	2.45	0.51
1:B:3194:LEU:HA	1:B:3197:LEU:HG	1.92	0.51
1:B:4092:ASP:OD1	1:B:4093:PHE:N	2.43	0.51
1:B:4941:GLY:HA2	1:B:4944:ARG:HE	1.76	0.51
1:E:747:CYS:HB2	1:E:808:TYR:CE2	2.46	0.51
1:E:858:THR:HG21	1:E:931:THR:HG22	1.92	0.51
1:E:996:TRP:O	1:E:1000:ARG:HG2	2.11	0.51
1:E:1087:ARG:HB3	1:E:1223:PHE:CD1	2.46	0.51
1:E:4063:ASP:HB2	1:E:4067:LYS:HE3	1.93	0.51
1:G:151:HIS:HB2	1:G:170:ILE:HB	1.90	0.51
1:G:248:GLU:HB2	1:G:373:LYS:HA	1.91	0.51
1:G:747:CYS:HB2	1:G:808:TYR:CE2	2.46	0.51
1:G:1432:THR:HG23	1:G:1572:ILE:HG23	1.91	0.51
1:G:1694:LEU:HB3	1:G:1715:LEU:HD12	1.92	0.51
1:G:3078:ARG:HG3	1:G:3152:PHE:CD1	2.44	0.51
1:G:4655:PHE:O	1:G:4659:ILE:HG12	2.11	0.51
1:J:72:SER:O	1:J:99:ARG:NH1	2.43	0.51
1:J:790:ARG:HD2	1:J:1624:LEU:HB3	1.92	0.51
1:J:3547:GLU:O	1:J:3551:GLU:HG2	2.10	0.51
1:J:4822:THR:O	1:J:4825:THR:OG1	2.23	0.51
2:D:13:ARG:HH11	2:D:13:ARG:C	2.12	0.51
1:B:526:LEU:HD11	1:B:540:PHE:HZ	1.75	0.51
1:B:747:CYS:HB2	1:B:808:TYR:CE2	2.46	0.51
1:B:2095:GLN:HA	1:B:2127:GLN:OE1	2.10	0.51
1:B:4655:PHE:O	1:B:4659:ILE:HG12	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:879:HIS:CE1	1:E:921:ASN:HD22	2.28	0.51
1:E:3132:THR:HA	1:E:3136:LEU:HB2	1.92	0.51
1:E:3163:VAL:HA	1:E:3166:TYR:HD2	1.75	0.51
1:E:4795:TYR:HD1	1:E:4796:MET:HE2	1.75	0.51
1:G:28:VAL:HB	1:G:33:LEU:HD23	1.92	0.51
1:G:526:LEU:HD11	1:G:540:PHE:HZ	1.75	0.51
1:G:659:TYR:HB2	1:G:1017:ARG:HH12	1.75	0.51
1:G:870:ILE:HD12	1:G:1051:TYR:CZ	2.45	0.51
1:G:904:HIS:CD2	1:G:907:LEU:H	2.27	0.51
1:G:3194:LEU:HA	1:G:3197:LEU:HG	1.92	0.51
1:G:4240:ASP:OD1	1:G:4675:LYS:NZ	2.40	0.51
1:J:28:VAL:HB	1:J:33:LEU:HD23	1.92	0.51
1:J:996:TRP:O	1:J:1000:ARG:HG2	2.11	0.51
1:J:1492:CYS:SG	1:J:1493:TYR:N	2.84	0.51
1:J:1694:LEU:HB3	1:J:1715:LEU:HD12	1.92	0.51
1:J:3163:VAL:HA	1:J:3166:TYR:HD2	1.75	0.51
3:K:68:THR:O	3:K:80:LEU:HD12	2.10	0.51
1:B:1816:GLY:O	1:B:1820:ARG:HG2	2.11	0.51
1:B:2893:GLU:O	1:B:2897:LYS:HG2	2.10	0.51
1:E:2381:GLU:O	1:E:2385:ARG:HG2	2.11	0.51
1:E:5014:TYR:HD1	1:E:5019:TRP:HE1	1.57	0.51
1:G:574:VAL:O	1:G:578:ILE:HG12	2.11	0.51
1:G:996:TRP:O	1:G:1000:ARG:HG2	2.11	0.51
1:J:714:TYR:HE1	1:J:1472:VAL:HG11	1.75	0.51
1:J:909:ASN:HA	1:J:965:TYR:HA	1.91	0.51
1:J:2381:GLU:O	1:J:2385:ARG:HG2	2.11	0.51
1:J:2559:LEU:O	1:J:2563:THR:HG23	2.10	0.51
1:J:2806:ARG:HH11	1:J:2810:LYS:HG3	1.76	0.51
1:B:659:TYR:HB2	1:B:1017:ARG:HH12	1.75	0.51
1:B:714:TYR:HE1	1:B:1472:VAL:HG11	1.75	0.51
1:B:2963:LEU:O	1:B:2967:MET:HG2	2.11	0.51
1:B:3536:ALA:HB2	1:B:3553:LEU:HD21	1.93	0.51
1:B:3683:GLN:HA	1:B:3686:GLU:HG2	1.92	0.51
1:B:4063:ASP:HB2	1:B:4067:LYS:HE3	1.93	0.51
1:E:574:VAL:O	1:E:578:ILE:HG12	2.11	0.51
1:E:904:HIS:CD2	1:E:907:LEU:H	2.27	0.51
1:G:2559:LEU:O	1:G:2563:THR:HG23	2.10	0.51
1:G:3683:GLN:HA	1:G:3686:GLU:HG2	1.92	0.51
1:G:5014:TYR:HD1	1:G:5019:TRP:HE1	1.57	0.51
1:J:470:SER:HA	1:J:473:ASN:HD21	1.76	0.51
1:B:470:SER:HA	1:B:473:ASN:ND2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:996:TRP:O	1:B:1000:ARG:HG2	2.11	0.51
1:E:1433:TYR:HB3	1:E:1575:LEU:HD23	1.91	0.51
1:E:3980:LEU:O	1:E:3986:TRP:NE1	2.43	0.51
1:E:4941:GLY:HA2	1:E:4944:ARG:HE	1.76	0.51
1:G:1087:ARG:HB3	1:G:1223:PHE:CD1	2.46	0.51
1:G:1860:LYS:O	1:G:1864:LYS:HG2	2.10	0.51
1:G:2522:LEU:HB3	1:G:2527:LEU:HD23	1.93	0.51
1:G:3132:THR:HA	1:G:3136:LEU:HB2	1.92	0.51
1:G:4795:TYR:HD1	1:G:4796:MET:HE2	1.76	0.51
1:J:157:ARG:NH2	1:J:162:LYS:O	2.37	0.51
1:B:907:LEU:O	1:B:963:ASN:ND2	2.44	0.51
1:B:1432:THR:HG23	1:B:1572:ILE:HG23	1.92	0.51
1:E:470:SER:HA	1:E:473:ASN:ND2	2.26	0.51
1:E:663:TYR:HD1	1:E:747:CYS:HB3	1.75	0.51
1:E:2777:TYR:CE2	1:E:2793:PRO:HD3	2.46	0.51
1:E:4651:THR:OG1	1:E:4803:HIS:NE2	2.32	0.51
1:G:76:ARG:O	1:G:79:GLN:HG3	2.11	0.51
1:G:470:SER:HA	1:G:473:ASN:HD21	1.76	0.51
1:G:3093:ARG:O	1:G:3097:GLU:HG2	2.11	0.51
1:G:3769:ARG:O	1:G:3773:ARG:NH1	2.44	0.51
1:J:574:VAL:O	1:J:578:ILE:HG12	2.11	0.51
3:C:68:THR:O	3:C:80:LEU:HD12	2.10	0.51
1:B:266:ARG:HG2	1:B:268:SER:H	1.76	0.50
1:B:1617:THR:HG22	1:B:1628:VAL:HG13	1.93	0.50
1:B:2206:THR:O	1:B:2210:VAL:HG23	2.11	0.50
1:B:2777:TYR:CE2	1:B:2793:PRO:HD3	2.46	0.50
1:E:76:ARG:O	1:E:79:GLN:HG3	2.11	0.50
1:E:526:LEU:HD11	1:E:540:PHE:HZ	1.75	0.50
1:E:659:TYR:HB2	1:E:1017:ARG:HH12	1.75	0.50
1:E:897:ARG:HB3	3:F:58:ASN:OD1	2.11	0.50
1:E:909:ASN:HA	1:E:965:TYR:HA	1.91	0.50
1:E:1042:ALA:O	1:E:1045:THR:OG1	2.22	0.50
1:E:1816:GLY:O	1:E:1820:ARG:HG2	2.11	0.50
1:E:2668:SER:HB3	1:E:2671:GLU:HG3	1.93	0.50
1:E:3093:ARG:O	1:E:3097:GLU:HG2	2.11	0.50
1:E:4581:LYS:HE2	1:E:4632:LEU:HD22	1.94	0.50
1:G:2095:GLN:HA	1:G:2127:GLN:OE1	2.10	0.50
1:G:2381:GLU:O	1:G:2385:ARG:HG2	2.11	0.50
1:G:4941:GLY:HA2	1:G:4944:ARG:HE	1.76	0.50
1:J:1858:ASP:O	1:J:1862:ILE:HG13	2.12	0.50
1:J:2963:LEU:O	1:J:2967:MET:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:3093:ARG:O	1:J:3097:GLU:HG2	2.11	0.50
1:J:3457:ASN:O	1:J:3461:GLN:HG2	2.11	0.50
1:B:548:VAL:HG21	1:B:582:HIS:HD2	1.76	0.50
1:B:790:ARG:HD2	1:B:1624:LEU:HB3	1.92	0.50
1:B:2806:ARG:HH11	1:B:2810:LYS:HG3	1.76	0.50
1:B:3384:LYS:NZ	1:B:3386:GLU:OE1	2.43	0.50
1:E:714:TYR:HE1	1:E:1472:VAL:HG11	1.75	0.50
1:E:1617:THR:HG22	1:E:1628:VAL:HG13	1.94	0.50
1:E:2013:LYS:NZ	1:E:3661:TRP:O	2.44	0.50
1:E:2095:GLN:HA	1:E:2127:GLN:OE1	2.10	0.50
1:E:2479:LEU:HA	1:E:2541:PHE:HZ	1.76	0.50
1:E:2559:LEU:O	1:E:2563:THR:HG23	2.10	0.50
1:E:3457:ASN:O	1:E:3461:GLN:HG2	2.11	0.50
1:E:4655:PHE:O	1:E:4659:ILE:HG12	2.11	0.50
1:G:3457:ASN:O	1:G:3461:GLN:HG2	2.11	0.50
1:J:1159:THR:HG22	1:J:1180:ARG:HA	1.94	0.50
1:J:2380:ILE:O	1:J:2384:ILE:HG13	2.11	0.50
1:J:2816:MET:HB3	1:J:2878:LEU:HD13	1.94	0.50
1:J:3683:GLN:HA	1:J:3686:GLU:HG2	1.92	0.50
1:B:590:LEU:HG	1:B:599:VAL:HG11	1.93	0.50
1:B:1159:THR:HG22	1:B:1180:ARG:HA	1.93	0.50
1:B:2668:SER:HB3	1:B:2671:GLU:HG3	1.93	0.50
1:B:2816:MET:HB3	1:B:2878:LEU:HD13	1.94	0.50
1:B:3036:LYS:HD2	1:B:3079:THR:HG21	1.92	0.50
1:B:3163:VAL:HA	1:B:3166:TYR:HD2	1.75	0.50
1:E:3194:LEU:HA	1:E:3197:LEU:HG	1.92	0.50
1:G:792:LEU:HD22	1:G:799:GLU:H	1.77	0.50
1:G:993:HIS:NE2	1:G:1022:VAL:O	2.41	0.50
1:G:1617:THR:HG22	1:G:1628:VAL:HG13	1.93	0.50
1:G:1808:ARG:HD3	1:G:1853:ILE:HG22	1.92	0.50
1:G:3034:LYS:HA	1:G:3037:GLU:HG3	1.94	0.50
1:G:3354:LEU:HB2	1:G:3415:TYR:CE2	2.47	0.50
1:G:3940:LYS:O	1:G:4002:LYS:NZ	2.36	0.50
1:J:792:LEU:HD22	1:J:799:GLU:H	1.77	0.50
1:J:2879:ALA:HA	1:J:2882:TYR:CD2	2.47	0.50
1:J:3034:LYS:HA	1:J:3037:GLU:HG3	1.94	0.50
1:J:3573:MET:O	1:J:3577:ARG:HG2	2.12	0.50
1:B:229:GLU:HA	1:B:249:GLY:HA3	1.92	0.50
1:B:1492:CYS:SG	1:B:1493:TYR:N	2.84	0.50
1:B:3921:ASP:O	1:B:3925:ARG:HG3	2.12	0.50
1:B:3935:TRP:NE1	1:E:80:GLU:OE1	2.33	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:790:ARG:HD2	1:E:1624:LEU:HB3	1.92	0.50
1:E:1464:PHE:HA	1:E:1468:LYS:HD2	1.92	0.50
1:E:2206:THR:O	1:E:2210:VAL:HG23	2.11	0.50
1:E:2380:ILE:O	1:E:2384:ILE:HG13	2.11	0.50
1:E:2522:LEU:HB3	1:E:2527:LEU:HD23	1.93	0.50
1:E:2645:THR:HB	1:E:2702:CYS:HA	1.93	0.50
1:E:2816:MET:HB3	1:E:2878:LEU:HD13	1.94	0.50
1:G:1816:GLY:O	1:G:1820:ARG:HG2	2.11	0.50
1:G:2777:TYR:CE2	1:G:2793:PRO:HD3	2.46	0.50
1:G:3573:MET:O	1:G:3577:ARG:HG2	2.12	0.50
1:J:229:GLU:HA	1:J:249:GLY:HA3	1.92	0.50
1:J:470:SER:HA	1:J:473:ASN:ND2	2.26	0.50
1:J:548:VAL:HG21	1:J:582:HIS:HD2	1.76	0.50
1:J:1816:GLY:O	1:J:1820:ARG:HG2	2.11	0.50
1:J:3036:LYS:HD2	1:J:3079:THR:HG21	1.92	0.50
1:J:3354:LEU:HB2	1:J:3415:TYR:CE2	2.47	0.50
1:J:3769:ARG:O	1:J:3773:ARG:NH1	2.44	0.50
1:J:3839:CYS:O	1:J:3925:ARG:NH2	2.44	0.50
3:F:105:ASN:HD21	3:F:107:TRP:HB3	1.77	0.50
1:B:50:GLU:O	1:B:52:THR:HG23	2.12	0.50
1:B:1727:ARG:O	1:B:1731:LEU:HG	2.12	0.50
1:B:2381:GLU:O	1:B:2385:ARG:HG2	2.11	0.50
1:B:4822:THR:O	1:B:4825:THR:OG1	2.23	0.50
1:E:1159:THR:HG22	1:E:1180:ARG:HA	1.94	0.50
1:E:2866:THR:HB	1:E:2872:GLN:HB2	1.94	0.50
1:E:2963:LEU:O	1:E:2967:MET:HG2	2.11	0.50
1:E:3034:LYS:HA	1:E:3037:GLU:HG3	1.94	0.50
1:E:4183:ILE:HD13	1:E:4193:ILE:HD11	1.93	0.50
1:G:858:THR:HG21	1:G:931:THR:HG22	1.92	0.50
1:G:1464:PHE:HA	1:G:1468:LYS:HD2	1.92	0.50
1:G:2479:LEU:HA	1:G:2541:PHE:HZ	1.76	0.50
1:G:2866:THR:HB	1:G:2872:GLN:HB2	1.94	0.50
1:G:3384:LYS:NZ	1:G:3386:GLU:OE1	2.43	0.50
1:G:3839:CYS:O	1:G:3925:ARG:NH2	2.44	0.50
1:G:3877:ASP:HB3	1:G:3880:PHE:HB3	1.93	0.50
1:G:3980:LEU:O	1:G:3986:TRP:NE1	2.43	0.50
1:J:1087:ARG:HB3	1:J:1223:PHE:CD1	2.46	0.50
1:J:1617:THR:HG22	1:J:1628:VAL:HG13	1.93	0.50
1:J:1727:ARG:O	1:J:1731:LEU:HG	2.11	0.50
1:J:2747:ILE:HG12	1:J:2755:ILE:HG13	1.94	0.50
1:B:1694:LEU:HB3	1:B:1715:LEU:HD12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1782:PHE:O	2:A:82:TYR:OH	2.22	0.50
1:B:2866:THR:HB	1:B:2872:GLN:HB2	1.94	0.50
1:B:3093:ARG:O	1:B:3097:GLU:HG2	2.11	0.50
1:B:3132:THR:HA	1:B:3136:LEU:HB2	1.92	0.50
1:B:3400:VAL:HG23	1:B:3403:ARG:HE	1.77	0.50
1:E:993:HIS:NE2	1:E:1022:VAL:O	2.41	0.50
1:E:1528:THR:HG23	1:E:1539:PHE:CE1	2.46	0.50
1:E:2879:ALA:HA	1:E:2882:TYR:CD2	2.47	0.50
1:E:3921:ASP:O	1:E:3925:ARG:HG3	2.12	0.50
1:G:1492:CYS:SG	1:G:1493:TYR:N	2.84	0.50
1:G:2013:LYS:NZ	1:G:3661:TRP:O	2.44	0.50
1:G:2645:THR:HB	1:G:2702:CYS:HA	1.93	0.50
1:G:4999:ASP:HB2	1:G:5002:GLU:CG	2.38	0.50
1:J:1065:ASN:HA	1:J:1068:ARG:HH21	1.77	0.50
1:J:1291:LEU:HD11	1:J:1564:PHE:CE2	2.46	0.50
1:J:2012:PHE:CZ	1:J:2031:LEU:HD23	2.47	0.50
1:B:77:ALA:HB2	1:G:3935:TRP:CH2	2.47	0.50
1:B:1858:ASP:O	1:B:1862:ILE:HG13	2.12	0.50
1:B:2013:LYS:NZ	1:B:3661:TRP:O	2.44	0.50
1:B:2354:VAL:HG11	1:B:2453:ILE:HD12	1.93	0.50
1:B:2522:LEU:HB3	1:B:2527:LEU:HD23	1.93	0.50
1:B:5014:TYR:HD1	1:B:5019:TRP:HE1	1.57	0.50
1:E:116:MET:HG3	1:E:139:GLU:HA	1.94	0.50
1:E:907:LEU:O	1:E:963:ASN:ND2	2.44	0.50
1:G:907:LEU:O	1:G:963:ASN:ND2	2.44	0.50
1:G:1159:THR:HG22	1:G:1180:ARG:HA	1.94	0.50
1:G:1858:ASP:O	1:G:1862:ILE:HG13	2.12	0.50
1:G:3281:LEU:HD13	1:G:3307:VAL:HG21	1.94	0.50
1:G:4063:ASP:HB2	1:G:4067:LYS:HE3	1.93	0.50
1:J:2866:THR:HB	1:J:2872:GLN:HB2	1.94	0.50
1:B:574:VAL:O	1:B:578:ILE:HG12	2.11	0.50
1:E:1858:ASP:O	1:E:1862:ILE:HG13	2.12	0.50
1:E:3839:CYS:O	1:E:3925:ARG:NH2	2.44	0.50
1:G:1065:ASN:HA	1:G:1068:ARG:HH21	1.77	0.50
1:G:2251:PHE:CD2	1:G:2286:LEU:HD22	2.47	0.50
1:G:2668:SER:HB3	1:G:2671:GLU:HG3	1.93	0.50
1:G:2816:MET:HB3	1:G:2878:LEU:HD13	1.94	0.50
1:G:2879:ALA:HA	1:G:2882:TYR:CD2	2.47	0.50
1:G:3921:ASP:O	1:G:3925:ARG:HG3	2.12	0.50
1:G:4569:LEU:HD13	1:G:4650:HIS:HA	1.94	0.50
1:J:307:ALA:HB1	1:J:312:THR:HG21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:747:CYS:SG	1:J:756:SER:HB2	2.52	0.50
1:J:897:ARG:HB3	3:K:58:ASN:OD1	2.12	0.50
1:J:2206:THR:O	1:J:2210:VAL:HG23	2.11	0.50
1:J:2645:THR:HB	1:J:2702:CYS:HA	1.93	0.50
1:J:2777:TYR:CE2	1:J:2793:PRO:HD3	2.46	0.50
1:J:2788:HIS:CE1	1:J:2790:MET:HB2	2.47	0.50
1:J:3032:SER:O	1:J:3036:LYS:HG3	2.12	0.50
1:J:3877:ASP:HB3	1:J:3880:PHE:HB3	1.93	0.50
1:J:4063:ASP:HB2	1:J:4067:LYS:HE3	1.93	0.50
2:A:13:ARG:HH11	2:A:13:ARG:C	2.12	0.50
3:C:18:LEU:HB2	3:C:82:MET:HB3	1.93	0.50
3:F:33:SER:OG	3:F:101:PRO:HA	2.12	0.50
3:K:33:SER:OG	3:K:101:PRO:HA	2.12	0.50
3:M:122:GLN:HE21	3:M:124:THR:HG1	1.54	0.50
1:B:663:TYR:HD1	1:B:747:CYS:HB3	1.75	0.50
1:B:3032:SER:O	1:B:3036:LYS:HG3	2.12	0.50
1:B:3514:LEU:HD11	1:B:3606:LEU:HD13	1.94	0.50
1:E:229:GLU:HA	1:E:249:GLY:HA3	1.92	0.50
1:E:3400:VAL:HG23	1:E:3403:ARG:HE	1.77	0.50
1:G:116:MET:HG3	1:G:139:GLU:HA	1.94	0.50
1:G:266:ARG:HG2	1:G:268:SER:H	1.76	0.50
1:G:1291:LEU:HD11	1:G:1564:PHE:CE2	2.46	0.50
1:G:4183:ILE:HD13	1:G:4193:ILE:HD11	1.93	0.50
1:J:924:MET:HE2	3:K:107:TRP:HB2	1.93	0.50
2:H:13:ARG:HH11	2:H:13:ARG:C	2.12	0.50
1:B:116:MET:HG3	1:B:139:GLU:HA	1.94	0.49
1:B:492:ASP:OD1	1:B:546:TRP:NE1	2.44	0.49
1:B:3839:CYS:O	1:B:3925:ARG:NH2	2.44	0.49
1:E:470:SER:HA	1:E:473:ASN:HD21	1.76	0.49
1:E:548:VAL:HG21	1:E:582:HIS:HD2	1.77	0.49
1:E:747:CYS:SG	1:E:756:SER:HB2	2.52	0.49
1:E:1727:ARG:O	1:E:1731:LEU:HG	2.12	0.49
1:G:470:SER:HA	1:G:473:ASN:ND2	2.26	0.49
1:G:747:CYS:SG	1:G:756:SER:HB2	2.52	0.49
1:G:790:ARG:HD2	1:G:1624:LEU:HB3	1.92	0.49
1:G:1578:ALA:HA	1:G:1584:ARG:HH12	1.77	0.49
1:G:2908:TYR:HA	1:G:2911:LEU:CD2	2.42	0.49
1:J:45:ARG:HD3	1:J:45:ARG:H	1.77	0.49
1:J:920:TYR:HE1	3:K:99:ARG:HE	1.58	0.49
1:J:2251:PHE:CD2	1:J:2286:LEU:HD22	2.46	0.49
1:J:4569:LEU:HD13	1:J:4650:HIS:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:TYR:CG	1:B:373:LYS:HG3	2.47	0.49
1:B:1578:ALA:HA	1:B:1584:ARG:HH12	1.78	0.49
1:B:2163:ARG:HA	1:B:2166:LEU:HG	1.94	0.49
1:B:2489:LYS:HE2	1:B:2491:SER:HB3	1.94	0.49
1:B:2908:TYR:HA	1:B:2911:LEU:CD2	2.42	0.49
1:B:3034:LYS:HA	1:B:3037:GLU:HG3	1.94	0.49
1:B:3354:LEU:HB2	1:B:3415:TYR:CE2	2.47	0.49
1:B:3573:MET:O	1:B:3577:ARG:HG2	2.11	0.49
1:B:4581:LYS:HE2	1:B:4632:LEU:HD22	1.93	0.49
1:B:5014:TYR:O	1:B:5017:ARG:NH2	2.43	0.49
1:E:266:ARG:HG2	1:E:268:SER:H	1.76	0.49
1:E:369:LEU:HB3	1:E:371:VAL:HG23	1.94	0.49
1:E:1291:LEU:HD11	1:E:1564:PHE:CE2	2.46	0.49
1:E:2012:PHE:CZ	1:E:2031:LEU:HD23	2.47	0.49
1:E:3354:LEU:HB2	1:E:3415:TYR:CE2	2.47	0.49
1:G:229:GLU:HA	1:G:249:GLY:HA3	1.92	0.49
1:G:2206:THR:O	1:G:2210:VAL:HG23	2.11	0.49
1:J:1699:GLU:HG3	1:J:1810:LYS:HZ2	1.77	0.49
1:J:2522:LEU:HB3	1:J:2527:LEU:HD23	1.93	0.49
1:J:3260:GLY:HA2	1:J:3325:ASN:ND2	2.27	0.49
1:J:3536:ALA:HB2	1:J:3553:LEU:HD21	1.93	0.49
1:J:4183:ILE:HD13	1:J:4193:ILE:HD11	1.93	0.49
1:B:1291:LEU:HD11	1:B:1564:PHE:CE2	2.46	0.49
1:B:2251:PHE:CD2	1:B:2286:LEU:HD22	2.47	0.49
1:B:3281:LEU:HD13	1:B:3307:VAL:HG21	1.93	0.49
1:E:2251:PHE:CD2	1:E:2286:LEU:HD22	2.47	0.49
1:E:3573:MET:O	1:E:3577:ARG:HG2	2.12	0.49
1:G:1037:ASP:O	1:G:1041:GLN:HG2	2.13	0.49
1:G:2747:ILE:HG12	1:G:2755:ILE:HG13	1.94	0.49
1:G:3536:ALA:HB2	1:G:3553:LEU:HD21	1.93	0.49
1:G:4581:LYS:HE2	1:G:4632:LEU:HD22	1.94	0.49
1:J:590:LEU:HG	1:J:599:VAL:HG11	1.93	0.49
1:J:1424:PRO:O	1:J:1428:LEU:HG	2.13	0.49
1:J:1578:ALA:HA	1:J:1584:ARG:HH12	1.78	0.49
1:J:2013:LYS:NZ	1:J:3661:TRP:O	2.44	0.49
1:J:2882:TYR:O	1:J:2886:TRP:HE3	1.95	0.49
1:J:3400:VAL:HG23	1:J:3403:ARG:HE	1.77	0.49
1:J:3511:VAL:HG23	1:J:3515:LYS:HD2	1.94	0.49
1:J:4581:LYS:HE2	1:J:4632:LEU:HD22	1.94	0.49
3:C:33:SER:OG	3:C:101:PRO:HA	2.12	0.49
1:B:470:SER:HA	1:B:473:ASN:HD21	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2012:PHE:CZ	1:B:2031:LEU:HD23	2.47	0.49
1:B:2874:MET:HE1	1:B:2939:ARG:HG3	1.94	0.49
1:E:50:GLU:O	1:E:52:THR:HG23	2.12	0.49
1:E:1065:ASN:OD1	1:E:1069:TRP:NE1	2.46	0.49
1:E:1578:ALA:HA	1:E:1584:ARG:HH12	1.78	0.49
1:E:2163:ARG:HA	1:E:2166:LEU:HG	1.94	0.49
1:E:3536:ALA:HB2	1:E:3553:LEU:HD21	1.93	0.49
1:E:3886:ARG:HD2	1:E:3889:GLN:HE21	1.78	0.49
1:E:3935:TRP:CH2	1:J:77:ALA:HB2	2.47	0.49
1:E:3937:TYR:HA	1:E:3940:LYS:HE2	1.94	0.49
1:G:50:GLU:O	1:G:52:THR:HG23	2.12	0.49
1:G:77:ALA:HB2	1:J:3935:TRP:CH2	2.47	0.49
1:G:307:ALA:HB1	1:G:312:THR:HG21	1.94	0.49
1:G:897:ARG:HB3	3:M:58:ASN:OD1	2.11	0.49
1:G:1065:ASN:OD1	1:G:1069:TRP:NE1	2.46	0.49
1:J:116:MET:HG3	1:J:139:GLU:HA	1.94	0.49
1:J:266:ARG:HG2	1:J:268:SER:H	1.76	0.49
3:K:105:ASN:HD21	3:K:107:TRP:HB3	1.77	0.49
1:B:747:CYS:SG	1:B:756:SER:HB2	2.52	0.49
1:B:1528:THR:HG23	1:B:1539:PHE:CE1	2.46	0.49
1:B:2879:ALA:HA	1:B:2882:TYR:CD2	2.47	0.49
1:B:4569:LEU:HD13	1:B:4650:HIS:HA	1.94	0.49
1:E:590:LEU:HG	1:E:599:VAL:HG11	1.93	0.49
1:E:881:LEU:O	1:E:885:THR:HG23	2.13	0.49
1:E:1613:LEU:H	1:E:1613:LEU:HD12	1.78	0.49
1:E:2354:VAL:HG11	1:E:2453:ILE:HD12	1.93	0.49
1:E:2747:ILE:HG12	1:E:2755:ILE:HG13	1.94	0.49
1:E:2788:HIS:CE1	1:E:2790:MET:HB2	2.47	0.49
1:E:3032:SER:O	1:E:3036:LYS:HG3	2.12	0.49
1:E:3268:HIS:CE1	1:E:3272:ILE:HD12	2.48	0.49
1:G:548:VAL:HG21	1:G:582:HIS:HD2	1.76	0.49
1:G:1727:ARG:O	1:G:1731:LEU:HG	2.12	0.49
1:G:2163:ARG:HA	1:G:2166:LEU:HG	1.94	0.49
1:G:2380:ILE:O	1:G:2384:ILE:HG13	2.11	0.49
1:G:2788:HIS:CE1	1:G:2790:MET:HB2	2.47	0.49
1:G:2882:TYR:O	1:G:2886:TRP:HE3	1.96	0.49
1:G:3886:ARG:O	1:G:3890:LEU:HG	2.12	0.49
1:J:1613:LEU:H	1:J:1613:LEU:HD12	1.78	0.49
1:J:2354:VAL:HG11	1:J:2453:ILE:HD12	1.93	0.49
1:J:2908:TYR:HA	1:J:2911:LEU:CD2	2.42	0.49
3:F:4:LEU:HD12	3:F:24:ALA:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:ALA:HB1	1:B:312:THR:HG21	1.94	0.49
1:B:792:LEU:HD22	1:B:799:GLU:H	1.77	0.49
1:B:881:LEU:O	1:B:885:THR:HG23	2.13	0.49
1:B:1424:PRO:O	1:B:1428:LEU:HG	2.13	0.49
1:E:1424:PRO:O	1:E:1428:LEU:HG	2.13	0.49
1:E:2489:LYS:HE2	1:E:2491:SER:HB3	1.94	0.49
1:E:3260:GLY:HA2	1:E:3325:ASN:ND2	2.27	0.49
1:E:3281:LEU:HD13	1:E:3307:VAL:HG21	1.94	0.49
1:E:3943:ILE:HG12	1:E:4009:GLN:HE22	1.77	0.49
1:G:1866:ILE:O	1:G:1926:LEU:N	2.45	0.49
1:G:2012:PHE:CZ	1:G:2031:LEU:HD23	2.47	0.49
1:G:2354:VAL:HG11	1:G:2453:ILE:HD12	1.93	0.49
1:G:5014:TYR:O	1:G:5017:ARG:NH2	2.43	0.49
1:J:246:TYR:CG	1:J:373:LYS:HG3	2.48	0.49
1:J:1065:ASN:OD1	1:J:1069:TRP:NE1	2.46	0.49
1:J:2190:VAL:HA	1:J:2193:GLN:HB3	1.95	0.49
1:B:897:ARG:HB3	3:C:58:ASN:OD1	2.13	0.49
1:B:2645:THR:HB	1:B:2702:CYS:HA	1.93	0.49
1:B:2827:ARG:NE	1:B:2935:TYR:OH	2.27	0.49
1:B:3511:VAL:HG23	1:B:3515:LYS:HD2	1.94	0.49
1:B:4219:PHE:HD1	1:B:4950:VAL:HG11	1.78	0.49
1:B:4795:TYR:HD1	1:B:4796:MET:HE2	1.77	0.49
1:E:307:ALA:HB1	1:E:312:THR:HG21	1.94	0.49
1:E:3727:ASP:HB3	1:E:3731:LYS:NZ	2.28	0.49
1:E:4219:PHE:HD1	1:E:4950:VAL:HG11	1.78	0.49
1:G:181:HIS:ND1	1:G:196:MET:HB2	2.28	0.49
1:G:251:ALA:O	1:G:255:HIS:ND1	2.46	0.49
1:G:2190:VAL:HA	1:G:2193:GLN:HB3	1.95	0.49
1:G:3032:SER:O	1:G:3036:LYS:HG3	2.12	0.49
1:J:1782:PHE:O	2:I:82:TYR:OH	2.22	0.49
1:J:2668:SER:HB3	1:J:2671:GLU:HG3	1.93	0.49
1:J:2827:ARG:NE	1:J:2935:TYR:OH	2.27	0.49
1:J:3268:HIS:CE1	1:J:3272:ILE:HD12	2.48	0.49
1:J:3921:ASP:O	1:J:3925:ARG:HG3	2.12	0.49
3:C:4:LEU:HD12	3:C:24:ALA:HB2	1.95	0.49
3:F:18:LEU:HB2	3:F:82:MET:HB3	1.94	0.49
3:K:4:LEU:HD12	3:K:24:ALA:HB2	1.95	0.49
3:K:18:LEU:HB2	3:K:82:MET:HB3	1.94	0.49
1:B:2190:VAL:HA	1:B:2193:GLN:HB3	1.95	0.49
1:B:3457:ASN:O	1:B:3461:GLN:HG2	2.12	0.49
1:B:3886:ARG:HD2	1:B:3889:GLN:HE21	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4096:ALA:O	1:B:4100:GLN:HG2	2.13	0.49
1:B:4183:ILE:HD13	1:B:4193:ILE:HD11	1.93	0.49
1:E:920:TYR:HE1	3:F:99:ARG:HE	1.58	0.49
1:E:1065:ASN:HA	1:E:1068:ARG:HH21	1.77	0.49
1:E:2443:ILE:HD12	1:E:2454:ARG:NH1	2.28	0.49
1:E:3514:LEU:HD11	1:E:3606:LEU:HD13	1.94	0.49
1:E:4569:LEU:HD13	1:E:4650:HIS:HA	1.94	0.49
1:G:590:LEU:HG	1:G:599:VAL:HG11	1.93	0.49
1:G:2653:LYS:HE2	1:G:2661:TRP:HA	1.94	0.49
1:G:4059:LEU:HD13	1:G:4167:ALA:HB2	1.95	0.49
1:G:4207:MET:HG2	1:G:4208:PRO:HD2	1.95	0.49
1:J:181:HIS:ND1	1:J:196:MET:HB2	2.28	0.49
1:J:1866:ILE:O	1:J:1926:LEU:N	2.45	0.49
1:J:2163:ARG:HA	1:J:2166:LEU:HG	1.94	0.49
1:J:2479:LEU:HA	1:J:2541:PHE:HZ	1.76	0.49
1:J:2673:HIS:CE1	1:J:2677:LYS:HE2	2.48	0.49
1:J:3937:TYR:HA	1:J:3940:LYS:HE2	1.94	0.49
1:B:181:HIS:ND1	1:B:196:MET:HB2	2.28	0.49
1:B:2575:ARG:NH1	1:B:2575:ARG:HA	2.28	0.49
1:B:2653:LYS:HE2	1:B:2661:TRP:HA	1.94	0.49
1:B:2788:HIS:CE1	1:B:2790:MET:HB2	2.47	0.49
1:B:2882:TYR:O	1:B:2886:TRP:HE3	1.95	0.49
1:B:3316:LEU:HD22	1:B:3346:VAL:HA	1.95	0.49
1:B:3670:GLU:HA	1:B:3673:MET:HG2	1.95	0.49
1:B:3935:TRP:CH2	1:E:77:ALA:HB2	2.47	0.49
1:E:3511:VAL:HG23	1:E:3515:LYS:HD2	1.94	0.49
1:E:3670:GLU:HA	1:E:3673:MET:HG2	1.95	0.49
1:G:1734:TYR:HD2	1:G:2141:ALA:HA	1.77	0.49
1:G:2821:TRP:HA	1:G:2938:THR:O	2.13	0.49
1:G:3260:GLY:HA2	1:G:3325:ASN:ND2	2.27	0.49
1:G:3514:LEU:HD11	1:G:3606:LEU:HD13	1.94	0.49
1:G:4128:PHE:HA	1:G:4131:ARG:HE	1.78	0.49
1:J:881:LEU:O	1:J:885:THR:HG23	2.13	0.49
1:J:907:LEU:O	1:J:963:ASN:ND2	2.45	0.49
1:J:2134:LEU:O	1:J:2138:LEU:HG	2.13	0.49
1:J:2470:ILE:HB	1:J:2502:MET:HE3	1.95	0.49
1:J:3281:LEU:HD13	1:J:3307:VAL:HG21	1.94	0.49
1:J:3727:ASP:HB3	1:J:3731:LYS:NZ	2.28	0.49
1:B:582:HIS:O	1:B:586:ILE:HG13	2.13	0.49
1:B:1433:TYR:CZ	1:B:1578:ALA:HB2	2.48	0.49
1:B:2380:ILE:O	1:B:2384:ILE:HG13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2479:LEU:HA	1:B:2541:PHE:HZ	1.76	0.49
1:B:2861:ASP:HB3	1:B:2928:LYS:HB2	1.95	0.49
1:B:2902:HIS:HB3	1:B:2905:LEU:HB2	1.95	0.49
1:B:3769:ARG:O	1:B:3773:ARG:NH1	2.44	0.49
1:B:3877:ASP:HB3	1:B:3880:PHE:HB3	1.94	0.49
1:E:45:ARG:HD3	1:E:45:ARG:H	1.77	0.49
1:E:792:LEU:HD22	1:E:799:GLU:H	1.77	0.49
1:E:2190:VAL:HA	1:E:2193:GLN:HB3	1.95	0.49
1:E:2823:ILE:HB	1:E:2935:TYR:HD1	1.78	0.49
1:E:3955:MET:HB2	1:E:4019:LEU:HD22	1.95	0.49
1:G:2443:ILE:HD12	1:G:2454:ARG:NH1	2.28	0.49
1:G:3937:TYR:HA	1:G:3940:LYS:HE2	1.94	0.49
1:J:2500:ALA:HB2	1:J:2553:TYR:HD1	1.78	0.49
1:J:2823:ILE:HB	1:J:2935:TYR:HD1	1.78	0.49
1:J:3670:GLU:HA	1:J:3673:MET:HG2	1.95	0.49
1:J:4207:MET:HG2	1:J:4208:PRO:HD2	1.95	0.49
1:J:4219:PHE:HD1	1:J:4950:VAL:HG11	1.78	0.49
1:B:2443:ILE:HD12	1:B:2454:ARG:NH1	2.28	0.48
1:B:2470:ILE:HB	1:B:2502:MET:HE3	1.95	0.48
1:B:4128:PHE:HA	1:B:4131:ARG:HE	1.78	0.48
1:E:181:HIS:ND1	1:E:196:MET:HB2	2.28	0.48
1:E:1008:SER:HB2	1:E:1017:ARG:NE	2.28	0.48
1:E:1433:TYR:CZ	1:E:1578:ALA:HB2	2.48	0.48
1:E:1439:VAL:HB	1:E:1514:LEU:HB3	1.95	0.48
1:E:3877:ASP:HB3	1:E:3880:PHE:HB3	1.94	0.48
1:G:1424:PRO:O	1:G:1428:LEU:HG	2.13	0.48
1:G:1528:THR:HG23	1:G:1539:PHE:CE1	2.46	0.48
1:G:2883:HIS:NE2	1:G:2906:VAL:O	2.47	0.48
1:G:2902:HIS:HB3	1:G:2905:LEU:HB2	1.95	0.48
1:G:3103:ILE:O	1:G:3107:VAL:HG13	2.13	0.48
1:G:3159:ASP:HA	1:G:3162:GLN:HE21	1.78	0.48
1:G:3192:GLU:O	1:G:3196:ARG:HG2	2.13	0.48
1:G:3670:GLU:HA	1:G:3673:MET:HG2	1.95	0.48
1:J:369:LEU:HB3	1:J:371:VAL:HG23	1.95	0.48
1:J:2443:ILE:HD12	1:J:2454:ARG:NH1	2.28	0.48
1:J:4059:LEU:HD13	1:J:4167:ALA:HB2	1.95	0.48
3:M:4:LEU:HD12	3:M:24:ALA:HB2	1.95	0.48
3:M:18:LEU:HB2	3:M:82:MET:HB3	1.94	0.48
1:B:1613:LEU:H	1:B:1613:LEU:HD12	1.78	0.48
1:B:2134:LEU:O	1:B:2138:LEU:HG	2.13	0.48
1:B:2823:ILE:HB	1:B:2935:TYR:HD1	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4059:LEU:HD13	1:B:4167:ALA:HB2	1.95	0.48
1:E:251:ALA:O	1:E:255:HIS:ND1	2.46	0.48
1:E:1866:ILE:O	1:E:1926:LEU:N	2.45	0.48
1:E:2575:ARG:NH1	1:E:2575:ARG:HA	2.28	0.48
1:G:2134:LEU:O	1:G:2138:LEU:HG	2.13	0.48
1:G:2861:ASP:HB3	1:G:2928:LYS:HB2	1.95	0.48
1:G:3268:HIS:CE1	1:G:3272:ILE:HD12	2.48	0.48
1:G:3943:ILE:HG12	1:G:4009:GLN:HE22	1.77	0.48
1:G:3955:MET:HB2	1:G:4019:LEU:HD22	1.95	0.48
1:G:4219:PHE:HD1	1:G:4950:VAL:HG11	1.78	0.48
1:J:50:GLU:O	1:J:52:THR:HG23	2.12	0.48
1:J:582:HIS:O	1:J:586:ILE:HG13	2.13	0.48
1:J:2821:TRP:HA	1:J:2938:THR:O	2.13	0.48
1:J:3889:GLN:HB3	1:J:3964:SER:HA	1.95	0.48
1:J:4096:ALA:O	1:J:4100:GLN:HG2	2.13	0.48
3:M:105:ASN:HD21	3:M:107:TRP:HB3	1.77	0.48
1:B:1065:ASN:OD1	1:B:1069:TRP:NE1	2.46	0.48
1:B:2747:ILE:HG12	1:B:2755:ILE:HG13	1.94	0.48
1:B:2888:ARG:O	1:B:2892:GLN:HG2	2.14	0.48
1:B:3268:HIS:CE1	1:B:3272:ILE:HD12	2.48	0.48
1:B:3937:TYR:HA	1:B:3940:LYS:HE2	1.94	0.48
1:B:4586:PRO:HB3	1:B:4628:VAL:HG21	1.96	0.48
1:E:652:ARG:HG2	1:E:750:LEU:HB3	1.95	0.48
1:E:838:HIS:CD2	1:E:1201:HIS:HB2	2.49	0.48
1:E:1225:PRO:HG2	1:E:1228:ILE:HD12	1.95	0.48
1:E:2376:LEU:O	1:E:2380:ILE:HG12	2.13	0.48
1:E:2908:TYR:HA	1:E:2911:LEU:CD2	2.42	0.48
1:E:4096:ALA:O	1:E:4100:GLN:HG2	2.13	0.48
1:E:4207:MET:HG2	1:E:4208:PRO:HD2	1.95	0.48
1:G:838:HIS:CD2	1:G:1201:HIS:HB2	2.49	0.48
1:G:881:LEU:O	1:G:885:THR:HG23	2.13	0.48
1:G:1225:PRO:HG2	1:G:1228:ILE:HD12	1.95	0.48
1:G:1433:TYR:CZ	1:G:1578:ALA:HB2	2.48	0.48
1:G:2673:HIS:CE1	1:G:2677:LYS:HE2	2.48	0.48
1:G:3889:GLN:HB3	1:G:3964:SER:HA	1.96	0.48
1:G:4586:PRO:HB3	1:G:4628:VAL:HG21	1.96	0.48
1:J:1037:ASP:O	1:J:1041:GLN:HG2	2.13	0.48
1:J:2376:LEU:O	1:J:2380:ILE:HG12	2.13	0.48
1:J:2902:HIS:HB3	1:J:2905:LEU:HB2	1.95	0.48
1:B:462:GLU:HG2	1:B:3710:LEU:HD13	1.96	0.48
1:B:838:HIS:CD2	1:B:1201:HIS:HB2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1037:ASP:O	1:B:1041:GLN:HG2	2.13	0.48
1:B:1065:ASN:HA	1:B:1068:ARG:HH21	1.77	0.48
1:B:1087:ARG:CZ	1:B:1222:GLY:HA3	2.43	0.48
1:B:1734:TYR:HD2	1:B:2141:ALA:HA	1.77	0.48
1:B:2500:ALA:HB2	1:B:2553:TYR:HD1	1.78	0.48
1:B:2883:HIS:NE2	1:B:2906:VAL:O	2.46	0.48
1:B:3103:ILE:O	1:B:3107:VAL:HG13	2.13	0.48
1:E:1037:ASP:O	1:E:1041:GLN:HG2	2.13	0.48
1:E:3316:LEU:HD22	1:E:3346:VAL:HA	1.95	0.48
1:G:582:HIS:O	1:G:586:ILE:HG13	2.13	0.48
1:G:1613:LEU:H	1:G:1613:LEU:HD12	1.78	0.48
1:G:2489:LYS:HE2	1:G:2491:SER:HB3	1.94	0.48
1:G:2823:ILE:HB	1:G:2935:TYR:HD1	1.78	0.48
1:G:4096:ALA:O	1:G:4100:GLN:HG2	2.13	0.48
1:J:1008:SER:HB2	1:J:1017:ARG:NE	2.28	0.48
1:J:1087:ARG:CZ	1:J:1222:GLY:HA3	2.43	0.48
1:J:1802:ILE:O	1:J:1804:LEU:HD22	2.14	0.48
1:J:2888:ARG:O	1:J:2892:GLN:HG2	2.14	0.48
1:J:3194:LEU:HD11	1:J:3275:PRO:HB2	1.96	0.48
1:B:931:THR:O	1:B:935:LEU:HG	2.14	0.48
1:B:1225:PRO:HG2	1:B:1228:ILE:HD12	1.95	0.48
1:B:1439:VAL:HB	1:B:1514:LEU:HB3	1.95	0.48
1:B:3727:ASP:HB3	1:B:3731:LYS:NZ	2.28	0.48
1:E:582:HIS:O	1:E:586:ILE:HG13	2.13	0.48
1:E:2595:LEU:HB2	1:E:2600:ARG:NE	2.25	0.48
1:E:2821:TRP:HA	1:E:2938:THR:O	2.13	0.48
1:E:2883:HIS:NE2	1:E:2906:VAL:O	2.47	0.48
1:E:2902:HIS:HB3	1:E:2905:LEU:HB2	1.95	0.48
1:E:3159:ASP:HA	1:E:3162:GLN:HE21	1.78	0.48
1:E:4128:PHE:HA	1:E:4131:ARG:HE	1.78	0.48
1:G:45:ARG:H	1:G:45:ARG:HD3	1.77	0.48
1:G:931:THR:O	1:G:935:LEU:HG	2.14	0.48
1:G:1802:ILE:O	1:G:1804:LEU:HD22	2.14	0.48
1:G:5003:HIS:HD2	1:G:5007:GLU:HB3	1.79	0.48
1:J:838:HIS:CD2	1:J:1201:HIS:HB2	2.49	0.48
1:J:1433:TYR:CZ	1:J:1578:ALA:HB2	2.48	0.48
1:J:2447:LYS:O	1:J:2451:LEU:HG	2.14	0.48
1:J:2823:ILE:HD12	1:J:2935:TYR:CD1	2.49	0.48
1:J:3639:THR:N	1:J:3640:PRO:HD2	2.29	0.48
1:J:3886:ARG:HD2	1:J:3889:GLN:HE21	1.78	0.48
1:J:3955:MET:HB2	1:J:4019:LEU:HD22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:7:ILE:HD11	2:I:73:LYS:HB2	1.96	0.48
1:B:251:ALA:O	1:B:255:HIS:ND1	2.46	0.48
1:B:1964:ARG:O	1:B:1968:LYS:HG3	2.14	0.48
1:B:3548:GLU:HG2	1:B:3552:PHE:CE2	2.49	0.48
1:B:3955:MET:HB2	1:B:4019:LEU:HD22	1.95	0.48
1:B:4207:MET:HG2	1:B:4208:PRO:HD2	1.95	0.48
1:E:2653:LYS:HE2	1:E:2661:TRP:HA	1.94	0.48
1:E:3194:LEU:HD11	1:E:3275:PRO:HB2	1.96	0.48
1:E:3889:GLN:HB3	1:E:3964:SER:HA	1.95	0.48
1:G:492:ASP:OD1	1:G:546:TRP:NE1	2.44	0.48
1:G:1161:ILE:HG12	1:G:1177:THR:HG22	1.96	0.48
1:G:2500:ALA:HB2	1:G:2553:TYR:HD1	1.78	0.48
1:G:3047:ALA:HB1	1:G:3095:PHE:CE1	2.49	0.48
1:G:3316:LEU:HD22	1:G:3346:VAL:HA	1.95	0.48
1:G:3727:ASP:HB3	1:G:3731:LYS:NZ	2.28	0.48
1:J:1945:TYR:O	1:J:1949:GLN:HG2	2.14	0.48
1:J:3159:ASP:HA	1:J:3162:GLN:HE21	1.78	0.48
1:B:45:ARG:HD3	1:B:45:ARG:H	1.77	0.48
1:B:2447:LYS:O	1:B:2451:LEU:HG	2.14	0.48
1:B:2821:TRP:HA	1:B:2938:THR:O	2.13	0.48
1:E:248:GLU:HB2	1:E:373:LYS:HA	1.96	0.48
1:E:998:ARG:HA	1:E:1001:VAL:HG22	1.95	0.48
1:E:1734:TYR:HD2	1:E:2141:ALA:HA	1.77	0.48
1:E:1964:ARG:O	1:E:1968:LYS:HG3	2.14	0.48
1:E:2861:ASP:HB3	1:E:2928:LYS:HB2	1.96	0.48
1:E:2882:TYR:O	1:E:2886:TRP:HE3	1.96	0.48
1:E:3639:THR:N	1:E:3640:PRO:HD2	2.29	0.48
1:E:3769:ARG:O	1:E:3773:ARG:NH1	2.44	0.48
1:E:4580:TYR:HA	1:E:4632:LEU:H	1.79	0.48
1:G:51:PRO:O	1:G:53:SER:N	2.47	0.48
1:G:462:GLU:HG2	1:G:3710:LEU:HD13	1.96	0.48
1:G:1861:GLN:O	1:G:1865:MET:HE2	2.14	0.48
1:G:1945:TYR:O	1:G:1949:GLN:HG2	2.14	0.48
1:G:2247:GLN:HG3	1:G:2279:SER:HA	1.96	0.48
1:G:2575:ARG:NH1	1:G:2575:ARG:HA	2.28	0.48
1:G:3511:VAL:HG23	1:G:3515:LYS:HD2	1.94	0.48
1:J:1002:ALA:HB1	3:K:1:GLN:HE21	1.79	0.48
1:J:1734:TYR:HD2	1:J:2141:ALA:HA	1.77	0.48
1:J:2312:MET:SD	1:J:2313:LEU:HD22	2.54	0.48
1:J:2352:VAL:O	1:J:2356:LEU:HG	2.14	0.48
1:J:2489:LYS:HE2	1:J:2491:SER:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:2861:ASP:HB3	1:J:2928:LYS:HB2	1.96	0.48
1:J:3192:GLU:O	1:J:3196:ARG:HG2	2.13	0.48
1:J:3514:LEU:HD11	1:J:3606:LEU:HD13	1.94	0.48
1:J:3943:ILE:HG12	1:J:4009:GLN:HE22	1.77	0.48
1:J:4580:TYR:HA	1:J:4632:LEU:H	1.79	0.48
1:J:4704:LEU:HA	1:J:4774:LYS:HE2	1.95	0.48
2:H:7:ILE:HD11	2:H:73:LYS:HB2	1.96	0.48
1:B:3284:TRP:HZ3	1:B:3304:CYS:HG	1.59	0.48
1:E:356:TRP:N	1:E:379:HIS:O	2.38	0.48
1:E:1229:ASN:HD22	1:E:1827:ARG:HG3	1.79	0.48
1:E:1258:ALA:HB3	1:E:1271:ARG:HB3	1.96	0.48
1:E:1945:TYR:O	1:E:1949:GLN:HG2	2.14	0.48
1:E:2134:LEU:O	1:E:2138:LEU:HG	2.13	0.48
1:G:246:TYR:CG	1:G:373:LYS:HG3	2.49	0.48
1:G:652:ARG:HG2	1:G:750:LEU:HB3	1.95	0.48
1:G:1087:ARG:CZ	1:G:1222:GLY:HA3	2.43	0.48
1:G:3309:SER:HA	1:G:3312:LEU:HG	1.96	0.48
1:J:251:ALA:O	1:J:255:HIS:ND1	2.46	0.48
1:J:4128:PHE:HA	1:J:4131:ARG:HE	1.78	0.48
1:J:4586:PRO:HB3	1:J:4628:VAL:HG21	1.96	0.48
3:K:6:GLU:HA	3:K:21:SER:O	2.14	0.48
3:M:33:SER:OG	3:M:101:PRO:HA	2.12	0.48
1:B:369:LEU:HB3	1:B:371:VAL:HG23	1.95	0.48
1:B:995:VAL:HA	1:B:998:ARG:HG2	1.96	0.48
1:B:1161:ILE:HG12	1:B:1177:THR:HG22	1.96	0.48
1:B:2312:MET:SD	1:B:2313:LEU:HD22	2.54	0.48
1:B:3260:GLY:HA2	1:B:3325:ASN:ND2	2.27	0.48
1:B:3943:ILE:HG12	1:B:4009:GLN:HE22	1.77	0.48
1:B:4580:TYR:HA	1:B:4632:LEU:H	1.79	0.48
1:E:931:THR:O	1:E:935:LEU:HG	2.14	0.48
1:E:1087:ARG:CZ	1:E:1222:GLY:HA3	2.43	0.48
1:E:1802:ILE:O	1:E:1804:LEU:HD22	2.14	0.48
1:E:2673:HIS:CE1	1:E:2677:LYS:HE2	2.48	0.48
1:E:3192:GLU:O	1:E:3196:ARG:HG2	2.13	0.48
1:E:4059:LEU:HD13	1:E:4167:ALA:HB2	1.95	0.48
1:G:369:LEU:HB3	1:G:371:VAL:HG23	1.94	0.48
1:G:952:LYS:HG2	1:G:970:LEU:HA	1.96	0.48
1:G:998:ARG:HA	1:G:1001:VAL:HG22	1.95	0.48
1:G:1258:ALA:HB3	1:G:1271:ARG:HB3	1.96	0.48
1:J:462:GLU:HG2	1:J:3710:LEU:HD13	1.96	0.48
1:J:652:ARG:HG2	1:J:750:LEU:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:995:VAL:HA	1:J:998:ARG:HG2	1.96	0.48
1:J:1067:SER:O	1:J:1071:ARG:HD2	2.14	0.48
1:J:2653:LYS:HE2	1:J:2661:TRP:HA	1.94	0.48
1:J:3086:GLU:HA	1:J:3089:LYS:HE3	1.96	0.48
1:J:3316:LEU:HD22	1:J:3346:VAL:HA	1.95	0.48
1:J:3428:ASN:O	1:J:3432:GLU:HG2	2.14	0.48
1:B:893:TYR:H	1:B:962:SER:HB2	1.79	0.48
1:B:1802:ILE:O	1:B:1804:LEU:HD22	2.14	0.48
1:B:1945:TYR:O	1:B:1949:GLN:HG2	2.14	0.48
1:B:2376:LEU:O	1:B:2380:ILE:HG12	2.13	0.48
1:B:2694:GLU:OE1	1:B:2697:ARG:NH2	2.47	0.48
1:B:3047:ALA:HB1	1:B:3095:PHE:CE1	2.49	0.48
1:B:3889:GLN:HB3	1:B:3964:SER:HA	1.95	0.48
1:G:248:GLU:HA	1:G:372:LEU:O	2.12	0.48
1:G:1067:SER:O	1:G:1071:ARG:HD2	2.14	0.48
1:G:1229:ASN:HD22	1:G:1827:ARG:HG3	1.79	0.48
1:G:1714:LEU:O	1:G:1718:ILE:HG12	2.14	0.48
1:G:2312:MET:SD	1:G:2313:LEU:HD22	2.54	0.48
1:G:3400:VAL:HG23	1:G:3403:ARG:HE	1.77	0.48
1:J:893:TYR:H	1:J:962:SER:HB2	1.78	0.48
1:J:1163:THR:HG22	1:J:1168:VAL:HG22	1.96	0.48
1:J:1297:PHE:HA	1:J:1522:LEU:HD22	1.96	0.48
1:J:1964:ARG:O	1:J:1968:LYS:HG3	2.14	0.48
1:J:2575:ARG:NH1	1:J:2575:ARG:HA	2.28	0.48
1:J:3107:VAL:HG12	1:J:3175:LEU:HD23	1.96	0.48
1:J:4021:LYS:O	1:J:4025:VAL:HG23	2.14	0.48
2:D:7:ILE:HD11	2:D:73:LYS:HB2	1.96	0.48
1:B:51:PRO:O	1:B:53:SER:N	2.47	0.47
1:B:952:LYS:HG2	1:B:970:LEU:HA	1.96	0.47
1:B:1163:THR:HG22	1:B:1168:VAL:HG22	1.96	0.47
1:B:1440:PHE:CZ	1:B:1563:GLN:HB2	2.49	0.47
1:B:2352:VAL:O	1:B:2356:LEU:HG	2.14	0.47
1:B:3192:GLU:O	1:B:3196:ARG:HG2	2.13	0.47
1:B:3811:GLU:O	1:B:3814:GLN:HG3	2.14	0.47
1:E:893:TYR:H	1:E:962:SER:HB2	1.78	0.47
1:E:1163:THR:HG22	1:E:1168:VAL:HG22	1.96	0.47
1:E:1440:PHE:CZ	1:E:1563:GLN:HB2	2.49	0.47
1:E:2352:VAL:O	1:E:2356:LEU:HG	2.14	0.47
1:E:2500:ALA:HB2	1:E:2553:TYR:HD1	1.78	0.47
1:E:4021:LYS:O	1:E:4025:VAL:HG23	2.14	0.47
1:E:4704:LEU:HA	1:E:4774:LYS:HE2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1964:ARG:O	1:G:1968:LYS:HG3	2.14	0.47
1:J:3103:ILE:O	1:J:3107:VAL:HG13	2.13	0.47
3:M:6:GLU:HA	3:M:21:SER:O	2.14	0.47
1:B:3051:ARG:HD2	1:B:3131:TYR:CE2	2.49	0.47
1:B:3445:TRP:HD1	1:B:3451:PHE:CE2	2.32	0.47
1:B:4023:MET:O	1:B:4027:LEU:HG	2.14	0.47
1:B:4704:LEU:HA	1:B:4774:LYS:HE2	1.95	0.47
1:B:5003:HIS:HD2	1:B:5007:GLU:HB3	1.79	0.47
1:E:462:GLU:HG2	1:E:3710:LEU:HD13	1.96	0.47
1:E:1297:PHE:HA	1:E:1522:LEU:HD22	1.96	0.47
1:E:2694:GLU:OE1	1:E:2697:ARG:NH2	2.47	0.47
1:E:2823:ILE:HD12	1:E:2935:TYR:CD1	2.49	0.47
1:E:2888:ARG:O	1:E:2892:GLN:HG2	2.14	0.47
1:E:4586:PRO:HB3	1:E:4628:VAL:HG21	1.96	0.47
1:G:2447:LYS:O	1:G:2451:LEU:HG	2.14	0.47
1:G:3445:TRP:HD1	1:G:3451:PHE:CE2	2.32	0.47
1:G:3548:GLU:HG2	1:G:3552:PHE:CE2	2.49	0.47
1:G:4704:LEU:HA	1:G:4774:LYS:HE2	1.95	0.47
1:G:4927:ILE:HD12	1:J:4936:ILE:HD13	1.96	0.47
1:J:952:LYS:HG2	1:J:970:LEU:HA	1.96	0.47
1:J:3047:ALA:HB1	1:J:3095:PHE:CE1	2.49	0.47
1:J:3309:SER:HA	1:J:3312:LEU:HG	1.95	0.47
1:B:652:ARG:HG2	1:B:750:LEU:HB3	1.95	0.47
1:B:867:LEU:HD12	1:B:871:ARG:HE	1.80	0.47
1:B:1229:ASN:HD22	1:B:1827:ARG:HG3	1.79	0.47
1:B:1714:LEU:O	1:B:1718:ILE:HG12	2.14	0.47
1:B:1866:ILE:O	1:B:1926:LEU:N	2.45	0.47
1:B:3137:LEU:HB3	1:B:3138:PRO:HD3	1.96	0.47
1:E:3103:ILE:O	1:E:3107:VAL:HG13	2.13	0.47
1:G:1163:THR:HG22	1:G:1168:VAL:HG22	1.96	0.47
1:G:2376:LEU:O	1:G:2380:ILE:HG12	2.13	0.47
1:G:2694:GLU:OE1	1:G:2697:ARG:NH2	2.47	0.47
1:G:2886:TRP:CD1	1:G:2889:LYS:HE2	2.50	0.47
1:G:2888:ARG:O	1:G:2892:GLN:HG2	2.14	0.47
1:G:3086:GLU:HA	1:G:3089:LYS:HE3	1.96	0.47
1:G:3194:LEU:HD11	1:G:3275:PRO:HB2	1.96	0.47
1:J:40:GLU:O	1:J:114:SER:OG	2.32	0.47
1:J:998:ARG:HA	1:J:1001:VAL:HG22	1.95	0.47
1:J:2883:HIS:NE2	1:J:2906:VAL:O	2.46	0.47
1:J:3051:ARG:HD2	1:J:3131:TYR:CE2	2.49	0.47
1:J:3946:GLN:OE1	1:J:3949:ARG:NH2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:5003:HIS:HD2	1:J:5007:GLU:HB3	1.79	0.47
