Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2024 – 09:41 AM EDT

PDB ID	:	2R7Z
Title	:	Cisplatin lesion containing RNA polymerase II elongation complex
Authors	:	Damsma, G.E.; Alt, A.; Brueckner, F.; Carell, T.; Cramer, P.
Deposited on	:	2007-09-10
Resolution	:	3.80 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

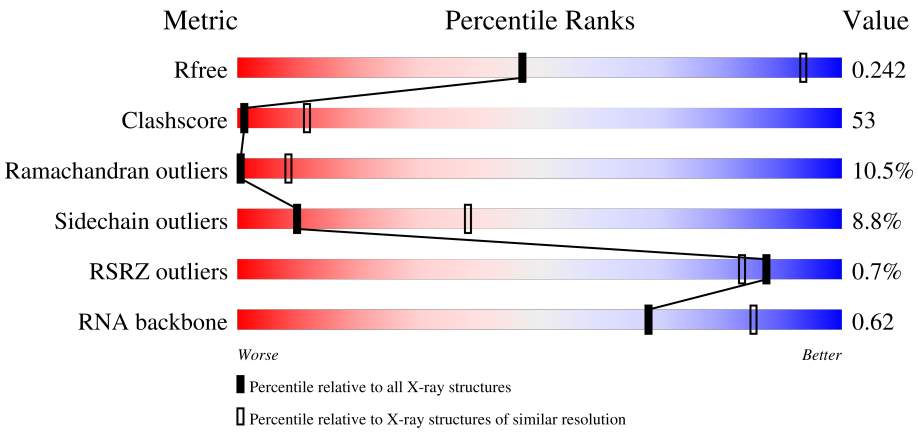
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)
RNA backbone	3102	1036 (4.60-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	T	17	65% 29% 6%
2	N	7	71% 29%
3	P	10	20% 70% 10%
4	A	1733	26% 45% 10% • 18%

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Mol	Chain	Length	Quality of chain
5	B	1224	% 27% 52% 11% • 9%
6	C	318	23% 48% 11% • 16%
7	D	221	28% 38% 11% • 20%
8	E	215	39% 55% 5%
9	F	155	19% 28% 6% • 46%
10	G	171	37% 54% 9%
11	H	146	2% 27% 52% 12% 9%
12	I	122	2% 34% 52% 11% • •
13	J	70	29% 47% 16% • 7%
14	K	120	% 28% 57% 11% 5%
15	L	70	11% 39% 13% • 34%

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 31804 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 DNA chain called 5'-D(*TP*AP*CP*TP*TP*GUP*CP*CP*CP*TP*CP*CP*TP*CP*AP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	T	17	336	163	53	104	16	0	0	0

- Molecule 2 is a DNA chain called 5'-D(*CP*AP*AP*GP*TP*AP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	N	7	143	69	30	38	6	0	0	0

- Molecule 3 is a RNA chain called 5'-R(*UP*UP*UP*GP*AP*GP*GP*AP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	P	10	216	97	41	69	9	0	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	A	1416	11140	7021	1946	2111	62	0	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	B	1108	8810	5580	1541	1634	55	0	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	C	266	2095	1317	348	417	13	0	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	D	177	1427	882	256	287	2	0	0	0

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	E	214	1752	1111	309	321	11	0	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	F	84	679	434	115	127	3	0	0	0

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	G	171	1340	861	222	249	8	0	0	0

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	H	133	1068	673	180	211	4	0	0	0

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	I	119	971	596	179	186	10	0	0	0

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	J	65	532	339	93	94	6	0	0	0

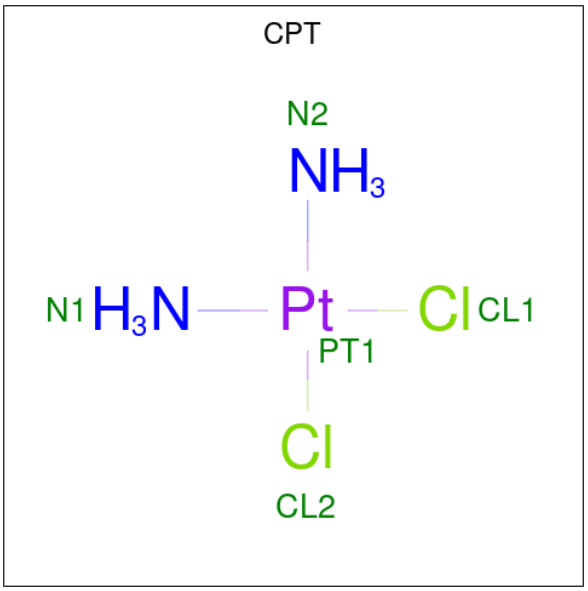
- Molecule 14 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	K	114	919	590	156	171	2	0	0	0

- Molecule 15 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	L	46	364	224	72	64	4	0	0	0

- Molecule 16 is Cisplatin (three-letter code: CPT) (formula: $Cl_2H_6N_2Pt$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Pt		
16	T	1	3	2	1	0	0

- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
17	A	2	2	2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	B	1	Total Zn 1 1	0	0
17	C	1	Total Zn 1 1	0	0
17	I	2	Total Zn 2 2	0	0
17	J	1	Total Zn 1 1	0	0
17	L	1	Total Zn 1 1	0	0

- Molecule 18 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

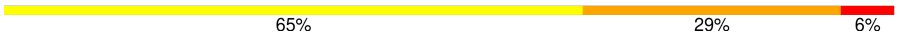
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total Mg 1 1	0	0

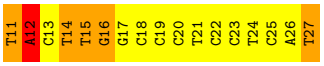
3 Residue-property plots (i)

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 electron 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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: 5'-D(*TP*AP*CP*TP*TP*GUP*CP*CP*CP*TP*CP*CP*TP*CP*AP*T)-3'

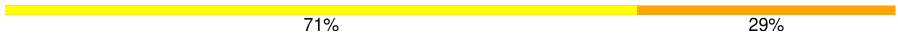
Chain T:





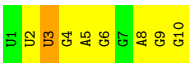
• Molecule 2: 5'-D(*CP*AP*AP*GP*TP*AP*G)-3'

Chain N:



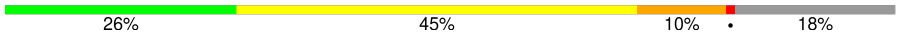
• Molecule 3: 5'-R(*UP*UP*UP*GP*AP*GP*GP*AP*GP*G)-3'

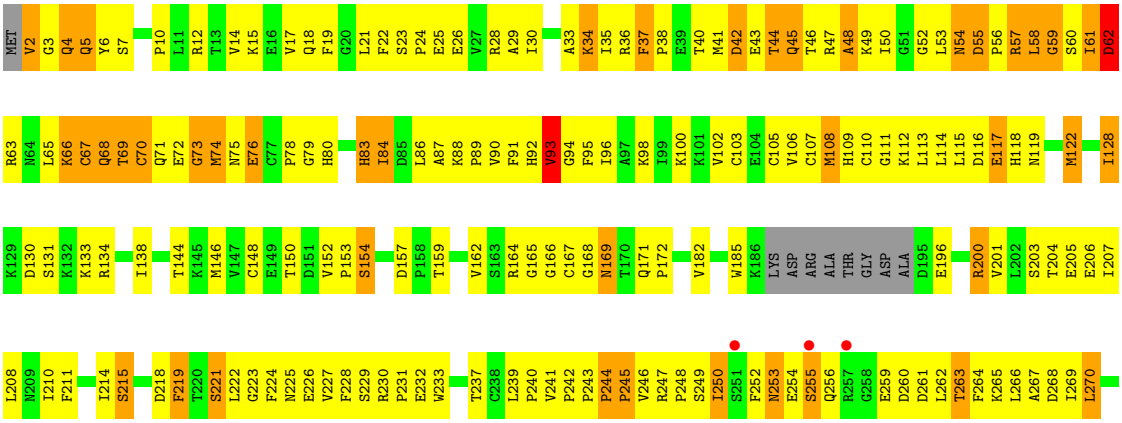
Chain P:



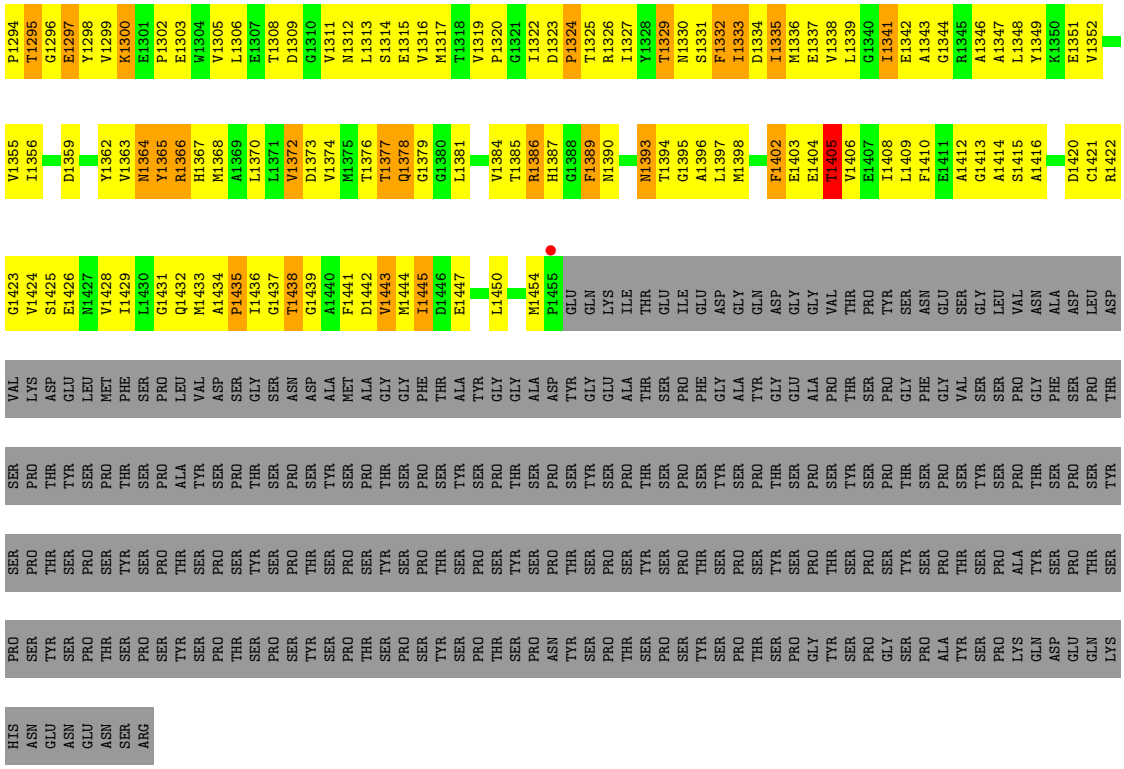
• Molecule 4: DNA-directed RNA polymerase II subunit RPB1

Chain A:



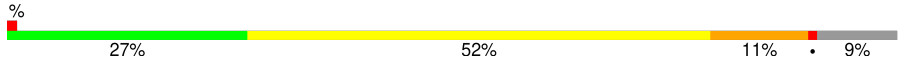


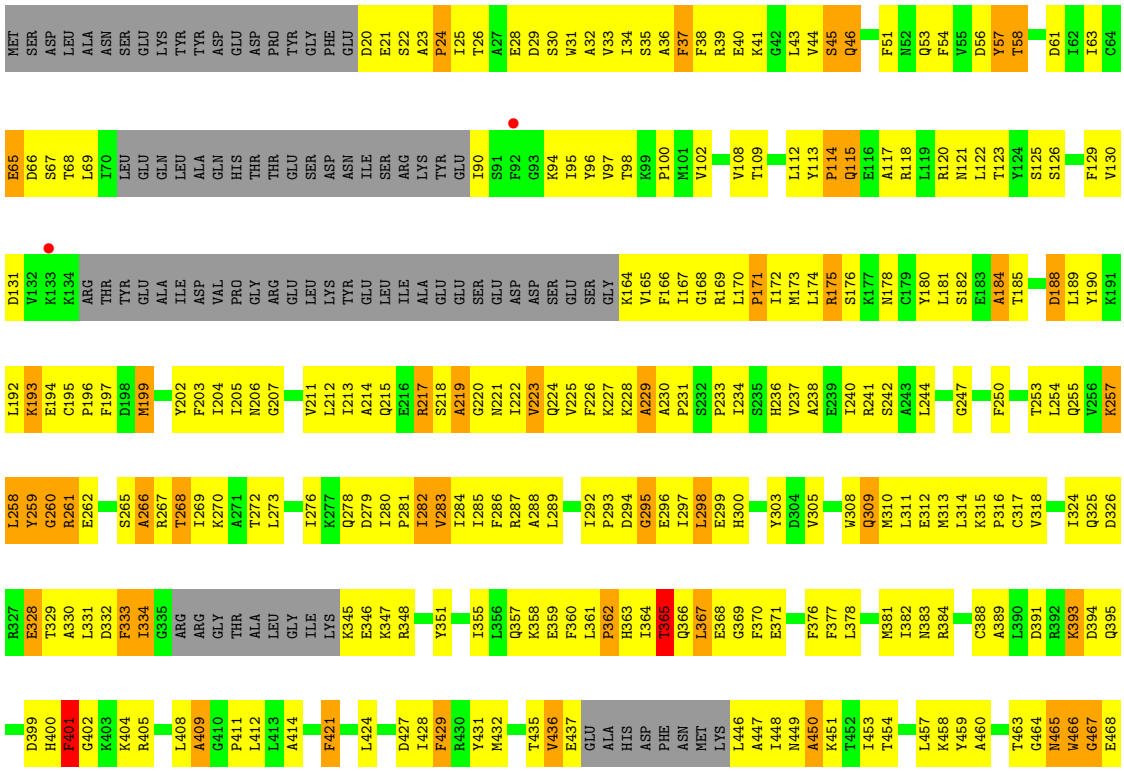
D1223 L1224 F1225 V1226 I1227 W1228 S1229 L1236 I1237 I1238 R1239 C1240 R1241 V1242 V1243 ARG PRO LYS SER LEU ASP ASP ALA GLU THR GLU A1254 E1255 E1256 M1259 L1260 K1261 K1262 I1263 E1264 N1265 M1267 L1268 I1271 T1272 L1273 R1274 E1277 M1278 I1279 E1280 R1281 V1282 V1283 M1284 R1289 K1290 V1291 P1292 S1293
T1161 V1162 I1163 P1164 E1165 D1166 E1167 E1168 I1169 I1170 Q1171 L1172 H1173 F1174 S1175 L1176 LEU ASP GLU GLU ALA GLU GLN SER PHE ASP Q1187 Q1188 S1189 P1190 W1191 L1192 L1195 E1196 L1197 D1198 A1201 M1202 K1205 D1206 L1207 T1208 M1209 G1210 Q1211 V1212 G1213 E1214 R1215 I1216 K1217 Q1218 T1219 F1220 K1221 N1222
ALA SER K1092 K1093 V1094 T1095 V1098 P1099 R1100 L1101 K1102 E1103 I1104 L1105 N1106 V1107 N1110 M1111 K1112 T1113 P1114 S1115 L1116 T1117 V1118 V1119 L1120 E1121 P1122 G1123 H1124 A1125 A1126 D1127 Q1128 E1129 Q1130 L1133 I1134 I1138 E1139 H1140 L1143 K1144 S1145 V1146 T1147 I1148 A1149 S1150 E1151 I1152 Y1153 Y1154 D1155
R1025 R1029 R1030 V1031 L1032 Q1033 E1034 Y1035 R1036 L1037 T1038 K1039 Q1040 A1041 F1042 D1043 W1044 V1045 L1046 S1047 N1048 I1049 E1050 A1051 Q1052 V1058 H1059 P1060 G1061 E1062 M1063 V1064 G1065 V1066 L1067 A1068 A1069 Q1070 S1071 I1072 G1073 E1074 P1075 A1076 T1077 Q1078 M1079 T1080 L1081 ASN THR PHE HIS PHE ALA GLY VAL
N959 I960 R961 R962 I963 I964 Q965 N966 A967 Q968 Q969 T970 F971 H972 I973 S979 D980 L981 V982 I983 K984 D985 I986 V987 L988 G989 V990 K991 D992 L993 Q994 E995 N996 L997 L998 V999 L1000 R1001 G1002 K1003 N1004 E1005 I1006 I1007 Q1008 N1009 A1010 Q1011 R1012 D1013 A1014 V1015 T1016 L1017 F1018 C1019 C1020 L1021 L1022
I886 G887 G888 S889 D890 R896 Y897 R898 V899 D900 L901 L902 N903 T904 D905 H906 T907 L908 D909 P910 S911 L912 L913 E914 S915 G916 S917 E918 I919 I920 G921 D922 Q926 L929 E932 Y933 K934 Q935 L936 V937 K938 D939 R940 K941 F942 L943 V946 F947 N953 W954 P955 L956 P957 V958
R821 I825 D826 T827 A828 V829 K830 T831 A832 E833 T834 G835 Y836 I837 Q838 R839 R840 L841 V842 K843 A844 L845 E846 D847 I848 M849 V850 H851 Y852 D853 N854 T855 T856 R857 N858 S859 L860 G861 N862 V863 I864 Q865 F866 I867 Y868 G869 E870 D871 G872 M873 D874 A875 I878 S882 L883 D884 T885
V747 S751 K752 G753 S754 N757 M761 S762 A763 C764 V765 G766 Q767 Q768 R774 I775 F779 V780 D781 R782 T783 L784 P785 H786 F787 S788 K789 S793 P794 E795 S796 K797 G798 F799 V800 E801 N802 S803 Y804 L805 R806 G807 L808 T809 P810 Q811 E812 F813 F814 F815 H816 A817 M818
T675 M676 I679 T680 E681 T682 I683 A684 E685 A686 D692 V693 T694 K695 E696 A697 Q698 A699 N700 L701 L702 T709 L710 R711 E712 S713 F714 E715 D716 N717 V718 V719 R720 F721 L722 N723 E724 A725 R726 D727 K728 A729 G730 R731 L732 N736 L737 K738 D739 L740 N741 N742 V743 K744 Q745 M746
L606 I607 I608 D609 I613 F614 G615 V616 V617 E618 K619 K620 T621 V622 G623 S624 S625 N626 G627 G628 L629 L630 H631 V632 V633 T634 R635 P639 Q640 V641 C642 F646 G647 N648 I649 Q650 K651 N654 F655 L658 H659 N660 G661 F662 S663 T664 G665 I666 G667 I670 A671 D672 G673 P674
L536 R537 I541 E542 L543 D544 Q545 V546 L547 N548 M549 L550 Y551 W552 W556 D557 G558 V559 I560 P561 T562 P563 A564 I565 I566 K567 P568 K569 P570 L571 W572 S573 G574 K575 Q576 I577 L578 S579 V580 N584 L588 Q589 R590 F591 D592 T595 T596 L597 L598 S599 P600 K601 D602 M605
R469 L470 N471 L472 S473 V474 T475 S476 P477 Y478 N479 A480 D481 F482 D485 E486 M487 N488 L489 H490 V491 P492 Q493 S494 E495 E496 T497 R498 A499 E500 Q503 L504 V507 I511 V512 S513 P514 Q515 S516 N517 K518 P519 C520 M521 G522 I523 V524 Q525 D526 T527 L528 I531 L534 T535
D408 S409 G410 D411 R412 I413 D414 L415 R416 Y417 S418 K419 R420 D423 I424 Q425 L426 Q427 Y428 G429 W430 K431 V432 E433 R434 H435 I436 M437 D438 M439 D440 P441 V442 L443 F444 N445 R446 Q447 P448 S449 L450 H451 K452 M453 S454 M455 M456 A457 H458 R459 V460 K461 V462 I463 P464 Y465 S466 T467 F468
N339 L340 M341 G342 K343 R344 V345 D346 F347 S348 A349 R350 T351 V352 I353 S354 G355 D356 P357 E360 L361 G365 V366 P367 K368 S369 K372 T373 L374 T375 Y376 P377 T381 P382 Y383 N384 I385 D386 R387 L388 L391 V392 R393 N394 G395 P396 H399 P400 G401 Y404 V405 I406 R407
L276 E277 T278 L279 E280 H281 N282 G283 A284 P285 H286 H287 A288 I289 E290 E291 A292 E293 Q297 F298 H299 V300 A301 T302 Y303 M304 D305 N306 D307 I308 A309 G310 Q311 P312 Q313 A314 L315 Q316 K317 S318 G319 R320 P321 V322 K323 S324 I325 R326 A327 R328 G331 K332 E333 G334 R335 I336 R337 G338

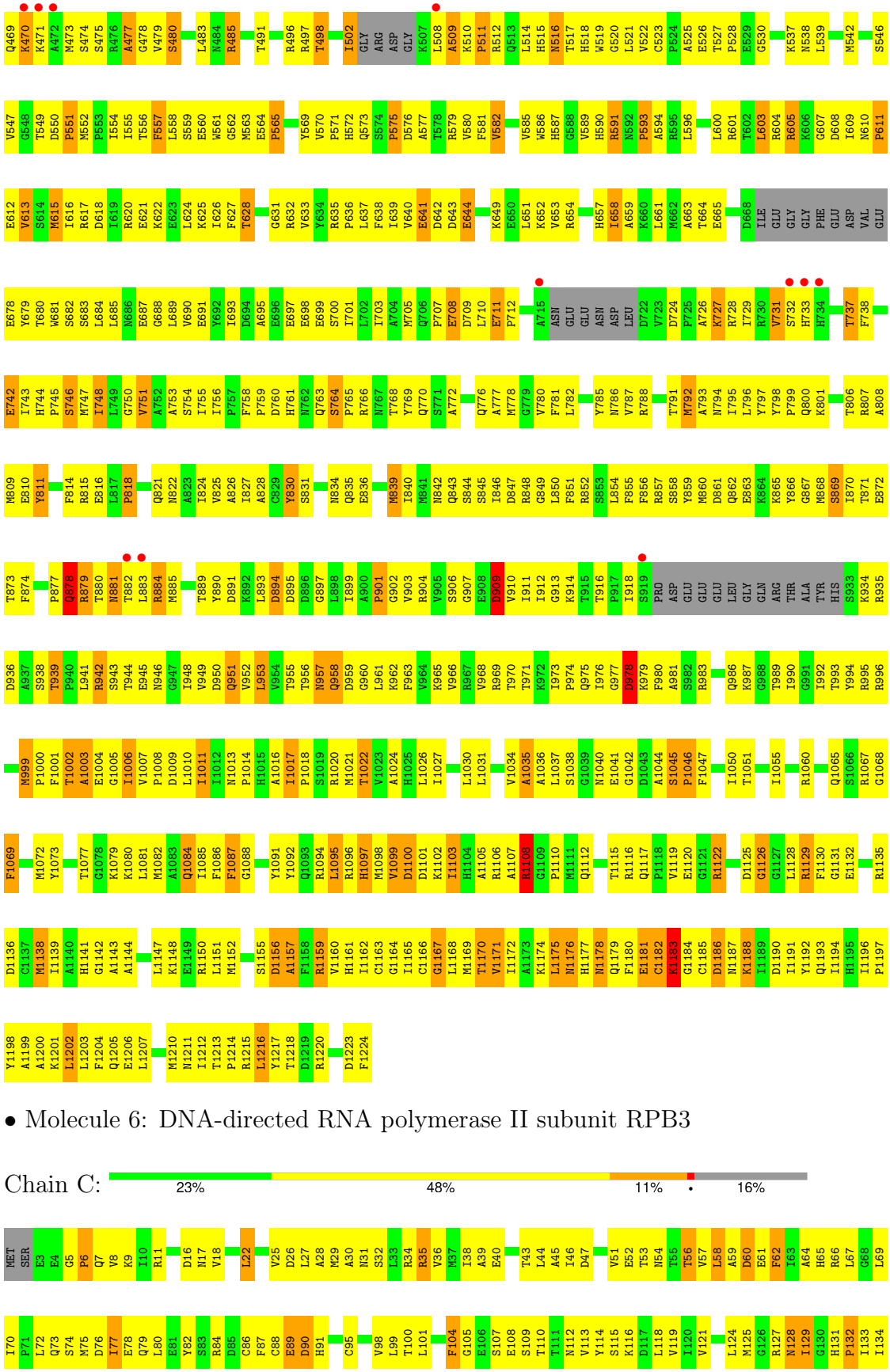


• Molecule 5: DNA-directed RNA polymerase II subunit RPB2

Chain B:

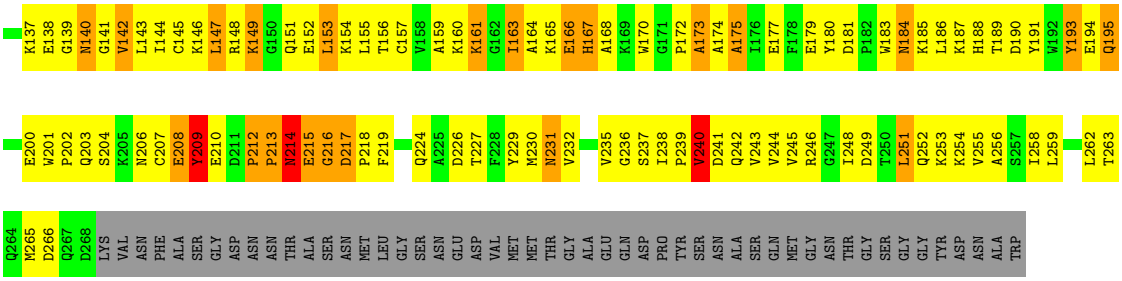






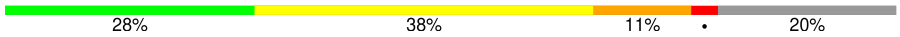
• Molecule 6: DNA-directed RNA polymerase II subunit RPB3

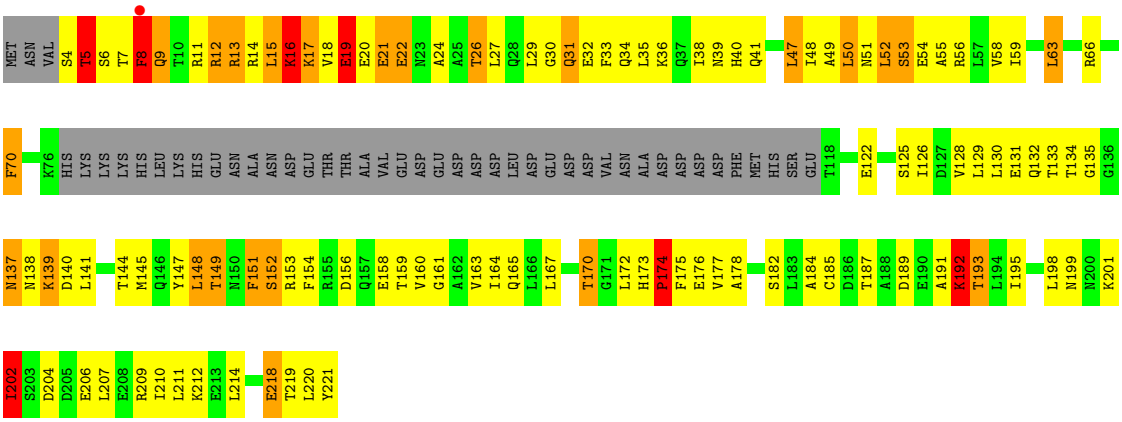
Chain C:



• Molecule 7: DNA-directed RNA polymerase II subunit RPB4

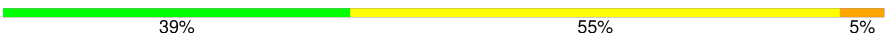
Chain D:

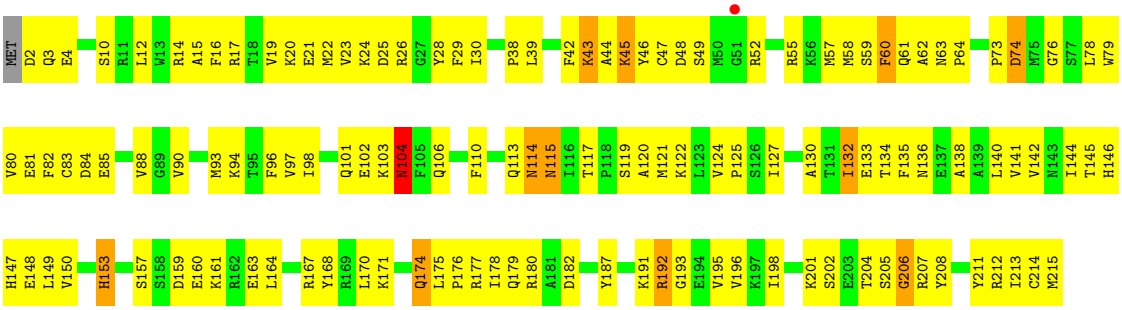




• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC1

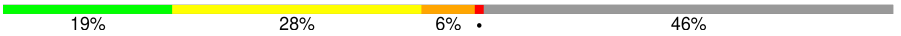
Chain E:

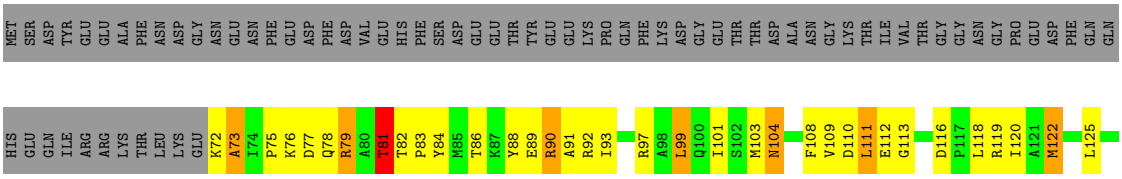




• Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:



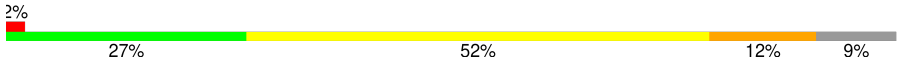


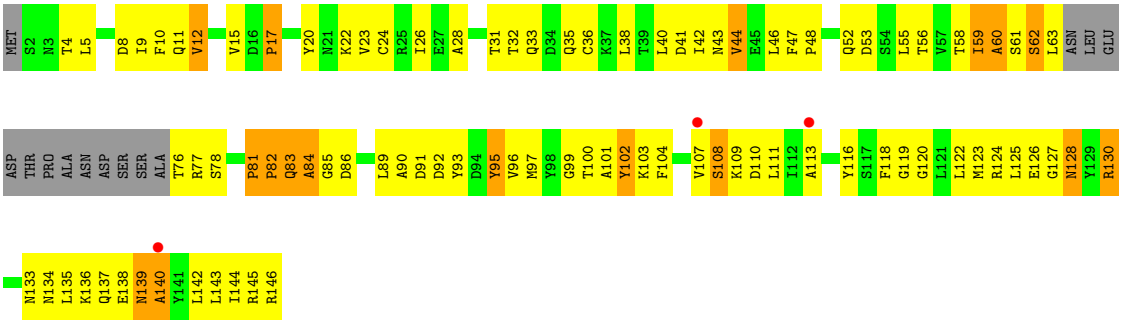
• Molecule 10: DNA-directed RNA polymerase II subunit RPB7

Chain G:

• Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC3

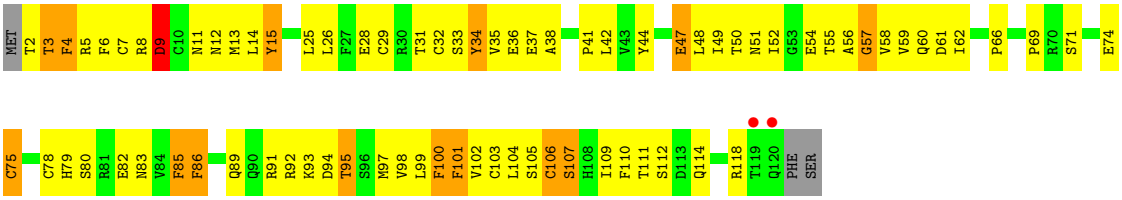
Chain H:





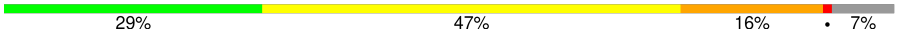
• Molecule 12: DNA-directed RNA polymerase II subunit RPB9

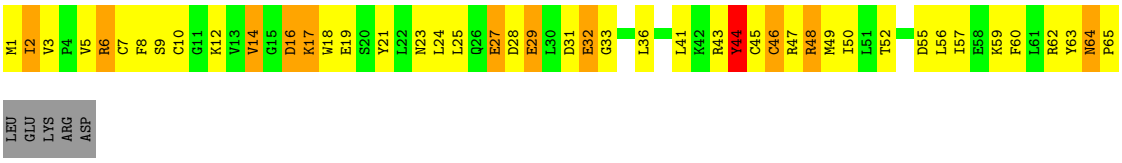
Chain I:



• Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC5

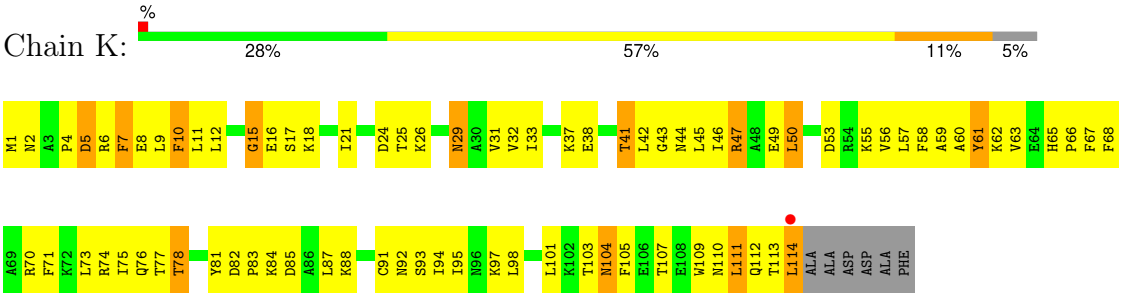
Chain J:





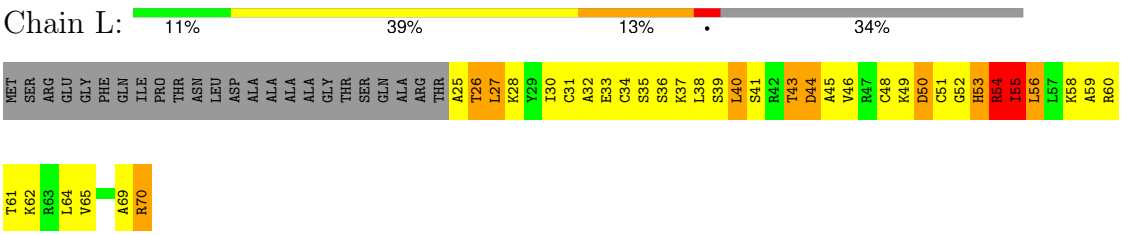
• Molecule 14: DNA-directed RNA polymerase II subunit RPB11

Chain K:



• Molecule 15: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	222.06Å 393.12Å 283.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.80 49.14 – 3.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.80) 99.8 (49.14-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.95 (at 3.77Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.215 , 0.240 0.216 , 0.242	Depositor DCC
R_{free} test set	2410 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å^2)	106.6	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 60.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.045 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.045 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	31804	wwPDB-VP
Average B, all atoms (Å^2)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: MG, ZN, CPT

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	T	1.41	5/373 (1.3%)	1.79	11/572 (1.9%)
2	N	1.38	0/161	1.10	0/247
3	P	0.95	0/242	0.98	0/377
4	A	0.43	0/11339	0.72	4/15334 (0.0%)
5	B	0.42	0/8981	0.68	0/12108
6	C	0.44	0/2133	0.72	0/2891
7	D	0.42	0/1437	0.69	1/1925 (0.1%)
8	E	0.41	0/1788	0.65	0/2406
9	F	0.49	0/691	0.77	0/933
10	G	0.45	0/1368	0.72	0/1844
11	H	0.38	0/1086	0.65	0/1470
12	I	0.36	0/989	0.65	0/1331
13	J	0.47	0/541	0.74	0/727
14	K	0.45	0/937	0.68	0/1265
15	L	0.47	0/366	0.71	0/485
All	All	0.46	5/32432 (0.0%)	0.73	16/43915 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	T	0	2
2	N	0	2
6	C	0	1
13	J	0	1
All	All	0	6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	16	DG	N3-C4	8.85	1.41	1.35
1	T	17	DG	N3-C4	7.68	1.40	1.35
1	T	17	DG	C2-N3	6.93	1.38	1.32
1	T	16	DG	N1-C2	5.71	1.42	1.37
1	T	14	DT	O3'-P	5.20	1.67	1.61

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	T	17	DG	O4'-C1'-N9	11.85	116.29	108.00
1	T	16	DG	O4'-C1'-N9	9.50	114.65	108.00
1	T	17	DG	N3-C2-N2	7.61	125.22	119.90
4	A	567	LYS	C-N-CD	6.05	141.11	128.40
1	T	16	DG	N1-C2-N3	-5.93	120.34	123.90
1	T	15	DT	C4'-C3'-C2'	5.50	108.05	103.10
1	T	17	DG	O4'-C4'-C3'	5.42	109.25	106.00
1	T	12	DA	O4'-C1'-N9	5.42	111.79	108.00
4	A	425	GLN	N-CA-C	-5.42	96.38	111.00
4	A	466	SER	N-CA-C	5.31	125.33	111.00
1	T	16	DG	C4'-C3'-C2'	-5.09	98.52	103.10
7	D	26	THR	N-CA-C	-5.06	97.33	111.00
1	T	27	DT	C4'-C3'-C2'	5.04	107.63	103.10
4	A	311	GLN	N-CA-C	5.01	124.53	111.00
1	T	17	DG	N1-C2-N3	-5.00	120.90	123.90
1	T	16	DG	C8-N9-C1'	5.00	133.50	127.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	C	82	TYR	Sidechain
13	J	44	TYR	Sidechain
2	N	5	DT	Sidechain
2	N	6	DA	Sidechain
1	T	11	DT	Sidechain
1	T	12	DA	Sidechain

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	T	336	0	195	46	0
2	N	143	0	80	20	0
3	P	216	0	108	13	0
4	A	11140	0	11217	1294	0
5	B	8810	0	8847	1025	0
6	C	2095	0	2052	253	0
7	D	1427	0	1451	136	0
8	E	1752	0	1776	149	0
9	F	679	0	701	79	0
10	G	1340	0	1357	152	0
11	H	1068	0	1040	131	0
12	I	971	0	930	102	0
13	J	532	0	543	106	0
14	K	919	0	929	115	0
15	L	364	0	388	57	0
16	T	3	0	0	1	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0
17	C	1	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	L	1	0	0	0	0
18	A	1	0	0	0	0
All	All	31804	0	31614	3347	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 53.

