Full wwPDB X-ray Structure Validation Report ⓘ

Jan 30, 2017 – 07:08 PM EST

PDB ID	:	5WTJ
Title	:	Crystal structure of an endonuclease
Authors	:	Liu, L.; Wang, Y.
Deposited on	:	2016-12-13
Resolution	:	3.50 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

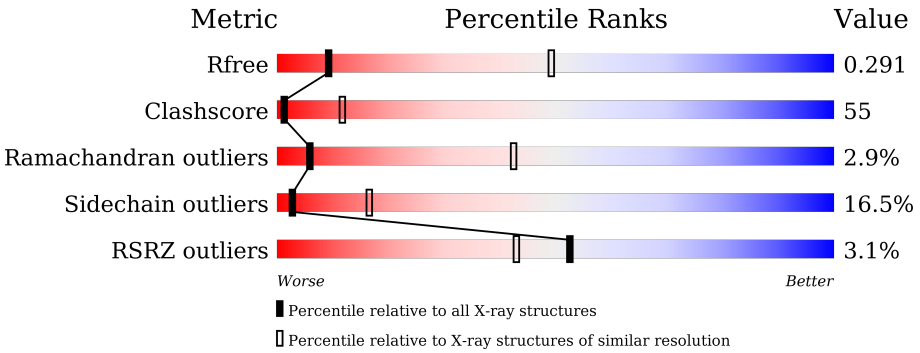
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 3.50 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}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	A	1397	% 30% 33% 9% · 27%
1	B	1397	3% 32% 31% 9% · 28%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15952 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 protein called CRISPR-associated endoribonuclease C2c2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1019	Total	C	N	O	S	Se	0	0	0
			8013	5109	1350	1538	5	11			
1	B	1012	Total	C	N	O	S	Se	0	0	0
			7938	5055	1326	1541	6	10			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1390	LEU	-	expression tag	UNP P0DOC6
A	1391	GLU	-	expression tag	UNP P0DOC6
A	1392	HIS	-	expression tag	UNP P0DOC6
A	1393	HIS	-	expression tag	UNP P0DOC6
A	1394	HIS	-	expression tag	UNP P0DOC6
A	1395	HIS	-	expression tag	UNP P0DOC6
A	1396	HIS	-	expression tag	UNP P0DOC6
A	1397	HIS	-	expression tag	UNP P0DOC6
B	1390	LEU	-	expression tag	UNP P0DOC6
B	1391	GLU	-	expression tag	UNP P0DOC6
B	1392	HIS	-	expression tag	UNP P0DOC6
B	1393	HIS	-	expression tag	UNP P0DOC6
B	1394	HIS	-	expression tag	UNP P0DOC6
B	1395	HIS	-	expression tag	UNP P0DOC6
B	1396	HIS	-	expression tag	UNP P0DOC6
B	1397	HIS	-	expression tag	UNP P0DOC6

- Molecule 2 is water.

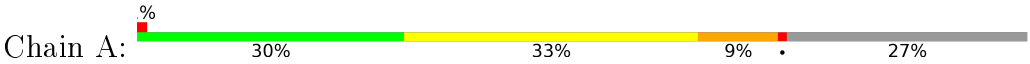
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	O	0	0
			1	1		

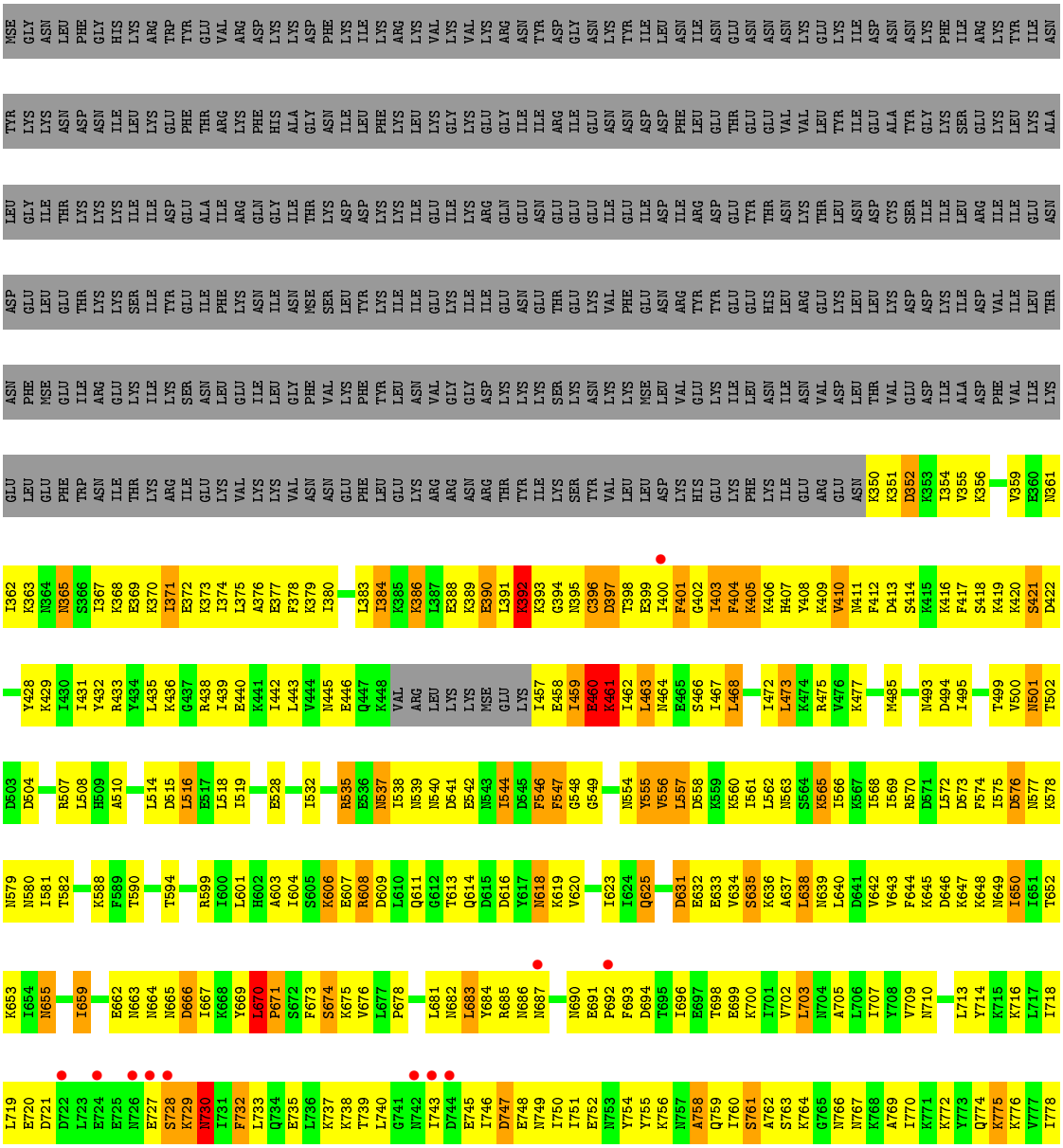
3 Residue-property plots (i)

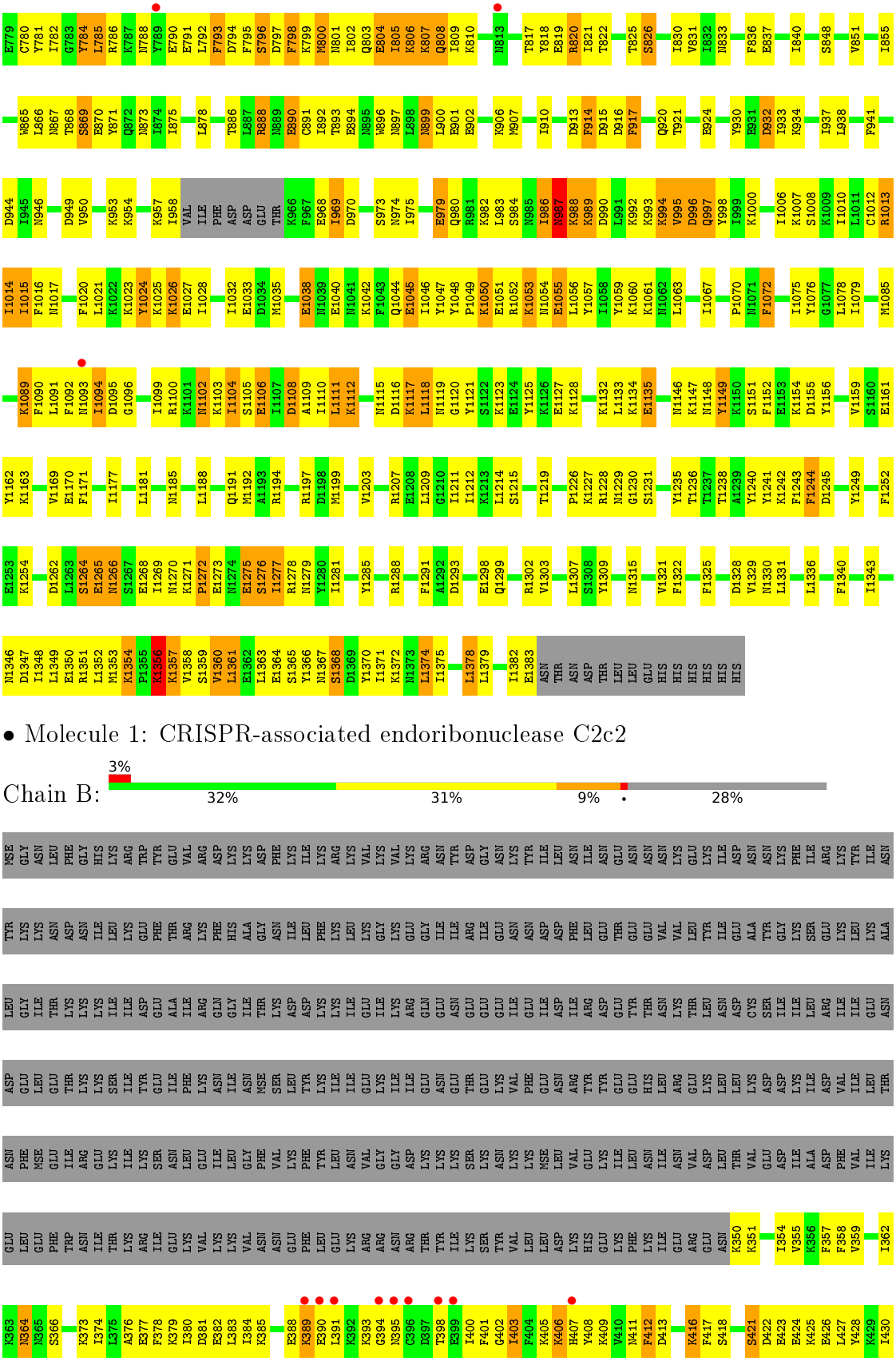
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: CRISPR-associated endoribonuclease C2c2

Chain A:

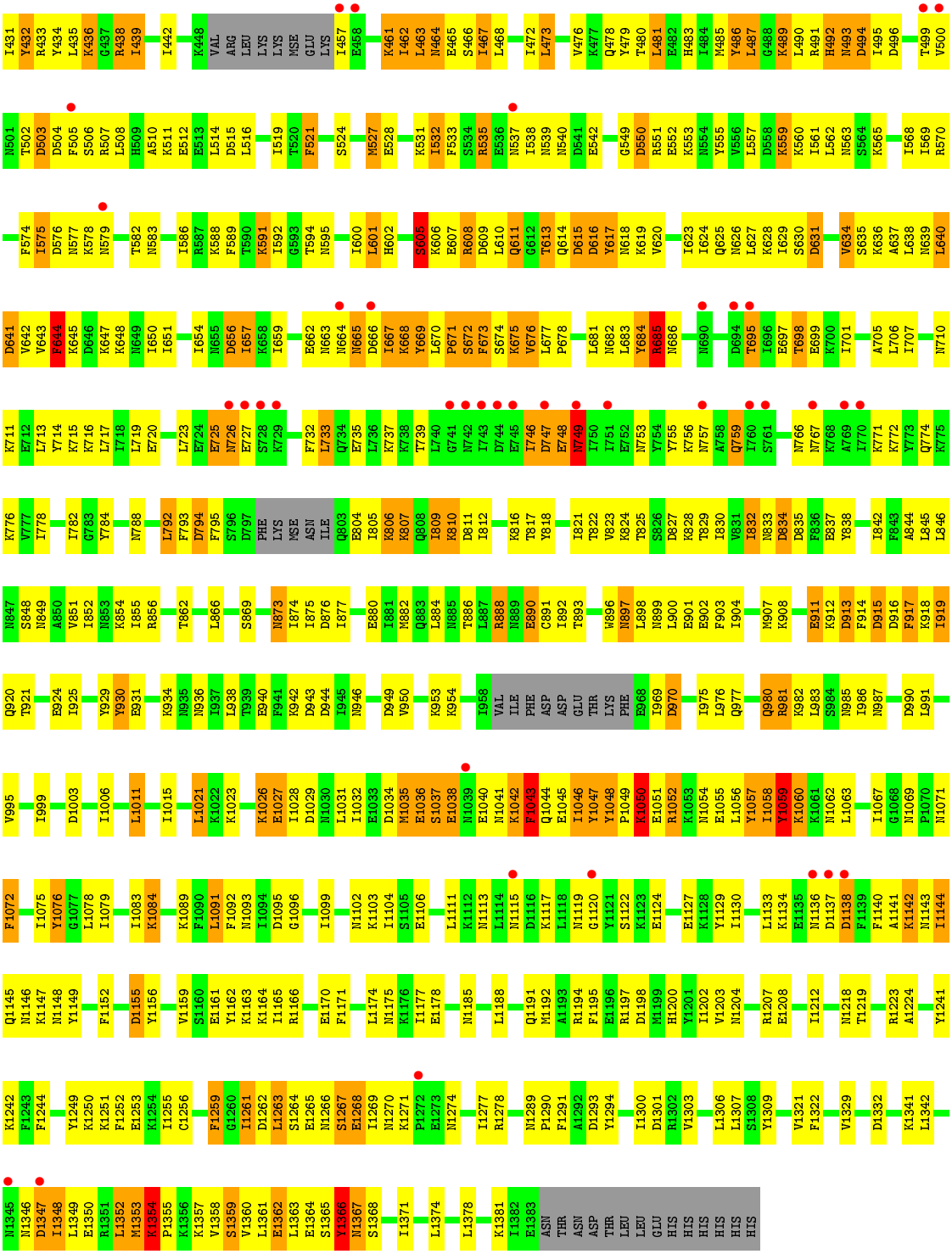






• Molecule 1: CRISPR-associated endoribonuclease C2c2

Chain B:


I431 Y432 R433 Y434 L435 K436 G437 R438 I439 I442 K448 VAL ARG LEU LYS LYS MSE GLU LYS I457 E458 K461 I462 L463 N464 E465 S466 I467 L468 I472 L473 V476 K477 Q478 Y479 T480 L481 E482 H483 I484 M485 Y486 L487 G488 K489 L490 R491 H492 N493 D494 I495 D496 T499 V500
N501 T502 D503 D504 F505 S506 R507 L508 H509 A510 K511 E512 E513 L514 D515 L516 I519 T520 F521 S524 M527 E528 K531 I532 F533 S534 R535 E536 N537 I538 N539 N540 D541 E542 G549 D550 R551 E552 K553 N554 Y555 V556 L557 D558 K559 K560 I561 L562 N563 S564 K565 I568 I569 R570
F574 I575 D576 N577 K578 N579 T582 N583 I586 R587 K588 F589 T590 K591 I592 G593 T594 N595 I600 L601 H602 S605 K606 E607 R608 D609 L610 Q611 G612 T613 Q614 D615 D616 Y617 N618 K619 V620 I623 I624 Q625 N626 L627 K628 I629 S630 D631 V634 S635 K636 A637 L638 N639 L640
D641 V642 V643 F644 K645 E646 K647 K648 N649 I650 I651 I654 N655 D656 I657 K658 I659 E662 N663 N664 N665 D666 I667 K668 Y669 L670 P671 S672 F673 S674 K675 V676 L677 P678 L681 N682 L683 Y684 R685 N686 W690 D694 T695 I696 E697 T698 E699 K700 I701 A705 L706 I707 N710
K711 E712 L713 Y714 K715 K716 L717 I718 L719 E720 L723 E724 E725 N726 E727 S728 K729 F732 L733 Q734 E735 L736 K737 K738 T739 L740 G741 N742 I743 D744 E745 I746 D747 E748 N749 I750 T751 E752 N753 Y754 Y755 K756 N757 A758 Q759 I760 S761 N766 N767 K768 A769 I770 K771 K772 Y773 Q774 K775
K776 V777 I778 I782 G783 Y784 N788 L792 F793 D794 F795 S796 D797 PHE LYS MSE ASN ILE Q803 E804 I805 K806 K807 Q808 I809 K810 D811 I812 K816 T817 Y818 I821 T822 V823 K824 T825 S826 D827 K828 T829 I830 V831 I832 N833 D834 D835 F836 E837 Y838 I842 F843 A844 L845 L846
N847 S848 N849 A850 V851 I852 N853 K854 I855 R856 T862 L866 S869 N873 I874 I875 D876 I877 E880 I881 M882 Q883 L884 N885 T886 L887 R888 N889 E890 C891 I892 T893 W896 N897 L898 N899 L900 E901 E902 F903 I904 M907 K908 E911 K912 D913 F914 D915 D916 F917 K918 I919
Q920 T921 E924 I925 Y929 Y930 E931 K934 N935 N936 I937 L938 T939 E940 F941 K942 D943 D944 I945 N946 D949 V950 K953 K954 I958 VAL ILE PHE ASP ASP GLU THR LYS PHE E968 I969 D970 I975 L976 Q977 Q980 R981 K982 L983 S984 N985 I986 N987 D990 L991
V995 I999 D1003 I1006 L1011 I1015 L1021 K1022 K1023 K1026 E1027 I1028 D1029 N1030 L1031 I1032 E1033 D1034 M1035 E1036 S1037 E1038 N1039 E1040 N1041 K1042 F1043 Q1044 E1045 I1046 Y1047 Y1048 P1049 K1050 E1051 R1052 K1053 N1054 E1055 L1056 Y1057 I1058 Y1059 K1060 K1061 N1062 L1063 I1067 G1068 N1069 P1070 N1071
F1072 I1075 Y1076 G1077 L1078 I1079 I1083 K1084 K1089 F1090 L1091 F1092 N1093 I1094 D1095 G1096 I1099 N1102 K1103 I1104 S1105 E1106 L1111 K1112 N1113 L1114 N1115 D1116 K1117 L1118 N1119 G1120 Y1121 S1122 K1123 E1124 E1127 K1128 Y1129 I1130 L1133 K1134 E1135 N1136 D1137 D1138 F1139 F1140 A1141 K1142 N1143 I1144
Q1145 N1146 K1147 N1148 Y1149 F1152 D1155 Y1156 V1159 S1160 E1161 Y1162 K1163 K1164 I1165 R1166 E1170 F1171 L1174 N1175 K1176 I1177 E1178 N1185 L1188 Q1191 M1192 A1193 R1194 F1195 E1196 R1197 D1198 M1199 H1200 Y1201 I1202 V1203 N1204 R1207 E1208 I1212 N1218 T1219 R1223 A1224 Y1241
K1242 F1243 F1244 Y1249 K1250 K1251 F1252 E1253 K1254 I1255 C1256 F1259 G1260 I1261 D1262 L1263 S1264 E1265 N1266 S1267 E1268 I1269 N1270 K1271 P1272 E1273 N1274 I1277 R1278 N1289 P1290 F1291 A1292 D1293 Y1294 I1300 D1301 R1302 V1303 L1306 L1307 S1308 Y1309 V1321 F1322 V1329 D1332 K1341 L1342
N1345 N1346 D1347 I1348 L1349 E1350 R1351 L1352 M1353 K1354 P1355 K1356 K1357 V1358 S1359 V1360 L1361 E1362 L1363 E1364 S1365 Y1366 N1367 S1368 I1371 L1374 L1378 K1381 I1382 E1383 ASN THR ASN ASP THR LEU LEU GLU HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	91.66Å 94.23Å 338.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.38 – 3.50 48.37 – 3.50	Depositor EDS
% Data completeness (in resolution range)	81.0 (48.38-3.50) 75.3 (48.37-3.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.71 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.263 , 0.291 0.262 , 0.291	Depositor DCC
R_{free} test set	1547 reflections (5.05%)	DCC
Wilson B-factor (Å^2)	18.6	Xtriage
Anisotropy	0.648	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , -0.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.053 for k,h,-l	Xtriage
F_o,F_c correlation	0.78	EDS
Total number of atoms	15952	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% 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

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.48	2/8117 (0.0%)	0.67	16/10925 (0.1%)
1	B	0.42	2/8038 (0.0%)	0.66	11/10824 (0.1%)
All	All	0.45	4/16155 (0.0%)	0.66	27/21749 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	7
All	All	0	9

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	671	PRO	N-CD	5.24	1.55	1.47
1	B	1038	GLU	CB-CG	-5.17	1.42	1.52
1	A	1272	PRO	N-CD	5.09	1.54	1.47
1	B	671	PRO	N-CD	5.09	1.54	1.47

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	634	VAL	CB-CA-C	-11.15	90.21	111.40
1	A	997	GLN	CB-CA-C	6.94	124.28	110.40
1	B	1021	LEU	CB-CG-CD1	-6.59	99.80	111.00
1	B	403	ILE	CB-CA-C	-6.57	98.46	111.60
1	A	758	ALA	CB-CA-C	-6.33	100.60	110.10
1	A	687	ASN	C-N-CD	6.25	141.53	128.40
1	B	1289	ASN	C-N-CD	6.16	141.34	128.40
1	A	730	ASN	CB-CA-C	6.03	122.47	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1354	LYS	C-N-CD	5.95	140.90	128.40
1	B	1354	LYS	C-N-CD	5.82	140.63	128.40
1	A	670	LEU	C-N-CD	5.70	140.37	128.40
1	A	1356	LYS	C-N-CA	5.64	135.81	121.70
1	A	576	ASP	N-CA-C	-5.54	96.05	111.00
1	A	501	ASN	N-CA-C	5.46	125.75	111.00
1	A	392	LYS	N-CA-C	5.34	125.43	111.00
1	A	944	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	573	ASP	CB-CG-OD2	5.25	123.02	118.30
1	B	631	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	1347	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	1138	ASP	CB-CG-OD2	5.19	122.97	118.30
1	B	1137	ASP	CB-CG-OD2	5.18	122.96	118.30
1	B	944	ASP	CB-CG-OD2	5.17	122.95	118.30
1	B	1347	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	995	VAL	CB-CA-C	-5.14	101.64	111.40
1	A	1272	PRO	CA-N-CD	-5.10	104.36	111.50
1	A	732	PHE	O-C-N	-5.03	114.66	122.70
1	B	481	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1051	GLU	Peptide
1	A	1356	LYS	Peptide
1	B	1091	LEU	Peptide
1	B	1129	TYR	Peptide
1	B	1268	GLU	Peptide
1	B	412	PHE	Peptide
1	B	605	SER	Peptide
1	B	644	PHE	Peptide
1	B	664	ASN	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8013	0	7662	834	3
1	B	7938	0	7580	876	1
2	A	1	0	0	0	0
All	All	15952	0	15242	1710	4

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 55.