2:H:30:LEU:HD12	2:H:36:PHE:HD2	1.79	0.47
3:F:102:ASN:HB2	3:F:104:TYR:CE2	2.49	0.47
1:B:993:HIS:CE1	1:B:1027:LEU:HD11	2.49	0.47
1:B:2673:HIS:CE1	1:B:2677:LYS:HE2	2.48	0.47
1:B:3828:PHE:O	1:B:3832:ILE:HG12	2.15	0.47
1:E:952:LYS:HG2	1:E:970:LEU:HA	1.96	0.47
1:E:2096:GLU:O	1:E:2100:HIS:ND1	2.48	0.47
1:E:2633:LEU:HB2	1:E:2689:LYS:HE2	1.96	0.47
1:E:3099:ALA:O	1:E:3103:ILE:HG12	2.14	0.47
1:E:5003:HIS:HD2	1:E:5007:GLU:HB3	1.79	0.47
1:G:1297:PHE:HA	1:G:1522:LEU:HD22	1.96	0.47
1:G:2747:ILE:HD11	1:G:2751:LEU:HD11	1.96	0.47
1:G:2823:ILE:HD12	1:G:2935:TYR:CD1	2.49	0.47
1:G:3946:GLN:OE1	1:G:3949:ARG:NH2	2.48	0.47
1:G:4580:TYR:HA	1:G:4632:LEU:H	1.79	0.47
1:J:1225:PRO:HG2	1:J:1228:ILE:HD12	1.95	0.47
1:J:2886:TRP:CD1	1:J:2889:LYS:HE2	2.50	0.47
1:J:4023:MET:O	1:J:4027:LEU:HG	2.15	0.47
2:A:7:ILE:HD11	2:A:73:LYS:HB2	1.96	0.47
3:F:6:GLU:HA	3:F:21:SER:O	2.14	0.47
3:K:102:ASN:HB2	3:K:104:TYR:CE2	2.49	0.47
1:B:1297:PHE:HA	1:B:1522:LEU:HD22	1.96	0.47
1:B:3159:ASP:HA	1:B:3162:GLN:HE21	1.78	0.47
1:B:3309:SER:HA	1:B:3312:LEU:HG	1.96	0.47
1:B:3428:ASN:O	1:B:3432:GLU:HG2	2.14	0.47
1:B:3442:PHE:HE1	1:B:3510:ILE:HG22	1.80	0.47
1:E:525:LEU:O	1:E:529:LEU:HG	2.15	0.47
1:E:3086:GLU:HA	1:E:3089:LYS:HE3	1.96	0.47
1:E:3428:ASN:O	1:E:3432:GLU:HG2	2.14	0.47
1:G:1007:TYR:O	1:G:1017:ARG:NH2	2.48	0.47
1:G:1439:VAL:HB	1:G:1514:LEU:HB3	1.95	0.47
1:G:1741:GLU:O	1:G:1745:ILE:HG13	2.15	0.47
1:G:2096:GLU:O	1:G:2100:HIS:ND1	2.48	0.47
1:G:3639:THR:N	1:G:3640:PRO:HD2	2.29	0.47
1:J:2595:LEU:HB2	1:J:2600:ARG:NE	2.25	0.47
1:J:3034:LYS:O	1:J:3037:GLU:HG3	2.15	0.47
1:J:3828:PHE:O	1:J:3832:ILE:HG12	2.14	0.47
3:C:6:GLU:HA	3:C:21:SER:O	2.14	0.47
1:B:1452:TRP:CZ3	1:B:1550:PRO:HG3	2.49	0.47
1:B:1699:GLU:HG3	1:B:1810:LYS:NZ	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1741:GLU:O	1:B:1745:ILE:HG13	2.15	0.47
1:B:1965:TYR:CZ	1:B:2031:LEU:HB2	2.50	0.47
1:E:51:PRO:O	1:E:53:SER:N	2.47	0.47
1:E:867:LEU:HD12	1:E:871:ARG:HE	1.79	0.47
1:E:2447:LYS:O	1:E:2451:LEU:HG	2.14	0.47
1:E:3137:LEU:HB3	1:E:3138:PRO:HD3	1.96	0.47
1:E:3445:TRP:HD1	1:E:3451:PHE:CE2	2.32	0.47
1:E:3676:ASP:HA	1:E:3679:LYS:HE2	1.97	0.47
1:G:404:ILE:HD13	1:G:481:GLU:HG3	1.96	0.47
1:G:867:LEU:HD12	1:G:871:ARG:HE	1.80	0.47
1:G:993:HIS:CE1	1:G:1027:LEU:HD11	2.49	0.47
1:G:1822:GLY:HA3	1:G:1838:PHE:HZ	1.79	0.47
1:G:2352:VAL:O	1:G:2356:LEU:HG	2.14	0.47
1:G:3034:LYS:O	1:G:3037:GLU:HG3	2.15	0.47
1:J:931:THR:O	1:J:935:LEU:HG	2.14	0.47
1:J:1452:TRP:CZ3	1:J:1550:PRO:HG3	2.49	0.47
1:J:2247:GLN:HG3	1:J:2279:SER:HA	1.96	0.47
1:J:2694:GLU:OE1	1:J:2697:ARG:NH2	2.47	0.47
1:J:3445:TRP:HD1	1:J:3451:PHE:CE2	2.33	0.47
1:J:4725:LEU:HA	1:J:4737:ILE:HG21	1.97	0.47
3:C:102:ASN:HB2	3:C:104:TYR:CE2	2.50	0.47
3:K:105:ASN:ND2	3:K:108:GLY:H	2.12	0.47
1:B:525:LEU:O	1:B:529:LEU:HG	2.15	0.47
1:B:920:TYR:O	1:B:923:GLN:HG2	2.15	0.47
1:B:1100:MET:HB2	1:B:1143:TRP:CH2	2.50	0.47
1:B:2499:LYS:HA	1:B:2502:MET:HG3	1.96	0.47
1:B:2633:LEU:HB2	1:B:2689:LYS:HE2	1.96	0.47
1:B:2823:ILE:HD12	1:B:2935:TYR:CD1	2.49	0.47
1:B:2886:TRP:CD1	1:B:2889:LYS:HE2	2.50	0.47
1:B:3099:ALA:O	1:B:3103:ILE:HG12	2.14	0.47
1:B:3107:VAL:HG12	1:B:3175:LEU:HD23	1.96	0.47
1:B:3107:VAL:HG12	1:B:3175:LEU:HB3	1.96	0.47
1:B:3172:ILE:O	1:B:3175:LEU:HG	2.15	0.47
1:B:3194:LEU:HD11	1:B:3275:PRO:HB2	1.96	0.47
1:B:3639:THR:N	1:B:3640:PRO:HD2	2.29	0.47
1:B:3891:LEU:O	1:B:3896:ASN:ND2	2.36	0.47
1:B:4021:LYS:O	1:B:4025:VAL:HG23	2.14	0.47
1:B:4661:TYR:OH	1:B:4786:ASP:OD2	2.30	0.47
1:E:1067:SER:O	1:E:1071:ARG:HD2	2.14	0.47
1:E:1452:TRP:CZ3	1:E:1550:PRO:HG3	2.50	0.47
1:E:2312:MET:SD	1:E:2313:LEU:HD22	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2747:ILE:HD11	1:E:2751:LEU:HD11	1.96	0.47
1:E:2792:ARG:HB2	1:E:2793:PRO:HD2	1.97	0.47
1:E:3047:ALA:HB1	1:E:3095:PHE:CE1	2.49	0.47
1:E:3107:VAL:HG12	1:E:3175:LEU:HD23	1.96	0.47
1:E:3172:ILE:O	1:E:3175:LEU:HG	2.15	0.47
1:E:3309:SER:HA	1:E:3312:LEU:HG	1.95	0.47
1:E:3548:GLU:HG2	1:E:3552:PHE:CE2	2.49	0.47
1:E:4020:GLN:HG2	1:E:4139:ILE:HD11	1.97	0.47
1:E:4023:MET:O	1:E:4027:LEU:HG	2.15	0.47
1:E:4088:ILE:HD12	1:E:4093:PHE:CD1	2.50	0.47
1:E:4936:ILE:HD13	1:J:4927:ILE:HD12	1.97	0.47
1:G:1440:PHE:CZ	1:G:1563:GLN:HB2	2.49	0.47
1:G:2439:GLU:O	1:G:2443:ILE:HG12	2.15	0.47
1:G:3051:ARG:HD2	1:G:3131:TYR:CE2	2.49	0.47
1:G:3099:ALA:O	1:G:3103:ILE:HG12	2.14	0.47
1:G:3107:VAL:HG12	1:G:3175:LEU:HB3	1.96	0.47
1:G:3172:ILE:O	1:G:3175:LEU:HG	2.15	0.47
1:G:3225:ARG:O	1:G:3229:ILE:HG23	2.15	0.47
1:G:3828:PHE:O	1:G:3832:ILE:HG12	2.15	0.47
1:J:993:HIS:CE1	1:J:1027:LEU:HD11	2.49	0.47
1:J:1440:PHE:CZ	1:J:1563:GLN:HB2	2.49	0.47
1:J:2633:LEU:HB2	1:J:2689:LYS:HE2	1.96	0.47
1:J:3099:ALA:O	1:J:3103:ILE:HG12	2.14	0.47
1:J:3137:LEU:HB3	1:J:3138:PRO:HD3	1.97	0.47
2:A:30:LEU:HD12	2:A:36:PHE:HD2	1.79	0.47
2:D:30:LEU:HD12	2:D:36:PHE:HD2	1.80	0.47
1:B:45:ARG:HB2	1:B:137:LEU:HB2	1.97	0.47
1:B:998:ARG:HA	1:B:1001:VAL:HG22	1.95	0.47
1:B:2247:GLN:HG3	1:B:2279:SER:HA	1.96	0.47
1:B:2439:GLU:O	1:B:2443:ILE:HG12	2.15	0.47
1:B:2747:ILE:HD11	1:B:2751:LEU:HD11	1.96	0.47
1:E:4094:GLN:HG3	1:E:4108:ILE:HG21	1.97	0.47
1:G:1452:TRP:CZ3	1:G:1550:PRO:HG3	2.49	0.47
1:G:1699:GLU:HG3	1:G:1810:LYS:NZ	2.30	0.47
1:G:2913:ALA:HA	1:G:2916:LYS:HB3	1.97	0.47
1:G:3816:MET:O	1:G:3820:LEU:HG	2.15	0.47
1:G:4725:LEU:HA	1:G:4737:ILE:HG21	1.97	0.47
1:J:51:PRO:O	1:J:53:SER:N	2.47	0.47
1:J:985:VAL:HG11	1:J:1040:CYS:SG	2.55	0.47
1:J:1822:GLY:HA3	1:J:1838:PHE:HZ	1.79	0.47
1:J:2096:GLU:O	1:J:2100:HIS:ND1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:2439:GLU:O	1:J:2443:ILE:HG12	2.15	0.47
1:J:2499:LYS:HA	1:J:2502:MET:HG3	1.96	0.47
1:B:977:LEU:HD12	1:B:1044:ARG:HD3	1.97	0.47
1:B:3180:ASN:OD1	1:B:3181:THR:N	2.48	0.47
1:B:3225:ARG:O	1:B:3229:ILE:HG23	2.15	0.47
1:B:3699:HIS:HA	1:B:3702:VAL:HG22	1.97	0.47
1:E:341:TYR:CE2	1:E:392:ARG:HB2	2.50	0.47
1:E:1100:MET:HB2	1:E:1143:TRP:CH2	2.50	0.47
1:E:1161:ILE:HG12	1:E:1177:THR:HG22	1.96	0.47
1:E:3811:GLU:O	1:E:3814:GLN:HG3	2.14	0.47
1:G:1814:MET:HA	1:G:1817:GLU:HG2	1.97	0.47
1:G:1965:TYR:CZ	1:G:2031:LEU:HB2	2.50	0.47
1:G:2499:LYS:HA	1:G:2502:MET:HG3	1.96	0.47
1:J:1161:ILE:HG12	1:J:1177:THR:HG22	1.96	0.47
1:J:1528:THR:HG23	1:J:1539:PHE:CE1	2.46	0.47
1:J:3107:VAL:HG12	1:J:3175:LEU:HB3	1.96	0.47
1:J:3172:ILE:O	1:J:3175:LEU:HG	2.15	0.47
1:J:3442:PHE:HE1	1:J:3510:ILE:HG22	1.80	0.47
1:J:3540:TYR:CZ	1:J:3549:VAL:HG21	2.50	0.47
1:J:3811:GLU:O	1:J:3814:GLN:HG3	2.14	0.47
1:J:4020:GLN:HG2	1:J:4139:ILE:HD11	1.97	0.47
3:K:15:GLY:H	3:K:85:LEU:HB2	1.80	0.47
3:M:102:ASN:HB2	3:M:104:TYR:CE2	2.49	0.47
1:B:1005:TRP:HE3	1:B:1021:LEU:HD11	1.80	0.47
1:B:1258:ALA:HB3	1:B:1271:ARG:HB3	1.96	0.47
1:B:2325:PRO:HB2	1:B:2421:ALA:HB1	1.97	0.47
1:B:2509:VAL:HG23	1:B:2510:TYR:H	1.79	0.47
1:B:2584:HIS:O	1:B:2588:ARG:HG3	2.15	0.47
1:B:2792:ARG:HB2	1:B:2793:PRO:HD2	1.97	0.47
1:E:977:LEU:HD12	1:E:1044:ARG:HD3	1.97	0.47
1:E:1007:TYR:O	1:E:1017:ARG:NH2	2.48	0.47
1:E:1100:MET:SD	1:E:1194:LEU:HG	2.55	0.47
1:E:1699:GLU:HG3	1:E:1810:LYS:NZ	2.30	0.47
1:E:1822:GLY:HA3	1:E:1838:PHE:HZ	1.79	0.47
1:E:2886:TRP:CD1	1:E:2889:LYS:HE2	2.50	0.47
1:E:2999:ALA:HB3	1:E:3000:LYS:HZ2	1.80	0.47
1:E:3003:LEU:HB2	1:E:3004:PRO:HD3	1.97	0.47
1:E:3699:HIS:HA	1:E:3702:VAL:HG22	1.97	0.47
1:G:525:LEU:O	1:G:529:LEU:HG	2.15	0.47
1:G:1619:ARG:HA	1:G:1626:TRP:HA	1.97	0.47
1:G:2792:ARG:HB2	1:G:2793:PRO:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3290:GLU:OE1	1:G:3309:SER:N	2.44	0.47
1:G:3811:GLU:O	1:G:3814:GLN:HG3	2.14	0.47
1:G:4094:GLN:HG3	1:G:4108:ILE:HG21	1.97	0.47
1:J:341:TYR:CE2	1:J:392:ARG:HB2	2.50	0.47
1:J:891:TRP:HA	1:J:902:ARG:HB3	1.97	0.47
1:J:1229:ASN:HD22	1:J:1827:ARG:HG3	1.79	0.47
1:J:1245:PHE:CD2	1:J:1290:ARG:HG2	2.51	0.47
1:J:1439:VAL:HB	1:J:1514:LEU:HB3	1.95	0.47
1:J:1699:GLU:HG3	1:J:1810:LYS:NZ	2.30	0.47
1:J:2747:ILE:HD11	1:J:2751:LEU:HD11	1.96	0.47
1:J:3704:HIS:O	1:J:3708:THR:HG23	2.15	0.47
1:J:4088:ILE:HD12	1:J:4093:PHE:CD1	2.50	0.47
1:B:985:VAL:HG11	1:B:1040:CYS:SG	2.55	0.46
1:B:1067:SER:O	1:B:1071:ARG:HD2	2.14	0.46
1:B:3034:LYS:O	1:B:3037:GLU:HG3	2.15	0.46
1:B:3057:PHE:HB2	1:B:3060:ASP:HB2	1.97	0.46
1:B:3540:TYR:CZ	1:B:3549:VAL:HG21	2.50	0.46
1:B:3704:HIS:O	1:B:3708:THR:HG23	2.15	0.46
1:B:3720:TYR:HA	1:B:3723:MET:HE2	1.97	0.46
1:E:985:VAL:HG11	1:E:1040:CYS:SG	2.55	0.46
1:E:993:HIS:CE1	1:E:1027:LEU:HD11	2.49	0.46
1:E:1699:GLU:HG3	1:E:1810:LYS:HZ2	1.81	0.46
1:E:1782:PHE:O	2:D:82:TYR:OH	2.24	0.46
1:E:3180:ASN:OD1	1:E:3181:THR:N	2.48	0.46
1:E:3225:ARG:O	1:E:3229:ILE:HG23	2.15	0.46
1:G:893:TYR:H	1:G:962:SER:HB2	1.78	0.46
1:G:3107:VAL:HG12	1:G:3175:LEU:HD23	1.96	0.46
1:J:404:ILE:HD13	1:J:481:GLU:HG3	1.97	0.46
1:J:867:LEU:HD12	1:J:871:ARG:HE	1.80	0.46
1:J:1007:TYR:O	1:J:1017:ARG:NH2	2.48	0.46
1:J:2509:VAL:HG23	1:J:2510:TYR:H	1.79	0.46
1:J:3548:GLU:HG2	1:J:3552:PHE:CE2	2.49	0.46
1:J:4666:VAL:HG11	1:J:4783:ILE:HD12	1.97	0.46
2:I:19:GLY:HA2	2:I:49:ARG:HD3	1.97	0.46
3:F:94:TYR:CD1	3:F:120:GLY:HA3	2.51	0.46
1:B:404:ILE:HD13	1:B:481:GLU:HG3	1.96	0.46
1:B:1822:GLY:HA3	1:B:1838:PHE:HZ	1.79	0.46
1:B:4088:ILE:HD12	1:B:4093:PHE:CD1	2.50	0.46
1:E:40:GLU:O	1:E:114:SER:OG	2.32	0.46
1:E:1005:TRP:HE3	1:E:1021:LEU:HD11	1.80	0.46
1:E:2389:ASP:OD2	1:E:2392:ARG:NE	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2443:ILE:HD12	1:E:2454:ARG:HH11	1.80	0.46
1:E:3034:LYS:O	1:E:3037:GLU:HG3	2.15	0.46
1:E:3051:ARG:HD2	1:E:3131:TYR:CE2	2.49	0.46
1:E:3107:VAL:HG12	1:E:3175:LEU:HB3	1.96	0.46
1:G:995:VAL:HA	1:G:998:ARG:HG2	1.96	0.46
1:G:1100:MET:HB2	1:G:1143:TRP:CH2	2.50	0.46
1:G:1758:ARG:NH1	1:G:2037:ASP:OD1	2.49	0.46
1:G:3137:LEU:HB3	1:G:3138:PRO:HD3	1.96	0.46
1:G:3428:ASN:O	1:G:3432:GLU:HG2	2.14	0.46
1:G:3704:HIS:O	1:G:3708:THR:HG23	2.15	0.46
1:G:3886:ARG:CD	1:G:3889:GLN:HE21	2.28	0.46
1:G:4088:ILE:HD12	1:G:4093:PHE:CD1	2.50	0.46
1:G:4666:VAL:HG11	1:G:4783:ILE:HD12	1.97	0.46
1:J:3225:ARG:O	1:J:3229:ILE:HG23	2.15	0.46
1:J:3443:ILE:HG22	1:J:3605:HIS:ND1	2.31	0.46
1:B:1100:MET:SD	1:B:1194:LEU:HG	2.56	0.46
1:B:1758:ARG:NH1	1:B:2037:ASP:OD1	2.49	0.46
1:B:2096:GLU:O	1:B:2100:HIS:ND1	2.48	0.46
1:B:3017:PHE:HB2	1:B:3074:SER:HB2	1.98	0.46
1:B:3996:PHE:O	1:B:4000:MET:HG3	2.16	0.46
1:B:4105:GLY:O	1:B:4109:GLN:HG2	2.16	0.46
1:B:4835:LYS:HD3	1:B:4835:LYS:N	2.31	0.46
1:B:4936:ILE:HD13	1:E:4927:ILE:HD12	1.97	0.46
1:E:891:TRP:HA	1:E:902:ARG:HB3	1.97	0.46
1:E:920:TYR:O	1:E:923:GLN:HG2	2.15	0.46
1:E:924:MET:HE1	3:F:106:PRO:HD2	1.98	0.46
1:E:1860:LYS:HG2	1:E:1864:LYS:HE2	1.98	0.46
1:E:2509:VAL:HG23	1:E:2510:TYR:H	1.79	0.46
1:E:3828:PHE:O	1:E:3832:ILE:HG12	2.15	0.46
1:G:1245:PHE:CD2	1:G:1290:ARG:HG2	2.50	0.46
1:G:3180:ASN:OD1	1:G:3181:THR:N	2.48	0.46
1:G:3540:TYR:CZ	1:G:3549:VAL:HG21	2.50	0.46
1:G:4105:GLY:O	1:G:4109:GLN:HG2	2.16	0.46
1:J:525:LEU:O	1:J:529:LEU:HG	2.15	0.46
1:J:1619:ARG:HA	1:J:1626:TRP:HA	1.97	0.46
1:J:1691:GLN:HE22	1:J:1803:PRO:HD2	1.81	0.46
1:J:1714:LEU:O	1:J:1718:ILE:HG12	2.14	0.46
1:J:3057:PHE:HB2	1:J:3060:ASP:HB2	1.97	0.46
3:C:94:TYR:CD1	3:C:120:GLY:HA3	2.51	0.46
3:M:15:GLY:H	3:M:85:LEU:HB2	1.80	0.46
3:M:94:TYR:CD1	3:M:120:GLY:HA3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:917:GLU:OE2	3:C:101:PRO:HB2	2.16	0.46
1:B:1814:MET:HA	1:B:1817:GLU:HG2	1.97	0.46
1:B:1860:LYS:HG2	1:B:1864:LYS:HE2	1.98	0.46
1:B:3086:GLU:HA	1:B:3089:LYS:HE3	1.96	0.46
1:B:3816:MET:O	1:B:3820:LEU:HG	2.15	0.46
1:B:4020:GLN:HG2	1:B:4139:ILE:HD11	1.97	0.46
1:E:995:VAL:HA	1:E:998:ARG:HG2	1.96	0.46
1:E:1934:SER:O	1:E:1938:GLN:HG2	2.16	0.46
1:E:4779:LYS:HA	1:E:4782:VAL:HG22	1.98	0.46
1:G:356:TRP:N	1:G:379:HIS:O	2.38	0.46
1:G:1860:LYS:HG2	1:G:1864:LYS:HE2	1.98	0.46
1:G:2633:LEU:HB2	1:G:2689:LYS:HE2	1.96	0.46
1:G:3511:VAL:HG22	1:G:3516:LYS:NZ	2.31	0.46
1:J:844:ARG:HH12	1:J:1071:ARG:HH21	1.63	0.46
1:J:3180:ASN:OD1	1:J:3181:THR:N	2.48	0.46
1:J:3181:THR:O	1:J:3185:LYS:HG2	2.16	0.46
1:B:356:TRP:N	1:B:379:HIS:O	2.38	0.46
1:B:1007:TYR:O	1:B:1017:ARG:NH2	2.48	0.46
1:B:2892:GLN:O	1:B:2895:GLU:HG2	2.16	0.46
1:B:2906:VAL:HG23	1:B:2911:LEU:HB3	1.97	0.46
1:B:3568:SER:O	1:B:3571:TRP:NE1	2.49	0.46
1:B:4745:LEU:O	1:B:4748:LEU:HG	2.15	0.46
1:E:844:ARG:HH12	1:E:1071:ARG:HH21	1.63	0.46
1:E:1477:GLY:HA2	1:E:1483:VAL:HA	1.98	0.46
1:E:1708:ARG:O	1:E:1712:TYR:HD1	1.99	0.46
1:E:1965:TYR:CZ	1:E:2031:LEU:HB2	2.50	0.46
1:E:2499:LYS:HA	1:E:2502:MET:HG3	1.96	0.46
1:E:3443:ILE:HG22	1:E:3605:HIS:ND1	2.31	0.46
1:E:3529:ASP:O	1:E:3533:ILE:HG12	2.16	0.46
1:E:3704:HIS:O	1:E:3708:THR:HG23	2.15	0.46
1:E:3946:GLN:OE1	1:E:3949:ARG:NH2	2.48	0.46
1:G:985:VAL:HG11	1:G:1040:CYS:SG	2.55	0.46
1:G:1691:GLN:HE22	1:G:1803:PRO:HD2	1.81	0.46
1:G:2325:PRO:HB2	1:G:2421:ALA:HB1	1.97	0.46
1:G:3443:ILE:HG22	1:G:3605:HIS:ND1	2.31	0.46
1:G:3529:ASP:O	1:G:3533:ILE:HG12	2.16	0.46
1:G:4992:LEU:O	1:G:4996:ILE:HG13	2.16	0.46
1:J:231:LEU:HD11	1:J:245:VAL:HB	1.97	0.46
1:J:1005:TRP:HE3	1:J:1021:LEU:HD11	1.80	0.46
1:J:1100:MET:SD	1:J:1194:LEU:HG	2.56	0.46
1:J:1100:MET:HB2	1:J:1143:TRP:CH2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1741:GLU:O	1:J:1745:ILE:HG13	2.15	0.46
1:J:1861:GLN:O	1:J:1865:MET:HE2	2.15	0.46
1:J:1934:SER:O	1:J:1938:GLN:HG2	2.16	0.46
1:J:2792:ARG:HB2	1:J:2793:PRO:HD2	1.97	0.46
1:J:3003:LEU:HB2	1:J:3004:PRO:HD3	1.97	0.46
1:J:3816:MET:O	1:J:3820:LEU:HG	2.15	0.46
3:C:15:GLY:H	3:C:85:LEU:HB2	1.80	0.46
1:B:276:TRP:HZ3	1:B:346:CYS:HA	1.81	0.46
1:B:920:TYR:HE1	3:C:99:ARG:HE	1.59	0.46
1:B:1002:ALA:HB1	3:C:1:GLN:HE21	1.80	0.46
1:B:1691:GLN:HE22	1:B:1803:PRO:HD2	1.81	0.46
1:B:4666:VAL:HG11	1:B:4783:ILE:HD12	1.97	0.46
1:E:1714:LEU:O	1:E:1718:ILE:HG12	2.14	0.46
1:E:1758:ARG:NH1	1:E:2037:ASP:OD1	2.49	0.46
1:E:2584:HIS:O	1:E:2588:ARG:HG3	2.15	0.46
1:E:2707:ALA:HB1	1:E:3009:TYR:HD1	1.81	0.46
1:E:2906:VAL:HG23	1:E:2911:LEU:HB3	1.97	0.46
1:E:3181:THR:O	1:E:3185:LYS:HG2	2.16	0.46
1:E:3996:PHE:O	1:E:4000:MET:HG3	2.16	0.46
1:E:4666:VAL:HG11	1:E:4783:ILE:HD12	1.97	0.46
1:E:4700:GLN:OE1	1:E:4703:ARG:NH1	2.49	0.46
1:E:4725:LEU:HA	1:E:4737:ILE:HG21	1.97	0.46
1:G:157:ARG:HH21	1:G:161:GLU:HB3	1.81	0.46
1:G:341:TYR:CE2	1:G:392:ARG:HB2	2.50	0.46
1:G:1100:MET:SD	1:G:1194:LEU:HG	2.55	0.46
1:G:1699:GLU:HG3	1:G:1810:LYS:HZ2	1.79	0.46
1:G:2588:ARG:HA	1:G:2591:ARG:HE	1.81	0.46
1:G:2702:CYS:O	1:G:2706:ILE:HG13	2.16	0.46
1:G:3676:ASP:HA	1:G:3679:LYS:HE2	1.96	0.46
1:J:918:ARG:O	1:J:922:LEU:HG	2.16	0.46
1:J:996:TRP:NE1	3:K:113:GLU:HB3	2.30	0.46
1:J:1561:VAL:HG23	1:J:1562:ILE:N	2.31	0.46
1:J:3290:GLU:OE1	1:J:3309:SER:N	2.44	0.46
1:J:3367:LYS:O	1:J:3371:LYS:HG2	2.16	0.46
1:J:3529:ASP:O	1:J:3533:ILE:HG12	2.16	0.46
2:D:19:GLY:HA2	2:D:49:ARG:HD3	1.97	0.46
1:B:2529:ASP:HB3	1:B:2554:LEU:HD21	1.98	0.46
1:B:2748:PRO:HB2	1:B:2750:LYS:HG2	1.98	0.46
1:B:3752:SER:O	1:B:3756:LYS:HG3	2.16	0.46
1:B:4094:GLN:HG3	1:B:4108:ILE:HG21	1.97	0.46
1:E:1561:VAL:HG23	1:E:1562:ILE:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2529:ASP:HB3	1:E:2554:LEU:HD21	1.98	0.46
1:E:2588:ARG:HA	1:E:2591:ARG:HE	1.81	0.46
1:E:2970:SER:HB3	1:E:2998:PHE:CE2	2.51	0.46
1:E:3442:PHE:HE1	1:E:3510:ILE:HG22	1.80	0.46
1:E:3568:SER:O	1:E:3571:TRP:NE1	2.49	0.46
1:E:4772:ASP:OD1	1:E:4772:ASP:N	2.49	0.46
1:G:45:ARG:HB2	1:G:137:LEU:HB2	1.97	0.46
1:G:891:TRP:HA	1:G:902:ARG:HB3	1.97	0.46
1:G:1578:ALA:HA	1:G:1584:ARG:NH1	2.31	0.46
1:G:2624:ARG:HB3	1:G:2674:LEU:HD13	1.98	0.46
1:G:2957:PHE:HE1	1:G:2961:GLN:HE21	1.64	0.46
1:G:3367:LYS:O	1:G:3371:LYS:HG2	2.16	0.46
1:G:3996:PHE:O	1:G:4000:MET:HG3	2.16	0.46
1:J:1758:ARG:NH1	1:J:2037:ASP:OD1	2.49	0.46
1:J:1860:LYS:HG2	1:J:1864:LYS:HE2	1.98	0.46
1:J:1965:TYR:CZ	1:J:2031:LEU:HB2	2.50	0.46
1:J:2325:PRO:HB2	1:J:2421:ALA:HB1	1.97	0.46
1:J:2443:ILE:HD12	1:J:2454:ARG:HH11	1.80	0.46
1:J:2610:LEU:O	1:J:2614:ILE:HG12	2.16	0.46
1:J:2957:PHE:HE1	1:J:2961:GLN:HE21	1.64	0.46
1:J:3511:VAL:HG22	1:J:3516:LYS:NZ	2.31	0.46
1:J:3980:LEU:CD1	1:J:4030:LEU:HD21	2.46	0.46
1:J:4094:GLN:HG3	1:J:4108:ILE:HG21	1.97	0.46
1:J:4779:LYS:HA	1:J:4782:VAL:HG22	1.98	0.46
1:B:677:ALA:HB1	2:A:40:ARG:HB3	1.98	0.46
1:B:3443:ILE:HG22	1:B:3605:HIS:ND1	2.31	0.46
1:B:3511:VAL:HG22	1:B:3516:LYS:NZ	2.31	0.46
1:B:3529:ASP:O	1:B:3533:ILE:HG12	2.16	0.46
1:B:3676:ASP:HA	1:B:3679:LYS:HE2	1.97	0.46
1:B:4725:LEU:HA	1:B:4737:ILE:HG21	1.97	0.46
1:E:276:TRP:HZ3	1:E:346:CYS:HA	1.81	0.46
1:E:404:ILE:HD13	1:E:481:GLU:HG3	1.96	0.46
1:E:2247:GLN:HG3	1:E:2279:SER:HA	1.96	0.46
1:E:2439:GLU:O	1:E:2443:ILE:HG12	2.15	0.46
1:E:4673:ARG:HH12	1:E:4698:LYS:HB2	1.81	0.46
1:E:4745:LEU:O	1:E:4748:LEU:HG	2.15	0.46
1:G:224:HIS:HA	1:G:388:LEU:HD22	1.98	0.46
1:G:231:LEU:HD11	1:G:245:VAL:HB	1.97	0.46
1:G:276:TRP:HZ3	1:G:346:CYS:HA	1.81	0.46
1:G:1557:THR:HG22	1:G:1557:THR:O	2.16	0.46
1:G:1934:SER:O	1:G:1938:GLN:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3354:LEU:HB2	1:G:3415:TYR:HE2	1.81	0.46
1:G:3442:PHE:HE1	1:G:3510:ILE:HG22	1.80	0.46
1:G:3568:SER:O	1:G:3571:TRP:NE1	2.49	0.46
1:G:4745:LEU:O	1:G:4748:LEU:HG	2.15	0.46
1:G:4835:LYS:HD3	1:G:4835:LYS:N	2.31	0.46
1:J:157:ARG:HH21	1:J:161:GLU:HB3	1.81	0.46
1:J:1087:ARG:HB3	1:J:1223:PHE:HA	1.98	0.46
1:J:3676:ASP:HA	1:J:3679:LYS:HE2	1.97	0.46
1:J:4745:LEU:O	1:J:4748:LEU:HG	2.15	0.46
1:J:4772:ASP:OD1	1:J:4772:ASP:N	2.49	0.46
2:A:19:GLY:HA2	2:A:49:ARG:HD3	1.97	0.46
2:I:30:LEU:HD12	2:I:36:PHE:HD2	1.79	0.46
3:C:105:ASN:ND2	3:C:108:GLY:H	2.14	0.46
1:B:157:ARG:HH21	1:B:161:GLU:HB3	1.81	0.46
1:B:231:LEU:HD11	1:B:245:VAL:HB	1.97	0.46
1:B:341:TYR:CE2	1:B:392:ARG:HB2	2.50	0.46
1:B:797:HIS:HE1	1:B:1626:TRP:HD1	1.63	0.46
1:B:1708:ARG:O	1:B:1712:TYR:HD1	1.99	0.46
1:B:1862:ILE:HA	1:B:1865:MET:HE3	1.97	0.46
1:B:2389:ASP:OD2	1:B:2392:ARG:NE	2.49	0.46
1:B:2913:ALA:HA	1:B:2916:LYS:HB3	1.97	0.46
1:E:73:LEU:HG	1:E:77:ALA:CB	2.46	0.46
1:E:918:ARG:O	1:E:922:LEU:HG	2.16	0.46
1:E:2624:ARG:HH22	1:E:2912:THR:CG2	2.28	0.46
1:E:2913:ALA:HA	1:E:2916:LYS:HB3	1.97	0.46
1:E:3540:TYR:CZ	1:E:3549:VAL:HG21	2.50	0.46
1:E:3816:MET:O	1:E:3820:LEU:HG	2.15	0.46
1:G:426:ARG:HG3	1:G:431:PRO:HD3	1.97	0.46
1:G:484:LEU:HD11	1:G:540:PHE:CE2	2.51	0.46
1:G:835:ARG:NH2	1:G:1203:ASN:HD22	2.09	0.46
1:G:2584:HIS:O	1:G:2588:ARG:HG3	2.15	0.46
1:G:2624:ARG:HH22	1:G:2912:THR:CG2	2.28	0.46
1:G:2883:HIS:CE1	1:G:2907:PRO:HA	2.51	0.46
1:G:3057:PHE:HB2	1:G:3060:ASP:HB2	1.97	0.46
1:G:3181:THR:O	1:G:3185:LYS:HG2	2.15	0.46
1:G:4700:GLN:OE1	1:G:4703:ARG:NH1	2.49	0.46
1:J:45:ARG:HB2	1:J:137:LEU:HB2	1.97	0.46
1:J:276:TRP:HZ3	1:J:346:CYS:HA	1.81	0.46
1:J:2702:CYS:O	1:J:2706:ILE:HG13	2.16	0.46
1:J:2892:GLN:O	1:J:2895:GLU:HG2	2.16	0.46
1:J:3648:ARG:HG2	1:J:3652:MET:HE1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:4673:ARG:HH12	1:J:4698:LYS:HB2	1.81	0.46
3:M:75:LYS:HE3	3:M:77:THR:OG1	2.16	0.46
1:B:195:PHE:HZ	1:G:2359:ARG:HH11	1.64	0.46
1:B:891:TRP:HA	1:B:902:ARG:HB3	1.97	0.46
1:B:901:LYS:HD3	1:B:903:LEU:HD11	1.98	0.46
1:B:1245:PHE:CD2	1:B:1290:ARG:HG2	2.51	0.46
1:B:1578:ALA:HA	1:B:1584:ARG:NH1	2.31	0.46
1:E:1691:GLN:HE22	1:E:1803:PRO:HD2	1.81	0.46
1:E:3199:ALA:O	1:E:3283:ARG:NE	2.49	0.46
1:E:3367:LYS:O	1:E:3371:LYS:HG2	2.16	0.46
1:E:3592:ILE:HA	1:E:3595:ARG:HE	1.81	0.46
1:E:3980:LEU:CD1	1:E:4030:LEU:HD21	2.46	0.46
1:G:677:ALA:HB1	2:H:40:ARG:HB3	1.98	0.46
1:G:920:TYR:O	1:G:923:GLN:HG2	2.15	0.46
1:G:2389:ASP:OD2	1:G:2392:ARG:NE	2.49	0.46
1:G:2443:ILE:HD12	1:G:2454:ARG:HH11	1.80	0.46
1:G:3199:ALA:O	1:G:3283:ARG:NE	2.49	0.46
1:G:3978:GLN:O	1:G:3982:HIS:ND1	2.49	0.46
1:G:4020:GLN:HG2	1:G:4139:ILE:HD11	1.97	0.46
1:J:1557:THR:HG22	1:J:1557:THR:O	2.16	0.46
1:J:1561:VAL:HG23	1:J:1562:ILE:H	1.81	0.46
1:J:2588:ARG:HA	1:J:2591:ARG:HE	1.81	0.46
1:J:2748:PRO:HB2	1:J:2750:LYS:HG2	1.98	0.46
1:J:3199:ALA:O	1:J:3283:ARG:NE	2.49	0.46
1:J:3568:SER:O	1:J:3571:TRP:NE1	2.49	0.46
1:J:4227:GLU:HA	1:J:4230:LYS:HB2	1.98	0.46
1:J:4835:LYS:HD3	1:J:4835:LYS:N	2.31	0.46
3:C:75:LYS:HE3	3:C:77:THR:OG1	2.16	0.46
3:F:40:ALA:HB3	3:F:43:LYS:HB2	1.98	0.46
3:F:105:ASN:ND2	3:F:108:GLY:H	2.14	0.46
3:K:75:LYS:HE3	3:K:77:THR:OG1	2.16	0.46
1:B:913:LEU:HB3	1:B:917:GLU:CB	2.46	0.45
1:B:1857:GLU:O	1:B:1861:GLN:HG3	2.16	0.45
1:B:2595:LEU:HB2	1:B:2600:ARG:NE	2.25	0.45
1:B:3367:LYS:O	1:B:3371:LYS:HG2	2.16	0.45
1:E:14:LEU:HD21	1:E:204:PRO:HG3	1.98	0.45
1:E:1087:ARG:HB3	1:E:1223:PHE:HA	1.98	0.45
1:E:1245:PHE:CD2	1:E:1290:ARG:HG2	2.50	0.45
1:E:1561:VAL:HG23	1:E:1562:ILE:H	1.81	0.45
1:E:1857:GLU:O	1:E:1861:GLN:HG3	2.16	0.45
1:E:2325:PRO:HB2	1:E:2421:ALA:HB1	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2610:LEU:O	1:E:2614:ILE:HG12	2.16	0.45
1:E:2748:PRO:HB2	1:E:2750:LYS:HG2	1.98	0.45
1:E:4661:TYR:OH	1:E:4786:ASP:OD2	2.30	0.45
1:E:4835:LYS:HD3	1:E:4835:LYS:N	2.31	0.45
1:G:901:LYS:HD3	1:G:903:LEU:HD11	1.98	0.45
1:G:2529:ASP:HB3	1:G:2554:LEU:HD21	1.98	0.45
1:G:2610:LEU:O	1:G:2614:ILE:HG12	2.16	0.45
1:G:2892:GLN:O	1:G:2895:GLU:HG2	2.16	0.45
1:G:2970:SER:HB3	1:G:2998:PHE:CE2	2.51	0.45
1:G:3017:PHE:HB2	1:G:3074:SER:HB2	1.98	0.45
1:J:73:LEU:HG	1:J:77:ALA:CB	2.46	0.45
1:J:920:TYR:O	1:J:923:GLN:HG2	2.16	0.45
1:J:1258:ALA:HB3	1:J:1271:ARG:HB3	1.96	0.45
1:J:2211:MET:HA	1:J:2214:VAL:HG12	1.98	0.45
1:J:2389:ASP:OD2	1:J:2392:ARG:NE	2.49	0.45
1:J:2913:ALA:HA	1:J:2916:LYS:HB3	1.97	0.45
1:J:3017:PHE:HB2	1:J:3074:SER:HB2	1.98	0.45
1:J:3727:ASP:HB3	1:J:3731:LYS:HZ1	1.80	0.45
1:J:3996:PHE:O	1:J:4000:MET:HG3	2.16	0.45
1:B:224:HIS:HA	1:B:388:LEU:HD22	1.98	0.45
1:B:426:ARG:HG3	1:B:431:PRO:HD3	1.97	0.45
1:B:1619:ARG:HA	1:B:1626:TRP:HA	1.97	0.45
1:B:1699:GLU:HG3	1:B:1810:LYS:HZ2	1.81	0.45
1:B:2707:ALA:HB1	1:B:3009:TYR:HD1	1.81	0.45
1:B:2965:ARG:HA	1:B:2968:ASP:OD2	2.16	0.45
1:B:2970:SER:HB3	1:B:2998:PHE:CE2	2.51	0.45
1:B:3592:ILE:HA	1:B:3595:ARG:HE	1.81	0.45
1:E:157:ARG:HH21	1:E:161:GLU:HB3	1.81	0.45
1:E:231:LEU:HD11	1:E:245:VAL:HB	1.97	0.45
1:E:484:LEU:HD11	1:E:540:PHE:CE2	2.51	0.45
1:E:1578:ALA:HA	1:E:1584:ARG:NH1	2.31	0.45
1:E:1814:MET:HA	1:E:1817:GLU:HG2	1.97	0.45
1:E:2359:ARG:HH11	1:J:195:PHE:HZ	1.64	0.45
1:E:2803:GLU:HA	1:E:2806:ARG:HE	1.81	0.45
1:E:2892:GLN:O	1:E:2895:GLU:HG2	2.16	0.45
1:E:2965:ARG:HA	1:E:2968:ASP:OD2	2.16	0.45
1:E:3057:PHE:HB2	1:E:3060:ASP:HB2	1.97	0.45
1:E:4647:SER:HG	1:E:4809:PHE:HZ	1.64	0.45
1:G:1005:TRP:HE3	1:G:1021:LEU:HD11	1.80	0.45
1:G:2509:VAL:HG23	1:G:2510:TYR:H	1.79	0.45
1:G:3003:LEU:HB2	1:G:3004:PRO:HD3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3592:ILE:HA	1:G:3595:ARG:HE	1.81	0.45
1:J:14:LEU:HD21	1:J:204:PRO:HG3	1.98	0.45
1:J:677:ALA:HB1	2:I:40:ARG:HB3	1.98	0.45
1:J:2584:HIS:O	1:J:2588:ARG:HG3	2.15	0.45
1:J:2707:ALA:HB1	1:J:3009:TYR:HD1	1.81	0.45
1:J:3354:LEU:HB2	1:J:3415:TYR:HE2	1.81	0.45
1:J:3699:HIS:HA	1:J:3702:VAL:HG22	1.97	0.45
1:J:3978:GLN:O	1:J:3982:HIS:ND1	2.49	0.45
3:K:94:TYR:CD1	3:K:120:GLY:HA3	2.50	0.45
1:B:73:LEU:HG	1:B:77:ALA:CB	2.46	0.45
1:B:484:LEU:HD11	1:B:540:PHE:CE2	2.51	0.45
1:B:918:ARG:O	1:B:922:LEU:HG	2.16	0.45
1:B:1561:VAL:HG23	1:B:1562:ILE:N	2.31	0.45
1:B:1934:SER:O	1:B:1938:GLN:HG2	2.16	0.45
1:B:2132:GLY:O	1:B:2136:ARG:HG3	2.16	0.45
1:B:2281:ILE:HG12	1:B:2282:ASP:OD1	2.17	0.45
1:B:3978:GLN:O	1:B:3982:HIS:ND1	2.49	0.45
1:E:45:ARG:HB2	1:E:137:LEU:HB2	1.97	0.45
1:E:2957:PHE:HE1	1:E:2961:GLN:HE21	1.64	0.45
1:E:3727:ASP:HB3	1:E:3731:LYS:HZ1	1.81	0.45
1:E:4679:ARG:NH1	1:E:5017:ARG:HD2	2.31	0.45
1:E:4992:LEU:O	1:E:4996:ILE:HG13	2.16	0.45
1:G:40:GLU:O	1:G:114:SER:OG	2.32	0.45
1:G:913:LEU:HB3	1:G:917:GLU:CB	2.46	0.45
1:G:977:LEU:HD12	1:G:1044:ARG:HD3	1.97	0.45
1:G:1561:VAL:HG23	1:G:1562:ILE:N	2.31	0.45
1:G:2803:GLU:HA	1:G:2806:ARG:HE	1.81	0.45
1:G:4922:PHE:O	1:G:4927:ILE:HG12	2.17	0.45
1:J:360:ALA:HA	1:J:377:ILE:CD1	2.47	0.45
1:J:379:HIS:ND1	1:J:381:GLU:HG2	2.31	0.45
1:J:484:LEU:HD11	1:J:540:PHE:CE2	2.51	0.45
1:J:2803:GLU:HA	1:J:2806:ARG:HE	1.81	0.45
1:J:2883:HIS:CE1	1:J:2907:PRO:HA	2.51	0.45
1:J:4222:VAL:HB	1:J:4950:VAL:HG13	1.98	0.45
1:J:4700:GLN:OE1	1:J:4703:ARG:NH1	2.49	0.45
3:F:75:LYS:HE3	3:F:77:THR:OG1	2.16	0.45
3:K:101:PRO:HD2	3:K:104:TYR:O	2.16	0.45
3:M:40:ALA:HB3	3:M:43:LYS:HB2	1.99	0.45
3:M:101:PRO:HD2	3:M:104:TYR:O	2.17	0.45
1:B:360:ALA:HA	1:B:377:ILE:CD1	2.47	0.45
1:B:2610:LEU:O	1:B:2614:ILE:HG12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2624:ARG:HB3	1:B:2674:LEU:HD13	1.98	0.45
1:B:2751:LEU:HD12	1:B:2823:ILE:HD11	1.98	0.45
1:B:2803:GLU:HA	1:B:2806:ARG:HE	1.81	0.45
1:B:3003:LEU:HB2	1:B:3004:PRO:HD3	1.97	0.45
1:B:3199:ALA:O	1:B:3283:ARG:NE	2.49	0.45
1:B:4234:PHE:CE1	1:B:4985:LEU:HG	2.52	0.45
1:B:4673:ARG:HH12	1:B:4698:LYS:HB2	1.81	0.45
1:B:4700:GLN:OE1	1:B:4703:ARG:NH1	2.49	0.45
1:E:2132:GLY:O	1:E:2136:ARG:HG3	2.16	0.45
1:E:2292:GLU:OE1	1:E:2292:GLU:N	2.42	0.45
1:E:4105:GLY:O	1:E:4109:GLN:HG2	2.16	0.45
1:G:1477:GLY:HA2	1:G:1483:VAL:HA	1.98	0.45
1:G:2906:VAL:HG23	1:G:2911:LEU:HB3	1.97	0.45
1:G:3284:TRP:HZ3	1:G:3304:CYS:HG	1.61	0.45
1:G:4779:LYS:HA	1:G:4782:VAL:HG22	1.98	0.45
1:J:977:LEU:HD12	1:J:1044:ARG:HD3	1.97	0.45
1:J:1708:ARG:O	1:J:1712:TYR:HD1	1.99	0.45
1:J:1814:MET:HA	1:J:1817:GLU:HG2	1.97	0.45
1:J:2624:ARG:HB3	1:J:2674:LEU:HD13	1.98	0.45
1:J:2794:TYR:HE1	1:J:2802:LYS:HE2	1.81	0.45
1:J:3775:ALA:HA	1:J:3778:MET:HG3	1.98	0.45
1:J:4001:MET:SD	1:J:4002:LYS:N	2.90	0.45
1:J:4661:TYR:OH	1:J:4786:ASP:OD2	2.30	0.45
2:H:19:GLY:HA2	2:H:49:ARG:HD3	1.97	0.45
1:B:379:HIS:ND1	1:B:381:GLU:HG2	2.31	0.45
1:B:1043:VAL:O	1:B:1047:LEU:HG	2.17	0.45
1:B:1561:VAL:HG23	1:B:1562:ILE:H	1.81	0.45
1:B:2794:TYR:HE1	1:B:2802:LYS:HE2	1.81	0.45
1:B:4992:LEU:O	1:B:4996:ILE:HG13	2.16	0.45
1:E:1557:THR:O	1:E:1557:THR:HG22	2.16	0.45
1:E:1712:TYR:O	1:E:1716:ILE:HG13	2.16	0.45
1:E:2794:TYR:HE1	1:E:2802:LYS:HE2	1.82	0.45
1:E:3978:GLN:O	1:E:3982:HIS:ND1	2.49	0.45
1:E:4222:VAL:HB	1:E:4950:VAL:HG13	1.98	0.45
1:E:4227:GLU:HA	1:E:4230:LYS:HB2	1.98	0.45
1:E:4813:LEU:O	1:E:4816:ILE:HG12	2.17	0.45
1:G:918:ARG:O	1:G:922:LEU:HG	2.16	0.45
1:G:1043:VAL:O	1:G:1047:LEU:HG	2.17	0.45
1:G:1623:ARG:HA	1:G:1623:ARG:NH1	2.32	0.45
1:G:3527:PRO:HB2	1:G:3573:MET:SD	2.57	0.45
1:G:3752:SER:O	1:G:3756:LYS:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3775:ALA:HA	1:G:3778:MET:HG3	1.98	0.45
1:G:4222:VAL:HB	1:G:4950:VAL:HG13	1.98	0.45
1:J:901:LYS:HD3	1:J:903:LEU:HD11	1.98	0.45
1:J:1043:VAL:O	1:J:1047:LEU:HG	2.17	0.45
1:J:1857:GLU:O	1:J:1861:GLN:HG3	2.16	0.45
1:J:2965:ARG:HA	1:J:2968:ASP:OD2	2.16	0.45
1:J:3592:ILE:HA	1:J:3595:ARG:HE	1.81	0.45
3:F:15:GLY:H	3:F:85:LEU:HB2	1.80	0.45
3:F:101:PRO:HD2	3:F:104:TYR:O	2.17	0.45
1:B:2443:ILE:HD12	1:B:2454:ARG:HH11	1.80	0.45
1:B:2957:PHE:HE1	1:B:2961:GLN:HE21	1.64	0.45
1:B:3457:ASN:OD1	1:B:3458:PHE:N	2.50	0.45
1:B:3648:ARG:HG2	1:B:3652:MET:CE	2.47	0.45
1:E:1619:ARG:HA	1:E:1626:TRP:HA	1.97	0.45
1:E:1623:ARG:NH1	1:E:1623:ARG:HA	2.32	0.45
1:E:1730:MET:O	1:E:1733:GLU:HG2	2.17	0.45
1:E:3511:VAL:HG22	1:E:3516:LYS:NZ	2.31	0.45
1:E:3648:ARG:HG2	1:E:3652:MET:CE	2.47	0.45
1:E:3752:SER:O	1:E:3756:LYS:HG3	2.16	0.45
1:E:3935:TRP:NE1	1:J:80:GLU:OE1	2.33	0.45
1:G:14:LEU:HD21	1:G:204:PRO:HG3	1.98	0.45
1:G:73:LEU:HG	1:G:77:ALA:CB	2.46	0.45
1:G:603:LEU:HA	1:G:606:LEU:HD12	1.99	0.45
1:G:924:MET:HE1	3:M:106:PRO:HD2	1.99	0.45
1:G:996:TRP:NE1	3:M:113:GLU:HB3	2.32	0.45
1:G:1708:ARG:O	1:G:1712:TYR:HD1	1.99	0.45
1:G:2619:LEU:HG	1:G:2623:LEU:HG	1.98	0.45
1:G:2965:ARG:HA	1:G:2968:ASP:OD2	2.16	0.45
1:G:3906:GLN:HB2	1:G:3912:THR:HA	1.99	0.45
1:J:2529:ASP:HB3	1:J:2554:LEU:HD21	1.98	0.45
1:J:4105:GLY:O	1:J:4109:GLN:HG2	2.16	0.45
1:J:4780:PHE:HA	1:J:4783:ILE:HG22	1.99	0.45
3:M:99:ARG:HD2	3:M:114:TYR:CD2	2.52	0.45
1:B:1623:ARG:NH1	1:B:1623:ARG:HA	2.32	0.45
1:B:2211:MET:HA	1:B:2214:VAL:HG12	1.98	0.45
1:B:2355:ARG:HD3	1:B:2358:ILE:HD11	1.98	0.45
1:B:2359:ARG:HH11	1:E:195:PHE:HZ	1.64	0.45
1:B:2588:ARG:HA	1:B:2591:ARG:HE	1.81	0.45
1:B:2619:LEU:HG	1:B:2623:LEU:HG	1.98	0.45
1:B:2702:CYS:O	1:B:2706:ILE:HG13	2.16	0.45
1:B:3181:THR:O	1:B:3185:LYS:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4679:ARG:NH1	1:B:5017:ARG:HD2	2.31	0.45
1:E:426:ARG:HG3	1:E:431:PRO:HD3	1.97	0.45
1:E:2667:THR:HG23	1:E:2672:LEU:HD11	1.99	0.45
1:E:2751:LEU:HD12	1:E:2823:ILE:HD11	1.98	0.45
1:G:850:ASP:OD1	1:G:1025:ARG:NH2	2.44	0.45
1:G:1493:TYR:HB3	1:G:1540:PHE:CD2	2.52	0.45
1:G:1857:GLU:O	1:G:1861:GLN:HG3	2.16	0.45
1:G:2858:GLN:HB2	1:G:2859:PRO:HD3	1.99	0.45
1:G:3699:HIS:HA	1:G:3702:VAL:HG22	1.97	0.45
1:G:4227:GLU:HA	1:G:4230:LYS:HB2	1.98	0.45
1:G:4679:ARG:NH1	1:G:5017:ARG:HD2	2.31	0.45
1:G:4813:LEU:O	1:G:4816:ILE:HG12	2.17	0.45
1:J:426:ARG:HG3	1:J:431:PRO:HD3	1.97	0.45
1:J:917:GLU:OE2	3:K:101:PRO:HB2	2.16	0.45
1:J:920:TYR:CG	3:K:101:PRO:HG3	2.52	0.45
1:J:2132:GLY:O	1:J:2136:ARG:HG3	2.16	0.45
1:J:2751:LEU:HD12	1:J:2823:ILE:HD11	1.98	0.45
1:J:3384:LYS:HG2	1:J:3386:GLU:H	1.82	0.45
1:J:4992:LEU:O	1:J:4996:ILE:HG13	2.16	0.45
1:B:996:TRP:NE1	3:C:113:GLU:HB3	2.32	0.45
1:B:1712:TYR:O	1:B:1716:ILE:HG13	2.16	0.45
1:B:2624:ARG:HH22	1:B:2912:THR:CG2	2.28	0.45
1:B:3245:VAL:HG13	1:B:3248:ARG:H	1.82	0.45
1:B:4927:ILE:HD12	1:G:4936:ILE:HD13	1.97	0.45
1:E:1741:GLU:O	1:E:1745:ILE:HG13	2.15	0.45
1:E:2702:CYS:O	1:E:2706:ILE:HG13	2.16	0.45
1:E:3527:PRO:HB2	1:E:3573:MET:SD	2.57	0.45
1:E:3924:LEU:HD21	1:E:3984:ARG:HH21	1.81	0.45
1:E:4922:PHE:O	1:E:4927:ILE:HG12	2.17	0.45
1:G:844:ARG:HH12	1:G:1071:ARG:HH21	1.63	0.45
1:G:870:ILE:HB	1:G:1051:TYR:OH	2.17	0.45
1:G:1008:SER:HB2	1:G:1017:ARG:NE	2.28	0.45
1:G:1712:TYR:O	1:G:1716:ILE:HG13	2.16	0.45
1:G:2281:ILE:HG12	1:G:2282:ASP:OD1	2.17	0.45
1:G:2667:THR:HG23	1:G:2672:LEU:HD11	1.99	0.45
1:G:2748:PRO:HB2	1:G:2750:LYS:HG2	1.98	0.45
1:G:2794:TYR:HE1	1:G:2802:LYS:HE2	1.82	0.45
1:G:2827:ARG:NE	1:G:2935:TYR:OH	2.27	0.45
1:G:4780:PHE:HA	1:G:4783:ILE:HG22	1.99	0.45
1:J:603:LEU:HA	1:J:606:LEU:HD12	1.99	0.45
1:J:1477:GLY:HA2	1:J:1483:VAL:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1493:TYR:HB3	1:J:1540:PHE:CD2	2.52	0.45
1:J:1578:ALA:HA	1:J:1584:ARG:NH1	2.31	0.45
1:J:3245:VAL:HG13	1:J:3248:ARG:H	1.82	0.45
1:J:3527:PRO:HB2	1:J:3573:MET:SD	2.57	0.45
1:J:3674:ILE:HG13	1:J:3732:SER:HB3	1.99	0.45
1:J:3906:GLN:HB2	1:J:3912:THR:HA	1.99	0.45
1:J:3924:LEU:HD21	1:J:3984:ARG:HH21	1.81	0.45
1:J:4234:PHE:CE1	1:J:4985:LEU:HG	2.52	0.45
1:J:4813:LEU:O	1:J:4816:ILE:HG12	2.17	0.45
1:B:850:ASP:OD1	1:B:1025:ARG:NH2	2.44	0.45
1:B:1477:GLY:HA2	1:B:1483:VAL:HA	1.98	0.45
1:B:1569:GLN:HB2	1:B:1572:ILE:HD12	1.99	0.45
1:B:2499:LYS:O	1:B:2503:VAL:HG12	2.17	0.45
1:B:4227:GLU:HA	1:B:4230:LYS:HB2	1.98	0.45
1:E:363:ASP:HB3	1:E:366:ALA:HB3	1.98	0.45
1:E:603:LEU:HA	1:E:606:LEU:HD12	1.99	0.45
1:E:2502:MET:SD	1:E:2503:VAL:N	2.90	0.45
1:E:3934:TYR:OH	1:E:3998:HIS:HB3	2.17	0.45
1:G:39:ALA:O	1:G:111:HIS:NE2	2.50	0.45
1:G:371:VAL:HG12	1:G:373:LYS:HB2	1.99	0.45
1:G:1561:VAL:HG23	1:G:1562:ILE:H	1.81	0.45
1:G:2499:LYS:O	1:G:2503:VAL:HG12	2.17	0.45
1:G:2707:ALA:HB1	1:G:3009:TYR:HD1	1.81	0.45
1:G:2994:GLU:O	1:G:2998:PHE:HD1	2.00	0.45
1:J:224:HIS:HA	1:J:388:LEU:HD22	1.98	0.45
1:J:913:LEU:HB3	1:J:917:GLU:CB	2.46	0.45
1:J:1620:ALA:HB3	1:J:1624:LEU:HB2	1.99	0.45
1:J:2499:LYS:O	1:J:2503:VAL:HG12	2.17	0.45
1:J:2906:VAL:HG23	1:J:2911:LEU:HB3	1.97	0.45
1:J:3648:ARG:HG2	1:J:3652:MET:CE	2.47	0.45
1:J:4679:ARG:NH1	1:J:5017:ARG:HD2	2.31	0.45
1:B:844:ARG:HH12	1:B:1071:ARG:HH21	1.63	0.45
1:B:870:ILE:HB	1:B:1051:TYR:OH	2.17	0.45
1:B:926:GLY:O	1:B:930:LYS:HG3	2.17	0.45
1:B:1087:ARG:HB3	1:B:1223:PHE:HA	1.98	0.45
1:B:1095:VAL:O	1:B:1145:SER:OG	2.25	0.45
1:B:2858:GLN:HB2	1:B:2859:PRO:HD3	1.99	0.45
1:B:3395:ARG:HG2	1:B:3450:ASN:OD1	2.17	0.45
1:B:3775:ALA:HA	1:B:3778:MET:HG3	1.98	0.45
1:B:4813:LEU:O	1:B:4816:ILE:HG12	2.17	0.45
1:B:4822:THR:O	1:B:4826:ILE:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4922:PHE:O	1:B:4927:ILE:HG12	2.17	0.45
1:E:996:TRP:NE1	3:F:113:GLU:HB3	2.32	0.45
1:E:2281:ILE:HG12	1:E:2282:ASP:OD1	2.17	0.45
1:E:2883:HIS:CE1	1:E:2907:PRO:HA	2.51	0.45
1:E:4780:PHE:HA	1:E:4783:ILE:HG22	1.99	0.45
1:G:379:HIS:ND1	1:G:381:GLU:HG2	2.31	0.45
1:G:1043:VAL:HA	1:G:1046:LEU:HG	1.99	0.45
1:G:1087:ARG:HB3	1:G:1223:PHE:HA	1.98	0.45
1:G:1569:GLN:HB2	1:G:1572:ILE:HD12	1.99	0.45
1:G:2694:GLU:O	1:G:2698:MET:HG3	2.17	0.45
1:G:3648:ARG:HG2	1:G:3652:MET:CE	2.47	0.45
1:G:3674:ILE:HG13	1:G:3732:SER:HB3	1.99	0.45
1:G:4673:ARG:HH12	1:G:4698:LYS:HB2	1.81	0.45
1:G:4772:ASP:OD1	1:G:4772:ASP:N	2.49	0.45
1:J:1154:ASP:HB3	1:J:1223:PHE:CE1	2.52	0.45
1:J:2694:GLU:O	1:J:2698:MET:HG3	2.17	0.45
1:J:3457:ASN:OD1	1:J:3458:PHE:N	2.50	0.45
1:B:603:LEU:HA	1:B:606:LEU:HD12	1.99	0.44
1:B:2502:MET:SD	1:B:2503:VAL:N	2.90	0.44
1:B:2823:ILE:O	1:B:2825:LYS:NZ	2.49	0.44
1:B:3980:LEU:CD1	1:B:4030:LEU:HD21	2.46	0.44
1:E:224:HIS:HA	1:E:388:LEU:HD22	1.98	0.44
1:E:1205:GLY:HA3	1:E:1225:PRO:HB2	1.99	0.44
1:E:1862:ILE:HA	1:E:1865:MET:HE3	1.99	0.44
1:E:3187:ARG:HD3	1:E:3271:GLU:HG3	1.99	0.44
1:E:3457:ASN:OD1	1:E:3458:PHE:N	2.50	0.44
1:G:2957:PHE:HE2	1:G:3034:LYS:HG3	1.82	0.44