All (3347) 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)
11:H:100:THR:HG23	11:H:138:GLU:HA	1.26	1.16
10:G:138:THR:HG22	10:G:139:ILE:H	1.09	1.12
4:A:53:LEU:HD23	4:A:54:ASN:H	0.99	1.12
4:A:1094:VAL:HG13	4:A:1113:THR:HG21	1.32	1.11
5:B:510:LYS:HG3	5:B:511:PRO:HD3	1.12	1.11
5:B:273:LEU:HB2	5:B:276:ILE:HD12	1.30	1.09
1:T:22:DC:H2"	1:T:23:DC:H5"	1.16	1.08
4:A:1438:THR:HB	5:B:1144:ALA:HB3	1.37	1.06
5:B:792:MET:HE2	5:B:857:ARG:HH12	1.16	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1017:LEU:HB2	8:E:206:GLY:H	1.17	1.05
5:B:806:THR:HG22	5:B:808:ALA:H	1.22	1.03
4:A:855:THR:HG21	4:A:857:ARG:HE	1.17	1.02
8:E:22:MET:HE3	8:E:26:ARG:HH21	1.18	1.02
12:I:111:THR:HG22	12:I:112:SER:H	1.25	1.02
5:B:882:THR:HG22	5:B:884:ARG:H	1.26	1.01
4:A:1161:THR:HG22	4:A:1163:ILE:H	1.26	1.01
5:B:589:VAL:HG12	5:B:590:HIS:H	1.22	1.01
5:B:172:ILE:HD13	5:B:178:ASN:HB3	1.42	1.01
7:D:40:HIS:HB3	10:G:73:LYS:HZ3	1.22	1.00
6:C:116:LYS:HD3	6:C:140:ASN:HB3	1.40	1.00
14:K:47:ARG:HB3	14:K:47:ARG:HH11	1.24	1.00
4:A:828:ALA:CB	5:B:530:GLY:HA2	1.92	1.00
6:C:43:THR:HG22	6:C:44:LEU:H	1.24	1.00
4:A:40:THR:HG22	4:A:41:MET:HG3	1.44	1.00
5:B:918:ILE:HB	5:B:935:ARG:HD2	1.43	0.99
4:A:475:THR:HG23	4:A:476:SER:H	1.27	0.99
1:T:22:DC:H2"	1:T:23:DC:C5'	1.92	0.99
4:A:535:THR:HG21	4:A:616:VAL:HA	1.46	0.98
4:A:53:LEU:HD23	4:A:54:ASN:N	1.76	0.98
8:E:19:VAL:O	8:E:23:VAL:HG23	1.63	0.98
5:B:510:LYS:CG	5:B:511:PRO:HD3	1.92	0.98
4:A:1445:ILE:H	4:A:1445:ILE:HD12	1.23	0.98
7:D:40:HIS:HB3	10:G:73:LYS:NZ	1.80	0.96
6:C:39:ALA:HA	6:C:164:ALA:HB3	1.45	0.96
6:C:44:LEU:HB2	6:C:77:ILE:HD11	1.48	0.95
5:B:879:ARG:HH11	5:B:883:LEU:HD22	1.29	0.95
4:A:399:HIS:HB3	4:A:400:PRO:HD3	1.46	0.95
10:G:7:LEU:HB2	10:G:74:TYR:CE2	2.02	0.95
6:C:166:GLU:HG3	14:K:10:PHE:HZ	1.32	0.95
5:B:563:MET:HE3	5:B:580:VAL:HB	1.49	0.95
5:B:365:THR:HG23	5:B:367:LEU:H	1.30	0.94
5:B:233:PRO:HG2	5:B:234:ILE:HD12	1.48	0.94
8:E:94:LYS:HE2	8:E:98:ILE:HD11	1.50	0.94
11:H:4:THR:HA	11:H:60:ALA:HB2	1.49	0.94
4:A:779:PHE:HE1	4:A:785:PRO:HD3	1.32	0.93
5:B:169:ARG:HB2	5:B:454:THR:HG23	1.47	0.93
4:A:1189:SER:O	4:A:1241:ARG:HD3	1.67	0.93
6:C:47:ASP:HA	15:L:69:ALA:HB3	1.51	0.93
4:A:1127:ASP:HB3	4:A:1130:GLN:HB3	1.48	0.93
5:B:98:THR:O	5:B:126:SER:HB2	1.69	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:903:ASN:HD22	4:A:904:THR:N	1.68	0.92
5:B:483:LEU:HD11	5:B:491:THR:HG23	1.51	0.91
6:C:45:ALA:HA	6:C:72:LEU:HD12	1.51	0.91
4:A:1004:ASN:ND2	8:E:167:ARG:HD2	1.86	0.91
5:B:579:ARG:HB2	5:B:586:TRP:NE1	1.85	0.91
4:A:828:ALA:HB2	5:B:530:GLY:HA2	1.51	0.91
5:B:217:ARG:HE	5:B:405:ARG:HB2	1.33	0.91
5:B:1159:ARG:HB3	5:B:1159:ARG:HH11	1.35	0.91
4:A:829:VAL:HG21	5:B:508:LEU:HD13	1.50	0.90
10:G:1:MET:SD	10:G:79:PHE:HD1	1.93	0.90
4:A:239:LEU:HD12	4:A:240:PRO:HD2	1.52	0.90
13:J:64:ASN:HB3	13:J:65:PRO:CD	2.00	0.90
5:B:577:ALA:HB1	5:B:589:VAL:HG11	1.52	0.90
5:B:579:ARG:HB2	5:B:586:TRP:HE1	1.35	0.90
6:C:98:VAL:O	6:C:99:LEU:HD23	1.72	0.90
9:F:86:THR:OG1	9:F:89:GLU:HG3	1.72	0.90
4:A:963:ILE:HD11	4:A:1048:ASN:HB3	1.54	0.89
5:B:510:LYS:HG3	5:B:511:PRO:CD	2.02	0.89
1:T:11:DT:H2"	1:T:12:DA:O5'	1.71	0.89
5:B:25:ILE:HD11	5:B:653:VAL:O	1.72	0.89
5:B:594:ALA:HA	5:B:617:ARG:HH12	1.38	0.89
13:J:44:TYR:HA	13:J:47:ARG:HB2	1.53	0.89
4:A:763:ALA:O	4:A:803:SER:HB3	1.72	0.89
13:J:5:VAL:HG12	13:J:6:ARG:HG3	1.53	0.89
14:K:53:ASP:HB3	14:K:56:VAL:HG23	1.53	0.89
4:A:567:LYS:CG	4:A:568:PRO:HD2	2.02	0.89
4:A:709:THR:HG22	4:A:711:ARG:H	1.36	0.89
5:B:364:ILE:HG12	5:B:585:VAL:HG13	1.55	0.89
4:A:1116:LEU:N	4:A:1308:THR:HG22	1.88	0.88
6:C:7:GLN:HG2	14:K:104:ASN:HD22	1.38	0.88
4:A:646:PHE:O	4:A:650:GLN:HG3	1.73	0.88
8:E:153:HIS:HB3	8:E:196:VAL:HG11	1.56	0.88
9:F:93:ILE:HD11	9:F:134:ILE:HD11	1.56	0.88
15:L:32:ALA:HB3	15:L:55:ILE:HD12	1.54	0.88
5:B:879:ARG:NH1	5:B:883:LEU:HD22	1.87	0.88
4:A:1312:ASN:O	4:A:1316:VAL:HG23	1.74	0.88
10:G:13:LEU:HD21	10:G:17:PHE:HB2	1.55	0.88
4:A:356:ASP:HB2	4:A:469:ARG:NH1	1.89	0.88
4:A:366:VAL:HG21	4:A:460:VAL:HG22	1.56	0.88
4:A:901:LEU:H	4:A:926:GLN:NE2	1.72	0.88
6:C:133:ILE:HD11	6:C:237:SER:HA	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:211:VAL:O	5:B:480:SER:HA	1.73	0.87
5:B:1166:CYS:HB2	5:B:1215:ARG:NH1	1.90	0.87
1:T:24:DT:H2"	1:T:25:DC:O5'	1.74	0.87
8:E:14:ARG:HH21	8:E:141:VAL:HG12	1.37	0.87
5:B:1002:THR:HG21	5:B:1006:ILE:HD12	1.57	0.87
4:A:49:LYS:NZ	4:A:61:ILE:HG13	1.89	0.87
5:B:1159:ARG:HB3	5:B:1159:ARG:NH1	1.89	0.87
4:A:321:PRO:O	4:A:322:VAL:HB	1.73	0.87
4:A:225:ASN:HD22	4:A:228:PHE:H	1.23	0.86
6:C:57:VAL:HG11	13:J:60:PHE:HB3	1.54	0.86
10:G:127:PRO:HG2	10:G:138:THR:HG21	1.58	0.86
5:B:1165:ILE:HG22	5:B:1166:CYS:N	1.90	0.86
4:A:441:PRO:HD2	4:A:498:ARG:NH2	1.90	0.86
9:F:82:THR:HG22	9:F:84:TYR:H	1.36	0.86
4:A:754:SER:H	4:A:757:ASN:HD22	1.23	0.86
5:B:594:ALA:HA	5:B:617:ARG:NH1	1.89	0.86
8:E:177:ARG:HD3	8:E:215:MET:HG3	1.57	0.86
4:A:427:GLN:HG3	4:A:430:TRP:CZ2	2.11	0.85
4:A:537:ARG:HD2	11:H:20:TYR:HE1	1.39	0.85
5:B:1159:ARG:HD3	5:B:1193:GLN:HG3	1.56	0.85
9:F:111:LEU:HD12	9:F:111:LEU:H	1.41	0.85
5:B:467:GLY:H	5:B:475:SER:HB3	1.40	0.85
5:B:516:ASN:HD22	5:B:516:ASN:N	1.74	0.85
8:E:22:MET:HE3	8:E:26:ARG:NH2	1.91	0.85
10:G:18:PHE:HA	10:G:22:MET:CE	2.07	0.84
5:B:798:TYR:HE2	6:C:62:PHE:CE2	1.95	0.84
10:G:138:THR:HG22	10:G:139:ILE:N	1.91	0.84
1:T:22:DC:C2'	1:T:23:DC:H5"	2.06	0.84
2:N:6:DA:H2"	2:N:7:DG:OP2	1.76	0.84
4:A:249:SER:O	4:A:250:ILE:HG13	1.76	0.84
6:C:32:SER:O	6:C:36:VAL:HG23	1.78	0.84
4:A:567:LYS:HB3	11:H:96:VAL:H	1.43	0.84
4:A:1283:VAL:HG12	4:A:1284:MET:H	1.42	0.83
11:H:4:THR:HA	11:H:60:ALA:CB	2.08	0.83
5:B:1224:PHE:HE2	8:E:171:LYS:HG3	1.43	0.83
5:B:1065:GLN:HE21	5:B:1067:ARG:N	1.75	0.83
10:G:23:LYS:HG3	10:G:56:ILE:HD11	1.61	0.83
10:G:34:VAL:HG12	10:G:45:ILE:HG21	1.60	0.83
11:H:42:ILE:HG23	11:H:95:TYR:HE1	1.40	0.83
5:B:1180:PHE:HB3	5:B:1191:ILE:HD12	1.61	0.83
12:I:26:LEU:HD23	12:I:37:GLU:HA	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:48:ILE:HG21	10:G:4:ILE:HB	1.60	0.83
1:T:18:DC:H2"	1:T:19:DC:O5'	1.79	0.83
8:E:117:THR:HG22	8:E:119:SER:H	1.44	0.83
4:A:93:VAL:HG22	4:A:301:ALA:HA	1.61	0.83
11:H:130:ARG:H	11:H:130:ARG:HD2	1.44	0.83
4:A:55:ASP:C	4:A:57:ARG:H	1.81	0.83
6:C:38:ILE:HA	6:C:173:ALA:HB2	1.61	0.83
11:H:100:THR:OG1	11:H:138:GLU:HG3	1.78	0.82
4:A:809:THR:HG23	4:A:812:GLU:OE1	1.78	0.82
4:A:1242:VAL:HG12	4:A:1243:VAL:H	1.45	0.82
6:C:43:THR:HG22	6:C:44:LEU:N	1.93	0.82
4:A:860:LEU:HD11	4:A:1393:ASN:HB2	1.59	0.82
4:A:56:PRO:O	4:A:57:ARG:HG3	1.80	0.82
10:G:14:HIS:ND1	10:G:15:PRO:HD2	1.94	0.82
8:E:16:PHE:CZ	8:E:20:LYS:HE2	2.14	0.82
1:T:20:DC:H2"	1:T:21:DT:O5'	1.80	0.82
4:A:1017:LEU:HB2	8:E:206:GLY:N	1.95	0.82
5:B:613:VAL:HG13	5:B:627:PHE:O	1.79	0.82
7:D:144:THR:O	7:D:148:LEU:HB2	1.79	0.82
13:J:12:LYS:O	13:J:14:VAL:HG23	1.79	0.82
4:A:70:CYS:O	4:A:72:GLU:HG2	1.79	0.82
4:A:743:VAL:O	4:A:747:VAL:HG23	1.79	0.82
5:B:801:LYS:O	13:J:52:THR:HG23	1.78	0.82
11:H:93:TYR:HB3	11:H:144:ILE:O	1.80	0.82
4:A:23:SER:HA	4:A:233:TRP:NE1	1.94	0.82
4:A:353:ILE:HG21	4:A:487:MET:HE3	1.61	0.82
4:A:458:HIS:CE1	4:A:507:VAL:HG21	2.15	0.82
5:B:23:ALA:HB1	5:B:24:PRO:HD2	1.62	0.82
5:B:189:LEU:HA	5:B:192:LEU:HD12	1.62	0.82
1:T:25:DC:H2"	1:T:26:DA:O5'	1.79	0.81
4:A:1127:ASP:HB3	4:A:1130:GLN:CB	2.09	0.81
13:J:57:ILE:HA	13:J:60:PHE:HD2	1.43	0.81
4:A:567:LYS:CD	4:A:568:PRO:HD2	2.11	0.81
5:B:792:MET:HE2	5:B:857:ARG:NH1	1.94	0.81
5:B:821:GLN:HE22	5:B:851:PHE:HA	1.45	0.81
5:B:839:MET:HE3	5:B:1010:LEU:HD21	1.63	0.81
4:A:886:ILE:HG22	4:A:887:GLY:N	1.95	0.80
5:B:53:GLN:HG2	5:B:547:VAL:HG22	1.61	0.80
5:B:521:LEU:HD22	5:B:633:VAL:HG12	1.60	0.80
6:C:6:PRO:HB3	6:C:25:VAL:HG12	1.64	0.80
5:B:563:MET:CE	5:B:580:VAL:HB	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:611:PRO:HB3	5:B:685:LEU:HD11	1.63	0.80
8:E:202:SER:OG	8:E:204:THR:HG22	1.81	0.80
4:A:858:ASN:ND2	4:A:860:LEU:H	1.80	0.80
5:B:710:LEU:HA	5:B:733:HIS:HB3	1.64	0.80
11:H:102:TYR:OH	11:H:122:LEU:HD22	1.81	0.80
6:C:172:PRO:O	6:C:235:VAL:HG23	1.81	0.80
5:B:244:LEU:HD21	5:B:366:GLN:NE2	1.97	0.80
11:H:59:ILE:HG22	11:H:60:ALA:N	1.97	0.80
4:A:868:TYR:HD2	4:A:1058:VAL:HG21	1.46	0.80
4:A:598:LEU:HA	11:H:122:LEU:HD13	1.64	0.79
7:D:35:LEU:HD23	7:D:174:PRO:HD2	1.65	0.79
4:A:524:VAL:HG12	4:A:525:GLN:H	1.47	0.79
4:A:475:THR:HG23	4:A:476:SER:N	1.96	0.79
5:B:782:LEU:HD12	5:B:788:ARG:HH11	1.46	0.79
3:P:3:U:H2'	3:P:4:G:C8	2.17	0.79
4:A:534:LEU:O	4:A:574:GLY:HA3	1.82	0.79
5:B:999:MET:HG3	5:B:1000:PRO:HD2	1.63	0.79
10:G:81:PRO:HG3	10:G:106:MET:SD	2.23	0.79
4:A:902:LEU:HG	4:A:926:GLN:HG3	1.64	0.79
12:I:55:THR:HG21	12:I:109:ILE:HD13	1.65	0.79
4:A:265:LYS:HD2	4:A:265:LYS:H	1.47	0.79
5:B:33:VAL:HG21	5:B:638:PHE:HZ	1.48	0.79
5:B:847:ASP:HB3	6:C:167:HIS:NE2	1.98	0.79
5:B:859:TYR:OH	5:B:941:LEU:HD12	1.83	0.78
4:A:741:ASN:HD22	4:A:744:LYS:H	1.31	0.78
5:B:882:THR:CG2	5:B:884:ARG:HB2	2.12	0.78
5:B:125:SER:HA	5:B:171:PRO:HA	1.63	0.78
5:B:549:THR:HG22	5:B:550:ASP:H	1.46	0.78
1:T:11:DT:H2"	1:T:12:DA:C5'	2.12	0.78
10:G:122:ASN:ND2	10:G:125:SER:HB3	1.98	0.78
12:I:85:PHE:H	12:I:85:PHE:HD2	1.27	0.78
7:D:49:ALA:HB2	7:D:174:PRO:HB3	1.66	0.78
8:E:213:ILE:HG12	8:E:214:CYS:H	1.47	0.78
14:K:45:LEU:HG	14:K:94:ILE:HD13	1.63	0.78
5:B:953:LEU:HD21	5:B:965:LYS:HB2	1.65	0.78
5:B:35:SER:HA	5:B:811:TYR:HE2	1.46	0.78
8:E:135:PHE:HB3	8:E:140:LEU:HD11	1.64	0.78
4:A:670:ILE:HG23	4:A:805:LEU:HD21	1.64	0.78
4:A:828:ALA:HB1	5:B:530:GLY:HA2	1.64	0.78
7:D:40:HIS:CB	10:G:73:LYS:NZ	2.47	0.78
14:K:65:HIS:CD2	14:K:67:PHE:H	2.01	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:886:ILE:HD11	4:A:943:LEU:HB3	1.64	0.78
5:B:217:ARG:NE	5:B:405:ARG:HB2	1.99	0.78
5:B:615:MET:HB3	5:B:626:ILE:HG12	1.66	0.78
7:D:189:ASP:O	7:D:193:THR:HB	1.84	0.78
4:A:446:ARG:CD	4:A:480:ALA:HB2	2.14	0.77
4:A:855:THR:HG23	4:A:857:ARG:HG3	1.66	0.77
13:J:1:MET:N	13:J:57:ILE:H	1.81	0.77
4:A:53:LEU:CD2	4:A:54:ASN:H	1.91	0.77
5:B:520:GLY:H	5:B:748:ILE:HG22	1.49	0.77
5:B:603:LEU:HD13	5:B:608:ASP:HB2	1.65	0.77
7:D:17:LYS:HE2	7:D:17:LYS:N	1.99	0.77
9:F:111:LEU:C	9:F:113:GLY:H	1.86	0.77
4:A:563:PRO:HG3	4:A:572:TRP:CZ2	2.19	0.77
14:K:47:ARG:HB3	14:K:47:ARG:NH1	1.99	0.77
4:A:779:PHE:CE1	4:A:785:PRO:HD3	2.18	0.77
4:A:885:THR:O	4:A:940:ARG:HD2	1.84	0.77
5:B:1017:ILE:HB	5:B:1018:PRO:HD3	1.65	0.77
8:E:179:GLN:HB2	8:E:182:ASP:HB2	1.67	0.77
12:I:75:CYS:HG	12:I:78:CYS:HG	1.32	0.77
4:A:1420:ASP:HB3	4:A:1422:ARG:HG3	1.65	0.77
10:G:15:PRO:HA	10:G:18:PHE:CD1	2.19	0.77
10:G:80:LYS:HD3	10:G:80:LYS:N	1.98	0.77
5:B:1085:ILE:N	5:B:1085:ILE:HD12	1.99	0.77
13:J:1:MET:N	13:J:56:LEU:N	2.33	0.77
4:A:49:LYS:HZ1	4:A:61:ILE:HG13	1.48	0.77
13:J:3:VAL:HG21	13:J:18:TRP:HB2	1.65	0.77
4:A:718:VAL:O	4:A:722:LEU:HD12	1.85	0.77
5:B:978:ASP:OD2	5:B:1098:MET:HG2	1.84	0.77
4:A:853:ASP:O	4:A:854:ASN:HB2	1.85	0.76
5:B:1065:GLN:HE21	5:B:1067:ARG:H	1.30	0.76
10:G:80:LYS:HD3	10:G:80:LYS:H	1.50	0.76
13:J:16:ASP:OD1	13:J:17:LYS:HD2	1.84	0.76
4:A:709:THR:HG23	12:I:94:ASP:HA	1.68	0.76
14:K:113:THR:O	14:K:114:LEU:HB2	1.83	0.76
5:B:996:ARG:NH2	6:C:175:ALA:H	1.84	0.76
6:C:66:ARG:NH1	13:J:2:ILE:HG21	2.00	0.76
9:F:103:MET:O	9:F:104:ASN:HB2	1.84	0.76
4:A:496:GLU:HG2	9:F:99:LEU:HD23	1.67	0.76
4:A:1208:THR:HG22	4:A:1210:GLY:H	1.51	0.76
5:B:1162:ILE:HD11	5:B:1194:ILE:HD13	1.66	0.76
10:G:18:PHE:HA	10:G:22:MET:HE3	1.65	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1116:LEU:HB2	4:A:1329:THR:OG1	1.86	0.76
5:B:705:MET:H	5:B:710:LEU:HD12	1.51	0.76
5:B:778:MET:CE	5:B:1094:ARG:HD3	2.15	0.76
4:A:414:ASP:OD1	4:A:416:ARG:HG2	1.86	0.76
5:B:862:GLN:HG2	5:B:963:PHE:HD1	1.51	0.76
5:B:467:GLY:N	5:B:475:SER:HB3	2.01	0.76
5:B:957:ASN:HD22	5:B:961:LEU:HD12	1.49	0.76
8:E:2:ASP:O	8:E:3:GLN:HG2	1.84	0.76
8:E:180:ARG:HH21	8:E:192:ARG:HB2	1.51	0.76
11:H:38:LEU:HD12	11:H:124:ARG:O	1.85	0.76
11:H:89:LEU:HB3	11:H:91:ASP:OD1	1.86	0.76
5:B:309:GLN:OE1	12:I:52:ILE:HD11	1.86	0.76
4:A:1341:ILE:HD12	4:A:1379:GLY:O	1.86	0.75
4:A:1424:VAL:HG13	4:A:1436:ILE:CD1	2.17	0.75
9:F:90:ARG:HD3	9:F:155:LEU:HD12	1.67	0.75
5:B:278:GLN:HG2	5:B:279:ASP:H	1.49	0.75
5:B:800:GLN:HB3	13:J:52:THR:HG21	1.66	0.75
5:B:882:THR:HG22	5:B:884:ARG:N	1.98	0.75
4:A:590:ARG:HH21	4:A:620:LYS:CB	1.99	0.75
13:J:8:PHE:H	13:J:49:MET:HE3	1.50	0.75
4:A:866:PHE:C	4:A:867:ILE:HD12	2.07	0.75
6:C:239:PRO:HB2	6:C:241:ASP:OD1	1.87	0.75
10:G:43:GLY:HA3	10:G:80:LYS:HB3	1.69	0.75
12:I:8:ARG:HG3	12:I:34:TYR:HE1	1.52	0.75
5:B:806:THR:HG22	5:B:808:ALA:N	2.01	0.75
8:E:14:ARG:HH21	8:E:141:VAL:CG1	1.99	0.75
13:J:44:TYR:H	13:J:44:TYR:HD2	1.34	0.75
4:A:567:LYS:HG3	4:A:568:PRO:HD2	1.67	0.75
5:B:363:HIS:O	5:B:364:ILE:HB	1.84	0.75
14:K:7:PHE:HA	14:K:10:PHE:CE2	2.22	0.75
4:A:466:SER:O	5:B:1103:ILE:HD11	1.86	0.74
4:A:537:ARG:HD2	11:H:20:TYR:CE1	2.21	0.74
5:B:758:PHE:HB3	5:B:761:HIS:HD2	1.52	0.74
12:I:111:THR:HG22	12:I:112:SER:N	2.02	0.74
3:P:3:U:H2'	3:P:4:G:H8	1.50	0.74
6:C:7:GLN:HG2	14:K:104:ASN:ND2	2.03	0.74
4:A:1239:ARG:HH22	4:A:1241:ARG:NH2	1.86	0.74
5:B:1072:MET:CE	5:B:1085:ILE:HB	2.18	0.74
6:C:147:LEU:HB2	6:C:151:GLN:HB2	1.69	0.74
14:K:65:HIS:HD2	14:K:67:PHE:H	1.36	0.74
4:A:981:LEU:CD2	4:A:1039:LYS:HA	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1341:ILE:HG23	4:A:1342:GLU:N	2.01	0.74
5:B:1152:MET:CE	5:B:1157:ALA:HA	2.18	0.74
4:A:1279:ILE:HD11	4:A:1316:VAL:CG2	2.17	0.74
5:B:214:ALA:HB3	5:B:498:THR:HA	1.69	0.74
5:B:1182:CYS:O	5:B:1182:CYS:SG	2.45	0.74
6:C:5:GLY:O	6:C:7:GLN:HG3	1.88	0.74
7:D:12:ARG:NH2	7:D:12:ARG:HB3	2.03	0.74
5:B:637:LEU:HD12	5:B:693:ILE:HD12	1.68	0.74
4:A:185:TRP:CZ3	4:A:200:ARG:HG2	2.22	0.74
5:B:971:THR:OG1	6:C:61:GLU:HG3	1.88	0.74
7:D:52:LEU:HD21	7:D:147:TYR:HE2	1.52	0.74
11:H:23:VAL:HG22	11:H:43:ASN:HA	1.70	0.74
4:A:19:PHE:O	4:A:1416:ALA:HA	1.86	0.74
4:A:528:LEU:O	4:A:531:ILE:HG22	1.88	0.74
4:A:1004:ASN:O	4:A:1008:GLN:HB2	1.87	0.74
5:B:770:GLN:OE1	5:B:983:ARG:HA	1.87	0.74
4:A:808:LEU:HD23	4:A:813:PHE:HA	1.70	0.73
4:A:836:TYR:CE2	4:A:840:ARG:HD2	2.22	0.73
4:A:855:THR:HG21	4:A:857:ARG:NE	2.00	0.73
4:A:982:THR:HB	4:A:985:ASP:H	1.53	0.73
4:A:1444:MET:HG2	10:G:60:ARG:HA	1.70	0.73
7:D:9:GLN:HE21	7:D:38:ILE:HD12	1.53	0.73
4:A:288:ALA:HA	4:A:291:GLU:OE2	1.89	0.73
4:A:567:LYS:HB3	11:H:95:TYR:HA	1.70	0.73
5:B:273:LEU:CB	5:B:276:ILE:HD12	2.16	0.73
4:A:164:ARG:HG3	4:A:165:GLY:N	2.03	0.73
4:A:518:LYS:HE2	4:A:624:SER:O	1.88	0.73
4:A:682:THR:HG23	4:A:728:LYS:HE3	1.70	0.73
5:B:1077:THR:HG22	14:K:44:ASN:ND2	2.03	0.73
5:B:1077:THR:HG22	14:K:44:ASN:HD21	1.52	0.73
5:B:287:ARG:HG2	5:B:292:ILE:HA	1.70	0.73
5:B:1065:GLN:NE2	5:B:1067:ARG:HG2	2.03	0.73
4:A:55:ASP:CG	4:A:55:ASP:O	2.22	0.73
5:B:642:ASP:HA	5:B:649:LYS:HA	1.68	0.73
4:A:283:GLY:O	4:A:285:PRO:HD3	1.88	0.73
4:A:351:THR:HB	5:B:1103:ILE:HD12	1.71	0.73
4:A:960:ILE:HA	4:A:963:ILE:HG22	1.69	0.73
4:A:628:GLY:O	4:A:632:VAL:HG23	1.88	0.73
4:A:849:MET:HE1	4:A:1061:GLY:HA2	1.70	0.73
5:B:521:LEU:HB3	5:B:633:VAL:HG11	1.70	0.73
7:D:12:ARG:HB3	7:D:12:ARG:HH21	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:J:43:ARG:HG3	13:J:45:CYS:SG	2.28	0.73
8:E:153:HIS:HB3	8:E:196:VAL:CG1	2.18	0.73
6:C:194:GLU:O	6:C:195:GLN:HG3	1.87	0.73
7:D:56:ARG:HB2	7:D:148:LEU:HD22	1.69	0.73
4:A:963:ILE:HD11	4:A:1048:ASN:CB	2.19	0.72
5:B:603:LEU:HB3	5:B:609:ILE:HD11	1.70	0.72
5:B:175:ARG:HG2	5:B:175:ARG:HH11	1.53	0.72
6:C:262:LEU:HD11	14:K:87:LEU:HD23	1.71	0.72
3:P:10:G:H4'	4:A:485:ASP:OD1	1.89	0.72
4:A:23:SER:HB3	4:A:233:TRP:CZ2	2.24	0.72
5:B:798:TYR:HE2	6:C:62:PHE:CZ	2.07	0.72
6:C:47:ASP:HA	15:L:69:ALA:CB	2.17	0.72
4:A:446:ARG:HD3	4:A:480:ALA:HB2	1.71	0.72
5:B:190:TYR:CE2	13:J:62:ARG:HB3	2.24	0.72
5:B:401:PHE:HA	5:B:404:LYS:HG3	1.70	0.72
5:B:737:THR:HG21	12:I:66:PRO:HA	1.71	0.72
5:B:1201:LYS:HE2	5:B:1205:GLN:OE1	1.89	0.72
11:H:81:PRO:CB	11:H:82:PRO:HD2	2.19	0.72
4:A:794:PRO:HG2	4:A:795:GLU:OE2	1.89	0.72
4:A:590:ARG:NH2	4:A:620:LYS:HB3	2.05	0.72
5:B:911:ILE:HD11	5:B:941:LEU:HD13	1.70	0.72
7:D:18:VAL:O	7:D:19:GLU:HB2	1.89	0.72
5:B:791:THR:HG22	5:B:858:SER:O	1.88	0.72
6:C:212:PRO:HB3	6:C:213:PRO:HD2	1.70	0.72
5:B:542:MET:HE2	5:B:743:ILE:HG13	1.72	0.72
5:B:613:VAL:HG22	5:B:628:THR:HA	1.70	0.72
5:B:810:GLU:HA	5:B:815:ARG:HH12	1.53	0.72
5:B:542:MET:CE	5:B:743:ILE:HG13	2.20	0.71
5:B:957:ASN:O	5:B:959:ASP:N	2.23	0.71
5:B:1001:PHE:CE1	5:B:1073:TYR:HB2	2.25	0.71
7:D:170:THR:CG2	7:D:172:LEU:HG	2.20	0.71
5:B:847:ASP:HB3	6:C:167:HIS:CD2	2.25	0.71
8:E:124:VAL:HG13	8:E:132:ILE:HB	1.71	0.71
4:A:87:ALA:HB3	4:A:276:LEU:HD23	1.70	0.71
5:B:980:PHE:HE1	5:B:990:ILE:HD11	1.53	0.71
3:P:8:A:O2'	3:P:9:G:H5'	1.91	0.71
4:A:798:GLY:HA2	4:A:815:PHE:CD1	2.25	0.71
1:T:16:DG:H4'	4:A:1403:GLU:OE2	1.91	0.71
4:A:34:LYS:HG2	4:A:36:ARG:HH21	1.54	0.71
4:A:244:PRO:HG2	4:A:245:PRO:HD3	1.71	0.71
4:A:1118:VAL:HG12	4:A:1327:ILE:HG13	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:996:ARG:HH22	6:C:175:ALA:H	1.35	0.71
7:D:35:LEU:H	7:D:35:LEU:HD12	1.55	0.71
1:T:23:DC:H2'	1:T:24:DT:C6	2.26	0.71
4:A:446:ARG:HB2	4:A:487:MET:SD	2.31	0.71
5:B:284:ILE:HD13	5:B:333:PHE:HD2	1.56	0.71
5:B:830:TYR:CE2	5:B:1000:PRO:HD3	2.26	0.71
7:D:134:THR:HG22	7:D:135:GLY:N	2.06	0.71
11:H:81:PRO:HB2	11:H:82:PRO:HD2	1.71	0.71
13:J:64:ASN:HB3	13:J:65:PRO:HD3	1.71	0.71
13:J:64:ASN:HD22	13:J:65:PRO:HD3	1.54	0.71
4:A:164:ARG:HG3	4:A:165:GLY:H	1.56	0.71
5:B:295:GLY:H	5:B:298:LEU:HD23	1.55	0.71
5:B:515:HIS:H	5:B:518:HIS:CD2	2.09	0.71
5:B:899:ILE:HD11	5:B:911:ILE:HA	1.73	0.71
10:G:115:MET:HB2	10:G:116:PRO:HD2	1.72	0.71
4:A:1279:ILE:HD11	4:A:1316:VAL:HG21	1.72	0.70
5:B:653:VAL:CG2	5:B:689:LEU:HB3	2.21	0.70
11:H:55:LEU:HD22	11:H:144:ILE:CG2	2.21	0.70
4:A:115:LEU:O	4:A:122:MET:HE3	1.92	0.70
11:H:83:GLN:C	11:H:85:GLY:H	1.92	0.70
4:A:265:LYS:HD2	4:A:265:LYS:N	2.04	0.70
5:B:221:ASN:N	5:B:241:ARG:O	2.24	0.70
5:B:393:LYS:HA	5:B:393:LYS:HE3	1.71	0.70
6:C:36:VAL:HG21	6:C:251:LEU:HD22	1.72	0.70
9:F:97:ARG:O	9:F:101:ILE:HG13	1.91	0.70
10:G:143:ILE:HG22	10:G:144:ARG:N	2.06	0.70
11:H:15:VAL:HG22	11:H:26:ILE:HD11	1.73	0.70
4:A:450:LEU:H	4:A:450:LEU:HD12	1.55	0.70
4:A:666:ILE:HD12	4:A:667:GLY:H	1.57	0.70
4:A:1118:VAL:HG23	4:A:1306:LEU:HB2	1.74	0.70
5:B:168:GLY:H	5:B:450:ALA:HB1	1.56	0.70
7:D:9:GLN:NE2	7:D:38:ILE:HD12	2.07	0.70
7:D:170:THR:HG21	7:D:172:LEU:HG	1.73	0.70
13:J:1:MET:H1	13:J:57:ILE:H	1.37	0.70
4:A:285:PRO:HG2	4:A:288:ALA:HB3	1.73	0.70
4:A:541:ILE:HD13	4:A:549:MET:CE	2.22	0.70
4:A:590:ARG:HH21	4:A:620:LYS:HB2	1.55	0.70
4:A:351:THR:HB	5:B:1103:ILE:CD1	2.22	0.70
5:B:977:GLY:HA3	5:B:1099:VAL:HB	1.74	0.70
6:C:145:CYS:HA	13:J:2:ILE:HD11	1.73	0.70
6:C:179:GLU:HG2	6:C:180:TYR:N	2.07	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:82:THR:HG22	9:F:84:TYR:N	2.06	0.70
10:G:1:MET:SD	10:G:79:PHE:CD1	2.83	0.70
13:J:3:VAL:HG21	13:J:18:TRP:CB	2.22	0.70
5:B:1159:ARG:HD3	5:B:1193:GLN:CG	2.22	0.70
4:A:981:LEU:HD21	4:A:1039:LYS:HA	1.73	0.70
10:G:145:VAL:HG12	10:G:146:LYS:N	2.05	0.70
4:A:567:LYS:NZ	11:H:46:LEU:HB2	2.07	0.70
4:A:853:ASP:OD1	4:A:855:THR:HB	1.90	0.70
4:A:1283:VAL:HG12	4:A:1284:MET:N	2.07	0.70
4:A:1349:TYR:HB2	4:A:1372:VAL:HG21	1.74	0.70
5:B:1165:ILE:HG22	5:B:1166:CYS:H	1.57	0.70
14:K:12:LEU:H	14:K:12:LEU:HD12	1.57	0.70
4:A:92:HIS:O	4:A:94:GLY:N	2.25	0.69
6:C:114:TYR:HB3	6:C:140:ASN:O	1.92	0.69
7:D:7:THR:HB	10:G:42:PHE:CZ	2.26	0.69
5:B:616:ILE:HD12	5:B:616:ILE:N	2.07	0.69
5:B:798:TYR:CE2	6:C:62:PHE:CE2	2.81	0.69
6:C:209:TYR:HD1	6:C:209:TYR:H	1.39	0.69
11:H:111:LEU:HD23	11:H:127:GLY:O	1.93	0.69
4:A:224:PHE:CZ	4:A:231:PRO:HG3	2.28	0.69
4:A:590:ARG:NH2	4:A:620:LYS:CB	2.55	0.69
4:A:1161:THR:HG22	4:A:1163:ILE:N	2.04	0.69
4:A:1373:ASP:HA	4:A:1376:THR:HG22	1.75	0.69
5:B:846:ILE:HG23	5:B:974:PRO:HG2	1.74	0.69
15:L:27:LEU:HD13	15:L:37:LYS:HE2	1.74	0.69
4:A:1329:THR:CG2	4:A:1331:SER:H	2.04	0.69
6:C:179:GLU:HG2	6:C:180:TYR:H	1.56	0.69
10:G:138:THR:CG2	10:G:139:ILE:H	1.92	0.69
4:A:855:THR:CG2	4:A:857:ARG:HE	2.01	0.69
4:A:1332:PHE:H	4:A:1332:PHE:HD2	1.39	0.69
4:A:382:PRO:HB3	4:A:428:TYR:HE2	1.57	0.69
5:B:950:ASP:O	5:B:951:GLN:HB2	1.91	0.69
6:C:66:ARG:HH21	13:J:5:VAL:HG23	1.57	0.69
11:H:89:LEU:C	11:H:91:ASP:H	1.96	0.69
4:A:311:GLN:O	4:A:312:PRO:C	2.31	0.69
4:A:567:LYS:HB3	11:H:96:VAL:N	2.07	0.69
4:A:567:LYS:HD3	11:H:95:TYR:CD2	2.27	0.69
4:A:567:LYS:HD2	4:A:568:PRO:HD2	1.74	0.69
5:B:411:PRO:O	5:B:414:ALA:HB3	1.93	0.69
5:B:653:VAL:HG22	5:B:689:LEU:HB3	1.75	0.69
5:B:701:ILE:HD11	5:B:703:ILE:HD11	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:770:GLN:CD	5:B:983:ARG:HA	2.13	0.69
7:D:7:THR:HB	10:G:42:PHE:CE2	2.28	0.69
11:H:4:THR:CA	11:H:60:ALA:HB2	2.22	0.69
14:K:47:ARG:HH11	14:K:47:ARG:CB	2.04	0.69
5:B:515:HIS:H	5:B:518:HIS:HD2	1.40	0.69
4:A:407:ARG:HB3	4:A:430:TRP:CE2	2.28	0.69
5:B:852:ARG:NH2	15:L:70:ARG:OXT	2.23	0.69
5:B:957:ASN:ND2	5:B:961:LEU:HD12	2.08	0.69
5:B:975:GLN:O	5:B:990:ILE:HD12	1.93	0.69
4:A:809:THR:H	4:A:812:GLU:HB2	1.58	0.68
4:A:1394:THR:HG21	4:A:1398:MET:SD	2.34	0.68
6:C:213:PRO:O	6:C:214:ASN:HB2	1.90	0.68
7:D:40:HIS:CE1	7:D:41:GLN:HG3	2.29	0.68
7:D:130:LEU:O	7:D:132:GLN:N	2.25	0.68
9:F:72:LYS:HD2	9:F:142:SER:HB3	1.75	0.68
4:A:7:SER:HB3	5:B:1193:GLN:NE2	2.08	0.68
4:A:679:ILE:HG12	4:A:732:LEU:HD12	1.75	0.68
5:B:1180:PHE:HB3	5:B:1191:ILE:CD1	2.23	0.68
6:C:244:VAL:O	6:C:248:ILE:HG13	1.94	0.68
4:A:341:MET:HE1	4:A:843:LYS:NZ	2.07	0.68
4:A:913:LEU:HD12	4:A:914:GLU:H	1.58	0.68
5:B:882:THR:HB	5:B:934:LYS:O	1.94	0.68
6:C:226:ASP:O	6:C:227:THR:HB	1.92	0.68
14:K:63:VAL:HG23	14:K:63:VAL:O	1.94	0.68
4:A:463:ILE:CD1	4:A:469:ARG:HG3	2.23	0.68
4:A:546:VAL:O	4:A:550:LEU:HG	1.94	0.68
4:A:567:LYS:CB	11:H:95:TYR:HA	2.24	0.68
5:B:44:VAL:HG11	5:B:199:MET:HG2	1.74	0.68
5:B:745:PRO:O	5:B:748:ILE:HG12	1.93	0.68
5:B:746:SER:HB2	5:B:1046:PRO:HG2	1.75	0.68
5:B:1095:LEU:H	5:B:1095:LEU:HD12	1.58	0.68
5:B:435:THR:C	5:B:437:GLU:H	1.97	0.68
6:C:164:ALA:HA	6:C:167:HIS:O	1.93	0.68
7:D:153:ARG:HB3	7:D:154:PHE:CE1	2.28	0.68
10:G:49:LEU:HG	10:G:76:ALA:HA	1.75	0.68
4:A:12:ARG:HD2	5:B:1218:THR:HB	1.74	0.68
5:B:542:MET:HG2	5:B:747:MET:HB3	1.74	0.68
5:B:603:LEU:HB3	5:B:609:ILE:CD1	2.23	0.68
5:B:642:ASP:O	5:B:644:GLU:N	2.26	0.68
7:D:53:SER:HB3	7:D:152:SER:CB	2.24	0.68
4:A:751:SER:O	4:A:752:LYS:HG2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:35:GLU:OE2	10:G:48:VAL:HG23	1.94	0.68
4:A:475:THR:CG2	4:A:476:SER:H	2.03	0.68
4:A:524:VAL:HG12	4:A:525:GLN:N	2.08	0.68
4:A:1066:VAL:O	4:A:1070:GLN:HG3	1.94	0.68
11:H:17:PRO:HB3	11:H:24:CYS:SG	2.34	0.68
4:A:106:VAL:HG13	4:A:112:LYS:O	1.94	0.68
5:B:589:VAL:HG12	5:B:590:HIS:N	2.03	0.68
7:D:130:LEU:C	7:D:132:GLN:H	1.97	0.68
12:I:34:TYR:CD2	12:I:35:VAL:N	2.62	0.68
5:B:1072:MET:HE3	5:B:1085:ILE:HB	1.75	0.67
8:E:78:LEU:HD21	8:E:80:VAL:HG23	1.74	0.67
11:H:59:ILE:HG22	11:H:60:ALA:H	1.59	0.67
4:A:107:CYS:N	4:A:114:LEU:HD21	2.09	0.67
4:A:591:PHE:HA	4:A:595:THR:HG21	1.74	0.67
4:A:901:LEU:O	4:A:921:GLY:N	2.28	0.67
4:A:1438:THR:HB	5:B:1144:ALA:CB	2.19	0.67
12:I:54:GLU:HB3	12:I:100:PHE:HE2	1.58	0.67
4:A:673:GLY:O	4:A:676:MET:HB2	1.95	0.67
5:B:65:GLU:HG3	5:B:66:ASP:H	1.59	0.67
5:B:184:ALA:HB1	5:B:188:ASP:HB3	1.76	0.67
5:B:516:ASN:HD22	5:B:516:ASN:H	1.39	0.67
5:B:693:ILE:HD13	5:B:701:ILE:HD13	1.76	0.67
5:B:705:MET:H	5:B:710:LEU:CD1	2.07	0.67
5:B:1166:CYS:HB2	5:B:1215:ARG:HH12	1.57	0.67
8:E:90:VAL:HG23	8:E:120:ALA:HA	1.76	0.67
8:E:198:ILE:HD11	8:E:212:ARG:HG3	1.75	0.67
15:L:32:ALA:HB3	15:L:55:ILE:CD1	2.21	0.67
4:A:107:CYS:SG	4:A:171:GLN:HG2	2.35	0.67
4:A:381:THR:HG23	4:A:383:TYR:H	1.59	0.67
4:A:1293:SER:OG	4:A:1294:PRO:HD2	1.94	0.67
4:A:1333:ILE:O	4:A:1337:GLU:HG3	1.95	0.67
5:B:758:PHE:CE1	5:B:1027:ILE:HG22	2.30	0.67
8:E:180:ARG:NH2	8:E:192:ARG:HB2	2.08	0.67
4:A:50:ILE:C	4:A:52:GLY:H	1.96	0.67
4:A:675:THR:O	4:A:679:ILE:HG13	1.95	0.67
4:A:1325:THR:O	8:E:148:GLU:HB2	1.94	0.67
5:B:800:GLN:HB3	13:J:52:THR:CG2	2.24	0.67
9:F:132:LEU:O	9:F:148:VAL:HG22	1.95	0.67
14:K:21:ILE:HG12	14:K:33:ILE:HG12	1.77	0.67
14:K:50:LEU:HD11	14:K:75:ILE:HD13	1.77	0.67
4:A:535:THR:CG2	4:A:616:VAL:HA	2.22	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1299:VAL:HG12	4:A:1300:LYS:N	2.10	0.67
4:A:1324:PRO:HB2	8:E:142:VAL:HG11	1.76	0.67
4:A:172:PRO:HD3	4:A:185:TRP:NE1	2.10	0.67
4:A:547:LEU:HD22	14:K:58:PHE:CD1	2.30	0.67
4:A:1063:MET:CG	4:A:1436:ILE:HG23	2.24	0.67
4:A:1206:ASP:O	4:A:1274:ARG:NH1	2.27	0.67
4:A:1444:MET:CG	10:G:60:ARG:HA	2.25	0.67
4:A:683:ILE:HG21	4:A:801:GLU:HG3	1.75	0.67
4:A:984:LYS:O	4:A:988:LEU:HB2	1.94	0.67
4:A:1143:LEU:HD12	4:A:1146:VAL:HG23	1.75	0.67
4:A:1206:ASP:HB3	4:A:1274:ARG:HH12	1.60	0.66
5:B:240:ILE:CG2	5:B:254:LEU:HB3	2.25	0.66
6:C:43:THR:CG2	6:C:44:LEU:H	2.03	0.66
4:A:356:ASP:HB2	4:A:469:ARG:HH12	1.58	0.66
4:A:679:ILE:O	4:A:683:ILE:HG13	1.95	0.66
4:A:849:MET:CE	4:A:1061:GLY:HA2	2.25	0.66
2:N:3:DA:H2"	2:N:4:DG:OP2	1.95	0.66
4:A:353:ILE:HD13	4:A:487:MET:HE2	1.77	0.66
4:A:1005:GLU:O	4:A:1009:ASN:HB2	1.95	0.66
4:A:1291:VAL:HG13	4:A:1292:PRO:HD2	1.77	0.66
5:B:756:ILE:O	5:B:759:PRO:HD3	1.96	0.66
5:B:778:MET:HE2	5:B:1094:ARG:HG2	1.77	0.66
9:F:125:LEU:HG	9:F:125:LEU:O	1.95	0.66
10:G:34:VAL:HG11	10:G:74:TYR:HE1	1.59	0.66
2:N:1:DC:H1'	2:N:2:DA:O5'	1.96	0.66
4:A:79:GLY:HA3	4:A:243:PRO:CG	2.26	0.66
4:A:225:ASN:ND2	4:A:228:PHE:H	1.90	0.66
4:A:567:LYS:HD3	11:H:95:TYR:CG	2.30	0.66
4:A:590:ARG:HG3	4:A:590:ARG:NH1	2.10	0.66
8:E:114:ASN:O	8:E:115:ASN:HB3	1.95	0.66
9:F:111:LEU:HD12	9:F:111:LEU:N	2.11	0.66
4:A:67:CYS:O	4:A:70:CYS:HB3	1.95	0.66
4:A:1121:GLU:HG2	4:A:1122:PRO:HD2	1.78	0.66
9:F:130:ILE:O	9:F:148:VAL:HG21	1.95	0.66
10:G:47:CYS:O	10:G:76:ALA:HB1	1.95	0.66
12:I:54:GLU:HB3	12:I:100:PHE:CE2	2.30	0.66
4:A:14:VAL:HG21	5:B:1216:LEU:HD12	1.78	0.66
4:A:499:ALA:O	4:A:503:GLN:HB2	1.96	0.66
5:B:37:PHE:CE1	5:B:41:LYS:HG3	2.31	0.66
6:C:67:LEU:HD11	6:C:155:LEU:CD1	2.26	0.66
7:D:128:VAL:O	7:D:132:GLN:HG3	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:23:LYS:HG3	10:G:56:ILE:CD1	2.25	0.66
12:I:8:ARG:HG3	12:I:34:TYR:CE1	2.31	0.66
13:J:2:ILE:HG12	13:J:57:ILE:HD12	1.77	0.66
13:J:48:ARG:HD2	13:J:49:MET:N	2.10	0.66
14:K:6:ARG:O	14:K:9:LEU:HG	1.96	0.66
4:A:982:THR:HG22	4:A:984:LYS:H	1.60	0.66
12:I:62:ILE:O	12:I:62:ILE:HG12	1.94	0.66
14:K:10:PHE:N	14:K:10:PHE:CD2	2.64	0.66
4:A:265:LYS:HZ3	4:A:322:VAL:HG13	1.59	0.66
4:A:340:LEU:HD21	5:B:1200:ALA:N	2.11	0.66
5:B:737:THR:CG2	12:I:66:PRO:HA	2.26	0.66
5:B:758:PHE:HB3	5:B:761:HIS:CD2	2.30	0.66
7:D:7:THR:O	7:D:9:GLN:N	2.29	0.66
7:D:52:LEU:HD21	7:D:147:TYR:CE2	2.31	0.66
5:B:121:ASN:HA	5:B:207:GLY:CA	2.26	0.65
5:B:798:TYR:CE2	6:C:62:PHE:HE2	2.15	0.65
6:C:73:GLN:HB3	6:C:131:HIS:H	1.61	0.65
4:A:68:GLN:C	4:A:70:CYS:H	1.99	0.65
4:A:248:PRO:O	4:A:260:ASP:HB2	1.95	0.65
4:A:376:TYR:OH	4:A:498:ARG:HD2	1.97	0.65
4:A:541:ILE:HG22	4:A:546:VAL:HG23	1.79	0.65
4:A:960:ILE:O	4:A:963:ILE:HG22	1.96	0.65
9:F:89:GLU:OE2	9:F:134:ILE:HG21	1.96	0.65
4:A:58:LEU:HD22	4:A:80:HIS:O	1.96	0.65
4:A:61:ILE:HG22	4:A:62:ASP:H	1.61	0.65
4:A:269:ILE:HD11	4:A:300:VAL:HA	1.77	0.65
4:A:1445:ILE:HD11	10:G:68:ALA:HB1	1.79	0.65
5:B:220:GLY:O	5:B:222:ILE:HG13	1.97	0.65
5:B:333:PHE:O	5:B:334:ILE:HG13	1.96	0.65
6:C:133:ILE:CD1	6:C:237:SER:HA	2.26	0.65
8:E:47:CYS:HA	8:E:52:ARG:O	1.97	0.65
13:J:3:VAL:HG21	13:J:18:TRP:CG	2.31	0.65
4:A:588:LEU:O	4:A:606:LEU:HA	1.95	0.65
5:B:69:LEU:HD22	5:B:429:PHE:CE1	2.32	0.65
5:B:1099:VAL:CG1	5:B:1100:ASP:N	2.60	0.65
6:C:18:VAL:HG12	6:C:18:VAL:O	1.96	0.65
4:A:868:TYR:CE1	4:A:1064:VAL:HG11	2.31	0.65
4:A:1224:LEU:HD12	4:A:1241:ARG:O	1.97	0.65
5:B:120:ARG:HG2	5:B:955:THR:HG21	1.79	0.65
11:H:100:THR:HG22	11:H:101:ALA:N	2.12	0.65
13:J:44:TYR:HA	13:J:47:ARG:CB	2.24	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:K:101:LEU:O	14:K:101:LEU:HD23	1.96	0.65
4:A:107:CYS:H	4:A:114:LEU:HD21	1.61	0.65
4:A:728:LYS:HA	4:A:731:ARG:HB2	1.79	0.65
5:B:1065:GLN:HB2	6:C:201:TRP:CZ3	2.32	0.65
6:C:183:TRP:O	6:C:185:LYS:N	2.29	0.65
15:L:70:ARG:HG2	15:L:70:ARG:HH11	1.62	0.65
4:A:298:PHE:HZ	4:A:314:ALA:HB2	1.61	0.65
4:A:306:ASN:HB2	4:A:324:SER:HB3	1.77	0.65
4:A:852:TYR:CD2	4:A:1060:PRO:HB2	2.32	0.65
4:A:548:ASN:HA	14:K:60:ALA:HB1	1.79	0.65
5:B:96:TYR:HB2	5:B:129:PHE:HB2	1.77	0.65
5:B:902:GLY:O	15:L:65:VAL:HG11	1.97	0.65
5:B:916:THR:O	5:B:935:ARG:HG3	1.97	0.65
6:C:232:VAL:HG21	6:C:244:VAL:HG22	1.79	0.65
1:T:23:DC:H2"	1:T:24:DT:H5'	1.78	0.65
4:A:224:PHE:CE2	4:A:231:PRO:HG3	2.32	0.65
4:A:1100:ARG:NH2	4:A:1351:GLU:HG2	2.12	0.65
4:A:1424:VAL:HG11	5:B:1139:ILE:HD13	1.78	0.65
5:B:102:VAL:HG23	5:B:112:LEU:HB2	1.79	0.65
5:B:708:GLU:O	5:B:710:LEU:N	2.30	0.65
5:B:797:TYR:HB2	5:B:852:ARG:O	1.97	0.65
14:K:49:GLU:HG3	14:K:94:ILE:HG12	1.79	0.65
4:A:680:THR:HA	4:A:683:ILE:HD12	1.79	0.64
4:A:698:GLN:HA	12:I:97:MET:O	1.97	0.64
4:A:746:MET:HE3	5:B:1018:PRO:HG2	1.79	0.64
4:A:901:LEU:H	4:A:926:GLN:HE21	1.45	0.64
4:A:1227:ILE:HG22	4:A:1228:TRP:H	1.62	0.64
5:B:172:ILE:HG22	5:B:173:MET:N	2.12	0.64
5:B:233:PRO:HG2	5:B:234:ILE:CD1	2.26	0.64
5:B:282:ILE:HD12	5:B:382:ILE:HD13	1.79	0.64
15:L:40:LEU:HD13	15:L:44:ASP:HB3	1.79	0.64
4:A:54:ASN:HB3	4:A:247:ARG:HH12	1.63	0.64
4:A:172:PRO:HD3	4:A:185:TRP:HE1	1.62	0.64
4:A:416:ARG:C	4:A:417:TYR:HD2	2.00	0.64
5:B:684:LEU:H	5:B:684:LEU:HD12	1.61	0.64
5:B:1166:CYS:O	5:B:1168:LEU:N	2.28	0.64
5:B:1197:PRO:HG2	5:B:1200:ALA:HB2	1.78	0.64
13:J:1:MET:H1	13:J:57:ILE:N	1.95	0.64
14:K:29:ASN:O	14:K:76:GLN:HG3	1.98	0.64
1:T:20:DC:H4'	4:A:447:GLN:NE2	2.12	0.64
4:A:84:ILE:HD11	4:A:270:LEU:HD22	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:102:VAL:HG11	4:A:211:PHE:CE2	2.32	0.64
4:A:560:ILE:HG13	11:H:78:SER:HB2	1.78	0.64
5:B:185:THR:H	5:B:188:ASP:HB2	1.62	0.64
5:B:467:GLY:H	5:B:475:SER:CB	2.08	0.64
5:B:562:GLY:HA3	5:B:590:HIS:CE1	2.31	0.64
5:B:593:PRO:HG2	5:B:617:ARG:NH2	2.12	0.64
15:L:28:LYS:HB2	15:L:39:SER:HA	1.79	0.64
4:A:965:GLN:O	4:A:968:GLN:HB2	1.97	0.64
5:B:114:PRO:HG2	5:B:115:GLN:H	1.63	0.64
5:B:1065:GLN:HG3	5:B:1067:ARG:H	1.62	0.64
6:C:208:GLU:O	6:C:210:GLU:N	2.30	0.64
10:G:91:VAL:HG23	10:G:141:SER:O	1.97	0.64
4:A:30:ILE:HG23	5:B:1170:THR:HG23	1.79	0.64
4:A:1002:GLY:HA3	4:A:1007:ILE:HG21	1.79	0.64
4:A:1227:ILE:HG22	4:A:1228:TRP:N	2.12	0.64
4:A:1410:PHE:HA	5:B:1212:ILE:HD11	1.79	0.64
6:C:214:ASN:HB3	6:C:217:ASP:OD2	1.98	0.64
4:A:768:GLN:HG2	4:A:816:HIS:HA	1.79	0.64
4:A:1100:ARG:HH21	4:A:1351:GLU:CG	2.11	0.64
4:A:1341:ILE:HG23	4:A:1342:GLU:H	1.62	0.64
7:D:202:ILE:HG21	7:D:207:LEU:HB2	1.79	0.64
5:B:824:ILE:CG2	5:B:1087:PHE:HE2	2.10	0.64
5:B:1138:MET:HA	5:B:1138:MET:HE3	1.80	0.64
13:J:8:PHE:H	13:J:49:MET:CE	2.11	0.64
13:J:36:LEU:HD12	13:J:47:ARG:NH1	2.13	0.64
4:A:399:HIS:CB	4:A:400:PRO:HD3	2.24	0.64
4:A:1299:VAL:HG12	4:A:1300:LYS:H	1.63	0.64
4:A:1329:THR:HG22	4:A:1331:SER:N	2.13	0.64
5:B:361:LEU:HD21	5:B:377:PHE:CD2	2.33	0.64
13:J:1:MET:H1	13:J:56:LEU:N	1.96	0.64
13:J:23:ASN:C	13:J:25:LEU:H	2.01	0.64
4:A:114:LEU:O	4:A:115:LEU:HG	1.98	0.64
5:B:465:ASN:HD22	5:B:465:ASN:N	1.95	0.64
5:B:515:HIS:HD2	5:B:517:THR:H	1.44	0.64
6:C:76:ASP:O	6:C:79:GLN:HG2	1.97	0.64
6:C:166:GLU:HG3	14:K:10:PHE:CZ	2.24	0.64
6:C:251:LEU:O	6:C:251:LEU:HD12	1.98	0.64
13:J:14:VAL:HG12	13:J:50:ILE:HD11	1.78	0.64
4:A:346:ASP:HB3	5:B:1108:ARG:H	1.63	0.64
7:D:170:THR:HB	7:D:172:LEU:H	1.62	0.64
4:A:341:MET:HE1	4:A:843:LYS:HZ3	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:720:ARG:O	4:A:724:GLU:HB2	1.98	0.63
5:B:378:LEU:O	5:B:382:ILE:HG13	1.98	0.63
8:E:213:ILE:HG12	8:E:214:CYS:N	2.13	0.63
11:H:41:ASP:O	11:H:42:ILE:HG13	1.98	0.63
11:H:82:PRO:O	11:H:84:ALA:N	2.27	0.63
4:A:55:ASP:N	4:A:56:PRO:HD3	2.12	0.63
5:B:744:HIS:HD2	5:B:746:SER:OG	1.81	0.63
5:B:822:ASN:ND2	13:J:52:THR:HG21	2.12	0.63
5:B:1183:LYS:N	5:B:1183:LYS:HE3	2.13	0.63
7:D:8:PHE:CZ	7:D:40:HIS:HA	2.33	0.63
4:A:406:ILE:HG22	4:A:412:ARG:HA	1.81	0.63
4:A:1329:THR:CG2	4:A:1331:SER:HB3	2.28	0.63
5:B:526:GLU:HG2	5:B:538:ASN:HD22	1.64	0.63
5:B:822:ASN:HD22	13:J:52:THR:HG21	1.62	0.63
5:B:850:LEU:HD12	5:B:851:PHE:N	2.12	0.63
5:B:1152:MET:HE3	5:B:1157:ALA:HA	1.79	0.63
6:C:105:GLY:HA3	6:C:149:LYS:O	1.99	0.63
7:D:31:GLN:O	7:D:34:GLN:HG3	1.99	0.63
10:G:3:PHE:CD1	10:G:80:LYS:NZ	2.65	0.63
1:T:23:DC:H2'	1:T:24:DT:H71	1.81	0.63
4:A:339:ASN:O	4:A:343:LYS:HG2	1.98	0.63
4:A:1166:ASP:OD2	4:A:1239:ARG:HD2	1.98	0.63
4:A:1198:ASP:O	4:A:1202:MET:HG2	1.99	0.63
5:B:44:VAL:CG1	5:B:199:MET:HG2	2.28	0.63
5:B:827:ILE:HD12	5:B:1086:PHE:HD2	1.64	0.63
5:B:1001:PHE:CZ	5:B:1073:TYR:HB2	2.33	0.63
6:C:177:GLU:HB2	6:C:231:ASN:HB3	1.81	0.63
11:H:42:ILE:HG23	11:H:95:TYR:CE1	2.30	0.63
4:A:35:ILE:HG22	4:A:84:ILE:HD12	1.81	0.63
4:A:1209:MET:SD	4:A:1236:LEU:HD22	2.38	0.63
4:A:1420:ASP:O	4:A:1421:CYS:HB2	1.98	0.63
5:B:65:GLU:HG3	5:B:66:ASP:N	2.14	0.63
5:B:95:ILE:HG13	5:B:130:VAL:HG22	1.80	0.63
5:B:345:LYS:O	5:B:347:LYS:HG2	1.98	0.63
5:B:879:ARG:HH11	5:B:883:LEU:CD2	2.06	0.63
15:L:40:LEU:HD22	15:L:44:ASP:CG	2.19	0.63
5:B:579:ARG:CB	5:B:586:TRP:HE1	2.08	0.63
5:B:1197:PRO:HG2	5:B:1200:ALA:CB	2.28	0.63
7:D:35:LEU:CD2	7:D:173:HIS:HB3	2.28	0.63
7:D:47:LEU:HD12	7:D:48:ILE:H	1.62	0.63
4:A:144:THR:O	4:A:146:MET:HG3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:356:ASP:OD2	14:K:65:HIS:HE1	1.82	0.63
4:A:438:ASP:O	4:A:439:ASN:HB2	1.97	0.63
4:A:1148:ILE:HG23	12:I:49:ILE:HB	1.80	0.63
10:G:15:PRO:HA	10:G:18:PHE:CE1	2.34	0.63
10:G:18:PHE:HA	10:G:22:MET:HE2	1.81	0.63
12:I:25:LEU:HB3	12:I:38:ALA:HB2	1.79	0.63
4:A:90:VAL:CG1	4:A:297:GLN:HA	2.28	0.63
4:A:1329:THR:HG22	4:A:1331:SER:H	1.63	0.63
4:A:1424:VAL:HG13	4:A:1436:ILE:HD11	1.80	0.63
9:F:109:VAL:HG12	9:F:110:ASP:N	2.14	0.63
4:A:341:MET:CE	4:A:843:LYS:NZ	2.61	0.63
4:A:381:THR:CG2	4:A:383:TYR:H	2.12	0.63
4:A:450:LEU:HD12	4:A:450:LEU:N	2.14	0.63
4:A:993:LEU:HD22	4:A:1046:LEU:HD22	1.80	0.63
5:B:424:LEU:O	5:B:428:ILE:HG13	1.99	0.63
5:B:866:TYR:HD1	5:B:870:ILE:O	1.82	0.63
5:B:1096:ARG:O	5:B:1097:HIS:HB2	1.99	0.63
5:B:1224:PHE:CE2	8:E:171:LYS:HG3	2.31	0.63
12:I:80:SER:HB2	12:I:103:CYS:SG	2.39	0.63
13:J:64:ASN:HB3	13:J:65:PRO:HD2	1.80	0.63
4:A:117:GLU:H	4:A:117:GLU:CD	2.01	0.62
4:A:857:ARG:HD3	4:A:861:GLY:O	1.99	0.62
4:A:870:GLU:HB2	8:E:204:THR:HG21	1.80	0.62
4:A:903:ASN:HD22	4:A:904:THR:H	1.47	0.62
5:B:324:ILE:HD13	5:B:330:ALA:HA	1.79	0.62
5:B:753:ALA:O	5:B:756:ILE:HG13	1.99	0.62
5:B:955:THR:HG22	5:B:956:THR:O	1.98	0.62
6:C:146:LYS:C	6:C:147:LEU:HD23	2.20	0.62
7:D:17:LYS:HE2	7:D:17:LYS:H	1.62	0.62
10:G:79:PHE:CE2	10:G:105:PRO:HD2	2.34	0.62
12:I:111:THR:CG2	12:I:112:SER:H	2.07	0.62
15:L:53:HIS:O	15:L:55:ILE:HG12	1.99	0.62
4:A:40:THR:CG2	4:A:41:MET:HG3	2.25	0.62
4:A:826:ASP:O	4:A:830:LYS:HB2	1.99	0.62
4:A:1370:LEU:O	4:A:1374:VAL:HG23	1.98	0.62
5:B:850:LEU:HD12	5:B:851:PHE:H	1.65	0.62
1:T:23:DC:H2"	1:T:24:DT:C5'	2.30	0.62
5:B:1081:LEU:HD12	5:B:1085:ILE:HD11	1.80	0.62
6:C:38:ILE:HA	6:C:173:ALA:CB	2.30	0.62
7:D:63:LEU:HD12	7:D:129:LEU:HG	1.81	0.62
1:T:19:DC:H2"	1:T:20:DC:O5'	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:2:U:C2'	3:P:3:U:O5'	2.48	0.62
4:A:7:SER:HB2	5:B:1175:LEU:HD22	1.81	0.62
4:A:382:PRO:CB	4:A:428:TYR:HE2	2.12	0.62
4:A:783:THR:HG21	4:A:815:PHE:CZ	2.35	0.62
4:A:901:LEU:HA	4:A:907:THR:OG1	1.99	0.62
5:B:400:HIS:O	5:B:402:GLY:N	2.32	0.62
5:B:999:MET:HG2	5:B:1007:VAL:HG22	1.80	0.62
10:G:1:MET:O	10:G:3:PHE:CE1	2.52	0.62
10:G:96:GLN:HG3	10:G:97:HIS:HD2	1.64	0.62
11:H:44:VAL:O	11:H:44:VAL:HG12	2.00	0.62
4:A:90:VAL:HG13	4:A:297:GLN:HA	1.81	0.62
4:A:298:PHE:CZ	4:A:314:ALA:HB2	2.35	0.62
4:A:1206:ASP:HB3	4:A:1274:ARG:NH1	2.15	0.62
5:B:376:PHE:HB3	5:B:586:TRP:CZ3	2.35	0.62
4:A:541:ILE:HG21	4:A:549:MET:HE3	1.81	0.62
4:A:590:ARG:O	4:A:591:PHE:HB2	2.00	0.62
4:A:1323:ASP:C	4:A:1325:THR:H	2.03	0.62
5:B:821:GLN:NE2	5:B:851:PHE:HA	2.14	0.62
6:C:100:THR:HG22	6:C:101:LEU:N	2.15	0.62
4:A:513:SER:HB2	4:A:520:CYS:HB3	1.80	0.62
4:A:782:ARG:NH2	5:B:699:GLU:O	2.32	0.62
4:A:856:THR:HB	4:A:865:GLN:HB2	1.81	0.62
5:B:579:ARG:HG2	5:B:579:ARG:HH11	1.65	0.62
5:B:1073:TYR:CE2	5:B:1080:LYS:HG2	2.35	0.62
7:D:134:THR:HG22	7:D:135:GLY:H	1.65	0.62
4:A:34:LYS:HB3	4:A:36:ARG:HE	1.65	0.62
4:A:746:MET:CE	5:B:1018:PRO:HG2	2.29	0.62
4:A:1208:THR:HG22	4:A:1210:GLY:N	2.14	0.62
5:B:429:PHE:HA	5:B:432:MET:HE3	1.82	0.62
5:B:899:ILE:CD1	5:B:911:ILE:HA	2.29	0.62
5:B:1008:PRO:HB2	5:B:1010:LEU:O	1.99	0.62
8:E:176:PRO:O	8:E:212:ARG:HA	1.99	0.62
10:G:51:TYR:C	10:G:51:TYR:CD2	2.72	0.62
1:T:11:DT:H2"	1:T:12:DA:H5'	1.81	0.62
4:A:17:VAL:HA	5:B:1215:ARG:O	1.99	0.62
4:A:23:SER:HA	4:A:233:TRP:CD1	2.35	0.62
4:A:1323:ASP:O	4:A:1325:THR:N	2.33	0.62
4:A:1454:MET:O	4:A:1454:MET:HG3	1.99	0.62
5:B:520:GLY:N	5:B:748:ILE:HG22	2.14	0.62
6:C:113:VAL:O	6:C:144:ILE:HB	2.00	0.62