All (1710) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:976:LEU:HD23	1:B:977:GLN:N	1.22	1.45
1:A:696:ILE:CB	1:A:699:GLU:HB3	1.55	1.35
1:B:817:THR:CG2	1:B:818:TYR:HA	1.54	1.35
1:B:914:PHE:HA	1:B:915:ASP:CB	1.47	1.34
1:B:914:PHE:CA	1:B:915:ASP:HB2	1.54	1.32
1:B:900:LEU:HD13	1:B:1056:LEU:CB	1.59	1.30
1:B:582:THR:CB	1:B:583:ASN:OD1	1.82	1.26
1:B:1049:PRO:HD2	1:B:1055:GLU:CB	1.65	1.26
1:B:351:LYS:HE2	1:B:483:HIS:CE1	1.70	1.26
1:A:1329:VAL:HG21	1:A:1353:MSE:CE	1.63	1.26
1:A:933:ILE:HG12	1:A:998:TYR:CD2	1.73	1.24
1:A:1118:LEU:HB3	1:A:1125:TYR:CZ	1.73	1.23
1:B:900:LEU:CD2	1:B:1056:LEU:HD12	1.68	1.22
1:A:1053:LYS:O	1:A:1055:GLU:HB3	1.37	1.22
1:A:732:PHE:HD1	1:A:784:TYR:CD2	1.55	1.22
1:A:560:LYS:O	1:A:561:ILE:HG12	1.36	1.21
1:B:634:VAL:HG21	1:B:891:CYS:SG	1.78	1.21
1:B:533:PHE:CE1	1:B:557:LEU:HD11	1.74	1.21
1:A:1118:LEU:HB3	1:A:1125:TYR:OH	1.40	1.20
1:A:570:ARG:HD3	1:A:577:ASN:OD1	1.40	1.20
1:B:481:LEU:HD23	1:B:1259:PHE:CE2	1.77	1.20
1:B:531:LYS:CB	1:B:562:LEU:HD11	1.73	1.19
1:B:671:PRO:HG3	1:B:774:GLN:NE2	1.54	1.18
1:A:418:SER:HB2	1:A:419:LYS:HA	1.26	1.18
1:A:762:ALA:HB2	1:A:770:ILE:HG13	1.19	1.17
1:B:976:LEU:CD2	1:B:977:GLN:H	1.57	1.17
1:A:501:ASN:O	1:A:502:THR:HG22	1.43	1.17
1:B:606:LYS:HD3	1:B:1219:THR:CG2	1.76	1.16
1:B:481:LEU:HD23	1:B:1259:PHE:CD2	1.81	1.16
1:A:1366:TYR:CD1	1:A:1367:ASN:HB2	1.81	1.15
1:A:561:ILE:HG22	1:A:562:LEU:HA	1.17	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:738:LYS:HE3	1:A:746:ILE:HD11	1.29	1.14
1:B:1047:TYR:HA	1:B:1057:TYR:HB3	1.20	1.14
1:A:404:PHE:CZ	1:A:439:ILE:HG21	1.81	1.14
1:A:732:PHE:CD1	1:A:784:TYR:CD2	2.35	1.14
1:B:817:THR:HG22	1:B:818:TYR:HA	1.20	1.13
1:A:404:PHE:HE2	1:A:439:ILE:HG13	1.06	1.12
1:B:583:ASN:ND2	1:B:586:ILE:HG13	1.63	1.11
1:B:557:LEU:HD22	1:B:575:ILE:HD11	1.13	1.11
1:A:797:ASP:O	1:A:798:PHE:HB2	1.46	1.11
1:B:490:LEU:HD22	1:B:495:ILE:HG21	1.27	1.11
1:B:900:LEU:HD13	1:B:1056:LEU:HB3	1.12	1.11
1:B:531:LYS:HB3	1:B:562:LEU:HD11	1.19	1.11
1:B:403:ILE:HA	1:B:406:LYS:HG3	1.19	1.11
1:A:375:LEU:HD22	1:A:380:ILE:HD11	1.32	1.11
1:B:533:PHE:CD1	1:B:557:LEU:HD11	1.86	1.11
1:A:1366:TYR:HD1	1:A:1367:ASN:HB2	1.12	1.10
1:B:634:VAL:CG2	1:B:891:CYS:SG	2.40	1.10
1:B:976:LEU:CD2	1:B:977:GLN:N	2.11	1.09
1:B:723:LEU:HD23	1:B:727:GLU:HG2	1.34	1.09
1:A:1053:LYS:C	1:A:1055:GLU:HB3	1.72	1.09
1:B:582:THR:HB	1:B:583:ASN:CG	1.70	1.09
1:B:897:ASN:HB2	1:B:1058:ILE:HD11	1.34	1.09
1:B:582:THR:CG2	1:B:583:ASN:OD1	2.00	1.09
1:B:1142:LYS:HG3	1:B:1145:GLN:H	1.10	1.08
1:B:1048:TYR:HD1	1:B:1052:ARG:CB	1.66	1.08
1:B:481:LEU:CD2	1:B:1259:PHE:CD2	2.37	1.08
1:B:606:LYS:HD3	1:B:1219:THR:HG23	1.13	1.08
1:B:1031:LEU:HD12	1:B:1043:PHE:CZ	1.88	1.08
1:B:1267:SER:HB2	1:B:1268:GLU:HA	1.25	1.08
1:B:648:LYS:HD2	1:B:650:ILE:HD12	1.12	1.08
1:B:684:TYR:HB3	1:B:685:ARG:HB2	1.33	1.07
1:B:1044:GLN:HA	1:B:1048:TYR:CE2	1.90	1.07
1:A:1111:LEU:HD21	1:A:1363:LEU:CD1	1.84	1.07
1:B:804:GLU:HA	1:B:807:LYS:HD3	1.11	1.07
1:B:919:ILE:H	1:B:919:ILE:HD12	1.18	1.07
1:A:696:ILE:CB	1:A:699:GLU:CB	2.33	1.07
1:B:1145:GLN:HB3	1:B:1146:ASN:HA	1.36	1.07
1:B:634:VAL:CG2	1:B:634:VAL:O	1.93	1.06
1:A:350:LYS:HA	1:A:352:ASP:H	1.19	1.06
1:B:461:LYS:HG3	1:B:462:ILE:HG23	1.31	1.06
1:B:582:THR:HG22	1:B:583:ASN:OD1	1.55	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:582:THR:CA	1:B:583:ASN:OD1	2.03	1.06
1:A:659:ILE:HG22	1:A:720:GLU:HA	1.37	1.06
1:B:1253:GLU:CD	1:B:1264:SER:HA	1.76	1.06
1:B:1366:TYR:O	1:B:1367:ASN:ND2	1.87	1.06
1:B:1046:ILE:H	1:B:1046:ILE:HD13	1.18	1.05
1:B:595:ASN:HD21	1:B:610:LEU:CB	1.67	1.05
1:A:464:ASN:HD21	1:A:467:ILE:HG13	1.21	1.05
1:A:394:GLY:HA2	1:A:395:ASN:HB3	1.29	1.05
1:A:375:LEU:HB3	1:A:380:ILE:HD12	1.36	1.05
1:B:557:LEU:HD22	1:B:575:ILE:CD1	1.87	1.05
1:A:1089:LYS:HD2	1:A:1089:LYS:H	1.22	1.05
1:B:897:ASN:CB	1:B:1058:ILE:HD11	1.85	1.05
1:A:404:PHE:CE2	1:A:439:ILE:HG13	1.91	1.04
1:A:547:PHE:HA	1:A:594:THR:HG22	1.40	1.04
1:B:897:ASN:HB3	1:B:1058:ILE:HD12	1.37	1.04
1:A:1118:LEU:CB	1:A:1125:TYR:CZ	2.39	1.04
1:B:583:ASN:HD22	1:B:586:ILE:HG13	0.88	1.03
1:A:367:ILE:O	1:A:371:ILE:HG22	1.57	1.03
1:B:533:PHE:CE1	1:B:557:LEU:CD1	2.41	1.03
1:B:900:LEU:HD22	1:B:1056:LEU:HD12	1.05	1.03
1:B:1048:TYR:HD1	1:B:1052:ARG:CA	1.71	1.03
1:A:671:PRO:HG3	1:A:774:GLN:HG2	1.39	1.03
1:A:439:ILE:HD13	1:A:442:ILE:HD12	1.42	1.02
1:A:384:ILE:HG22	1:A:388:GLU:CB	1.90	1.02
1:A:351:LYS:H	1:A:354:ILE:HD12	1.25	1.02
1:B:582:THR:HA	1:B:583:ASN:OD1	1.59	1.02
1:B:897:ASN:HB3	1:B:1058:ILE:CD1	1.89	1.02
1:B:351:LYS:CE	1:B:483:HIS:CE1	2.43	1.01
1:A:738:LYS:HE3	1:A:746:ILE:CD1	1.89	1.01
1:A:557:LEU:HD22	1:A:558:ASP:H	1.24	1.01
1:B:557:LEU:CD2	1:B:575:ILE:HD11	1.91	1.01
1:A:1367:ASN:ND2	1:A:1371:ILE:HD11	1.76	1.01
1:A:732:PHE:HA	1:A:784:TYR:CZ	1.94	1.01
1:B:439:ILE:O	1:B:442:ILE:HB	1.58	1.01
1:B:634:VAL:HG23	1:B:634:VAL:O	1.19	1.00
1:A:1264:SER:O	1:A:1265:GLU:HB2	1.54	1.00
1:B:1048:TYR:CD1	1:B:1052:ARG:CB	2.43	1.00
1:A:541:ASP:OD1	1:A:1273:GLU:HB2	1.59	1.00
1:B:1142:LYS:HG2	1:B:1143:ASN:HA	1.39	1.00
1:B:685:ARG:HG2	1:B:685:ARG:HH11	1.20	1.00
1:B:461:LYS:HG3	1:B:462:ILE:CG2	1.89	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:817:THR:HG23	1:B:818:TYR:HA	1.37	1.00
1:A:802:ILE:HA	1:A:805:ILE:CB	1.92	1.00
1:A:670:LEU:H	1:A:670:LEU:HD13	1.25	0.99
1:A:683:LEU:HD22	1:A:793:PHE:CE2	1.97	0.99
1:A:762:ALA:CB	1:A:770:ILE:HG13	1.91	0.99
1:B:1111:LEU:HD22	1:B:1359:SER:OG	1.61	0.99
1:A:561:ILE:CG2	1:A:562:LEU:HA	1.93	0.99
1:B:892:ILE:HD12	1:B:893:THR:N	1.78	0.99
1:A:669:TYR:HD1	1:A:755:TYR:CD2	1.79	0.99
1:B:1060:LYS:HE2	1:B:1060:LYS:N	1.77	0.99
1:A:1356:LYS:HB3	1:A:1368:SER:OG	1.62	0.98
1:A:1277:ILE:CD1	1:A:1281:ILE:HD13	1.92	0.98
1:B:1048:TYR:N	1:B:1057:TYR:HB2	1.79	0.98
1:B:630:SER:HA	1:B:631:ASP:HB2	1.45	0.98
1:B:533:PHE:CD1	1:B:557:LEU:CD1	2.46	0.98
1:B:381:ASP:O	1:B:384:ILE:HG22	1.63	0.98
1:B:532:ILE:HG22	1:B:562:LEU:CD1	1.94	0.98
1:B:900:LEU:HD23	1:B:901:GLU:N	1.76	0.97
1:B:897:ASN:CB	1:B:1058:ILE:CD1	2.41	0.97
1:A:1096:GLY:HA2	1:A:1099:ILE:HG13	1.46	0.97
1:A:1329:VAL:HG21	1:A:1353:MSE:HE3	1.40	0.97
1:A:667:ILE:HG13	1:A:718:ILE:HD12	1.45	0.97
1:A:732:PHE:HD1	1:A:784:TYR:CE2	1.81	0.97
1:B:532:ILE:N	1:B:562:LEU:HD12	1.79	0.97
1:B:900:LEU:CD1	1:B:1056:LEU:HB3	1.95	0.97
1:B:557:LEU:CD2	1:B:575:ILE:CD1	2.42	0.97
1:B:725:GLU:O	1:B:726:ASN:ND2	1.97	0.97
1:B:817:THR:HG22	1:B:818:TYR:CA	1.95	0.97
1:B:616:ASP:O	1:B:620:VAL:HG13	1.64	0.97
1:A:738:LYS:HE2	1:A:746:ILE:CG1	1.95	0.96
1:B:463:LEU:HD22	1:B:464:ASN:N	1.80	0.96
1:A:683:LEU:CD2	1:A:793:PHE:CD2	2.48	0.96
1:A:375:LEU:HB3	1:A:380:ILE:CD1	1.96	0.96
1:B:1047:TYR:CA	1:B:1057:TYR:HB3	1.95	0.95
1:B:606:LYS:HB2	1:B:1219:THR:OG1	1.66	0.95
1:B:1142:LYS:HG2	1:B:1143:ASN:CA	1.96	0.95
1:A:665:ASN:HD22	1:A:669:TYR:HE2	1.07	0.95
1:A:361:ASN:HB3	1:A:367:ILE:HG13	1.47	0.95
1:A:738:LYS:CE	1:A:746:ILE:HD11	1.96	0.95
1:B:1329:VAL:HG21	1:B:1353:MSE:HE3	1.49	0.95
1:A:404:PHE:HZ	1:A:439:ILE:HG21	1.13	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1053:LYS:C	1:A:1055:GLU:CB	2.35	0.94
1:A:1149:TYR:OH	1:A:1361:LEU:HD22	1.67	0.94
1:A:411:ASN:H	1:A:413:ASP:H	1.15	0.94
1:B:583:ASN:HD22	1:B:586:ILE:CG1	1.80	0.94
1:B:1049:PRO:CD	1:B:1055:GLU:CB	2.44	0.94
1:A:669:TYR:CD1	1:A:755:TYR:HD2	1.84	0.94
1:B:682:ASN:O	1:B:685:ARG:HB3	1.68	0.94
1:B:491:ARG:HE	1:B:1207:ARG:HH21	1.14	0.94
1:A:376:ALA:O	1:A:379:LYS:HG2	1.67	0.93
1:A:439:ILE:CD1	1:A:442:ILE:HD12	1.96	0.93
1:A:669:TYR:HD1	1:A:755:TYR:HD2	0.98	0.93
1:B:1047:TYR:C	1:B:1057:TYR:HB2	1.89	0.93
1:B:1048:TYR:HD1	1:B:1052:ARG:HA	1.31	0.93
1:B:461:LYS:CB	1:B:462:ILE:HG13	1.98	0.93
1:B:674:SER:HB3	1:B:876:ASP:OD1	1.69	0.93
1:A:1350:GLU:HA	1:A:1352:LEU:H	1.28	0.93
1:B:1142:LYS:CG	1:B:1145:GLN:H	1.82	0.93
1:B:749:ASN:ND2	1:B:749:ASN:O	2.00	0.93
1:A:1015:ILE:HG22	1:A:1016:PHE:HD1	1.33	0.93
1:B:1044:GLN:HA	1:B:1048:TYR:HE2	1.24	0.93
1:B:804:GLU:CA	1:B:807:LYS:HD3	1.99	0.93
1:A:805:ILE:O	1:A:807:LYS:N	2.01	0.92
1:B:648:LYS:HD2	1:B:650:ILE:CD1	1.98	0.92
1:B:588:LYS:HD3	1:B:618:ASN:HD21	1.33	0.92
1:B:562:LEU:HD13	1:B:565:LYS:HZ1	1.34	0.92
1:A:560:LYS:O	1:A:561:ILE:CG1	2.18	0.91
1:A:792:LEU:HD12	1:A:793:PHE:CD1	2.05	0.91
1:A:613:THR:HG23	1:A:614:GLN:HA	1.50	0.91
1:A:463:LEU:H	1:A:463:LEU:HD12	1.34	0.91