1:G:3457:ASN:OD1	1:G:3458:PHE:N	2.50	0.44
1:J:1623:ARG:NH1	1:J:1623:ARG:HA	2.32	0.44
1:J:1712:TYR:O	1:J:1716:ILE:HG13	2.16	0.44
1:J:1730:MET:O	1:J:1733:GLU:HG2	2.17	0.44
1:J:2624:ARG:HH22	1:J:2912:THR:CG2	2.28	0.44
1:J:3187:ARG:HD3	1:J:3271:GLU:HG3	1.99	0.44
1:J:3752:SER:O	1:J:3756:LYS:HG3	2.16	0.44
3:M:105:ASN:ND2	3:M:108:GLY:H	2.14	0.44
1:B:1557:THR:HG22	1:B:1557:THR:O	2.16	0.44
1:B:2994:GLU:O	1:B:2998:PHE:HD1	2.00	0.44
1:B:3510:ILE:O	1:B:3514:LEU:HD23	2.17	0.44
1:B:4001:MET:SD	1:B:4002:LYS:N	2.90	0.44
1:B:4779:LYS:HA	1:B:4782:VAL:HG22	1.98	0.44
1:E:677:ALA:HB1	2:D:40:ARG:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:917:GLU:OE2	3:F:101:PRO:HB2	2.17	0.44
1:E:1154:ASP:HB3	1:E:1223:PHE:CE1	2.52	0.44
1:E:2858:GLN:HB2	1:E:2859:PRO:HD3	1.99	0.44
1:E:3284:TRP:HA	1:E:3287:ARG:HD3	2.00	0.44
1:E:3384:LYS:HG2	1:E:3386:GLU:H	1.82	0.44
1:E:3775:ALA:HA	1:E:3778:MET:HG3	1.98	0.44
1:E:4001:MET:SD	1:E:4002:LYS:N	2.90	0.44
1:G:475:GLN:HB3	1:G:533:ASN:HD22	1.82	0.44
1:G:2978:GLU:OE1	1:G:3053:ARG:NH1	2.51	0.44
1:G:3384:LYS:HG2	1:G:3386:GLU:H	1.82	0.44
1:G:3395:ARG:HG2	1:G:3450:ASN:OD1	2.17	0.44
1:G:3944:GLU:O	1:G:3948:LYS:HG3	2.17	0.44
1:J:1042:ALA:O	1:J:1045:THR:OG1	2.22	0.44
1:J:1043:VAL:HA	1:J:1046:LEU:HG	1.99	0.44
1:J:1431:THR:HG21	1:J:1523:ALA:HB2	1.99	0.44
1:J:2292:GLU:OE1	1:J:2292:GLU:N	2.42	0.44
1:J:2502:MET:SD	1:J:2503:VAL:N	2.90	0.44
1:J:2667:THR:HG23	1:J:2672:LEU:HD11	1.99	0.44
3:C:101:PRO:HD2	3:C:104:TYR:O	2.17	0.44
1:B:40:GLU:O	1:B:114:SER:OG	2.32	0.44
1:B:815:VAL:O	1:B:1007:TYR:OH	2.24	0.44
1:B:1008:SER:HB2	1:B:1017:ARG:NE	2.28	0.44
1:B:1205:GLY:HA3	1:B:1225:PRO:HB2	1.99	0.44
1:B:1620:ALA:HB3	1:B:1624:LEU:HB2	1.99	0.44
1:B:1782:PHE:HB2	2:A:37:ASP:OD2	2.18	0.44
1:B:1808:ARG:NH1	1:B:1853:ILE:O	2.49	0.44
1:B:2667:THR:HG23	1:B:2672:LEU:HD11	1.99	0.44
1:B:2957:PHE:HE2	1:B:3034:LYS:HG3	1.82	0.44
1:B:3046:LEU:HD11	1:B:3064:VAL:HG13	2.00	0.44
1:B:3527:PRO:HB2	1:B:3573:MET:SD	2.57	0.44
1:B:3934:TYR:OH	1:B:3998:HIS:HB3	2.17	0.44
1:E:39:ALA:O	1:E:111:HIS:NE2	2.50	0.44
1:E:206:CYS:HB2	1:E:271:GLY:O	2.17	0.44
1:E:870:ILE:HB	1:E:1051:TYR:OH	2.17	0.44
1:E:1493:TYR:HB3	1:E:1540:PHE:CD2	2.52	0.44
1:E:2619:LEU:HG	1:E:2623:LEU:HG	1.98	0.44
1:E:3354:LEU:HB2	1:E:3415:TYR:HE2	1.81	0.44
1:E:3395:ARG:HG2	1:E:3450:ASN:OD1	2.18	0.44
1:G:2142:TYR:CE2	1:G:2197:LEU:HB2	2.52	0.44
1:G:2336:ARG:HB2	1:G:2435:ARG:HD2	1.99	0.44
1:G:2355:ARG:HD3	1:G:2358:ILE:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2595:LEU:HB2	1:G:2600:ARG:NE	2.25	0.44
1:G:4001:MET:SD	1:G:4002:LYS:N	2.90	0.44
1:G:4822:THR:O	1:G:4826:ILE:HG13	2.17	0.44
1:J:926:GLY:O	1:J:930:LYS:HG3	2.18	0.44
1:J:2355:ARG:HD3	1:J:2358:ILE:HD11	1.98	0.44
1:J:2970:SER:HB3	1:J:2998:PHE:CE2	2.51	0.44
1:J:3284:TRP:HA	1:J:3287:ARG:HD3	2.00	0.44
1:J:3510:ILE:O	1:J:3514:LEU:HD23	2.18	0.44
1:B:14:LEU:HD21	1:B:204:PRO:HG3	1.98	0.44
1:B:39:ALA:O	1:B:111:HIS:NE2	2.50	0.44
1:B:467:LYS:HE3	1:B:467:LYS:HB3	1.87	0.44
1:B:1493:TYR:HB3	1:B:1540:PHE:CD2	2.52	0.44
1:B:1730:MET:O	1:B:1733:GLU:HG2	2.17	0.44
1:B:4222:VAL:HB	1:B:4950:VAL:HG13	1.98	0.44
1:E:835:ARG:NH2	1:E:1203:ASN:HD22	2.09	0.44
1:E:1861:GLN:O	1:E:1865:MET:HE2	2.17	0.44
1:E:2367:ALA:HB3	1:E:2426:TYR:CE1	2.53	0.44
1:E:2499:LYS:O	1:E:2503:VAL:HG12	2.17	0.44
1:E:2694:GLU:O	1:E:2698:MET:HG3	2.17	0.44
1:E:3046:LEU:HD11	1:E:3064:VAL:HG13	2.00	0.44
1:E:3206:LEU:HD12	1:E:3280:TYR:CD2	2.53	0.44
1:E:4234:PHE:CE1	1:E:4985:LEU:HG	2.52	0.44
1:G:360:ALA:HA	1:G:377:ILE:CD1	2.46	0.44
1:G:1154:ASP:HB3	1:G:1223:PHE:CE1	2.52	0.44
1:G:2211:MET:HA	1:G:2214:VAL:HG12	1.98	0.44
1:G:3051:ARG:HH22	1:G:3102:ASP:HB2	1.83	0.44
1:G:3245:VAL:HG13	1:G:3248:ARG:H	1.82	0.44
1:J:206:CYS:HB2	1:J:271:GLY:O	2.17	0.44
1:J:2142:TYR:CE2	1:J:2197:LEU:HB2	2.52	0.44
1:J:2281:ILE:HG12	1:J:2282:ASP:OD1	2.17	0.44
1:J:2994:GLU:O	1:J:2998:PHE:HD1	2.00	0.44
1:J:4822:THR:O	1:J:4826:ILE:HG13	2.17	0.44
1:J:4996:ILE:HD13	6:J:5103:CFF:C8	2.48	0.44
3:C:40:ALA:HB3	3:C:43:LYS:HB2	1.99	0.44
3:M:36:TRP:HB2	3:M:48:VAL:HB	1.99	0.44
1:B:206:CYS:HB2	1:B:271:GLY:O	2.17	0.44
1:B:1154:ASP:HB3	1:B:1223:PHE:CE1	2.53	0.44
1:B:1438:ARG:HG3	1:B:1513:ASP:HB3	2.00	0.44
1:E:874:LEU:O	1:E:878:ILE:HG12	2.18	0.44
1:E:1215:ALA:HA	1:E:1219:LEU:HB3	2.00	0.44
1:E:3017:PHE:HB2	1:E:3074:SER:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:206:CYS:HB2	1:G:271:GLY:O	2.17	0.44
1:G:926:GLY:O	1:G:930:LYS:HG3	2.17	0.44
1:G:1620:ALA:HB3	1:G:1624:LEU:HB2	1.99	0.44
1:G:2132:GLY:O	1:G:2136:ARG:HG3	2.16	0.44
1:G:3206:LEU:HD12	1:G:3280:TYR:CD2	2.53	0.44
1:G:3924:LEU:HD21	1:G:3984:ARG:HH21	1.81	0.44
1:G:4242:ILE:HD12	6:G:5103:CFF:H141	1.99	0.44
1:J:2367:ALA:HB3	1:J:2426:TYR:CE1	2.53	0.44
1:J:2858:GLN:HB2	1:J:2859:PRO:HD3	1.99	0.44
3:F:36:TRP:HB2	3:F:48:VAL:HB	1.99	0.44
1:B:475:GLN:HB3	1:B:533:ASN:HD22	1.82	0.44
1:B:920:TYR:CG	3:C:101:PRO:HG3	2.53	0.44
1:B:1814:MET:SD	1:B:1841:VAL:HG13	2.58	0.44
1:B:3089:LYS:O	1:B:3092:LEU:HG	2.18	0.44
1:B:3674:ILE:HG13	1:B:3732:SER:HB3	1.99	0.44
1:E:901:LYS:HD3	1:E:903:LEU:HD11	1.98	0.44
1:E:1431:THR:HG21	1:E:1523:ALA:HB2	1.99	0.44
1:E:2211:MET:HA	1:E:2214:VAL:HG12	1.98	0.44
1:E:2994:GLU:O	1:E:2998:PHE:HD1	2.00	0.44
1:E:3046:LEU:HD23	1:E:3071:LEU:HD12	2.00	0.44
1:E:4247:ILE:O	1:E:4251:ILE:HG13	2.18	0.44
1:E:4822:THR:O	1:E:4826:ILE:HG13	2.17	0.44
1:G:40:GLU:HG2	1:G:42:PHE:H	1.83	0.44
1:G:874:LEU:O	1:G:878:ILE:HG12	2.18	0.44
1:G:2751:LEU:HD12	1:G:2823:ILE:HD11	1.98	0.44
1:G:3923:LEU:HD11	1:G:3962:PHE:CE1	2.53	0.44
1:J:2859:PRO:HB2	1:J:2932:MET:SD	2.58	0.44
1:J:2957:PHE:HE2	1:J:3034:LYS:HG3	1.82	0.44
1:J:3537:LYS:HE2	1:J:3537:LYS:HB3	1.90	0.44
3:K:36:TRP:HB2	3:K:48:VAL:HB	1.99	0.44
3:K:99:ARG:HD2	3:K:114:TYR:CD2	2.53	0.44
3:M:100:VAL:HG22	3:M:105:ASN:HB2	2.00	0.44
1:B:1025:ARG:HG2	1:B:1026:LEU:HD12	2.00	0.44
1:B:2142:TYR:CE2	1:B:2197:LEU:HB2	2.52	0.44
1:B:3384:LYS:HG2	1:B:3386:GLU:H	1.82	0.44
1:E:292:ALA:HB2	1:E:312:THR:HG22	2.00	0.44
1:E:379:HIS:ND1	1:E:381:GLU:HG2	2.31	0.44
1:E:475:GLN:HB3	1:E:533:ASN:HD22	1.82	0.44
1:E:492:ASP:OD1	1:E:546:TRP:NE1	2.44	0.44
1:E:917:GLU:OE1	3:F:101:PRO:HB2	2.17	0.44
1:E:1043:VAL:O	1:E:1047:LEU:HG	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1254:HIS:CD2	1:E:1283:LEU:HG	2.53	0.44
1:E:1438:ARG:HG3	1:E:1513:ASP:HB3	2.00	0.44
1:E:2624:ARG:HB3	1:E:2674:LEU:HD13	1.98	0.44
1:E:2874:MET:HG3	1:E:2937:VAL:CG2	2.48	0.44
1:E:3416:VAL:HG23	1:E:3423:TRP:HZ3	1.83	0.44
1:E:3674:ILE:HG13	1:E:3732:SER:HB3	1.99	0.44
1:G:1076:ARG:HG2	1:G:1605:TRP:CZ3	2.53	0.44
1:G:1215:ALA:HA	1:G:1219:LEU:HB3	2.00	0.44
1:G:2859:PRO:HB2	1:G:2932:MET:SD	2.58	0.44
1:G:4234:PHE:CE1	1:G:4985:LEU:HG	2.52	0.44
1:J:1076:ARG:HG2	1:J:1605:TRP:CZ3	2.53	0.44
1:J:2619:LEU:HG	1:J:2623:LEU:HG	1.98	0.44
1:J:2978:GLU:OE1	1:J:3053:ARG:NH1	2.51	0.44
1:J:3046:LEU:HD11	1:J:3064:VAL:HG13	2.00	0.44
1:J:3051:ARG:HH22	1:J:3102:ASP:HB2	1.82	0.44
3:C:99:ARG:HD2	3:C:114:TYR:CD2	2.52	0.44
3:F:99:ARG:HD2	3:F:114:TYR:CD2	2.52	0.44
1:B:1035:ASN:OD1	3:C:109:THR:OG1	2.36	0.44
1:B:2336:ARG:HB2	1:B:2435:ARG:HD2	1.99	0.44
1:B:2694:GLU:O	1:B:2698:MET:HG3	2.17	0.44
1:B:2874:MET:HG3	1:B:2937:VAL:CG2	2.48	0.44
1:B:3046:LEU:HD23	1:B:3071:LEU:HD12	2.00	0.44
1:B:3284:TRP:HA	1:B:3287:ARG:HD3	2.00	0.44
1:B:3354:LEU:HB2	1:B:3415:TYR:HE2	1.81	0.44
1:B:3955:MET:CE	1:B:4015:GLU:HG2	2.48	0.44
1:E:926:GLY:O	1:E:930:LYS:HG3	2.18	0.44
1:E:1786:LEU:HD22	2:D:87:HIS:CD2	2.52	0.44
1:E:2182:ILE:O	1:E:2186:MET:HG3	2.18	0.44
1:E:2957:PHE:HE2	1:E:3034:LYS:HG3	1.82	0.44
1:E:4996:ILE:HD13	6:E:5103:CFF:C8	2.48	0.44
1:G:871:ARG:NH1	1:G:922:LEU:HD22	2.33	0.44
1:G:917:GLU:OE2	3:M:101:PRO:HB2	2.17	0.44
1:G:3187:ARG:HD3	1:G:3271:GLU:HG3	1.99	0.44
1:G:3233:PRO:HD2	1:G:3239:MET:SD	2.58	0.44
1:G:3962:PHE:O	1:G:3966:THR:HG23	2.18	0.44
1:J:516:LYS:HB2	1:J:516:LYS:HE2	1.82	0.44
1:J:870:ILE:HB	1:J:1051:TYR:OH	2.17	0.44
1:J:871:ARG:NH1	1:J:922:LEU:HD22	2.33	0.44
1:J:1438:ARG:HG3	1:J:1513:ASP:HB3	2.00	0.44
1:J:2336:ARG:HB2	1:J:2435:ARG:HD2	1.99	0.44
1:J:2788:HIS:HE1	1:J:2790:MET:HB2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:3089:LYS:O	1:J:3092:LEU:HG	2.18	0.44
1:J:3204:ALA:HB2	1:J:3304:CYS:SG	2.58	0.44
1:J:3934:TYR:OH	1:J:3998:HIS:HB3	2.17	0.44
1:J:4003:LEU:HB2	1:J:4013:LEU:HD13	2.00	0.44
3:C:36:TRP:HB2	3:C:48:VAL:HB	1.99	0.44
1:B:118:LEU:HA	1:B:137:LEU:HD23	2.00	0.44
1:B:835:ARG:NH2	1:B:1203:ASN:HD22	2.09	0.44
1:B:2367:ALA:HB3	1:B:2426:TYR:CE1	2.53	0.44
1:B:3104:GLU:O	1:B:3107:VAL:HG22	2.18	0.44
1:B:3206:LEU:HD12	1:B:3280:TYR:CD2	2.53	0.44
1:B:3416:VAL:HG23	1:B:3423:TRP:HZ3	1.83	0.44
1:B:3924:LEU:HD21	1:B:3984:ARG:HH21	1.81	0.44
1:B:3944:GLU:O	1:B:3948:LYS:HG3	2.17	0.44
1:E:913:LEU:HB3	1:E:917:GLU:CB	2.46	0.44
1:E:1515:VAL:HB	1:E:1532:ASN:HA	2.00	0.44
1:E:2978:GLU:OE1	1:E:3053:ARG:NH1	2.51	0.44
1:G:118:LEU:HA	1:G:137:LEU:HD23	2.00	0.44
1:G:195:PHE:HZ	1:J:2359:ARG:HH11	1.65	0.44
1:G:411:TYR:HB2	1:G:486:LEU:HD21	2.00	0.44
1:G:3089:LYS:O	1:G:3092:LEU:HG	2.18	0.44
1:G:3510:ILE:O	1:G:3514:LEU:HD23	2.18	0.44
1:G:4247:ILE:O	1:G:4251:ILE:HG13	2.18	0.44
1:G:4865:LYS:HB3	1:G:4873:ASP:OD2	2.18	0.44
1:J:1569:GLN:HB2	1:J:1572:ILE:HD12	1.99	0.44
1:J:3206:LEU:HD12	1:J:3280:TYR:CD2	2.53	0.44
3:K:40:ALA:HB3	3:K:43:LYS:HB2	1.98	0.44
1:B:1215:ALA:HA	1:B:1219:LEU:HB3	2.00	0.43
1:B:1515:VAL:HB	1:B:1532:ASN:HA	2.00	0.43
1:B:3946:GLN:OE1	1:B:3949:ARG:NH2	2.48	0.43
1:B:4558:ASN:O	1:B:4562:LEU:HG	2.19	0.43
1:E:1025:ARG:HG2	1:E:1026:LEU:HD12	2.00	0.43
1:E:1727:ARG:HD3	1:E:1730:MET:SD	2.58	0.43
1:E:2142:TYR:CE2	1:E:2197:LEU:HB2	2.52	0.43
1:E:2920:ARG:HH11	1:E:2924:GLN:HE21	1.66	0.43
1:E:3051:ARG:HH22	1:E:3102:ASP:HB2	1.83	0.43
1:E:3245:VAL:HG13	1:E:3248:ARG:H	1.82	0.43
1:E:3944:GLU:O	1:E:3948:LYS:HG3	2.18	0.43
1:E:4003:LEU:HB2	1:E:4013:LEU:HD13	2.00	0.43
1:G:1025:ARG:HG2	1:G:1026:LEU:HD12	2.00	0.43
1:G:1035:ASN:OD1	3:M:109:THR:OG1	2.36	0.43
1:G:1431:THR:HG21	1:G:1523:ALA:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1730:MET:O	1:G:1733:GLU:HG2	2.17	0.43
1:G:2502:MET:SD	1:G:2503:VAL:N	2.90	0.43
1:G:2625:ARG:NE	1:G:2625:ARG:HA	2.33	0.43
1:G:2625:ARG:NH1	1:G:2906:VAL:HG12	2.33	0.43
1:G:2626:LEU:HD12	1:G:2626:LEU:HA	1.86	0.43
1:G:2788:HIS:HE1	1:G:2790:MET:HB2	1.83	0.43
1:G:2926:LEU:O	1:G:2930:LEU:HG	2.18	0.43
1:G:3046:LEU:HD23	1:G:3071:LEU:HD12	2.00	0.43
1:G:4652:LEU:O	1:G:4656:LEU:HG	2.18	0.43
1:J:39:ALA:O	1:J:111:HIS:NE2	2.50	0.43
1:J:356:TRP:N	1:J:379:HIS:O	2.38	0.43
1:J:1025:ARG:HG2	1:J:1026:LEU:HD12	2.00	0.43
1:J:1814:MET:SD	1:J:1841:VAL:HG13	2.58	0.43
1:J:2182:ILE:O	1:J:2186:MET:HG3	2.18	0.43
1:J:3944:GLU:O	1:J:3948:LYS:HG3	2.17	0.43
1:J:4865:LYS:HB3	1:J:4873:ASP:OD2	2.18	0.43
1:J:4922:PHE:O	1:J:4927:ILE:HG12	2.17	0.43
1:B:40:GLU:HG2	1:B:42:PHE:H	1.83	0.43
1:B:2625:ARG:HA	1:B:2625:ARG:NE	2.33	0.43
1:B:3051:ARG:HH22	1:B:3102:ASP:HB2	1.82	0.43
1:B:3347:SER:HB2	1:B:3414:ARG:NH2	2.34	0.43
1:B:3906:GLN:HB2	1:B:3912:THR:HA	1.99	0.43
1:B:4003:LEU:HB2	1:B:4013:LEU:HD13	2.00	0.43
1:B:4652:LEU:O	1:B:4656:LEU:HG	2.18	0.43
1:E:1076:ARG:HG2	1:E:1605:TRP:CZ3	2.53	0.43
1:G:1727:ARG:HD3	1:G:1730:MET:SD	2.58	0.43
1:G:3046:LEU:HD11	1:G:3064:VAL:HG13	2.00	0.43
1:G:3892:CYS:SG	1:G:3903:LEU:HD12	2.58	0.43
1:J:40:GLU:HG2	1:J:42:PHE:H	1.83	0.43
1:J:379:HIS:CE1	1:J:381:GLU:HG2	2.54	0.43
1:J:1254:HIS:CD2	1:J:1283:LEU:HG	2.53	0.43
1:J:3018:LEU:HD21	1:J:3150:HIS:NE2	2.33	0.43
1:J:3046:LEU:HD23	1:J:3071:LEU:HD12	2.00	0.43
1:J:3233:PRO:HD2	1:J:3239:MET:SD	2.58	0.43
3:F:47:LEU:O	3:F:62:SER:OG	2.37	0.43
1:B:292:ALA:HB2	1:B:312:THR:HG22	2.00	0.43
1:B:871:ARG:NH1	1:B:922:LEU:HD22	2.33	0.43
1:B:1748:PHE:HD1	1:B:1749:PRO:HD2	1.84	0.43
1:B:2182:ILE:O	1:B:2186:MET:HG3	2.18	0.43
1:B:2978:GLU:OE1	1:B:3053:ARG:NH1	2.51	0.43
1:B:3187:ARG:HD3	1:B:3271:GLU:HG3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4865:LYS:HB3	1:B:4873:ASP:OD2	2.18	0.43
1:B:4953:ASP:O	1:B:4956:THR:OG1	2.28	0.43
1:E:871:ARG:NH1	1:E:922:LEU:HD22	2.33	0.43
1:E:1569:GLN:HB2	1:E:1572:ILE:HD12	1.99	0.43
1:E:1620:ALA:HB3	1:E:1624:LEU:HB2	1.99	0.43
1:E:1778:SER:HB2	1:E:1798:LEU:HB2	2.01	0.43
1:E:1814:MET:SD	1:E:1841:VAL:HG13	2.58	0.43
1:E:2355:ARG:HD3	1:E:2358:ILE:HD11	1.98	0.43
1:E:2449:GLU:HA	1:E:2452:ARG:HD3	2.00	0.43
1:E:2821:TRP:CG	1:E:2874:MET:SD	3.12	0.43
1:E:3906:GLN:HB2	1:E:3912:THR:HA	1.99	0.43
1:G:917:GLU:OE1	3:M:101:PRO:HB2	2.17	0.43
1:G:1254:HIS:CD2	1:G:1283:LEU:HG	2.53	0.43
1:G:1748:PHE:HD1	1:G:1749:PRO:HD2	1.84	0.43
1:G:2755:ILE:HG22	1:G:2810:LYS:NZ	2.34	0.43
1:G:2821:TRP:CG	1:G:2874:MET:SD	3.12	0.43
1:G:2823:ILE:O	1:G:2825:LYS:NZ	2.49	0.43
1:G:2874:MET:HG3	1:G:2937:VAL:CG2	2.48	0.43
1:G:2970:SER:HA	1:G:2973:PHE:CD2	2.53	0.43
1:G:3104:GLU:O	1:G:3107:VAL:HG22	2.18	0.43
1:J:411:TYR:HB2	1:J:486:LEU:HD21	2.00	0.43
1:J:1205:GLY:HA3	1:J:1225:PRO:HB2	2.00	0.43
1:J:3104:GLU:O	1:J:3107:VAL:HG22	2.18	0.43
3:F:52:THR:OG1	3:F:56:SER:HB2	2.19	0.43
3:F:122:GLN:HE21	3:F:124:THR:HG1	1.61	0.43
1:B:874:LEU:O	1:B:878:ILE:HG12	2.18	0.43
1:B:1861:GLN:O	1:B:1865:MET:HE2	2.18	0.43
1:B:2575:ARG:HB3	1:B:2578:MET:HG2	2.01	0.43
1:B:3437:MET:O	1:B:3441:ILE:HG13	2.18	0.43
1:E:379:HIS:CE1	1:E:381:GLU:HG2	2.54	0.43
1:E:3104:GLU:O	1:E:3107:VAL:HG22	2.18	0.43
1:E:3321:ARG:NH1	1:E:3325:ASN:OD1	2.51	0.43
1:E:4892:ARG:NH2	1:J:4918:ILE:HD13	2.34	0.43
1:G:43:GLY:HA2	1:G:443:LEU:HD23	2.00	0.43
1:G:470:SER:O	1:G:474:ARG:HG3	2.18	0.43
1:G:797:HIS:HE1	1:G:1626:TRP:HD1	1.63	0.43
1:G:1205:GLY:HA3	1:G:1225:PRO:HB2	1.99	0.43
1:G:1778:SER:HB2	1:G:1798:LEU:HB2	2.01	0.43
1:G:1782:PHE:HB2	2:H:37:ASP:OD2	2.18	0.43
1:G:1814:MET:SD	1:G:1841:VAL:HG13	2.58	0.43
1:G:2367:ALA:HB3	1:G:2426:TYR:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4727:LYS:HD3	1:G:4728:HIS:CE1	2.53	0.43
1:J:874:LEU:HD21	1:J:1051:TYR:OH	2.19	0.43
1:J:1727:ARG:HD3	1:J:1730:MET:SD	2.58	0.43
1:J:4727:LYS:HD3	1:J:4728:HIS:CE1	2.54	0.43
3:C:71:ARG:CB	3:C:78:VAL:HG22	2.49	0.43
3:F:94:TYR:HD1	3:F:120:GLY:HA3	1.84	0.43
3:K:47:LEU:O	3:K:62:SER:OG	2.37	0.43
3:K:94:TYR:HD1	3:K:120:GLY:HA3	1.84	0.43
1:B:43:GLY:HA2	1:B:443:LEU:HD23	2.00	0.43
1:B:247:TYR:CB	1:B:374:LYS:HB2	2.47	0.43
1:B:874:LEU:HD21	1:B:1051:TYR:OH	2.19	0.43
1:B:2821:TRP:CG	1:B:2874:MET:SD	3.12	0.43
1:B:2859:PRO:HB2	1:B:2932:MET:SD	2.58	0.43
1:B:3321:ARG:NH1	1:B:3325:ASN:OD1	2.51	0.43
1:B:3727:ASP:HB3	1:B:3731:LYS:HZ1	1.84	0.43
1:B:4780:PHE:HA	1:B:4783:ILE:HG22	1.99	0.43
1:E:43:GLY:HA2	1:E:443:LEU:HD23	2.00	0.43
1:E:1035:ASN:OD1	3:F:109:THR:OG1	2.36	0.43
1:E:1748:PHE:HD1	1:E:1749:PRO:HD2	1.84	0.43
1:E:1771:LEU:HB3	1:E:2153:MET:HE1	2.01	0.43
1:E:2819:TRP:NE1	1:E:2881:ASN:OD1	2.42	0.43
1:G:3284:TRP:HA	1:G:3287:ARG:HD3	2.00	0.43
1:J:118:LEU:HA	1:J:137:LEU:HD23	2.00	0.43
1:J:475:GLN:HB3	1:J:533:ASN:HD22	1.82	0.43
1:J:2449:GLU:HA	1:J:2452:ARG:HD3	2.00	0.43
1:J:2755:ILE:HG22	1:J:2810:LYS:NZ	2.34	0.43
1:J:2821:TRP:CG	1:J:2874:MET:SD	3.12	0.43
1:J:3347:SER:HB2	1:J:3414:ARG:NH2	2.34	0.43
3:K:64:LYS:N	3:K:64:LYS:HD3	2.34	0.43
1:B:250:GLY:N	1:B:253:CYS:SG	2.92	0.43
1:B:913:LEU:HD13	3:C:104:TYR:OH	2.19	0.43
1:B:1043:VAL:HA	1:B:1046:LEU:HG	1.99	0.43
1:B:1698:LEU:HG	1:B:1712:TYR:CZ	2.54	0.43
1:B:2175:GLU:O	1:B:2179:ILE:HG12	2.19	0.43
1:B:2920:ARG:HH11	1:B:2924:GLN:HE21	1.66	0.43
1:B:4996:ILE:HD13	6:B:5103:CFF:C8	2.48	0.43
1:E:920:TYR:CG	3:F:101:PRO:HG3	2.53	0.43
1:E:1043:VAL:HA	1:E:1046:LEU:HG	1.99	0.43
1:E:1782:PHE:HB2	2:D:37:ASP:OD2	2.18	0.43
1:E:2318:TYR:HA	1:E:2395:PRO:HA	2.01	0.43
1:E:2336:ARG:HB2	1:E:2435:ARG:HD2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3347:SER:HB2	1:E:3414:ARG:NH2	2.34	0.43
1:E:4654:ALA:O	1:E:4658:ILE:HG12	2.19	0.43
1:G:379:HIS:CE1	1:G:381:GLU:HG2	2.54	0.43
1:G:516:LYS:HE2	1:G:516:LYS:HB2	1.82	0.43
1:G:1230:MET:HE3	1:G:1827:ARG:HE	1.83	0.43
1:G:1438:ARG:HG3	1:G:1513:ASP:HB3	2.00	0.43
1:G:2182:ILE:O	1:G:2186:MET:HG3	2.18	0.43
1:J:43:GLY:HA2	1:J:443:LEU:HD23	2.00	0.43
1:J:470:SER:O	1:J:474:ARG:HG3	2.18	0.43
1:J:1130:GLN:HG2	1:J:1138:PRO:HA	2.00	0.43
1:J:1782:PHE:HB2	2:I:37:ASP:OD2	2.18	0.43
1:J:2121:PHE:CG	1:J:3701:LEU:HD13	2.54	0.43
1:J:2970:SER:HA	1:J:2973:PHE:CD2	2.53	0.43
1:J:4242:ILE:HA	1:J:4245:MET:HG2	2.00	0.43
1:J:4796:MET:O	1:J:4800:LEU:HG	2.19	0.43
2:I:41:ASP:OD1	2:I:42:ARG:N	2.52	0.43
3:C:52:THR:OG1	3:C:56:SER:HB2	2.19	0.43
3:C:94:TYR:HD1	3:C:120:GLY:HA3	1.84	0.43
1:B:1727:ARG:HD3	1:B:1730:MET:SD	2.58	0.43
1:B:2755:ILE:HG22	1:B:2810:LYS:NZ	2.34	0.43
1:B:2866:THR:OG1	1:B:2867:LEU:N	2.50	0.43
1:B:4242:ILE:HA	1:B:4245:MET:HG2	2.00	0.43
1:B:4918:ILE:HD13	1:G:4892:ARG:NH2	2.33	0.43
1:E:470:SER:O	1:E:474:ARG:HG3	2.18	0.43
1:E:688:LEU:HD23	1:E:712:TYR:HD1	1.83	0.43
1:E:771:PHE:HB3	1:E:1472:VAL:HG23	2.01	0.43
1:E:1230:MET:HE3	1:E:1827:ARG:HE	1.84	0.43
1:E:3089:LYS:O	1:E:3092:LEU:HG	2.18	0.43
1:E:3510:ILE:O	1:E:3514:LEU:HD23	2.18	0.43
1:E:4698:LYS:HB2	1:E:4698:LYS:HE3	1.86	0.43
1:G:250:GLY:N	1:G:253:CYS:SG	2.92	0.43
1:G:874:LEU:HD21	1:G:1051:TYR:OH	2.19	0.43
1:G:2449:GLU:HA	1:G:2452:ARG:HD3	2.00	0.43
1:G:2754:PHE:HE1	1:G:2933:ASN:ND2	2.17	0.43
1:G:3437:MET:O	1:G:3441:ILE:HG13	2.18	0.43
1:G:3765:TYR:O	1:G:3769:ARG:HG3	2.18	0.43
1:G:3934:TYR:OH	1:G:3998:HIS:HB3	2.18	0.43
1:G:4182:GLU:OE1	1:G:4983:HIS:NE2	2.52	0.43
1:G:4211:LYS:O	1:G:4215:ARG:HG3	2.19	0.43
1:J:292:ALA:HB2	1:J:312:THR:HG22	2.00	0.43
1:J:492:ASP:OD1	1:J:546:TRP:NE1	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1215:ALA:HA	1:J:1219:LEU:HB3	2.00	0.43
1:J:2318:TYR:HA	1:J:2395:PRO:HA	2.01	0.43
1:J:3416:VAL:HG23	1:J:3423:TRP:HZ3	1.83	0.43
1:J:3437:MET:O	1:J:3441:ILE:HG13	2.18	0.43
1:J:4823:LEU:O	1:J:4827:LEU:HG	2.19	0.43
2:D:41:ASP:OD1	2:D:42:ARG:N	2.52	0.43
3:C:64:LYS:HD3	3:C:64:LYS:N	2.34	0.43
1:B:182:LEU:HD11	1:B:189:LEU:HB3	2.01	0.43
1:B:379:HIS:CE1	1:B:381:GLU:HG2	2.54	0.43
1:B:771:PHE:HB3	1:B:1472:VAL:HG23	2.01	0.43
1:B:1076:ARG:HG2	1:B:1605:TRP:CZ3	2.53	0.43
1:B:1254:HIS:CD2	1:B:1283:LEU:HG	2.53	0.43
1:B:1431:THR:HG21	1:B:1523:ALA:HB2	1.99	0.43
1:B:1778:SER:HB2	1:B:1798:LEU:HB2	2.01	0.43
1:B:2735:PHE:CG	1:B:2907:PRO:HG3	2.54	0.43
1:B:2926:LEU:O	1:B:2930:LEU:HG	2.19	0.43
1:B:3233:PRO:HD2	1:B:3239:MET:SD	2.58	0.43
1:B:4247:ILE:O	1:B:4251:ILE:HG13	2.18	0.43
1:E:17:ASP:HB2	1:E:98:HIS:CE1	2.54	0.43
1:E:1965:TYR:CE2	1:E:2031:LEU:HD22	2.54	0.43
1:E:2625:ARG:NH1	1:E:2906:VAL:HG12	2.33	0.43
1:E:2823:ILE:O	1:E:2825:LYS:NZ	2.49	0.43
1:E:3233:PRO:HD2	1:E:3239:MET:SD	2.58	0.43
1:E:4211:LYS:O	1:E:4215:ARG:HG3	2.19	0.43
1:E:4558:ASN:O	1:E:4562:LEU:HG	2.18	0.43
1:E:4823:LEU:O	1:E:4827:LEU:HG	2.19	0.43
1:E:4865:LYS:HB3	1:E:4873:ASP:OD2	2.18	0.43
1:G:2575:ARG:HB3	1:G:2578:MET:HG2	2.01	0.43
1:G:2648:TYR:CE2	1:G:2706:ILE:HG12	2.54	0.43
1:G:4558:ASN:O	1:G:4562:LEU:HG	2.18	0.43
1:G:4930:ALA:HB1	1:J:4937:ILE:HD11	2.01	0.43
1:J:51:PRO:C	1:J:53:SER:H	2.22	0.43
1:J:636:ASN:OD1	1:J:637:LEU:N	2.52	0.43
1:J:2625:ARG:NH1	1:J:2906:VAL:HG12	2.33	0.43
1:J:2874:MET:HG3	1:J:2937:VAL:CG2	2.48	0.43
1:J:3765:TYR:O	1:J:3769:ARG:HG3	2.18	0.43
1:J:4211:LYS:O	1:J:4215:ARG:HG3	2.19	0.43
3:F:71:ARG:CB	3:F:78:VAL:HG22	2.49	0.43
3:M:47:LEU:O	3:M:62:SER:OG	2.37	0.43
1:B:360:ALA:HA	1:B:377:ILE:HD13	2.01	0.43
1:B:411:TYR:HB2	1:B:486:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:917:GLU:HB3	3:C:104:TYR:OH	2.18	0.43
1:B:973:SER:HA	1:B:1044:ARG:NH2	2.28	0.43
1:B:1495:VAL:HB	1:B:1500:PHE:CZ	2.54	0.43
1:B:2001:PRO:O	1:B:2005:GLN:HG3	2.19	0.43
1:B:2648:TYR:CE2	1:B:2706:ILE:HG12	2.54	0.43
1:B:3342:ALA:HA	1:B:3345:ILE:HG22	2.01	0.43
1:E:118:LEU:HA	1:E:137:LEU:HD23	2.00	0.43
1:E:850:ASP:OD1	1:E:1025:ARG:NH2	2.44	0.43
1:E:894:GLY:HA3	1:E:903:LEU:HD22	2.01	0.43
1:E:1039:LEU:HD11	3:F:107:TRP:CZ2	2.54	0.43
1:E:1658:ASP:OD1	1:E:1658:ASP:N	2.52	0.43
1:E:3018:LEU:HD21	1:E:3150:HIS:NE2	2.34	0.43
1:E:3068:LEU:HD23	1:E:3139:VAL:HG21	2.00	0.43
1:E:3069:HIS:O	1:E:3073:ARG:HG3	2.19	0.43
1:E:3281:LEU:HG	1:E:3315:LEU:HD12	2.01	0.43
1:E:3537:LYS:HE2	1:E:3537:LYS:HB3	1.90	0.43
1:G:3416:VAL:HG23	1:G:3423:TRP:HZ3	1.83	0.43
1:G:4822:THR:O	1:G:4825:THR:OG1	2.23	0.43
1:J:182:LEU:HD11	1:J:189:LEU:HB3	2.01	0.43
1:J:471:LEU:HD13	1:J:474:ARG:HH21	1.84	0.43
1:J:548:VAL:HG21	1:J:582:HIS:CD2	2.54	0.43
1:J:688:LEU:HD23	1:J:712:TYR:HD1	1.83	0.43
1:J:917:GLU:OE1	3:K:101:PRO:HB2	2.18	0.43
1:J:1000:ARG:HB3	1:J:1005:TRP:HB2	2.00	0.43
1:J:2754:PHE:HE1	1:J:2933:ASN:ND2	2.17	0.43
1:J:3068:LEU:HD23	1:J:3139:VAL:HG21	2.00	0.43
1:J:3342:ALA:HA	1:J:3345:ILE:HG22	2.01	0.43
1:J:3398:PHE:CD1	1:J:3451:PHE:HD1	2.37	0.43
2:A:29:MET:N	2:A:29:MET:SD	2.92	0.43
3:M:64:LYS:HD3	3:M:64:LYS:N	2.34	0.43
1:B:880:GLU:HA	1:B:967:PRO:HB2	2.01	0.43
1:B:1658:ASP:OD1	1:B:1658:ASP:N	2.52	0.43
1:B:1965:TYR:CE2	1:B:2031:LEU:HD22	2.54	0.43
1:B:2596:THR:HB	1:B:2599:GLN:HG3	2.01	0.43
1:B:4654:ALA:O	1:B:4658:ILE:HG12	2.19	0.43
1:B:4727:LYS:HD3	1:B:4728:HIS:CE1	2.54	0.43
1:E:40:GLU:HG2	1:E:42:PHE:H	1.83	0.43
1:E:2351:ASN:O	1:E:2355:ARG:HG2	2.19	0.43
1:E:2735:PHE:CG	1:E:2907:PRO:HG3	2.54	0.43
1:E:2788:HIS:HE1	1:E:2790:MET:HB2	1.83	0.43
1:E:2859:PRO:HB2	1:E:2932:MET:SD	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2926:LEU:O	1:E:2930:LEU:HG	2.19	0.43
1:E:3342:ALA:HA	1:E:3345:ILE:HG22	2.01	0.43
1:E:3670:GLU:O	1:E:3673:MET:HB2	2.19	0.43
1:E:3955:MET:CE	1:E:4015:GLU:HG2	2.48	0.43
1:G:51:PRO:C	1:G:53:SER:H	2.22	0.43
1:G:548:VAL:HG21	1:G:582:HIS:CD2	2.54	0.43
1:G:1042:ALA:O	1:G:1045:THR:OG1	2.22	0.43
1:G:2025:GLU:HA	1:G:2028:ARG:HE	1.84	0.43
1:G:2121:PHE:CG	1:G:3701:LEU:HD13	2.54	0.43
1:G:3069:HIS:O	1:G:3073:ARG:HG3	2.19	0.43
1:G:3204:ALA:HB2	1:G:3304:CYS:SG	2.58	0.43
1:G:3724:ALA:O	1:G:3728:ILE:HG13	2.19	0.43
1:G:4054:ASN:O	1:G:4058:ILE:HG13	2.19	0.43
1:G:4823:LEU:O	1:G:4827:LEU:HG	2.19	0.43
1:J:245:VAL:HG23	1:J:376:ALA:HB3	2.00	0.43
1:J:360:ALA:HA	1:J:377:ILE:HD13	2.01	0.43
1:J:1778:SER:HB2	1:J:1798:LEU:HB2	2.01	0.43
1:J:1965:TYR:CE2	1:J:2031:LEU:HD22	2.54	0.43
1:J:2025:GLU:HA	1:J:2028:ARG:HE	1.84	0.43
1:J:2742:THR:HG21	1:J:2815:ALA:N	2.34	0.43
1:J:3395:ARG:HG2	1:J:3450:ASN:OD1	2.17	0.43
1:J:4054:ASN:O	1:J:4058:ILE:HG13	2.19	0.43
1:J:4654:ALA:O	1:J:4658:ILE:HG12	2.19	0.43
1:B:2351:ASN:O	1:B:2355:ARG:HG2	2.19	0.42
1:E:828:GLU:HG3	1:E:840:VAL:HG21	2.01	0.42
1:E:973:SER:HA	1:E:1044:ARG:NH2	2.28	0.42
1:E:1123:VAL:HG13	1:E:1132:TRP:HB3	2.01	0.42
1:E:1130:GLN:HG2	1:E:1138:PRO:HA	2.00	0.42
1:E:2740:VAL:HG12	1:E:2742:THR:HB	2.01	0.42
1:E:2755:ILE:HG22	1:E:2810:LYS:NZ	2.34	0.42
1:E:3204:ALA:HB2	1:E:3304:CYS:SG	2.58	0.42
1:E:3219:TYR:O	1:E:3227:ARG:NH2	2.38	0.42
1:E:4080:TYR:CG	1:E:4096:ALA:HB2	2.54	0.42
1:G:17:ASP:HB2	1:G:98:HIS:CE1	2.54	0.42
1:G:547:VAL:O	1:G:551:LEU:HG	2.20	0.42
1:G:1000:ARG:HB3	1:G:1005:TRP:HB2	2.00	0.42
1:G:1039:LEU:HD11	3:M:107:TRP:CZ2	2.54	0.42
1:G:2318:TYR:HA	1:G:2395:PRO:HA	2.01	0.42
1:G:3018:LEU:HD21	1:G:3150:HIS:NE2	2.34	0.42
1:G:3068:LEU:HD23	1:G:3139:VAL:HG21	2.00	0.42
1:G:4003:LEU:HB2	1:G:4013:LEU:HD13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4160:LEU:HA	1:G:4163:PHE:HD2	1.84	0.42
1:G:4716:TRP:CD1	6:G:5103:CFF:C4	3.02	0.42
1:J:984:LEU:HD23	1:J:987:ARG:NH2	2.34	0.42
1:J:1748:PHE:HD1	1:J:1749:PRO:HD2	1.84	0.42
1:J:2625:ARG:HA	1:J:2625:ARG:NE	2.33	0.42
1:J:3670:GLU:O	1:J:3673:MET:HB2	2.19	0.42
1:J:4247:ILE:O	1:J:4251:ILE:HG13	2.18	0.42
1:J:4652:LEU:O	1:J:4656:LEU:HG	2.18	0.42
1:B:688:LEU:HD23	1:B:712:TYR:HD1	1.83	0.42
1:B:2449:GLU:HA	1:B:2452:ARG:HD3	2.00	0.42
1:B:2625:ARG:NH1	1:B:2906:VAL:HG12	2.33	0.42
1:B:2788:HIS:HE1	1:B:2790:MET:HB2	1.83	0.42
1:B:3204:ALA:HB2	1:B:3304:CYS:SG	2.58	0.42
1:B:3281:LEU:HG	1:B:3315:LEU:HD12	2.01	0.42
1:B:3729:MET:HE2	1:B:3800:LEU:HD11	2.01	0.42
1:B:4772:ASP:N	1:B:4772:ASP:OD1	2.49	0.42
1:E:51:PRO:C	1:E:53:SER:H	2.22	0.42
1:E:2175:GLU:O	1:E:2179:ILE:HG12	2.19	0.42
1:E:2648:TYR:CE2	1:E:2706:ILE:HG12	2.54	0.42
1:E:2821:TRP:CD1	1:E:2874:MET:SD	3.13	0.42
1:E:3729:MET:HE2	1:E:3800:LEU:HD11	2.01	0.42
1:E:4796:MET:O	1:E:4800:LEU:HG	2.19	0.42
1:G:1495:VAL:HB	1:G:1500:PHE:CZ	2.54	0.42
1:G:1515:VAL:HB	1:G:1532:ASN:HA	2.00	0.42
1:G:2742:THR:HG21	1:G:2815:ALA:N	2.34	0.42
1:G:3164:SER:O	1:G:3168:THR:HG23	2.19	0.42
1:G:3670:GLU:O	1:G:3673:MET:HB2	2.19	0.42
1:G:3955:MET:CE	1:G:4015:GLU:HG2	2.48	0.42
1:J:17:ASP:HB2	1:J:98:HIS:CE1	2.54	0.42
1:J:828:GLU:HG3	1:J:840:VAL:HG21	2.01	0.42
1:J:2821:TRP:CD1	1:J:2874:MET:SD	3.12	0.42
1:J:2920:ARG:HH11	1:J:2924:GLN:HE21	1.66	0.42
1:J:2926:LEU:O	1:J:2930:LEU:HG	2.19	0.42
1:J:3156:VAL:HG23	1:J:3157:ILE:HG13	2.01	0.42
1:J:4546:VAL:HA	1:J:4549:VAL:HG22	2.01	0.42
2:A:41:ASP:OD1	2:A:42:ARG:N	2.52	0.42
2:H:41:ASP:OD1	2:H:42:ARG:N	2.52	0.42
1:B:470:SER:O	1:B:474:ARG:HG3	2.18	0.42
1:B:548:VAL:HG21	1:B:582:HIS:CD2	2.54	0.42
1:B:636:ASN:OD1	1:B:637:LEU:N	2.52	0.42
1:B:2754:PHE:HE1	1:B:2933:ASN:ND2	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2958:GLY:O	1:B:2962:GLN:HG2	2.20	0.42
1:B:3724:ALA:O	1:B:3728:ILE:HG13	2.19	0.42
1:B:3765:TYR:O	1:B:3769:ARG:HG3	2.18	0.42
1:E:471:LEU:HD13	1:E:474:ARG:HH21	1.84	0.42
1:E:1128:ARG:HE	1:E:1130:GLN:NE2	2.17	0.42
1:E:1786:LEU:HD22	2:D:87:HIS:HD2	1.84	0.42
1:E:2754:PHE:HE1	1:E:2933:ASN:ND2	2.17	0.42
1:E:3164:SER:O	1:E:3168:THR:HG23	2.20	0.42
1:E:3437:MET:O	1:E:3441:ILE:HG13	2.18	0.42
1:E:3765:TYR:O	1:E:3769:ARG:HG3	2.18	0.42
1:E:3945:GLU:O	1:E:3949:ARG:HG3	2.19	0.42
1:E:4242:ILE:HA	1:E:4245:MET:HG2	2.00	0.42
1:E:4546:VAL:HA	1:E:4549:VAL:HG22	2.01	0.42
1:E:4727:LYS:HD3	1:E:4728:HIS:CE1	2.53	0.42
1:G:471:LEU:HD13	1:G:474:ARG:HH21	1.84	0.42
1:G:920:TYR:CG	3:M:101:PRO:HG3	2.53	0.42
1:G:984:LEU:HD23	1:G:987:ARG:NH2	2.34	0.42
1:G:1808:ARG:NH1	1:G:1853:ILE:O	2.49	0.42
1:G:1965:TYR:CE2	1:G:2031:LEU:HD22	2.54	0.42
1:G:3321:ARG:NH1	1:G:3325:ASN:OD1	2.51	0.42
1:G:3342:ALA:HA	1:G:3345:ILE:HG22	2.01	0.42
1:J:547:VAL:O	1:J:551:LEU:HG	2.20	0.42
1:J:2648:TYR:CE2	1:J:2706:ILE:HG12	2.54	0.42
1:J:3144:PHE:CD2	1:J:3197:LEU:HB3	2.55	0.42
1:J:3281:LEU:HG	1:J:3315:LEU:HD12	2.01	0.42
1:J:3321:ARG:NH1	1:J:3325:ASN:OD1	2.51	0.42
1:J:3955:MET:CE	1:J:4015:GLU:HG2	2.48	0.42
3:C:47:LEU:O	3:C:62:SER:OG	2.37	0.42
3:K:52:THR:OG1	3:K:56:SER:HB2	2.19	0.42
1:B:17:ASP:HB2	1:B:98:HIS:CE1	2.54	0.42
1:B:822:ARG:NH2	1:B:824:GLU:OE1	2.52	0.42
1:B:917:GLU:OE1	3:C:101:PRO:HB2	2.19	0.42
1:B:1247:PRO:HA	1:B:1598:GLN:HA	2.01	0.42
1:B:2121:PHE:CG	1:B:3701:LEU:HD13	2.54	0.42
1:B:2742:THR:HG21	1:B:2815:ALA:N	2.34	0.42
1:B:3068:LEU:HD23	1:B:3139:VAL:HG21	2.00	0.42
1:B:4160:LEU:HA	1:B:4163:PHE:HD2	1.84	0.42
1:E:46:LEU:HA	1:E:136:GLY:CA	2.49	0.42
1:E:548:VAL:HG21	1:E:582:HIS:CD2	2.54	0.42
1:E:2121:PHE:CG	1:E:3701:LEU:HD13	2.54	0.42
1:E:2742:THR:HG21	1:E:2815:ALA:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2970:SER:HA	1:E:2973:PHE:CD2	2.53	0.42
1:E:4652:LEU:O	1:E:4656:LEU:HG	2.18	0.42
1:G:636:ASN:OD1	1:G:637:LEU:N	2.52	0.42
1:G:913:LEU:HD13	3:M:104:TYR:OH	2.19	0.42
1:G:1099:GLU:O	1:G:1100:MET:HE2	2.20	0.42
1:G:2351:ASN:O	1:G:2355:ARG:HG2	2.19	0.42
1:G:2474:LEU:HD23	1:G:2499:LYS:NZ	2.35	0.42
1:G:2821:TRP:CD1	1:G:2874:MET:SD	3.12	0.42
1:G:4541:TRP:O	1:G:4544:LEU:HG	2.20	0.42
1:G:4796:MET:O	1:G:4800:LEU:HG	2.19	0.42
1:J:850:ASP:OD1	1:J:1025:ARG:NH2	2.44	0.42
1:J:1123:VAL:HG13	1:J:1132:TRP:HB3	2.01	0.42
1:J:1786:LEU:HD22	2:I:87:HIS:CD2	2.55	0.42
1:J:1862:ILE:HA	1:J:1865:MET:HE3	2.01	0.42
1:J:2596:THR:HB	1:J:2599:GLN:HG3	2.01	0.42
1:J:2740:VAL:HG12	1:J:2742:THR:HB	2.01	0.42
1:J:3287:ARG:N	1:J:3287:ARG:HD2	2.35	0.42
1:J:3378:GLN:O	1:J:3381:LEU:HG	2.20	0.42
1:J:3963:ASN:O	1:J:3967:GLU:HG2	2.19	0.42
2:H:29:MET:SD	2:H:29:MET:N	2.92	0.42
3:M:52:THR:OG1	3:M:56:SER:HB2	2.19	0.42
3:M:71:ARG:CB	3:M:78:VAL:HG22	2.49	0.42
1:B:46:LEU:HA	1:B:136:GLY:CA	2.49	0.42
1:B:245:VAL:HG23	1:B:376:ALA:HB3	2.00	0.42
1:B:914:PRO:HB2	1:B:916:PRO:HD2	2.02	0.42
1:B:1126:GLY:HA3	1:B:1143:TRP:CZ3	2.55	0.42
1:B:2474:LEU:HD23	1:B:2499:LYS:NZ	2.35	0.42
1:B:2821:TRP:CD1	1:B:2874:MET:SD	3.13	0.42
1:B:3018:LEU:HD21	1:B:3150:HIS:NE2	2.34	0.42
1:B:3069:HIS:O	1:B:3073:ARG:HG3	2.19	0.42
1:B:3164:SER:O	1:B:3168:THR:HG23	2.19	0.42
1:B:3287:ARG:N	1:B:3287:ARG:HD2	2.35	0.42
1:E:914:PRO:HB2	1:E:916:PRO:HD2	2.02	0.42
1:E:1099:GLU:O	1:E:1100:MET:HE2	2.20	0.42
1:E:2575:ARG:HB3	1:E:2578:MET:HG2	2.01	0.42
1:E:3287:ARG:N	1:E:3287:ARG:HD2	2.35	0.42
1:G:16:THR:O	1:G:98:HIS:ND1	2.53	0.42
1:G:822:ARG:NH2	1:G:824:GLU:OE1	2.52	0.42
1:G:914:PRO:HB2	1:G:916:PRO:HD2	2.02	0.42
1:G:1100:MET:HB2	1:G:1143:TRP:CZ2	2.55	0.42
1:G:2001:PRO:O	1:G:2005:GLN:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2691:TYR:HA	1:G:2696:TYR:CE1	2.55	0.42
1:G:3144:PHE:CD2	1:G:3197:LEU:HB3	2.55	0.42
1:G:3287:ARG:HD2	1:G:3287:ARG:N	2.35	0.42
1:G:3347:SER:HB2	1:G:3414:ARG:NH2	2.34	0.42
1:G:4080:TYR:CG	1:G:4096:ALA:HB2	2.54	0.42
1:J:248:GLU:HG2	1:J:372:LEU:HB2	2.01	0.42
1:J:250:GLY:N	1:J:253:CYS:SG	2.92	0.42
1:J:914:PRO:HB2	1:J:916:PRO:HD2	2.02	0.42
1:J:1128:ARG:HE	1:J:1130:GLN:NE2	2.18	0.42
1:J:1515:VAL:HB	1:J:1532:ASN:HA	2.00	0.42
1:J:1526:LEU:HD23	1:J:1526:LEU:H	1.84	0.42
1:J:2866:THR:OG1	1:J:2867:LEU:N	2.50	0.42
1:J:2879:ALA:HA	1:J:2882:TYR:HD2	1.84	0.42
1:J:3321:ARG:O	1:J:3324:VAL:HG12	2.20	0.42
1:J:3352:GLU:OE1	1:J:3352:GLU:N	2.49	0.42
2:D:29:MET:N	2:D:29:MET:SD	2.92	0.42
1:B:248:GLU:HG2	1:B:372:LEU:HB2	2.01	0.42
1:B:797:HIS:HE1	1:B:1626:TRP:CD1	2.37	0.42
1:B:1130:GLN:HG2	1:B:1138:PRO:HA	2.00	0.42
1:B:1786:LEU:HD22	2:A:87:HIS:CD2	2.55	0.42
1:B:2883:HIS:CE1	1:B:2907:PRO:HA	2.52	0.42
1:B:2970:SER:HA	1:B:2973:PHE:CD2	2.53	0.42
1:B:3670:GLU:O	1:B:3673:MET:HB2	2.19	0.42
1:B:3945:GLU:O	1:B:3949:ARG:HG3	2.19	0.42
1:B:4054:ASN:O	1:B:4058:ILE:HG13	2.19	0.42
1:B:4064:MET:HA	1:B:4103:PHE:HE1	1.85	0.42
1:B:4546:VAL:HA	1:B:4549:VAL:HG22	2.01	0.42
1:B:4937:ILE:HD11	1:E:4930:ALA:HB1	2.02	0.42
1:E:36:CYS:HB3	1:E:52:THR:HG21	2.02	0.42
1:E:182:LEU:HD11	1:E:189:LEU:HB3	2.01	0.42
1:E:411:TYR:HB2	1:E:486:LEU:HD21	2.00	0.42
1:E:468:LEU:O	1:E:472:ARG:HG2	2.20	0.42
1:E:880:GLU:HA	1:E:967:PRO:HB2	2.01	0.42
1:E:880:GLU:O	1:E:884:LEU:HG	2.20	0.42
1:E:917:GLU:HB3	3:F:104:TYR:OH	2.18	0.42
1:E:1495:VAL:HB	1:E:1500:PHE:CZ	2.54	0.42
1:E:3724:ALA:O	1:E:3728:ILE:HG13	2.19	0.42
1:E:4064:MET:HA	1:E:4103:PHE:HE1	1.85	0.42
1:G:292:ALA:HB2	1:G:312:THR:HG22	2.00	0.42
1:G:474:ARG:O	1:G:478:PHE:HD1	2.03	0.42
1:G:1526:LEU:H	1:G:1526:LEU:HD23	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1698:LEU:HG	1:G:1712:TYR:CZ	2.54	0.42
1:G:1786:LEU:HD22	2:H:87:HIS:CD2	2.55	0.42
1:G:2175:GLU:O	1:G:2179:ILE:HG12	2.19	0.42
1:G:2735:PHE:CG	1:G:2907:PRO:HG3	2.54	0.42
1:G:2740:VAL:HG12	1:G:2742:THR:HB	2.01	0.42
1:G:3038:MET:O	1:G:3042:LEU:HD23	2.20	0.42
1:G:3923:LEU:HD22	1:G:3965:LEU:HD11	2.01	0.42
1:G:4013:LEU:O	1:G:4017:LEU:HG	2.20	0.42
1:G:4088:ILE:HG21	1:G:4125:PHE:HB3	2.01	0.42
1:G:4242:ILE:HA	1:G:4245:MET:HG2	2.00	0.42
1:J:1698:LEU:HG	1:J:1712:TYR:CZ	2.54	0.42
1:J:2823:ILE:O	1:J:2825:LYS:NZ	2.49	0.42
1:J:4558:ASN:O	1:J:4562:LEU:HG	2.18	0.42
1:J:4658:ILE:CD1	1:J:4792:LEU:HB3	2.50	0.42
1:J:4859:PHE:HE1	1:J:4909:TYR:HB3	1.85	0.42
2:I:29:MET:N	2:I:29:MET:SD	2.92	0.42
3:F:64:LYS:N	3:F:64:LYS:HD3	2.34	0.42
3:M:94:TYR:HD1	3:M:120:GLY:HA3	1.83	0.42
1:B:36:CYS:HB3	1:B:52:THR:HG21	2.02	0.42
1:B:1123:VAL:HG13	1:B:1132:TRP:HB3	2.01	0.42
1:B:2318:TYR:HA	1:B:2395:PRO:HA	2.01	0.42
1:B:2791:LEU:HD12	1:B:2791:LEU:HA	1.93	0.42
1:B:2914:LYS:HD2	1:B:2915:GLU:N	2.35	0.42
1:B:3144:PHE:CD2	1:B:3197:LEU:HB3	2.55	0.42
1:B:4003:LEU:HB3	1:B:4013:LEU:HB2	2.02	0.42
1:B:4013:LEU:O	1:B:4017:LEU:HG	2.20	0.42
1:E:372:LEU:H	1:E:372:LEU:HD22	1.84	0.42
1:E:547:VAL:O	1:E:551:LEU:HG	2.19	0.42
1:E:822:ARG:NH2	1:E:824:GLU:OE1	2.52	0.42
1:E:874:LEU:HD21	1:E:1051:TYR:OH	2.19	0.42
1:E:984:LEU:HD23	1:E:987:ARG:NH2	2.34	0.42
1:E:1932:PRO:O	1:E:1936:LYS:HG3	2.20	0.42
1:E:2025:GLU:HA	1:E:2028:ARG:HE	1.84	0.42
1:E:3321:ARG:O	1:E:3324:VAL:HG12	2.20	0.42
1:E:3378:GLN:O	1:E:3381:LEU:HG	2.19	0.42
1:E:3521:GLY:HA2	1:E:3524:MET:HG2	2.02	0.42
1:E:4003:LEU:HB3	1:E:4013:LEU:HB2	2.02	0.42
1:E:4054:ASN:O	1:E:4058:ILE:HG13	2.19	0.42
1:E:4658:ILE:CD1	1:E:4792:LEU:HB3	2.50	0.42
1:G:182:LEU:HD11	1:G:189:LEU:HB3	2.01	0.42
1:G:1130:GLN:HG2	1:G:1138:PRO:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2920:ARG:HH11	1:G:2924:GLN:HE21	1.66	0.42
1:G:4654:ALA:O	1:G:4658:ILE:HG12	2.19	0.42
1:J:468:LEU:O	1:J:472:ARG:HG2	2.20	0.42
1:J:771:PHE:HB3	1:J:1472:VAL:HG23	2.01	0.42
1:J:822:ARG:NH2	1:J:824:GLU:OE1	2.52	0.42
1:J:894:GLY:HA3	1:J:903:LEU:HD22	2.01	0.42
1:J:1088:TRP:HA	1:J:1224:GLU:O	2.20	0.42
1:J:1495:VAL:HB	1:J:1500:PHE:CZ	2.54	0.42
1:J:2175:GLU:O	1:J:2179:ILE:HG12	2.19	0.42
1:J:3038:MET:O	1:J:3042:LEU:HD23	2.20	0.42
1:J:3069:HIS:O	1:J:3073:ARG:HG3	2.19	0.42
1:J:3164:SER:O	1:J:3168:THR:HG23	2.19	0.42
3:F:100:VAL:HG22	3:F:105:ASN:HB2	2.00	0.42