10:G:91:VAL:HA	10:G:101:VAL:HA	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:I:82:GLU:HB3	12:I:104:LEU:HD12	1.81	0.62
4:A:265:LYS:HE2	4:A:322:VAL:CG1	2.29	0.62
4:A:761:MET:HA	4:A:804:TYR:HB2	1.82	0.62
4:A:1017:LEU:HB3	8:E:205:SER:HA	1.82	0.62
5:B:1073:TYR:OH	6:C:179:GLU:HG3	1.99	0.62
7:D:33:PHE:CE1	10:G:80:LYS:HE3	2.35	0.62
11:H:91:ASP:C	11:H:93:TYR:H	2.04	0.62
4:A:1124:HIS:HB3	4:A:1130:GLN:HG2	1.82	0.61
5:B:766:ARG:HH22	5:B:1020:ARG:HH11	1.48	0.61
6:C:101:LEU:HD22	6:C:118:LEU:HD21	1.81	0.61
7:D:14:ARG:O	7:D:16:LYS:HD3	2.00	0.61
4:A:663:SER:OG	4:A:664:THR:N	2.32	0.61
4:A:903:ASN:ND2	4:A:904:THR:N	2.46	0.61
5:B:1084:GLN:NE2	5:B:1084:GLN:H	1.98	0.61
6:C:66:ARG:NH2	13:J:5:VAL:HG23	2.15	0.61
7:D:153:ARG:NH2	7:D:184:ALA:HA	2.15	0.61
8:E:195:VAL:HG22	8:E:213:ILE:HG13	1.81	0.61
5:B:807:ARG:HG2	5:B:1045:SER:OG	1.99	0.61
8:E:157:SER:OG	8:E:160:GLU:HG3	2.01	0.61
4:A:728:LYS:O	4:A:732:LEU:HG	2.00	0.61
4:A:842:VAL:HG11	5:B:1136:ASP:OD2	2.00	0.61
4:A:961:ARG:HH11	4:A:961:ARG:HG3	1.66	0.61
4:A:1356:ILE:HD13	4:A:1363:VAL:HG21	1.81	0.61
5:B:69:LEU:HD13	5:B:429:PHE:HD1	1.65	0.61
5:B:569:TYR:CE1	5:B:589:VAL:HG21	2.35	0.61
7:D:47:LEU:CD1	7:D:48:ILE:H	2.13	0.61
10:G:117:GLN:C	10:G:119:LEU:H	2.03	0.61
10:G:153:GLN:HG2	10:G:154:VAL:HG23	1.82	0.61
4:A:19:PHE:HB3	4:A:1413:GLY:HA2	1.81	0.61
4:A:718:VAL:HG12	4:A:722:LEU:HD11	1.82	0.61
4:A:1039:LYS:HE3	4:A:1043:ASP:OD2	2.01	0.61
5:B:37:PHE:CD1	5:B:41:LYS:HG3	2.36	0.61
5:B:705:MET:N	5:B:710:LEU:HD12	2.14	0.61
7:D:5:THR:HG23	10:G:9:LEU:HD13	1.82	0.61
11:H:61:SER:O	11:H:62:SER:HB3	2.01	0.61
4:A:21:LEU:HD11	4:A:1414:ALA:HA	1.83	0.61
4:A:138:ILE:CD1	4:A:222:LEU:HD23	2.31	0.61
4:A:269:ILE:HD13	4:A:300:VAL:HG22	1.81	0.61
4:A:321:PRO:O	4:A:322:VAL:CB	2.48	0.61
4:A:784:LEU:HD11	4:A:815:PHE:CE2	2.35	0.61
5:B:1164:GLY:HA3	5:B:1190:ASP:OD2	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:108:PHE:HE1	9:F:131:PRO:HG3	1.66	0.61
10:G:128:PRO:O	10:G:138:THR:HG23	2.01	0.61
4:A:29:ALA:HB1	5:B:1184:GLY:CA	2.31	0.61
4:A:87:ALA:CB	4:A:276:LEU:HD23	2.31	0.61
4:A:353:ILE:HG21	4:A:487:MET:CE	2.31	0.61
4:A:470:LEU:HD22	4:A:487:MET:CE	2.30	0.61
4:A:870:GLU:HG2	8:E:208:TYR:CG	2.35	0.61
4:A:1035:TYR:O	4:A:1037:LEU:N	2.34	0.61
5:B:295:GLY:N	5:B:298:LEU:HD23	2.16	0.61
6:C:147:LEU:HD23	6:C:147:LEU:N	2.14	0.61
3:P:2:U:H2'	3:P:3:U:O5'	2.00	0.61
4:A:172:PRO:HB3	4:A:185:TRP:CE2	2.35	0.61
4:A:1444:MET:HG2	10:G:60:ARG:CA	2.29	0.61
5:B:359:GLU:O	5:B:362:PRO:HD3	2.00	0.61
5:B:1165:ILE:CG2	5:B:1166:CYS:N	2.61	0.61
6:C:186:LEU:HD21	6:C:224:GLN:O	2.01	0.61
4:A:4:GLN:O	4:A:5:GLN:HB2	2.00	0.61
4:A:896:ARG:NH2	4:A:1030:ARG:NH2	2.49	0.61
5:B:508:LEU:O	5:B:509:ALA:CB	2.49	0.61
5:B:654:ARG:HH11	5:B:654:ARG:HG3	1.65	0.61
5:B:1096:ARG:O	5:B:1097:HIS:CB	2.48	0.61
6:C:238:ILE:HG22	6:C:243:VAL:HG23	1.83	0.61
6:C:241:ASP:O	6:C:245:VAL:HG23	2.00	0.61
1:T:11:DT:O2	2:N:7:DG:N2	2.33	0.61
4:A:427:GLN:HG3	4:A:430:TRP:CE2	2.36	0.61
4:A:1373:ASP:HA	4:A:1376:THR:CG2	2.30	0.61
4:A:1450:LEU:O	4:A:1450:LEU:HG	2.01	0.61
5:B:121:ASN:HA	5:B:207:GLY:HA2	1.83	0.61
6:C:45:ALA:HA	6:C:72:LEU:CD1	2.28	0.61
7:D:17:LYS:H	7:D:17:LYS:CE	2.14	0.61
8:E:15:ALA:O	8:E:19:VAL:HG23	2.01	0.61
4:A:337:ARG:HD3	5:B:1132:GLU:OE1	2.00	0.60
4:A:345:VAL:HG23	4:A:346:ASP:O	2.01	0.60
4:A:1094:VAL:HG13	4:A:1113:THR:CG2	2.21	0.60
5:B:955:THR:CG2	5:B:956:THR:N	2.64	0.60
6:C:100:THR:HG22	6:C:101:LEU:H	1.65	0.60
4:A:152:VAL:HG13	4:A:153:PRO:HD2	1.82	0.60
4:A:269:ILE:CD1	4:A:300:VAL:HA	2.30	0.60
4:A:1424:VAL:HG22	4:A:1436:ILE:HD11	1.83	0.60
5:B:872:GLU:CD	5:B:914:LYS:HE2	2.21	0.60
5:B:948:ILE:HG22	5:B:949:VAL:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:145:VAL:CG1	10:G:146:LYS:N	2.64	0.60
4:A:694:THR:O	4:A:698:GLN:HG3	2.02	0.60
4:A:1063:MET:SD	4:A:1436:ILE:HG12	2.42	0.60
5:B:842:ASN:ND2	5:B:845:SER:OG	2.35	0.60
5:B:1097:HIS:H	5:B:1098:MET:HE2	1.66	0.60
8:E:10:SER:O	8:E:14:ARG:HG3	2.00	0.60
13:J:9:SER:HB2	13:J:45:CYS:HB2	1.83	0.60
2:N:2:DA:OP1	2:N:2:DA:H3'	2.01	0.60
4:A:29:ALA:HB1	5:B:1184:GLY:HA2	1.84	0.60
4:A:50:ILE:O	4:A:52:GLY:N	2.32	0.60
4:A:882:SER:HB3	4:A:953:ASN:OD1	2.00	0.60
8:E:124:VAL:HA	8:E:132:ILE:HD12	1.82	0.60
9:F:119:ARG:HH11	9:F:119:ARG:HG3	1.66	0.60
13:J:44:TYR:CD2	13:J:44:TYR:N	2.68	0.60
4:A:384:ASN:CG	4:A:388:LEU:HD12	2.22	0.60
4:A:896:ARG:HD3	4:A:897:TYR:CE1	2.36	0.60
4:A:1121:GLU:CG	4:A:1122:PRO:HD2	2.31	0.60
8:E:135:PHE:HD2	8:E:140:LEU:HD21	1.66	0.60
3:P:3:U:O2'	4:A:320:ARG:NH2	2.35	0.60
4:A:49:LYS:HZ1	4:A:61:ILE:N	1.99	0.60
4:A:1030:ARG:HG3	4:A:1034:GLU:OE2	2.00	0.60
5:B:582:VAL:HG23	5:B:626:ILE:HB	1.82	0.60
5:B:1182:CYS:O	5:B:1183:LYS:O	2.20	0.60
11:H:81:PRO:CB	11:H:82:PRO:CD	2.80	0.60
4:A:377:PRO:HG3	4:A:493:GLN:HG3	1.83	0.60
4:A:384:ASN:OD1	4:A:388:LEU:HD12	2.01	0.60
4:A:590:ARG:HG3	4:A:590:ARG:HH11	1.65	0.60
4:A:672:ASP:HB2	4:A:736:ASN:OD1	2.01	0.60
4:A:958:VAL:HG11	4:A:1049:ILE:HG23	1.83	0.60
4:A:1410:PHE:HA	5:B:1212:ILE:CD1	2.31	0.60
5:B:601:ARG:O	5:B:605:ARG:HG3	2.01	0.60
5:B:611:PRO:HG2	5:B:685:LEU:HD21	1.83	0.60
5:B:912:ILE:HB	5:B:939:THR:OG1	2.01	0.60
4:A:1290:LYS:O	4:A:1291:VAL:HG23	2.02	0.60
4:A:1323:ASP:OD1	4:A:1325:THR:HB	2.02	0.60
5:B:294:ASP:O	5:B:296:GLU:N	2.31	0.60
8:E:48:ASP:CG	8:E:49:SER:H	2.05	0.60
5:B:570:VAL:CG2	5:B:573:GLN:HB3	2.31	0.60
5:B:825:VAL:CG1	5:B:826:ALA:N	2.65	0.60
5:B:1115:THR:O	5:B:1116:ARG:HB2	2.02	0.60
4:A:567:LYS:HZ1	11:H:46:LEU:HB2	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:903:ASN:HD22	4:A:903:ASN:C	2.04	0.60
5:B:882:THR:HG21	5:B:884:ARG:HB2	1.84	0.60
5:B:1163:CYS:SG	5:B:1165:ILE:HB	2.41	0.60
10:G:45:ILE:O	10:G:45:ILE:HG22	2.02	0.60
15:L:38:LEU:O	15:L:39:SER:HB3	2.02	0.60
4:A:344:ARG:HA	5:B:1129:ARG:HA	1.84	0.59
4:A:466:SER:HA	14:K:2:ASN:HD22	1.67	0.59
4:A:781:ASP:O	4:A:789:LYS:HA	2.02	0.59
4:A:1032:LEU:O	4:A:1036:ARG:HD3	2.01	0.59
4:A:1102:LYS:HG2	4:A:1106:ASN:HD21	1.65	0.59
5:B:522:VAL:HG11	5:B:537:LYS:HB3	1.82	0.59
5:B:744:HIS:CG	5:B:745:PRO:HD2	2.36	0.59
5:B:799:PRO:HB3	5:B:818:PRO:HG2	1.83	0.59
6:C:124:LEU:O	6:C:127:ARG:HG2	2.02	0.59
7:D:172:LEU:HD22	7:D:176:GLU:OE1	2.01	0.59
4:A:841:LEU:O	4:A:845:LEU:HG	2.02	0.59
4:A:858:ASN:C	4:A:858:ASN:HD22	2.04	0.59
4:A:960:ILE:HA	4:A:963:ILE:CG2	2.32	0.59
4:A:1102:LYS:HG2	4:A:1106:ASN:ND2	2.16	0.59
4:A:1149:ALA:HB2	12:I:47:GLU:HA	1.83	0.59
6:C:66:ARG:NH2	13:J:3:VAL:O	2.35	0.59
8:E:14:ARG:NH2	8:E:141:VAL:HG12	2.13	0.59
9:F:111:LEU:C	9:F:113:GLY:N	2.53	0.59
10:G:91:VAL:HB	10:G:139:ILE:O	2.01	0.59
14:K:21:ILE:HG23	14:K:31:VAL:HG11	1.84	0.59
15:L:31:CYS:SG	15:L:34:CYS:SG	3.00	0.59
4:A:53:LEU:HD22	4:A:54:ASN:HD22	1.66	0.59
4:A:1151:GLU:HA	12:I:44:TYR:O	2.01	0.59
4:A:1317:MET:O	4:A:1322:ILE:HD11	2.01	0.59
5:B:115:GLN:HG2	5:B:193:LYS:HB2	1.82	0.59
5:B:192:LEU:O	5:B:193:LYS:HB2	2.02	0.59
5:B:408:LEU:O	5:B:411:PRO:HD2	2.02	0.59
8:E:161:LYS:HD2	8:E:195:VAL:HG23	1.84	0.59
11:H:40:LEU:HD13	11:H:123:MET:HB2	1.85	0.59
12:I:55:THR:HG22	12:I:58:VAL:HG21	1.84	0.59
4:A:86:LEU:HG	4:A:237:THR:O	2.03	0.59
4:A:1153:TYR:CE1	12:I:42:LEU:HD13	2.36	0.59
6:C:98:VAL:C	6:C:99:LEU:HD23	2.22	0.59
7:D:63:LEU:HD13	7:D:133:THR:OG1	2.02	0.59
8:E:17:ARG:O	8:E:21:GLU:HG3	2.02	0.59
10:G:27:LYS:O	10:G:30:LEU:HB3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:34:VAL:HG11	10:G:74:TYR:CE1	2.37	0.59
10:G:51:TYR:O	10:G:54:ILE:HG13	2.02	0.59
10:G:119:LEU:HD12	10:G:131:GLN:O	2.03	0.59
15:L:55:ILE:O	15:L:56:LEU:HB2	2.02	0.59
4:A:37:PHE:HB2	4:A:52:GLY:HA3	1.84	0.59
4:A:869:GLY:O	8:E:204:THR:HG21	2.01	0.59
4:A:1015:VAL:HG12	4:A:1019:CYS:SG	2.43	0.59
4:A:1445:ILE:H	4:A:1445:ILE:CD1	2.00	0.59
5:B:57:TYR:N	5:B:57:TYR:HD1	2.01	0.59
5:B:167:ILE:HG22	5:B:453:ILE:HD12	1.84	0.59
5:B:347:LYS:HG3	5:B:348:ARG:H	1.67	0.59
12:I:55:THR:CG2	12:I:58:VAL:HG21	2.33	0.59
12:I:106:CYS:O	12:I:107:SER:HB2	2.01	0.59
4:A:399:HIS:HB3	4:A:400:PRO:CD	2.27	0.59
4:A:1116:LEU:HD11	4:A:1118:VAL:HG13	1.84	0.59
4:A:1343:ALA:HB2	8:E:150:VAL:HG22	1.83	0.59
5:B:824:ILE:HG23	5:B:1087:PHE:HE2	1.67	0.59
5:B:1000:PRO:O	5:B:1007:VAL:HG23	2.02	0.59
8:E:144:ILE:HG13	8:E:145:THR:N	2.17	0.59
4:A:1114:PRO:HB2	4:A:1311:VAL:HG23	1.84	0.59
9:F:130:ILE:O	9:F:148:VAL:CG2	2.51	0.59
10:G:1:MET:SD	10:G:1:MET:C	2.81	0.59
4:A:37:PHE:N	4:A:37:PHE:CD1	2.69	0.59
4:A:42:ASP:HA	4:A:46:THR:O	2.03	0.59
4:A:1041:ALA:O	4:A:1045:VAL:HG23	2.01	0.59
4:A:1341:ILE:CG2	4:A:1342:GLU:N	2.66	0.59
6:C:77:ILE:HG23	6:C:161:LYS:HE3	1.85	0.59
4:A:252:PHE:O	4:A:253:ASN:HB2	2.03	0.59
4:A:341:MET:CE	4:A:843:LYS:HZ3	2.16	0.59
4:A:1349:TYR:CA	4:A:1372:VAL:HG21	2.32	0.59
5:B:35:SER:O	5:B:39:ARG:HG3	2.03	0.59
5:B:827:ILE:HD12	5:B:1086:PHE:CD2	2.37	0.59
6:C:69:LEU:N	6:C:69:LEU:HD12	2.18	0.59
8:E:178:ILE:HG22	8:E:213:ILE:O	2.03	0.59
1:T:13:DC:H2'	1:T:14:DT:H71	1.85	0.59
4:A:49:LYS:HZ3	4:A:61:ILE:HG13	1.63	0.59
4:A:63:ARG:HA	4:A:74:MET:SD	2.43	0.59
4:A:503:GLN:NE2	9:F:90:ARG:HH21	2.00	0.59
4:A:596:THR:O	4:A:598:LEU:N	2.35	0.59
4:A:954:TRP:HB3	4:A:955:PRO:HD2	1.85	0.59
5:B:542:MET:HB3	5:B:636:PRO:HD2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:918:ILE:HG21	5:B:935:ARG:NH1	2.17	0.59
4:A:2:VAL:HG21	5:B:1157:ALA:C	2.23	0.58
4:A:84:ILE:CD1	4:A:270:LEU:HD22	2.32	0.58
4:A:222:LEU:O	4:A:224:PHE:N	2.36	0.58
4:A:1313:LEU:HD23	4:A:1338:VAL:HG21	1.85	0.58
5:B:502:ILE:H	5:B:502:ILE:HD12	1.68	0.58
5:B:642:ASP:HB3	5:B:649:LYS:CD	2.32	0.58
6:C:8:VAL:HG12	6:C:9:LYS:N	2.18	0.58
10:G:106:MET:CG	10:G:107:LYS:N	2.66	0.58
4:A:741:ASN:HD21	4:A:743:VAL:HB	1.68	0.58
4:A:774:ARG:HB2	4:A:797:LYS:O	2.02	0.58
4:A:890:ASP:H	4:A:1296:GLY:HA3	1.68	0.58
4:A:1130:GLN:HE21	4:A:1134:ILE:HD11	1.67	0.58
4:A:1410:PHE:HD2	5:B:1212:ILE:HD12	1.69	0.58
5:B:168:GLY:N	5:B:450:ALA:HB1	2.17	0.58
5:B:326:ASP:OD2	5:B:328:GLU:HB2	2.02	0.58
11:H:83:GLN:O	11:H:85:GLY:N	2.36	0.58
15:L:40:LEU:HD22	15:L:44:ASP:CB	2.34	0.58
4:A:547:LEU:HD22	14:K:58:PHE:CE1	2.38	0.58
4:A:852:TYR:CE2	4:A:1060:PRO:HB2	2.39	0.58
4:A:1409:LEU:HD13	5:B:1207:LEU:HD21	1.85	0.58
5:B:792:MET:HG3	5:B:855:PHE:HE1	1.68	0.58
11:H:93:TYR:CD2	11:H:143:LEU:HB3	2.38	0.58
13:J:14:VAL:HG12	13:J:14:VAL:O	2.03	0.58
13:J:45:CYS:O	13:J:48:ARG:HG3	2.03	0.58
4:A:185:TRP:HZ3	4:A:200:ARG:HG2	1.65	0.58
5:B:1065:GLN:NE2	5:B:1067:ARG:H	1.99	0.58
6:C:66:ARG:NH1	13:J:2:ILE:CG2	2.67	0.58
6:C:174:ALA:O	6:C:175:ALA:HB3	2.04	0.58
10:G:49:LEU:HD21	10:G:77:VAL:HG23	1.85	0.58
10:G:149:GLY:O	10:G:159:ALA:HB1	2.02	0.58
13:J:44:TYR:HD2	13:J:44:TYR:N	1.99	0.58
14:K:53:ASP:OD1	14:K:55:LYS:HB2	2.02	0.58
5:B:254:LEU:HD23	5:B:381:MET:HE1	1.85	0.58
5:B:293:PRO:HG2	5:B:296:GLU:HB3	1.86	0.58
9:F:111:LEU:O	9:F:113:GLY:N	2.34	0.58
14:K:31:VAL:HG12	14:K:32:VAL:N	2.17	0.58
4:A:369:SER:HB2	14:K:2:ASN:OD1	2.03	0.58
4:A:541:ILE:HG21	4:A:549:MET:CE	2.33	0.58
4:A:785:PRO:HG2	4:A:786:HIS:HD2	1.68	0.58
4:A:910:PRO:HB3	4:A:917:SER:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1114:PRO:O	4:A:1115:SER:O	2.21	0.58
5:B:20:ASP:O	5:B:22:SER:N	2.37	0.58
6:C:31:ASN:O	6:C:34:ARG:HB3	2.04	0.58
14:K:6:ARG:O	14:K:8:GLU:N	2.37	0.58
1:T:22:DC:OP1	5:B:1122:ARG:HB3	2.04	0.58
4:A:666:ILE:HG23	5:B:1026:LEU:HB3	1.86	0.58
4:A:858:ASN:ND2	4:A:861:GLY:H	2.01	0.58
5:B:265:SER:O	5:B:266:ALA:HB3	2.03	0.58
5:B:345:LYS:O	5:B:347:LYS:N	2.35	0.58
5:B:1006:ILE:HG23	13:J:45:CYS:SG	2.44	0.58
6:C:238:ILE:CG2	6:C:242:GLN:HB2	2.34	0.58
8:E:177:ARG:HD3	8:E:215:MET:CG	2.31	0.58
4:A:63:ARG:HA	4:A:74:MET:CE	2.34	0.58
4:A:152:VAL:CG1	4:A:153:PRO:HD2	2.33	0.58
4:A:1017:LEU:CB	8:E:205:SER:HA	2.34	0.58
4:A:1334:ASP:O	4:A:1337:GLU:N	2.36	0.58
5:B:828:ALA:HB2	5:B:1085:ILE:HG23	1.85	0.58
5:B:863:GLU:OE2	5:B:873:THR:HA	2.03	0.58
7:D:145:MET:O	7:D:149:THR:HB	2.03	0.58
12:I:55:THR:HG22	12:I:55:THR:O	2.02	0.58
1:T:21:DT:H2"	1:T:22:DC:O5'	2.03	0.58
4:A:92:HIS:CD2	4:A:304:MET:HE3	2.39	0.58
4:A:372:LYS:HA	4:A:435:HIS:ND1	2.19	0.58
4:A:675:THR:OG1	4:A:736:ASN:ND2	2.37	0.58
4:A:1313:LEU:HD23	4:A:1338:VAL:CG2	2.34	0.58
5:B:980:PHE:CA	5:B:1095:LEU:HD11	2.34	0.58
4:A:55:ASP:C	4:A:57:ARG:N	2.52	0.58
4:A:347:PHE:HE2	4:A:375:THR:HG23	1.69	0.58
4:A:445:ASN:HB2	4:A:454:SER:O	2.03	0.58
5:B:969:ARG:NH1	6:C:61:GLU:OE1	2.37	0.58
6:C:107:SER:C	6:C:109:SER:H	2.07	0.58
6:C:249:ASP:O	6:C:252:GLN:HB3	2.04	0.58
9:F:89:GLU:O	9:F:93:ILE:HG13	2.04	0.58
11:H:22:LYS:O	11:H:23:VAL:HG23	2.04	0.58
4:A:494:SER:O	4:A:497:THR:N	2.37	0.57
4:A:541:ILE:HD13	4:A:549:MET:HE1	1.85	0.57
4:A:1116:LEU:CD1	4:A:1118:VAL:HG13	2.34	0.57
5:B:172:ILE:HD13	5:B:178:ASN:CB	2.25	0.57
8:E:145:THR:HG21	8:E:187:TYR:CD2	2.39	0.57
13:J:1:MET:N	13:J:56:LEU:H	2.00	0.57
13:J:64:ASN:CB	13:J:65:PRO:CD	2.78	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:L:27:LEU:HB3	15:L:37:LYS:HD3	1.86	0.57
4:A:49:LYS:HE2	4:A:61:ILE:HD12	1.84	0.57
4:A:685:GLU:HG3	4:A:686:ALA:N	2.18	0.57
5:B:54:PHE:HA	5:B:58:THR:HB	1.85	0.57
5:B:57:TYR:N	5:B:57:TYR:CD1	2.69	0.57
5:B:525:ALA:O	5:B:768:THR:HG23	2.05	0.57
5:B:576:ASP:HA	5:B:622:LYS:NZ	2.20	0.57
10:G:106:MET:HG2	10:G:107:LYS:N	2.19	0.57
4:A:577:ILE:O	4:A:580:VAL:HG23	2.04	0.57
4:A:626:ASN:O	4:A:631:HIS:CD2	2.57	0.57
4:A:701:LEU:HD21	12:I:114:GLN:HB2	1.86	0.57
5:B:758:PHE:HZ	5:B:1031:LEU:HD22	1.69	0.57
5:B:1031:LEU:HD11	5:B:1042:GLY:HA3	1.85	0.57
7:D:54:GLU:O	7:D:58:VAL:HG23	2.03	0.57
3:P:3:U:H4'	4:A:323:LYS:NZ	2.19	0.57
4:A:382:PRO:HB3	4:A:428:TYR:CE2	2.38	0.57
4:A:863:VAL:HG11	4:A:866:PHE:CD2	2.38	0.57
4:A:1447:GLU:OE2	10:G:23:LYS:HB2	2.04	0.57
5:B:100:PRO:HD2	5:B:180:TYR:CE1	2.40	0.57
8:E:101:GLN:NE2	8:E:127:ILE:HG21	2.19	0.57
10:G:79:PHE:HE2	10:G:105:PRO:HG2	1.69	0.57
11:H:58:THR:HB	11:H:143:LEU:HD13	1.86	0.57
13:J:47:ARG:HG2	13:J:47:ARG:HH11	1.69	0.57
14:K:65:HIS:CD2	14:K:67:PHE:HB2	2.39	0.57
4:A:34:LYS:HG2	4:A:36:ARG:NH2	2.19	0.57
4:A:102:VAL:O	4:A:105:CYS:HB2	2.04	0.57
4:A:268:ASP:HB3	4:A:299:HIS:CE1	2.39	0.57
4:A:1313:LEU:O	4:A:1315:GLU:N	2.37	0.57
4:A:1341:ILE:O	4:A:1344:GLY:N	2.38	0.57
5:B:217:ARG:HD2	5:B:217:ARG:C	2.24	0.57
9:F:118:LEU:HD12	9:F:118:LEU:O	2.05	0.57
4:A:138:ILE:HD13	4:A:222:LEU:HD23	1.86	0.57
4:A:215:SER:O	4:A:218:ASP:HB2	2.04	0.57
4:A:565:ILE:O	4:A:570:PRO:HA	2.05	0.57
4:A:647:GLY:O	4:A:651:LYS:HG3	2.04	0.57
4:A:868:TYR:CD2	4:A:1058:VAL:HG21	2.35	0.57
7:D:175:PHE:HZ	10:G:85:GLU:HG3	1.68	0.57
9:F:90:ARG:HD3	9:F:155:LEU:CD1	2.35	0.57
11:H:142:LEU:C	11:H:143:LEU:HD12	2.25	0.57
4:A:34:LYS:CG	4:A:36:ARG:HH21	2.18	0.57
4:A:844:ALA:O	4:A:845:LEU:HD23	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1220:PHE:O	4:A:1221:LYS:HB2	2.03	0.57
5:B:557:PHE:C	5:B:557:PHE:CD2	2.77	0.57
5:B:579:ARG:N	5:B:589:VAL:HG13	2.18	0.57
5:B:604:ARG:NH1	5:B:691:GLU:OE2	2.38	0.57
6:C:213:PRO:HG2	6:C:214:ASN:H	1.69	0.57
7:D:52:LEU:O	7:D:54:GLU:N	2.36	0.57
8:E:94:LYS:CE	8:E:98:ILE:HD11	2.30	0.57
9:F:90:ARG:HG3	9:F:91:ALA:N	2.18	0.57
10:G:143:ILE:CG2	10:G:144:ARG:N	2.67	0.57
4:A:71:GLN:C	4:A:73:GLY:H	2.08	0.57
4:A:477:PRO:HG2	4:A:521:MET:HG2	1.87	0.57
4:A:600:PRO:C	4:A:602:ASP:H	2.05	0.57
4:A:1336:MET:CE	4:A:1381:LEU:HG	2.35	0.57
5:B:794:ASN:C	5:B:795:ILE:HD12	2.25	0.57
5:B:955:THR:HG22	5:B:956:THR:N	2.20	0.57
5:B:1069:PHE:H	5:B:1069:PHE:HD1	1.52	0.57
4:A:385:ILE:HG22	4:A:386:ASP:N	2.20	0.57
5:B:357:GLN:O	5:B:366:GLN:HA	2.04	0.57
5:B:594:ALA:CA	5:B:617:ARG:HH12	2.15	0.57
5:B:847:ASP:C	5:B:849:GLY:H	2.07	0.57
6:C:212:PRO:CB	6:C:213:PRO:HD2	2.35	0.57
8:E:134:THR:C	8:E:135:PHE:HD1	2.08	0.57
4:A:477:PRO:CG	4:A:521:MET:HG2	2.35	0.57
4:A:1116:LEU:H	4:A:1308:THR:HG22	1.69	0.57
4:A:1239:ARG:HH22	4:A:1241:ARG:HH22	1.51	0.57
5:B:31:TRP:CE3	5:B:34:ILE:HD12	2.40	0.57
5:B:190:TYR:HD2	13:J:62:ARG:O	1.88	0.57
5:B:1099:VAL:O	5:B:1101:ASP:N	2.38	0.57
6:C:238:ILE:HG23	6:C:242:GLN:HB2	1.85	0.57
7:D:17:LYS:O	7:D:17:LYS:HG2	2.04	0.57
10:G:1:MET:SD	10:G:1:MET:O	2.63	0.57
4:A:44:THR:O	4:A:45:GLN:HB2	2.04	0.56
4:A:442:VAL:O	4:A:457:ALA:HA	2.05	0.56
4:A:590:ARG:HB3	4:A:605:MET:N	2.20	0.56
5:B:552:MET:HA	5:B:555:ILE:HB	1.87	0.56
15:L:34:CYS:SG	15:L:34:CYS:O	2.63	0.56
4:A:93:VAL:HG11	4:A:305:ASP:HB3	1.86	0.56
4:A:115:LEU:HB2	4:A:122:MET:HE2	1.87	0.56
4:A:444:PHE:CB	4:A:458:HIS:HD2	2.17	0.56
4:A:886:ILE:CG2	4:A:887:GLY:N	2.67	0.56
4:A:946:VAL:HG13	8:E:201:LYS:HB3	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:642:ASP:HB3	5:B:649:LYS:HD2	1.87	0.56
6:C:70:ILE:HG12	6:C:142:VAL:HG11	1.87	0.56
10:G:59:GLY:HA3	10:G:70:PHE:CD2	2.41	0.56
4:A:168:GLY:O	4:A:169:ASN:C	2.44	0.56
4:A:886:ILE:HD11	4:A:943:LEU:CB	2.35	0.56
5:B:603:LEU:HD13	5:B:608:ASP:CB	2.33	0.56
5:B:616:ILE:HG23	5:B:700:SER:OG	2.06	0.56
5:B:635:ARG:NH2	5:B:742:GLU:OE2	2.38	0.56
5:B:792:MET:HA	5:B:856:PHE:O	2.06	0.56
5:B:912:ILE:O	5:B:938:SER:HB3	2.05	0.56
5:B:1102:LYS:O	5:B:1103:ILE:C	2.44	0.56
6:C:73:GLN:NE2	6:C:75:MET:HB2	2.20	0.56
6:C:181:ASP:OD1	6:C:186:LEU:HD13	2.05	0.56
8:E:3:GLN:HG3	8:E:4:GLU:N	2.20	0.56
8:E:55:ARG:HD2	8:E:83:CYS:O	2.05	0.56
9:F:135:ARG:HD3	9:F:143:PHE:CD2	2.39	0.56
10:G:25:TYR:HE2	10:G:29:LYS:HD2	1.70	0.56
11:H:110:ASP:O	11:H:128:ASN:ND2	2.38	0.56
12:I:14:LEU:HA	12:I:28:GLU:O	2.06	0.56
13:J:21:TYR:CE1	13:J:36:LEU:HD21	2.40	0.56
4:A:282:ASN:O	4:A:284:ALA:N	2.38	0.56
5:B:97:VAL:HG12	5:B:178:ASN:HD21	1.70	0.56
5:B:1183:LYS:HA	5:B:1186:ASP:HA	1.88	0.56
6:C:77:ILE:HA	6:C:129:ILE:HD11	1.88	0.56
10:G:74:TYR:H	10:G:74:TYR:HD2	1.51	0.56
11:H:89:LEU:O	11:H:91:ASP:N	2.36	0.56
14:K:49:GLU:HG3	14:K:94:ILE:CG1	2.35	0.56
4:A:42:ASP:HB3	4:A:45:GLN:H	1.70	0.56
5:B:195:CYS:SG	5:B:196:PRO:HD2	2.46	0.56
5:B:880:THR:O	5:B:881:ASN:HB2	2.05	0.56
5:B:1072:MET:HE1	5:B:1085:ILE:HB	1.87	0.56
6:C:40:GLU:HA	6:C:163:ILE:HG21	1.87	0.56
7:D:7:THR:HG21	7:D:32:GLU:CD	2.25	0.56
7:D:195:ILE:HG22	7:D:198:LEU:HG	1.85	0.56
4:A:356:ASP:HB2	4:A:469:ARG:HH11	1.71	0.56
4:A:384:ASN:O	4:A:385:ILE:C	2.43	0.56
4:A:860:LEU:CD1	4:A:1393:ASN:HB2	2.31	0.56
5:B:94:LYS:HG2	5:B:95:ILE:N	2.20	0.56
5:B:225:VAL:HG12	5:B:238:ALA:HB2	1.88	0.56
5:B:839:MET:HG3	5:B:1010:LEU:HD11	1.86	0.56
5:B:1085:ILE:HD12	5:B:1085:ILE:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:254:LYS:O	6:C:258:ILE:HD13	2.05	0.56
7:D:40:HIS:CB	10:G:73:LYS:HZ3	2.05	0.56
9:F:143:PHE:C	9:F:143:PHE:HD1	2.09	0.56
11:H:23:VAL:HG13	11:H:42:ILE:O	2.05	0.56
3:P:3:U:H4'	4:A:323:LYS:HZ3	1.71	0.56
4:A:75:ASN:O	4:A:76:GLU:CB	2.54	0.56
4:A:965:GLN:HA	4:A:968:GLN:HG3	1.87	0.56
5:B:39:ARG:NH2	5:B:665:GLU:HG2	2.20	0.56
5:B:258:LEU:HG	5:B:258:LEU:O	2.05	0.56
5:B:620:ARG:NH2	12:I:89:GLN:NE2	2.54	0.56
5:B:707:PRO:O	5:B:711:GLU:HG3	2.06	0.56
5:B:906:SER:O	5:B:941:LEU:HD23	2.05	0.56
7:D:160:VAL:O	7:D:164:ILE:HG13	2.06	0.56
13:J:64:ASN:ND2	13:J:65:PRO:HD3	2.21	0.56
4:A:262:LEU:O	4:A:264:PHE:N	2.39	0.56
4:A:1341:ILE:CG2	4:A:1342:GLU:H	2.18	0.56
5:B:113:TYR:CD2	5:B:192:LEU:HD22	2.41	0.56
5:B:981:ALA:HB2	5:B:987:LYS:HA	1.87	0.56
10:G:117:GLN:O	10:G:119:LEU:N	2.37	0.56
4:A:68:GLN:O	4:A:70:CYS:N	2.34	0.56
4:A:269:ILE:HG12	4:A:299:HIS:HB3	1.86	0.56
4:A:1063:MET:HG3	4:A:1436:ILE:HG23	1.88	0.56
5:B:176:SER:O	5:B:182:SER:HB3	2.05	0.56
5:B:299:GLU:HB3	5:B:571:PRO:HG3	1.87	0.56
5:B:365:THR:HG23	5:B:367:LEU:N	2.13	0.56
9:F:138:LEU:HB3	9:F:139:PRO:HD2	1.87	0.56
14:K:10:PHE:N	14:K:10:PHE:HD2	2.03	0.56
14:K:46:ILE:O	14:K:50:LEU:HB2	2.04	0.56
1:T:12:DA:H2"	1:T:13:DC:O5'	2.05	0.56
4:A:442:VAL:HB	4:A:489:LEU:HD11	1.87	0.56
4:A:947:PHE:HD2	4:A:954:TRP:CZ2	2.24	0.56
4:A:1100:ARG:HH21	4:A:1351:GLU:HG2	1.69	0.56
4:A:1164:PRO:HG2	4:A:1165:GLU:H	1.71	0.56
5:B:260:GLY:O	5:B:267:ARG:HD3	2.06	0.56
5:B:305:VAL:O	5:B:305:VAL:HG12	2.05	0.56
5:B:405:ARG:CZ	5:B:632:ARG:HG2	2.36	0.56
5:B:516:ASN:N	5:B:516:ASN:ND2	2.47	0.56
5:B:731:VAL:HG12	5:B:732:SER:N	2.20	0.56
5:B:1087:PHE:HD2	5:B:1088:GLY:N	2.04	0.56
6:C:203:GLN:HG2	6:C:207:CYS:SG	2.46	0.56
6:C:248:ILE:HD13	14:K:101:LEU:HD22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:81:THR:HB	9:F:136:ARG:HH11	1.70	0.56
9:F:111:LEU:H	9:F:111:LEU:CD1	2.15	0.56
12:I:33:SER:O	12:I:35:VAL:HG23	2.06	0.56
4:A:335:ARG:NH1	5:B:1202:LEU:HD13	2.21	0.55
4:A:605:MET:HE3	4:A:614:PHE:O	2.06	0.55
4:A:1149:ALA:CB	12:I:47:GLU:HA	2.36	0.55
4:A:1214:GLU:O	4:A:1218:GLN:HG2	2.05	0.55
5:B:637:LEU:HD21	5:B:742:GLU:OE2	2.05	0.55
5:B:758:PHE:CE2	5:B:1044:ALA:HA	2.40	0.55
5:B:861:ASP:OD1	5:B:862:GLN:N	2.39	0.55
11:H:135:LEU:HD13	11:H:137:GLN:HE21	1.71	0.55
12:I:85:PHE:CD1	12:I:99:LEU:HD13	2.41	0.55
14:K:42:LEU:HD21	14:K:46:ILE:HD11	1.88	0.55
14:K:45:LEU:HG	14:K:94:ILE:CD1	2.33	0.55
14:K:58:PHE:HB3	14:K:76:GLN:HB3	1.87	0.55
1:T:12:DA:C2	2:N:6:DA:C2	2.94	0.55
4:A:44:THR:O	4:A:44:THR:HG22	2.06	0.55
4:A:482:PHE:O	5:B:989:THR:HG23	2.06	0.55
5:B:222:ILE:O	5:B:240:ILE:HA	2.06	0.55
5:B:259:TYR:HB2	5:B:268:THR:HG23	1.88	0.55
5:B:310:MET:O	5:B:313:MET:HB2	2.06	0.55
5:B:906:SER:HA	5:B:946:ASN:HB2	1.88	0.55
5:B:1196:ILE:HB	5:B:1197:PRO:HD2	1.88	0.55
6:C:152:GLU:HG2	6:C:153:LEU:H	1.72	0.55
10:G:14:HIS:CD2	10:G:16:SER:HB2	2.41	0.55
13:J:1:MET:H1	13:J:56:LEU:CA	2.20	0.55
3:P:2:U:O2'	3:P:3:U:H5'	2.06	0.55
4:A:709:THR:HG21	12:I:93:LYS:O	2.06	0.55
4:A:768:GLN:CG	4:A:816:HIS:HA	2.36	0.55
4:A:867:ILE:HG22	4:A:872:GLY:N	2.22	0.55
5:B:226:PHE:HA	5:B:395:GLN:HG3	1.86	0.55
5:B:515:HIS:CD2	5:B:517:THR:H	2.23	0.55
5:B:1065:GLN:HE21	5:B:1067:ARG:HG2	1.72	0.55
8:E:78:LEU:HD23	8:E:78:LEU:C	2.27	0.55
8:E:198:ILE:CD1	8:E:212:ARG:HG3	2.36	0.55
10:G:9:LEU:HG	10:G:10:ASN:N	2.20	0.55
11:H:116:TYR:HE2	11:H:140:ALA:CB	2.19	0.55
4:A:22:PHE:CE1	5:B:1213:THR:HG22	2.42	0.55
4:A:278:THR:O	4:A:278:THR:HG22	2.07	0.55
4:A:416:ARG:O	4:A:417:TYR:HD2	1.89	0.55
5:B:332:ASP:O	5:B:334:ILE:N	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:446:LEU:O	5:B:447:ALA:HB3	2.06	0.55
5:B:1135:ARG:O	5:B:1139:ILE:HG13	2.07	0.55
8:E:124:VAL:HG13	8:E:132:ILE:CB	2.35	0.55
12:I:71:SER:OG	12:I:83:ASN:HB2	2.07	0.55
4:A:34:LYS:CB	4:A:36:ARG:HE	2.18	0.55
4:A:567:LYS:HB3	11:H:95:TYR:CA	2.35	0.55
4:A:1260:LEU:O	4:A:1260:LEU:HG	2.07	0.55
10:G:44:TYR:O	10:G:78:VAL:HG12	2.07	0.55
4:A:317:LYS:O	4:A:318:SER:CB	2.55	0.55
4:A:1349:TYR:CB	4:A:1372:VAL:HG21	2.36	0.55
4:A:1402:PHE:CE1	4:A:1403:GLU:HG3	2.42	0.55
4:A:1445:ILE:HD12	10:G:59:GLY:O	2.07	0.55
5:B:94:LYS:O	5:B:130:VAL:HG13	2.07	0.55
5:B:778:MET:CE	5:B:1094:ARG:CD	2.85	0.55
8:E:42:PHE:HZ	8:E:58:MET:HE3	1.72	0.55
10:G:1:MET:HE3	10:G:80:LYS:O	2.06	0.55
11:H:127:GLY:O	11:H:128:ASN:HB2	2.06	0.55
4:A:154:SER:HB3	4:A:162:VAL:HG21	1.89	0.55
4:A:590:ARG:HH11	4:A:590:ARG:CG	2.19	0.55
4:A:816:HIS:CD2	5:B:764:SER:HB2	2.42	0.55
4:A:843:LYS:HD3	4:A:846:GLU:OE2	2.07	0.55
4:A:845:LEU:HD22	4:A:1374:VAL:HG21	1.89	0.55
4:A:1155:ASP:OD2	4:A:1161:THR:HG23	2.06	0.55
5:B:215:GLN:HA	5:B:215:GLN:NE2	2.21	0.55
5:B:358:LYS:HA	5:B:366:GLN:HB3	1.89	0.55
5:B:637:LEU:O	5:B:690:VAL:HG13	2.06	0.55
6:C:31:ASN:O	6:C:34:ARG:N	2.40	0.55
2:N:1:DC:H1'	2:N:2:DA:C5'	2.37	0.55
4:A:10:PRO:O	5:B:1193:GLN:HB3	2.06	0.55
4:A:93:VAL:HG13	4:A:301:ALA:HB1	1.89	0.55
4:A:767:GLN:HB2	4:A:799:PHE:HD1	1.71	0.55
4:A:785:PRO:HG2	4:A:786:HIS:CD2	2.41	0.55
4:A:1035:TYR:O	4:A:1037:LEU:HD23	2.07	0.55
5:B:361:LEU:N	5:B:362:PRO:CD	2.70	0.55
5:B:806:THR:CG2	5:B:808:ALA:HB3	2.37	0.55
7:D:176:GLU:C	7:D:178:ALA:H	2.10	0.55
15:L:25:ALA:O	15:L:26:THR:HB	2.07	0.55
4:A:265:LYS:HE2	4:A:322:VAL:HG13	1.89	0.55
4:A:308:ILE:HG22	4:A:309:ALA:H	1.71	0.55
4:A:709:THR:HB	4:A:712:GLU:HG3	1.88	0.55
4:A:981:LEU:HD23	4:A:1039:LYS:HA	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:351:TYR:CE1	5:B:355:ILE:HD11	2.42	0.55
5:B:866:TYR:O	5:B:868:MET:N	2.40	0.55
6:C:45:ALA:O	6:C:159:ALA:HA	2.07	0.55
6:C:147:LEU:HD12	6:C:151:GLN:O	2.07	0.55
9:F:76:LYS:O	9:F:79:ARG:HD3	2.07	0.55
4:A:853:ASP:OD1	4:A:855:THR:CB	2.55	0.55
5:B:69:LEU:HD22	5:B:429:PHE:HE1	1.71	0.55
5:B:473:MET:O	5:B:475:SER:N	2.40	0.55
5:B:640:VAL:O	5:B:640:VAL:HG12	2.07	0.55
5:B:758:PHE:CE1	5:B:1027:ILE:CG2	2.90	0.55
5:B:874:PHE:HA	5:B:913:GLY:O	2.06	0.55
5:B:1172:ILE:HG22	5:B:1172:ILE:O	2.07	0.55
10:G:73:LYS:HE2	10:G:74:TYR:O	2.07	0.55
5:B:953:LEU:CD2	5:B:965:LYS:HB2	2.35	0.54
5:B:1099:VAL:HG12	5:B:1100:ASP:H	1.71	0.54
6:C:11:ARG:HD3	6:C:209:TYR:CE2	2.42	0.54
12:I:52:ILE:HG13	12:I:52:ILE:O	2.06	0.54
15:L:30:ILE:O	15:L:56:LEU:HA	2.07	0.54
15:L:49:LYS:O	15:L:50:ASP:CB	2.54	0.54
15:L:58:LYS:O	15:L:58:LYS:HG2	2.06	0.54
1:T:20:DC:H4'	4:A:447:GLN:HE22	1.71	0.54
4:A:19:PHE:HE1	4:A:1396:ALA:HB3	1.71	0.54
4:A:718:VAL:O	4:A:721:PHE:HB2	2.08	0.54
4:A:1191:TRP:CD1	4:A:1256:GLU:HB2	2.41	0.54
4:A:1291:VAL:HG13	4:A:1292:PRO:CD	2.35	0.54
4:A:1308:THR:HG23	4:A:1309:ASP:N	2.22	0.54
4:A:1336:MET:HE3	4:A:1381:LEU:HG	1.88	0.54
5:B:180:TYR:HD1	5:B:180:TYR:H	1.54	0.54
5:B:570:VAL:HG23	5:B:573:GLN:HB3	1.88	0.54
12:I:60:GLN:NE2	12:I:107:SER:OG	2.40	0.54
13:J:5:VAL:O	13:J:6:ARG:O	2.26	0.54
4:A:3:GLY:O	4:A:4:GLN:CB	2.56	0.54
4:A:61:ILE:HG22	4:A:62:ASP:N	2.23	0.54
4:A:244:PRO:CG	4:A:245:PRO:HD3	2.38	0.54
4:A:767:GLN:NE2	4:A:774:ARG:HB3	2.22	0.54
4:A:808:LEU:HG	4:A:812:GLU:HB3	1.89	0.54
4:A:1441:PHE:CE2	9:F:89:GLU:HG2	2.42	0.54
5:B:865:LYS:HE2	5:B:871:THR:OG1	2.06	0.54
5:B:1006:ILE:HD13	13:J:44:TYR:CE2	2.43	0.54
5:B:1223:ASP:O	5:B:1224:PHE:HB2	2.08	0.54
7:D:56:ARG:HD3	7:D:149:THR:HA	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:124:VAL:HG13	8:E:132:ILE:HD12	1.88	0.54
1:T:12:DA:H2"	1:T:13:DC:C5'	2.37	0.54
1:T:18:DC:P	1:T:18:DC:H3'	2.48	0.54
4:A:219:PHE:O	4:A:222:LEU:O	2.25	0.54
5:B:459:TYR:CE1	5:B:469:GLN:HG2	2.42	0.54
6:C:73:GLN:HE21	6:C:75:MET:N	2.05	0.54
4:A:69:THR:C	4:A:71:GLN:N	2.61	0.54
4:A:366:VAL:CG2	4:A:460:VAL:HG22	2.34	0.54
4:A:979:SER:OG	4:A:980:ASP:N	2.41	0.54
4:A:1074:GLU:N	4:A:1075:PRO:HD2	2.23	0.54
5:B:1004:GLU:O	6:C:177:GLU:HG2	2.08	0.54
5:B:1038:SER:C	5:B:1040:ASN:H	2.10	0.54
7:D:40:HIS:CB	10:G:73:LYS:HZ2	2.18	0.54
7:D:209:ARG:O	7:D:212:LYS:HB2	2.08	0.54
9:F:119:ARG:HG3	9:F:119:ARG:NH1	2.23	0.54
4:A:3:GLY:O	4:A:4:GLN:HB2	2.08	0.54
4:A:182:VAL:HG22	4:A:201:VAL:HA	1.89	0.54
4:A:1435:PRO:HA	4:A:1439:GLY:O	2.06	0.54
5:B:39:ARG:HH21	5:B:665:GLU:CD	2.11	0.54
5:B:309:GLN:CD	12:I:52:ILE:HD11	2.28	0.54
5:B:825:VAL:HG12	5:B:826:ALA:N	2.21	0.54
4:A:265:LYS:NZ	4:A:322:VAL:HG13	2.23	0.54
4:A:401:GLY:C	4:A:435:HIS:CD2	2.81	0.54
4:A:829:VAL:C	4:A:831:THR:H	2.10	0.54
4:A:1346:ALA:HB3	8:E:149:LEU:HD13	1.89	0.54
5:B:796:LEU:HD12	5:B:852:ARG:O	2.08	0.54
5:B:1069:PHE:HA	5:B:1085:ILE:O	2.07	0.54
7:D:39:ASN:ND2	7:D:41:GLN:HB2	2.23	0.54
12:I:51:ASN:O	12:I:54:GLU:HG3	2.08	0.54
15:L:39:SER:O	15:L:40:LEU:HG	2.08	0.54
4:A:41:MET:HB3	4:A:48:ALA:O	2.08	0.54
4:A:774:ARG:NH2	4:A:797:LYS:HB2	2.23	0.54
4:A:774:ARG:O	4:A:775:ILE:C	2.46	0.54
4:A:831:THR:HG23	4:A:832:ALA:N	2.21	0.54
5:B:130:VAL:HB	5:B:167:ILE:CD1	2.38	0.54
5:B:185:THR:O	5:B:188:ASP:HB2	2.07	0.54
5:B:205:ILE:N	5:B:205:ILE:HD12	2.23	0.54
5:B:1152:MET:HE1	5:B:1157:ALA:HA	1.89	0.54
6:C:8:VAL:HG12	6:C:9:LYS:H	1.73	0.54
6:C:46:ILE:HD12	6:C:67:LEU:HB3	1.89	0.54
7:D:167:LEU:O	7:D:170:THR:OG1	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:85:GLU:HB2	8:E:88:VAL:HG22	1.89	0.54
9:F:143:PHE:C	9:F:143:PHE:CD1	2.78	0.54
11:H:102:TYR:N	11:H:102:TYR:CD2	2.76	0.54
14:K:65:HIS:HD2	14:K:67:PHE:N	2.05	0.54
4:A:910:PRO:HB3	4:A:917:SER:N	2.22	0.54
5:B:576:ASP:HA	5:B:622:LYS:HZ2	1.73	0.54
5:B:653:VAL:HG22	5:B:689:LEU:HD13	1.90	0.54
5:B:658:ILE:HG22	5:B:659:ALA:N	2.22	0.54
5:B:948:ILE:O	5:B:968:VAL:HG13	2.08	0.54
5:B:1099:VAL:HG12	5:B:1100:ASP:N	2.23	0.54
6:C:116:LYS:HD3	6:C:140:ASN:CB	2.27	0.54
12:I:103:CYS:HB3	12:I:106:CYS:SG	2.48	0.54
14:K:15:GLY:O	14:K:16:GLU:HG3	2.08	0.54
4:A:172:PRO:HG3	4:A:185:TRP:CZ2	2.43	0.53
4:A:401:GLY:C	4:A:435:HIS:HD2	2.10	0.53
4:A:472:LEU:O	4:A:475:THR:HG22	2.07	0.53
4:A:899:VAL:HB	4:A:929:LEU:CD1	2.38	0.53
4:A:1254:ALA:O	4:A:1255:GLU:HB2	2.07	0.53
4:A:1329:THR:HG23	4:A:1331:SER:H	1.73	0.53
5:B:1001:PHE:CD2	6:C:34:ARG:NH2	2.76	0.53
7:D:7:THR:HG21	7:D:32:GLU:OE2	2.08	0.53
7:D:39:ASN:HD22	7:D:41:GLN:HB2	1.73	0.53
9:F:89:GLU:HB3	9:F:134:ILE:CD1	2.39	0.53
11:H:99:GLY:HA3	11:H:118:PHE:HA	1.89	0.53
4:A:130:ASP:O	4:A:133:LYS:N	2.39	0.53
4:A:714:PHE:O	4:A:718:VAL:HG23	2.08	0.53
4:A:806:ARG:HH12	5:B:729:ILE:CD1	2.20	0.53
5:B:39:ARG:HG2	5:B:39:ARG:HH11	1.73	0.53
5:B:1084:GLN:OE1	6:C:189:THR:CG2	2.57	0.53
6:C:259:LEU:HD13	14:K:91:CYS:HB2	1.90	0.53
11:H:58:THR:HG22	11:H:59:ILE:N	2.23	0.53
13:J:27:GLU:C	13:J:29:GLU:H	2.12	0.53
4:A:167:CYS:O	4:A:167:CYS:SG	2.66	0.53
4:A:347:PHE:CE2	4:A:375:THR:HG23	2.43	0.53
4:A:940:ARG:HG2	4:A:940:ARG:HH11	1.72	0.53
4:A:1225:PHE:HE2	4:A:1227:ILE:HD11	1.72	0.53
5:B:485:ARG:NH2	5:B:782:LEU:HD11	2.23	0.53
5:B:1162:ILE:O	5:B:1171:VAL:HG21	2.08	0.53
6:C:142:VAL:H	13:J:16:ASP:HB3	1.72	0.53
7:D:52:LEU:C	7:D:54:GLU:H	2.11	0.53
10:G:88:ASP:OD2	10:G:88:ASP:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:5:LEU:HD22	11:H:133:ASN:O	2.09	0.53
4:A:335:ARG:HA	4:A:339:ASN:HB2	1.90	0.53
4:A:846:GLU:OE1	4:A:1425:SER:OG	2.27	0.53
4:A:858:ASN:HD22	4:A:861:GLY:H	1.56	0.53
5:B:810:GLU:HB2	5:B:815:ARG:HH22	1.74	0.53
6:C:35:ARG:NH1	14:K:41:THR:H	2.06	0.53
6:C:101:LEU:HD13	6:C:118:LEU:HD23	1.90	0.53
6:C:125:MET:HB2	6:C:127:ARG:NH2	2.23	0.53
8:E:124:VAL:HG13	8:E:132:ILE:CG1	2.39	0.53
10:G:61:ILE:HG23	10:G:66:GLY:O	2.08	0.53
11:H:56:THR:HB	11:H:145:ARG:HG2	1.90	0.53
4:A:130:ASP:O	4:A:131:SER:C	2.47	0.53
4:A:504:LEU:HD12	4:A:504:LEU:N	2.24	0.53
5:B:449:ASN:C	5:B:451:LYS:H	2.12	0.53
5:B:1176:ASN:C	5:B:1178:ASN:H	2.10	0.53
7:D:49:ALA:HB2	7:D:174:PRO:CB	2.37	0.53
7:D:53:SER:HB3	7:D:152:SER:HB2	1.91	0.53
10:G:102:GLN:HG3	10:G:106:MET:O	2.08	0.53
14:K:50:LEU:HD11	14:K:75:ILE:CD1	2.37	0.53
4:A:68:GLN:HE22	4:A:80:HIS:CG	2.27	0.53
4:A:84:ILE:O	4:A:84:ILE:HG23	2.07	0.53
4:A:332:LYS:O	4:A:333:GLU:HB2	2.09	0.53
4:A:416:ARG:C	4:A:417:TYR:CD2	2.81	0.53
4:A:504:LEU:HD11	9:F:91:ALA:HB1	1.91	0.53
4:A:541:ILE:HD13	4:A:549:MET:HE3	1.91	0.53
4:A:665:GLY:HA2	5:B:1026:LEU:HD22	1.91	0.53
4:A:971:PHE:CE2	4:A:1040:GLN:HG2	2.44	0.53
4:A:1329:THR:H	4:A:1335:ILE:HD11	1.73	0.53
8:E:207:ARG:CB	8:E:207:ARG:HH11	2.20	0.53
12:I:85:PHE:CD2	12:I:85:PHE:N	2.74	0.53
13:J:44:TYR:CA	13:J:47:ARG:HB2	2.33	0.53
4:A:658:LEU:HD13	5:B:831:SER:HA	1.90	0.53
4:A:786:HIS:CD2	4:A:786:HIS:N	2.74	0.53
4:A:1372:VAL:O	4:A:1376:THR:HG22	2.07	0.53
5:B:483:LEU:HD11	5:B:491:THR:CG2	2.32	0.53
9:F:86:THR:HG23	9:F:89:GLU:OE1	2.09	0.53
15:L:48:CYS:HB3	15:L:51:CYS:O	2.08	0.53
4:A:42:ASP:C	4:A:44:THR:H	2.12	0.53
4:A:464:PRO:HG2	4:A:465:TYR:HD1	1.72	0.53
4:A:503:GLN:HE21	9:F:90:ARG:HH21	1.55	0.53
4:A:1120:LEU:CD1	4:A:1120:LEU:H	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1198:ASP:HB3	4:A:1201:ALA:HB3	1.90	0.53
4:A:1283:VAL:CG1	4:A:1284:MET:H	2.17	0.53
4:A:1289:ARG:NH1	4:A:1326:ARG:NH1	2.56	0.53
5:B:287:ARG:NH1	5:B:324:ILE:O	2.41	0.53
5:B:745:PRO:O	5:B:747:MET:N	2.41	0.53
8:E:78:LEU:HD21	8:E:80:VAL:CG2	2.37	0.53
10:G:34:VAL:CG1	10:G:45:ILE:HG21	2.36	0.53
11:H:15:VAL:HG22	11:H:26:ILE:CD1	2.39	0.53
11:H:83:GLN:C	11:H:85:GLY:N	2.60	0.53
11:H:103:LYS:HG2	11:H:104:PHE:N	2.24	0.53
14:K:55:LYS:HB3	14:K:81:TYR:CD1	2.44	0.53
4:A:682:THR:CG2	4:A:728:LYS:HE3	2.37	0.53
5:B:126:SER:O	5:B:169:ARG:HA	2.09	0.53
5:B:286:PHE:CD1	5:B:297:ILE:HG23	2.44	0.53
5:B:744:HIS:ND1	5:B:745:PRO:HD2	2.24	0.53
8:E:207:ARG:HH11	8:E:207:ARG:HB3	1.74	0.53
10:G:85:GLU:HG2	10:G:86:VAL:N	2.24	0.53
12:I:2:THR:O	12:I:3:THR:C	2.46	0.53
13:J:7:CYS:SG	13:J:46:CYS:HA	2.49	0.53
1:T:19:DC:H2"	1:T:20:DC:C5'	2.39	0.53
4:A:567:LYS:HB2	4:A:568:PRO:CD	2.39	0.53
4:A:1076:ALA:HA	4:A:1079:MET:CE	2.38	0.53
4:A:1140:HIS:CE1	4:A:1272:THR:HG23	2.43	0.53
4:A:1325:THR:HG23	8:E:146:HIS:O	2.08	0.53
5:B:1001:PHE:CE2	6:C:34:ARG:NE	2.77	0.53
6:C:144:ILE:O	6:C:145:CYS:HB3	2.09	0.53
12:I:13:MET:CE	12:I:14:LEU:H	2.22	0.53
14:K:82:ASP:OD1	14:K:84:LYS:N	2.41	0.53
4:A:50:ILE:C	4:A:52:GLY:N	2.60	0.52
4:A:157:ASP:C	4:A:159:THR:H	2.12	0.52
4:A:352:VAL:O	4:A:467:THR:HB	2.09	0.52
4:A:524:VAL:CG1	4:A:525:GLN:H	2.21	0.52
4:A:665:GLY:HA2	5:B:1026:LEU:CD2	2.39	0.52
4:A:899:VAL:HB	4:A:929:LEU:HD12	1.90	0.52
4:A:901:LEU:HG	4:A:926:GLN:HE21	1.74	0.52
4:A:901:LEU:HB2	4:A:926:GLN:HG2	1.90	0.52
4:A:1356:ILE:HG21	4:A:1363:VAL:HG23	1.90	0.52
5:B:33:VAL:HG21	5:B:638:PHE:CZ	2.36	0.52
5:B:112:LEU:HD12	5:B:113:TYR:H	1.73	0.52
5:B:315:LYS:N	5:B:316:PRO:HD2	2.24	0.52
5:B:999:MET:HB3	5:B:1007:VAL:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:13:LEU:CD2	10:G:17:PHE:HB2	2.34	0.52
13:J:27:GLU:O	13:J:29:GLU:N	2.39	0.52
4:A:18:GLN:O	5:B:1215:ARG:HG2	2.10	0.52
4:A:24:PRO:HD2	4:A:233:TRP:HE1	1.74	0.52
4:A:79:GLY:HA3	4:A:243:PRO:HG3	1.91	0.52
4:A:523:ILE:CD1	4:A:649:ILE:HG21	2.38	0.52
4:A:527:THR:CG2	4:A:650:GLN:HA	2.40	0.52
4:A:1120:LEU:CD1	4:A:1120:LEU:N	2.72	0.52
4:A:1409:LEU:CD1	5:B:1207:LEU:HD21	2.39	0.52
6:C:53:THR:O	6:C:153:LEU:HA	2.09	0.52
7:D:151:PHE:CD1	7:D:151:PHE:N	2.77	0.52
8:E:83:CYS:HG	8:E:110:PHE:HZ	1.54	0.52
8:E:192:ARG:HH11	8:E:192:ARG:HG3	1.73	0.52
10:G:34:VAL:HG12	10:G:45:ILE:CG2	2.34	0.52
4:A:997:LEU:N	4:A:997:LEU:HD23	2.23	0.52
5:B:464:GLY:HA2	5:B:479:VAL:O	2.09	0.52
6:C:39:ALA:CA	6:C:164:ALA:HB3	2.29	0.52
9:F:118:LEU:O	9:F:122:MET:HG3	2.09	0.52
10:G:143:ILE:HG23	10:G:169:GLY:O	2.09	0.52
4:A:35:ILE:CG2	4:A:84:ILE:HD12	2.39	0.52
4:A:1329:THR:HG21	4:A:1331:SER:HB3	1.92	0.52
4:A:1364:ASN:O	4:A:1365:TYR:C	2.47	0.52
5:B:130:VAL:HB	5:B:167:ILE:HD12	1.91	0.52
5:B:558:LEU:HD21	5:B:600:LEU:HD11	1.91	0.52
5:B:811:TYR:N	5:B:811:TYR:CD1	2.78	0.52
5:B:880:THR:HB	5:B:934:LYS:HD2	1.92	0.52
8:E:16:PHE:CE2	8:E:20:LYS:HE2	2.44	0.52
9:F:116:ASP:O	9:F:120:ILE:HG13	2.10	0.52
11:H:12:VAL:HA	11:H:28:ALA:HB2	1.92	0.52
4:A:255:SER:OG	5:B:918:ILE:HG23	2.09	0.52
4:A:567:LYS:HD2	4:A:568:PRO:CD	2.40	0.52
4:A:699:ALA:HB3	4:A:701:LEU:HG	1.91	0.52
4:A:1348:LEU:O	4:A:1352:VAL:HG23	2.09	0.52
4:A:1377:THR:O	4:A:1379:GLY:N	2.42	0.52
5:B:860:MET:HG2	5:B:861:ASP:N	2.25	0.52
5:B:1095:LEU:H	5:B:1095:LEU:CD1	2.19	0.52
6:C:252:GLN:HG3	14:K:95:ILE:HG23	1.92	0.52
7:D:66:ARG:O	7:D:70:PHE:HB2	2.09	0.52
9:F:77:ASP:C	9:F:79:ARG:H	2.12	0.52
11:H:126:GLU:C	11:H:130:ARG:HH22	2.13	0.52
1:T:16:DG:N2	2:N:2:DA:C2	2.78	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:298:PHE:CD2	4:A:299:HIS:N	2.78	0.52
4:A:853:ASP:OD2	4:A:855:THR:CG2	2.58	0.52
4:A:1389:PHE:CD1	4:A:1389:PHE:C	2.82	0.52
4:A:1445:ILE:HD12	4:A:1445:ILE:N	2.07	0.52
5:B:25:ILE:HD11	5:B:653:VAL:C	2.29	0.52
5:B:638:PHE:HB3	5:B:651:LEU:HD22	1.90	0.52
5:B:763:GLN:HG2	5:B:765:PRO:HD2	1.92	0.52
5:B:1031:LEU:CD2	5:B:1044:ALA:HB2	2.40	0.52
11:H:40:LEU:HD22	11:H:123:MET:CE	2.40	0.52
13:J:1:MET:H3	13:J:56:LEU:H	1.57	0.52
14:K:61:TYR:C	14:K:61:TYR:CD2	2.80	0.52
4:A:254:GLU:O	4:A:256:GLN:N	2.41	0.52
6:C:263:THR:C	6:C:265:MET:H	2.12	0.52
9:F:75:PRO:HG2	9:F:78:GLN:HB2	1.92	0.52
10:G:7:LEU:HB2	10:G:74:TYR:HE2	1.67	0.52
10:G:83:LYS:HG2	10:G:149:GLY:HA2	1.91	0.52
11:H:36:CYS:HA	11:H:126:GLU:O	2.09	0.52
12:I:7:CYS:HB3	12:I:14:LEU:HD21	1.90	0.52
4:A:40:THR:HG22	4:A:41:MET:CG	2.28	0.52
4:A:262:LEU:HD12	4:A:328:ARG:NH2	2.24	0.52
4:A:438:ASP:OD1	4:A:461:LYS:HA	2.10	0.52
4:A:982:THR:N	4:A:985:ASP:HB2	2.25	0.52
4:A:1021:LEU:O	4:A:1025:ARG:HG2	2.10	0.52
4:A:1313:LEU:HB3	4:A:1338:VAL:HG21	1.92	0.52
5:B:29:ASP:OD1	5:B:658:ILE:HD13	2.10	0.52
5:B:846:ILE:HA	5:B:850:LEU:HB3	1.91	0.52
5:B:899:ILE:CG2	5:B:949:VAL:HG21	2.40	0.52
5:B:983:ARG:HD2	5:B:1091:TYR:HB3	1.92	0.52
7:D:191:ALA:C	7:D:193:THR:H	2.12	0.52
11:H:107:VAL:O	11:H:108:SER:O	2.28	0.52
4:A:767:GLN:HE21	4:A:774:ARG:HB3	1.75	0.52
4:A:1011:GLN:NE2	4:A:1015:VAL:HG21	2.25	0.52
4:A:1259:MET:C	4:A:1261:LYS:H	2.12	0.52
5:B:213:ILE:HD12	5:B:497:ARG:HB3	1.92	0.52
5:B:616:ILE:HG13	5:B:697:GLU:HG3	1.92	0.52
5:B:782:LEU:HD12	5:B:788:ARG:NH1	2.20	0.52
5:B:806:THR:HB	5:B:809:MET:HG3	1.92	0.52
5:B:890:TYR:CZ	5:B:910:VAL:HG21	2.45	0.52
6:C:161:LYS:O	6:C:170:TRP:NE1	2.42	0.52
7:D:210:ILE:O	7:D:214:LEU:HG	2.10	0.52
11:H:58:THR:HG22	11:H:59:ILE:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:113:ALA:HB2	11:H:126:GLU:HG3	1.91	0.52
15:L:28:LYS:HB2	15:L:39:SER:CA	2.39	0.52
1:T:23:DC:H2'	1:T:24:DT:H6	1.71	0.52
4:A:148:CYS:O	4:A:168:GLY:HA2	2.09	0.52
5:B:843:GLN:HB2	5:B:993:THR:HB	1.91	0.52
6:C:86:CYS:O	6:C:88:CYS:N	2.41	0.52
6:C:175:ALA:CB	13:J:43:ARG:HH12	2.23	0.52
6:C:175:ALA:CB	13:J:43:ARG:NH1	2.72	0.52
10:G:7:LEU:HD11	10:G:45:ILE:HD11	1.92	0.52
11:H:89:LEU:C	11:H:91:ASP:N	2.63	0.52
11:H:104:PHE:CE2	11:H:136:LYS:HG2	2.45	0.52
12:I:6:PHE:HA	12:I:14:LEU:HG	1.92	0.52
12:I:82:GLU:HB3	12:I:104:LEU:CD1	2.39	0.52
14:K:41:THR:HG22	14:K:42:LEU:N	2.25	0.52
4:A:230:ARG:H	4:A:233:TRP:HE3	1.52	0.51
4:A:360:GLU:HG3	4:A:459:ARG:HH12	1.73	0.51
4:A:825:ILE:O	4:A:829:VAL:HG23	2.10	0.51