1:A:459:ILE:H	1:A:459:ILE:HD12	1.33	0.91
1:A:638:LEU:HD22	1:A:639:ASN:N	1.85	0.91
1:B:1348:ILE:HG22	1:B:1348:ILE:O	1.68	0.91
1:B:535:ARG:HD3	1:B:540:ASN:O	1.71	0.91
1:B:1141:ALA:HB3	1:B:1142:LYS:C	1.90	0.91
1:A:439:ILE:HD13	1:A:442:ILE:CD1	2.01	0.90
1:B:1048:TYR:H	1:B:1057:TYR:H	1.18	0.90
1:A:792:LEU:HD12	1:A:793:PHE:CE1	2.07	0.90
1:A:801:ASN:HA	1:A:804:GLU:CG	2.01	0.90
1:B:1124:GLU:CB	1:B:1127:GLU:CB	2.49	0.90
1:A:544:ILE:HG21	1:A:555:TYR:CE2	2.06	0.90
1:B:1099:ILE:HA	1:B:1103:LYS:CB	2.02	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:900:LEU:HD23	1:B:901:GLU:H	1.33	0.90
1:A:1015:ILE:HG22	1:A:1016:PHE:CD1	2.07	0.89
1:A:1215:SER:OG	1:A:1242:LYS:HB2	1.71	0.89
1:B:1048:TYR:CD1	1:B:1052:ARG:HA	2.07	0.89
1:A:1177:ILE:HD11	1:A:1374:LEU:HD11	1.53	0.89
1:A:368:LYS:HG3	1:A:369:GLU:N	1.86	0.89
1:A:1055:GLU:N	1:A:1055:GLU:OE2	2.05	0.89
1:A:568:ILE:HD13	1:A:625:GLN:HE22	1.36	0.89
1:B:684:TYR:CB	1:B:685:ARG:HB2	2.01	0.89
1:A:362:ILE:HG12	1:A:367:ILE:HD12	1.52	0.89
1:A:732:PHE:HA	1:A:784:TYR:CE2	2.08	0.89
1:B:1031:LEU:HD12	1:B:1043:PHE:HZ	1.34	0.89
1:B:434:TYR:CE2	1:B:468:LEU:HD23	2.08	0.89
1:B:616:ASP:O	1:B:620:VAL:HG22	1.71	0.89
1:A:519:ILE:HD13	1:A:601:LEU:CD2	2.03	0.88
1:B:1031:LEU:CD1	1:B:1043:PHE:HZ	1.86	0.88
1:B:1357:LYS:HD3	1:B:1362:GLU:OE1	1.73	0.88
1:B:434:TYR:CE2	1:B:468:LEU:CD2	2.56	0.88
1:A:1367:ASN:HD21	1:A:1371:ILE:HD11	1.35	0.88
1:A:638:LEU:HD13	1:A:638:LEU:H	1.37	0.88
1:B:976:LEU:HD23	1:B:977:GLN:CA	2.02	0.88
1:B:900:LEU:HD13	1:B:1056:LEU:HB2	1.55	0.88
1:B:897:ASN:HB3	1:B:1059:TYR:CE2	2.08	0.88
1:A:399:GLU:HG3	1:A:400:ILE:HD13	1.53	0.88
1:A:518:LEU:HD23	1:A:855:ILE:HD11	1.53	0.88
1:A:933:ILE:HG12	1:A:998:TYR:HD2	1.30	0.88
1:B:648:LYS:CD	1:B:650:ILE:HD12	2.01	0.88
1:A:1277:ILE:HD12	1:A:1281:ILE:HD13	1.54	0.88
1:B:1269:ILE:HB	1:B:1270:ASN:HB2	1.55	0.88
1:A:659:ILE:CG2	1:A:720:GLU:HA	2.03	0.87
1:B:1360:VAL:O	1:B:1361:LEU:HD23	1.74	0.87
1:B:1367:ASN:O	1:B:1371:ILE:HG22	1.74	0.87
1:B:647:LYS:CB	1:B:648:LYS:HG3	2.03	0.87
1:B:809:ILE:O	1:B:812:ILE:N	2.07	0.87
1:A:462:ILE:HG22	1:A:463:LEU:N	1.88	0.87
1:A:989:LYS:O	1:A:993:LYS:HG2	1.75	0.87
1:A:738:LYS:HE2	1:A:746:ILE:HG13	1.57	0.87
1:A:417:PHE:O	1:A:418:SER:OG	1.91	0.87
1:A:807:LYS:O	1:A:808:GLN:C	2.11	0.87
1:B:900:LEU:HD22	1:B:1056:LEU:CD1	2.00	0.86
1:A:797:ASP:O	1:A:798:PHE:CB	2.24	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:818:TYR:N	1:A:819:GLU:HA	1.90	0.86
1:A:1096:GLY:HA2	1:A:1099:ILE:CG1	2.05	0.86
1:B:1043:PHE:C	1:B:1046:ILE:HD11	1.96	0.86
1:A:1104:ILE:O	1:A:1108:ASP:HB2	1.76	0.86
1:A:371:ILE:CD1	1:A:431:ILE:HD11	2.04	0.86
1:B:969:ILE:CB	1:B:970:ASP:HB3	2.05	0.86
1:B:1145:GLN:CB	1:B:1146:ASN:HA	2.01	0.86
1:A:637:ALA:HB3	1:A:820:ARG:HH12	1.40	0.85
1:A:1367:ASN:ND2	1:A:1371:ILE:CD1	2.40	0.85
1:B:1329:VAL:HG21	1:B:1353:MSE:CE	2.06	0.85
1:B:434:TYR:HE2	1:B:468:LEU:CD2	1.89	0.85
1:A:547:PHE:CA	1:A:594:THR:HG22	2.06	0.85
1:A:738:LYS:CE	1:A:746:ILE:CG1	2.55	0.85
1:B:804:GLU:HA	1:B:807:LYS:CD	2.04	0.85
1:A:351:LYS:N	1:A:354:ILE:HD12	1.90	0.85
1:A:933:ILE:CG1	1:A:998:TYR:CD2	2.59	0.85
1:B:1142:LYS:HG3	1:B:1145:GLN:N	1.90	0.85
1:B:608:ARG:HA	1:B:609:ASP:C	1.95	0.85
1:B:723:LEU:CD2	1:B:727:GLU:HG2	2.07	0.85
1:A:807:LYS:O	1:A:810:LYS:N	2.09	0.85
1:B:457:ILE:O	1:B:457:ILE:HG22	1.76	0.85
1:A:758:ALA:HA	1:A:761:SER:HB2	1.59	0.85
1:B:897:ASN:HB3	1:B:1059:TYR:HE2	1.38	0.85
1:B:1360:VAL:C	1:B:1361:LEU:HD23	1.97	0.85
1:B:684:TYR:HB3	1:B:685:ARG:CB	2.06	0.85
1:A:738:LYS:HB2	1:A:746:ILE:HG12	1.58	0.85
1:B:461:LYS:HB3	1:B:462:ILE:HG13	1.58	0.85
1:B:1058:ILE:HG13	1:B:1059:TYR:CD2	2.12	0.84
1:B:1266:ASN:O	1:B:1267:SER:OG	1.93	0.84
1:A:1364:GLU:O	1:A:1365:SER:OG	1.96	0.84
1:A:457:ILE:O	1:A:457:ILE:HG22	1.77	0.84
1:A:667:ILE:HA	1:A:670:LEU:HD11	1.57	0.84
1:B:576:ASP:OD1	1:B:577:ASN:N	2.09	0.84
1:B:975:ILE:HG22	1:B:976:LEU:HB2	1.60	0.84
1:B:1358:VAL:HG12	1:B:1365:SER:HB3	1.57	0.84
1:B:1329:VAL:HG11	1:B:1353:MSE:HE2	1.60	0.84
1:B:914:PHE:HA	1:B:915:ASP:HB2	0.84	0.84
1:B:1059:TYR:N	1:B:1060:LYS:HB2	1.92	0.84
1:B:398:THR:HA	1:B:401:PHE:CB	2.08	0.83
1:B:673:PHE:CD1	1:B:714:TYR:CD2	2.66	0.83
1:A:1054:ASN:N	1:A:1055:GLU:HA	1.94	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:LYS:HG3	1:A:369:GLU:H	1.41	0.83
1:B:1142:LYS:N	1:B:1143:ASN:HA	1.94	0.83
1:A:1348:ILE:O	1:A:1348:ILE:HG22	1.78	0.83
1:A:459:ILE:HD13	1:A:460:GLU:H	1.44	0.83
1:A:946:ASN:HA	1:A:949:ASP:HB3	1.59	0.83
1:B:1364:GLU:O	1:B:1365:SER:OG	1.95	0.83
1:A:350:LYS:HA	1:A:352:ASP:N	1.93	0.83
1:A:696:ILE:CB	1:A:699:GLU:N	2.42	0.83
1:B:1031:LEU:CD1	1:B:1043:PHE:CZ	2.61	0.83
1:B:532:ILE:HG22	1:B:562:LEU:HD12	1.61	0.83
1:A:445:ASN:HD22	1:A:460:GLU:HA	1.42	0.82
1:B:494:ASP:O	1:B:495:ILE:HD13	1.79	0.82
1:B:673:PHE:HD1	1:B:714:TYR:CD2	1.96	0.82
1:A:468:LEU:O	1:A:472:ILE:HG13	1.79	0.82
1:B:1041:ASN:O	1:B:1042:LYS:O	1.97	0.82
1:A:801:ASN:HA	1:A:804:GLU:HG3	1.61	0.82
1:B:378:PHE:CZ	1:B:435:LEU:CD1	2.63	0.82
1:A:1366:TYR:CD1	1:A:1367:ASN:CB	2.62	0.82
1:A:420:LYS:O	1:A:421:SER:OG	1.97	0.82
1:A:461:LYS:HA	1:A:461:LYS:NZ	1.94	0.82
1:A:696:ILE:CB	1:A:699:GLU:H	1.93	0.82
1:B:461:LYS:HB2	1:B:461:LYS:HZ2	1.44	0.82
1:A:737:LYS:HD2	1:A:750:ILE:HG22	1.62	0.82
1:B:1047:TYR:HA	1:B:1057:TYR:CB	2.08	0.82
1:A:892:ILE:O	1:A:896:TRP:HB3	1.79	0.82
1:B:897:ASN:CB	1:B:1059:TYR:HE2	1.93	0.82
1:B:644:PHE:HE2	1:B:651:ILE:HD11	1.44	0.82
1:B:461:LYS:NZ	1:B:461:LYS:HB2	1.95	0.81
1:B:900:LEU:CD2	1:B:1056:LEU:CD1	2.56	0.81
1:A:395:ASN:OD1	1:A:396:CYS:N	2.14	0.81
1:A:968:GLU:HA	1:A:969:ILE:CB	2.10	0.81
1:B:1130:ILE:HG12	1:B:1133:LEU:HD12	1.61	0.81
1:B:560:LYS:HE2	1:B:563:ASN:CB	2.10	0.81
1:B:358:PHE:O	1:B:362:ILE:HG12	1.80	0.81
1:B:1142:LYS:NZ	1:B:1142:LYS:HB3	1.94	0.81
1:A:375:LEU:CD2	1:A:380:ILE:HD11	2.08	0.81
1:A:568:ILE:HD13	1:A:625:GLN:NE2	1.95	0.81
1:B:1091:LEU:HA	1:B:1092:PHE:C	1.99	0.81
1:A:807:LYS:O	1:A:809:ILE:N	2.13	0.81
1:B:888:ARG:NH1	1:B:1011:LEU:HD21	1.96	0.80
1:B:595:ASN:ND2	1:B:610:LEU:CB	2.44	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:LYS:H	1:A:395:ASN:HB3	1.45	0.80
1:B:986:ILE:HD12	1:B:986:ILE:O	1.81	0.80
1:A:351:LYS:H	1:A:354:ILE:CD1	1.94	0.80
1:B:504:ASP:HA	1:B:507:ARG:HD3	1.63	0.80
1:A:514:LEU:HD12	1:A:514:LEU:O	1.81	0.80
1:A:933:ILE:CG1	1:A:998:TYR:CE2	2.65	0.80
1:B:914:PHE:CA	1:B:915:ASP:CB	2.34	0.80
1:A:1106:GLU:O	1:A:1110:ILE:HG13	1.82	0.80
1:B:1130:ILE:O	1:B:1134:LYS:HG3	1.82	0.80
1:A:683:LEU:HD23	1:A:684:TYR:N	1.97	0.79
1:A:659:ILE:HG22	1:A:720:GLU:CA	2.12	0.79
1:A:1215:SER:OG	1:A:1242:LYS:CB	2.30	0.79
1:A:519:ILE:HD13	1:A:601:LEU:HD23	1.64	0.79
1:A:644:PHE:HB3	1:A:647:LYS:O	1.80	0.79
1:A:608:ARG:NH2	1:A:836:PHE:HB2	1.97	0.79
1:A:933:ILE:HG12	1:A:998:TYR:CE2	2.18	0.79
1:B:467:ILE:HD12	1:B:467:ILE:O	1.82	0.79
1:B:588:LYS:HD3	1:B:618:ASN:ND2	1.96	0.79
1:A:738:LYS:CE	1:A:746:ILE:CD1	2.58	0.79
1:B:405:LYS:HA	1:B:408:TYR:CB	2.12	0.79
1:A:1045:GLU:HB3	1:A:1091:LEU:HD22	1.65	0.79
1:A:1361:LEU:H	1:A:1361:LEU:HD12	1.48	0.79
1:A:738:LYS:CE	1:A:746:ILE:HG13	2.12	0.79
1:A:685:ARG:O	1:A:685:ARG:HD2	1.83	0.78
1:B:1357:LYS:CD	1:B:1362:GLU:OE1	2.31	0.78
1:A:391:LEU:O	1:A:392:LYS:CB	2.31	0.78
1:B:434:TYR:HE2	1:B:468:LEU:HD23	1.43	0.78
1:B:427:LEU:H	1:B:427:LEU:HD12	1.46	0.78
1:A:399:GLU:CG	1:A:400:ILE:HD13	2.13	0.78
1:A:464:ASN:ND2	1:A:467:ILE:HG13	1.97	0.78
1:A:1040:GLU:HG2	1:A:1042:LYS:HG2	1.66	0.78
1:B:533:PHE:HE1	1:B:557:LEU:CD1	1.96	0.78
1:B:432:TYR:CE1	1:B:436:LYS:NZ	2.51	0.78
1:A:1111:LEU:HD21	1:A:1363:LEU:HD12	1.65	0.78
1:A:683:LEU:HD21	1:A:793:PHE:CD2	2.18	0.78
1:A:404:PHE:HZ	1:A:439:ILE:CG2	1.92	0.78
1:A:683:LEU:CD2	1:A:793:PHE:CE2	2.65	0.77
1:B:888:ARG:HH12	1:B:1011:LEU:HD21	1.48	0.77
1:B:465:GLU:O	1:B:466:SER:OG	2.03	0.77
1:B:532:ILE:CG2	1:B:562:LEU:HD12	2.15	0.77
1:A:557:LEU:CD2	1:A:558:ASP:H	1.97	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1060:LYS:HE2	1:B:1060:LYS:CA	2.14	0.77
1:A:1090:PHE:CB	1:A:1162:TYR:HE1	1.97	0.77
1:B:1091:LEU:CB	1:B:1093:ASN:HB2	2.15	0.77
1:B:461:LYS:CG	1:B:462:ILE:HG13	2.15	0.77
1:B:975:ILE:CG2	1:B:976:LEU:HB2	2.15	0.77
1:A:1112:LYS:HA	1:A:1115:ASN:HB2	1.66	0.77
1:A:1277:ILE:HD11	1:A:1281:ILE:HD13	1.64	0.77
1:B:357:PHE:HE2	1:B:427:LEU:HD21	1.49	0.77
1:A:913:ASP:HA	1:A:1013:ARG:NH2	2.00	0.77