1:B:51:PRO:C	1:B:53:SER:H	2.22	0.42
1:B:371:VAL:HG12	1:B:373:LYS:HB2	2.01	0.42
1:B:828:GLU:HG3	1:B:840:VAL:HG21	2.01	0.42
1:B:1000:ARG:HB3	1:B:1005:TRP:HB2	2.01	0.42
1:B:2158:CYS:O	1:B:2162:ILE:HG13	2.20	0.42
1:B:2626:LEU:CG	1:B:2640:PRO:HB3	2.50	0.42
1:B:2691:TYR:HA	1:B:2696:TYR:CE1	2.55	0.42
1:B:3021:PRO:HD3	1:B:3036:LYS:NZ	2.34	0.42
1:B:3450:ASN:HA	1:B:3453:ARG:HG2	2.02	0.42
1:B:3521:GLY:HA2	1:B:3524:MET:HG2	2.02	0.42
1:B:4080:TYR:CG	1:B:4096:ALA:HB2	2.54	0.42
1:B:4188:ARG:HD2	1:B:4191:GLU:HG3	2.02	0.42
1:B:4211:LYS:O	1:B:4215:ARG:HG3	2.19	0.42
1:B:4796:MET:O	1:B:4800:LEU:HG	2.19	0.42
1:B:4859:PHE:HE1	1:B:4909:TYR:HB3	1.85	0.42
1:E:516:LYS:HE2	1:E:516:LYS:HB2	1.82	0.42
1:E:1698:LEU:HG	1:E:1712:TYR:CZ	2.54	0.42
1:E:2625:ARG:HA	1:E:2625:ARG:NE	2.34	0.42
1:E:3156:VAL:HG23	1:E:3157:ILE:HG13	2.01	0.42
1:E:4124:ASN:OD1	1:E:4125:PHE:N	2.53	0.42
1:G:2158:CYS:O	1:G:2162:ILE:HG13	2.20	0.42
1:G:2605:ASP:HA	1:G:2608:MET:HG2	2.02	0.42
1:G:2819:TRP:NE1	1:G:2881:ASN:OD1	2.42	0.42
1:G:2914:LYS:HD2	1:G:2915:GLU:N	2.35	0.42
1:G:4802:GLY:HA2	1:G:4808:PHE:HB2	2.02	0.42
1:J:247:TYR:CB	1:J:374:LYS:HB2	2.47	0.42
1:J:874:LEU:O	1:J:878:ILE:HG12	2.18	0.42
1:J:880:GLU:O	1:J:884:LEU:HG	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:2001:PRO:O	1:J:2005:GLN:HG3	2.19	0.42
1:J:2351:ASN:O	1:J:2355:ARG:HG2	2.19	0.42
1:J:2626:LEU:CG	1:J:2640:PRO:HB3	2.50	0.42
1:J:2735:PHE:CG	1:J:2907:PRO:HG3	2.54	0.42
1:J:3219:TYR:O	1:J:3227:ARG:NH2	2.38	0.42
1:J:4080:TYR:CG	1:J:4096:ALA:HB2	2.54	0.42
3:C:4:LEU:HD22	3:C:118:GLY:HA3	2.01	0.42
1:B:471:LEU:HD13	1:B:474:ARG:HH21	1.84	0.42
1:B:1037:ASP:N	1:B:1037:ASP:OD1	2.53	0.42
1:B:1666:THR:HG22	1:B:1670:TYR:CE2	2.55	0.42
1:B:1830:VAL:HB	1:B:1837:GLN:HG3	2.02	0.42
1:B:2025:GLU:HA	1:B:2028:ARG:HE	1.84	0.42
1:B:3321:ARG:O	1:B:3324:VAL:HG12	2.20	0.42
1:E:587:ILE:HD12	1:E:624:ASN:HB3	2.02	0.42
1:E:1000:ARG:HB3	1:E:1005:TRP:HB2	2.00	0.42
1:E:1037:ASP:OD1	1:E:1037:ASP:N	2.53	0.42
1:E:1088:TRP:HA	1:E:1224:GLU:O	2.20	0.42
1:E:2452:ARG:O	1:E:2456:ILE:HG13	2.20	0.42
1:E:2806:ARG:NH1	1:E:2810:LYS:HG3	2.35	0.42
1:E:3062:PRO:HA	1:E:3065:VAL:HG22	2.02	0.42
1:E:4088:ILE:HG21	1:E:4125:PHE:HB3	2.01	0.42
1:G:1088:TRP:HA	1:G:1224:GLU:O	2.20	0.42
1:G:3156:VAL:HG23	1:G:3157:ILE:HG13	2.01	0.42
1:G:3349:ALA:HB1	1:G:3353:LEU:HD12	2.02	0.42
1:G:3450:ASN:HA	1:G:3453:ARG:HG2	2.02	0.42
1:G:3521:GLY:HA2	1:G:3524:MET:HG2	2.02	0.42
1:J:453:GLU:HA	1:J:454:PRO:HD3	1.96	0.42
1:J:1099:GLU:O	1:J:1100:MET:HE2	2.20	0.42
1:J:1100:MET:HB2	1:J:1143:TRP:CZ2	2.55	0.42
1:J:2158:CYS:O	1:J:2162:ILE:HG13	2.20	0.42
1:J:2605:ASP:HA	1:J:2608:MET:HG2	2.02	0.42
1:J:2759:ALA:HB1	1:J:2806:ARG:HA	2.02	0.42
1:J:3517:MET:SD	1:J:3517:MET:N	2.93	0.42
1:J:4003:LEU:HB3	1:J:4013:LEU:HB2	2.02	0.42
1:J:4182:GLU:OE1	1:J:4983:HIS:NE2	2.52	0.42
1:J:4691:GLN:HB2	1:J:4703:ARG:HH22	1.85	0.42
3:K:122:GLN:HE21	3:K:124:THR:HG1	1.61	0.42
1:B:1128:ARG:HE	1:B:1130:GLN:NE2	2.18	0.42
1:B:1230:MET:HE3	1:B:1827:ARG:HE	1.85	0.42
1:B:2598:ALA:O	1:B:2602:VAL:HG23	2.20	0.42
1:B:3349:ALA:HB1	1:B:3353:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:16:THR:O	1:E:98:HIS:ND1	2.53	0.42
1:E:467:LYS:HE3	1:E:467:LYS:HB3	1.87	0.42
1:E:1126:GLY:HA3	1:E:1143:TRP:CZ3	2.55	0.42
1:E:1247:PRO:HA	1:E:1598:GLN:HA	2.01	0.42
1:E:1808:ARG:NH1	1:E:1853:ILE:O	2.49	0.42
1:E:1830:VAL:HB	1:E:1837:GLN:HG3	2.02	0.42
1:E:2862:LEU:HD23	1:E:2864:GLY:H	1.85	0.42
1:E:3250:MET:HA	1:E:3253:ILE:HG22	2.02	0.42
1:E:3962:PHE:O	1:E:3966:THR:HG23	2.20	0.42
1:E:4541:TRP:O	1:E:4544:LEU:HG	2.20	0.42
1:G:36:CYS:HB3	1:G:52:THR:HG21	2.02	0.42
1:G:48:PHE:HD2	1:G:50:GLU:OE1	2.03	0.42
1:G:688:LEU:HD23	1:G:712:TYR:HD1	1.83	0.42
1:G:984:LEU:HD23	1:G:987:ARG:HH21	1.85	0.42
1:G:3281:LEU:HG	1:G:3315:LEU:HD12	2.01	0.42
1:G:3321:ARG:O	1:G:3324:VAL:HG12	2.20	0.42
1:G:3432:GLU:O	1:G:3435:PHE:HB3	2.20	0.42
1:G:3727:ASP:HB3	1:G:3731:LYS:HZ1	1.85	0.42
1:G:4003:LEU:HB3	1:G:4013:LEU:HB2	2.02	0.42
1:G:4064:MET:HA	1:G:4103:PHE:HE1	1.85	0.42
1:J:371:VAL:HG12	1:J:373:LYS:HB2	2.01	0.42
1:J:1666:THR:HG22	1:J:1670:TYR:CE2	2.55	0.42
1:J:2121:PHE:O	1:J:3725:TYR:OH	2.35	0.42
1:J:2452:ARG:O	1:J:2456:ILE:HG13	2.20	0.42
1:J:2575:ARG:HB3	1:J:2578:MET:HG2	2.01	0.42
1:J:3670:GLU:OE1	1:J:3732:SER:HB3	2.20	0.42
1:J:3945:GLU:O	1:J:3949:ARG:HG3	2.19	0.42
1:J:4013:LEU:O	1:J:4017:LEU:HG	2.20	0.42
1:J:4064:MET:HA	1:J:4103:PHE:HE1	1.85	0.42
1:J:4124:ASN:OD1	1:J:4125:PHE:N	2.53	0.42
1:J:4160:LEU:HA	1:J:4163:PHE:HD2	1.84	0.42
1:B:880:GLU:O	1:B:884:LEU:HG	2.19	0.41
1:B:894:GLY:HA3	1:B:903:LEU:HD22	2.01	0.41
1:B:2230:THR:HG22	1:B:2234:ARG:HH11	1.85	0.41
1:B:2605:ASP:HA	1:B:2608:MET:HG2	2.02	0.41
1:B:2764:GLU:HA	1:B:2855:TYR:CE2	2.55	0.41
1:B:3352:GLU:OE1	1:B:3352:GLU:N	2.49	0.41
1:B:3378:GLN:O	1:B:3381:LEU:HG	2.20	0.41
1:B:4541:TRP:O	1:B:4544:LEU:HG	2.20	0.41
1:E:250:GLY:N	1:E:253:CYS:SG	2.92	0.41
1:E:541:SER:HA	1:E:574:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:913:LEU:HD13	3:F:104:TYR:OH	2.20	0.41
1:E:2691:TYR:HA	1:E:2696:TYR:CE1	2.55	0.41
1:E:2764:GLU:HA	1:E:2855:TYR:CE2	2.55	0.41
1:E:2823:ILE:HA	1:E:2936:ALA:O	2.20	0.41
1:E:2866:THR:OG1	1:E:2867:LEU:N	2.50	0.41
1:E:3398:PHE:CD1	1:E:3451:PHE:HD1	2.37	0.41
1:E:4859:PHE:HE1	1:E:4909:TYR:HB3	1.85	0.41
1:G:363:ASP:HB3	1:G:366:ALA:HB3	2.02	0.41
1:G:880:GLU:HA	1:G:967:PRO:HB2	2.01	0.41
1:G:1154:ASP:OD1	1:G:1159:THR:OG1	2.22	0.41
1:G:1666:THR:HG22	1:G:1670:TYR:CE2	2.55	0.41
1:G:2487:GLN:HB3	1:G:2546:MET:HE1	2.02	0.41
1:G:2598:ALA:O	1:G:2602:VAL:HG23	2.20	0.41
1:G:3378:GLN:O	1:G:3381:LEU:HG	2.20	0.41
1:G:4546:VAL:HA	1:G:4549:VAL:HG22	2.01	0.41
1:G:4651:THR:OG1	1:G:4803:HIS:NE2	2.32	0.41
1:J:2914:LYS:HD2	1:J:2915:GLU:N	2.35	0.41
2:H:30:LEU:N	2:H:34:LYS:O	2.51	0.41
3:F:4:LEU:HD22	3:F:118:GLY:HA3	2.01	0.41
3:K:71:ARG:CB	3:K:78:VAL:HG22	2.49	0.41
1:B:358:THR:HG21	1:B:382:GLY:HA2	2.01	0.41
1:B:2189:LYS:HA	1:B:2192:TYR:CZ	2.55	0.41
1:B:2740:VAL:HG12	1:B:2742:THR:HB	2.01	0.41
1:B:2760:GLU:HA	1:B:2802:LYS:NZ	2.35	0.41
1:B:2806:ARG:NH1	1:B:2810:LYS:HG3	2.35	0.41
1:B:2862:LEU:HD23	1:B:2864:GLY:H	1.85	0.41
1:B:3062:PRO:HA	1:B:3065:VAL:HG22	2.02	0.41
1:B:3533:ILE:O	1:B:3537:LYS:HG3	2.20	0.41
1:B:3996:PHE:HZ	1:B:4019:LEU:HG	1.85	0.41
1:B:4802:GLY:HA2	1:B:4808:PHE:HB2	2.02	0.41
1:B:4823:LEU:O	1:B:4827:LEU:HG	2.19	0.41
1:E:1274:HIS:O	1:E:1559:GLN:NE2	2.53	0.41
1:E:2464:ASP:HA	1:E:2467:VAL:HG12	2.03	0.41
1:E:2760:GLU:HA	1:E:2802:LYS:NZ	2.35	0.41
1:E:2914:LYS:HD2	1:E:2915:GLU:N	2.35	0.41
1:E:3144:PHE:CD2	1:E:3197:LEU:HB3	2.55	0.41
1:E:3604:TYR:O	1:E:3607:GLU:HG3	2.20	0.41
1:E:3996:PHE:HZ	1:E:4019:LEU:HG	1.85	0.41
1:E:4904:PRO:HB3	1:E:4913:ARG:HD3	2.02	0.41
1:G:358:THR:HG21	1:G:382:GLY:HA2	2.01	0.41
1:G:437:PRO:HB2	1:G:440:ALA:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:541:SER:HA	1:G:574:VAL:HG12	2.02	0.41
1:G:894:GLY:HA3	1:G:903:LEU:HD22	2.01	0.41
1:G:2626:LEU:CG	1:G:2640:PRO:HB3	2.50	0.41
1:G:2759:ALA:HB1	1:G:2806:ARG:HA	2.02	0.41
1:J:46:LEU:HA	1:J:136:GLY:CA	2.49	0.41
1:J:48:PHE:HD2	1:J:50:GLU:OE1	2.03	0.41
1:J:340:LYS:O	1:J:344:SER:OG	2.32	0.41
1:J:467:LYS:HE3	1:J:467:LYS:HB3	1.87	0.41
1:J:514:SER:O	1:J:518:ILE:HG13	2.20	0.41
1:J:1126:GLY:HA3	1:J:1143:TRP:CZ3	2.55	0.41
1:J:1230:MET:HE3	1:J:1827:ARG:HE	1.85	0.41
1:J:2474:LEU:HD23	1:J:2499:LYS:NZ	2.35	0.41
1:J:2760:GLU:HA	1:J:2802:LYS:NZ	2.35	0.41
1:J:2764:GLU:HA	1:J:2855:TYR:CE2	2.55	0.41
1:J:2788:HIS:CD2	1:J:2789:PRO:HD2	2.55	0.41
1:J:2823:ILE:HA	1:J:2936:ALA:O	2.20	0.41
1:J:2862:LEU:HD23	1:J:2864:GLY:H	1.85	0.41
1:J:3432:GLU:O	1:J:3435:PHE:HB3	2.20	0.41
1:J:3531:ASP:O	1:J:3535:LEU:HD23	2.20	0.41
2:A:30:LEU:N	2:A:34:LYS:O	2.51	0.41
1:B:363:ASP:HB3	1:B:366:ALA:HB3	2.02	0.41
1:B:547:VAL:O	1:B:551:LEU:HG	2.20	0.41
1:B:984:LEU:HD23	1:B:987:ARG:NH2	2.34	0.41
1:B:1088:TRP:HA	1:B:1224:GLU:O	2.20	0.41
1:B:1101:ARG:NH1	1:B:1114:GLU:HB3	2.34	0.41
1:B:3398:PHE:CD1	1:B:3451:PHE:HD1	2.37	0.41
1:B:3670:GLU:OE1	1:B:3732:SER:HB3	2.20	0.41
1:B:4124:ASN:OD1	1:B:4125:PHE:N	2.53	0.41
1:B:4998:LYS:HG3	1:B:5003:HIS:CE1	2.56	0.41
1:E:453:GLU:HA	1:E:454:PRO:HD3	1.96	0.41
1:E:1078:GLU:HA	1:E:1237:TRP:CD1	2.55	0.41
1:E:1666:THR:HG22	1:E:1670:TYR:CE2	2.55	0.41
1:E:2005:GLN:O	1:E:2009:LEU:HD23	2.21	0.41
1:E:2198:MET:HA	1:E:2203:MET:HE1	2.03	0.41
1:E:2596:THR:HB	1:E:2599:GLN:HG3	2.01	0.41
1:E:2605:ASP:HA	1:E:2608:MET:HG2	2.02	0.41
1:E:2636:PHE:O	1:E:2640:PRO:HD2	2.21	0.41
1:E:2958:GLY:O	1:E:2962:GLN:HG2	2.20	0.41
1:E:3531:ASP:O	1:E:3535:LEU:HD23	2.20	0.41
1:E:3963:ASN:O	1:E:3967:GLU:HG2	2.19	0.41
1:E:4188:ARG:HD2	1:E:4191:GLU:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:771:PHE:HB3	1:G:1472:VAL:HG23	2.01	0.41
1:G:2189:LYS:HA	1:G:2192:TYR:CZ	2.55	0.41
1:G:2596:THR:HB	1:G:2599:GLN:HG3	2.01	0.41
1:G:3250:MET:HA	1:G:3253:ILE:HG22	2.02	0.41
1:G:3398:PHE:CD1	1:G:3451:PHE:HD1	2.37	0.41
1:G:3531:ASP:O	1:G:3535:LEU:HD23	2.20	0.41
1:G:4123:ILE:H	1:G:4123:ILE:HD12	1.85	0.41
1:J:36:CYS:HB3	1:J:52:THR:HG21	2.02	0.41
1:J:541:SER:HA	1:J:574:VAL:HG12	2.02	0.41
1:J:587:ILE:HD12	1:J:624:ASN:HB3	2.02	0.41
1:J:984:LEU:HD23	1:J:987:ARG:HH21	1.85	0.41
1:J:2368:LEU:HD11	1:J:2376:LEU:HD12	2.02	0.41
1:J:2691:TYR:HA	1:J:2696:TYR:CE1	2.55	0.41
1:J:3724:ALA:O	1:J:3728:ILE:HG13	2.19	0.41
1:J:3752:SER:HB2	1:J:3755:GLU:HG3	2.01	0.41
1:J:3996:PHE:HZ	1:J:4019:LEU:HG	1.85	0.41
1:J:4060:LYS:HA	1:J:4063:ASP:OD2	2.21	0.41
1:J:4088:ILE:HG21	1:J:4125:PHE:HB3	2.01	0.41
2:I:62:GLY:HA3	2:I:74:LEU:HD21	2.03	0.41
1:B:16:THR:O	1:B:98:HIS:ND1	2.53	0.41
1:B:48:PHE:HD2	1:B:50:GLU:OE1	2.03	0.41
1:B:113:HIS:NE2	1:B:402:ARG:HB3	2.35	0.41
1:B:474:ARG:O	1:B:478:PHE:HD1	2.03	0.41
1:B:984:LEU:O	1:B:988:LEU:HG	2.21	0.41
1:B:1100:MET:HB2	1:B:1143:TRP:CZ2	2.55	0.41
1:B:1274:HIS:O	1:B:1559:GLN:NE2	2.53	0.41
1:B:1498:GLY:HA2	1:B:1501:VAL:HG12	2.03	0.41
1:B:1927:LEU:HD22	1:B:2101:MET:HG3	2.03	0.41
1:B:1932:PRO:O	1:B:1936:LYS:HG3	2.20	0.41
1:B:2452:ARG:O	1:B:2456:ILE:HG13	2.20	0.41
1:B:2636:PHE:O	1:B:2640:PRO:HD2	2.21	0.41
1:B:3156:VAL:HG23	1:B:3157:ILE:HG13	2.02	0.41
1:B:3537:LYS:HE2	1:B:3537:LYS:HB3	1.90	0.41
1:B:3963:ASN:O	1:B:3967:GLU:HG2	2.19	0.41
1:B:4088:ILE:HG21	1:B:4125:PHE:HB3	2.01	0.41
1:B:4123:ILE:H	1:B:4123:ILE:HD12	1.85	0.41
1:E:2438:PRO:HB2	1:E:2443:ILE:HD11	2.03	0.41
1:E:2474:LEU:HD23	1:E:2499:LYS:NZ	2.35	0.41
1:E:3670:GLU:OE1	1:E:3732:SER:HB3	2.20	0.41
1:E:3752:SER:HB2	1:E:3755:GLU:HG3	2.01	0.41
1:G:46:LEU:HA	1:G:136:GLY:CA	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:468:LEU:O	1:G:472:ARG:HG2	2.20	0.41
1:G:797:HIS:HE1	1:G:1626:TRP:CD1	2.37	0.41
1:G:1078:GLU:HA	1:G:1237:TRP:CD1	2.55	0.41
1:G:2005:GLN:O	1:G:2009:LEU:HD23	2.21	0.41
1:G:3963:ASN:O	1:G:3967:GLU:HG2	2.21	0.41
1:G:3996:PHE:HZ	1:G:4019:LEU:HG	1.85	0.41
1:G:4996:ILE:HD13	6:G:5103:CFF:C8	2.51	0.41
1:J:100:THR:HG21	1:J:162:LYS:HD3	2.03	0.41
1:J:973:SER:HA	1:J:1044:ARG:NH2	2.28	0.41
1:J:3604:TYR:O	1:J:3607:GLU:HG3	2.20	0.41
1:J:4802:GLY:HA2	1:J:4808:PHE:HB2	2.02	0.41
1:J:4904:PRO:HB3	1:J:4913:ARG:HD3	2.02	0.41
1:B:437:PRO:HB2	1:B:440:ALA:HB3	2.03	0.41
1:B:514:SER:O	1:B:518:ILE:HG13	2.20	0.41
1:B:587:ILE:HD12	1:B:624:ASN:HB3	2.02	0.41
1:B:871:ARG:HH11	1:B:922:LEU:HD22	1.86	0.41
1:B:1099:GLU:O	1:B:1100:MET:HE2	2.20	0.41
1:B:1526:LEU:HD23	1:B:1526:LEU:H	1.84	0.41
1:B:2005:GLN:O	1:B:2009:LEU:HD23	2.21	0.41
1:B:2558:VAL:O	1:B:2562:ILE:HG12	2.21	0.41
1:B:2823:ILE:HA	1:B:2936:ALA:O	2.20	0.41
1:B:2950:SER:HA	1:B:2953:LYS:HB2	2.03	0.41
1:B:3038:MET:O	1:B:3042:LEU:HD23	2.20	0.41
1:B:3413:ILE:HD11	1:B:3512:ALA:HB2	2.03	0.41
1:B:3604:TYR:O	1:B:3607:GLU:HG3	2.20	0.41
1:B:3752:SER:HB2	1:B:3755:GLU:HG3	2.01	0.41
1:B:4651:THR:OG1	1:B:4803:HIS:NE2	2.32	0.41
1:B:4658:ILE:CD1	1:B:4792:LEU:HB3	2.50	0.41
1:B:4904:PRO:HB3	1:B:4913:ARG:HD3	2.02	0.41
1:E:360:ALA:HB3	1:E:375:LYS:HB3	2.03	0.41
1:E:984:LEU:HD23	1:E:987:ARG:HH21	1.85	0.41
1:E:1100:MET:HB2	1:E:1143:TRP:CZ2	2.55	0.41
1:E:1758:ARG:NH1	1:E:2037:ASP:HA	2.36	0.41
1:E:1828:ASP:N	1:E:1828:ASP:OD1	2.54	0.41
1:E:1927:LEU:HD22	1:E:2101:MET:HG3	2.02	0.41
1:E:3391:GLU:HA	1:E:3394:VAL:HG22	2.03	0.41
1:E:3450:ASN:HA	1:E:3453:ARG:HG2	2.02	0.41
1:E:4691:GLN:HB2	1:E:4703:ARG:HH22	1.85	0.41
1:G:871:ARG:HD3	1:G:925:SER:HB2	2.02	0.41
1:G:1126:GLY:HA3	1:G:1143:TRP:CZ3	2.55	0.41
1:G:1247:PRO:HA	1:G:1598:GLN:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1274:HIS:O	1:G:1559:GLN:NE2	2.53	0.41
1:G:1498:GLY:HA2	1:G:1501:VAL:HG12	2.03	0.41
1:G:2273:LEU:HD11	1:G:2334:PHE:HB2	2.03	0.41
1:G:2368:LEU:HD11	1:G:2376:LEU:HD12	2.02	0.41
1:G:2764:GLU:HA	1:G:2855:TYR:CE2	2.55	0.41
1:G:3062:PRO:HA	1:G:3065:VAL:HG22	2.02	0.41
1:G:3945:GLU:O	1:G:3949:ARG:HG3	2.19	0.41
1:G:4124:ASN:OD1	1:G:4125:PHE:N	2.53	0.41
1:G:4642:ALA:O	1:G:4646:LEU:HD23	2.21	0.41
1:G:4658:ILE:CD1	1:G:4792:LEU:HB3	2.50	0.41
1:J:363:ASP:HB3	1:J:366:ALA:HB3	2.02	0.41
1:J:917:GLU:HB3	3:K:104:TYR:OH	2.19	0.41
1:J:1035:ASN:OD1	3:K:109:THR:OG1	2.37	0.41
1:J:2273:LEU:HD11	1:J:2334:PHE:HB2	2.03	0.41
1:J:2464:ASP:HA	1:J:2467:VAL:HG12	2.03	0.41
1:J:2866:THR:O	1:J:2867:LEU:HB2	2.21	0.41
1:J:3962:PHE:O	1:J:3966:THR:HG23	2.20	0.41
1:J:4642:ALA:O	1:J:4646:LEU:HD23	2.21	0.41
2:D:62:GLY:HA3	2:D:74:LEU:HD21	2.03	0.41
1:B:119:SER:OG	1:B:120:CYS:N	2.54	0.41
1:B:3015:LEU:HD21	1:B:3025:LEU:HD12	2.03	0.41
1:B:3250:MET:HA	1:B:3253:ILE:HG22	2.02	0.41
1:E:100:THR:HG21	1:E:162:LYS:HD3	2.03	0.41
1:E:358:THR:HG21	1:E:382:GLY:HA2	2.02	0.41
1:E:664:PHE:CE1	1:E:746:CYS:HB2	2.56	0.41
1:E:3131:TYR:CE2	1:E:3136:LEU:HG	2.56	0.41
1:E:3785:ALA:HA	1:E:3787:LYS:HE2	2.03	0.41
1:E:4013:LEU:O	1:E:4017:LEU:HG	2.20	0.41
1:E:4060:LYS:HA	1:E:4063:ASP:OD2	2.21	0.41
1:E:4698:LYS:HG3	1:E:4699:GLY:N	2.36	0.41
1:G:113:HIS:NE2	1:G:402:ARG:HB3	2.35	0.41
1:G:880:GLU:O	1:G:884:LEU:HG	2.19	0.41
1:G:2230:THR:HG22	1:G:2234:ARG:HH11	1.85	0.41
1:G:3400:VAL:HG23	1:G:3403:ARG:HH21	1.84	0.41
1:G:3413:ILE:HD11	1:G:3512:ALA:HB2	2.03	0.41
1:G:3533:ILE:O	1:G:3537:LYS:HG3	2.20	0.41
1:G:3752:SER:HB2	1:G:3755:GLU:HG3	2.01	0.41
1:G:4698:LYS:HG3	1:G:4699:GLY:N	2.36	0.41
1:G:4904:PRO:HB3	1:G:4913:ARG:HD3	2.02	0.41
1:J:113:HIS:NE2	1:J:402:ARG:HB3	2.35	0.41
1:J:358:THR:HG21	1:J:382:GLY:HA2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:437:PRO:HB2	1:J:440:ALA:HB3	2.03	0.41
1:J:474:ARG:O	1:J:478:PHE:HD1	2.03	0.41
1:J:835:ARG:NH2	1:J:1203:ASN:HD22	2.09	0.41
1:J:880:GLU:HA	1:J:967:PRO:HB2	2.01	0.41
1:J:1288:PHE:HB2	1:J:1600:LEU:HB2	2.03	0.41
1:J:2950:SER:HA	1:J:2953:LYS:HB2	2.03	0.41
1:J:2958:GLY:O	1:J:2962:GLN:HG2	2.20	0.41
1:J:3062:PRO:HA	1:J:3065:VAL:HG22	2.02	0.41
1:J:3349:ALA:HB1	1:J:3353:LEU:HD12	2.02	0.41
1:J:3384:LYS:HG2	1:J:3386:GLU:N	2.36	0.41
1:J:4188:ARG:HD2	1:J:4191:GLU:HG3	2.02	0.41
1:B:2866:THR:O	1:B:2867:LEU:HB2	2.21	0.41
1:B:4060:LYS:HA	1:B:4063:ASP:OD2	2.21	0.41
1:E:1534:LYS:HE3	1:E:1534:LYS:HB2	1.95	0.41
1:E:1683:HIS:CG	1:E:1797:ARG:HH21	2.39	0.41
1:E:2001:PRO:O	1:E:2005:GLN:HG3	2.19	0.41
1:E:2368:LEU:HD11	1:E:2376:LEU:HD12	2.02	0.41
1:E:3038:MET:O	1:E:3042:LEU:HD23	2.20	0.41
1:E:3244:PRO:HB2	1:E:3248:ARG:HE	1.86	0.41
1:E:3413:ILE:HD11	1:E:3512:ALA:HB2	2.03	0.41
1:E:3533:ILE:O	1:E:3537:LYS:HG3	2.20	0.41
1:E:3923:LEU:HD11	1:E:3962:PHE:CZ	2.56	0.41
1:E:4642:ALA:O	1:E:4646:LEU:HD23	2.21	0.41
1:G:828:GLU:HG3	1:G:840:VAL:HG21	2.01	0.41
1:G:1123:VAL:HG13	1:G:1132:TRP:HB3	2.01	0.41
1:G:1128:ARG:HE	1:G:1130:GLN:NE2	2.17	0.41
1:G:1927:LEU:HD22	1:G:2101:MET:HG3	2.02	0.41
1:G:2866:THR:HG21	1:G:2872:GLN:NE2	2.36	0.41
1:G:3244:PRO:HB2	1:G:3248:ARG:HE	1.86	0.41
1:G:3522:LEU:HA	1:G:3525:CYS:SG	2.61	0.41
1:G:3779:VAL:O	1:G:3783:ILE:HG13	2.21	0.41
1:G:4060:LYS:HA	1:G:4063:ASP:OD2	2.21	0.41
1:G:4243:PHE:HE2	1:G:4668:LEU:HA	1.86	0.41
1:J:16:THR:O	1:J:98:HIS:ND1	2.53	0.41
1:J:664:PHE:CE1	1:J:746:CYS:HB2	2.56	0.41
1:J:1247:PRO:HA	1:J:1598:GLN:HA	2.01	0.41
1:J:1932:PRO:O	1:J:1936:LYS:HG3	2.20	0.41
1:J:2598:ALA:O	1:J:2602:VAL:HG23	2.20	0.41
1:J:3413:ILE:HD11	1:J:3512:ALA:HB2	2.03	0.41
1:J:4698:LYS:HG3	1:J:4699:GLY:N	2.36	0.41
2:A:62:GLY:HA3	2:A:74:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:100:VAL:HG22	3:C:105:ASN:HB2	2.02	0.41
1:B:246:TYR:HE1	1:B:375:LYS:HZ3	1.68	0.41
1:B:573:GLU:CD	1:B:573:GLU:H	2.24	0.41
1:B:659:TYR:CE2	1:B:661:LYS:HB2	2.56	0.41
1:B:984:LEU:HD23	1:B:987:ARG:HH21	1.85	0.41
1:B:1288:PHE:HB2	1:B:1600:LEU:HB2	2.03	0.41
1:B:1293:LEU:HD11	1:B:1594:ARG:HG2	2.03	0.41
1:B:2438:PRO:HB2	1:B:2443:ILE:HD11	2.03	0.41
1:B:2694:GLU:O	1:B:2697:ARG:HG3	2.20	0.41
1:B:2788:HIS:CD2	1:B:2789:PRO:HD2	2.55	0.41
1:B:3923:LEU:HD11	1:B:3962:PHE:CZ	2.56	0.41
1:B:4698:LYS:HG3	1:B:4699:GLY:N	2.36	0.41
1:B:4892:ARG:NH2	1:E:4918:ILE:HD13	2.35	0.41
1:E:437:PRO:HB2	1:E:440:ALA:HB3	2.02	0.41
1:E:1079:LYS:HE3	1:E:1107:PRO:HB3	2.03	0.41
1:E:1526:LEU:HD23	1:E:1526:LEU:H	1.84	0.41
1:E:2158:CYS:O	1:E:2162:ILE:HG13	2.20	0.41
1:E:2866:THR:O	1:E:2867:LEU:HB2	2.21	0.41
1:E:3015:LEU:HD21	1:E:3025:LEU:HD12	2.03	0.41
1:E:3432:GLU:O	1:E:3435:PHE:HB3	2.20	0.41
1:E:4664:LEU:HD22	1:E:4665:LYS:HD3	2.03	0.41
1:G:984:LEU:O	1:G:988:LEU:HG	2.21	0.41
1:G:1932:PRO:O	1:G:1936:LYS:HG3	2.20	0.41
1:G:2452:ARG:O	1:G:2456:ILE:HG13	2.20	0.41
1:G:2464:ASP:HA	1:G:2467:VAL:HG12	2.03	0.41
1:G:2814:LYS:HA	1:G:2817:ILE:HG12	2.03	0.41
1:G:2823:ILE:HA	1:G:2936:ALA:O	2.20	0.41
1:G:3604:TYR:O	1:G:3607:GLU:HG3	2.20	0.41
1:G:3891:LEU:O	1:G:3896:ASN:ND2	2.47	0.41
1:J:1037:ASP:OD1	1:J:1037:ASP:N	2.53	0.41
1:J:1683:HIS:CG	1:J:1797:ARG:HH21	2.39	0.41
1:J:2005:GLN:O	1:J:2009:LEU:HD23	2.21	0.41
1:J:2333:ASP:HA	1:J:2336:ARG:HG2	2.02	0.41
1:J:2515:GLN:O	1:J:2519:LEU:HG	2.21	0.41
1:J:2819:TRP:NE1	1:J:2881:ASN:OD1	2.42	0.41
1:J:3391:GLU:HA	1:J:3394:VAL:HG22	2.03	0.41
1:J:3923:LEU:HD11	1:J:3962:PHE:CZ	2.56	0.41
1:J:4123:ILE:H	1:J:4123:ILE:HD12	1.85	0.41
1:J:4243:PHE:HE2	1:J:4668:LEU:HA	1.86	0.41
1:J:4541:TRP:O	1:J:4544:LEU:HG	2.20	0.41
1:J:4960:ILE:HB	1:J:4983:HIS:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:100:VAL:HG22	3:K:105:ASN:HB2	2.03	0.41
1:B:77:ALA:HB2	1:G:3935:TRP:CZ2	2.56	0.41
1:B:213:TYR:C	1:B:341:TYR:HB2	2.41	0.41
1:B:468:LEU:O	1:B:472:ARG:HG2	2.20	0.41
1:B:667:MET:HB2	1:B:790:ARG:HB2	2.03	0.41
1:B:684:VAL:HG13	1:B:781:VAL:HG12	2.03	0.41
1:B:1042:ALA:O	1:B:1046:LEU:HG	2.21	0.41
1:B:1078:GLU:HA	1:B:1237:TRP:CD1	2.55	0.41
1:B:1683:HIS:CG	1:B:1797:ARG:HH21	2.39	0.41
1:B:1737:PRO:HG2	1:B:1769:THR:HG22	2.03	0.41
1:B:1758:ARG:NH1	1:B:2037:ASP:HA	2.36	0.41
1:B:2230:THR:O	1:B:2234:ARG:HG3	2.21	0.41
1:B:2273:LEU:HD11	1:B:2334:PHE:HB2	2.03	0.41
1:B:2368:LEU:HD11	1:B:2376:LEU:HD12	2.02	0.41
1:B:2819:TRP:NE1	1:B:2881:ASN:OD1	2.42	0.41
1:B:2866:THR:HG21	1:B:2872:GLN:NE2	2.36	0.41
1:B:2874:MET:HE1	1:B:2939:ARG:NH1	2.35	0.41
1:B:3131:TYR:CE2	1:B:3136:LEU:HG	2.56	0.41
1:B:3391:GLU:HA	1:B:3394:VAL:HG22	2.03	0.41
1:B:3400:VAL:HG23	1:B:3403:ARG:HH21	1.84	0.41
1:B:3432:GLU:O	1:B:3435:PHE:HB3	2.20	0.41
1:B:3531:ASP:O	1:B:3535:LEU:HD23	2.20	0.41
1:B:3962:PHE:HZ	1:B:3992:PHE:CE2	2.39	0.41
1:B:3962:PHE:O	1:B:3966:THR:HG23	2.20	0.41
1:B:4664:LEU:HD22	1:B:4665:LYS:HD3	2.03	0.41
1:E:113:HIS:NE2	1:E:402:ARG:HB3	2.35	0.41
1:E:172:VAL:HG22	1:E:179:TYR:HA	2.03	0.41
1:E:445:LEU:HD21	1:E:522:LEU:HD23	2.03	0.41
1:E:514:SER:O	1:E:518:ILE:HG13	2.20	0.41
1:E:636:ASN:OD1	1:E:637:LEU:N	2.52	0.41
1:E:710:ASP:OD1	1:E:711:LEU:N	2.54	0.41
1:E:733:PRO:HG2	1:E:762:CYS:HB3	2.03	0.41
1:E:816:LEU:HB2	1:E:819:GLU:HB2	2.03	0.41
1:E:871:ARG:HD3	1:E:925:SER:HB2	2.02	0.41
1:E:1288:PHE:HB2	1:E:1600:LEU:HB2	2.03	0.41
1:E:1737:PRO:HG2	1:E:1769:THR:HG22	2.03	0.41
1:E:1780:PRO:HD3	1:E:1801:ALA:H	1.86	0.41
1:E:2189:LYS:HA	1:E:2192:TYR:CZ	2.55	0.41
1:E:2230:THR:HG22	1:E:2234:ARG:HH11	1.85	0.41
1:E:2515:GLN:O	1:E:2519:LEU:HG	2.21	0.41
1:E:2558:VAL:O	1:E:2562:ILE:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2598:ALA:O	1:E:2602:VAL:HG23	2.20	0.41
1:E:2694:GLU:O	1:E:2697:ARG:HG3	2.20	0.41
1:E:2866:THR:HG21	1:E:2872:GLN:NE2	2.36	0.41
1:E:2879:ALA:HA	1:E:2882:TYR:HD2	1.85	0.41
1:E:2950:SER:HA	1:E:2953:LYS:HB2	2.03	0.41
1:E:3021:PRO:HD3	1:E:3036:LYS:NZ	2.34	0.41
1:E:3191:GLY:HA2	1:E:3194:LEU:HG	2.03	0.41
1:E:3400:VAL:HG23	1:E:3403:ARG:HH21	1.84	0.41
1:E:3935:TRP:CZ2	1:J:77:ALA:HB2	2.56	0.41
1:E:4160:LEU:HA	1:E:4163:PHE:HD2	1.84	0.41
1:E:4802:GLY:HA2	1:E:4808:PHE:HB2	2.02	0.41
1:E:4998:LYS:HG3	1:E:5003:HIS:CE1	2.56	0.41
1:G:57:ASN:HA	1:G:308:HIS:CD2	2.56	0.41
1:G:213:TYR:C	1:G:341:TYR:HB2	2.41	0.41
1:G:514:SER:O	1:G:518:ILE:HG13	2.20	0.41
1:G:667:MET:HB2	1:G:790:ARG:HB2	2.03	0.41
1:G:1079:LYS:HE3	1:G:1107:PRO:HB3	2.03	0.41
1:G:1288:PHE:HB2	1:G:1600:LEU:HB2	2.03	0.41
1:G:2515:GLN:O	1:G:2519:LEU:HG	2.21	0.41
1:G:2716:ASP:OD1	1:G:2716:ASP:N	2.54	0.41
1:G:2760:GLU:HA	1:G:2802:LYS:NZ	2.35	0.41
1:G:2862:LEU:HD23	1:G:2864:GLY:H	1.85	0.41
1:G:2950:SER:HA	1:G:2953:LYS:HB2	2.03	0.41
1:G:2958:GLY:O	1:G:2962:GLN:HG2	2.19	0.41
1:G:3670:GLU:OE1	1:G:3732:SER:HB3	2.20	0.41
1:G:4664:LEU:HD22	1:G:4665:LYS:HD3	2.03	0.41
1:G:4859:PHE:HE1	1:G:4909:TYR:HB3	1.85	0.41
1:G:4960:ILE:HB	1:G:4983:HIS:HB3	2.03	0.41
1:J:866:HIS:HB3	1:J:870:ILE:HG12	2.03	0.41
1:J:984:LEU:O	1:J:988:LEU:HG	2.21	0.41
1:J:1078:GLU:HA	1:J:1237:TRP:CD1	2.55	0.41
1:J:1079:LYS:HE3	1:J:1107:PRO:HB3	2.03	0.41
1:J:1095:VAL:O	1:J:1145:SER:OG	2.25	0.41
1:J:1478:ASP:OD1	1:J:1482:ASN:N	2.53	0.41
1:J:2636:PHE:O	1:J:2640:PRO:HD2	2.21	0.41
1:J:2866:THR:HG21	1:J:2872:GLN:NE2	2.36	0.41
1:J:3015:LEU:HD21	1:J:3025:LEU:HD12	2.03	0.41
1:J:3250:MET:HA	1:J:3253:ILE:HG22	2.02	0.41
1:J:3450:ASN:HA	1:J:3453:ARG:HG2	2.02	0.41
1:J:4664:LEU:HD22	1:J:4665:LYS:HD3	2.03	0.41
2:D:30:LEU:N	2:D:34:LYS:O	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:4:LEU:HD22	3:K:118:GLY:HA3	2.01	0.41
3:M:4:LEU:HD22	3:M:118:GLY:HA3	2.01	0.41
1:B:14:LEU:HD21	1:B:165:VAL:HG12	2.03	0.41
1:B:541:SER:HA	1:B:574:VAL:HG12	2.02	0.41
1:B:1240:LYS:HE2	1:B:1240:LYS:HB3	1.93	0.41
1:B:1459:GLN:HE22	1:B:1469:VAL:HA	1.87	0.41
1:B:2295:LEU:HA	1:B:2298:VAL:HG12	2.03	0.41
1:B:3522:LEU:HA	1:B:3525:CYS:SG	2.61	0.41
1:B:3935:TRP:CZ2	1:E:77:ALA:HB2	2.56	0.41
1:E:659:TYR:CE2	1:E:661:LYS:HB2	2.56	0.41
1:E:2788:HIS:CD2	1:E:2789:PRO:HD2	2.55	0.41
1:E:2814:LYS:HA	1:E:2817:ILE:HG12	2.03	0.41
1:E:3522:LEU:HA	1:E:3525:CYS:SG	2.61	0.41
1:G:219:VAL:HG12	1:G:261:ARG:HB2	2.03	0.41
1:G:221:ARG:NH2	1:G:255:HIS:O	2.49	0.41
1:G:467:LYS:HE3	1:G:467:LYS:HB3	1.87	0.41
1:G:573:GLU:CD	1:G:573:GLU:H	2.24	0.41
1:G:917:GLU:HB3	3:M:104:TYR:OH	2.18	0.41
1:G:2333:ASP:HA	1:G:2336:ARG:HG2	2.02	0.41
1:G:2636:PHE:O	1:G:2640:PRO:HD2	2.21	0.41
1:G:2788:HIS:CD2	1:G:2789:PRO:HD2	2.55	0.41
1:G:4998:LYS:HG3	1:G:5003:HIS:CE1	2.56	0.41
1:J:445:LEU:HD21	1:J:522:LEU:HD23	2.03	0.41
1:J:924:MET:HE1	3:K:106:PRO:HD2	2.02	0.41
1:J:1718:ILE:HG13	1:J:1719:HIS:ND1	2.36	0.41
1:J:2230:THR:HG22	1:J:2234:ARG:HH11	1.85	0.41
1:J:2558:VAL:O	1:J:2562:ILE:HG12	2.21	0.41
1:J:3172:ILE:HG21	1:J:3194:LEU:HD23	2.03	0.41
3:C:105:ASN:C	3:C:107:TRP:H	2.24	0.41
1:B:266:ARG:NH2	1:B:269:TRP:O	2.54	0.40
1:B:1079:LYS:HE3	1:B:1107:PRO:HB3	2.03	0.40
1:B:1466:LEU:O	1:B:1469:VAL:HG22	2.21	0.40
1:B:1478:ASP:OD1	1:B:1482:ASN:N	2.53	0.40
1:B:2303:ALA:O	1:B:2307:LEU:HD23	2.22	0.40
1:B:2333:ASP:HA	1:B:2336:ARG:HG2	2.02	0.40
1:B:2620:GLN:HA	1:B:2623:LEU:HD12	2.04	0.40
1:B:2999:ALA:HB3	1:B:3000:LYS:HZ2	1.87	0.40
1:B:3785:ALA:HA	1:B:3787:LYS:HE2	2.03	0.40
1:B:3847:PHE:HZ	1:B:3937:TYR:HH	1.67	0.40
1:B:4642:ALA:O	1:B:4646:LEU:HD23	2.21	0.40
1:E:266:ARG:NH2	1:E:269:TRP:O	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1466:LEU:O	1:E:1469:VAL:HG22	2.21	0.40
1:E:1718:ILE:HG13	1:E:1719:HIS:ND1	2.36	0.40
1:E:2230:THR:O	1:E:2234:ARG:HG3	2.21	0.40
1:E:4243:PHE:HE2	1:E:4668:LEU:HA	1.86	0.40
1:E:4567:LEU:HD13	1:E:4815:ASP:HB3	2.03	0.40
1:G:535:ALA:O	1:G:539:LEU:HG	2.21	0.40
1:G:587:ILE:HD12	1:G:624:ASN:HB3	2.02	0.40
1:G:973:SER:HA	1:G:1044:ARG:NH2	2.28	0.40
1:G:2303:ALA:O	1:G:2307:LEU:HD23	2.22	0.40
1:G:2558:VAL:O	1:G:2562:ILE:HG12	2.21	0.40
1:G:2755:ILE:HG22	1:G:2810:LYS:HZ1	1.87	0.40
1:G:2866:THR:O	1:G:2867:LEU:HB2	2.21	0.40
1:G:3015:LEU:HD21	1:G:3025:LEU:HD12	2.03	0.40
1:G:3131:TYR:CE2	1:G:3136:LEU:HG	2.56	0.40
1:G:3398:PHE:HA	1:G:3401:LEU:HG	2.03	0.40
1:G:4040:ILE:O	1:G:4044:MET:HG2	2.22	0.40
1:J:535:ALA:O	1:J:539:LEU:HG	2.21	0.40
1:J:1293:LEU:HD11	1:J:1594:ARG:HG2	2.03	0.40
1:J:1293:LEU:HD21	1:J:1594:ARG:HD3	2.03	0.40
1:J:1658:ASP:OD1	1:J:1658:ASP:N	2.52	0.40
1:J:2694:GLU:O	1:J:2697:ARG:HG3	2.20	0.40
1:J:3521:GLY:HA2	1:J:3524:MET:HG2	2.02	0.40
1:J:3533:ILE:O	1:J:3537:LYS:HG3	2.20	0.40
2:D:23:VAL:HB	2:D:45:PRO:HB2	2.03	0.40
2:I:23:VAL:HB	2:I:45:PRO:HB2	2.03	0.40
1:B:871:ARG:HD3	1:B:925:SER:HB2	2.02	0.40
1:B:927:GLU:HA	1:B:930:LYS:HD2	2.02	0.40
1:B:1434:TYR:HA	1:B:1518:CYS:O	2.22	0.40
1:B:2247:GLN:NE2	1:B:2281:ILE:O	2.38	0.40
1:B:2464:ASP:HA	1:B:2467:VAL:HG12	2.03	0.40
1:B:2470:ILE:HB	1:B:2502:MET:CE	2.52	0.40
1:B:2487:GLN:HB3	1:B:2546:MET:HE1	2.03	0.40
1:B:3244:PRO:HB2	1:B:3248:ARG:HE	1.86	0.40
1:B:3540:TYR:HB3	1:B:3604:TYR:CD2	2.56	0.40
1:B:4661:TYR:OH	1:B:4788:SER:HB2	2.21	0.40
1:B:4960:ILE:HB	1:B:4983:HIS:HB3	2.03	0.40
1:E:2121:PHE:CZ	1:E:3701:LEU:HB2	2.56	0.40
1:E:3349:ALA:HB1	1:E:3353:LEU:HD12	2.02	0.40
1:E:4123:ILE:H	1:E:4123:ILE:HD12	1.85	0.40
1:E:4182:GLU:OE1	1:E:4983:HIS:NE2	2.52	0.40
1:G:439:GLU:HG2	1:G:440:ALA:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1570:LYS:O	1:G:1572:ILE:HG13	2.22	0.40
1:G:1658:ASP:N	1:G:1658:ASP:OD1	2.52	0.40
1:G:1718:ILE:HG13	1:G:1719:HIS:ND1	2.36	0.40
1:G:1786:LEU:HD22	2:H:87:HIS:HD2	1.87	0.40
1:G:1828:ASP:N	1:G:1828:ASP:OD1	2.54	0.40
1:G:2438:PRO:HB2	1:G:2443:ILE:HD11	2.03	0.40
1:G:2620:GLN:HA	1:G:2623:LEU:HD12	2.04	0.40
1:G:2694:GLU:O	1:G:2697:ARG:HG3	2.20	0.40
1:G:3384:LYS:HG2	1:G:3386:GLU:N	2.36	0.40
1:G:3517:MET:SD	1:G:3517:MET:N	2.93	0.40
1:G:4168:GLU:O	1:G:4172:GLU:HG2	2.22	0.40
1:J:573:GLU:H	1:J:573:GLU:CD	2.24	0.40
1:J:871:ARG:HH11	1:J:922:LEU:HD22	1.86	0.40
1:J:1274:HIS:O	1:J:1559:GLN:NE2	2.53	0.40
1:J:1570:LYS:O	1:J:1572:ILE:HG13	2.21	0.40
1:J:2962:GLN:O	1:J:2966:TRP:HD1	2.05	0.40
1:J:3540:TYR:HB3	1:J:3604:TYR:CD2	2.56	0.40
1:J:4661:TYR:OH	1:J:4788:SER:HB2	2.21	0.40
3:C:85:LEU:HB3	3:C:125:VAL:HG13	2.03	0.40
3:M:85:LEU:HB3	3:M:125:VAL:HG13	2.03	0.40
1:B:172:VAL:HG22	1:B:179:TYR:HA	2.03	0.40
1:B:710:ASP:OD1	1:B:711:LEU:N	2.54	0.40
1:B:1119:GLU:HA	1:B:1133:HIS:CE1	2.56	0.40
1:B:2369:ARG:HD2	1:B:2369:ARG:HA	1.95	0.40
1:B:2759:ALA:HB1	1:B:2806:ARG:HA	2.02	0.40
1:B:3191:GLY:HA2	1:B:3194:LEU:HG	2.03	0.40
1:E:219:VAL:HG12	1:E:261:ARG:HB2	2.03	0.40
1:E:927:GLU:HA	1:E:930:LYS:HD2	2.02	0.40
1:E:1123:VAL:CG1	1:E:1132:TRP:HB3	2.52	0.40
1:E:1427:ILE:HD13	1:E:1427:ILE:HA	1.93	0.40
1:E:1434:TYR:HA	1:E:1518:CYS:O	2.22	0.40
1:E:1478:ASP:OD1	1:E:1482:ASN:N	2.52	0.40
1:E:1497:GLY:HA2	1:E:1500:PHE:HD2	1.86	0.40
1:E:1498:GLY:HA2	1:E:1501:VAL:HG12	2.03	0.40
1:E:2295:LEU:HA	1:E:2298:VAL:HG12	2.03	0.40
1:E:2738:ARG:H	1:E:2738:ARG:HD3	1.87	0.40
1:E:2759:ALA:HB1	1:E:2806:ARG:HA	2.02	0.40
1:E:2765:LYS:HA	1:E:2765:LYS:HD3	1.87	0.40
1:E:3540:TYR:HB3	1:E:3604:TYR:CD2	2.56	0.40
1:G:67:PHE:HE2	1:G:118:LEU:HB2	1.86	0.40
1:G:659:TYR:CE2	1:G:661:LYS:HB2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:927:GLU:HA	1:G:930:LYS:HD2	2.02	0.40
1:G:1101:ARG:HB3	1:G:1123:VAL:HG21	2.04	0.40
1:G:1293:LEU:HD11	1:G:1594:ARG:HG2	2.03	0.40
1:G:1466:LEU:O	1:G:1469:VAL:HG22	2.21	0.40
1:G:2121:PHE:CZ	1:G:3701:LEU:HB2	2.57	0.40
1:G:2230:THR:O	1:G:2234:ARG:HG3	2.21	0.40
1:G:3391:GLU:HA	1:G:3394:VAL:HG22	2.03	0.40
1:G:3445:TRP:HD1	1:G:3451:PHE:CD2	2.40	0.40
1:G:4128:PHE:HA	1:G:4131:ARG:NE	2.36	0.40
1:G:4188:ARG:HD2	1:G:4191:GLU:HG3	2.02	0.40
1:G:4661:TYR:OH	1:G:4786:ASP:OD2	2.30	0.40
1:G:4691:GLN:HB2	1:G:4703:ARG:HH22	1.85	0.40
1:J:213:TYR:C	1:J:341:TYR:HB2	2.41	0.40
1:J:871:ARG:HD3	1:J:925:SER:HB2	2.03	0.40
1:J:1740:PRO:HA	1:J:1743:ARG:HG2	2.03	0.40
1:J:2189:LYS:HA	1:J:2192:TYR:CZ	2.55	0.40
1:J:2230:THR:O	1:J:2234:ARG:HG3	2.21	0.40
1:J:3400:VAL:HG23	1:J:3403:ARG:HH21	1.84	0.40
1:J:3445:TRP:HD1	1:J:3451:PHE:CD2	2.40	0.40
1:J:4168:GLU:O	1:J:4172:GLU:HG2	2.22	0.40
1:J:4867:GLU:OE1	1:J:4872:PRO:HD2	2.22	0.40
1:B:487:VAL:O	1:B:491:ILE:HG13	2.22	0.40
1:B:719:LEU:C	1:B:730:VAL:HG12	2.42	0.40
1:B:1123:VAL:CG1	1:B:1132:TRP:HB3	2.52	0.40
1:B:2155:LEU:HD12	1:B:2188:ASN:HD22	1.87	0.40
1:B:2962:GLN:O	1:B:2966:TRP:HD1	2.05	0.40
1:B:3696:ASP:OD2	1:B:3773:ARG:NH2	2.54	0.40
1:B:4668:LEU:O	1:B:4672:LYS:HG3	2.21	0.40
1:B:4691:GLN:HB2	1:B:4703:ARG:HH22	1.85	0.40
1:B:4867:GLU:OE1	1:B:4872:PRO:HD2	2.22	0.40
1:E:213:TYR:C	1:E:341:TYR:HB2	2.41	0.40
1:E:535:ALA:O	1:E:539:LEU:HG	2.21	0.40
1:E:573:GLU:CD	1:E:573:GLU:H	2.24	0.40
1:E:719:LEU:C	1:E:730:VAL:HG12	2.42	0.40
1:E:1440:PHE:HZ	1:E:1563:GLN:HB2	1.87	0.40
1:E:4128:PHE:HA	1:E:4131:ARG:NE	2.36	0.40
1:E:4661:TYR:OH	1:E:4788:SER:HB2	2.21	0.40
1:E:4937:ILE:HD11	1:J:4930:ALA:HB1	2.03	0.40
1:G:664:PHE:CE1	1:G:746:CYS:HB2	2.56	0.40
1:G:1042:ALA:O	1:G:1046:LEU:HG	2.21	0.40
1:G:1830:VAL:HB	1:G:1837:GLN:HG3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2740:VAL:HG11	1:G:2815:ALA:HA	2.04	0.40
1:G:2948:THR:O	1:G:2953:LYS:HE3	2.22	0.40
1:G:3546:ASP:N	1:G:3546:ASP:OD1	2.55	0.40
1:G:4668:LEU:O	1:G:4672:LYS:HG3	2.21	0.40
1:J:733:PRO:HG2	1:J:762:CYS:HB3	2.03	0.40
1:J:1123:VAL:CG1	1:J:1132:TRP:HB3	2.52	0.40
1:J:1440:PHE:HZ	1:J:1563:GLN:HB2	1.87	0.40
1:J:1808:ARG:NH1	1:J:1853:ILE:O	2.49	0.40
1:J:2198:MET:HA	1:J:2203:MET:HE1	2.02	0.40
1:J:2716:ASP:OD1	1:J:2716:ASP:N	2.54	0.40
1:J:2765:LYS:HD3	1:J:2765:LYS:HA	1.87	0.40
1:J:3398:PHE:HA	1:J:3401:LEU:HG	2.03	0.40
1:J:3785:ALA:HA	1:J:3787:LYS:HE2	2.03	0.40
1:J:4668:LEU:O	1:J:4672:LYS:HG3	2.21	0.40
2:H:8:SER:O	2:H:70:GLN:HG3	2.21	0.40
2:H:62:GLY:HA3	2:H:74:LEU:HD21	2.03	0.40
3:F:85:LEU:HB3	3:F:125:VAL:HG13	2.04	0.40
3:K:85:LEU:HB3	3:K:125:VAL:HG13	2.03	0.40
1:B:67:PHE:HE2	1:B:118:LEU:HB2	1.86	0.40
1:B:246:TYR:HD1	1:B:375:LYS:HA	1.85	0.40
1:B:363:ASP:HA	1:B:364:PRO:HD2	1.96	0.40
1:B:451:TYR:OH	1:B:474:ARG:HD2	2.22	0.40
1:B:816:LEU:HB2	1:B:819:GLU:HB2	2.03	0.40
1:B:1780:PRO:HD3	1:B:1801:ALA:H	1.86	0.40
1:B:2948:THR:O	1:B:2953:LYS:HE3	2.22	0.40
1:E:48:PHE:HD2	1:E:50:GLU:OE1	2.03	0.40
1:E:67:PHE:HE2	1:E:118:LEU:HB2	1.86	0.40
1:E:119:SER:OG	1:E:120:CYS:N	2.54	0.40
1:E:1042:ALA:O	1:E:1046:LEU:HG	2.21	0.40
1:E:1095:VAL:O	1:E:1145:SER:OG	2.25	0.40
1:E:1293:LEU:HD21	1:E:1594:ARG:HD3	2.03	0.40
1:E:1459:GLN:HE22	1:E:1469:VAL:HA	1.87	0.40
1:E:1944:GLU:HG3	1:E:2126:ARG:NH1	2.37	0.40
1:E:2487:GLN:HB3	1:E:2546:MET:CE	2.52	0.40
1:E:2716:ASP:OD1	1:E:2716:ASP:N	2.54	0.40
1:E:3172:ILE:HG21	1:E:3194:LEU:HD23	2.03	0.40
1:E:3962:PHE:HZ	1:E:3992:PHE:CE2	2.39	0.40
1:E:4960:ILE:HB	1:E:4983:HIS:HB3	2.03	0.40
1:G:100:THR:HG21	1:G:162:LYS:HD3	2.03	0.40
1:G:445:LEU:HD21	1:G:522:LEU:HD23	2.03	0.40
1:G:516:LYS:NZ	1:G:555:GLU:HG3	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:710:ASP:OD1	1:G:711:LEU:N	2.54	0.40
1:G:871:ARG:HH11	1:G:922:LEU:HD22	1.86	0.40
1:G:1758:ARG:NH1	1:G:2037:ASP:HA	2.36	0.40
1:G:1944:GLU:HG3	1:G:2126:ARG:NH1	2.37	0.40
1:G:2155:LEU:HD12	1:G:2188:ASN:HD22	1.87	0.40
1:G:2487:GLN:HB3	1:G:2546:MET:CE	2.52	0.40
1:G:2928:LYS:HA	1:G:2928:LYS:HD3	1.85	0.40
1:J:659:TYR:CE2	1:J:661:LYS:HB2	2.56	0.40
1:J:719:LEU:C	1:J:730:VAL:HG12	2.42	0.40
1:J:1042:ALA:O	1:J:1046:LEU:HG	2.21	0.40
1:J:1101:ARG:HB3	1:J:1123:VAL:HG21	2.04	0.40
1:J:1498:GLY:HA2	1:J:1501:VAL:HG12	2.03	0.40
1:J:2121:PHE:CZ	1:J:3701:LEU:HB2	2.56	0.40
1:J:2627:VAL:HG22	1:J:2678:LEU:HD13	2.04	0.40
1:J:2991:HIS:O	1:J:2995:ILE:HG13	2.22	0.40
1:J:3021:PRO:HD3	1:J:3036:LYS:NZ	2.34	0.40
1:J:3131:TYR:CE2	1:J:3136:LEU:HG	2.56	0.40
1:J:3779:VAL:O	1:J:3783:ILE:HG13	2.21	0.40
1:J:4040:ILE:O	1:J:4044:MET:HG2	2.22	0.40
1:J:4694:ASP:N	1:J:4694:ASP:OD1	2.55	0.40
1:J:4998:LYS:HG3	1:J:5003:HIS:CE1	2.56	0.40
2:I:48:PHE:CZ	2:I:55:VAL:HG12	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	4280/5027 (85%)	4178 (98%)	100 (2%)	2 (0%)	100	100
1	E	4280/5027 (85%)	4178 (98%)	100 (2%)	2 (0%)	100	100
1	G	4280/5027 (85%)	4178 (98%)	100 (2%)	2 (0%)	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	4280/5027 (85%)	4178 (98%)	100 (2%)	2 (0%)	100	100
2	A	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
2	D	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
2	H	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
2	I	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
3	C	124/137 (90%)	117 (94%)	7 (6%)	0	100	100
3	F	124/137 (90%)	117 (94%)	7 (6%)	0	100	100
3	K	124/137 (90%)	117 (94%)	7 (6%)	0	100	100
3	M	124/137 (90%)	117 (94%)	7 (6%)	0	100	100
All	All	18036/21084 (86%)	17584 (98%)	444 (2%)	8 (0%)	100	100