4:A:868:TYR:CE1	4:A:1064:VAL:CG1	2.92	0.51
4:A:961:ARG:HG3	4:A:961:ARG:NH1	2.24	0.51
4:A:1168:GLU:O	4:A:1172:LEU:HG	2.10	0.51
5:B:368:GLU:O	5:B:370:PHE:N	2.42	0.51
5:B:753:ALA:HA	5:B:756:ILE:CD1	2.40	0.51
5:B:899:ILE:HD11	5:B:910:VAL:O	2.10	0.51
5:B:945:GLU:O	5:B:946:ASN:HB3	2.10	0.51
5:B:992:ILE:HG12	5:B:993:THR:N	2.25	0.51
5:B:1180:PHE:O	5:B:1181:GLU:O	2.27	0.51
12:I:110:PHE:H	12:I:110:PHE:HD2	1.58	0.51
4:A:320:ARG:NH1	4:A:320:ARG:HG3	2.25	0.51
4:A:451:HIS:CD2	4:A:1074:GLU:HG3	2.45	0.51
4:A:471:ASN:OD1	4:A:472:LEU:N	2.43	0.51
4:A:765:VAL:HG23	4:A:802:ASN:O	2.10	0.51
4:A:958:VAL:HG22	4:A:1052:GLN:HB3	1.92	0.51
5:B:20:ASP:C	5:B:22:SER:H	2.14	0.51
5:B:189:LEU:O	5:B:192:LEU:N	2.39	0.51
5:B:549:THR:HB	5:B:628:THR:OG1	2.10	0.51
5:B:687:GLU:O	5:B:689:LEU:HG	2.11	0.51
5:B:843:GLN:O	5:B:846:ILE:N	2.43	0.51
6:C:59:ALA:O	6:C:62:PHE:HB3	2.10	0.51
6:C:99:LEU:HA	6:C:119:VAL:O	2.10	0.51
7:D:137:ASN:C	7:D:137:ASN:HD22	2.13	0.51
15:L:28:LYS:HB2	15:L:39:SER:CB	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:19:DC:C4	1:T:20:DC:N4	2.79	0.51
4:A:35:ILE:HD13	4:A:241:VAL:HG11	1.93	0.51
4:A:511:ILE:O	4:A:519:PRO:HA	2.10	0.51
4:A:567:LYS:CE	11:H:46:LEU:HB2	2.40	0.51
4:A:730:GLY:O	4:A:732:LEU:N	2.43	0.51
4:A:903:ASN:ND2	4:A:903:ASN:C	2.63	0.51
6:C:248:ILE:HG23	14:K:98:LEU:HD22	1.92	0.51
7:D:17:LYS:H	7:D:17:LYS:CD	2.23	0.51
7:D:185:CYS:CB	7:D:211:LEU:HD22	2.40	0.51
8:E:175:LEU:HD23	8:E:176:PRO:HD2	1.91	0.51
2:N:6:DA:C2'	2:N:7:DG:OP2	2.55	0.51
4:A:18:GLN:HB2	5:B:1215:ARG:HB2	1.93	0.51
4:A:69:THR:O	4:A:71:GLN:N	2.43	0.51
4:A:853:ASP:OD2	4:A:855:THR:HG22	2.10	0.51
6:C:29:MET:HE1	14:K:98:LEU:HG	1.93	0.51
7:D:21:GLU:HB2	7:D:22:GLU:OE1	2.11	0.51
15:L:46:VAL:O	15:L:46:VAL:HG12	2.10	0.51
1:T:18:DC:H3'	1:T:18:DC:OP1	2.11	0.51
4:A:23:SER:HB3	4:A:233:TRP:CE2	2.46	0.51
4:A:244:PRO:O	4:A:246:VAL:N	2.43	0.51
4:A:261:ASP:O	4:A:264:PHE:HB2	2.11	0.51
4:A:388:LEU:O	4:A:392:VAL:HG23	2.10	0.51
4:A:567:LYS:HE3	11:H:46:LEU:HB2	1.93	0.51
4:A:1208:THR:O	4:A:1212:VAL:HG23	2.10	0.51
5:B:288:ALA:HA	5:B:331:LEU:HD12	1.91	0.51
5:B:610:ASN:O	5:B:612:GLU:N	2.44	0.51
5:B:1045:SER:O	5:B:1046:PRO:O	2.27	0.51
6:C:253:LYS:O	6:C:256:ALA:HB3	2.10	0.51
11:H:47:PHE:CD2	11:H:95:TYR:HD1	2.28	0.51
4:A:34:LYS:HD3	4:A:34:LYS:H	1.75	0.51
4:A:93:VAL:CG2	4:A:301:ALA:HA	2.36	0.51
4:A:320:ARG:HG3	4:A:320:ARG:HH11	1.74	0.51
4:A:470:LEU:HD12	4:A:471:ASN:O	2.11	0.51
4:A:831:THR:CG2	4:A:832:ALA:N	2.72	0.51
5:B:640:VAL:O	5:B:641:GLU:C	2.49	0.51
5:B:1085:ILE:N	5:B:1085:ILE:CD1	2.69	0.51
5:B:1103:ILE:O	5:B:1122:ARG:NH1	2.43	0.51
9:F:116:ASP:HB3	9:F:119:ARG:HB2	1.93	0.51
13:J:48:ARG:HE	13:J:49:MET:HE2	1.75	0.51
4:A:367:PRO:HD3	4:A:467:THR:O	2.10	0.51
4:A:913:LEU:HD12	4:A:914:GLU:N	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1209:MET:CE	4:A:1236:LEU:HB3	2.40	0.51
4:A:1332:PHE:CD2	4:A:1332:PHE:N	2.74	0.51
5:B:33:VAL:HG12	5:B:681:TRP:HZ3	1.76	0.51
5:B:792:MET:H	5:B:857:ARG:HA	1.74	0.51
5:B:980:PHE:CD2	5:B:1094:ARG:HA	2.46	0.51
5:B:1099:VAL:C	5:B:1101:ASP:H	2.14	0.51
7:D:47:LEU:HD12	7:D:48:ILE:N	2.25	0.51
4:A:108:MET:N	4:A:108:MET:SD	2.84	0.51
4:A:276:LEU:HD13	4:A:293:GLU:HA	1.93	0.51
4:A:567:LYS:CG	4:A:568:PRO:CD	2.83	0.51
4:A:567:LYS:CB	4:A:568:PRO:CD	2.88	0.51
4:A:577:ILE:C	4:A:579:SER:N	2.62	0.51
4:A:666:ILE:HD11	5:B:1067:ARG:O	2.11	0.51
4:A:1144:LYS:HB2	4:A:1268:LEU:O	2.11	0.51
4:A:1265:ASN:C	4:A:1267:MET:N	2.64	0.51
4:A:1364:ASN:HD22	4:A:1364:ASN:C	2.14	0.51
5:B:102:VAL:CG2	5:B:112:LEU:HD22	2.41	0.51
6:C:36:VAL:HG21	6:C:251:LEU:HB2	1.93	0.51
4:A:317:LYS:O	4:A:318:SER:HB3	2.11	0.51
4:A:1125:ALA:C	4:A:1127:ASP:H	2.14	0.51
4:A:1444:MET:CE	9:F:135:ARG:HB2	2.41	0.51
5:B:197:PHE:CZ	5:B:816:GLU:HG2	2.46	0.51
5:B:882:THR:CB	5:B:934:LYS:O	2.59	0.51
5:B:903:VAL:HG12	5:B:904:ARG:N	2.26	0.51
5:B:996:ARG:NH2	6:C:175:ALA:N	2.56	0.51
5:B:1011:ILE:O	5:B:1011:ILE:HG22	2.10	0.51
7:D:134:THR:CG2	7:D:135:GLY:N	2.74	0.51
8:E:28:TYR:CE1	8:E:78:LEU:HD13	2.46	0.51
11:H:130:ARG:HD2	11:H:130:ARG:N	2.21	0.51
12:I:34:TYR:HD2	12:I:35:VAL:N	2.08	0.51
4:A:227:VAL:HG21	7:D:14:ARG:HH12	1.76	0.51
4:A:382:PRO:CA	4:A:428:TYR:HE2	2.24	0.51
4:A:466:SER:HB2	5:B:1099:VAL:HG11	1.93	0.51
4:A:852:TYR:CD1	9:F:136:ARG:HB3	2.45	0.51
5:B:516:ASN:H	5:B:516:ASN:ND2	2.08	0.51
5:B:521:LEU:HD13	5:B:633:VAL:CG1	2.41	0.51
5:B:1002:THR:O	5:B:1004:GLU:N	2.44	0.51
6:C:259:LEU:HD13	14:K:91:CYS:CB	2.41	0.51
8:E:83:CYS:SG	8:E:110:PHE:HZ	2.34	0.51
1:T:13:DC:H2"	1:T:14:DT:O5'	2.11	0.50
4:A:37:PHE:HD1	4:A:37:PHE:H	1.58	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:166:GLY:O	4:A:167:CYS:SG	2.69	0.50
4:A:849:MET:HB3	4:A:1063:MET:SD	2.50	0.50
5:B:44:VAL:O	5:B:45:SER:C	2.49	0.50
5:B:234:ILE:HD12	5:B:234:ILE:N	2.26	0.50
5:B:680:THR:O	5:B:684:LEU:HD12	2.11	0.50
5:B:859:TYR:CZ	5:B:941:LEU:HD12	2.46	0.50
5:B:894:ASP:HB2	15:L:58:LYS:NZ	2.25	0.50
5:B:957:ASN:O	5:B:960:GLY:N	2.44	0.50
5:B:1050:ILE:HG22	5:B:1051:THR:N	2.25	0.50
7:D:34:GLN:C	7:D:36:LYS:H	2.14	0.50
4:A:7:SER:HB3	5:B:1193:GLN:HE21	1.76	0.50
4:A:69:THR:C	4:A:71:GLN:H	2.15	0.50
4:A:89:PRO:O	4:A:204:THR:HG21	2.10	0.50
4:A:92:HIS:HD2	4:A:304:MET:HE3	1.75	0.50
4:A:283:GLY:O	4:A:285:PRO:CD	2.58	0.50
4:A:852:TYR:CD2	4:A:1060:PRO:CB	2.95	0.50
4:A:870:GLU:HG2	8:E:208:TYR:CD2	2.46	0.50
4:A:878:ILE:HG21	4:A:955:PRO:HB2	1.93	0.50
4:A:1143:LEU:O	4:A:1146:VAL:HG23	2.12	0.50
5:B:205:ILE:O	5:B:207:GLY:N	2.44	0.50
5:B:284:ILE:HG23	5:B:324:ILE:HD12	1.93	0.50
5:B:579:ARG:HG2	5:B:579:ARG:NH1	2.26	0.50
5:B:1198:TYR:O	5:B:1201:LYS:HB3	2.10	0.50
6:C:101:LEU:HD22	6:C:118:LEU:CD2	2.41	0.50
13:J:43:ARG:HG2	13:J:46:CYS:SG	2.52	0.50
4:A:537:ARG:NH1	11:H:120:GLY:O	2.43	0.50
4:A:907:THR:HG23	4:A:908:LEU:N	2.26	0.50
5:B:657:HIS:CE1	5:B:689:LEU:HD11	2.47	0.50
5:B:661:LEU:HD23	5:B:679:TYR:O	2.11	0.50
7:D:153:ARG:C	7:D:154:PHE:CD1	2.85	0.50
11:H:76:THR:O	11:H:76:THR:HG22	2.10	0.50
15:L:40:LEU:HD13	15:L:44:ASP:CB	2.40	0.50
4:A:18:GLN:CB	5:B:1215:ARG:HB2	2.42	0.50
4:A:446:ARG:HB3	4:A:478:TYR:HB3	1.93	0.50
4:A:492:PRO:O	4:A:493:GLN:NE2	2.45	0.50
5:B:446:LEU:N	5:B:446:LEU:HD23	2.26	0.50
8:E:198:ILE:HD11	8:E:212:ARG:CG	2.42	0.50
4:A:106:VAL:HG13	4:A:112:LYS:N	2.26	0.50
4:A:146:MET:HB3	4:A:171:GLN:O	2.12	0.50
4:A:172:PRO:HB3	4:A:185:TRP:CD2	2.46	0.50
4:A:471:ASN:O	4:A:474:VAL:HG12	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:535:THR:HG23	4:A:575:LYS:HE2	1.93	0.50
4:A:942:PHE:C	4:A:942:PHE:CD2	2.85	0.50
4:A:1116:LEU:N	4:A:1308:THR:CG2	2.69	0.50
4:A:1343:ALA:O	4:A:1346:ALA:HB3	2.12	0.50
4:A:1445:ILE:HD11	10:G:68:ALA:CB	2.39	0.50
5:B:797:TYR:C	5:B:798:TYR:HD2	2.15	0.50
5:B:885:MET:HA	5:B:936:ASP:HB2	1.94	0.50
5:B:1162:ILE:HG22	5:B:1163:CYS:H	1.76	0.50
6:C:22:LEU:HD13	6:C:230:MET:CE	2.41	0.50
6:C:66:ARG:NH1	6:C:144:ILE:O	2.43	0.50
9:F:99:LEU:HD12	9:F:103:MET:HG3	1.94	0.50
11:H:103:LYS:HG2	11:H:104:PHE:H	1.75	0.50
4:A:146:MET:HA	4:A:171:GLN:HB2	1.91	0.50
4:A:600:PRO:HG2	4:A:601:LYS:H	1.75	0.50
4:A:873:MET:C	4:A:1058:VAL:HG23	2.31	0.50
4:A:1006:ILE:CD1	8:E:163:GLU:HG3	2.42	0.50
4:A:1152:ILE:HG13	12:I:44:TYR:HD2	1.76	0.50
5:B:69:LEU:HD13	5:B:429:PHE:CD1	2.47	0.50
5:B:190:TYR:HE2	13:J:62:ARG:HB3	1.72	0.50
5:B:240:ILE:HG23	5:B:240:ILE:O	2.10	0.50
5:B:780:VAL:HG21	13:J:56:LEU:HD11	1.92	0.50
5:B:956:THR:CG2	5:B:960:GLY:HA2	2.42	0.50
6:C:174:ALA:O	6:C:175:ALA:CB	2.59	0.50
6:C:187:LYS:C	6:C:189:THR:H	2.15	0.50
7:D:56:ARG:HA	7:D:148:LEU:HD13	1.94	0.50
10:G:80:LYS:O	10:G:80:LYS:HG2	2.12	0.50
4:A:204:THR:O	4:A:206:GLU:N	2.45	0.50
4:A:265:LYS:NZ	4:A:322:VAL:HG22	2.27	0.50
4:A:331:GLY:O	4:A:332:LYS:O	2.30	0.50
4:A:335:ARG:HA	4:A:339:ASN:HD22	1.76	0.50
4:A:982:THR:O	4:A:985:ASP:HB2	2.12	0.50
4:A:1146:VAL:HG11	4:A:1207:LEU:HD12	1.94	0.50
5:B:766:ARG:NH2	5:B:1020:ARG:HD3	2.26	0.50
8:E:20:LYS:NZ	8:E:60:PHE:CE1	2.79	0.50
10:G:4:ILE:HG12	10:G:77:VAL:HG22	1.92	0.50
12:I:101:PHE:N	12:I:101:PHE:CD1	2.79	0.50
15:L:27:LEU:HD13	15:L:37:LYS:CE	2.41	0.50
4:A:37:PHE:N	4:A:37:PHE:HD1	2.09	0.50
4:A:241:VAL:HG13	4:A:266:LEU:HD13	1.93	0.50
4:A:265:LYS:CE	4:A:322:VAL:HG13	2.42	0.50
4:A:325:ILE:HG21	5:B:1210:MET:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:598:LEU:O	4:A:599:SER:C	2.49	0.50
4:A:670:ILE:HG23	4:A:805:LEU:CD2	2.40	0.50
4:A:888:GLY:O	4:A:940:ARG:NH2	2.45	0.50
4:A:901:LEU:N	4:A:926:GLN:NE2	2.52	0.50
4:A:1431:GLY:HA3	5:B:1152:MET:SD	2.52	0.50
5:B:25:ILE:HG23	5:B:658:ILE:CD1	2.41	0.50
5:B:172:ILE:CG2	5:B:173:MET:N	2.75	0.50
5:B:299:GLU:OE2	5:B:572:HIS:HE1	1.94	0.50
5:B:546:SER:OG	5:B:631:GLY:N	2.38	0.50
5:B:1020:ARG:HB2	5:B:1022:THR:HG22	1.94	0.50
6:C:167:HIS:HA	14:K:6:ARG:HH12	1.76	0.50
6:C:242:GLN:HB3	6:C:246:ARG:HG3	1.94	0.50
8:E:17:ARG:O	8:E:20:LYS:HB2	2.11	0.50
10:G:17:PHE:N	10:G:17:PHE:CD2	2.78	0.50
12:I:59:VAL:C	12:I:61:ASP:H	2.15	0.50
14:K:60:ALA:O	14:K:73:LEU:HD12	2.11	0.50
4:A:98:LYS:O	4:A:102:VAL:HG23	2.12	0.50
4:A:119:ASN:O	4:A:122:MET:HB3	2.11	0.50
4:A:351:THR:HG22	5:B:1103:ILE:HA	1.94	0.50
4:A:630:ILE:HG23	4:A:642:CYS:SG	2.52	0.50
4:A:816:HIS:CD2	5:B:764:SER:H	2.29	0.50
4:A:1111:MET:CE	4:A:1330:ASN:OD1	2.60	0.50
5:B:117:ALA:HA	5:B:122:LEU:HD12	1.93	0.50
5:B:347:LYS:HG3	5:B:348:ARG:N	2.27	0.50
5:B:582:VAL:HA	5:B:626:ILE:O	2.12	0.50
5:B:1106:ARG:HD3	5:B:1126:GLY:O	2.12	0.50
8:E:205:SER:O	8:E:207:ARG:N	2.45	0.50
10:G:1:MET:CE	10:G:80:LYS:O	2.60	0.50
12:I:86:PHE:CE1	12:I:100:PHE:HB2	2.47	0.50
14:K:46:ILE:HG21	14:K:87:LEU:HD11	1.94	0.50
4:A:58:LEU:O	4:A:59:GLY:O	2.30	0.49
4:A:88:LYS:HE3	4:A:280:GLU:OE2	2.12	0.49
4:A:345:VAL:HG11	5:B:1130:PHE:HB2	1.95	0.49
4:A:973:ILE:HD13	4:A:1036:ARG:O	2.11	0.49
4:A:1062:GLU:OE2	9:F:88:TYR:OH	2.30	0.49
5:B:824:ILE:CG2	5:B:1087:PHE:CE2	2.93	0.49
6:C:251:LEU:O	6:C:255:VAL:HG23	2.11	0.49
12:I:26:LEU:CD2	12:I:37:GLU:HA	2.39	0.49
13:J:14:VAL:CG1	13:J:50:ILE:HD11	2.41	0.49
14:K:7:PHE:O	14:K:11:LEU:HB2	2.12	0.49
14:K:53:ASP:C	14:K:55:LYS:H	2.16	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:49:LYS:NZ	4:A:61:ILE:CG1	2.71	0.49
5:B:378:LEU:O	5:B:378:LEU:HD12	2.12	0.49
5:B:621:GLU:HG3	5:B:621:GLU:O	2.12	0.49
6:C:18:VAL:CG2	6:C:240:VAL:HB	2.42	0.49
10:G:38:CYS:SG	10:G:44:TYR:CE1	3.03	0.49
11:H:116:TYR:HB2	11:H:123:MET:HB3	1.95	0.49
4:A:244:PRO:HG2	4:A:245:PRO:CD	2.41	0.49
4:A:332:LYS:HG3	4:A:333:GLU:HG2	1.94	0.49
4:A:696:GLU:OE2	4:A:702:LEU:HD21	2.13	0.49
4:A:1164:PRO:HG2	4:A:1165:GLU:HG3	1.94	0.49
4:A:1319:VAL:HG13	4:A:1320:PRO:HD2	1.93	0.49
5:B:977:GLY:HA3	5:B:1099:VAL:CB	2.42	0.49
5:B:1183:LYS:C	5:B:1185:CYS:H	2.16	0.49
6:C:73:GLN:HE21	6:C:75:MET:H	1.59	0.49
8:E:12:LEU:HD21	8:E:58:MET:SD	2.53	0.49
10:G:14:HIS:CE1	10:G:15:PRO:HD2	2.46	0.49
4:A:840:ARG:O	4:A:841:LEU:C	2.51	0.49
4:A:1098:VAL:N	4:A:1099:PRO:HD2	2.27	0.49
5:B:171:PRO:HD2	5:B:457:LEU:HD13	1.95	0.49
5:B:658:ILE:O	5:B:661:LEU:HB2	2.11	0.49
5:B:846:ILE:CG2	5:B:974:PRO:HG2	2.41	0.49
5:B:918:ILE:HG21	5:B:935:ARG:HH11	1.76	0.49
5:B:1161:HIS:HB3	5:B:1171:VAL:HG11	1.95	0.49
6:C:70:ILE:HD11	6:C:144:ILE:HG12	1.93	0.49
8:E:79:TRP:CD1	8:E:96:PHE:HE1	2.30	0.49
8:E:168:TYR:HB3	8:E:170:LEU:HG	1.94	0.49
13:J:7:CYS:HB3	13:J:10:CYS:SG	2.51	0.49
14:K:58:PHE:HE2	14:K:74:ARG:HE	1.57	0.49
4:A:302:THR:HA	4:A:305:ASP:O	2.12	0.49
4:A:417:TYR:CD2	4:A:417:TYR:N	2.80	0.49
4:A:527:THR:HG21	4:A:650:GLN:HA	1.95	0.49
4:A:590:ARG:HB2	4:A:605:MET:HB3	1.94	0.49
4:A:779:PHE:O	4:A:780:VAL:C	2.51	0.49
4:A:929:LEU:CD2	4:A:983:ILE:HG21	2.42	0.49
5:B:35:SER:HA	5:B:811:TYR:CE2	2.37	0.49
5:B:121:ASN:ND2	5:B:207:GLY:HA3	2.28	0.49
5:B:175:ARG:HG2	5:B:175:ARG:NH1	2.24	0.49
5:B:882:THR:HG22	5:B:884:ARG:HB2	1.93	0.49
6:C:137:LYS:HB3	6:C:138:GLU:OE1	2.13	0.49
10:G:96:GLN:HA	10:G:121:PHE:CE2	2.48	0.49
11:H:40:LEU:HD12	11:H:122:LEU:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:58:THR:HB	11:H:143:LEU:HB2	1.95	0.49
14:K:47:ARG:C	14:K:47:ARG:HD2	2.32	0.49
4:A:2:VAL:HG21	5:B:1157:ALA:O	2.11	0.49
4:A:262:LEU:C	4:A:264:PHE:N	2.66	0.49
4:A:316:GLN:O	4:A:317:LYS:C	2.51	0.49
4:A:1317:MET:HG3	4:A:1327:ILE:HG21	1.93	0.49
5:B:224:GLN:O	5:B:238:ALA:HA	2.12	0.49
5:B:237:VAL:HG22	5:B:257:LYS:HA	1.95	0.49
5:B:1166:CYS:HB2	5:B:1215:ARG:HH11	1.75	0.49
10:G:1:MET:O	10:G:3:PHE:CD1	2.65	0.49
4:A:54:ASN:HB3	4:A:247:ARG:HH22	1.78	0.49
4:A:412:ARG:HH22	5:B:1108:ARG:HH22	1.61	0.49
4:A:526:ASP:OD1	5:B:1013:ASN:ND2	2.44	0.49
4:A:590:ARG:NH2	4:A:620:LYS:HB2	2.22	0.49
4:A:798:GLY:HA2	4:A:815:PHE:HD1	1.72	0.49
4:A:852:TYR:HA	4:A:1060:PRO:HB3	1.94	0.49
4:A:1189:SER:OG	4:A:1190:PRO:HD2	2.13	0.49
4:A:1334:ASP:O	4:A:1336:MET:N	2.45	0.49
4:A:1394:THR:HG22	4:A:1395:GLY:N	2.27	0.49
5:B:31:TRP:CZ3	5:B:34:ILE:HD12	2.48	0.49
6:C:70:ILE:HD11	6:C:144:ILE:CG1	2.43	0.49
6:C:70:ILE:HD13	6:C:115:SER:HB3	1.94	0.49
6:C:184:ASN:HD21	6:C:187:LYS:HA	1.77	0.49
7:D:27:LEU:HD13	7:D:173:HIS:HD2	1.78	0.49
7:D:130:LEU:C	7:D:132:GLN:N	2.65	0.49
8:E:135:PHE:CB	8:E:140:LEU:HD11	2.37	0.49
4:A:55:ASP:N	4:A:56:PRO:CD	2.76	0.49
4:A:63:ARG:HA	4:A:74:MET:HE2	1.94	0.49
4:A:417:TYR:O	4:A:418:SER:C	2.50	0.49
5:B:364:ILE:HG12	5:B:585:VAL:CG1	2.36	0.49
5:B:843:GLN:O	5:B:844:SER:C	2.51	0.49
8:E:24:LYS:HB3	8:E:30:ILE:HD12	1.95	0.49
12:I:100:PHE:N	12:I:100:PHE:CD1	2.81	0.49
14:K:110:ASN:C	14:K:112:GLN:H	2.16	0.49
4:A:381:THR:HG21	4:A:383:TYR:CD1	2.47	0.49
4:A:537:ARG:HH12	11:H:122:LEU:HG	1.77	0.49
4:A:711:ARG:NH1	12:I:95:THR:HB	2.27	0.49
4:A:909:ASP:C	4:A:911:SER:H	2.16	0.49
4:A:1001:ARG:O	4:A:1002:GLY:O	2.31	0.49
4:A:1273:LEU:HD12	4:A:1273:LEU:N	2.28	0.49
5:B:654:ARG:H	5:B:657:HIS:HD2	1.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:758:PHE:CZ	5:B:1031:LEU:HD22	2.48	0.49
5:B:806:THR:HG22	5:B:808:ALA:CB	2.43	0.49
5:B:973:ILE:HG23	5:B:974:PRO:HD2	1.95	0.49
5:B:1156:ASP:HB3	5:B:1197:PRO:HA	1.95	0.49
6:C:191:TYR:CD2	6:C:201:TRP:CD1	3.01	0.49
6:C:258:ILE:HD12	6:C:258:ILE:N	2.28	0.49
11:H:40:LEU:HD22	11:H:123:MET:HE3	1.94	0.49
4:A:474:VAL:HG22	4:A:478:TYR:HE1	1.77	0.49
4:A:597:LEU:HD12	4:A:597:LEU:N	2.28	0.49
4:A:699:ALA:O	4:A:700:ASN:HB3	2.13	0.49
4:A:767:GLN:OE1	4:A:799:PHE:HB2	2.13	0.49
4:A:1305:VAL:HG12	4:A:1306:LEU:N	2.28	0.49
5:B:661:LEU:HD11	5:B:684:LEU:HD21	1.93	0.49
5:B:796:LEU:HD21	5:B:821:GLN:HE21	1.77	0.49
5:B:824:ILE:HG12	13:J:48:ARG:HH12	1.77	0.49
5:B:1068:GLY:O	5:B:1069:PHE:O	2.31	0.49
5:B:1202:LEU:HD23	5:B:1206:GLU:HG3	1.93	0.49
6:C:40:GLU:HA	6:C:163:ILE:CG2	2.43	0.49
7:D:47:LEU:HD11	10:G:3:PHE:CD2	2.48	0.49
7:D:202:ILE:CG2	7:D:207:LEU:HB2	2.43	0.49
12:I:100:PHE:N	12:I:100:PHE:HD1	2.11	0.49
2:N:5:DT:H2"	2:N:6:DA:OP2	2.13	0.48
4:A:18:GLN:HB3	5:B:1215:ARG:HG3	1.93	0.48
4:A:105:CYS:O	4:A:114:LEU:HG	2.13	0.48
4:A:150:THR:HG22	4:A:150:THR:O	2.13	0.48
4:A:416:ARG:HG3	4:A:417:TYR:CD2	2.48	0.48
4:A:655:PHE:O	4:A:658:LEU:HB3	2.13	0.48
5:B:181:LEU:HD22	5:B:189:LEU:HD22	1.95	0.48
5:B:652:LYS:HB3	5:B:689:LEU:CD2	2.43	0.48
5:B:894:ASP:HB2	15:L:58:LYS:HZ3	1.78	0.48
5:B:996:ARG:NH1	6:C:38:ILE:HG23	2.27	0.48
6:C:113:VAL:HG23	6:C:147:LEU:HD21	1.95	0.48
6:C:183:TRP:CE2	6:C:207:CYS:HB3	2.47	0.48
8:E:42:PHE:HZ	8:E:58:MET:CE	2.25	0.48
9:F:109:VAL:HG12	9:F:110:ASP:H	1.78	0.48
10:G:117:GLN:C	10:G:119:LEU:N	2.67	0.48
13:J:57:ILE:HA	13:J:60:PHE:CD2	2.34	0.48
15:L:52:GLY:O	15:L:54:ARG:N	2.46	0.48
15:L:70:ARG:HG2	15:L:70:ARG:NH1	2.27	0.48
4:A:35:ILE:HG22	4:A:35:ILE:O	2.11	0.48
4:A:244:PRO:O	4:A:247:ARG:N	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:266:LEU:HD21	4:A:303:TYR:CE1	2.48	0.48
4:A:285:PRO:CG	4:A:288:ALA:HB3	2.43	0.48
4:A:353:ILE:HB	4:A:470:LEU:HD23	1.96	0.48
4:A:722:LEU:HD21	4:A:794:PRO:HB3	1.95	0.48
4:A:912:LEU:O	4:A:979:SER:N	2.44	0.48
4:A:1210:GLY:O	4:A:1214:GLU:HG2	2.13	0.48
5:B:253:THR:HG22	5:B:254:LEU:N	2.27	0.48
5:B:265:SER:O	5:B:266:ALA:CB	2.61	0.48
5:B:435:THR:CG2	5:B:437:GLU:HB2	2.43	0.48
5:B:1034:VAL:HG12	5:B:1035:ALA:N	2.27	0.48
7:D:51:ASN:O	7:D:52:LEU:O	2.31	0.48
7:D:59:ILE:HG21	7:D:145:MET:SD	2.53	0.48
7:D:219:THR:HG22	7:D:220:LEU:O	2.13	0.48
8:E:168:TYR:CB	8:E:170:LEU:HG	2.43	0.48
10:G:25:TYR:CE2	10:G:29:LYS:HD2	2.48	0.48
11:H:62:SER:O	11:H:63:LEU:C	2.52	0.48
11:H:127:GLY:HA3	11:H:130:ARG:NH2	2.28	0.48
12:I:55:THR:HG22	12:I:58:VAL:CG2	2.44	0.48
14:K:47:ARG:HD2	14:K:47:ARG:O	2.13	0.48
1:T:24:DT:H2"	1:T:25:DC:C5'	2.44	0.48
1:T:26:DA:H2"	1:T:27:DT:O5'	2.11	0.48
4:A:470:LEU:HD22	4:A:487:MET:HE3	1.94	0.48
4:A:921:GLY:O	4:A:922:ASP:C	2.51	0.48
5:B:95:ILE:CG1	5:B:130:VAL:HG22	2.42	0.48
5:B:840:ILE:HD13	5:B:994:TYR:CE1	2.49	0.48
5:B:942:ARG:O	5:B:944:THR:N	2.46	0.48
7:D:47:LEU:CD1	10:G:3:PHE:HD2	2.26	0.48
7:D:144:THR:HG21	10:G:46:LEU:HD13	1.95	0.48
9:F:81:THR:HB	9:F:136:ARG:NH1	2.28	0.48
11:H:128:ASN:CG	11:H:128:ASN:O	2.51	0.48
4:A:441:PRO:HD2	4:A:498:ARG:CZ	2.43	0.48
4:A:444:PHE:HB3	4:A:458:HIS:CD2	2.49	0.48
4:A:1115:SER:O	4:A:1311:VAL:HG22	2.14	0.48
4:A:1441:PHE:CZ	9:F:89:GLU:HA	2.48	0.48
5:B:56:ASP:CB	5:B:57:TYR:HD1	2.26	0.48
5:B:769:TYR:O	5:B:772:ALA:N	2.45	0.48
5:B:827:ILE:O	5:B:1085:ILE:HG23	2.13	0.48
5:B:1132:GLU:O	5:B:1135:ARG:HB3	2.13	0.48
6:C:132:PRO:O	6:C:134:ILE:HG13	2.14	0.48
6:C:215:GLU:O	6:C:216:GLY:C	2.51	0.48
11:H:139:ASN:O	11:H:140:ALA:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:I:34:TYR:CD2	12:I:34:TYR:C	2.87	0.48
4:A:41:MET:O	4:A:50:ILE:HG13	2.14	0.48
4:A:44:THR:O	4:A:45:GLN:CB	2.62	0.48
4:A:567:LYS:HD3	11:H:95:TYR:HA	1.95	0.48
4:A:663:SER:HA	5:B:1014:PRO:HB3	1.95	0.48
4:A:1007:ILE:O	4:A:1010:ALA:N	2.46	0.48
4:A:1437:GLY:HA3	9:F:88:TYR:CD2	2.49	0.48
5:B:63:ILE:HA	5:B:421:PHE:CE2	2.49	0.48
6:C:142:VAL:O	6:C:142:VAL:HG12	2.13	0.48
7:D:12:ARG:HH21	7:D:12:ARG:CB	2.22	0.48
11:H:8:ASP:HB3	11:H:10:PHE:CE1	2.49	0.48
12:I:29:CYS:SG	12:I:32:CYS:SG	3.12	0.48
4:A:1242:VAL:HG12	4:A:1243:VAL:N	2.21	0.48
4:A:1385:THR:HG22	4:A:1386:ARG:N	2.29	0.48
5:B:65:GLU:HG3	5:B:66:ASP:OD1	2.13	0.48
5:B:843:GLN:O	5:B:846:ILE:HB	2.14	0.48
6:C:184:ASN:ND2	6:C:187:LYS:HA	2.29	0.48
8:E:39:LEU:O	8:E:42:PHE:HB3	2.12	0.48
9:F:97:ARG:HG3	9:F:101:ILE:HD11	1.95	0.48
10:G:88:ASP:HB3	10:G:144:ARG:HA	1.95	0.48
12:I:15:TYR:N	12:I:15:TYR:CD1	2.82	0.48
13:J:8:PHE:N	13:J:49:MET:HE3	2.24	0.48
4:A:116:ASP:O	4:A:118:HIS:N	2.47	0.48
4:A:289:ILE:C	4:A:291:GLU:H	2.17	0.48
4:A:1134:ILE:O	4:A:1138:ILE:HG13	2.13	0.48
5:B:51:PHE:CD2	5:B:173:MET:HB3	2.48	0.48
5:B:521:LEU:HD13	5:B:633:VAL:HG12	1.95	0.48
5:B:589:VAL:CG1	5:B:590:HIS:H	2.04	0.48
5:B:654:ARG:HG3	5:B:654:ARG:NH1	2.28	0.48
5:B:1002:THR:O	5:B:1005:GLY:N	2.43	0.48
10:G:14:HIS:CD2	10:G:16:SER:CB	2.96	0.48
11:H:101:ALA:HB2	11:H:116:TYR:CE1	2.49	0.48
14:K:85:ASP:O	14:K:88:LYS:HB2	2.13	0.48
15:L:33:GLU:OE2	15:L:55:ILE:HD11	2.14	0.48
4:A:19:PHE:HB3	4:A:1413:GLY:CA	2.43	0.48
4:A:666:ILE:HD12	4:A:667:GLY:N	2.26	0.48
4:A:836:TYR:CD2	4:A:840:ARG:HD2	2.49	0.48
4:A:886:ILE:HG13	4:A:943:LEU:CD1	2.43	0.48
4:A:1076:ALA:HA	4:A:1079:MET:HE3	1.95	0.48
4:A:1389:PHE:CD1	4:A:1390:ASN:N	2.82	0.48
4:A:1444:MET:HE1	9:F:135:ARG:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:309:GLN:O	5:B:312:GLU:HB3	2.13	0.48
5:B:1156:ASP:O	5:B:1157:ALA:O	2.32	0.48
7:D:16:LYS:HD3	7:D:16:LYS:H	1.78	0.48
11:H:44:VAL:HG13	11:H:48:PRO:HA	1.96	0.48
3:P:8:A:C2'	3:P:9:G:H5'	2.44	0.48
4:A:35:ILE:HD12	4:A:83:HIS:O	2.13	0.48
4:A:699:ALA:O	4:A:700:ASN:CB	2.61	0.48
4:A:898:ARG:O	4:A:1029:ARG:NH1	2.46	0.48
4:A:1162:VAL:O	4:A:1162:VAL:HG12	2.14	0.48
4:A:1279:ILE:HD11	4:A:1316:VAL:HG22	1.95	0.48
5:B:261:ARG:NH1	5:B:261:ARG:HB3	2.29	0.48
5:B:314:LEU:O	5:B:317:CYS:HB3	2.14	0.48
5:B:683:SER:O	5:B:687:GLU:HB2	2.14	0.48
5:B:1174:LYS:O	5:B:1176:ASN:N	2.47	0.48
6:C:6:PRO:CB	6:C:25:VAL:HG12	2.41	0.48
12:I:50:THR:HG22	12:I:52:ILE:H	1.79	0.48
15:L:52:GLY:O	15:L:53:HIS:C	2.51	0.48
3:P:5:A:H2'	3:P:6:G:C8	2.49	0.48
4:A:224:PHE:CE1	4:A:231:PRO:HG3	2.49	0.48
4:A:622:VAL:O	4:A:622:VAL:HG13	2.14	0.48
4:A:939:ASP:OD2	4:A:1020:CYS:HA	2.14	0.48
4:A:1120:LEU:N	4:A:1120:LEU:HD12	2.29	0.48
4:A:1162:VAL:HG11	12:I:41:PRO:HG3	1.96	0.48
5:B:280:ILE:CG2	5:B:285:ILE:HG13	2.43	0.48
5:B:863:GLU:O	5:B:961:LEU:HD22	2.14	0.48
5:B:1183:LYS:N	5:B:1183:LYS:CE	2.76	0.48
7:D:151:PHE:CE2	10:G:89:GLY:HA2	2.49	0.48
14:K:7:PHE:HA	14:K:10:PHE:HE2	1.76	0.48
4:A:22:PHE:HB2	5:B:1211:ASN:ND2	2.28	0.47
4:A:72:GLU:O	4:A:73:GLY:O	2.32	0.47
4:A:92:HIS:O	4:A:93:VAL:C	2.52	0.47
4:A:148:CYS:HB3	4:A:168:GLY:HA2	1.96	0.47
4:A:218:ASP:HA	4:A:221:SER:OG	2.14	0.47
4:A:474:VAL:HG22	4:A:474:VAL:O	2.13	0.47
4:A:809:THR:O	4:A:813:PHE:N	2.37	0.47
4:A:1094:VAL:HG12	4:A:1095:THR:N	2.29	0.47
5:B:25:ILE:HG23	5:B:658:ILE:HD11	1.96	0.47
5:B:806:THR:HG22	5:B:808:ALA:HB3	1.96	0.47
5:B:1183:LYS:HE3	5:B:1183:LYS:O	2.14	0.47
6:C:166:GLU:O	6:C:167:HIS:HB2	2.14	0.47
11:H:40:LEU:CD1	11:H:123:MET:HB2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:K:6:ARG:C	14:K:8:GLU:H	2.16	0.47
15:L:28:LYS:HG3	15:L:39:SER:OG	2.13	0.47
15:L:40:LEU:CD1	15:L:44:ASP:HB3	2.44	0.47
4:A:361:LEU:HD12	4:A:474:VAL:HB	1.96	0.47
4:A:445:ASN:HB2	4:A:455:MET:HG2	1.96	0.47
4:A:1019:CYS:O	4:A:1022:LEU:N	2.47	0.47
5:B:190:TYR:CD2	13:J:62:ARG:HB3	2.49	0.47
5:B:300:HIS:O	5:B:303:TYR:HE2	1.97	0.47
5:B:611:PRO:CB	5:B:685:LEU:HD11	2.41	0.47
6:C:112:ASN:HB2	6:C:114:TYR:CE1	2.49	0.47
10:G:66:GLY:O	10:G:67:SER:C	2.52	0.47
11:H:4:THR:HG22	11:H:5:LEU:H	1.79	0.47
11:H:118:PHE:N	11:H:118:PHE:CD1	2.82	0.47
11:H:135:LEU:HD13	11:H:137:GLN:NE2	2.28	0.47
1:T:16:DG:H5”	4:A:1403:GLU:HG2	1.95	0.47
4:A:335:ARG:NH1	5:B:1202:LEU:HD22	2.30	0.47
4:A:365:GLY:O	4:A:468:PHE:HA	2.13	0.47
4:A:382:PRO:HD3	4:A:428:TYR:CD2	2.49	0.47
4:A:399:HIS:CB	4:A:400:PRO:CD	2.86	0.47
4:A:626:ASN:O	4:A:631:HIS:HD2	1.97	0.47
4:A:811:GLN:O	4:A:812:GLU:C	2.53	0.47
4:A:946:VAL:HG22	8:E:201:LYS:HD2	1.95	0.47
4:A:1316:VAL:O	4:A:1316:VAL:HG12	2.13	0.47
5:B:269:ILE:HG22	5:B:282:ILE:HG23	1.94	0.47
5:B:604:ARG:NH2	5:B:613:VAL:O	2.48	0.47
6:C:175:ALA:HB1	13:J:43:ARG:NH1	2.30	0.47
6:C:209:TYR:CD1	6:C:209:TYR:N	2.76	0.47
12:I:4:PHE:CD1	12:I:4:PHE:C	2.88	0.47
12:I:105:SER:O	12:I:106:CYS:HB3	2.14	0.47
13:J:16:ASP:O	13:J:18:TRP:N	2.47	0.47
2:N:6:DA:O5’	2:N:6:DA:H2’	2.14	0.47
4:A:626:ASN:C	4:A:628:GLY:H	2.16	0.47
4:A:996:ASN:C	4:A:998:LEU:HD12	2.35	0.47
4:A:1030:ARG:NH1	4:A:1035:TYR:OH	2.48	0.47
4:A:1220:PHE:CE2	4:A:1263:ILE:HG23	2.49	0.47
4:A:1409:LEU:HD13	5:B:1207:LEU:CD2	2.43	0.47
5:B:90:ILE:CD1	5:B:432:MET:SD	3.02	0.47
5:B:293:PRO:HG2	5:B:296:GLU:CB	2.44	0.47
5:B:796:LEU:HD11	5:B:821:GLN:NE2	2.29	0.47
5:B:840:ILE:HB	5:B:1011:ILE:HB	1.96	0.47
6:C:52:GLU:CD	6:C:154:LYS:HD2	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:34:GLN:C	7:D:36:LYS:N	2.67	0.47
7:D:176:GLU:O	7:D:178:ALA:N	2.48	0.47
8:E:43:LYS:O	8:E:45:LYS:N	2.45	0.47
9:F:93:ILE:HD11	9:F:134:ILE:CD1	2.37	0.47
10:G:44:TYR:O	10:G:78:VAL:HA	2.13	0.47
10:G:138:THR:HG22	10:G:139:ILE:HG13	1.96	0.47
12:I:92:ARG:HG2	12:I:94:ASP:OD1	2.14	0.47
13:J:7:CYS:HA	13:J:49:MET:HE3	1.97	0.47
13:J:23:ASN:C	13:J:25:LEU:N	2.66	0.47
4:A:961:ARG:HG2	4:A:965:GLN:HE21	1.79	0.47
4:A:1261:LYS:O	4:A:1264:GLU:HB3	2.13	0.47
4:A:1436:ILE:O	4:A:1437:GLY:C	2.51	0.47
5:B:29:ASP:HB3	5:B:658:ILE:CD1	2.44	0.47
5:B:167:ILE:HG22	5:B:167:ILE:O	2.15	0.47
5:B:401:PHE:HB2	5:B:517:THR:OG1	2.14	0.47
5:B:781:PHE:HE2	5:B:793:ALA:HB1	1.79	0.47
7:D:191:ALA:O	7:D:193:THR:N	2.47	0.47
8:E:19:VAL:HG11	8:E:80:VAL:HG11	1.96	0.47
12:I:49:ILE:HG22	12:I:49:ILE:O	2.13	0.47
12:I:80:SER:CB	12:I:103:CYS:SG	3.02	0.47
15:L:38:LEU:HD11	15:L:49:LYS:HE2	1.95	0.47
1:T:20:DC:H2"	1:T:21:DT:C5'	2.44	0.47
4:A:24:PRO:HD2	4:A:233:TRP:NE1	2.29	0.47
4:A:404:TYR:HB2	4:A:433:GLU:HB2	1.97	0.47
4:A:444:PHE:HB2	4:A:458:HIS:HD2	1.80	0.47
4:A:466:SER:CA	14:K:2:ASN:HD22	2.28	0.47
4:A:623:GLY:C	4:A:625:SER:H	2.17	0.47
4:A:738:LYS:HB2	4:A:740:LEU:HG	1.96	0.47
4:A:853:ASP:OD1	4:A:855:THR:N	2.47	0.47
4:A:873:MET:C	4:A:1058:VAL:CG2	2.83	0.47
5:B:37:PHE:CE2	5:B:542:MET:HA	2.50	0.47
5:B:575:PRO:HG2	5:B:576:ASP:H	1.78	0.47
5:B:680:THR:O	5:B:684:LEU:CD1	2.63	0.47
5:B:847:ASP:C	5:B:849:GLY:N	2.67	0.47
7:D:19:GLU:O	7:D:21:GLU:N	2.48	0.47
12:I:83:ASN:HA	12:I:102:VAL:O	2.14	0.47
4:A:15:LYS:HD3	5:B:1220:ARG:HH21	1.80	0.47
4:A:23:SER:O	4:A:25:GLU:N	2.47	0.47
4:A:310:GLY:O	4:A:312:PRO:HD2	2.14	0.47
4:A:591:PHE:HA	4:A:595:THR:CG2	2.44	0.47
4:A:808:LEU:HD23	4:A:813:PHE:CA	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:899:VAL:CG2	4:A:908:LEU:HD21	2.45	0.47
4:A:947:PHE:CD2	4:A:954:TRP:CZ2	3.02	0.47
4:A:993:LEU:HD23	4:A:1022:LEU:HD21	1.95	0.47
4:A:1280:GLU:O	4:A:1282:VAL:HG23	2.15	0.47
4:A:1364:ASN:HD22	4:A:1365:TYR:N	2.13	0.47
4:A:1373:ASP:CA	4:A:1376:THR:HG22	2.44	0.47
4:A:1389:PHE:CZ	4:A:1402:PHE:CE2	3.02	0.47
5:B:465:ASN:N	5:B:465:ASN:ND2	2.63	0.47
5:B:857:ARG:HD2	5:B:945:GLU:OE1	2.15	0.47
5:B:909:ASP:OD1	5:B:909:ASP:N	2.47	0.47
5:B:953:LEU:HD23	5:B:953:LEU:O	2.14	0.47
6:C:105:GLY:O	6:C:149:LYS:O	2.32	0.47
6:C:174:ALA:HA	13:J:10:CYS:O	2.15	0.47
10:G:1:MET:HG2	10:G:85:GLU:OE1	2.14	0.47
10:G:101:VAL:CG1	10:G:102:GLN:N	2.77	0.47
4:A:244:PRO:CB	4:A:245:PRO:HD3	2.45	0.47
4:A:340:LEU:HD13	4:A:1429:ILE:HG23	1.97	0.47
4:A:547:LEU:HD22	14:K:58:PHE:HD1	1.76	0.47
5:B:435:THR:C	5:B:437:GLU:N	2.66	0.47
5:B:824:ILE:HG22	5:B:824:ILE:O	2.14	0.47
5:B:970:THR:HG22	5:B:971:THR:N	2.30	0.47
9:F:82:THR:CG2	9:F:84:TYR:H	2.18	0.47
12:I:106:CYS:O	12:I:107:SER:CB	2.62	0.47
14:K:57:LEU:HD12	14:K:77:THR:O	2.15	0.47
15:L:38:LEU:CD1	15:L:49:LYS:HE2	2.45	0.47
4:A:14:VAL:HG21	5:B:1216:LEU:CD1	2.44	0.47
4:A:377:PRO:HD3	4:A:493:GLN:OE1	2.14	0.47
4:A:384:ASN:O	4:A:386:ASP:N	2.47	0.47
4:A:472:LEU:O	4:A:475:THR:HB	2.15	0.47
4:A:528:LEU:HD23	4:A:751:SER:HA	1.96	0.47
4:A:1205:LYS:O	4:A:1206:ASP:C	2.54	0.47
4:A:1315:GLU:C	4:A:1317:MET:H	2.18	0.47
5:B:29:ASP:CG	5:B:658:ILE:HD13	2.35	0.47
5:B:360:PHE:C	5:B:360:PHE:CD2	2.88	0.47
5:B:376:PHE:CE2	5:B:569:TYR:HD2	2.33	0.47
5:B:798:TYR:CD2	5:B:798:TYR:N	2.82	0.47
6:C:46:ILE:HG23	6:C:157:CYS:HB3	1.96	0.47
6:C:69:LEU:N	6:C:69:LEU:CD1	2.78	0.47
7:D:24:ALA:C	7:D:26:THR:H	2.18	0.47
10:G:125:SER:OG	10:G:128:PRO:HA	2.14	0.47
11:H:100:THR:CG2	11:H:101:ALA:N	2.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:351:THR:CB	5:B:1103:ILE:HD12	2.44	0.47
4:A:618:GLU:O	4:A:621:THR:N	2.36	0.47
4:A:737:LEU:HD23	4:A:737:LEU:HA	1.69	0.47
4:A:871:ASP:OD2	4:A:873:MET:HB2	2.15	0.47
4:A:1362:TYR:CD1	4:A:1363:VAL:N	2.83	0.47
5:B:118:ARG:HH11	5:B:204:ILE:HD11	1.80	0.47
5:B:844:SER:O	5:B:847:ASP:HB2	2.14	0.47
5:B:986:GLN:OE1	5:B:986:GLN:HA	2.13	0.47
5:B:1007:VAL:CG2	5:B:1008:PRO:HD2	2.45	0.47
5:B:1160:VAL:CG1	5:B:1161:HIS:N	2.78	0.47
5:B:1201:LYS:HE2	5:B:1205:GLN:CD	2.35	0.47
8:E:94:LYS:HG3	8:E:98:ILE:HD11	1.97	0.47
8:E:157:SER:C	8:E:159:ASP:N	2.68	0.47
11:H:11:GLN:HA	11:H:53:ASP:O	2.15	0.47
15:L:40:LEU:HB3	15:L:41:SER:H	1.52	0.47
4:A:247:ARG:HH11	4:A:247:ARG:HG3	1.81	0.46
4:A:252:PHE:O	4:A:253:ASN:CB	2.63	0.46
4:A:757:ASN:HA	5:B:1021:MET:SD	2.55	0.46
4:A:862:ASN:HA	8:E:174:GLN:HB3	1.97	0.46
4:A:1438:THR:HG22	9:F:92:ARG:HD2	1.97	0.46
5:B:90:ILE:HD11	5:B:432:MET:SD	2.55	0.46
5:B:230:ALA:N	5:B:231:PRO:HD2	2.30	0.46
5:B:293:PRO:CG	5:B:296:GLU:OE1	2.63	0.46
5:B:1138:MET:HA	5:B:1138:MET:CE	2.45	0.46
6:C:77:ILE:C	6:C:79:GLN:H	2.18	0.46
8:E:90:VAL:O	8:E:90:VAL:HG22	2.15	0.46
8:E:94:LYS:HG3	8:E:98:ILE:CD1	2.45	0.46
8:E:164:LEU:HD11	8:E:211:TYR:CE1	2.50	0.46
11:H:24:CYS:HB2	11:H:44:VAL:HG21	1.96	0.46
12:I:5:ARG:HG2	12:I:6:PHE:O	2.15	0.46
12:I:8:ARG:CG	12:I:34:TYR:HE1	2.26	0.46
4:A:315:LEU:HD13	5:B:471:LYS:HB3	1.97	0.46
4:A:469:ARG:HH11	4:A:469:ARG:HB3	1.80	0.46
4:A:596:THR:C	4:A:598:LEU:N	2.69	0.46
4:A:1029:ARG:HH11	4:A:1029:ARG:HG3	1.80	0.46
4:A:1280:GLU:O	4:A:1281:ARG:C	2.53	0.46
5:B:38:PHE:CD1	5:B:811:TYR:CD2	3.04	0.46
5:B:40:GLU:HG2	5:B:40:GLU:O	2.14	0.46
5:B:181:LEU:HD22	5:B:189:LEU:CD2	2.45	0.46
5:B:388:CYS:O	5:B:391:ASP:N	2.43	0.46
5:B:616:ILE:N	5:B:616:ILE:CD1	2.76	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:957:ASN:O	5:B:958:GLN:C	2.53	0.46
10:G:79:PHE:HE2	10:G:105:PRO:CG	2.28	0.46
10:G:87:VAL:HG21	10:G:103:VAL:HG11	1.97	0.46
1:T:11:DT:C2'	1:T:12:DA:H5'	2.46	0.46
4:A:332:LYS:H	4:A:337:ARG:HB3	1.79	0.46
4:A:349:ALA:C	5:B:1128:LEU:HD11	2.35	0.46
4:A:500:GLU:OE2	4:A:1438:THR:HG21	2.15	0.46
4:A:629:LEU:O	4:A:633:VAL:HG23	2.15	0.46
4:A:665:GLY:O	4:A:667:GLY:N	2.48	0.46
4:A:726:ARG:O	4:A:729:ALA:HB3	2.14	0.46
4:A:1072:ILE:HD11	4:A:1368:MET:HG2	1.97	0.46
5:B:43:LEU:HD11	5:B:811:TYR:O	2.15	0.46
5:B:94:LYS:HG2	5:B:95:ILE:H	1.78	0.46
5:B:121:ASN:OD1	5:B:963:PHE:HZ	1.99	0.46
5:B:212:LEU:HD12	5:B:409:ALA:HB1	1.98	0.46
5:B:603:LEU:HB3	5:B:609:ILE:CG1	2.46	0.46
5:B:664:THR:HG23	5:B:678:GLU:N	2.29	0.46
5:B:1001:PHE:CE2	6:C:34:ARG:CZ	2.99	0.46
5:B:1034:VAL:HG21	5:B:1055:ILE:HG23	1.96	0.46
5:B:1142:GLY:C	5:B:1144:ALA:H	2.18	0.46
6:C:43:THR:CG2	6:C:44:LEU:N	2.64	0.46
6:C:66:ARG:CZ	13:J:2:ILE:HG21	2.44	0.46
8:E:29:PHE:O	8:E:30:ILE:HG13	2.15	0.46
13:J:48:ARG:HD2	13:J:48:ARG:C	2.35	0.46
4:A:713:SER:O	4:A:717:ASN:ND2	2.49	0.46
4:A:971:PHE:HE2	4:A:1040:GLN:HG2	1.81	0.46
5:B:580:VAL:HG13	5:B:624:LEU:HB3	1.97	0.46
5:B:593:PRO:O	5:B:594:ALA:C	2.53	0.46
5:B:1125:ASP:O	5:B:1126:GLY:O	2.34	0.46
5:B:1167:GLY:H	5:B:1217:TYR:HE1	1.64	0.46
6:C:6:PRO:HB3	6:C:25:VAL:CG1	2.41	0.46
6:C:27:LEU:O	6:C:30:ALA:N	2.49	0.46
6:C:69:LEU:CD1	6:C:69:LEU:H	2.28	0.46
8:E:85:GLU:O	8:E:88:VAL:HG23	2.15	0.46
12:I:29:CYS:SG	12:I:31:THR:HB	2.56	0.46
4:A:65:LEU:O	4:A:66:LYS:C	2.53	0.46
4:A:210:ILE:O	4:A:214:ILE:HG13	2.14	0.46
4:A:253:ASN:HB3	5:B:935:ARG:NH2	2.31	0.46
4:A:264:PHE:O	4:A:267:ALA:HB3	2.15	0.46
4:A:528:LEU:HD23	4:A:751:SER:CA	2.46	0.46
4:A:854:ASN:HB2	4:A:1000:LEU:HD21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:29:ASP:HB3	5:B:658:ILE:HD13	1.98	0.46
5:B:641:GLU:HA	5:B:641:GLU:OE1	2.15	0.46
5:B:871:THR:HG22	5:B:872:GLU:N	2.30	0.46
5:B:1166:CYS:O	5:B:1166:CYS:SG	2.74	0.46
6:C:18:VAL:HG23	6:C:240:VAL:HB	1.96	0.46
6:C:189:THR:HG22	6:C:190:ASP:N	2.31	0.46
9:F:75:PRO:O	9:F:77:ASP:O	2.32	0.46
4:A:65:LEU:O	4:A:66:LYS:O	2.34	0.46
4:A:206:GLU:O	4:A:210:ILE:HG13	2.16	0.46
4:A:512:VAL:HA	4:A:519:PRO:HA	1.97	0.46
4:A:608:ILE:HD12	4:A:613:ILE:CD1	2.45	0.46
4:A:1000:LEU:HD23	4:A:1000:LEU:HA	1.81	0.46
4:A:1349:TYR:N	4:A:1372:VAL:HG21	2.31	0.46
5:B:31:TRP:CE3	5:B:31:TRP:HA	2.50	0.46
5:B:102:VAL:O	5:B:109:THR:HA	2.16	0.46
5:B:283:VAL:O	5:B:286:PHE:N	2.49	0.46
5:B:555:ILE:HD11	5:B:587:HIS:CE1	2.51	0.46
5:B:797:TYR:O	13:J:1:MET:HG2	2.15	0.46
5:B:1034:VAL:O	5:B:1037:LEU:N	2.45	0.46
7:D:156:ASP:C	7:D:158:GLU:H	2.19	0.46
8:E:93:MET:SD	8:E:97:VAL:HG23	2.55	0.46
11:H:4:THR:O	11:H:5:LEU:HD23	2.16	0.46
4:A:218:ASP:O	4:A:219:PHE:C	2.53	0.46
4:A:265:LYS:HE2	4:A:322:VAL:HG11	1.98	0.46
4:A:1437:GLY:CA	9:F:88:TYR:CD2	2.99	0.46
5:B:39:ARG:NH2	5:B:665:GLU:CD	2.69	0.46
5:B:165:VAL:HG11	5:B:448:ILE:CD1	2.46	0.46
5:B:361:LEU:HD11	5:B:377:PHE:CD2	2.50	0.46
5:B:903:VAL:O	5:B:948:ILE:HG23	2.16	0.46
6:C:77:ILE:CG2	6:C:161:LYS:HE3	2.45	0.46
6:C:125:MET:HB2	6:C:127:ARG:HH21	1.81	0.46
11:H:128:ASN:O	11:H:128:ASN:OD1	2.34	0.46
14:K:107:THR:O	14:K:111:LEU:HG	2.16	0.46
4:A:75:ASN:O	4:A:76:GLU:HB3	2.15	0.46
4:A:416:ARG:HG3	4:A:417:TYR:CE2	2.51	0.46
4:A:556:TRP:CZ3	4:A:558:GLY:HA2	2.51	0.46
4:A:738:LYS:C	4:A:740:LEU:H	2.19	0.46
4:A:806:ARG:NH1	5:B:729:ILE:HG13	2.31	0.46
4:A:1239:ARG:NH1	4:A:1239:ARG:HB3	2.31	0.46
7:D:7:THR:HB	10:G:42:PHE:HZ	1.77	0.46
7:D:27:LEU:HD13	7:D:173:HIS:CD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:185:CYS:HB2	7:D:211:LEU:HD22	1.96	0.46
8:E:46:TYR:CD2	8:E:58:MET:HG2	2.51	0.46
8:E:55:ARG:C	8:E:57:MET:N	2.69	0.46
4:A:61:ILE:CG2	4:A:62:ASP:H	2.22	0.46
4:A:351:THR:HB	5:B:1103:ILE:HD11	1.97	0.46
4:A:909:ASP:O	4:A:911:SER:N	2.49	0.46
5:B:227:LYS:HB2	5:B:395:GLN:OE1	2.16	0.46
5:B:758:PHE:HB2	5:B:1024:ALA:HB1	1.98	0.46
5:B:893:LEU:HD22	5:B:897:GLY:C	2.36	0.46
5:B:980:PHE:HE2	5:B:1094:ARG:HB2	1.81	0.46
7:D:153:ARG:HB3	7:D:154:PHE:CD1	2.51	0.46
8:E:20:LYS:NZ	8:E:60:PHE:HE1	2.13	0.46
11:H:138:GLU:O	11:H:139:ASN:C	2.53	0.46
12:I:69:PRO:HG2	12:I:85:PHE:CD2	2.50	0.46
4:A:10:PRO:HD2	5:B:1191:ILE:O	2.16	0.46
4:A:128:ILE:O	4:A:134:ARG:HG3	2.16	0.46
4:A:259:GLU:OE1	4:A:263:THR:HG21	2.16	0.46
4:A:298:PHE:HD2	4:A:299:HIS:N	2.13	0.46
4:A:346:ASP:CG	5:B:1108:ARG:HA	2.36	0.46
4:A:683:ILE:HG21	4:A:801:GLU:CG	2.45	0.46
4:A:711:ARG:O	4:A:714:PHE:HB3	2.15	0.46
4:A:960:ILE:CA	4:A:963:ILE:HG22	2.41	0.46
5:B:221:ASN:OD1	5:B:242:SER:HA	2.16	0.46
5:B:228:LYS:O	5:B:229:ALA:O	2.34	0.46
5:B:412:LEU:HB3	5:B:466:TRP:CZ2	2.51	0.46
5:B:555:ILE:HG22	5:B:556:THR:N	2.31	0.46
5:B:591:ARG:O	5:B:593:PRO:HD3	2.16	0.46
5:B:780:VAL:HG21	13:J:56:LEU:CD1	2.46	0.46
5:B:825:VAL:HG21	5:B:1092:TYR:HE1	1.80	0.46
5:B:883:LEU:O	5:B:885:MET:N	2.49	0.46
5:B:975:GLN:HG2	5:B:976:ILE:N	2.31	0.46
7:D:138:ASN:OD1	7:D:141:LEU:HB2	2.15	0.46
12:I:12:ASN:HB3	12:I:13:MET:H	1.55	0.46
14:K:55:LYS:HB3	14:K:81:TYR:CE1	2.51	0.46
2:N:1:DC:H1'	2:N:2:DA:H5'	1.98	0.45
2:N:3:DA:H1'	2:N:4:DG:H5'	1.97	0.45
4:A:92:HIS:O	4:A:95:PHE:N	2.46	0.45
4:A:254:GLU:HB2	5:B:935:ARG:HH12	1.80	0.45
5:B:118:ARG:CG	5:B:204:ILE:HD13	2.46	0.45
5:B:520:GLY:HA2	5:B:748:ILE:HG22	1.98	0.45
5:B:764:SER:HB3	5:B:765:PRO:CD	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:863:GLU:OE1	5:B:962:LYS:HD2	2.16	0.45
10:G:1:MET:O	10:G:1:MET:CE	2.64	0.45
11:H:31:THR:O	11:H:31:THR:HG22	2.16	0.45
12:I:80:SER:OG	12:I:105:SER:HB2	2.16	0.45
4:A:252:PHE:O	4:A:256:GLN:NE2	2.49	0.45
4:A:254:GLU:HB2	5:B:935:ARG:HH22	1.81	0.45
4:A:340:LEU:CD2	5:B:1199:ALA:HB3	2.47	0.45
4:A:474:VAL:C	4:A:477:PRO:HD2	2.35	0.45
4:A:573:SER:O	4:A:576:GLN:HB2	2.14	0.45
4:A:1195:LEU:HD11	4:A:1267:MET:CE	2.45	0.45
4:A:1397:LEU:HB2	4:A:1426:GLU:OE1	2.16	0.45
5:B:240:ILE:HG22	5:B:254:LEU:HB3	1.98	0.45
5:B:324:ILE:CG2	5:B:325:GLN:N	2.79	0.45
5:B:745:PRO:C	5:B:747:MET:N	2.69	0.45
5:B:778:MET:HE1	5:B:1094:ARG:HD3	1.95	0.45
5:B:1040:ASN:O	5:B:1042:GLY:N	2.50	0.45
7:D:12:ARG:O	7:D:14:ARG:HG3	2.16	0.45
2:N:2:DA:H2"	2:N:3:DA:OP2	2.15	0.45
4:A:203:SER:OG	4:A:206:GLU:HB2	2.17	0.45
4:A:347:PHE:H	5:B:1107:ALA:HA	1.80	0.45
4:A:464:PRO:O	4:A:465:TYR:O	2.35	0.45
4:A:577:ILE:O	4:A:579:SER:N	2.48	0.45
4:A:913:LEU:HD21	4:A:915:SER:OG	2.15	0.45
5:B:126:SER:CB	5:B:172:ILE:HD11	2.45	0.45
5:B:521:LEU:HB3	5:B:633:VAL:CG1	2.42	0.45
5:B:593:PRO:HG2	5:B:617:ARG:CZ	2.45	0.45
5:B:750:GLY:O	5:B:751:VAL:C	2.54	0.45
5:B:1004:GLU:HB2	5:B:1006:ILE:HG13	1.97	0.45
5:B:1161:HIS:NE2	5:B:1175:LEU:HD21	2.31	0.45
5:B:1162:ILE:HD11	5:B:1194:ILE:CD1	2.43	0.45
8:E:55:ARG:C	8:E:57:MET:H	2.19	0.45
10:G:30:LEU:HD22	10:G:72:VAL:HG11	1.97	0.45
14:K:12:LEU:HD12	14:K:12:LEU:N	2.29	0.45
1:T:18:DC:H5'	4:A:832:ALA:O	2.17	0.45
4:A:399:HIS:O	4:A:401:GLY:N	2.49	0.45
4:A:650:GLN:HB3	4:A:654:ASN:HD21	1.82	0.45
4:A:898:ARG:HB2	4:A:933:TYR:CE1	2.52	0.45
4:A:1095:THR:HG21	4:A:1103:GLU:OE1	2.16	0.45
4:A:1323:ASP:C	4:A:1325:THR:N	2.70	0.45
5:B:32:ALA:O	5:B:35:SER:HB2	2.16	0.45
5:B:39:ARG:HG2	5:B:39:ARG:NH1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1202:LEU:O	5:B:1206:GLU:HG3	2.16	0.45
10:G:132:SER:HB3	10:G:135:ASP:HB2	1.97	0.45
11:H:95:TYR:CE2	11:H:97:MET:HG3	2.52	0.45
13:J:19:GLU:O	13:J:23:ASN:HB2	2.16	0.45
4:A:552:TRP:NE1	14:K:62:LYS:HB3	2.31	0.45
4:A:1438:THR:CB	5:B:1144:ALA:HB3	2.27	0.45
5:B:844:SER:O	5:B:847:ASP:N	2.46	0.45
6:C:252:GLN:CG	14:K:95:ILE:HG23	2.46	0.45
7:D:29:LEU:O	7:D:30:GLY:C	2.52	0.45
8:E:22:MET:CE	8:E:26:ARG:HE	2.30	0.45
10:G:108:VAL:HG13	10:G:159:ALA:O	2.17	0.45
12:I:32:CYS:SG	12:I:33:SER:N	2.89	0.45
14:K:31:VAL:CG1	14:K:32:VAL:N	2.80	0.45
14:K:58:PHE:CE2	14:K:74:ARG:NE	2.76	0.45
1:T:23:DC:H2"	1:T:24:DT:O5'	2.16	0.45
4:A:73:GLY:O	4:A:75:ASN:N	2.50	0.45
4:A:313:GLN:O	4:A:314:ALA:HB3	2.16	0.45
4:A:666:ILE:HD12	4:A:666:ILE:N	2.32	0.45
4:A:889:SER:HB3	4:A:1297:GLU:HG2	1.98	0.45
5:B:53:GLN:HG2	5:B:547:VAL:CG2	2.38	0.45
5:B:131:ASP:HA	5:B:164:LYS:HB3	1.97	0.45
5:B:189:LEU:HD12	5:B:196:PRO:HA	1.99	0.45
5:B:212:LEU:HD12	5:B:409:ALA:CB	2.47	0.45
5:B:449:ASN:O	5:B:451:LYS:N	2.50	0.45
5:B:1160:VAL:HG12	5:B:1161:HIS:N	2.32	0.45
6:C:76:ASP:OD2	6:C:128:ASN:N	2.48	0.45
6:C:143:LEU:HD21	6:C:146:LYS:CE	2.47	0.45
7:D:195:ILE:CG2	7:D:198:LEU:HG	2.46	0.45
10:G:45:ILE:HD13	10:G:78:VAL:HG13	1.98	0.45
14:K:53:ASP:HB3	14:K:56:VAL:CG2	2.35	0.45
14:K:88:LYS:O	14:K:91:CYS:HB2	2.17	0.45
3:P:5:A:H2'	3:P:6:G:H8	1.82	0.45
4:A:341:MET:CE	4:A:843:LYS:HZ1	2.30	0.45
4:A:1146:VAL:HG11	4:A:1207:LEU:CD1	2.47	0.45
4:A:1355:VAL:O	4:A:1355:VAL:HG12	2.17	0.45
4:A:1404:GLU:HB2	4:A:1408:ILE:HG13	1.98	0.45
5:B:282:ILE:CD1	5:B:382:ILE:HD13	2.47	0.45
5:B:311:LEU:O	5:B:312:GLU:C	2.55	0.45