1:A:350:LYS:CA	1:A:352:ASP:H	1.97	0.77
1:B:1253:GLU:OE1	1:B:1264:SER:HA	1.83	0.77
1:B:1256:CYS:HB3	1:B:1261:ILE:HG13	1.67	0.77
1:B:1332:ASP:HB2	1:B:1354:LYS:HE3	1.66	0.77
1:B:467:ILE:HG23	1:B:468:LEU:CD1	2.15	0.77
1:B:659:ILE:CB	1:B:719:LEU:O	2.32	0.77
1:B:685:ARG:HG2	1:B:685:ARG:NH1	1.94	0.76
1:B:1047:TYR:CA	1:B:1057:TYR:CB	2.63	0.76
1:B:412:PHE:CB	1:B:413:ASP:HA	2.15	0.76
1:A:1118:LEU:CB	1:A:1125:TYR:CE2	2.68	0.76
1:B:1355:PRO:HB2	1:B:1368:SER:HB2	1.67	0.76
1:B:562:LEU:HD13	1:B:565:LYS:NZ	1.99	0.76
1:A:1119:ASN:HB3	1:A:1120:GLY:HA2	1.68	0.76
1:A:544:ILE:CG2	1:A:555:TYR:CE2	2.69	0.76
1:A:461:LYS:HA	1:A:461:LYS:HZ2	1.48	0.76
1:B:606:LYS:CB	1:B:1219:THR:OG1	2.34	0.76
1:A:418:SER:CB	1:A:419:LYS:HA	2.06	0.76
1:B:817:THR:CG2	1:B:818:TYR:CA	2.49	0.76
1:A:1366:TYR:HD1	1:A:1367:ASN:CB	1.95	0.75
1:B:552:GLU:HA	1:B:553:LYS:CB	2.15	0.75
1:A:411:ASN:N	1:A:412:PHE:HA	2.01	0.75
1:B:378:PHE:CZ	1:B:435:LEU:HD13	2.22	0.75
1:A:501:ASN:O	1:A:502:THR:CG2	2.28	0.75
1:B:892:ILE:HD12	1:B:893:THR:CA	2.17	0.75
1:A:411:ASN:N	1:A:413:ASP:H	1.85	0.75
1:A:614:GLN:CB	1:A:618:ASN:HB2	2.16	0.75
1:A:643:VAL:O	1:A:645:LYS:CB	2.35	0.75
1:A:703:LEU:O	1:A:707:ILE:HG12	1.87	0.75
1:A:1111:LEU:HD23	1:A:1359:SER:OG	1.86	0.75
1:B:804:GLU:O	1:B:806:LYS:N	2.19	0.75
1:B:464:ASN:O	1:B:467:ILE:HG22	1.86	0.75
1:B:532:ILE:CG2	1:B:562:LEU:CD1	2.64	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:LEU:HD23	1:A:383:LEU:O	1.87	0.74
1:A:802:ILE:CA	1:A:805:ILE:CB	2.64	0.74
1:A:806:LYS:O	1:A:809:ILE:HB	1.86	0.74
1:A:398:THR:OG1	1:A:443:LEU:CD1	2.35	0.74
1:A:902:GLU:OE2	1:A:1057:TYR:HD2	1.70	0.74
1:B:374:ILE:HA	1:B:377:GLU:CB	2.17	0.74
1:A:676:VAL:HG12	1:A:778:ILE:HG23	1.70	0.74
1:A:1358:VAL:CB	1:A:1365:SER:HB3	2.18	0.74
1:A:613:THR:CG2	1:A:614:GLN:HA	2.18	0.74
1:B:1141:ALA:N	1:B:1142:LYS:HA	2.02	0.74
1:B:531:LYS:HB2	1:B:562:LEU:HD11	1.68	0.74
1:B:986:ILE:HD13	1:B:991:LEU:HD12	1.68	0.74
1:A:1118:LEU:HB2	1:A:1125:TYR:CE2	2.23	0.74
1:A:1371:ILE:HG22	1:A:1375:ILE:CD1	2.17	0.74
1:B:1142:LYS:HG2	1:B:1143:ASN:C	2.08	0.74
1:B:532:ILE:CA	1:B:562:LEU:HD12	2.17	0.74
1:B:403:ILE:HA	1:B:406:LYS:CG	2.10	0.74
1:B:463:LEU:HD13	1:B:463:LEU:O	1.87	0.74
1:B:1147:LYS:N	1:B:1148:ASN:HA	2.03	0.74
1:B:582:THR:HB	1:B:583:ASN:ND2	2.01	0.74
1:A:1350:GLU:HA	1:A:1352:LEU:N	2.01	0.73
1:A:462:ILE:CG2	1:A:463:LEU:N	2.51	0.73
1:B:376:ALA:HA	1:B:379:LYS:CB	2.19	0.73
1:B:616:ASP:O	1:B:620:VAL:CG1	2.35	0.73
1:A:1010:ILE:HG23	1:A:1014:ILE:HD12	1.68	0.73
1:B:1047:TYR:C	1:B:1057:TYR:CB	2.57	0.73
1:B:657:ILE:HD13	1:B:657:ILE:N	2.04	0.73
1:B:749:ASN:HD21	1:B:753:ASN:HD22	1.35	0.73
1:A:1092:PHE:CB	1:A:1093:ASN:OD1	2.37	0.73
1:A:515:ASP:O	1:A:519:ILE:HG13	1.88	0.73
1:A:1354:LYS:NZ	1:A:1354:LYS:HB2	2.04	0.73
1:A:547:PHE:HA	1:A:594:THR:CG2	2.17	0.73
1:A:667:ILE:HG13	1:A:718:ILE:CD1	2.19	0.73
1:B:532:ILE:N	1:B:562:LEU:CD1	2.51	0.73
1:B:919:ILE:CD1	1:B:919:ILE:H	1.94	0.73
1:B:606:LYS:CD	1:B:1219:THR:CG2	2.62	0.73
1:B:1099:ILE:HG23	1:B:1103:LYS:CB	2.19	0.72
1:B:462:ILE:HD12	1:B:462:ILE:N	2.03	0.72
1:A:638:LEU:CD1	1:A:638:LEU:H	2.03	0.72
1:B:1031:LEU:O	1:B:1043:PHE:CE2	2.42	0.72
1:B:1265:GLU:CB	1:B:1266:ASN:HB3	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:532:ILE:HG22	1:B:562:LEU:HD13	1.69	0.72
1:A:973:SER:HB3	1:A:974:ASN:HA	1.71	0.72
1:B:481:LEU:CD2	1:B:1259:PHE:CE2	2.66	0.72
1:A:1367:ASN:CG	1:A:1371:ILE:CD1	2.57	0.72
1:A:608:ARG:HG2	1:A:608:ARG:HH11	1.55	0.72
1:A:802:ILE:O	1:A:805:ILE:CB	2.37	0.72
1:B:1059:TYR:HA	1:B:1060:LYS:C	2.09	0.72
1:B:640:LEU:HD13	1:B:701:ILE:HG23	1.70	0.72
1:A:1329:VAL:CG2	1:A:1353:MSE:HE3	2.18	0.72
1:B:1079:ILE:N	1:B:1079:ILE:HD12	2.03	0.72
1:A:371:ILE:HD13	1:A:431:ILE:HD11	1.70	0.72
1:B:1048:TYR:N	1:B:1057:TYR:H	1.87	0.72
1:A:1111:LEU:HD21	1:A:1363:LEU:HD11	1.70	0.72
1:A:557:LEU:HD22	1:A:558:ASP:N	2.02	0.72
1:B:720:GLU:OE2	1:B:723:LEU:CD1	2.38	0.72
1:A:1328:ASP:HB3	1:A:1371:ILE:HG21	1.72	0.71
1:B:976:LEU:HD23	1:B:977:GLN:H	0.74	0.71
1:A:666:ASP:O	1:A:667:ILE:HG22	1.91	0.71
1:B:514:LEU:HG	1:B:862:THR:HG21	1.73	0.71
1:B:1031:LEU:O	1:B:1043:PHE:HE2	1.73	0.71
1:B:903:PHE:CE2	1:B:1021:LEU:HD11	2.25	0.71
1:A:1264:SER:O	1:A:1265:GLU:CB	2.33	0.71
1:B:677:LEU:HD11	1:B:707:ILE:HD12	1.73	0.71
1:A:643:VAL:O	1:A:644:PHE:C	2.29	0.71
1:B:481:LEU:HD21	1:B:1259:PHE:CD2	2.22	0.71
1:A:1361:LEU:HD13	1:A:1363:LEU:HD11	1.72	0.71
1:A:703:LEU:HD12	1:A:707:ILE:HD11	1.71	0.71
1:A:775:LYS:HB2	1:A:775:LYS:NZ	2.06	0.71
1:A:400:ILE:HD13	1:A:400:ILE:N	2.05	0.71
1:A:896:TRP:CG	1:A:897:ASN:N	2.55	0.71
1:B:351:LYS:HE2	1:B:483:HIS:HE1	1.50	0.71
1:A:1236:THR:HG23	1:A:1242:LYS:HG2	1.72	0.71
1:A:368:LYS:HA	1:A:371:ILE:CG2	2.20	0.71
1:B:1192:MSE:HE3	1:B:1278:ARG:HG2	1.72	0.71
1:A:638:LEU:HD13	1:A:638:LEU:N	2.05	0.71
1:B:467:ILE:HG23	1:B:468:LEU:HD12	1.72	0.71
1:B:1191:GLN:HE22	1:B:1194:ARG:HH21	1.36	0.70
1:B:1048:TYR:HB2	1:B:1052:ARG:HA	1.72	0.70
1:A:445:ASN:OD1	1:A:446:GLU:N	2.24	0.70
1:B:644:PHE:HE2	1:B:651:ILE:CD1	2.04	0.70
1:A:1014:ILE:HG22	1:A:1015:ILE:N	2.04	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1356:LYS:HD2	1:A:1357:LYS:HB3	1.73	0.70
1:A:361:ASN:CB	1:A:367:ILE:HG13	2.21	0.70
1:B:489:LYS:HG2	1:B:489:LYS:O	1.91	0.70
1:A:1054:ASN:N	1:A:1055:GLU:CA	2.54	0.70
1:A:519:ILE:CD1	1:A:601:LEU:HD23	2.22	0.70
1:B:438:ARG:HA	1:B:438:ARG:NE	2.06	0.70
1:B:904:ILE:HG12	1:B:1021:LEU:HD13	1.73	0.70
1:B:461:LYS:CG	1:B:462:ILE:HG23	2.16	0.70
1:A:1346:ASN:HD22	1:A:1349:LEU:HD22	1.56	0.70
1:A:399:GLU:CD	1:A:400:ILE:HD13	2.12	0.70
1:A:696:ILE:CB	1:A:699:GLU:CA	2.70	0.70
1:B:1263:LEU:HA	1:B:1270:ASN:HD22	1.56	0.70
1:A:1276:SER:OG	1:A:1279:ASN:HB2	1.91	0.69
1:A:801:ASN:HA	1:A:804:GLU:HG2	1.74	0.69
1:A:1118:LEU:HB3	1:A:1125:TYR:CE2	2.28	0.69
1:B:1171:PHE:HB3	1:B:1174:LEU:HD12	1.74	0.69
1:B:1349:LEU:CD2	1:B:1350:GLU:HG2	2.22	0.69
1:B:416:LYS:N	1:B:417:PHE:HA	2.07	0.69
1:A:371:ILE:O	1:A:371:ILE:HD12	1.92	0.69
1:B:426:GLU:O	1:B:430:ILE:HG23	1.93	0.69
1:B:436:LYS:NZ	1:B:436:LYS:HB3	2.07	0.69
1:A:933:ILE:HG13	1:A:998:TYR:CE2	2.26	0.69
1:B:533:PHE:HD1	1:B:557:LEU:CD1	2.06	0.69
1:A:1329:VAL:HG21	1:A:1353:MSE:HE2	1.70	0.69
1:A:570:ARG:HD3	1:A:577:ASN:CG	2.12	0.69
1:A:683:LEU:C	1:A:683:LEU:HD23	2.13	0.69
1:A:796:SER:N	1:A:797:ASP:HA	2.08	0.69
1:B:616:ASP:O	1:B:620:VAL:CG2	2.40	0.69
1:B:897:ASN:CG	1:B:1059:TYR:HE2	1.96	0.69
1:B:634:VAL:O	1:B:638:LEU:CB	2.41	0.69
1:A:1329:VAL:HG21	1:A:1353:MSE:HE1	1.69	0.69
1:A:670:LEU:H	1:A:670:LEU:CD1	2.02	0.69
1:B:1075:ILE:HD11	1:B:1290:PRO:HG2	1.74	0.69
1:B:914:PHE:CD1	1:B:916:ASP:CB	2.75	0.69
1:B:921:THR:OG1	1:B:924:GLU:CB	2.41	0.69
1:B:1267:SER:HA	1:B:1270:ASN:O	1.93	0.68
1:B:1348:ILE:CG2	1:B:1348:ILE:O	2.38	0.68
1:A:1149:TYR:OH	1:A:1361:LEU:CD2	2.41	0.68
1:B:1044:GLN:O	1:B:1046:ILE:HD13	1.93	0.68
1:B:1059:TYR:CA	1:B:1060:LYS:CB	2.72	0.68
1:A:362:ILE:HG12	1:A:367:ILE:CD1	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:LYS:O	1:A:371:ILE:HG23	1.93	0.68
1:A:608:ARG:HG2	1:A:608:ARG:NH1	2.06	0.68
1:B:897:ASN:HB2	1:B:1058:ILE:CD1	2.12	0.68
1:A:516:LEU:HD11	1:A:1197:ARG:HE	1.58	0.68
1:B:1058:ILE:HD12	1:B:1059:TYR:CE2	2.28	0.68
1:A:464:ASN:OD1	1:A:467:ILE:HG12	1.94	0.68
1:A:738:LYS:HB2	1:A:746:ILE:CG1	2.24	0.68
1:A:351:LYS:HA	1:A:354:ILE:HD12	1.76	0.68
1:B:485:MSE:HE2	1:B:1202:ILE:HD11	1.75	0.67
1:B:614:GLN:O	1:B:615:ASP:O	2.12	0.67
1:A:431:ILE:HG12	1:A:472:ILE:HD13	1.75	0.67
1:B:432:TYR:HE1	1:B:436:LYS:NZ	1.91	0.67
1:A:1017:ASN:HB3	1:A:1020:PHE:HB2	1.76	0.67
1:B:1035:MSE:O	1:B:1038:GLU:OE1	2.12	0.67
1:B:1044:GLN:HA	1:B:1048:TYR:CZ	2.29	0.67
1:B:1364:GLU:HG2	1:B:1365:SER:N	2.09	0.67
1:A:519:ILE:HD13	1:A:601:LEU:HD21	1.75	0.67
1:B:1269:ILE:CB	1:B:1270:ASN:HB2	2.23	0.67
1:B:358:PHE:CZ	1:B:427:LEU:HG	2.28	0.67
1:A:495:ILE:HD11	1:A:508:LEU:HD22	1.76	0.67
1:B:1056:LEU:O	1:B:1058:ILE:HG22	1.94	0.67
1:B:510:ALA:HB3	1:B:866:LEU:HD21	1.75	0.67
1:A:404:PHE:HD1	1:A:404:PHE:H	1.40	0.67
1:A:459:ILE:N	1:A:459:ILE:HD12	2.03	0.67
1:B:463:LEU:HD22	1:B:463:LEU:C	2.15	0.67
1:B:351:LYS:HE3	1:B:483:HIS:ND1	2.10	0.67
1:B:424:GLU:HA	1:B:427:LEU:HD13	1.76	0.67
1:B:1291:PHE:HZ	1:B:1378:LEU:HD12	1.59	0.66
1:A:518:LEU:CD2	1:A:855:ILE:HD11	2.22	0.66
1:A:900:LEU:HB3	1:A:1056:LEU:HD22	1.76	0.66