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2867	LEU
1	E	2867	LEU
1	G	2867	LEU
1	J	2867	LEU
1	B	52	THR
1	E	52	THR
1	G	52	THR
1	J	52	THR

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	3659/4270 (86%)	3650 (100%)	9 (0%)	92	94
1	E	3659/4270 (86%)	3650 (100%)	9 (0%)	92	94
1	G	3659/4270 (86%)	3650 (100%)	9 (0%)	92	94
1	J	3659/4270 (86%)	3650 (100%)	9 (0%)	92	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	A	88/88 (100%)	87 (99%)	1 (1%)	70 79
2	D	88/88 (100%)	87 (99%)	1 (1%)	70 79
2	H	88/88 (100%)	87 (99%)	1 (1%)	70 79
2	I	88/88 (100%)	87 (99%)	1 (1%)	70 79
3	C	104/114 (91%)	104 (100%)	0	100 100
3	F	104/114 (91%)	104 (100%)	0	100 100
3	K	104/114 (91%)	104 (100%)	0	100 100
3	M	104/114 (91%)	104 (100%)	0	100 100
All	All	15404/17888 (86%)	15364 (100%)	40 (0%)	90 92

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	45	ARG
1	B	886	ARG
1	B	1025	ARG
1	B	1954	ARG
1	B	2690	LYS
1	B	2738	ARG
1	B	2827	ARG
1	B	2914	LYS
1	B	3694	LYS
1	E	45	ARG
1	E	886	ARG
1	E	1025	ARG
1	E	1954	ARG
1	E	2690	LYS
1	E	2738	ARG
1	E	2827	ARG
1	E	2914	LYS
1	E	3694	LYS
1	G	45	ARG
1	G	886	ARG
1	G	1025	ARG
1	G	1954	ARG
1	G	2690	LYS
1	G	2738	ARG
1	G	2827	ARG
1	G	2914	LYS