5:B:315:LYS:HE3	12:I:4:PHE:CD2	2.52	0.45
5:B:1096:ARG:HA	5:B:1098:MET:HE2	1.99	0.45
6:C:107:SER:O	6:C:109:SER:N	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:145:THR:HG21	8:E:187:TYR:CE2	2.51	0.45
9:F:73:ALA:HA	9:F:143:PHE:CE1	2.52	0.45
10:G:143:ILE:CG2	10:G:144:ARG:H	2.29	0.45
12:I:82:GLU:O	12:I:104:LEU:HG	2.16	0.45
14:K:53:ASP:C	14:K:55:LYS:N	2.70	0.45
4:A:28:ARG:O	4:A:29:ALA:C	2.55	0.45
4:A:146:MET:CA	4:A:171:GLN:HB2	2.47	0.45
4:A:320:ARG:HH21	4:A:323:LYS:HZ1	1.65	0.45
4:A:1226:VAL:HG12	4:A:1227:ILE:N	2.32	0.45
4:A:1299:VAL:CG1	4:A:1300:LYS:H	2.28	0.45
5:B:270:LYS:HA	5:B:281:PRO:HA	1.99	0.45
5:B:466:TRP:O	5:B:468:GLU:N	2.48	0.45
5:B:512:ARG:HG2	5:B:512:ARG:HH11	1.82	0.45
5:B:979:LYS:HG2	5:B:1095:LEU:HD13	1.99	0.45
5:B:1038:SER:C	5:B:1040:ASN:N	2.70	0.45
12:I:69:PRO:HG2	12:I:85:PHE:CE2	2.52	0.45
15:L:36:SER:O	15:L:37:LYS:C	2.55	0.45
15:L:43:THR:HG22	15:L:43:THR:O	2.15	0.45
4:A:445:ASN:HA	4:A:478:TYR:CE2	2.52	0.45
4:A:683:ILE:HD13	4:A:801:GLU:CG	2.47	0.45
4:A:871:ASP:OD1	4:A:1366:ARG:NH2	2.49	0.45
4:A:936:LEU:O	4:A:939:ASP:HB2	2.17	0.45
4:A:1394:THR:CG2	4:A:1398:MET:SD	3.04	0.45
5:B:436:VAL:O	5:B:436:VAL:HG12	2.17	0.45
5:B:828:ALA:O	5:B:834:ASN:ND2	2.48	0.45
6:C:179:GLU:CG	6:C:180:TYR:N	2.78	0.45
6:C:183:TRP:CZ2	6:C:207:CYS:HB3	2.51	0.45
6:C:226:ASP:O	6:C:227:THR:CB	2.61	0.45
6:C:259:LEU:HD21	14:K:92:ASN:CG	2.38	0.45
12:I:58:VAL:O	12:I:58:VAL:HG12	2.16	0.45
13:J:12:LYS:O	13:J:14:VAL:CG2	2.59	0.45
14:K:17:SER:O	14:K:18:LYS:C	2.54	0.45
4:A:34:LYS:CD	4:A:34:LYS:N	2.80	0.45
4:A:1152:ILE:HG22	4:A:1192:LEU:O	2.17	0.45
4:A:1170:ILE:HG22	4:A:1174:PHE:HE1	1.82	0.45
4:A:1224:LEU:HD11	4:A:1240:CYS:HB2	1.99	0.45
4:A:1299:VAL:CG1	4:A:1300:LYS:N	2.78	0.45
5:B:281:PRO:O	5:B:283:VAL:N	2.50	0.45
5:B:284:ILE:HG23	5:B:324:ILE:CD1	2.47	0.45
5:B:519:TRP:HE1	5:B:635:ARG:NH2	2.15	0.45
5:B:882:THR:O	5:B:883:LEU:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1007:VAL:HG22	5:B:1008:PRO:HD2	1.98	0.45
5:B:1096:ARG:O	5:B:1097:HIS:CG	2.70	0.45
5:B:1151:LEU:N	5:B:1151:LEU:CD1	2.80	0.45
6:C:29:MET:CE	14:K:98:LEU:HG	2.47	0.45
6:C:31:ASN:O	6:C:32:SER:C	2.55	0.45
8:E:24:LYS:HG3	8:E:25:ASP:N	2.32	0.45
8:E:133:GLU:HB3	8:E:135:PHE:HE1	1.81	0.45
10:G:7:LEU:CD1	10:G:45:ILE:HD11	2.47	0.45
11:H:82:PRO:C	11:H:84:ALA:H	2.15	0.45
14:K:56:VAL:HA	14:K:77:THR:HG22	1.98	0.45
4:A:106:VAL:HG13	4:A:112:LYS:H	1.82	0.44
4:A:231:PRO:C	4:A:233:TRP:H	2.20	0.44
4:A:774:ARG:H	4:A:774:ARG:HG2	1.49	0.44
4:A:788:SER:O	4:A:789:LYS:O	2.35	0.44
4:A:920:LEU:HD23	4:A:920:LEU:C	2.37	0.44
4:A:963:ILE:HD13	4:A:1049:ILE:CG1	2.46	0.44
4:A:1120:LEU:H	4:A:1120:LEU:HD13	1.82	0.44
5:B:550:ASP:OD1	5:B:551:PRO:HD2	2.17	0.44
5:B:558:LEU:O	5:B:561:TRP:N	2.49	0.44
5:B:563:MET:HE2	5:B:587:HIS:C	2.37	0.44
5:B:695:ALA:O	5:B:698:GLU:HB3	2.17	0.44
5:B:797:TYR:HE1	5:B:854:LEU:CD2	2.30	0.44
5:B:799:PRO:CB	5:B:818:PRO:HG2	2.47	0.44
6:C:27:LEU:O	6:C:28:ALA:C	2.56	0.44
7:D:195:ILE:O	7:D:198:LEU:HG	2.17	0.44
8:E:114:ASN:O	8:E:115:ASN:CB	2.63	0.44
9:F:128:LYS:HD3	9:F:149:GLU:O	2.17	0.44
10:G:152:SER:O	10:G:153:GLN:HB2	2.17	0.44
11:H:91:ASP:C	11:H:93:TYR:N	2.70	0.44
13:J:64:ASN:CB	13:J:65:PRO:HD3	2.44	0.44
4:A:23:SER:O	4:A:26:GLU:N	2.50	0.44
4:A:157:ASP:C	4:A:159:THR:N	2.70	0.44
4:A:568:PRO:HG2	4:A:569:LYS:H	1.83	0.44
4:A:994:GLN:HA	4:A:997:LEU:HG	1.99	0.44
4:A:1428:VAL:HG22	5:B:1147:LEU:HD21	1.98	0.44
4:A:1433:MET:CE	10:G:63:PRO:HB2	2.47	0.44
5:B:596:LEU:O	5:B:600:LEU:HG	2.17	0.44
5:B:600:LEU:O	5:B:609:ILE:HD12	2.17	0.44
5:B:1177:HIS:O	5:B:1179:GLN:N	2.51	0.44
6:C:239:PRO:O	6:C:241:ASP:N	2.50	0.44
7:D:48:ILE:HG21	10:G:4:ILE:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:151:PHE:N	7:D:151:PHE:HD1	2.15	0.44
8:E:21:GLU:O	8:E:24:LYS:HG2	2.17	0.44
11:H:91:ASP:O	11:H:93:TYR:N	2.47	0.44
11:H:116:TYR:HE2	11:H:140:ALA:HB1	1.82	0.44
11:H:130:ARG:HB3	11:H:133:ASN:HB2	1.99	0.44
14:K:93:SER:O	14:K:97:LYS:HG3	2.17	0.44
1:T:24:DT:OP2	5:B:942:ARG:NH2	2.50	0.44
4:A:35:ILE:HA	4:A:52:GLY:O	2.17	0.44
4:A:53:LEU:CD2	4:A:54:ASN:HD22	2.30	0.44
4:A:114:LEU:HD13	4:A:171:GLN:OE1	2.17	0.44
4:A:138:ILE:HD12	4:A:222:LEU:HD23	1.98	0.44
4:A:353:ILE:HB	4:A:470:LEU:CD2	2.47	0.44
4:A:373:THR:HG21	5:B:1105:ALA:HB3	1.98	0.44
5:B:527:THR:OG1	5:B:528:PRO:HD2	2.18	0.44
5:B:840:ILE:CG2	5:B:994:TYR:HD1	2.30	0.44
5:B:952:VAL:HG12	5:B:953:LEU:N	2.33	0.44
5:B:995:ARG:HH12	6:C:165:LYS:HG2	1.82	0.44
5:B:1030:LEU:HD12	5:B:1030:LEU:HA	1.83	0.44
6:C:26:ASP:O	6:C:27:LEU:C	2.56	0.44
6:C:238:ILE:HD11	6:C:246:ARG:NH1	2.32	0.44
8:E:61:GLN:HG2	8:E:62:ALA:N	2.32	0.44
14:K:103:THR:O	14:K:105:PHE:N	2.50	0.44
4:A:108:MET:O	4:A:109:HIS:HB2	2.18	0.44
4:A:472:LEU:O	4:A:475:THR:CG2	2.65	0.44
4:A:648:ASN:O	4:A:649:ILE:C	2.55	0.44
4:A:784:LEU:HB3	4:A:785:PRO:HD2	1.98	0.44
4:A:1100:ARG:NH2	4:A:1351:GLU:CG	2.76	0.44
4:A:1130:GLN:HA	4:A:1133:LEU:HD12	2.00	0.44
4:A:1162:VAL:CG1	12:I:41:PRO:HG3	2.48	0.44
5:B:882:THR:HG21	5:B:935:ARG:HA	2.00	0.44
6:C:193:TYR:C	6:C:193:TYR:CD1	2.90	0.44
6:C:208:GLU:C	6:C:210:GLU:H	2.21	0.44
14:K:49:GLU:OE2	14:K:97:LYS:HE3	2.16	0.44
14:K:57:LEU:N	14:K:76:GLN:O	2.50	0.44
2:N:4:DG:H1'	2:N:5:DT:H5'	1.99	0.44
4:A:262:LEU:C	4:A:264:PHE:H	2.21	0.44
4:A:341:MET:CE	5:B:1135:ARG:NH1	2.80	0.44
4:A:412:ARG:NH2	5:B:1108:ARG:NH2	2.65	0.44
4:A:563:PRO:HG3	4:A:572:TRP:CE2	2.52	0.44
4:A:1068:ALA:HA	4:A:1367:HIS:ND1	2.32	0.44
4:A:1148:ILE:O	12:I:48:LEU:N	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1277:GLU:C	4:A:1279:ILE:H	2.20	0.44
5:B:519:TRP:CD1	5:B:519:TRP:C	2.91	0.44
5:B:615:MET:HA	5:B:625:LYS:O	2.18	0.44
5:B:810:GLU:HA	5:B:815:ARG:NH1	2.29	0.44
5:B:846:ILE:HG23	5:B:974:PRO:CG	2.46	0.44
6:C:61:GLU:HA	6:C:64:ALA:HB3	2.00	0.44
7:D:29:LEU:HD22	10:G:82:PHE:CE2	2.53	0.44
8:E:48:ASP:CG	8:E:49:SER:N	2.71	0.44
8:E:55:ARG:NH1	8:E:113:GLN:NE2	2.66	0.44
11:H:81:PRO:HB2	11:H:82:PRO:CD	2.44	0.44
13:J:36:LEU:HB2	13:J:47:ARG:NH1	2.33	0.44
14:K:24:ASP:OD1	14:K:26:LYS:N	2.51	0.44
14:K:68:PHE:HB3	14:K:70:ARG:NH1	2.32	0.44
4:A:464:PRO:HG2	4:A:465:TYR:CD1	2.51	0.44
4:A:1260:LEU:O	4:A:1260:LEU:CG	2.64	0.44
4:A:1450:LEU:O	4:A:1450:LEU:CG	2.65	0.44
5:B:36:ALA:HA	5:B:39:ARG:HD2	1.99	0.44
5:B:402:GLY:HA2	5:B:695:ALA:HB3	1.99	0.44
5:B:842:ASN:HB3	5:B:1009:ASP:HA	2.00	0.44
5:B:1216:LEU:C	5:B:1217:TYR:HD1	2.21	0.44
7:D:153:ARG:HG2	7:D:218:GLU:HG3	1.99	0.44
8:E:138:ALA:HA	8:E:141:VAL:HG23	2.00	0.44
10:G:48:VAL:HG13	10:G:74:TYR:HD1	1.82	0.44
12:I:78:CYS:O	12:I:80:SER:N	2.51	0.44
2:N:1:DC:H2"	2:N:2:DA:OP2	2.16	0.44
4:A:456:MET:HB3	4:A:507:VAL:HG22	2.00	0.44
4:A:1265:ASN:O	4:A:1267:MET:N	2.51	0.44
4:A:1385:THR:HG22	4:A:1386:ARG:H	1.82	0.44
5:B:23:ALA:HB1	5:B:24:PRO:CD	2.42	0.44
5:B:203:PHE:HB3	5:B:205:ILE:CD1	2.48	0.44
5:B:244:LEU:HD13	5:B:247:GLY:O	2.18	0.44
5:B:278:GLN:HG2	5:B:279:ASP:N	2.26	0.44
5:B:615:MET:C	5:B:616:ILE:HD12	2.36	0.44
5:B:661:LEU:C	5:B:663:ALA:H	2.20	0.44
5:B:745:PRO:C	5:B:747:MET:H	2.21	0.44
6:C:200:GLU:O	6:C:202:PRO:HD3	2.18	0.44
7:D:51:ASN:O	7:D:54:GLU:HB3	2.18	0.44
7:D:156:ASP:C	7:D:158:GLU:N	2.71	0.44
4:A:14:VAL:CG2	5:B:1216:LEU:HD12	2.46	0.44
4:A:56:PRO:O	4:A:57:ARG:CG	2.57	0.44
4:A:626:ASN:O	4:A:628:GLY:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:808:LEU:CD2	4:A:813:PHE:HA	2.45	0.44
4:A:834:THR:HG21	4:A:1077:THR:OG1	2.18	0.44
4:A:844:ALA:C	4:A:845:LEU:HD23	2.38	0.44
4:A:903:ASN:ND2	4:A:905:ASP:H	2.16	0.44
4:A:1105:LEU:HD22	4:A:1384:VAL:HG21	1.99	0.44
4:A:1118:VAL:CG2	4:A:1306:LEU:HB2	2.45	0.44
4:A:1191:TRP:CE3	4:A:1191:TRP:HA	2.53	0.44
4:A:1289:ARG:HD2	4:A:1303:GLU:OE2	2.18	0.44
5:B:525:ALA:O	5:B:768:THR:HA	2.17	0.44
7:D:50:LEU:HD13	7:D:55:ALA:CB	2.48	0.44
8:E:180:ARG:NH2	8:E:192:ARG:HD2	2.32	0.44
10:G:101:VAL:HG12	10:G:102:GLN:N	2.33	0.44
14:K:59:ALA:HA	14:K:74:ARG:O	2.17	0.44
14:K:78:THR:O	14:K:81:TYR:HB3	2.18	0.44
15:L:28:LYS:CB	15:L:39:SER:HA	2.47	0.44
4:A:23:SER:O	4:A:24:PRO:C	2.53	0.44
4:A:130:ASP:HB3	4:A:133:LYS:HB2	2.00	0.44
4:A:343:LYS:CE	5:B:1156:ASP:OD2	2.66	0.44
4:A:345:VAL:CG1	5:B:1130:PHE:HB2	2.48	0.44
4:A:845:LEU:HB3	4:A:848:ILE:HD12	2.00	0.44
4:A:1293:SER:OG	4:A:1295:THR:CG2	2.66	0.44
4:A:1313:LEU:HD23	4:A:1338:VAL:HB	2.00	0.44
5:B:37:PHE:HE1	5:B:41:LYS:HG3	1.78	0.44
5:B:123:THR:OG1	5:B:458:LYS:HE2	2.18	0.44
5:B:196:PRO:HG2	5:B:197:PHE:H	1.82	0.44
5:B:222:ILE:HG22	5:B:223:VAL:N	2.32	0.44
5:B:314:LEU:O	5:B:318:VAL:HG23	2.18	0.44
5:B:361:LEU:HD11	5:B:377:PHE:CE2	2.52	0.44
5:B:552:MET:C	5:B:554:ILE:H	2.22	0.44
5:B:981:ALA:HB3	5:B:1095:LEU:HD21	1.99	0.44
6:C:62:PHE:O	6:C:66:ARG:HG3	2.18	0.44
6:C:121:VAL:O	6:C:121:VAL:HG12	2.17	0.44
6:C:241:ASP:OD1	6:C:242:GLN:N	2.48	0.44
7:D:18:VAL:O	7:D:18:VAL:HG23	2.18	0.44
8:E:55:ARG:HB2	8:E:84:ASP:OD2	2.18	0.44
14:K:58:PHE:HB3	14:K:76:GLN:HE21	1.83	0.44
4:A:224:PHE:HD2	4:A:229:SER:O	2.00	0.43
4:A:418:SER:O	4:A:420:ARG:N	2.51	0.43
4:A:576:GLN:HG3	11:H:119:GLY:HA3	2.00	0.43
4:A:836:TYR:CZ	4:A:840:ARG:HD2	2.53	0.43
4:A:1339:LEU:HD13	8:E:147:HIS:CD2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1429:ILE:O	5:B:1197:PRO:HG3	2.18	0.43
5:B:1147:LEU:CD2	5:B:1151:LEU:HD22	2.48	0.43
4:A:427:GLN:HB2	4:A:430:TRP:CE2	2.53	0.43
4:A:504:LEU:HD11	9:F:91:ALA:CB	2.48	0.43
4:A:552:TRP:HE1	14:K:62:LYS:HB3	1.83	0.43
4:A:666:ILE:N	5:B:1026:LEU:HD13	2.33	0.43
4:A:768:GLN:NE2	4:A:816:HIS:HD1	2.16	0.43
4:A:996:ASN:O	4:A:998:LEU:HD12	2.17	0.43
4:A:1434:ALA:O	4:A:1436:ILE:N	2.50	0.43
4:A:1444:MET:O	9:F:133:VAL:N	2.51	0.43
5:B:840:ILE:HD13	5:B:994:TYR:HE1	1.83	0.43
5:B:1072:MET:HE3	5:B:1085:ILE:HD13	1.99	0.43
5:B:1110:PRO:HG2	5:B:1119:VAL:HG22	2.00	0.43
8:E:207:ARG:CB	8:E:207:ARG:NH1	2.81	0.43
11:H:116:TYR:O	11:H:122:LEU:HA	2.17	0.43
12:I:8:ARG:HB2	12:I:9:ASP:OD1	2.18	0.43
14:K:87:LEU:O	14:K:88:LYS:C	2.56	0.43
15:L:49:LYS:O	15:L:50:ASP:HB3	2.17	0.43
4:A:270:LEU:HD12	4:A:270:LEU:O	2.18	0.43
4:A:396:PRO:HG3	4:A:416:ARG:HB3	1.99	0.43
4:A:412:ARG:HH22	5:B:1108:ARG:NH2	2.16	0.43
4:A:427:GLN:O	4:A:428:TYR:C	2.56	0.43
4:A:490:HIS:HB3	5:B:1150:ARG:NH1	2.32	0.43
4:A:886:ILE:HG13	4:A:943:LEU:HD12	1.99	0.43
4:A:1120:LEU:O	4:A:1323:ASP:HB2	2.18	0.43
5:B:38:PHE:HD1	5:B:811:TYR:CD2	2.36	0.43
5:B:166:PHE:C	5:B:167:ILE:HG13	2.39	0.43
5:B:333:PHE:O	5:B:334:ILE:CG1	2.66	0.43
5:B:558:LEU:O	5:B:560:GLU:N	2.50	0.43
5:B:681:TRP:HA	5:B:684:LEU:HD13	2.00	0.43
5:B:806:THR:C	5:B:808:ALA:N	2.69	0.43
6:C:114:TYR:HB2	6:C:116:LYS:HG2	2.01	0.43
7:D:134:THR:CG2	7:D:135:GLY:H	2.29	0.43
7:D:139:LYS:HE2	7:D:139:LYS:HB2	1.88	0.43
8:E:81:GLU:HG2	8:E:82:PHE:N	2.33	0.43
8:E:102:GLU:O	8:E:104:ASN:N	2.51	0.43
9:F:79:ARG:NH2	9:F:150:GLU:OE1	2.39	0.43
10:G:21:ARG:HD3	10:G:21:ARG:HA	1.68	0.43
11:H:100:THR:HG22	11:H:101:ALA:H	1.81	0.43
4:A:54:ASN:HB3	4:A:247:ARG:NH1	2.31	0.43
4:A:108:MET:HB3	4:A:210:ILE:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:115:LEU:HB2	4:A:122:MET:CE	2.49	0.43
4:A:680:THR:HA	4:A:683:ILE:CD1	2.48	0.43
4:A:814:PHE:O	4:A:817:ALA:HB3	2.19	0.43
4:A:1227:ILE:CG2	4:A:1228:TRP:N	2.81	0.43
5:B:129:PHE:HE2	5:B:166:PHE:CD1	2.36	0.43
5:B:284:ILE:HD13	5:B:333:PHE:CD2	2.43	0.43
5:B:785:TYR:CD1	5:B:786:ASN:N	2.86	0.43
5:B:992:ILE:HD11	14:K:66:PRO:HB2	1.99	0.43
8:E:28:TYR:CD1	8:E:78:LEU:HD13	2.53	0.43
8:E:171:LYS:HD3	8:E:171:LYS:N	2.33	0.43
10:G:115:MET:HB2	10:G:116:PRO:CD	2.47	0.43
11:H:4:THR:HG22	11:H:5:LEU:N	2.33	0.43
11:H:95:TYR:HE2	11:H:97:MET:CG	2.31	0.43
14:K:65:HIS:CG	14:K:66:PRO:HD2	2.53	0.43
15:L:55:ILE:O	15:L:56:LEU:CB	2.64	0.43
1:T:12:DA:C2'	1:T:13:DC:H5'	2.49	0.43
4:A:78:PRO:HA	5:B:1201:LYS:NZ	2.33	0.43
4:A:548:ASN:OD1	14:K:60:ALA:HB1	2.18	0.43
4:A:1209:MET:HE1	4:A:1236:LEU:HB3	2.00	0.43
5:B:34:ILE:O	5:B:37:PHE:N	2.52	0.43
5:B:582:VAL:HG12	5:B:587:HIS:NE2	2.33	0.43
5:B:882:THR:O	5:B:883:LEU:CB	2.67	0.43
5:B:1147:LEU:HD23	5:B:1151:LEU:HD22	2.00	0.43
9:F:99:LEU:O	9:F:103:MET:HG2	2.19	0.43
1:T:12:DA:H2"	1:T:13:DC:H5'	2.00	0.43
4:A:68:GLN:C	4:A:70:CYS:N	2.68	0.43
4:A:709:THR:CG2	4:A:711:ARG:HB2	2.49	0.43
4:A:853:ASP:O	4:A:854:ASN:CB	2.62	0.43
4:A:963:ILE:HD13	4:A:1049:ILE:HG12	2.01	0.43
4:A:1042:PHE:CE2	4:A:1046:LEU:HD11	2.53	0.43
4:A:1114:PRO:HG2	4:A:1115:SER:H	1.82	0.43
4:A:1206:ASP:C	4:A:1274:ARG:NH1	2.71	0.43
5:B:280:ILE:HG21	5:B:285:ILE:HG13	2.00	0.43
5:B:393:LYS:HA	5:B:393:LYS:CE	2.45	0.43
5:B:520:GLY:CA	5:B:748:ILE:HG22	2.48	0.43
5:B:785:TYR:CD1	5:B:785:TYR:C	2.91	0.43
13:J:31:ASP:O	13:J:32:GLU:C	2.57	0.43
15:L:61:THR:HG22	15:L:62:LYS:N	2.33	0.43
4:A:29:ALA:HB1	5:B:1184:GLY:HA3	2.01	0.43
4:A:399:HIS:NE2	4:A:462:VAL:HG11	2.33	0.43
4:A:1394:THR:HG22	4:A:1395:GLY:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:37:PHE:HE2	5:B:542:MET:HA	1.84	0.43
5:B:97:VAL:HG12	5:B:178:ASN:ND2	2.32	0.43
5:B:1034:VAL:O	5:B:1036:ALA:N	2.51	0.43
5:B:1115:THR:HG22	5:B:1117:GLN:HG3	2.01	0.43
7:D:48:ILE:CG2	10:G:4:ILE:HB	2.39	0.43
4:A:116:ASP:C	4:A:118:HIS:N	2.70	0.43
4:A:415:LEU:HD23	4:A:415:LEU:HA	1.83	0.43
4:A:535:THR:HG21	4:A:616:VAL:CA	2.33	0.43
4:A:596:THR:C	4:A:598:LEU:H	2.22	0.43
4:A:600:PRO:C	4:A:602:ASP:N	2.72	0.43
4:A:1102:LYS:O	4:A:1106:ASN:ND2	2.51	0.43
4:A:1435:PRO:O	4:A:1436:ILE:HG13	2.19	0.43
5:B:259:TYR:HD1	5:B:259:TYR:H	1.67	0.43
5:B:308:TRP:N	5:B:308:TRP:CD1	2.85	0.43
5:B:826:ALA:HB2	5:B:1008:PRO:HB3	1.99	0.43
5:B:879:ARG:HA	5:B:879:ARG:HD3	1.81	0.43
6:C:107:SER:C	6:C:109:SER:N	2.72	0.43
8:E:28:TYR:CE1	8:E:78:LEU:CD1	3.02	0.43
8:E:177:ARG:O	8:E:212:ARG:CD	2.66	0.43
9:F:84:TYR:N	9:F:84:TYR:CD1	2.87	0.43
10:G:80:LYS:N	10:G:80:LYS:CD	2.78	0.43
10:G:110:VAL:HG22	10:G:161:GLY:O	2.19	0.43
11:H:10:PHE:N	11:H:10:PHE:CD1	2.87	0.43
4:A:47:ARG:HH12	4:A:254:GLU:CG	2.31	0.43
4:A:89:PRO:C	4:A:204:THR:HG21	2.39	0.43
4:A:91:PHE:HB2	4:A:297:GLN:HE22	1.84	0.43
4:A:106:VAL:CG1	4:A:112:LYS:N	2.82	0.43
4:A:466:SER:HB2	5:B:1099:VAL:CG1	2.49	0.43
4:A:475:THR:CG2	4:A:476:SER:N	2.67	0.43
4:A:709:THR:HB	4:A:712:GLU:H	1.84	0.43
4:A:850:VAL:HG21	4:A:1058:VAL:HG11	2.01	0.43
4:A:1017:LEU:HD12	4:A:1017:LEU:O	2.18	0.43
5:B:95:ILE:HG13	5:B:130:VAL:CG2	2.47	0.43
5:B:125:SER:CA	5:B:171:PRO:HA	2.42	0.43
5:B:761:HIS:HB2	5:B:1024:ALA:HB2	2.00	0.43
5:B:763:GLN:O	5:B:765:PRO:N	2.52	0.43
5:B:814:PHE:C	5:B:816:GLU:N	2.73	0.43
5:B:848:ARG:NH1	13:J:8:PHE:O	2.52	0.43
5:B:872:GLU:OE2	5:B:914:LYS:HE2	2.18	0.43
5:B:1187:ASN:O	5:B:1188:LYS:CB	2.66	0.43
5:B:1196:ILE:HD12	5:B:1200:ALA:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:22:LEU:HD13	6:C:230:MET:HE1	2.00	0.43
6:C:47:ASP:CA	15:L:69:ALA:CB	2.93	0.43
7:D:4:SER:C	7:D:5:THR:OG1	2.56	0.43
9:F:82:THR:HA	9:F:83:PRO:HD3	1.87	0.43
9:F:89:GLU:HB3	9:F:134:ILE:HD11	2.01	0.43
11:H:93:TYR:N	11:H:93:TYR:CD1	2.87	0.43
12:I:98:VAL:HG12	12:I:99:LEU:N	2.33	0.43
13:J:1:MET:H1	13:J:56:LEU:HB2	1.83	0.43
13:J:57:ILE:CA	13:J:60:PHE:HD2	2.24	0.43
4:A:12:ARG:NE	5:B:1192:TYR:HE2	2.17	0.43
4:A:1402:PHE:CD1	4:A:1403:GLU:HG3	2.54	0.43
4:A:1434:ALA:HA	4:A:1435:PRO:HD3	1.82	0.43
5:B:236:HIS:CE1	5:B:389:ALA:HA	2.54	0.43
5:B:508:LEU:O	5:B:509:ALA:HB2	2.19	0.43
5:B:542:MET:HB3	5:B:636:PRO:CD	2.48	0.43
5:B:918:ILE:HD12	5:B:935:ARG:HD3	2.01	0.43
6:C:16:ASP:C	6:C:17:ASN:ND2	2.71	0.43
6:C:65:HIS:O	6:C:69:LEU:HD13	2.19	0.43
9:F:77:ASP:C	9:F:79:ARG:N	2.72	0.43
15:L:46:VAL:CG1	15:L:56:LEU:HD12	2.48	0.43
4:A:61:ILE:O	4:A:63:ARG:N	2.52	0.42
4:A:340:LEU:HD21	5:B:1199:ALA:HB3	2.01	0.42
4:A:899:VAL:HG22	4:A:908:LEU:HD21	2.00	0.42
4:A:1006:ILE:HD11	8:E:163:GLU:HG3	2.00	0.42
4:A:1225:PHE:CE2	4:A:1227:ILE:HD11	2.53	0.42
5:B:56:ASP:HB2	5:B:57:TYR:HD1	1.84	0.42
5:B:100:PRO:HD2	5:B:180:TYR:HE1	1.81	0.42
5:B:522:VAL:HG12	5:B:523:CYS:N	2.34	0.42
5:B:603:LEU:HB3	5:B:609:ILE:HG13	2.01	0.42
5:B:840:ILE:HG21	5:B:994:TYR:HD1	1.84	0.42
5:B:1081:LEU:O	5:B:1082:MET:C	2.57	0.42
6:C:191:TYR:HD2	6:C:201:TRP:CD1	2.37	0.42
8:E:60:PHE:C	8:E:60:PHE:CD2	2.91	0.42
11:H:127:GLY:HA3	11:H:130:ARG:HH22	1.83	0.42
15:L:46:VAL:HG13	15:L:56:LEU:HD12	1.99	0.42
4:A:110:CYS:HB3	4:A:167:CYS:SG	2.59	0.42
4:A:557:ASP:O	4:A:559:VAL:HG23	2.19	0.42
4:A:830:LYS:HG2	4:A:1098:VAL:HG21	2.01	0.42
4:A:843:LYS:HD3	4:A:843:LYS:HA	1.75	0.42
4:A:964:ILE:O	4:A:967:ALA:HB3	2.19	0.42
4:A:1010:ALA:O	4:A:1013:ASP:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1191:TRP:HD1	4:A:1256:GLU:HB2	1.83	0.42
4:A:1261:LYS:HA	4:A:1264:GLU:HB3	2.00	0.42
5:B:189:LEU:O	5:B:192:LEU:HB2	2.19	0.42
5:B:496:ARG:NH1	5:B:539:LEU:HB2	2.33	0.42
5:B:542:MET:CG	5:B:747:MET:HB3	2.46	0.42
5:B:549:THR:HG22	5:B:550:ASP:N	2.23	0.42
5:B:1084:GLN:OE1	6:C:189:THR:HG22	2.18	0.42
5:B:1107:ALA:O	5:B:1108:ARG:O	2.36	0.42
5:B:1162:ILE:HG22	5:B:1163:CYS:N	2.33	0.42
6:C:213:PRO:O	6:C:214:ASN:CB	2.65	0.42
7:D:192:LYS:HE3	7:D:204:ASP:OD1	2.19	0.42
8:E:147:HIS:CD2	8:E:149:LEU:H	2.36	0.42
12:I:13:MET:O	12:I:14:LEU:HD23	2.19	0.42
14:K:8:GLU:O	14:K:37:LYS:HD2	2.20	0.42
4:A:215:SER:HB3	4:A:218:ASP:OD2	2.19	0.42
4:A:391:LEU:O	4:A:394:ASN:HB2	2.20	0.42
4:A:806:ARG:HD3	5:B:728:ARG:HA	2.01	0.42
4:A:914:GLU:HB2	4:A:979:SER:O	2.18	0.42
4:A:932:GLU:O	4:A:935:GLN:HB3	2.20	0.42
4:A:1074:GLU:H	4:A:1075:PRO:HD2	1.82	0.42
4:A:1111:MET:HE2	4:A:1330:ASN:OD1	2.19	0.42
4:A:1214:GLU:OE1	4:A:1214:GLU:HA	2.19	0.42
5:B:100:PRO:HD3	5:B:172:ILE:HD12	2.00	0.42
5:B:129:PHE:HE2	5:B:166:PHE:HD1	1.67	0.42
5:B:240:ILE:CD1	5:B:377:PHE:HE2	2.32	0.42
5:B:860:MET:HG2	5:B:861:ASP:H	1.84	0.42
5:B:1202:LEU:HD22	5:B:1206:GLU:CD	2.40	0.42
6:C:138:GLU:OE1	6:C:138:GLU:N	2.48	0.42
7:D:63:LEU:O	7:D:129:LEU:HD11	2.20	0.42
4:A:452:LYS:HE3	5:B:1141:HIS:ND1	2.34	0.42
4:A:573:SER:O	4:A:574:GLY:C	2.57	0.42
4:A:1107:VAL:HG12	4:A:1107:VAL:O	2.19	0.42
5:B:37:PHE:CD1	5:B:37:PHE:C	2.92	0.42
5:B:822:ASN:O	13:J:48:ARG:NH1	2.52	0.42
5:B:848:ARG:HD2	13:J:7:CYS:O	2.19	0.42
6:C:66:ARG:NH2	13:J:5:VAL:CG2	2.81	0.42
7:D:122:GLU:HA	7:D:125:SER:OG	2.19	0.42
8:E:164:LEU:HD21	8:E:211:TYR:CG	2.54	0.42
10:G:79:PHE:HZ	10:G:106:MET:CE	2.33	0.42
11:H:145:ARG:O	11:H:146:ARG:HB2	2.19	0.42
12:I:56:ALA:O	12:I:57:GLY:O	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:I:74:GLU:HA	12:I:80:SER:O	2.19	0.42
13:J:63:TYR:O	13:J:64:ASN:HB2	2.18	0.42
1:T:24:DT:OP1	5:B:857:ARG:NH2	2.52	0.42
4:A:47:ARG:HH12	4:A:254:GLU:HG2	1.84	0.42
4:A:302:THR:CG2	4:A:303:TYR:N	2.81	0.42
4:A:344:ARG:NE	5:B:1120:GLU:HB2	2.35	0.42
4:A:899:VAL:CG2	4:A:1029:ARG:HG2	2.49	0.42
4:A:961:ARG:O	4:A:965:GLN:HG3	2.18	0.42
5:B:180:TYR:CD1	5:B:180:TYR:N	2.86	0.42
5:B:199:MET:SD	5:B:199:MET:N	2.76	0.42
5:B:424:LEU:HD22	5:B:453:ILE:HD11	2.00	0.42
5:B:742:GLU:O	5:B:743:ILE:C	2.58	0.42
6:C:160:LYS:O	6:C:161:LYS:O	2.37	0.42
7:D:47:LEU:CD1	10:G:3:PHE:CD2	3.02	0.42
8:E:16:PHE:HZ	8:E:20:LYS:HE2	1.74	0.42
9:F:72:LYS:O	9:F:73:ALA:CB	2.67	0.42
11:H:55:LEU:HD22	11:H:144:ILE:HG21	1.98	0.42
11:H:81:PRO:HB3	11:H:82:PRO:HD2	1.99	0.42
14:K:18:LYS:NZ	14:K:38:GLU:HG2	2.34	0.42
14:K:63:VAL:O	14:K:63:VAL:CG2	2.63	0.42
14:K:109:TRP:O	14:K:112:GLN:HB2	2.19	0.42
2:N:5:DT:H6	2:N:5:DT:H2'	1.53	0.42
4:A:84:ILE:HD11	4:A:270:LEU:HD13	2.02	0.42
4:A:241:VAL:HA	4:A:242:PRO:HD2	1.83	0.42
4:A:534:LEU:O	4:A:534:LEU:HG	2.19	0.42
4:A:574:GLY:O	4:A:575:LYS:C	2.58	0.42
4:A:577:ILE:O	4:A:578:LEU:C	2.55	0.42
4:A:664:THR:CG2	4:A:665:GLY:N	2.83	0.42
4:A:857:ARG:CZ	9:F:139:PRO:HG3	2.49	0.42
4:A:1036:ARG:HG2	4:A:1036:ARG:HH11	1.85	0.42
4:A:1444:MET:HB2	4:A:1444:MET:HE3	1.86	0.42
5:B:112:LEU:HD21	5:B:117:ALA:HB2	2.02	0.42
5:B:121:ASN:HD22	5:B:207:GLY:HA3	1.84	0.42
5:B:197:PHE:HZ	5:B:816:GLU:HG2	1.85	0.42
5:B:498:THR:HB	5:B:537:LYS:O	2.20	0.42
5:B:763:GLN:O	5:B:764:SER:C	2.58	0.42
5:B:776:GLN:O	5:B:1095:LEU:HA	2.19	0.42
5:B:806:THR:O	5:B:809:MET:HG3	2.19	0.42
5:B:831:SER:HB3	5:B:994:TYR:OH	2.20	0.42
5:B:1110:PRO:O	5:B:1119:VAL:HG13	2.20	0.42
6:C:133:ILE:CD1	6:C:237:SER:CA	2.94	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:161:GLY:O	7:D:165:GLN:HG3	2.20	0.42
8:E:124:VAL:HG13	8:E:132:ILE:CD1	2.50	0.42
10:G:99:PHE:CZ	10:G:143:ILE:HD13	2.54	0.42
12:I:4:PHE:C	12:I:4:PHE:HD1	2.22	0.42
13:J:41:LEU:N	13:J:41:LEU:HD23	2.34	0.42
15:L:34:CYS:O	15:L:36:SER:N	2.53	0.42
2:N:3:DA:H1'	2:N:4:DG:C8	2.55	0.42
4:A:207:ILE:O	4:A:211:PHE:HD1	2.02	0.42
4:A:793:SER:HB2	4:A:794:PRO:HD2	2.01	0.42
4:A:872:GLY:O	4:A:1058:VAL:HG23	2.20	0.42
4:A:1197:LEU:HD11	4:A:1238:ILE:HD11	2.01	0.42
5:B:661:LEU:C	5:B:663:ALA:N	2.73	0.42
6:C:235:VAL:HG21	13:J:6:ARG:NH2	2.35	0.42
6:C:259:LEU:HD12	6:C:259:LEU:HA	1.93	0.42
7:D:47:LEU:CD1	7:D:48:ILE:N	2.81	0.42
8:E:136:ASN:OD1	8:E:138:ALA:N	2.53	0.42
14:K:43:GLY:HA2	14:K:71:PHE:CZ	2.55	0.42
4:A:33:ALA:O	4:A:83:HIS:HD2	2.02	0.42
4:A:341:MET:HE1	5:B:1135:ARG:NH1	2.34	0.42
4:A:683:ILE:HD13	4:A:801:GLU:HG3	2.02	0.42
4:A:901:LEU:HD13	4:A:919:ILE:HG23	2.02	0.42
4:A:1120:LEU:HD23	4:A:1124:HIS:O	2.19	0.42
4:A:1364:ASN:C	4:A:1364:ASN:ND2	2.73	0.42
5:B:468:GLU:HB3	5:B:469:GLN:H	1.70	0.42
5:B:469:GLN:HB2	5:B:470:LYS:H	1.52	0.42
5:B:563:MET:HE2	5:B:587:HIS:O	2.19	0.42
5:B:579:ARG:HD2	5:B:586:TRP:CZ2	2.55	0.42
5:B:889:THR:HG22	5:B:891:ASP:H	1.84	0.42
6:C:44:LEU:HD21	6:C:159:ALA:CB	2.50	0.42
6:C:80:LEU:HD11	6:C:95:CYS:C	2.40	0.42
6:C:104:PHE:HD2	6:C:105:GLY:H	1.67	0.42
9:F:72:LYS:O	9:F:73:ALA:HB3	2.20	0.42
12:I:13:MET:HE2	12:I:14:LEU:H	1.84	0.42
13:J:47:ARG:NH1	13:J:47:ARG:HG2	2.31	0.42
14:K:65:HIS:HD2	14:K:67:PHE:HB2	1.84	0.42
14:K:83:PRO:O	14:K:84:LYS:C	2.58	0.42
4:A:399:HIS:CG	4:A:400:PRO:N	2.87	0.42
4:A:434:ARG:HE	4:A:437:MET:HG3	1.85	0.42
4:A:525:GLN:HG3	5:B:836:GLU:HG2	2.02	0.42
4:A:883:LEU:CD2	4:A:1021:LEU:HB2	2.50	0.42
4:A:1007:ILE:C	4:A:1009:ASN:H	2.24	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1173:HIS:C	4:A:1174:PHE:CD1	2.93	0.42
5:B:169:ARG:HB2	5:B:454:THR:CG2	2.33	0.42
5:B:234:ILE:HG21	5:B:237:VAL:CG2	2.50	0.42
5:B:903:VAL:CG1	5:B:904:ARG:N	2.83	0.42
5:B:1216:LEU:O	5:B:1217:TYR:HD1	2.01	0.42
6:C:56:THR:HG22	6:C:58:LEU:HD23	2.01	0.42
6:C:80:LEU:HD11	6:C:95:CYS:CA	2.49	0.42
6:C:112:ASN:CB	6:C:114:TYR:CE1	3.02	0.42
6:C:248:ILE:HG13	6:C:248:ILE:H	1.65	0.42
9:F:97:ARG:HA	9:F:97:ARG:HD2	1.79	0.42
11:H:33:GLN:C	11:H:35:GLN:H	2.22	0.42
11:H:113:ALA:HB1	11:H:125:LEU:O	2.20	0.42
12:I:2:THR:O	12:I:2:THR:HG22	2.20	0.42
13:J:3:VAL:CG2	13:J:18:TRP:CG	3.01	0.42
4:A:91:PHE:HB3	4:A:96:ILE:HG12	2.02	0.42
4:A:407:ARG:HB3	4:A:430:TRP:NE1	2.34	0.42
4:A:418:SER:C	4:A:420:ARG:N	2.72	0.42
4:A:433:GLU:OE1	5:B:1108:ARG:NH1	2.53	0.42
4:A:600:PRO:O	4:A:602:ASP:N	2.52	0.42
4:A:1120:LEU:O	4:A:1323:ASP:N	2.52	0.42
4:A:1346:ALA:CB	8:E:149:LEU:HD13	2.50	0.42
5:B:376:PHE:HE2	5:B:569:TYR:HD2	1.68	0.42
5:B:956:THR:HG22	5:B:957:ASN:N	2.35	0.42
7:D:195:ILE:HG22	7:D:195:ILE:O	2.20	0.42
8:E:22:MET:HB2	8:E:187:TYR:CE1	2.55	0.42
12:I:59:VAL:C	12:I:61:ASP:N	2.73	0.42
12:I:92:ARG:HB3	12:I:95:THR:OG1	2.19	0.42
4:A:49:LYS:HZ2	4:A:60:SER:HA	1.84	0.41
4:A:249:SER:O	4:A:250:ILE:CG1	2.60	0.41
4:A:353:ILE:HG21	4:A:487:MET:HG3	2.01	0.41
4:A:463:ILE:HB	4:A:464:PRO:HD2	2.01	0.41
4:A:590:ARG:HD2	4:A:605:MET:CB	2.50	0.41
4:A:639:PRO:HG2	4:A:640:GLN:H	1.84	0.41
4:A:1127:ASP:O	4:A:1130:GLN:HB3	2.20	0.41
4:A:1385:THR:C	4:A:1387:HIS:N	2.72	0.41
5:B:39:ARG:NH2	5:B:665:GLU:CG	2.83	0.41
5:B:581:PHE:HA	5:B:585:VAL:O	2.19	0.41
5:B:603:LEU:HD22	5:B:603:LEU:HA	1.87	0.41
5:B:1177:HIS:C	5:B:1179:GLN:H	2.24	0.41
6:C:187:LYS:HG3	6:C:219:PHE:CE1	2.54	0.41
7:D:16:LYS:O	7:D:16:LYS:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:79:ARG:HG3	9:F:144:GLU:OE1	2.19	0.41
12:I:50:THR:HG22	12:I:51:ASN:N	2.35	0.41
14:K:6:ARG:HD3	14:K:6:ARG:HA	1.94	0.41
14:K:68:PHE:N	14:K:68:PHE:CD2	2.85	0.41
4:A:59:GLY:HA2	4:A:67:CYS:SG	2.61	0.41
4:A:606:LEU:O	4:A:613:ILE:HB	2.20	0.41
4:A:715:GLU:O	4:A:717:ASN:N	2.53	0.41
4:A:730:GLY:C	4:A:732:LEU:N	2.73	0.41
4:A:886:ILE:CD1	4:A:943:LEU:HB3	2.42	0.41
5:B:286:PHE:O	5:B:289:LEU:HB2	2.20	0.41
5:B:331:LEU:HD12	5:B:331:LEU:N	2.35	0.41
5:B:412:LEU:HB3	5:B:466:TRP:HZ2	1.85	0.41
5:B:558:LEU:C	5:B:560:GLU:N	2.74	0.41
5:B:807:ARG:HG2	5:B:1045:SER:HG	1.83	0.41
5:B:1202:LEU:O	5:B:1203:LEU:C	2.57	0.41
6:C:236:GLY:C	6:C:238:ILE:N	2.71	0.41
8:E:192:ARG:HG3	8:E:192:ARG:NH1	2.34	0.41
9:F:147:SER:OG	9:F:150:GLU:HG3	2.20	0.41
4:A:106:VAL:HA	4:A:114:LEU:HD21	2.03	0.41
4:A:208:LEU:HD23	4:A:208:LEU:C	2.40	0.41
4:A:635:ARG:HH11	4:A:635:ARG:HA	1.85	0.41
4:A:836:TYR:OH	4:A:1403:GLU:OE2	2.35	0.41
4:A:858:ASN:ND2	4:A:860:LEU:N	2.59	0.41
4:A:867:ILE:CG2	4:A:872:GLY:N	2.84	0.41
4:A:996:ASN:HA	4:A:998:LEU:HD12	2.02	0.41
4:A:1138:ILE:CG2	4:A:1316:VAL:HG13	2.51	0.41
4:A:1283:VAL:CG1	4:A:1284:MET:N	2.77	0.41
4:A:1409:LEU:HD23	4:A:1409:LEU:HA	1.92	0.41
5:B:298:LEU:N	5:B:298:LEU:CD2	2.83	0.41
5:B:542:MET:HE1	5:B:743:ILE:HG21	2.01	0.41
5:B:1097:HIS:H	5:B:1098:MET:CE	2.31	0.41
5:B:1119:VAL:HG23	5:B:1126:GLY:HA2	2.02	0.41
5:B:1169:MET:CE	5:B:1204:PHE:HB2	2.50	0.41
6:C:58:LEU:CD2	6:C:58:LEU:N	2.83	0.41
6:C:104:PHE:HD2	6:C:105:GLY:N	2.19	0.41
8:E:62:ALA:HB3	8:E:78:LEU:HD22	2.01	0.41
8:E:117:THR:O	8:E:120:ALA:HB3	2.20	0.41
10:G:79:PHE:CE2	10:G:105:PRO:HG2	2.53	0.41
10:G:96:GLN:HB3	10:G:121:PHE:CE2	2.55	0.41
10:G:111:THR:HB	10:G:114:LEU:HB2	2.01	0.41
11:H:42:ILE:CG2	11:H:43:ASN:N	2.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:L:28:LYS:HB2	15:L:39:SER:HB2	2.02	0.41
15:L:40:LEU:HD23	15:L:40:LEU:HA	1.91	0.41
4:A:6:TYR:CD1	4:A:7:SER:N	2.88	0.41
4:A:516:SER:O	4:A:517:ASN:C	2.58	0.41
4:A:567:LYS:CD	11:H:95:TYR:HA	2.50	0.41
4:A:711:ARG:HH11	12:I:95:THR:HB	1.85	0.41
4:A:775:ILE:HG21	4:A:783:THR:HG23	2.02	0.41
4:A:986:ILE:O	4:A:990:VAL:HG23	2.19	0.41
4:A:996:ASN:HB3	4:A:1050:GLU:OE2	2.20	0.41
4:A:1007:ILE:C	4:A:1009:ASN:N	2.73	0.41
5:B:172:ILE:HG22	5:B:173:MET:H	1.84	0.41
5:B:405:ARG:NH2	5:B:632:ARG:HD3	2.35	0.41
5:B:604:ARG:O	5:B:607:GLY:N	2.54	0.41
5:B:801:LYS:O	13:J:52:THR:CG2	2.60	0.41
5:B:824:ILE:HG12	13:J:48:ARG:NH1	2.36	0.41
5:B:1147:LEU:O	5:B:1148:LYS:C	2.57	0.41
5:B:1182:CYS:C	5:B:1183:LYS:HE3	2.41	0.41
6:C:145:CYS:HA	13:J:2:ILE:CD1	2.43	0.41
6:C:242:GLN:C	6:C:244:VAL:H	2.24	0.41
6:C:243:VAL:O	6:C:243:VAL:HG12	2.20	0.41
9:F:88:TYR:CD1	9:F:88:TYR:N	2.88	0.41
10:G:26:LEU:O	10:G:27:LYS:C	2.59	0.41
15:L:65:VAL:O	15:L:65:VAL:HG23	2.21	0.41
4:A:53:LEU:O	4:A:54:ASN:C	2.59	0.41
4:A:54:ASN:HA	4:A:58:LEU:HD12	2.03	0.41
4:A:472:LEU:O	4:A:475:THR:CB	2.69	0.41
4:A:683:ILE:O	4:A:686:ALA:N	2.53	0.41
4:A:1362:TYR:HD1	4:A:1363:VAL:N	2.18	0.41
5:B:211:VAL:HG23	5:B:483:LEU:HB2	2.02	0.41
5:B:218:SER:O	5:B:219:ALA:O	2.38	0.41
5:B:401:PHE:HD2	5:B:521:LEU:HD12	1.85	0.41
5:B:605:ARG:NH1	5:B:639:ILE:HD13	2.35	0.41
5:B:618:ASP:OD1	5:B:621:GLU:HB3	2.20	0.41
5:B:726:ALA:O	5:B:727:LYS:O	2.39	0.41
5:B:865:LYS:NZ	5:B:869:SER:HA	2.35	0.41
5:B:1084:GLN:CD	5:B:1084:GLN:N	2.74	0.41
6:C:17:ASN:N	6:C:240:VAL:HG11	2.35	0.41
6:C:100:THR:CG2	6:C:101:LEU:N	2.83	0.41
6:C:131:HIS:HA	6:C:132:PRO:HD3	1.93	0.41
6:C:175:ALA:HB2	13:J:10:CYS:HB2	2.03	0.41
6:C:229:TYR:N	6:C:229:TYR:CD1	2.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:24:LYS:HB2	8:E:24:LYS:HE3	1.77	0.41
10:G:15:PRO:O	10:G:16:SER:C	2.59	0.41
10:G:126:ASN:HD22	10:G:126:ASN:HA	1.54	0.41
10:G:145:VAL:CG1	10:G:146:LYS:H	2.32	0.41
11:H:100:THR:HG1	11:H:138:GLU:HG3	1.84	0.41
14:K:31:VAL:O	14:K:74:ARG:HA	2.21	0.41
15:L:55:ILE:HG12	15:L:55:ILE:H	1.41	0.41
4:A:42:ASP:HB3	4:A:45:GLN:CA	2.51	0.41
4:A:224:PHE:CD2	4:A:231:PRO:HG3	2.56	0.41
4:A:438:ASP:OD1	4:A:462:VAL:HG23	2.21	0.41
4:A:971:PHE:CD1	4:A:971:PHE:N	2.88	0.41
4:A:973:ILE:HD11	4:A:1038:THR:HG23	2.03	0.41
4:A:1138:ILE:HG21	4:A:1316:VAL:HG13	2.03	0.41
4:A:1212:VAL:O	4:A:1216:ILE:HG13	2.19	0.41
5:B:34:ILE:O	5:B:35:SER:C	2.59	0.41
5:B:616:ILE:HG13	5:B:697:GLU:HA	2.02	0.41
5:B:770:GLN:HG2	5:B:983:ARG:O	2.20	0.41
5:B:843:GLN:N	5:B:994:TYR:O	2.37	0.41
5:B:862:GLN:HG2	5:B:963:PHE:CD1	2.42	0.41
6:C:242:GLN:C	6:C:244:VAL:N	2.72	0.41
6:C:254:LYS:HE2	6:C:254:LYS:HB3	1.89	0.41
10:G:14:HIS:HD2	10:G:16:SER:CB	2.33	0.41
14:K:5:ASP:O	14:K:6:ARG:C	2.58	0.41
1:T:15:DT:H73	16:T:67:CPT:N1	2.35	0.41
1:T:19:DC:H2"	1:T:20:DC:H5'	2.02	0.41
4:A:52:GLY:O	4:A:56:PRO:HG2	2.21	0.41
4:A:53:LEU:CD2	4:A:54:ASN:N	2.64	0.41
4:A:243:PRO:CB	4:A:244:PRO:HD2	2.50	0.41
4:A:298:PHE:O	4:A:299:HIS:C	2.59	0.41
4:A:302:THR:HG22	4:A:303:TYR:N	2.35	0.41
4:A:404:TYR:CD2	4:A:414:ASP:HA	2.56	0.41
4:A:845:LEU:O	4:A:846:GLU:C	2.59	0.41
4:A:1127:ASP:HB3	4:A:1130:GLN:HB2	1.95	0.41
4:A:1315:GLU:C	4:A:1317:MET:N	2.73	0.41
4:A:1365:TYR:O	4:A:1367:HIS:N	2.54	0.41
4:A:1385:THR:C	4:A:1387:HIS:H	2.23	0.41
5:B:313:MET:O	5:B:316:PRO:HG2	2.20	0.41
5:B:383:ASN:O	5:B:384:ARG:C	2.58	0.41
5:B:466:TRP:CE3	5:B:466:TRP:HA	2.54	0.41
6:C:167:HIS:HD2	6:C:168:ALA:H	1.69	0.41
8:E:124:VAL:CG1	8:E:132:ILE:HB	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:163:GLU:O	8:E:164:LEU:C	2.58	0.41
15:L:43:THR:C	15:L:45:ALA:H	2.22	0.41
4:A:224:PHE:CD2	4:A:231:PRO:HD3	2.56	0.41
4:A:316:GLN:HB2	4:A:322:VAL:HG23	2.02	0.41
4:A:360:GLU:O	4:A:361:LEU:C	2.57	0.41
4:A:361:LEU:CD1	4:A:474:VAL:HB	2.51	0.41
4:A:860:LEU:CB	4:A:862:ASN:OD1	2.69	0.41
4:A:1273:LEU:N	4:A:1273:LEU:CD1	2.83	0.41
4:A:1364:ASN:O	4:A:1366:ARG:HG3	2.21	0.41
4:A:1405:THR:HB	4:A:1406:VAL:H	1.58	0.41
4:A:1409:LEU:O	4:A:1412:ALA:HB3	2.20	0.41
4:A:1423:GLY:O	4:A:1424:VAL:C	2.59	0.41
5:B:172:ILE:CG2	5:B:173:MET:H	2.34	0.41
5:B:1079:LYS:N	6:C:27:LEU:HD21	2.36	0.41
6:C:179:GLU:CG	6:C:180:TYR:H	2.28	0.41
7:D:138:ASN:C	7:D:140:ASP:N	2.74	0.41
7:D:173:HIS:NE2	7:D:201:LYS:NZ	2.69	0.41
10:G:1:MET:HG2	10:G:85:GLU:CD	2.41	0.41
14:K:55:LYS:CB	14:K:81:TYR:CE1	3.04	0.41
4:A:42:ASP:HB3	4:A:45:GLN:N	2.33	0.41
4:A:43:GLU:O	4:A:44:THR:CB	2.68	0.41
4:A:58:LEU:HD13	4:A:243:PRO:HA	2.02	0.41
4:A:71:GLN:O	4:A:73:GLY:N	2.50	0.41
4:A:252:PHE:HB2	4:A:256:GLN:CD	2.40	0.41
4:A:322:VAL:O	4:A:322:VAL:HG12	2.21	0.41
4:A:512:VAL:O	4:A:512:VAL:HG12	2.21	0.41
4:A:567:LYS:CB	4:A:568:PRO:HD2	2.50	0.41
4:A:818:MET:HA	5:B:514:LEU:HB3	2.02	0.41
4:A:838:GLN:O	4:A:842:VAL:HG23	2.21	0.41
4:A:935:GLN:O	4:A:938:LYS:N	2.54	0.41
4:A:1072:ILE:O	4:A:1075:PRO:HG2	2.21	0.41
4:A:1348:LEU:HG	4:A:1372:VAL:HG23	2.01	0.41
5:B:26:THR:O	5:B:29:ASP:HB2	2.21	0.41
5:B:255:GLN:HB2	5:B:272:THR:HB	2.01	0.41
5:B:334:ILE:HG22	5:B:334:ILE:O	2.21	0.41
5:B:431:TYR:CD2	5:B:447:ALA:HB2	2.56	0.41
5:B:526:GLU:CG	5:B:538:ASN:HD22	2.31	0.41
5:B:729:ILE:O	5:B:729:ILE:HG22	2.21	0.41
5:B:830:TYR:O	5:B:831:SER:C	2.59	0.41
5:B:979:LYS:HG2	5:B:1095:LEU:CD1	2.50	0.41
5:B:1002:THR:O	5:B:1003:ALA:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1106:ARG:HG3	5:B:1107:ALA:N	2.35	0.41
6:C:69:LEU:HD12	6:C:69:LEU:H	1.85	0.41
7:D:53:SER:H	7:D:148:LEU:CD2	2.34	0.41
7:D:192:LYS:HZ2	7:D:192:LYS:HB3	1.85	0.41
8:E:102:GLU:C	8:E:104:ASN:N	2.71	0.41
8:E:124:VAL:N	8:E:125:PRO:HD2	2.35	0.41
8:E:157:SER:C	8:E:159:ASP:H	2.23	0.41
10:G:154:VAL:HG12	10:G:155:SER:N	2.36	0.41
11:H:118:PHE:O	11:H:120:GLY:N	2.53	0.41
11:H:143:LEU:HD12	11:H:143:LEU:N	2.36	0.41
12:I:62:ILE:O	12:I:62:ILE:CG1	2.66	0.41
12:I:85:PHE:HD1	12:I:99:LEU:HD13	1.83	0.41
14:K:68:PHE:HB3	14:K:70:ARG:HH11	1.84	0.41
4:A:388:LEU:HD22	4:A:432:VAL:HB	2.02	0.41
4:A:412:ARG:NH2	5:B:1108:ARG:NH1	2.69	0.41
4:A:666:ILE:HD11	5:B:1086:PHE:HE1	1.86	0.41
4:A:860:LEU:HB3	4:A:862:ASN:OD1	2.21	0.41
4:A:971:PHE:O	4:A:972:HIS:C	2.59	0.41
4:A:1119:TYR:O	4:A:1120:LEU:O	2.39	0.41
4:A:1347:ALA:O	4:A:1348:LEU:C	2.59	0.41
4:A:1443:VAL:C	4:A:1444:MET:HG3	2.40	0.41
5:B:170:LEU:HA	5:B:171:PRO:HD2	1.89	0.41
5:B:212:LEU:HD13	5:B:409:ALA:HA	2.03	0.41
5:B:329:THR:O	5:B:332:ASP:HB3	2.20	0.41
5:B:465:ASN:ND2	5:B:477:ALA:HB2	2.35	0.41
5:B:615:MET:O	5:B:697:GLU:HG3	2.20	0.41
5:B:777:ALA:HA	5:B:1095:LEU:HA	2.02	0.41
5:B:806:THR:HG21	5:B:808:ALA:HB3	2.02	0.41
5:B:878:GLN:O	5:B:879:ARG:C	2.58	0.41
5:B:895:ASP:C	5:B:897:GLY:H	2.24	0.41
5:B:977:GLY:HA3	5:B:1099:VAL:CG2	2.50	0.41
8:E:55:ARG:O	8:E:57:MET:N	2.53	0.41
10:G:22:MET:C	10:G:24:GLN:N	2.74	0.41
10:G:99:PHE:CD1	10:G:99:PHE:C	2.95	0.41
12:I:54:GLU:OE2	12:I:118:ARG:CZ	2.69	0.41
1:T:11:DT:H1'	1:T:12:DA:H5'	2.02	0.40
4:A:335:ARG:O	4:A:336:ILE:C	2.60	0.40
4:A:522:GLY:HA2	4:A:630:ILE:CD1	2.51	0.40
4:A:901:LEU:HD22	4:A:919:ILE:HG22	2.03	0.40
4:A:1242:VAL:O	4:A:1243:VAL:HB	2.21	0.40
5:B:174:LEU:HD22	5:B:202:TYR:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:174:LEU:HD21	5:B:204:ILE:HD11	2.03	0.40
5:B:258:LEU:O	5:B:258:LEU:CG	2.67	0.40
5:B:877:PRO:C	5:B:878:GLN:HG3	2.42	0.40
5:B:1001:PHE:HD2	6:C:34:ARG:NH2	2.17	0.40
6:C:80:LEU:CD1	6:C:95:CYS:HA	2.51	0.40
6:C:167:HIS:CE1	15:L:70:ARG:HA	2.57	0.40
6:C:186:LEU:HB3	6:C:188:HIS:CD2	2.56	0.40
6:C:217:ASP:HA	6:C:218:PRO:HD3	1.89	0.40
7:D:158:GLU:O	7:D:161:GLY:N	2.51	0.40
11:H:5:LEU:N	11:H:60:ALA:HB2	2.37	0.40
11:H:127:GLY:O	11:H:128:ASN:CB	2.69	0.40
13:J:59:LYS:H	13:J:59:LYS:HG2	1.72	0.40
14:K:46:ILE:O	14:K:46:ILE:HG22	2.21	0.40
2:N:3:DA:C1'	2:N:4:DG:H5'	2.52	0.40
4:A:42:ASP:HB3	4:A:45:GLN:HA	2.03	0.40
4:A:486:GLU:O	4:A:487:MET:HG2	2.21	0.40
4:A:781:ASP:O	4:A:782:ARG:HB3	2.21	0.40
4:A:1237:ILE:HG22	4:A:1238:ILE:N	2.36	0.40
5:B:129:PHE:CE2	5:B:166:PHE:HD1	2.39	0.40
5:B:552:MET:C	5:B:554:ILE:N	2.74	0.40
5:B:758:PHE:O	5:B:760:ASP:N	2.54	0.40
6:C:54:ASN:HB2	6:C:153:LEU:CD1	2.52	0.40
7:D:63:LEU:HD22	7:D:63:LEU:HA	1.66	0.40
8:E:191:LYS:O	8:E:193:GLY:N	2.55	0.40
10:G:79:PHE:CE2	10:G:105:PRO:CG	3.03	0.40
15:L:25:ALA:O	15:L:26:THR:CB	2.69	0.40
2:N:5:DT:H1'	2:N:6:DA:H5'	2.03	0.40
4:A:7:SER:CB	5:B:1193:GLN:NE2	2.83	0.40
4:A:18:GLN:H	5:B:1215:ARG:HB2	1.86	0.40
4:A:219:PHE:CD2	4:A:231:PRO:HD2	2.56	0.40
4:A:325:ILE:HG22	5:B:1210:MET:HE1	2.02	0.40
4:A:711:ARG:O	4:A:714:PHE:N	2.51	0.40
4:A:935:GLN:O	4:A:936:LEU:C	2.59	0.40
4:A:964:ILE:O	4:A:967:ALA:N	2.55	0.40
4:A:1215:ARG:HH11	4:A:1215:ARG:HG2	1.87	0.40
4:A:1317:MET:HE1	4:A:1338:VAL:HG11	2.02	0.40
4:A:1434:ALA:CB	4:A:1436:ILE:HD12	2.52	0.40
5:B:33:VAL:O	5:B:36:ALA:HB3	2.22	0.40
5:B:610:ASN:C	5:B:612:GLU:H	2.25	0.40
5:B:616:ILE:CG1	5:B:697:GLU:HA	2.51	0.40
5:B:858:SER:HA	5:B:966:VAL:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:52:GLU:HB3	6:C:154:LYS:HB2	2.03	0.40
6:C:59:ALA:O	6:C:62:PHE:CB	2.69	0.40
6:C:204:SER:C	6:C:206:ASN:N	2.73	0.40
7:D:29:LEU:N	7:D:29:LEU:HD23	2.35	0.40
9:F:77:ASP:O	9:F:79:ARG:N	2.54	0.40
11:H:9:ILE:HA	11:H:55:LEU:O	2.21	0.40
13:J:1:MET:H2	13:J:57:ILE:H	1.65	0.40
4:A:289:ILE:C	4:A:291:GLU:N	2.74	0.40
4:A:535:THR:CG2	4:A:575:LYS:HE2	2.50	0.40
4:A:693:VAL:HA	4:A:696:GLU:HB3	2.03	0.40
4:A:853:ASP:OD1	4:A:853:ASP:C	2.60	0.40
4:A:863:VAL:HG11	4:A:866:PHE:CE2	2.56	0.40
5:B:118:ARG:HG2	5:B:204:ILE:HD13	2.03	0.40
5:B:205:ILE:N	5:B:205:ILE:CD1	2.84	0.40
5:B:294:ASP:C	5:B:296:GLU:H	2.22	0.40
5:B:564:GLU:HA	5:B:565:PRO:HD2	1.93	0.40
5:B:766:ARG:HA	5:B:766:ARG:HD3	1.91	0.40
5:B:796:LEU:HD12	5:B:797:TYR:N	2.37	0.40
5:B:797:TYR:HE1	5:B:854:LEU:HD21	1.86	0.40
5:B:839:MET:CE	5:B:1010:LEU:HD21	2.42	0.40
5:B:895:ASP:C	5:B:897:GLY:N	2.74	0.40
5:B:1060:ARG:HD2	5:B:1060:ARG:HA	1.74	0.40
6:C:67:LEU:HD11	6:C:155:LEU:HD13	2.02	0.40
7:D:159:THR:O	7:D:163:VAL:HG23	2.21	0.40
9:F:154:ASP:HB3	9:F:155:LEU:H	1.67	0.40
10:G:119:LEU:HD13	10:G:132:SER:HB2	2.03	0.40
12:I:34:TYR:HE2	12:I:36:GLU:HB3	1.86	0.40
13:J:52:THR:O	13:J:52:THR:HG22	2.20	0.40
4:A:57:ARG:O	4:A:68:GLN:NE2	2.42	0.40
4:A:95:PHE:O	4:A:96:ILE:C	2.59	0.40
4:A:103:CYS:C	4:A:105:CYS:N	2.75	0.40
4:A:431:LYS:HE3	4:A:431:LYS:HB2	1.95	0.40
4:A:463:ILE:HD13	4:A:469:ARG:HG3	2.00	0.40
4:A:534:LEU:CD1	4:A:541:ILE:HD11	2.51	0.40
4:A:551:TYR:CE2	14:K:62:LYS:HE2	2.57	0.40
4:A:709:THR:HG22	4:A:711:ARG:N	2.18	0.40
4:A:783:THR:HG21	4:A:815:PHE:CE2	2.56	0.40
4:A:804:TYR:OH	5:B:763:GLN:HA	2.21	0.40
4:A:878:ILE:HG23	4:A:956:LEU:N	2.36	0.40
4:A:986:ILE:HG22	4:A:987:VAL:N	2.37	0.40
4:A:1121:GLU:O	4:A:1122:PRO:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1215:ARG:HG2	4:A:1215:ARG:NH1	2.37	0.40
4:A:1313:LEU:HD23	4:A:1338:VAL:CB	2.52	0.40
4:A:1377:THR:O	4:A:1378:GLN:C	2.59	0.40
5:B:126:SER:HB3	5:B:172:ILE:CD1	2.51	0.40
5:B:203:PHE:CD1	5:B:203:PHE:N	2.89	0.40
5:B:308:TRP:HA	5:B:311:LEU:HD12	2.03	0.40
5:B:889:THR:CG2	5:B:891:ASP:OD2	2.69	0.40
5:B:1035:ALA:HB1	5:B:1040:ASN:O	2.21	0.40
5:B:1110:PRO:HG2	5:B:1119:VAL:CG2	2.51	0.40
5:B:1163:CYS:HB3	5:B:1166:CYS:O	2.22	0.40
6:C:62:PHE:O	6:C:65:HIS:HB3	2.22	0.40
6:C:89:GLU:O	6:C:90:ASP:HB3	2.21	0.40
6:C:165:LYS:O	14:K:6:ARG:NH1	2.53	0.40
8:E:63:ASN:HA	8:E:64:PRO:HD3	1.78	0.40
8:E:120:ALA:O	8:E:122:LYS:N	2.55	0.40
12:I:13:MET:HG3	12:I:14:LEU:N	2.37	0.40
13:J:36:LEU:HD12	13:J:47:ARG:HH12	1.82	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 X-ray entries followed by that with respect to entries of similar resolution.