1:A:1322:PHE:HB3	1:A:1331:LEU:HD21	1.77	0.66
1:A:1366:TYR:CE1	1:A:1367:ASN:HB2	2.29	0.66
1:A:351:LYS:CA	1:A:354:ILE:HD12	2.25	0.66
1:A:493:ASN:OD1	1:A:603:ALA:CB	2.42	0.66
1:B:351:LYS:CE	1:B:483:HIS:ND1	2.59	0.66
1:A:794:ASP:O	1:A:795:PHE:HD1	1.78	0.66
1:B:1059:TYR:CA	1:B:1060:LYS:HB2	2.26	0.66
1:B:1144:ILE:C	1:B:1145:GLN:HG3	2.15	0.66
1:B:358:PHE:CB	1:B:480:THR:HG21	2.25	0.66
1:B:606:LYS:HB2	1:B:1219:THR:CG2	2.25	0.66
1:B:914:PHE:HA	1:B:915:ASP:HB3	1.72	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:638:LEU:HG	1:A:891:CYS:CB	2.25	0.66
1:B:550:ASP:N	1:B:550:ASP:OD1	2.28	0.66
1:B:606:LYS:HD3	1:B:1219:THR:HG21	1.76	0.66
1:A:637:ALA:CB	1:A:820:ARG:HH12	2.08	0.66
1:B:644:PHE:CE2	1:B:651:ILE:HD11	2.29	0.66
1:A:394:GLY:HA2	1:A:395:ASN:CB	2.12	0.66
1:A:398:THR:OG1	1:A:443:LEU:HD13	1.95	0.66
1:B:1358:VAL:CG1	1:B:1365:SER:HB3	2.26	0.66
1:A:1008:SER:O	1:A:1012:CYS:SG	2.50	0.66
1:A:1050:LYS:HA	1:A:1050:LYS:HE2	1.76	0.66
1:B:1358:VAL:HG22	1:B:1359:SER:H	1.60	0.66
1:B:565:LYS:HA	1:B:568:ILE:HD12	1.77	0.66
1:B:1355:PRO:CB	1:B:1368:SER:HB2	2.24	0.66
1:A:544:ILE:HD13	1:A:555:TYR:CD2	2.30	0.65
1:A:570:ARG:CD	1:A:577:ASN:OD1	2.33	0.65
1:B:1142:LYS:HG2	1:B:1144:ILE:N	2.11	0.65
1:B:1192:MSE:CE	1:B:1278:ARG:HG2	2.26	0.65
1:B:1357:LYS:HA	1:B:1363:LEU:O	1.96	0.65
1:A:439:ILE:CD1	1:A:442:ILE:CD1	2.66	0.65
1:B:892:ILE:C	1:B:892:ILE:HD12	2.15	0.65
1:A:1371:ILE:CG2	1:A:1375:ILE:HD11	2.25	0.65
1:A:792:LEU:O	1:A:792:LEU:HD13	1.95	0.65
1:A:666:ASP:N	1:A:666:ASP:OD1	2.29	0.65
1:B:503:ASP:OD1	1:B:503:ASP:N	2.29	0.65
1:A:1102:ASN:O	1:A:1106:GLU:HB2	1.96	0.65
1:A:806:LYS:N	1:A:809:ILE:CD1	2.59	0.65
1:B:615:ASP:N	1:B:615:ASP:OD2	2.24	0.65
1:A:738:LYS:HB2	1:A:746:ILE:CD1	2.26	0.65
1:A:792:LEU:C	1:A:792:LEU:HD13	2.17	0.65
1:B:489:LYS:HD3	1:B:508:LEU:HD13	1.79	0.65
1:A:705:ALA:O	1:A:709:VAL:HG23	1.97	0.65
1:B:421:SER:HB3	1:B:424:GLU:OE1	1.97	0.65
1:B:380:ILE:O	1:B:384:ILE:HB	1.97	0.65
1:A:462:ILE:HG22	1:A:464:ASN:N	2.12	0.65
1:B:1048:TYR:N	1:B:1057:TYR:CB	2.58	0.65
1:B:1329:VAL:HG11	1:B:1353:MSE:CE	2.27	0.65
1:B:557:LEU:HD21	1:B:575:ILE:CD1	2.26	0.65
1:B:917:PHE:O	1:B:918:LYS:HG3	1.95	0.65
1:A:463:LEU:O	1:A:463:LEU:HD13	1.97	0.64
1:A:892:ILE:O	1:A:896:TRP:CB	2.44	0.64
1:B:1099:ILE:CA	1:B:1103:LYS:CB	2.75	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1358:VAL:O	1:B:1359:SER:HB2	1.97	0.64
1:B:913:ASP:O	1:B:915:ASP:HB2	1.96	0.64
1:B:946:ASN:HA	1:B:949:ASP:HB3	1.79	0.64
1:B:492:HIS:CE1	1:B:1200:HIS:CD2	2.84	0.64
1:A:459:ILE:CD1	1:A:460:GLU:H	2.11	0.64
1:A:518:LEU:HD23	1:A:855:ILE:CD1	2.27	0.64
1:B:1045:GLU:O	1:B:1057:TYR:CD2	2.50	0.64
1:B:987:ASN:HB3	1:B:990:ASP:HB2	1.79	0.64
1:A:576:ASP:O	1:A:578:LYS:N	2.31	0.64
1:A:410:VAL:C	1:A:412:PHE:HA	2.18	0.64
1:A:535:ARG:HH11	1:A:535:ARG:CG	2.11	0.64
1:A:732:PHE:CD1	1:A:784:TYR:CE2	2.72	0.64
1:A:806:LYS:N	1:A:809:ILE:HD12	2.12	0.64
1:B:490:LEU:HA	1:B:495:ILE:HG13	1.79	0.64
1:B:842:ILE:O	1:B:846:LEU:CD1	2.46	0.64
1:A:1356:LYS:HB3	1:A:1368:SER:HG	1.61	0.64
1:B:914:PHE:N	1:B:915:ASP:HB2	2.12	0.64
1:A:1298:GLU:HA	1:A:1343:ILE:CB	2.28	0.64
1:A:987:ASN:HD21	1:A:990:ASP:HB2	1.62	0.64
1:B:1277:ILE:HG22	1:B:1294:TYR:HE1	1.62	0.64
1:B:1023:LYS:HA	1:B:1026:LYS:HB3	1.79	0.64
1:B:1071:ASN:HD22	1:B:1075:ILE:HG13	1.63	0.64
1:B:463:LEU:HD23	1:B:468:LEU:HD13	1.79	0.63
1:B:665:ASN:O	1:B:666:ASP:OD1	2.16	0.63
1:B:852:ILE:HG22	1:B:882:MSE:HE2	1.81	0.63
1:B:975:ILE:CG2	1:B:976:LEU:CB	2.76	0.63
1:A:732:PHE:CE1	1:A:784:TYR:CD2	2.86	0.63
1:A:888:ARG:HG2	1:A:888:ARG:O	1.98	0.63
1:B:1059:TYR:HA	1:B:1060:LYS:CB	2.29	0.63
1:B:492:HIS:HE1	1:B:1200:HIS:CD2	2.16	0.63
1:A:821:ILE:HG22	1:A:822:THR:N	2.13	0.63
1:B:900:LEU:CD2	1:B:901:GLU:H	2.09	0.63
1:A:670:LEU:N	1:A:670:LEU:HD13	2.08	0.63
1:A:868:THR:HG23	1:A:869:SER:N	2.13	0.63
1:B:1358:VAL:HG22	1:B:1359:SER:N	2.13	0.63
1:B:400:ILE:O	1:B:403:ILE:CB	2.46	0.63
1:A:1048:TYR:HD1	1:A:1049:PRO:O	1.81	0.63
1:A:1348:ILE:O	1:A:1348:ILE:CG2	2.46	0.63
1:A:473:LEU:HD22	1:A:477:LYS:HE3	1.81	0.63
1:A:738:LYS:HE2	1:A:746:ILE:HG12	1.80	0.63
1:A:399:GLU:HG3	1:A:400:ILE:CD1	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:913:ASP:HA	1:A:1013:ARG:HH22	1.60	0.63
1:B:490:LEU:HD22	1:B:495:ILE:CG2	2.17	0.63
1:B:684:TYR:N	1:B:685:ARG:HB2	2.13	0.63
1:A:463:LEU:N	1:A:463:LEU:HD12	2.06	0.63
1:A:554:ASN:N	1:A:555:TYR:HA	2.14	0.63
1:A:608:ARG:CG	1:A:608:ARG:HH11	2.12	0.63
1:A:659:ILE:HG22	1:A:719:LEU:O	1.99	0.63
1:A:685:ARG:HH11	1:A:685:ARG:HG2	1.64	0.63
1:A:735:GLU:O	1:A:739:THR:HG23	1.99	0.63
1:A:732:PHE:HA	1:A:784:TYR:OH	1.98	0.63
1:A:439:ILE:HD12	1:A:442:ILE:HD12	1.81	0.62
1:B:1140:PHE:C	1:B:1142:LYS:HA	2.20	0.62
1:A:1026:LYS:HB2	1:A:1026:LYS:NZ	2.13	0.62
1:A:1346:ASN:HB3	1:A:1349:LEU:HB2	1.81	0.62
1:B:1099:ILE:O	1:B:1103:LYS:N	2.32	0.62
1:B:364:ASN:H	1:B:364:ASN:ND2	1.96	0.62
1:A:756:LYS:HA	1:A:759:GLN:HG2	1.82	0.62
1:B:897:ASN:CG	1:B:1059:TYR:CE2	2.73	0.62
1:A:1354:LYS:HB2	1:A:1354:LYS:HZ2	1.63	0.62
1:A:1367:ASN:O	1:A:1371:ILE:HD12	1.98	0.62
1:B:643:VAL:O	1:B:643:VAL:HG12	2.00	0.62
1:B:842:ILE:O	1:B:846:LEU:HD12	2.00	0.62
1:A:1371:ILE:HG22	1:A:1375:ILE:HD12	1.80	0.62
1:A:350:LYS:HA	1:A:351:LYS:HB3	1.81	0.62
1:B:378:PHE:CE2	1:B:435:LEU:HD13	2.34	0.62
1:A:1359:SER:HB3	1:A:1363:LEU:HD12	1.82	0.62
1:A:1371:ILE:CG2	1:A:1375:ILE:CD1	2.76	0.62
1:B:913:ASP:O	1:B:915:ASP:CB	2.47	0.62
1:A:1285:TYR:HA	1:A:1288:ARG:HG2	1.81	0.62
1:B:1191:GLN:NE2	1:B:1194:ARG:HH21	1.98	0.62
1:B:892:ILE:HD12	1:B:893:THR:HA	1.81	0.62
1:B:907:MSE:O	1:B:911:GLU:HG2	1.99	0.62
1:A:623:ILE:HG23	1:A:830:ILE:HB	1.82	0.61
1:B:892:ILE:CD1	1:B:893:THR:N	2.58	0.61
1:A:775:LYS:HZ3	1:A:775:LYS:HB2	1.64	0.61
1:A:1060:LYS:NZ	1:A:1170:GLU:OE2	2.33	0.61
1:A:599:ARG:NH2	1:A:606:LYS:O	2.34	0.61
1:B:1144:ILE:O	1:B:1144:ILE:HG22	2.01	0.61
1:B:684:TYR:CA	1:B:685:ARG:HB2	2.30	0.61
1:B:900:LEU:HD13	1:B:1056:LEU:CD1	2.30	0.61
1:B:1048:TYR:CD1	1:B:1052:ARG:CA	2.63	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:936:ASN:O	1:B:940:GLU:HG3	1.99	0.61
1:A:1090:PHE:CB	1:A:1162:TYR:CE1	2.82	0.61
1:A:384:ILE:HD11	1:A:463:LEU:CD1	2.31	0.61
1:A:401:PHE:HA	1:A:403:ILE:HD13	1.82	0.61
1:A:632:GLU:O	1:A:634:VAL:N	2.34	0.61
1:B:1045:GLU:O	1:B:1057:TYR:HD2	1.83	0.61
1:A:638:LEU:HG	1:A:891:CYS:HA	1.82	0.61
1:B:900:LEU:CD1	1:B:1056:LEU:CD1	2.78	0.61
1:B:519:ILE:HD11	1:B:600:ILE:HB	1.81	0.61
1:A:638:LEU:C	1:A:638:LEU:HD22	2.21	0.61
1:A:655:ASN:OD1	1:A:655:ASN:N	2.33	0.61
1:B:748:GLU:O	1:B:749:ASN:HB3	2.01	0.61
1:B:697:GLU:O	1:B:701:ILE:HG12	2.01	0.61
1:A:1148:ASN:ND2	1:A:1151:SER:HB3	2.16	0.61
1:A:384:ILE:CD1	1:A:463:LEU:CD1	2.79	0.61
1:B:582:THR:CB	1:B:583:ASN:CG	2.41	0.61
1:A:1050:LYS:CE	1:A:1050:LYS:HA	2.29	0.61
1:A:1277:ILE:HD12	1:A:1277:ILE:O	2.01	0.61
1:B:1058:ILE:HB	1:B:1059:TYR:CE1	2.35	0.61
1:B:439:ILE:C	1:B:442:ILE:HB	2.21	0.61
1:B:1048:TYR:CE1	1:B:1052:ARG:CB	2.84	0.60
1:B:809:ILE:O	1:B:810:LYS:C	2.37	0.60
1:B:1046:ILE:N	1:B:1046:ILE:HD13	2.02	0.60
1:B:809:ILE:O	1:B:811:ASP:N	2.33	0.60
1:A:1207:ARG:HD3	1:A:1214:LEU:HD22	1.82	0.60
1:A:1349:LEU:O	1:A:1351:ARG:HB3	2.01	0.60
1:B:1360:VAL:HG12	1:B:1360:VAL:O	2.00	0.60
1:B:1358:VAL:CG2	1:B:1359:SER:H	2.14	0.60
1:A:914:PHE:H	1:A:1013:ARG:HH22	1.48	0.60
1:B:667:ILE:O	1:B:667:ILE:HG12	2.00	0.60
1:A:713:LEU:HD21	1:A:785:LEU:HD21	1.83	0.60
1:A:933:ILE:HG13	1:A:998:TYR:HE2	1.66	0.60
1:B:1291:PHE:CD1	1:B:1381:LYS:HB3	2.36	0.60
1:A:957:LYS:O	1:A:958:ILE:HD12	2.01	0.60
1:B:1274:ASN:O	1:B:1277:ILE:HG12	2.02	0.60
1:A:389:LYS:O	1:A:390:GLU:CB	2.50	0.60
1:A:561:ILE:HG22	1:A:562:LEU:CA	2.11	0.60
1:B:1091:LEU:O	1:B:1162:TYR:HE1	1.85	0.60
1:B:723:LEU:HD23	1:B:727:GLU:CG	2.23	0.60
1:B:983:LEU:O	1:B:986:ILE:HG13	2.01	0.60
1:A:1013:ARG:O	1:A:1014:ILE:HB	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1063:LEU:HD12	1:A:1171:PHE:CZ	2.37	0.60
1:A:920:GLN:NE2	1:A:1006:ILE:CD1	2.65	0.60
1:B:1058:ILE:CD1	1:B:1059:TYR:CE2	2.85	0.60
1:B:1191:GLN:HG3	1:B:1307:LEU:HD21	1.84	0.60
1:B:434:TYR:HE2	1:B:468:LEU:CG	2.15	0.60
1:B:467:ILE:HG23	1:B:468:LEU:HD13	1.83	0.60
1:B:533:PHE:HE1	1:B:557:LEU:HD13	1.64	0.60
1:B:917:PHE:HD1	1:B:917:PHE:H	1.50	0.60
1:B:1079:ILE:H	1:B:1079:ILE:HD12	1.67	0.59
1:B:583:ASN:HB2	1:B:586:ILE:HB	1.82	0.59
1:A:667:ILE:HG23	1:A:667:ILE:O	2.01	0.59