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Mol	Chain	Res	Type
1	G	3694	LYS
1	J	45	ARG
1	J	886	ARG
1	J	1025	ARG
1	J	1954	ARG
1	J	2690	LYS
1	J	2738	ARG
1	J	2827	ARG
1	J	2914	LYS
1	J	3694	LYS
2	A	18	LYS
2	D	18	LYS
2	H	18	LYS
2	I	18	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	797	HIS
1	B	879	HIS
1	B	1203	ASN
1	B	1206	GLN
1	B	1459	GLN
1	B	1691	GLN
1	B	2268	GLN
1	B	3008	GLN
1	B	3162	GLN
1	B	3889	GLN
1	B	3927	GLN
1	E	797	HIS
1	E	879	HIS
1	E	963	ASN
1	E	1203	ASN
1	E	1206	GLN
1	E	1459	GLN
1	E	1691	GLN
1	E	2268	GLN
1	E	3162	GLN
1	E	3889	GLN
1	E	3927	GLN
1	G	797	HIS
1	G	879	HIS

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Mol	Chain	Res	Type
1	G	1203	ASN
1	G	1206	GLN
1	G	1459	GLN
1	G	1691	GLN
1	G	2268	GLN
1	G	3162	GLN
1	G	3889	GLN
1	G	3927	GLN
1	J	797	HIS
1	J	879	HIS
1	J	1203	ASN
1	J	1206	GLN
1	J	1459	GLN
1	J	1691	GLN
1	J	2268	GLN
1	J	3162	GLN
1	J	3889	GLN
1	J	3927	GLN
2	A	65	GLN
2	A	87	HIS
2	D	65	GLN
2	D	87	HIS
2	H	65	GLN
2	H	87	HIS
2	I	65	GLN
2	I	87	HIS
3	C	1	GLN
3	F	1	GLN
3	K	1	GLN
3	K	122	GLN
3	M	1	GLN
3	M	122	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	CFF	J	5103	-	8,15,15	1.02	0	8,23,23	2.44	2 (25%)
5	ATP	B	5102	-	26,33,33	0.60	0	31,52,52	0.77	2 (6%)
5	ATP	G	5102	-	26,33,33	0.61	0	31,52,52	0.77	2 (6%)
6	CFF	B	5103	-	8,15,15	1.03	0	8,23,23	2.47	2 (25%)
5	ATP	E	5102	-	26,33,33	0.60	0	31,52,52	0.77	2 (6%)
6	CFF	E	5103	-	8,15,15	1.02	0	8,23,23	2.45	2 (25%)
6	CFF	G	5103	-	8,15,15	2.43	3 (37%)	8,23,23	1.22	1 (12%)
5	ATP	J	5102	-	26,33,33	0.61	0	31,52,52	0.77	2 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CFF	J	5103	-	-	-	0/2/2/2
5	ATP	B	5102	-	-	6/18/38/38	0/3/3/3
5	ATP	G	5102	-	-	6/18/38/38	0/3/3/3
6	CFF	B	5103	-	-	-	0/2/2/2
5	ATP	E	5102	-	-	6/18/38/38	0/3/3/3
6	CFF	E	5103	-	-	-	0/2/2/2
6	CFF	G	5103	-	-	-	0/2/2/2
5	ATP	J	5102	-	-	6/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	5103	CFF	C5-C4	4.60	1.45	1.39
6	G	5103	CFF	C5-C6	4.35	1.48	1.41
6	G	5103	CFF	C6-N1	2.26	1.41	1.38