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
4	A	1406/1733 (81%)	988 (70%)	277 (20%)	141 (10%)	0 9
5	B	1090/1224 (89%)	754 (69%)	217 (20%)	119 (11%)	0 8
6	C	264/318 (83%)	181 (69%)	50 (19%)	33 (12%)	0 6
7	D	173/221 (78%)	125 (72%)	28 (16%)	20 (12%)	0 6
8	E	212/215 (99%)	157 (74%)	38 (18%)	17 (8%)	1 14
9	F	82/155 (53%)	62 (76%)	15 (18%)	5 (6%)	1 20
10	G	169/171 (99%)	131 (78%)	30 (18%)	8 (5%)	2 24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
11	H	129/146 (88%)	90 (70%)	19 (15%)	20 (16%)	0 4
12	I	117/122 (96%)	84 (72%)	23 (20%)	10 (8%)	1 12
13	J	63/70 (90%)	36 (57%)	15 (24%)	12 (19%)	0 2
14	K	112/120 (93%)	86 (77%)	20 (18%)	6 (5%)	2 22
15	L	44/70 (63%)	17 (39%)	14 (32%)	13 (30%)	0 0
All	All	3861/4565 (85%)	2711 (70%)	746 (19%)	404 (10%)	0 8

All (404) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	42	ASP
4	A	44	THR
4	A	48	ALA
4	A	54	ASN
4	A	55	ASP
4	A	57	ARG
4	A	62	ASP
4	A	66	LYS
4	A	67	CYS
4	A	73	GLY
4	A	74	MET
4	A	93	VAL
4	A	154	SER
4	A	223	GLY
4	A	250	ILE
4	A	253	ASN
4	A	255	SER
4	A	286	HIS
4	A	311	GLN
4	A	312	PRO
4	A	318	SER
4	A	322	VAL
4	A	332	LYS
4	A	335	ARG
4	A	336	ILE
4	A	385	ILE
4	A	423	ASP
4	A	536	LEU
4	A	567	LYS
4	A	597	LEU