1:A:683:LEU:HD22	1:A:793:PHE:HE2	1.63	0.59
1:A:733:LEU:HD12	1:A:751:ILE:CD1	2.32	0.59
1:A:493:ASN:O	1:A:494:ASP:HB3	2.01	0.59
1:B:975:ILE:HG23	1:B:976:LEU:CB	2.32	0.59
1:A:738:LYS:CB	1:A:746:ILE:HG12	2.29	0.59
1:B:1277:ILE:HG22	1:B:1294:TYR:CE1	2.37	0.59
1:B:381:ASP:O	1:B:384:ILE:CG2	2.45	0.59
1:B:400:ILE:HD13	1:B:400:ILE:N	2.16	0.59
1:B:1141:ALA:HB3	1:B:1142:LYS:O	2.02	0.59
1:B:1075:ILE:CD1	1:B:1290:PRO:HG2	2.32	0.59
1:B:424:GLU:O	1:B:427:LEU:HD13	2.01	0.59
1:A:394:GLY:CA	1:A:395:ASN:HB3	2.18	0.59
1:A:932:ASP:OD1	1:A:932:ASP:N	2.34	0.59
1:B:1060:LYS:HE2	1:B:1060:LYS:H	1.62	0.59
1:B:1212:ILE:HG12	1:B:1252:PHE:HB2	1.84	0.59
1:A:393:LYS:H	1:A:394:GLY:HA2	1.68	0.59
1:A:958:ILE:HG22	1:A:958:ILE:O	2.02	0.59
1:B:405:LYS:O	1:B:409:LYS:N	2.36	0.59
1:B:630:SER:CA	1:B:631:ASP:HB2	2.28	0.59
1:B:666:ASP:C	1:B:667:ILE:HG22	2.23	0.59
1:A:1367:ASN:CG	1:A:1371:ILE:HD12	2.23	0.59
1:B:666:ASP:O	1:B:667:ILE:C	2.39	0.59
1:A:793:PHE:N	1:A:793:PHE:HD1	2.00	0.59
1:B:606:LYS:O	1:B:606:LYS:HG2	2.03	0.59
1:A:1152:PHE:HA	1:A:1155:ASP:HB2	1.85	0.58
1:A:404:PHE:O	1:A:408:TYR:N	2.33	0.58
1:A:459:ILE:O	1:A:460:GLU:HB3	2.03	0.58
1:A:683:LEU:HD22	1:A:793:PHE:CD2	2.28	0.58
1:B:461:LYS:HG3	1:B:462:ILE:CG1	2.32	0.58
1:B:568:ILE:HA	1:B:625:GLN:HE22	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:GLY:N	1:A:549:GLY:HA2	2.18	0.58
1:A:696:ILE:HA	1:A:698:THR:N	2.18	0.58
1:A:1266:ASN:OD1	1:A:1266:ASN:N	2.35	0.58
1:A:555:TYR:O	1:A:581:ILE:HD12	2.02	0.58
1:A:727:GLU:CB	1:A:728:SER:HA	2.33	0.58
1:B:1147:LYS:CB	1:B:1148:ASN:HA	2.32	0.58
1:A:1152:PHE:O	1:A:1156:TYR:N	2.35	0.58
1:A:368:LYS:O	1:A:371:ILE:CG2	2.52	0.58
1:A:436:LYS:O	1:A:440:GLU:N	2.30	0.58
1:A:457:ILE:CG2	1:A:457:ILE:O	2.51	0.58
1:A:667:ILE:CG1	1:A:718:ILE:HD12	2.24	0.58
1:A:401:PHE:HB3	1:A:404:PHE:HE1	1.68	0.58
1:B:491:ARG:HE	1:B:1207:ARG:NH2	1.95	0.58
1:A:399:GLU:CD	1:A:400:ILE:CD1	2.72	0.58
1:A:411:ASN:CB	1:A:414:SER:H	2.17	0.58
1:A:535:ARG:HH11	1:A:535:ARG:HB2	1.68	0.58
1:B:897:ASN:CB	1:B:1059:TYR:CE2	2.77	0.58
1:B:524:SER:O	1:B:527:MSE:HG3	2.04	0.58
1:A:659:ILE:CG2	1:A:720:GLU:CA	2.79	0.58
1:B:748:GLU:OE1	1:B:749:ASN:OD1	2.22	0.58
1:A:678:PRO:O	1:A:682:ASN:N	2.35	0.58
1:A:848:SER:HB2	1:A:851:VAL:HG23	1.86	0.58
1:B:432:TYR:HA	1:B:435:LEU:HD12	1.86	0.58
1:B:439:ILE:O	1:B:442:ILE:CB	2.41	0.58
1:B:630:SER:HA	1:B:631:ASP:CB	2.29	0.58
1:A:673:PHE:HD1	1:A:714:TYR:CD2	2.22	0.58
1:B:1271:LYS:O	1:B:1274:ASN:N	2.37	0.58
1:B:532:ILE:CG2	1:B:562:LEU:HD13	2.32	0.58
1:A:1118:LEU:N	1:A:1125:TYR:CE1	2.72	0.57
1:A:1271:LYS:HB3	1:A:1275:GLU:HB3	1.85	0.57
1:A:560:LYS:C	1:A:561:ILE:CG1	2.65	0.57
1:B:1058:ILE:HG13	1:B:1059:TYR:CE2	2.38	0.57
1:B:373:LYS:O	1:B:377:GLU:N	2.37	0.57
1:A:1015:ILE:CG2	1:A:1016:PHE:CD1	2.86	0.57
1:A:1119:ASN:CB	1:A:1120:GLY:HA2	2.29	0.57
1:A:1383:GLU:HA	1:A:1383:GLU:OE2	2.04	0.57
1:A:590:THR:O	1:A:594:THR:HG23	2.05	0.57
1:A:649:ASN:O	1:A:652:THR:N	2.37	0.57
1:A:979:GLU:CG	1:A:982:LYS:CB	2.82	0.57
1:B:562:LEU:CD1	1:B:565:LYS:HZ1	2.13	0.57
1:A:673:PHE:O	1:A:675:LYS:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:638:LEU:HG	1:A:891:CYS:CA	2.34	0.57
1:A:973:SER:HB3	1:A:975:ILE:H	1.68	0.57
1:A:1322:PHE:HE2	1:A:1352:LEU:HD12	1.69	0.57
1:B:1051:GLU:HB3	1:B:1054:ASN:HB2	1.86	0.57
1:B:929:TYR:CE2	1:B:1006:ILE:HD11	2.40	0.57
1:B:1269:ILE:CA	1:B:1270:ASN:HB2	2.34	0.57
1:B:574:PHE:HB3	1:B:586:ILE:HG12	1.85	0.57
1:A:568:ILE:CD1	1:A:625:GLN:NE2	2.67	0.57
1:A:637:ALA:HB3	1:A:820:ARG:NH1	2.16	0.57
1:A:720:GLU:HG2	1:A:721:ASP:O	2.03	0.57
1:A:749:ASN:O	1:A:749:ASN:OD1	2.22	0.57
1:A:461:LYS:HA	1:A:461:LYS:CE	2.32	0.57
1:A:631:ASP:N	1:A:631:ASP:OD1	2.37	0.57
1:B:1079:ILE:O	1:B:1083:ILE:HG13	2.04	0.57
1:B:528:GLU:O	1:B:565:LYS:NZ	2.35	0.57
1:B:671:PRO:CB	1:B:675:LYS:HZ2	2.17	0.57
1:B:886:THR:O	1:B:890:GLU:HB2	2.03	0.57
1:B:975:ILE:HG23	1:B:976:LEU:CA	2.34	0.57
1:A:1102:ASN:OD1	1:A:1102:ASN:N	2.36	0.57
1:A:659:ILE:CG2	1:A:719:LEU:C	2.73	0.57
1:A:804:GLU:O	1:A:805:ILE:O	2.22	0.57
1:B:606:LYS:HB2	1:B:1219:THR:HG21	1.86	0.57
1:B:533:PHE:HD1	1:B:557:LEU:HD12	1.68	0.57
1:B:753:ASN:O	1:B:757:ASN:N	2.36	0.57
1:B:1059:TYR:CD1	1:B:1059:TYR:N	2.73	0.57
1:B:1263:LEU:HA	1:B:1270:ASN:ND2	2.19	0.57
1:B:1156:TYR:OH	1:B:1365:SER:HA	2.05	0.57
1:B:384:ILE:HG23	1:B:385:LYS:N	2.19	0.57
1:B:478:GLN:O	1:B:478:GLN:HG2	2.04	0.57
1:B:588:LYS:HZ2	1:B:614:GLN:CB	2.17	0.57
1:B:774:GLN:O	1:B:778:ILE:HG12	2.05	0.57
1:A:1315:ASN:ND2	1:A:1336:LEU:O	2.38	0.57
1:A:729:LYS:O	1:A:730:ASN:HB2	2.05	0.57
1:B:537:ASN:O	1:B:538:ILE:HG22	2.04	0.57
1:B:606:LYS:HB2	1:B:1219:THR:CB	2.34	0.57
1:A:685:ARG:NH1	1:A:685:ARG:HG2	2.20	0.56
1:A:917:PHE:CD1	1:A:917:PHE:N	2.73	0.56
1:B:605:SER:HB3	1:B:1219:THR:OG1	2.04	0.56
1:A:1099:ILE:O	1:A:1103:LYS:HB2	2.05	0.56
1:A:541:ASP:OD1	1:A:1273:GLU:CB	2.43	0.56
1:A:793:PHE:N	1:A:793:PHE:CD1	2.73	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:921:THR:OG1	1:A:924:GLU:CB	2.53	0.56
1:B:1091:LEU:HA	1:B:1093:ASN:N	2.20	0.56
1:A:902:GLU:HG3	1:A:1057:TYR:CD2	2.40	0.56
1:A:1105:SER:O	1:A:1109:ALA:N	2.37	0.56
1:A:412:PHE:O	1:A:413:ASP:HB3	2.06	0.56
1:A:733:LEU:HD12	1:A:751:ILE:HD11	1.88	0.56
1:A:946:ASN:O	1:A:950:VAL:N	2.37	0.56
1:A:937:ILE:HG21	1:A:953:LYS:HZ1	1.69	0.56
1:B:606:LYS:CD	1:B:1219:THR:HG21	2.34	0.56
1:A:900:LEU:CG	1:A:1056:LEU:HD22	2.35	0.56
1:A:401:PHE:HB3	1:A:402:GLY:HA2	1.86	0.56
1:A:640:LEU:N	1:A:640:LEU:HD23	2.20	0.56
1:B:1059:TYR:H	1:B:1060:LYS:HB2	1.67	0.56
1:B:666:ASP:O	1:B:667:ILE:CG2	2.53	0.56
1:B:669:TYR:HB3	1:B:755:TYR:OH	2.06	0.56
1:B:900:LEU:CD2	1:B:901:GLU:N	2.62	0.56
1:B:975:ILE:CG2	1:B:976:LEU:CA	2.83	0.56
1:A:648:LYS:CB	1:A:650:ILE:CD1	2.84	0.56
1:B:560:LYS:CE	1:B:563:ASN:CB	2.84	0.56
1:B:975:ILE:HG23	1:B:976:LEU:HA	1.86	0.56
1:A:632:GLU:C	1:A:634:VAL:N	2.59	0.56
1:A:648:LYS:CB	1:A:650:ILE:HG13	2.35	0.56
1:A:772:LYS:O	1:A:776:LYS:HG3	2.06	0.56
1:B:674:SER:HB3	1:B:876:ASP:CG	2.25	0.56
1:A:1079:ILE:HD11	1:A:1177:ILE:HD12	1.86	0.56
1:B:930:TYR:OH	1:B:953:LYS:HB3	2.06	0.56
1:A:1192:MSE:HE2	1:A:1278:ARG:HB2	1.86	0.56
1:A:435:LEU:O	1:A:439:ILE:HG12	2.06	0.56
1:A:649:ASN:O	1:A:652:THR:HB	2.06	0.56
1:A:820:ARG:HB3	1:A:820:ARG:CZ	2.35	0.56
1:B:609:ASP:O	1:B:611:GLN:N	2.31	0.56
1:A:729:LYS:O	1:A:729:LYS:HD3	2.06	0.56
1:B:1259:PHE:N	1:B:1259:PHE:CD1	2.73	0.56
1:B:358:PHE:HB3	1:B:480:THR:HG21	1.87	0.56
1:A:1049:PRO:HD2	1:A:1056:LEU:O	2.05	0.56
1:B:1141:ALA:HB3	1:B:1143:ASN:N	2.20	0.56
1:B:1267:SER:CB	1:B:1268:GLU:HA	2.07	0.56
1:B:659:ILE:CB	1:B:719:LEU:HB3	2.36	0.56
1:A:404:PHE:CZ	1:A:439:ILE:CG2	2.71	0.55
1:B:1041:ASN:C	1:B:1042:LYS:O	2.44	0.55
1:B:823:VAL:HG12	1:B:824:LYS:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1123:LYS:O	1:A:1127:GLU:CB	2.54	0.55
1:B:481:LEU:HD21	1:B:1259:PHE:HD2	1.69	0.55
1:B:535:ARG:CD	1:B:540:ASN:O	2.50	0.55
1:A:507:ARG:HG2	1:A:866:LEU:HD22	1.88	0.55
1:A:547:PHE:N	1:A:547:PHE:CD1	2.72	0.55
1:A:732:PHE:CD1	1:A:784:TYR:CG	2.93	0.55
1:B:981:ARG:HG3	1:B:982:LYS:N	2.21	0.55
1:A:580:ASN:O	1:A:581:ILE:C	2.44	0.55
1:A:902:GLU:OE2	1:A:1057:TYR:CD2	2.58	0.55
1:B:892:ILE:HD11	1:B:1015:ILE:HD12	1.89	0.55
1:B:1047:TYR:CD1	1:B:1047:TYR:N	2.73	0.55
1:A:1093:ASN:O	1:A:1094:ILE:HB	2.07	0.55
1:A:729:LYS:HD2	1:A:788:ASN:OD1	2.07	0.55
1:B:1350:GLU:HA	1:B:1352:LEU:HD13	1.89	0.55
1:B:461:LYS:HG3	1:B:462:ILE:HG13	1.88	0.55
1:A:1228:ARG:HD2	1:A:1265:GLU:HG3	1.89	0.55
1:A:798:PHE:CD1	1:A:799:LYS:N	2.73	0.55
1:A:806:LYS:H	1:A:809:ILE:CD1	2.18	0.55
1:B:1322:PHE:HZ	1:B:1342:LEU:HD21	1.71	0.55
1:B:1115:ASN:OD1	1:B:1360:VAL:HG23	2.06	0.55
1:B:398:THR:O	1:B:402:GLY:N	2.32	0.55
1:B:552:GLU:CA	1:B:553:LYS:CB	2.85	0.55
1:B:657:ILE:H	1:B:657:ILE:HD13	1.72	0.55
1:A:1356:LYS:CB	1:A:1368:SER:OG	2.45	0.55
1:A:404:PHE:CD1	1:A:404:PHE:N	2.73	0.55
1:A:673:PHE:HD1	1:A:714:TYR:HD2	1.53	0.55
1:A:738:LYS:HE3	1:A:746:ILE:CG1	2.30	0.55
1:A:1277:ILE:CD1	1:A:1281:ILE:CD1	2.77	0.55
1:A:1188:LEU:HD22	1:A:1303:VAL:HG21	1.89	0.55
1:A:401:PHE:CD1	1:A:401:PHE:N	2.73	0.55
1:A:735:GLU:HB3	1:A:784:TYR:HE2	1.72	0.55
1:B:667:ILE:O	1:B:667:ILE:HG23	2.06	0.55
1:B:917:PHE:N	1:B:917:PHE:CD1	2.73	0.55
1:A:464:ASN:HD21	1:A:467:ILE:CG1	2.07	0.54
1:B:1188:LEU:HD22	1:B:1303:VAL:HG21	1.88	0.54