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	5103	CFF	C5-C6-N1	-5.86	111.95	118.20
6	E	5103	CFF	C5-C6-N1	-5.82	111.99	118.20
6	J	5103	CFF	C5-C6-N1	-5.80	112.01	118.20
6	B	5103	CFF	C4-C5-C6	3.49	122.20	119.96
6	E	5103	CFF	C4-C5-C6	3.44	122.17	119.96
6	J	5103	CFF	C4-C5-C6	3.43	122.17	119.96
6	G	5103	CFF	C5-C6-N1	-2.39	115.65	118.20
5	B	5102	ATP	C5-C6-N6	2.30	123.85	120.35
5	J	5102	ATP	C5-C6-N6	2.28	123.82	120.35
5	G	5102	ATP	C5-C6-N6	2.26	123.79	120.35
5	E	5102	ATP	C5-C6-N6	2.25	123.76	120.35
5	G	5102	ATP	PB-O3B-PG	2.05	139.88	132.83
5	E	5102	ATP	PB-O3B-PG	2.04	139.84	132.83
5	J	5102	ATP	PB-O3B-PG	2.04	139.82	132.83
5	B	5102	ATP	PB-O3B-PG	2.04	139.81	132.83

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	5102	ATP	PB-O3B-PG-O2G
5	B	5102	ATP	PB-O3B-PG-O3G
5	B	5102	ATP	C5'-O5'-PA-O1A
5	B	5102	ATP	C5'-O5'-PA-O2A
5	E	5102	ATP	PB-O3B-PG-O2G
5	E	5102	ATP	PB-O3B-PG-O3G
5	E	5102	ATP	C5'-O5'-PA-O1A
5	E	5102	ATP	C5'-O5'-PA-O2A
5	G	5102	ATP	PB-O3B-PG-O2G
5	G	5102	ATP	PB-O3B-PG-O3G
5	G	5102	ATP	C5'-O5'-PA-O1A
5	G	5102	ATP	C5'-O5'-PA-O2A
5	J	5102	ATP	PB-O3B-PG-O2G
5	J	5102	ATP	PB-O3B-PG-O3G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	J	5102	ATP	C5'-O5'-PA-O1A
5	J	5102	ATP	C5'-O5'-PA-O2A
5	B	5102	ATP	C5'-O5'-PA-O3A
5	E	5102	ATP	C5'-O5'-PA-O3A
5	G	5102	ATP	C5'-O5'-PA-O3A
5	J	5102	ATP	C5'-O5'-PA-O3A
5	B	5102	ATP	O4'-C4'-C5'-O5'
5	E	5102	ATP	O4'-C4'-C5'-O5'
5	G	5102	ATP	O4'-C4'-C5'-O5'
5	J	5102	ATP	O4'-C4'-C5'-O5'

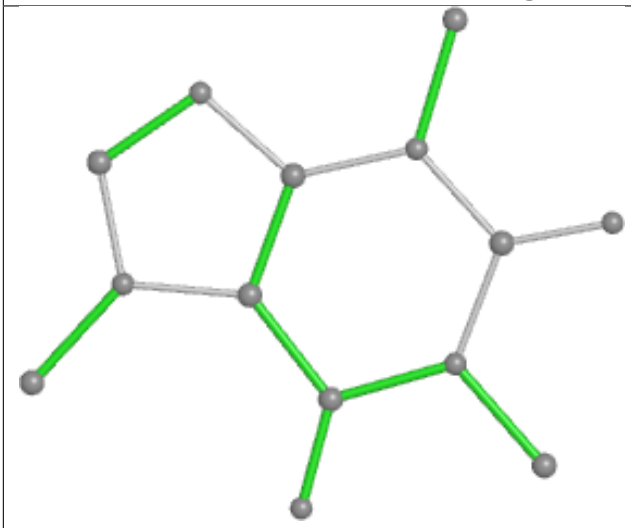
There are no ring outliers.

8 monomers are involved in 11 short contacts:

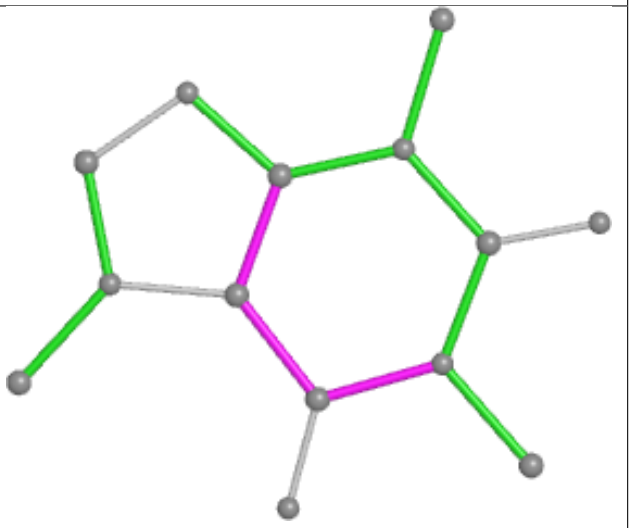
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	5103	CFF	1	0
5	B	5102	ATP	1	0
5	G	5102	ATP	1	0
6	B	5103	CFF	1	0
5	E	5102	ATP	1	0
6	E	5103	CFF	1	0
6	G	5103	CFF	4	0
5	J	5102	ATP	1	0