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Mol	Chain	Res	Type
4	A	626	ASN
4	A	780	VAL
4	A	789	LYS
4	A	968	GLN
4	A	1002	GLY
4	A	1036	ARG
4	A	1115	SER
4	A	1120	LEU
4	A	1122	PRO
4	A	1223	ASP
4	A	1314	SER
4	A	1365	TYR
4	A	1366	ARG
4	A	1378	GLN
4	A	1405	THR
5	B	21	GLU
5	B	45	SER
5	B	108	VAL
5	B	206	ASN
5	B	219	ALA
5	B	229	ALA
5	B	258	LEU
5	B	259	TYR
5	B	266	ALA
5	B	334	ILE
5	B	367	LEU
5	B	401	PHE
5	B	474	SER
5	B	509	ALA
5	B	643	ASP
5	B	709	ASP
5	B	727	LYS
5	B	731	VAL
5	B	751	VAL
5	B	764	SER
5	B	943	SER
5	B	951	GLN
5	B	958	GLN
5	B	1046	PRO
5	B	1069	PHE
5	B	1097	HIS
5	B	1100	ASP

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Mol	Chain	Res	Type
5	B	1108	ARG
5	B	1156	ASP
5	B	1157	ALA
5	B	1171	VAL
5	B	1175	LEU
5	B	1178	ASN
5	B	1181	GLU
5	B	1182	CYS
5	B	1183	LYS
5	B	1188	LYS
6	C	87	PHE
6	C	141	GLY
6	C	149	LYS
6	C	161	LYS
6	C	173	ALA
6	C	184	ASN
6	C	209	TYR
6	C	214	ASN
6	C	215	GLU
7	D	5	THR
7	D	8	PHE
7	D	19	GLU
7	D	20	GLU
7	D	21	GLU
7	D	52	LEU
7	D	131	GLU
7	D	192	LYS
7	D	199	ASN
8	E	44	ALA
8	E	130	ALA
8	E	192	ARG
8	E	206	GLY
10	G	62	LEU
10	G	63	PRO
10	G	118	ASP
10	G	139	ILE
11	H	108	SER
11	H	128	ASN
12	I	3	THR
12	I	9	ASP
12	I	47	GLU
13	J	2	ILE

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Mol	Chain	Res	Type
13	J	6	ARG
13	J	17	LYS
13	J	29	GLU
13	J	32	GLU
13	J	55	ASP
13	J	64	ASN
14	K	7	PHE
15	L	35	SER
15	L	50	ASP
15	L	53	HIS
15	L	60	ARG
4	A	58	LEU
4	A	59	GLY
4	A	69	THR
4	A	76	GLU
4	A	113	LEU
4	A	117	GLU
4	A	205	GLU
4	A	226	GLU
4	A	263	THR
4	A	283	GLY
4	A	410	GLY
4	A	465	TYR
4	A	517	ASN
4	A	543	LEU
4	A	601	LYS
4	A	609	ASP
4	A	619	LYS
4	A	661	GLY
4	A	666	ILE
4	A	716	ASP
4	A	731	ARG
4	A	775	ILE
4	A	847	ASP
4	A	875	ALA
4	A	986	ILE
4	A	1124	HIS
4	A	1212	VAL
4	A	1221	LYS
4	A	1255	GLU
5	B	58	THR
5	B	67	SER

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Mol	Chain	Res	Type
5	B	68	THR
5	B	260	GLY
5	B	282	ILE
5	B	328	GLU
5	B	369	GLY
5	B	394	ASP
5	B	450	ALA
5	B	467	GLY
5	B	470	LYS
5	B	477	ALA
5	B	591	ARG
5	B	605	ARG
5	B	613	VAL
5	B	712	PRO
5	B	792	MET
5	B	867	GLY
5	B	884	ARG
5	B	907	GLY
5	B	1003	ALA
5	B	1041	GLU
5	B	1103	ILE
5	B	1126	GLY
5	B	1131	GLY
5	B	1155	SER
5	B	1167	GLY
5	B	1186	ASP
6	C	78	GLU
6	C	84	ARG
6	C	108	GLU
6	C	110	THR
6	C	156	THR
6	C	175	ALA
6	C	216	GLY
6	C	231	ASN
7	D	9	GLN
7	D	53	SER
7	D	177	VAL
8	E	73	PRO
8	E	74	ASP
8	E	106	GLN
8	E	121	MET
8	E	174	GLN

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Mol	Chain	Res	Type
9	F	73	ALA
9	F	81	THR
9	F	154	ASP
10	G	167	TYR
11	H	59	ILE
11	H	62	SER
11	H	81	PRO
11	H	82	PRO
11	H	84	ALA
11	H	90	ALA
11	H	140	ALA
12	I	11	ASN
12	I	57	GLY
12	I	79	HIS
12	I	91	ARG
12	I	106	CYS
13	J	28	ASP
14	K	15	GLY
14	K	104	ASN
15	L	43	THR
15	L	54	ARG
4	A	4	GLN
4	A	232	GLU
4	A	298	PHE
4	A	321	PRO
4	A	331	GLY
4	A	399	HIS
4	A	418	SER
4	A	846	GLU
4	A	854	ASN
4	A	871	ASP
4	A	1016	THR
4	A	1324	PRO
4	A	1335	ILE
4	A	1377	THR
4	A	1393	ASN
4	A	1402	PHE
5	B	46	GLN
5	B	184	ALA
5	B	193	LYS
5	B	257	LYS
5	B	460	ALA

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Mol	Chain	Res	Type
5	B	559	SER
5	B	641	GLU
5	B	708	GLU
5	B	711	GLU
5	B	738	PHE
5	B	746	SER
5	B	754	SER
5	B	878	GLN
5	B	879	ARG
5	B	881	ASN
5	B	942	ARG
5	B	1016	ALA
5	B	1035	ALA
5	B	1143	ALA
6	C	90	ASP
6	C	153	LEU
6	C	212	PRO
6	C	213	PRO
6	C	240	VAL
7	D	6	SER
7	D	218	GLU
8	E	43	LYS
8	E	45	LYS
8	E	59	SER
8	E	103	LYS
8	E	115	ASN
9	F	112	GLU
10	G	35	GLU
11	H	32	THR
11	H	109	LYS
12	I	107	SER
13	J	27	GLU
14	K	111	LEU
15	L	44	ASP
15	L	55	ILE
15	L	59	ALA
4	A	45	GLN
4	A	70	CYS
4	A	128	ILE
4	A	169	ASN
4	A	219	PHE
4	A	400	PRO

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Mol	Chain	Res	Type
4	A	424	ILE
4	A	592	ASP
4	A	852	TYR
4	A	916	GLY
4	A	958	VAL
4	A	1126	ALA
4	A	1229	SER
4	A	1281	ARG
4	A	1302	PRO
4	A	1438	THR
5	B	65	GLU
5	B	171	PRO
5	B	333	PHE
5	B	365	THR
5	B	409	ALA
5	B	478	GLY
5	B	480	SER
5	B	869	SER
5	B	909	ASP
5	B	1017	ILE
6	C	60	ASP
6	C	132	PRO
6	C	167	HIS
6	C	208	GLU
6	C	217	ASP
7	D	13	ARG
8	E	76	GLY
10	G	154	VAL
11	H	17	PRO
11	H	60	ALA
11	H	77	ARG
11	H	92	ASP
11	H	139	ASN
12	I	95	THR
13	J	24	LEU
13	J	33	GLY
14	K	29	ASN
15	L	64	LEU
4	A	61	ILE
4	A	84	ILE
4	A	245	PRO
4	A	544	ASP

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Mol	Chain	Res	Type
4	A	591	PHE
4	A	599	SER
4	A	782	ARG
4	A	910	PRO
4	A	920	LEU
4	A	1114	PRO
4	A	1116	LEU
4	A	1128	GLN
4	A	1165	GLU
4	A	1242	VAL
4	A	1297	GLU
4	A	1300	LYS
5	B	24	PRO
5	B	28	GLU
5	B	114	PRO
5	B	115	GLN
5	B	262	GLU
5	B	295	GLY
5	B	309	GLN
5	B	346	GLU
5	B	362	PRO
5	B	421	PHE
5	B	436	VAL
5	B	551	PRO
5	B	565	PRO
5	B	978	ASP
5	B	1045	SER
6	C	142	VAL
6	C	148	ARG
7	D	15	LEU
7	D	31	GLN
7	D	174	PRO
8	E	104	ASN
9	F	104	ASN
11	H	52	GLN
14	K	4	PRO
15	L	40	LEU
4	A	5	GLN
4	A	111	GLY
4	A	419	LYS
4	A	492	PRO
4	A	598	LEU

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Mol	Chain	Res	Type
4	A	753	GLY
4	A	1071	SER
5	B	283	VAL
5	B	611	PRO
5	B	688	GLY
5	B	1011	ILE
6	C	195	GLN
7	D	16	LYS
11	H	12	VAL
11	H	83	GLN
15	L	26	THR
15	L	56	LEU
4	A	568	PRO
4	A	600	PRO
4	A	627	GLY
4	A	1341	ILE
5	B	575	PRO
7	D	202	ILE
10	G	20	PRO
4	A	244	PRO
4	A	1435	PRO
5	B	818	PRO
6	C	51	VAL
6	C	139	GLY
13	J	14	VAL
4	A	196	GLU
4	A	284	ALA
4	A	1031	VAL
4	A	1164	PRO
5	B	511	PRO
5	B	1214	PRO
6	C	6	PRO
8	E	38	PRO
4	A	357	PRO
4	A	765	VAL
5	B	658	ILE
5	B	901	PRO
11	H	44	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	
4	A	1239/1520 (82%)	1124 (91%)	115 (9%)	9	35
5	B	962/1061 (91%)	887 (92%)	75 (8%)	12	42
6	C	234/274 (85%)	211 (90%)	23 (10%)	8	33
7	D	159/200 (80%)	129 (81%)	30 (19%)	1	10
8	E	196/197 (100%)	190 (97%)	6 (3%)	40	65
9	F	74/137 (54%)	65 (88%)	9 (12%)	5	25
10	G	152/152 (100%)	139 (91%)	13 (9%)	10	40
11	H	117/128 (91%)	112 (96%)	5 (4%)	29	58
12	I	113/116 (97%)	104 (92%)	9 (8%)	12	42
13	J	60/65 (92%)	56 (93%)	4 (7%)	16	47
14	K	99/102 (97%)	89 (90%)	10 (10%)	7	32
15	L	40/57 (70%)	36 (90%)	4 (10%)	7	32
All	All	3445/4009 (86%)	3142 (91%)	303 (9%)	10	38

All (303) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	2	VAL
4	A	34	LYS
4	A	37	PHE
4	A	38	PRO
4	A	62	ASP
4	A	68	GLN
4	A	83	HIS
4	A	93	VAL
4	A	100	LYS
4	A	108	MET
4	A	122	MET
4	A	200	ARG
4	A	215	SER
4	A	221	SER

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Mol	Chain	Res	Type
4	A	270	LEU
4	A	302	THR
4	A	312	PRO
4	A	320	ARG
4	A	321	PRO
4	A	326	ARG
4	A	335	ARG
4	A	345	VAL
4	A	354	SER
4	A	381	THR
4	A	396	PRO
4	A	406	ILE
4	A	407	ARG
4	A	408	ASP
4	A	412	ARG
4	A	418	SER
4	A	442	VAL
4	A	443	LEU
4	A	445	ASN
4	A	449	SER
4	A	450	LEU
4	A	451	HIS
4	A	460	VAL
4	A	462	VAL
4	A	469	ARG
4	A	470	LEU
4	A	487	MET
4	A	493	GLN
4	A	503	GLN
4	A	512	VAL
4	A	515	GLN
4	A	518	LYS
4	A	560	ILE
4	A	562	THR
4	A	584	ASN
4	A	590	ARG
4	A	618	GLU
4	A	626	ASN
4	A	635	ARG
4	A	659	HIS
4	A	666	ILE
4	A	670	ILE

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Mol	Chain	Res	Type
4	A	692	ASP
4	A	711	ARG
4	A	727	ASP
4	A	739	ASP
4	A	768	GLN
4	A	774	ARG
4	A	779	PHE
4	A	821	ARG
4	A	834	THR
4	A	858	ASN
4	A	871	ASP
4	A	873	MET
4	A	903	ASN
4	A	907	THR
4	A	929	LEU
4	A	939	ASP
4	A	940	ARG
4	A	942	PHE
4	A	969	GLN
4	A	992	ASP
4	A	1001	ARG
4	A	1017	LEU
4	A	1029	ARG
4	A	1035	TYR
4	A	1037	LEU
4	A	1067	LEU
4	A	1110	ASN
4	A	1111	MET
4	A	1116	LEU
4	A	1120	LEU
4	A	1122	PRO
4	A	1127	ASP
4	A	1138	ILE
4	A	1146	VAL
4	A	1152	ILE
4	A	1155	ASP
4	A	1173	HIS
4	A	1187	GLN
4	A	1206	ASP
4	A	1240	CYS
4	A	1264	GLU
4	A	1271	ILE

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Mol	Chain	Res	Type
4	A	1291	VAL
4	A	1295	THR
4	A	1298	TYR
4	A	1329	THR
4	A	1332	PHE
4	A	1333	ILE
4	A	1359	ASP
4	A	1364	ASN
4	A	1372	VAL
4	A	1386	ARG
4	A	1389	PHE
4	A	1405	THR
4	A	1415	SER
4	A	1432	GLN
4	A	1442	ASP
4	A	1443	VAL
4	A	1445	ILE
5	B	30	SER
5	B	37	PHE
5	B	46	GLN
5	B	57	TYR
5	B	61	ASP
5	B	175	ARG
5	B	188	ASP
5	B	194	GLU
5	B	199	MET
5	B	217	ARG
5	B	223	VAL
5	B	250	PHE
5	B	261	ARG
5	B	268	THR
5	B	298	LEU
5	B	365	THR
5	B	371	GLU
5	B	393	LYS
5	B	399	ASP
5	B	401	PHE
5	B	427	ASP
5	B	429	PHE
5	B	463	THR
5	B	465	ASN
5	B	466	TRP

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Mol	Chain	Res	Type
5	B	485	ARG
5	B	498	THR
5	B	502	ILE
5	B	516	ASN
5	B	557	PHE
5	B	582	VAL
5	B	593	PRO
5	B	603	LEU
5	B	615	MET
5	B	628	THR
5	B	644	GLU
5	B	682	SER
5	B	724	ASP
5	B	737	THR
5	B	742	GLU
5	B	748	ILE
5	B	755	ILE
5	B	787	VAL
5	B	811	TYR
5	B	830	TYR
5	B	835	GLN
5	B	839	MET
5	B	878	GLN
5	B	894	ASP
5	B	901	PRO
5	B	909	ASP
5	B	939	THR
5	B	953	LEU
5	B	957	ASN
5	B	978	ASP
5	B	999	MET
5	B	1002	THR
5	B	1006	ILE
5	B	1022	THR
5	B	1047	PHE
5	B	1084	GLN
5	B	1087	PHE
5	B	1095	LEU
5	B	1099	VAL
5	B	1108	ARG
5	B	1112	GLN
5	B	1122	ARG

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Mol	Chain	Res	Type
5	B	1129	ARG
5	B	1138	MET
5	B	1159	ARG
5	B	1170	THR
5	B	1176	ASN
5	B	1183	LYS
5	B	1202	LEU
5	B	1216	LEU
6	C	22	LEU
6	C	35	ARG
6	C	56	THR
6	C	58	LEU
6	C	60	ASP
6	C	62	PHE
6	C	74	SER
6	C	77	ILE
6	C	89	GLU
6	C	91	HIS
6	C	104	PHE
6	C	128	ASN
6	C	129	ILE
6	C	140	ASN
6	C	147	LEU
6	C	163	ILE
6	C	166	GLU
6	C	193	TYR
6	C	209	TYR
6	C	214	ASN
6	C	240	VAL
6	C	251	LEU
6	C	266	ASP
7	D	5	THR
7	D	8	PHE
7	D	11	ARG
7	D	12	ARG
7	D	13	ARG
7	D	15	LEU
7	D	16	LYS
7	D	17	LYS
7	D	19	GLU
7	D	22	GLU
7	D	47	LEU

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Mol	Chain	Res	Type
7	D	50	LEU
7	D	63	LEU
7	D	70	PHE
7	D	126	ILE
7	D	137	ASN
7	D	139	LYS
7	D	148	LEU
7	D	149	THR
7	D	151	PHE
7	D	152	SER
7	D	170	THR
7	D	174	PRO
7	D	182	SER
7	D	187	THR
7	D	192	LYS
7	D	193	THR
7	D	202	ILE
7	D	206	GLU
7	D	221	TYR
8	E	60	PHE
8	E	74	ASP
8	E	104	ASN
8	E	114	ASN
8	E	132	ILE
8	E	153	HIS
9	F	79	ARG
9	F	81	THR
9	F	90	ARG
9	F	99	LEU
9	F	111	LEU
9	F	122	MET
9	F	143	PHE
9	F	148	VAL
9	F	153	VAL
10	G	1	MET
10	G	13	LEU
10	G	21	ARG
10	G	45	ILE
10	G	52	ASP
10	G	74	TYR
10	G	78	VAL
10	G	79	PHE

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Mol	Chain	Res	Type
10	G	80	LYS
10	G	87	VAL
10	G	88	ASP
10	G	126	ASN
10	G	171	ILE
11	H	86	ASP
11	H	95	TYR
11	H	102	TYR
11	H	130	ARG
11	H	134	ASN
12	I	4	PHE
12	I	9	ASP
12	I	15	TYR
12	I	34	TYR
12	I	75	CYS
12	I	85	PHE
12	I	86	PHE
12	I	100	PHE
12	I	101	PHE
13	J	16	ASP
13	J	44	TYR
13	J	46	CYS
13	J	48	ARG
14	K	1	MET
14	K	5	ASP
14	K	10	PHE
14	K	25	THR
14	K	41	THR
14	K	47	ARG
14	K	50	LEU
14	K	61	TYR
14	K	78	THR
14	K	114	LEU
15	L	27	LEU
15	L	54	ARG
15	L	55	ILE
15	L	70	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (95) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	54	ASN

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Mol	Chain	Res	Type
4	A	92	HIS
4	A	225	ASN
4	A	299	HIS
4	A	339	ASN
4	A	435	HIS
4	A	447	GLN
4	A	451	HIS
4	A	493	GLN
4	A	503	GLN
4	A	517	ASN
4	A	631	HIS
4	A	654	ASN
4	A	736	ASN
4	A	741	ASN
4	A	757	ASN
4	A	768	GLN
4	A	786	HIS
4	A	858	ASN
4	A	903	ASN
4	A	926	GLN
4	A	965	GLN
4	A	994	GLN
4	A	1106	ASN
4	A	1130	GLN
4	A	1140	HIS
4	A	1173	HIS
4	A	1364	ASN
5	B	121	ASN
5	B	178	ASN
5	B	215	GLN
5	B	236	HIS
5	B	350	GLN
5	B	363	HIS
5	B	366	GLN
5	B	465	ASN
5	B	484	ASN
5	B	513	GLN
5	B	515	HIS
5	B	516	ASN
5	B	518	HIS
5	B	538	ASN
5	B	734	HIS

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Mol	Chain	Res	Type
5	B	744	HIS
5	B	763	GLN
5	B	821	GLN
5	B	842	ASN
5	B	957	ASN
5	B	1015	HIS
5	B	1065	GLN
5	B	1076	HIS
5	B	1117	GLN
5	B	1161	HIS
5	B	1179	GLN
5	B	1193	GLN
5	B	1211	ASN
6	C	17	ASN
6	C	24	ASN
6	C	73	GLN
6	C	79	GLN
6	C	112	ASN
6	C	123	ASN
6	C	167	HIS
6	C	252	GLN
7	D	9	GLN
7	D	39	ASN
7	D	40	HIS
7	D	74	GLN
7	D	137	ASN
7	D	143	ASN
7	D	179	GLN
8	E	8	ASN
8	E	32	GLN
8	E	101	GLN
8	E	104	ASN
8	E	113	GLN
8	E	114	ASN
8	E	143	ASN
8	E	147	HIS
10	G	14	HIS
10	G	53	ASN
10	G	97	HIS
10	G	122	ASN
10	G	126	ASN
11	H	131	ASN

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Mol	Chain	Res	Type
11	H	137	GLN
12	I	12	ASN
12	I	60	GLN
12	I	89	GLN
12	I	90	GLN
13	J	64	ASN
14	K	44	ASN
14	K	65	HIS
14	K	76	GLN
14	K	89	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	P	9/10 (90%)	1 (11%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	P	3	U

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 9 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
16	CPT	T	67	1	0,2,4	-	-	-		

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	T	67	CPT	1	0

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 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	T	17/17 (100%)	-0.41	0	100	100	110, 139, 169, 175	0
2	N	7/7 (100%)	0.35	0	100	100	148, 156, 169, 171	0
3	P	10/10 (100%)	-0.28	0	100	100	118, 128, 165, 172	0
4	A	1416/1733 (81%)	-0.33	7 (0%)	91	87	44, 103, 161, 199	0
5	B	1108/1224 (90%)	-0.26	13 (1%)	79	72	47, 116, 176, 199	0
6	C	266/318 (83%)	-0.40	0	100	100	64, 100, 144, 162	0
7	D	177/221 (80%)	-0.19	1 (0%)	89	85	70, 120, 177, 190	0
8	E	214/215 (99%)	-0.24	1 (0%)	91	87	79, 144, 185, 197	0
9	F	84/155 (54%)	-0.54	0	100	100	53, 81, 115, 132	0
10	G	171/171 (100%)	-0.31	0	100	100	82, 103, 141, 150	0
11	H	133/146 (91%)	0.15	3 (2%)	60	52	119, 149, 180, 188	0
12	I	119/122 (97%)	-0.11	2 (1%)	70	62	94, 150, 183, 199	0
13	J	65/70 (92%)	-0.60	0	100	100	71, 96, 131, 140	0
14	K	114/120 (95%)	-0.41	1 (0%)	84	79	64, 101, 130, 149	0
15	L	46/70 (65%)	-0.11	0	100	100	96, 154, 172, 178	0
All	All	3947/4599 (85%)	-0.29	28 (0%)	87	83	44, 111, 175, 199	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	1176	LEU	10.4
4	A	1175	SER	5.0
5	B	471	LYS	4.9
4	A	1455	PRO	3.7
5	B	470	LYS	3.7
4	A	257	ARG	3.1
11	H	140	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
5	B	508	LEU	2.8
5	B	734	HIS	2.8
5	B	883	LEU	2.8
5	B	882	THR	2.7
4	A	255	SER	2.6
5	B	133	LYS	2.6
5	B	919	SER	2.5
8	E	51	GLY	2.4
12	I	119	THR	2.3
11	H	107	VAL	2.3
4	A	251	SER	2.2
12	I	120	GLN	2.2
7	D	8	PHE	2.1
5	B	733	HIS	2.1
5	B	92	PHE	2.1
4	A	1092	LYS	2.1
5	B	715	ALA	2.1
5	B	472	ALA	2.1
5	B	732	SER	2.1
11	H	113	ALA	2.0
14	K	114	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
16	CPT	T	67	3/5	0.96	0.23	131,131,131,132	0
18	MG	A	1736	1/1	0.97	0.21	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
17	ZN	A	1734	1/1	0.98	0.09	108,108,108,108	0
17	ZN	C	319	1/1	0.99	0.14	60,60,60,60	0
17	ZN	I	203	1/1	0.99	0.14	113,113,113,113	0
17	ZN	I	204	1/1	0.99	0.07	196,196,196,196	0
17	ZN	J	101	1/1	0.99	0.22	68,68,68,68	0
17	ZN	L	105	1/1	0.99	0.10	127,127,127,127	0
17	ZN	B	1307	1/1	0.99	0.19	71,71,71,71	0
17	ZN	A	1735	1/1	1.00	0.13	65,65,65,65	0

6.5 Other polymers (i)

There are no such residues in this entry.