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

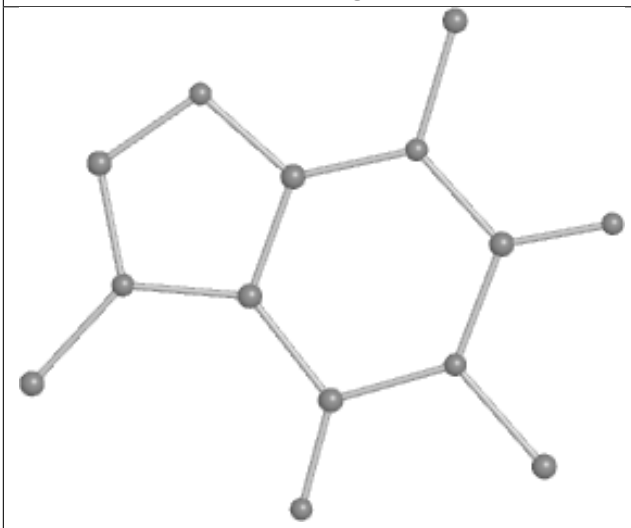
Ligand CFF J 5103



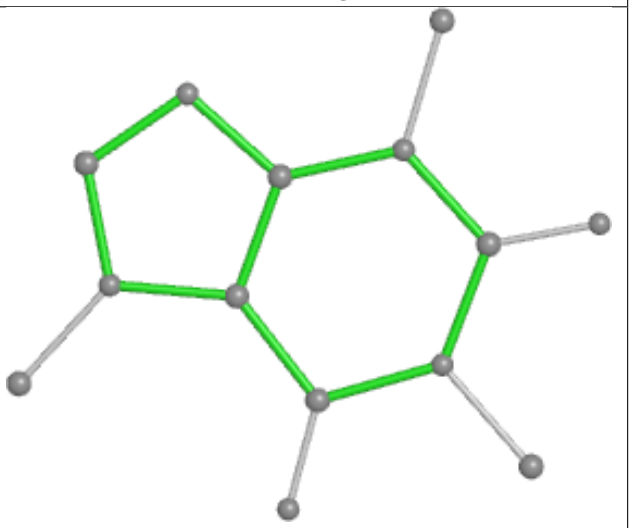
Bond lengths



Bond angles

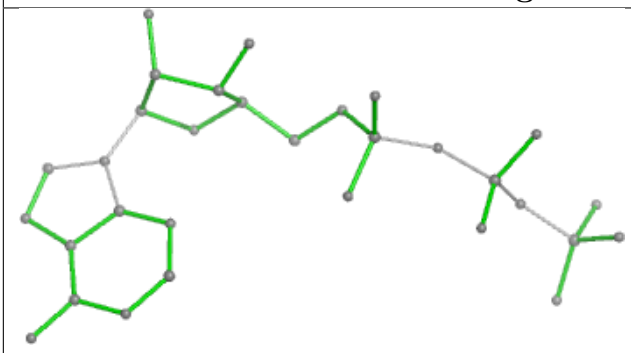


Torsions

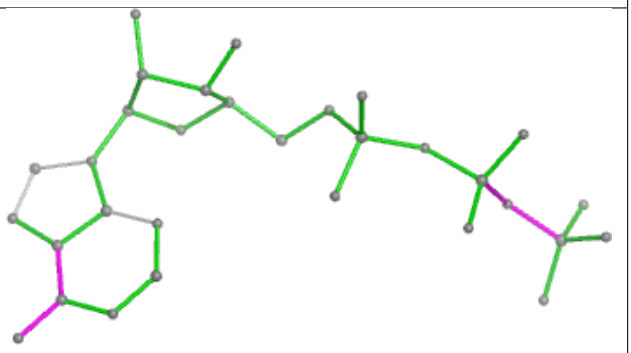


Rings

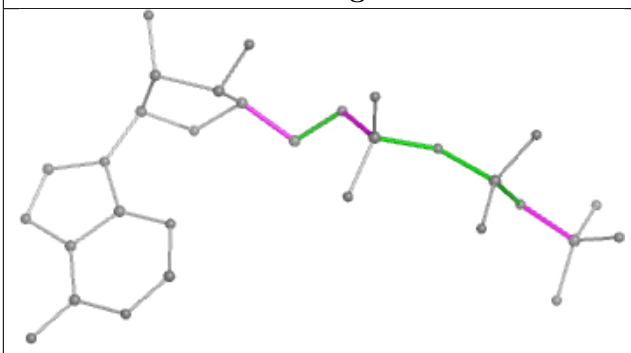
Ligand ATP B 5102



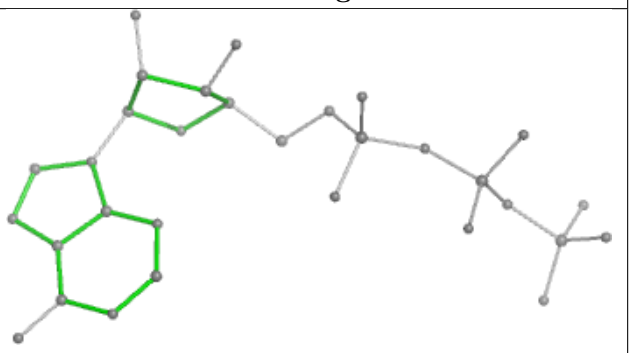
Bond lengths



Bond angles

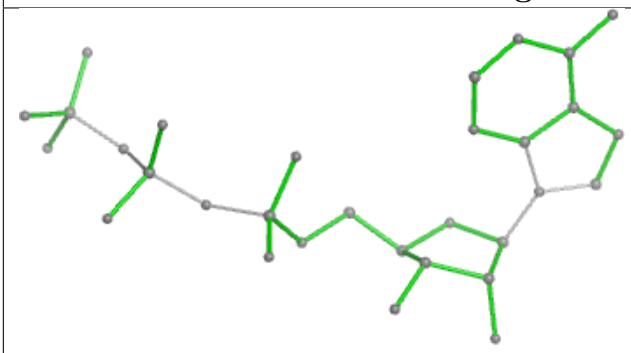


Torsions

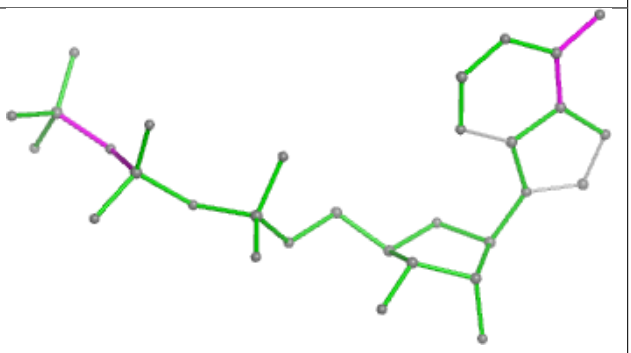


Rings

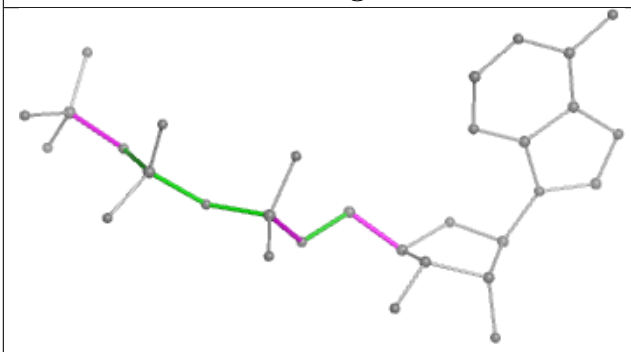
Ligand ATP G 5102



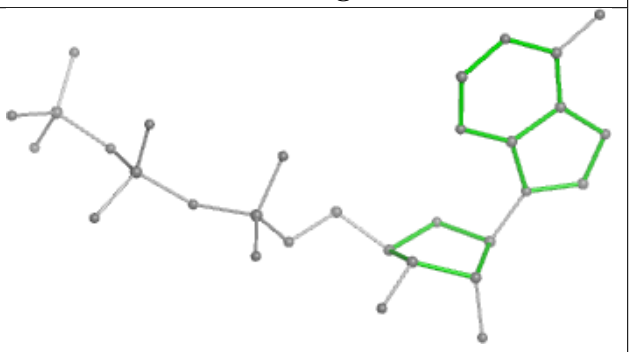
Bond lengths



Bond angles

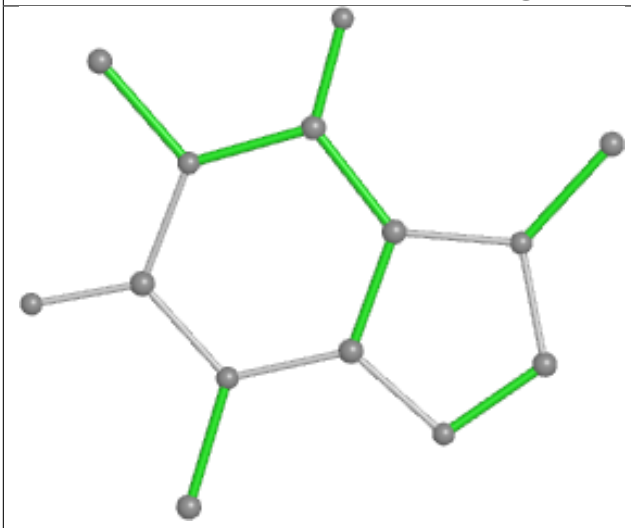


Torsions

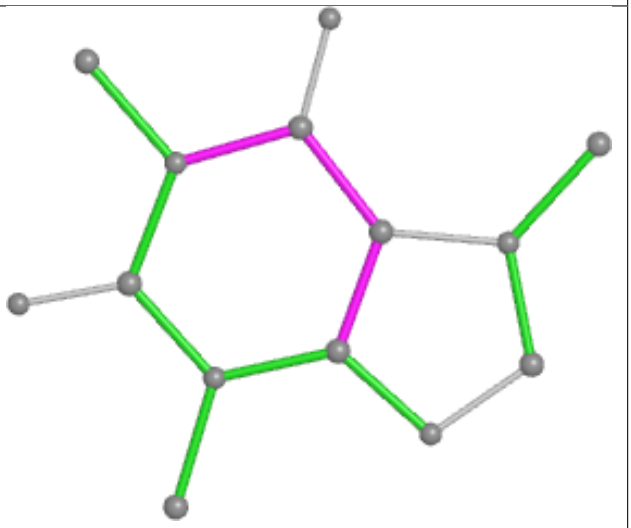


Rings

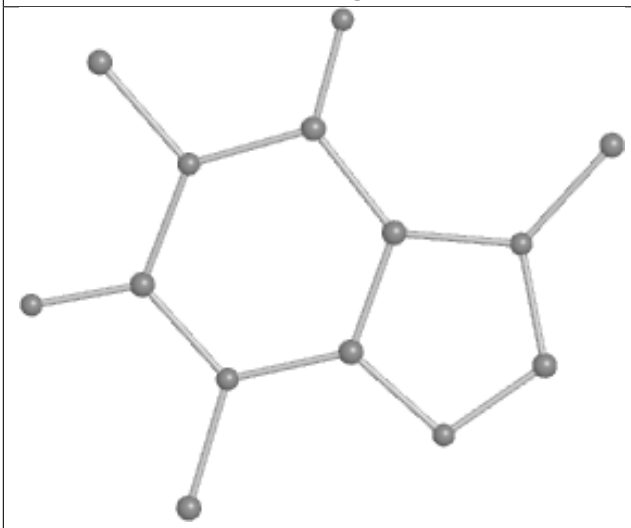
Ligand CFF B 5103



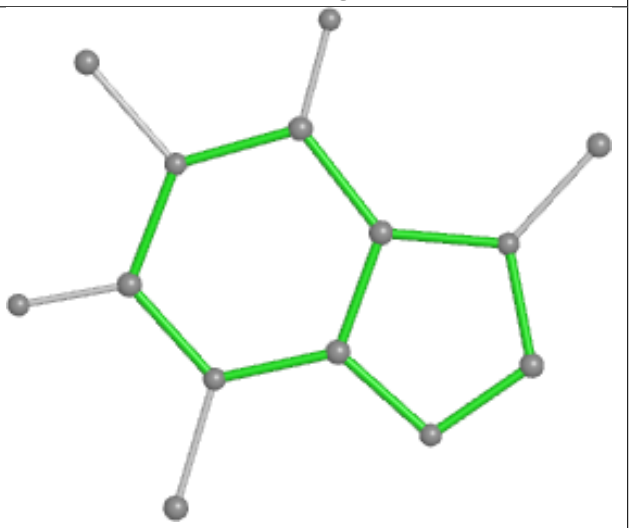
Bond lengths



Bond angles

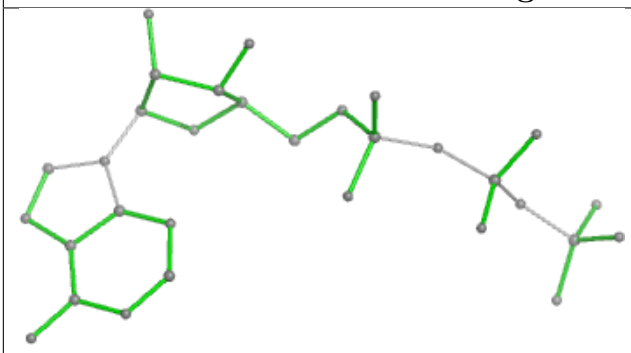


Torsions

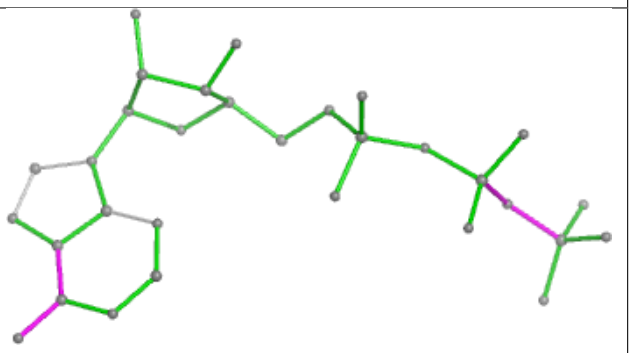


Rings

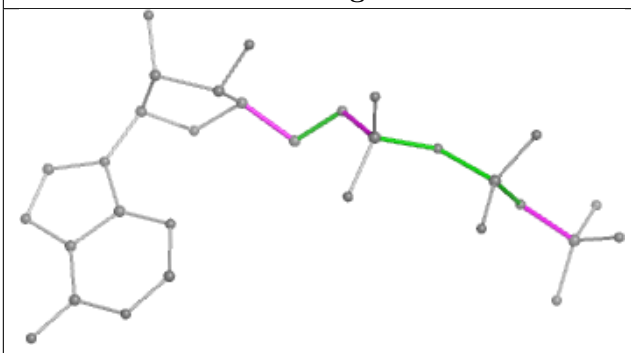
Ligand ATP E 5102



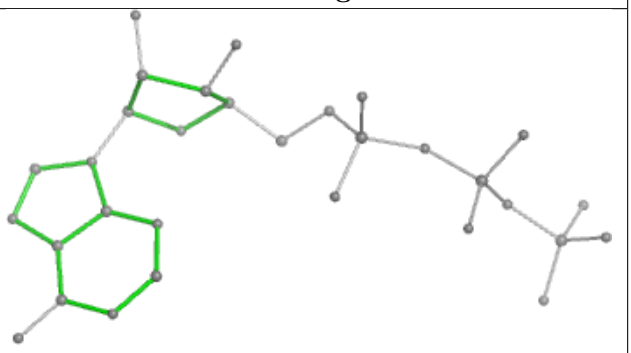
Bond lengths



Bond angles

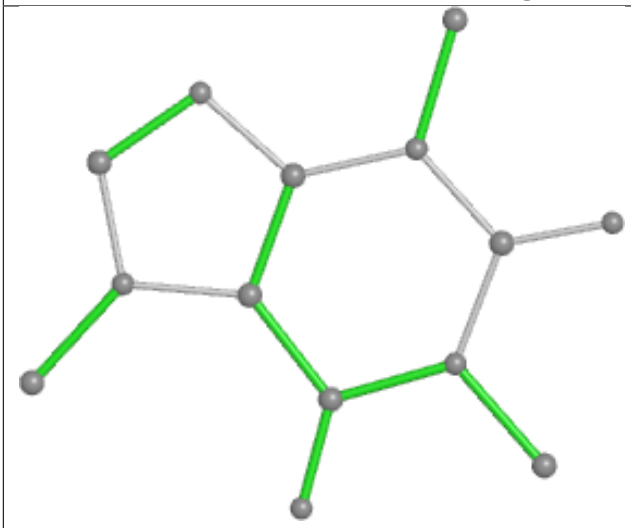


Torsions

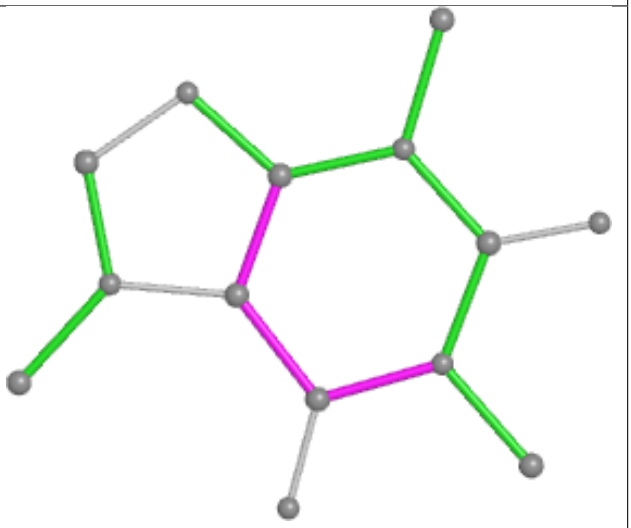


Rings

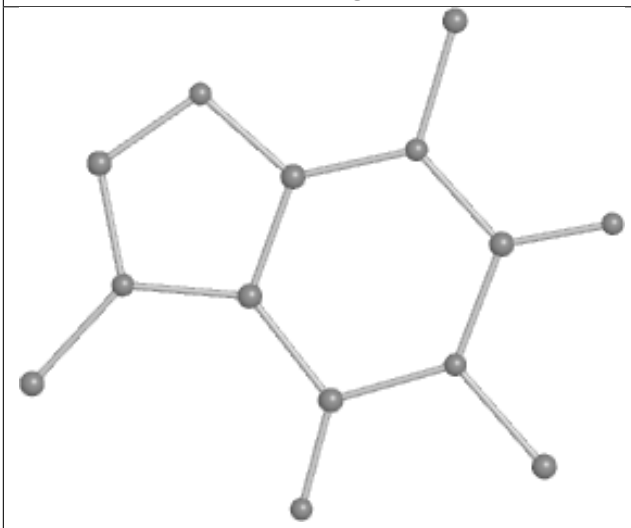
Ligand CFF E 5103



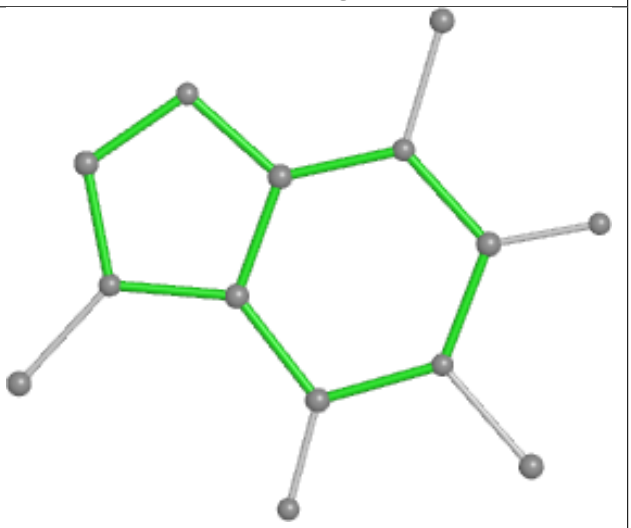
Bond lengths



Bond angles

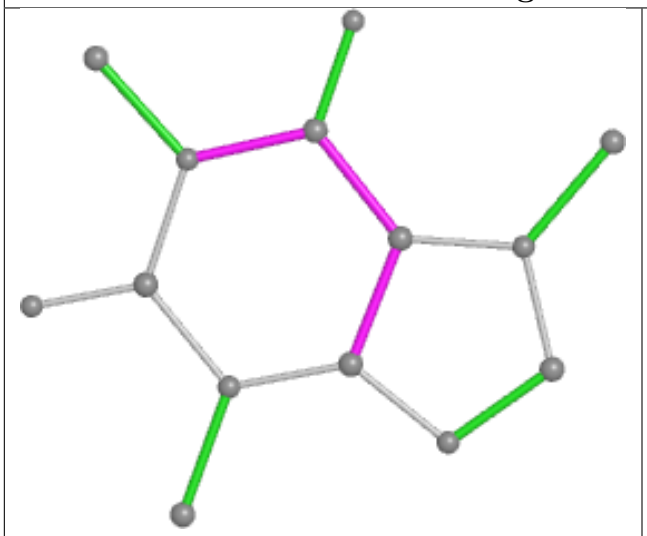


Torsions

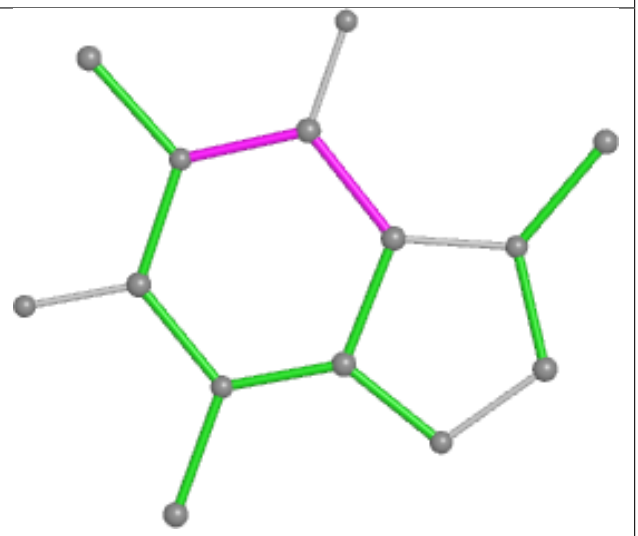


Rings

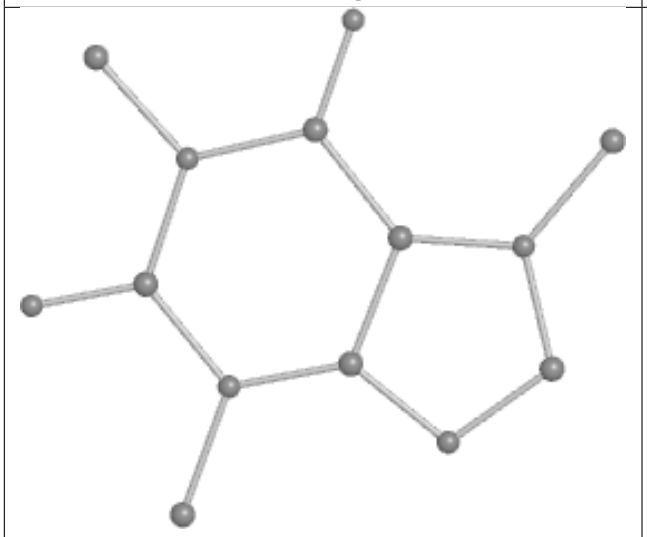
Ligand CFF G 5103



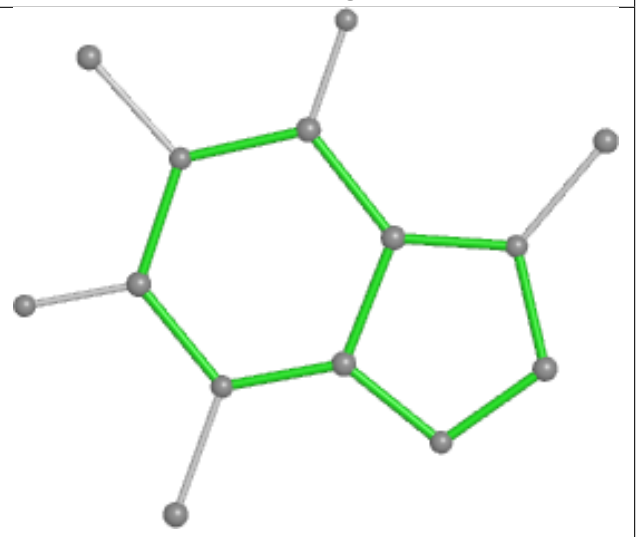
Bond lengths



Bond angles

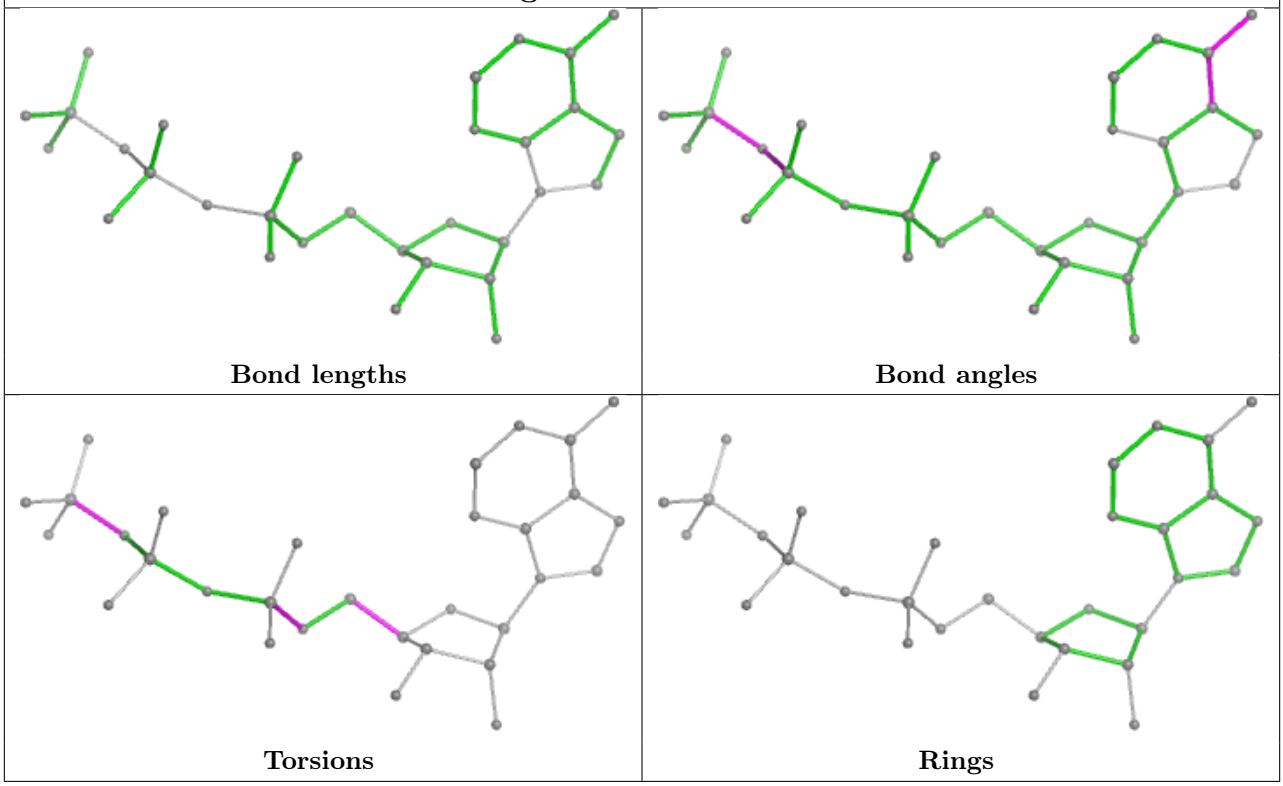


Torsions



Rings

Ligand ATP J 5102



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.

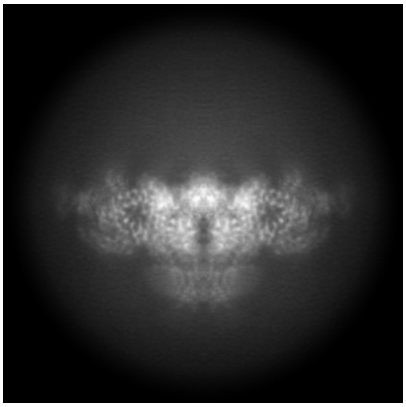
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-19467. These allow visual inspection of the internal detail of the map and identification of artifacts.

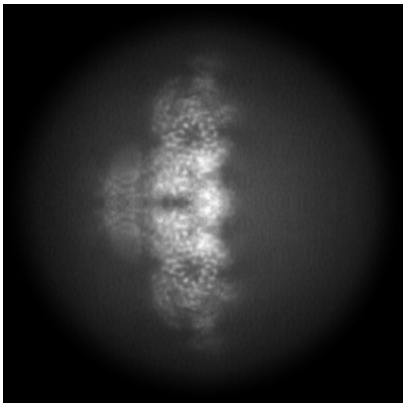
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

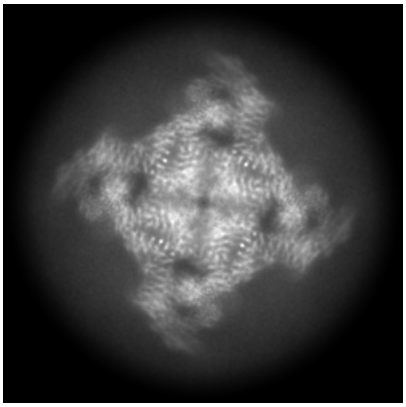
6.1.1 Primary map



X



Y

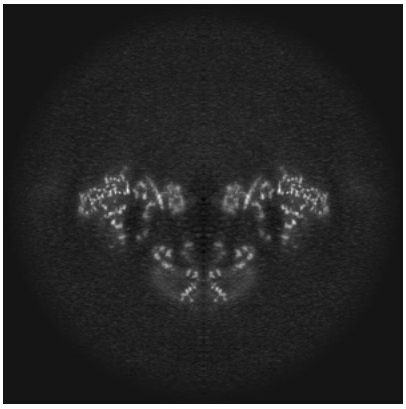


Z

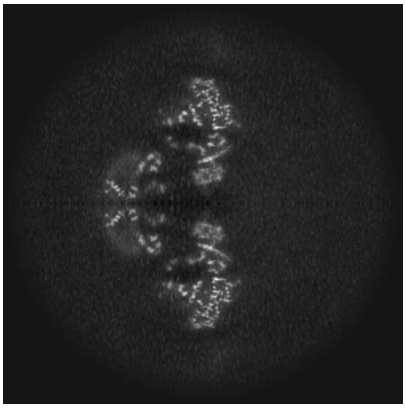
The images above show the map projected in three orthogonal directions.

6.2 Central slices

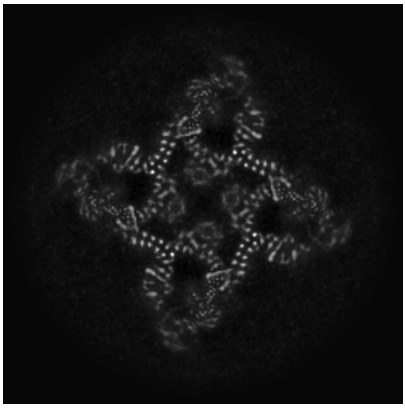
6.2.1 Primary map



X Index: 168



Y Index: 168

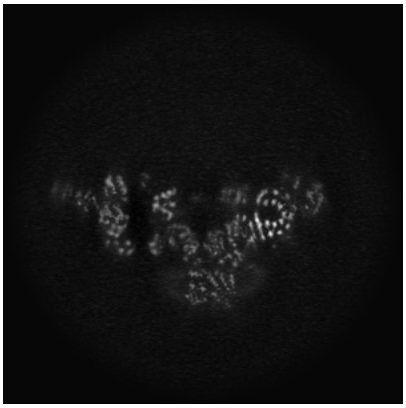


Z Index: 168

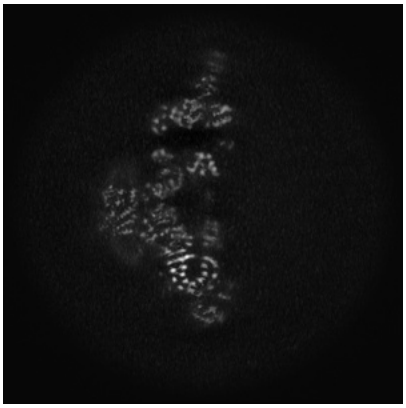
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

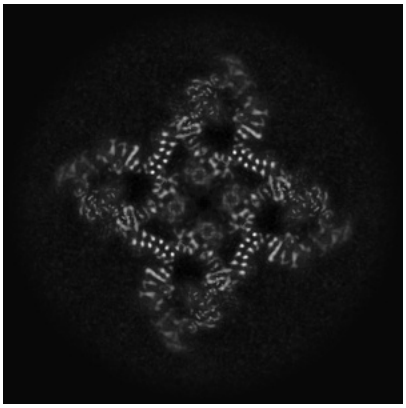
6.3.1 Primary map



X Index: 157



Y Index: 157

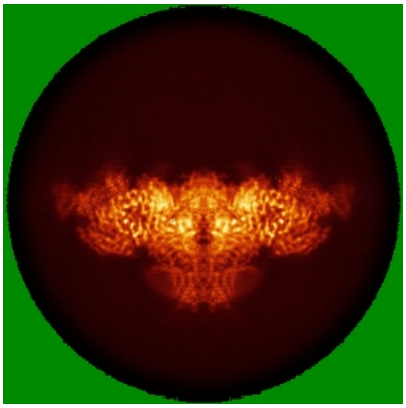


Z Index: 167

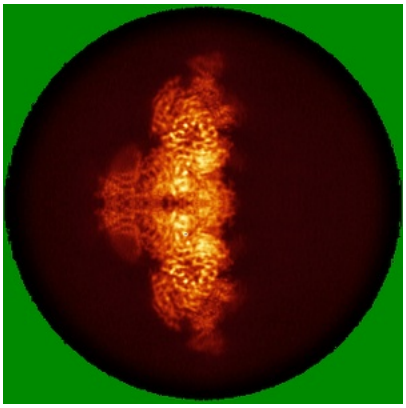
The images above show the largest variance slices of the map in three orthogonal directions.

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

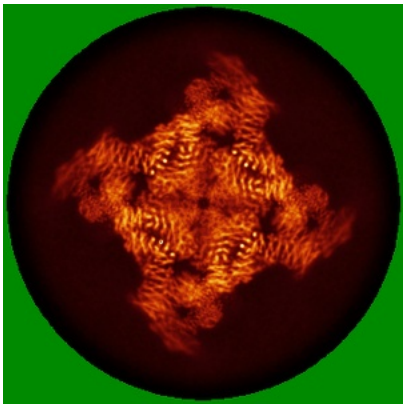
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.28. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

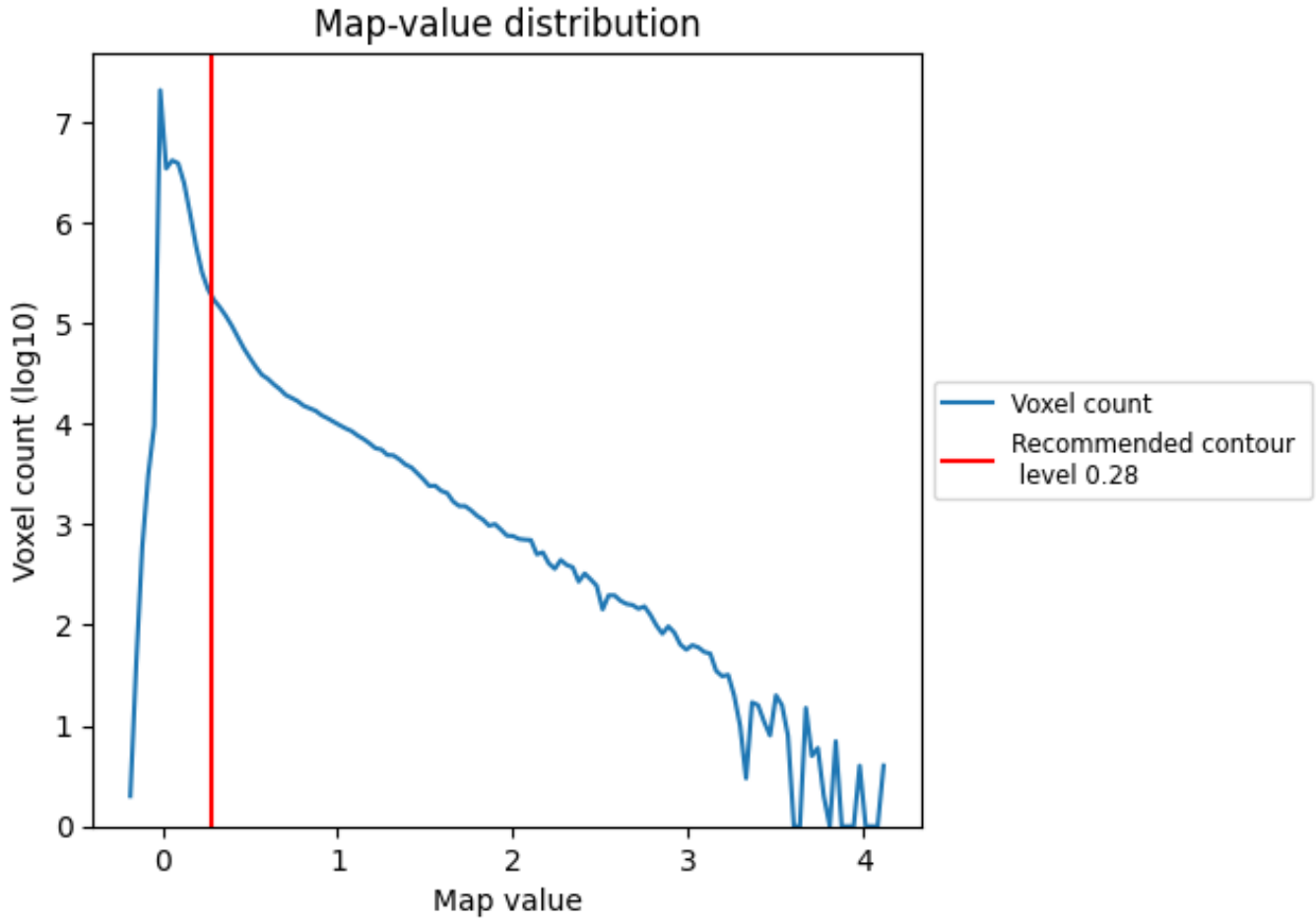
6.6 Mask visualisation (i)

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

7 Map analysis

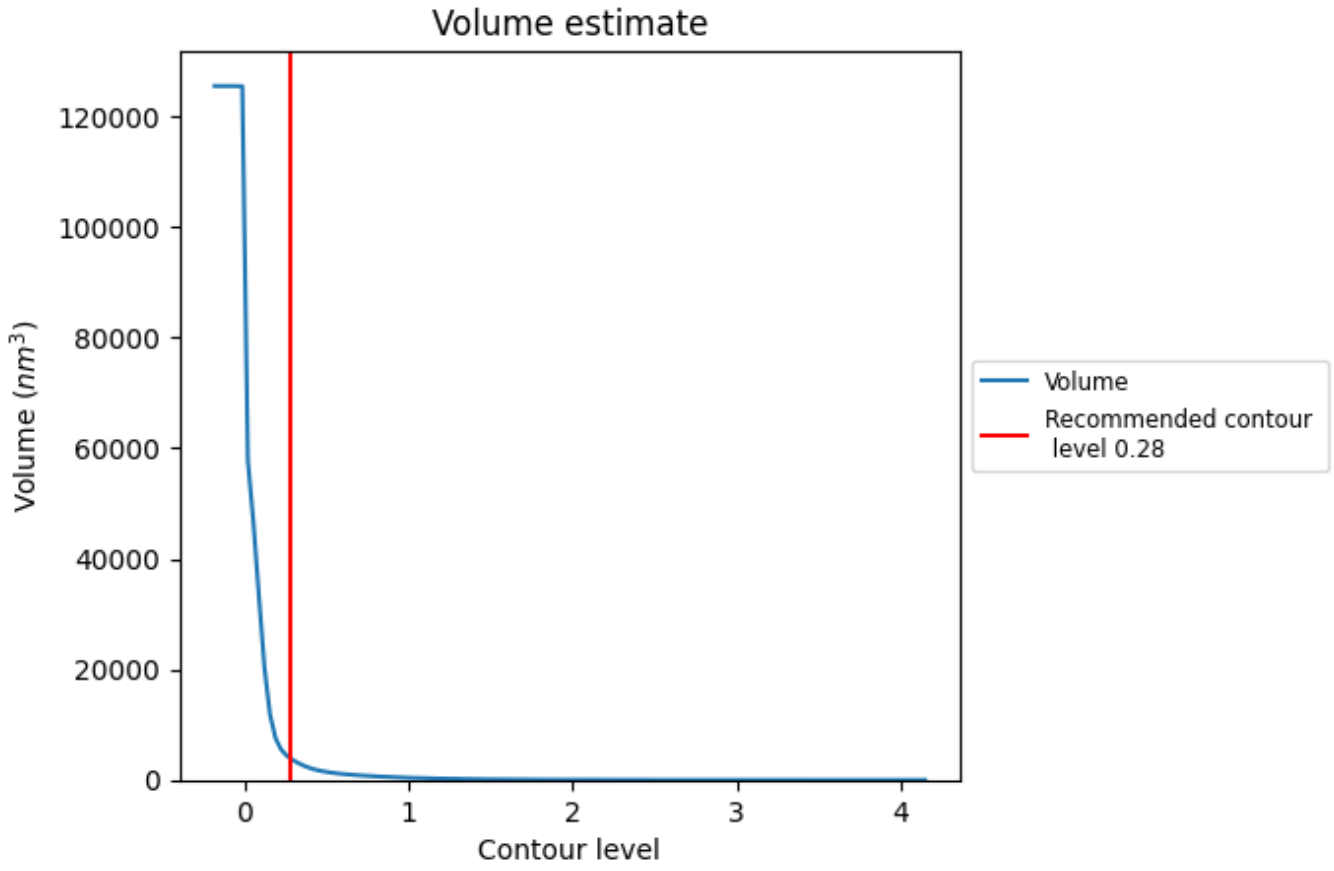
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

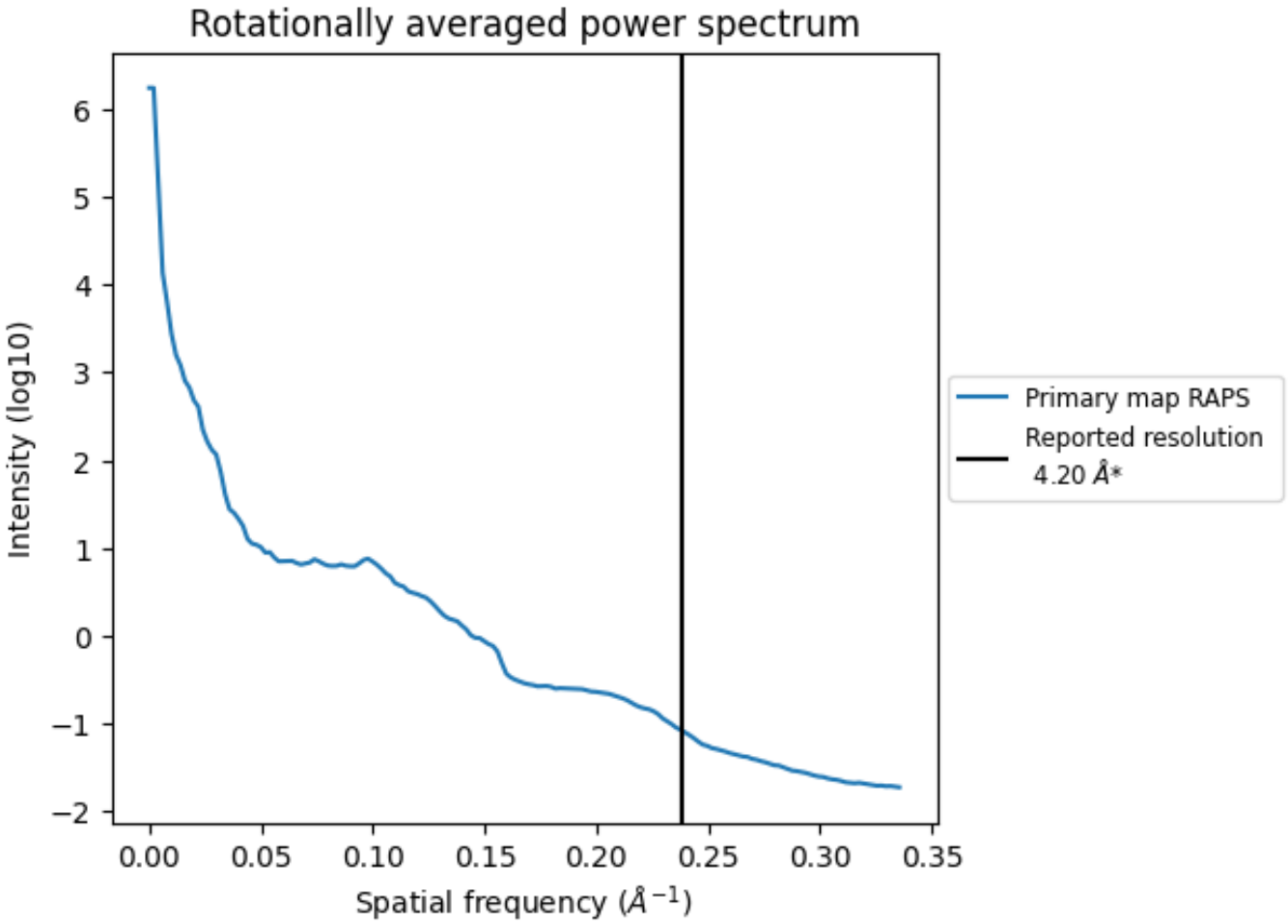
7.2 Volume estimate



The volume at the recommended contour level is 3900 nm^3; this corresponds to an approximate mass of 3523 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

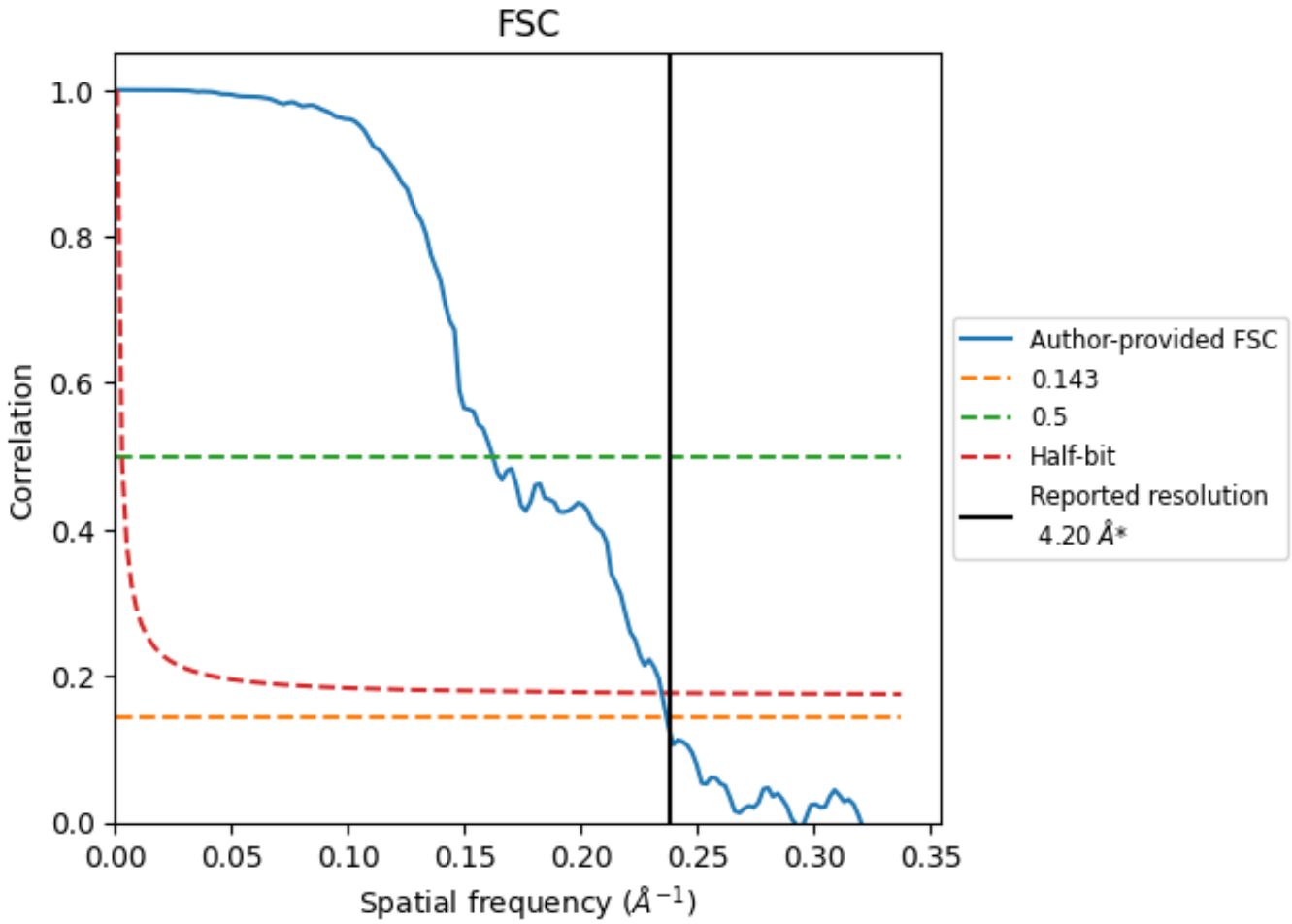


*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

8.2 Resolution estimates (i)

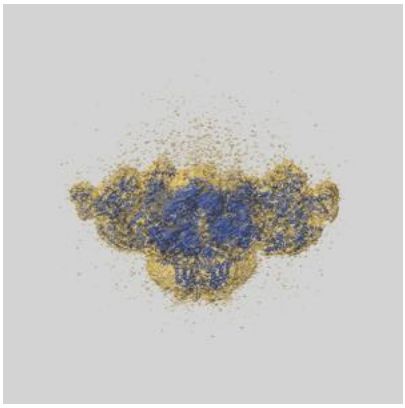
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.22	6.17	4.26
Unmasked-calculated*	-	-	-

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

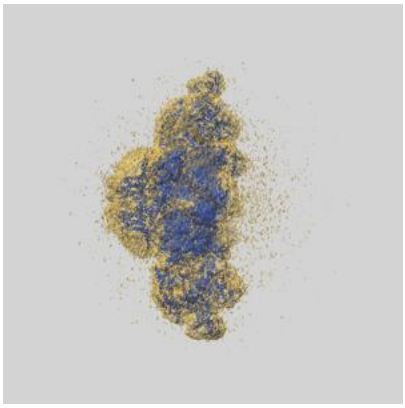
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-19467 and PDB model 8RRW. Per-residue inclusion information can be found in section 3 on page 8.

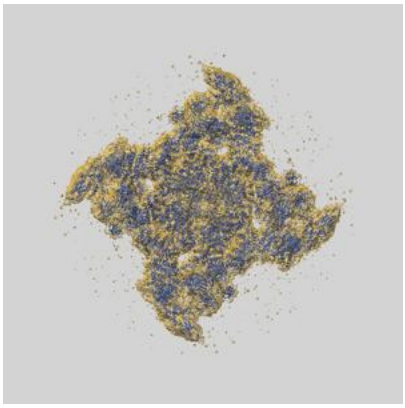
9.1 Map-model overlay



X



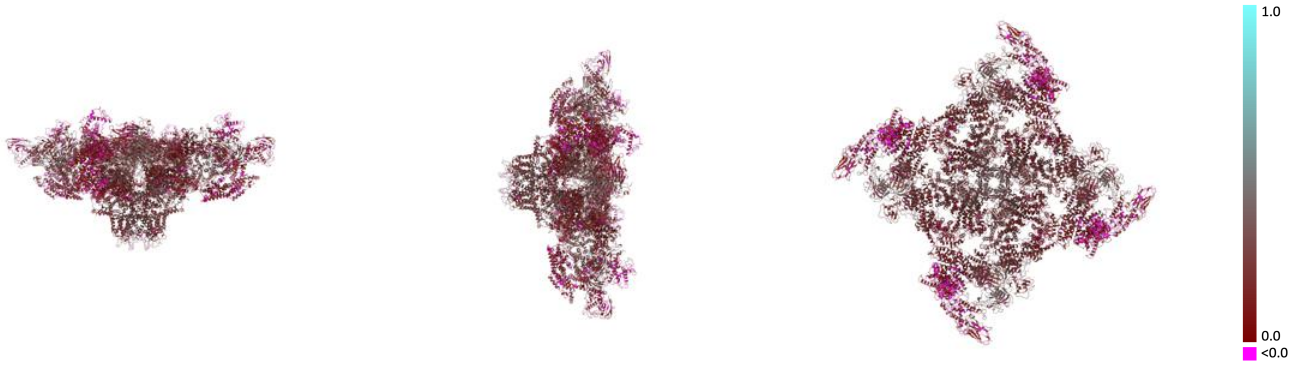
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.28 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

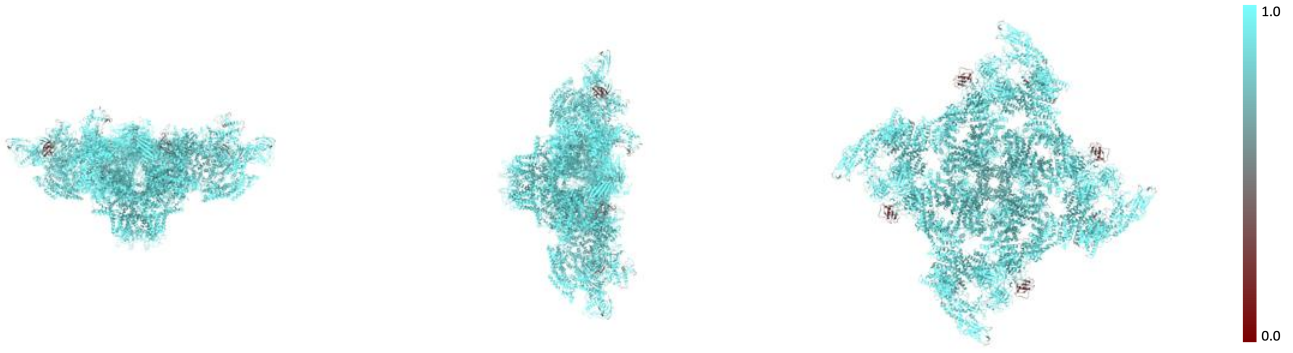
9.2 Q-score mapped to coordinate model



X Y Z

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

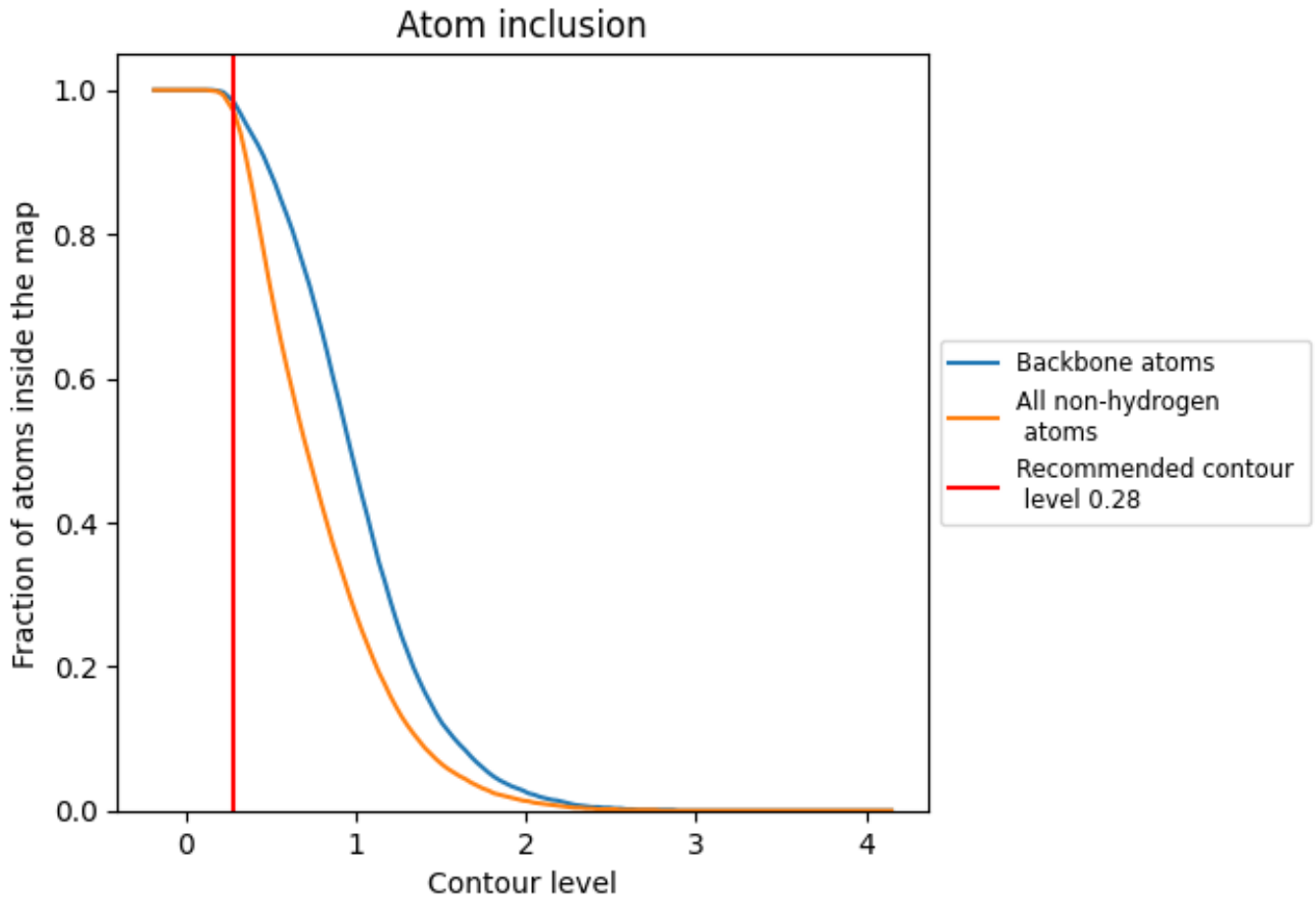
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.28).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 97% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.28) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9720	0.2010
A	0.5280	0.2090
B	0.9840	0.2030
C	0.9250	0.1360
D	0.5240	0.2080
E	0.9840	0.2030
F	0.9240	0.1370
G	0.9840	0.2030
H	0.5320	0.2130
I	0.5300	0.2090
J	0.9840	0.2030
K	0.9250	0.1380
M	0.9250	0.1360