1:B:493:ASN:N	1:B:493:ASN:OD1	2.40	0.54
1:B:631:ASP:OD2	1:B:888:ARG:HA	2.07	0.54
1:B:986:ILE:HD12	1:B:986:ILE:C	2.27	0.54
1:A:1044:GLN:HA	1:A:1048:TYR:CE1	2.42	0.54
1:A:1357:LYS:HD2	1:A:1357:LYS:C	2.26	0.54
1:A:738:LYS:NZ	1:A:743:ILE:HA	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:786:ARG:O	1:A:790:GLU:HB2	2.06	0.54
1:A:792:LEU:CD1	1:A:793:PHE:CD1	2.85	0.54
1:B:1130:ILE:HG22	1:B:1130:ILE:O	2.05	0.54
1:B:659:ILE:CB	1:B:719:LEU:C	2.75	0.54
1:A:1096:GLY:HA2	1:A:1099:ILE:HG12	1.88	0.54
1:A:461:LYS:CA	1:A:461:LYS:CE	2.85	0.54
1:A:647:LYS:CB	1:A:648:LYS:CB	2.86	0.54
1:B:463:LEU:HD13	1:B:463:LEU:C	2.27	0.54
1:B:671:PRO:HB3	1:B:675:LYS:NZ	2.22	0.54
1:A:544:ILE:CG2	1:A:555:TYR:HE2	2.21	0.54
1:A:694:ASP:CB	1:A:800:MSE:HG2	2.38	0.54
1:A:941:PHE:O	1:A:946:ASN:ND2	2.41	0.54
1:B:1136:ASN:OD1	1:B:1149:TYR:CE1	2.61	0.54
1:B:538:ILE:O	1:B:538:ILE:HG23	2.08	0.54
1:B:608:ARG:HA	1:B:609:ASP:O	2.08	0.54
1:A:1032:ILE:HD13	1:A:1048:TYR:HD2	1.72	0.54
1:A:637:ALA:CB	1:A:820:ARG:NH1	2.69	0.54
1:B:1036:GLU:CB	1:B:1038:GLU:OE1	2.56	0.54
1:B:1256:CYS:O	1:B:1261:ILE:HG13	2.08	0.54
1:B:427:LEU:O	1:B:431:ILE:HG12	2.07	0.54
1:A:409:LYS:CA	1:A:410:VAL:CB	2.85	0.54
1:A:632:GLU:C	1:A:634:VAL:H	2.11	0.54
1:A:774:GLN:O	1:A:778:ILE:HG12	2.07	0.54
1:B:1044:GLN:HA	1:B:1048:TYR:OH	2.08	0.54
1:B:835:ASP:O	1:B:838:TYR:HB3	2.08	0.54
1:A:355:VAL:O	1:A:359:VAL:HG23	2.08	0.54
1:A:368:LYS:CA	1:A:371:ILE:HG22	2.38	0.54
1:A:375:LEU:HB3	1:A:380:ILE:HD11	1.86	0.54
1:A:1128:LYS:O	1:A:1132:LYS:NZ	2.41	0.54
1:A:568:ILE:CD1	1:A:625:GLN:HE22	2.16	0.54
1:A:733:LEU:O	1:A:737:LYS:HG3	2.08	0.54
1:A:409:LYS:CB	1:A:410:VAL:CB	2.85	0.53
1:B:913:ASP:C	1:B:915:ASP:HB2	2.28	0.53
1:B:671:PRO:CG	1:B:774:GLN:NE2	2.49	0.53
1:B:830:ILE:HG21	1:B:877:ILE:HG12	1.90	0.53
1:B:980:GLN:HG2	1:B:980:GLN:O	2.06	0.53
1:A:375:LEU:HD22	1:A:380:ILE:CD1	2.22	0.53
1:A:393:LYS:N	1:A:394:GLY:HA2	2.22	0.53
1:A:987:ASN:OD1	1:A:988:LYS:N	2.42	0.53
1:B:1265:GLU:CB	1:B:1266:ASN:CB	2.87	0.53
1:B:710:ASN:HA	1:B:713:LEU:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:PHE:CE2	1:A:435:LEU:HD12	2.43	0.53
1:A:383:LEU:O	1:A:386:LYS:HB2	2.09	0.53
1:B:1111:LEU:CD2	1:B:1359:SER:OG	2.46	0.53
1:A:1089:LYS:HD2	1:A:1089:LYS:N	1.94	0.53
1:A:461:LYS:NZ	1:A:461:LYS:O	2.35	0.53
1:A:662:GLU:HG3	1:A:663:ASN:N	2.24	0.53
1:A:673:PHE:CD1	1:A:714:TYR:HD2	2.26	0.53
1:B:393:LYS:N	1:B:394:GLY:HA2	2.24	0.53
1:B:609:ASP:C	1:B:611:GLN:H	2.12	0.53
1:B:684:TYR:N	1:B:685:ARG:CB	2.72	0.53
1:A:1299:GLN:HE22	1:A:1302:ARG:HH11	1.55	0.53
1:A:1177:ILE:HG23	1:A:1378:LEU:HD21	1.91	0.53
1:A:535:ARG:HG2	1:A:535:ARG:NH1	2.23	0.53
1:A:801:ASN:O	1:A:803:GLN:N	2.38	0.53
1:B:354:ILE:HG22	1:B:358:PHE:CE2	2.44	0.53
1:B:784:TYR:HE1	1:B:788:ASN:OD1	1.91	0.53
1:A:1291:PHE:O	1:A:1383:GLU:N	2.40	0.53
1:A:1359:SER:OG	1:A:1360:VAL:N	2.37	0.53
1:A:665:ASN:ND2	1:A:669:TYR:HE2	1.91	0.53
1:A:968:GLU:CA	1:A:969:ILE:CB	2.85	0.53
1:B:1141:ALA:CB	1:B:1142:LYS:C	2.73	0.53
1:B:884:LEU:O	1:B:888:ARG:N	2.41	0.53
1:A:613:THR:CG2	1:A:614:GLN:CA	2.85	0.53
1:B:1048:TYR:H	1:B:1057:TYR:N	1.98	0.53
1:A:900:LEU:CB	1:A:1056:LEU:HD22	2.38	0.53
1:A:973:SER:HB3	1:A:974:ASN:CA	2.38	0.53
1:B:1262:ASP:C	1:B:1263:LEU:HD12	2.30	0.53
1:B:1332:ASP:OD2	1:B:1354:LYS:HE2	2.09	0.53
1:B:654:ILE:O	1:B:657:ILE:HG12	2.09	0.53
1:A:1192:MSE:HE2	1:A:1278:ARG:CB	2.39	0.52
1:A:636:LYS:HA	1:A:638:LEU:CD1	2.39	0.52
1:A:1032:ILE:HD13	1:A:1048:TYR:CD2	2.45	0.52
1:A:738:LYS:HA	1:A:746:ILE:HG12	1.90	0.52
1:B:631:ASP:O	1:B:635:SER:HB3	2.09	0.52
1:A:411:ASN:N	1:A:412:PHE:CA	2.72	0.52
1:B:491:ARG:NH1	1:B:1208:GLU:OE1	2.43	0.52
1:B:807:LYS:H	1:B:807:LYS:HD2	1.73	0.52
1:A:1049:PRO:CD	1:A:1056:LEU:O	2.57	0.52
1:A:371:ILE:HD11	1:A:472:ILE:HG21	1.91	0.52
1:A:631:ASP:HB2	1:A:635:SER:HB3	1.91	0.52
1:B:1149:TYR:HA	1:B:1152:PHE:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1111:LEU:O	1:A:1115:ASN:N	2.40	0.52
1:A:409:LYS:N	1:A:410:VAL:CB	2.73	0.52
1:A:637:ALA:O	1:A:640:LEU:N	2.37	0.52
1:A:663:ASN:OD1	1:A:664:ASN:HB2	2.09	0.52
1:B:493:ASN:O	1:B:495:ILE:HG12	2.09	0.52
1:B:666:ASP:C	1:B:667:ILE:CG2	2.78	0.52
1:B:668:LYS:O	1:B:670:LEU:N	2.42	0.52
1:A:1052:ARG:HH12	1:A:1054:ASN:CB	2.22	0.52
1:A:1060:LYS:NZ	1:A:1170:GLU:CD	2.63	0.52
1:A:368:LYS:HA	1:A:371:ILE:HG22	1.92	0.52
1:A:659:ILE:HG22	1:A:719:LEU:C	2.30	0.52
1:A:669:TYR:CD1	1:A:755:TYR:CD2	2.71	0.52
1:B:1141:ALA:N	1:B:1142:LYS:CA	2.71	0.52
1:B:1062:ASN:ND2	1:B:1175:ASN:OD1	2.42	0.52
1:B:1357:LYS:CG	1:B:1362:GLU:OE1	2.57	0.52
1:B:673:PHE:O	1:B:674:SER:C	2.47	0.52
1:B:748:GLU:O	1:B:749:ASN:CB	2.57	0.52
1:A:407:HIS:O	1:A:411:ASN:HA	2.10	0.52
1:A:461:LYS:C	1:A:461:LYS:HZ1	2.12	0.52
1:A:664:ASN:HB3	1:A:665:ASN:OD1	2.10	0.52
1:B:388:GLU:CB	1:B:389:LYS:HA	2.38	0.52
1:B:408:TYR:O	1:B:411:ASN:N	2.43	0.52
1:B:436:LYS:CB	1:B:436:LYS:NZ	2.73	0.52
1:B:634:VAL:HG21	1:B:891:CYS:HG	1.69	0.52
1:B:900:LEU:O	1:B:902:GLU:N	2.42	0.52
1:A:1007:LYS:O	1:A:1010:ILE:HB	2.09	0.52
1:A:1052:ARG:NH1	1:A:1054:ASN:CB	2.73	0.52
1:A:1367:ASN:OD1	1:A:1371:ILE:HD12	2.09	0.52
1:A:439:ILE:HD13	1:A:442:ILE:HD11	1.90	0.52
1:B:1142:LYS:HZ1	1:B:1142:LYS:HB3	1.75	0.52
1:B:1358:VAL:CG2	1:B:1359:SER:N	2.73	0.52
1:B:531:LYS:CB	1:B:562:LEU:CD1	2.67	0.52
1:B:975:ILE:HG22	1:B:976:LEU:CB	2.37	0.52
1:A:821:ILE:CG2	1:A:822:THR:N	2.73	0.52
1:B:1269:ILE:N	1:B:1270:ASN:CB	2.73	0.52
1:B:427:LEU:N	1:B:427:LEU:HD12	2.21	0.52
1:B:807:LYS:HD2	1:B:807:LYS:N	2.24	0.52
1:A:418:SER:CB	1:A:419:LYS:CA	2.85	0.52
1:A:546:PHE:CD2	1:A:546:PHE:N	2.73	0.52
1:A:662:GLU:CG	1:A:663:ASN:N	2.73	0.52
1:B:1051:GLU:HB2	1:B:1055:GLU:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1069:ASN:HB3	1:B:1071:ASN:OD1	2.10	0.52
1:B:1079:ILE:N	1:B:1079:ILE:CD1	2.73	0.52
1:B:427:LEU:O	1:B:430:ILE:HG13	2.09	0.52
1:B:434:TYR:HE2	1:B:468:LEU:HG	1.75	0.52
1:B:683:LEU:O	1:B:684:TYR:C	2.47	0.52
1:B:492:HIS:HE1	1:B:1200:HIS:HD2	1.56	0.51
1:B:1357:LYS:NZ	1:B:1362:GLU:OE1	2.33	0.51
1:B:1044:GLN:C	1:B:1046:ILE:HD13	2.30	0.51
1:B:434:TYR:CE2	1:B:468:LEU:HG	2.45	0.51
1:B:746:ILE:HB	1:B:747:ASP:OD1	2.10	0.51
1:A:532:ILE:O	1:A:557:LEU:HD23	2.11	0.51
1:A:1010:ILE:O	1:A:1014:ILE:HB	2.10	0.51
1:A:888:ARG:HH11	1:A:888:ARG:HB2	1.75	0.51
1:A:994:LYS:HE3	1:A:994:LYS:O	2.11	0.51
1:B:1047:TYR:O	1:B:1048:TYR:HD2	1.93	0.51
1:B:378:PHE:N	1:B:379:LYS:HA	2.25	0.51
1:B:1059:TYR:N	1:B:1060:LYS:CB	2.72	0.51
1:B:1142:LYS:N	1:B:1143:ASN:CA	2.72	0.51
1:A:1024:TYR:CE1	1:A:1028:ILE:HD12	2.46	0.51
1:A:1329:VAL:CG2	1:A:1353:MSE:CE	2.59	0.51
1:A:1367:ASN:CG	1:A:1371:ILE:HD11	2.24	0.51
1:A:671:PRO:HG3	1:A:774:GLN:CG	2.26	0.51
1:B:1142:LYS:HZ2	1:B:1142:LYS:HB3	1.73	0.51
1:B:416:LYS:N	1:B:417:PHE:CA	2.74	0.51
1:B:682:ASN:C	1:B:685:ARG:HB3	2.31	0.51
1:B:837:GLU:HG2	1:B:874:ILE:HG12	1.93	0.51
1:A:638:LEU:CD2	1:A:639:ASN:ND2	2.73	0.51
1:B:1046:ILE:CD1	1:B:1046:ILE:H	1.97	0.51
1:B:1263:LEU:N	1:B:1263:LEU:CD1	2.73	0.51
1:B:438:ARG:NE	1:B:438:ARG:CA	2.73	0.51
1:B:640:LEU:HD22	1:B:701:ILE:CG2	2.41	0.51
1:A:399:GLU:OE2	1:A:400:ILE:CD1	2.59	0.51
1:A:548:GLY:N	1:A:549:GLY:CA	2.73	0.51
1:A:807:LYS:C	1:A:809:ILE:N	2.59	0.51
1:B:1078:LEU:HD23	1:B:1374:LEU:HD12	1.93	0.51
1:B:1291:PHE:CZ	1:B:1378:LEU:HD12	2.41	0.51
1:A:350:LYS:CA	1:A:351:LYS:HB3	2.41	0.51
1:A:384:ILE:CD1	1:A:463:LEU:HD11	2.41	0.51
1:A:643:VAL:O	1:A:645:LYS:N	2.44	0.51
1:A:979:GLU:HG2	1:A:982:LYS:CB	2.41	0.51
1:B:1349:LEU:HD21	1:B:1350:GLU:HG2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:489:LYS:HD3	1:B:508:LEU:CD1	2.41	0.51
1:B:642:VAL:HG22	1:B:642:VAL:O	2.10	0.51
1:A:461:LYS:NZ	1:A:461:LYS:CA	2.73	0.51
1:A:576:ASP:O	1:A:579:ASN:N	2.44	0.51
1:B:1075:ILE:HG23	1:B:1177:ILE:HG21	1.92	0.51
1:B:439:ILE:CD1	1:B:439:ILE:N	2.73	0.51
1:B:531:LYS:C	1:B:562:LEU:CD1	2.80	0.51
1:B:560:LYS:HD3	1:B:563:ASN:CB	2.41	0.51
1:A:375:LEU:CB	1:A:380:ILE:CD1	2.82	0.50
1:A:535:ARG:HG3	1:A:537:ASN:O	2.11	0.50
1:A:638:LEU:HD22	1:A:639:ASN:ND2	2.25	0.50
1:A:662:GLU:CD	1:A:663:ASN:H	2.15	0.50
1:A:871:TYR:O	1:A:875:ILE:HG13	2.11	0.50
1:B:976:LEU:CG	1:B:977:GLN:H	2.20	0.50
1:A:383:LEU:HD23	1:A:383:LEU:C	2.31	0.50
1:B:1042:LYS:O	1:B:1044:GLN:N	2.44	0.50
1:B:1366:TYR:CD1	1:B:1366:TYR:C	2.85	0.50
1:B:461:LYS:CG	1:B:462:ILE:CG1	2.86	0.50
1:B:569:ILE:HG22	1:B:575:ILE:HB	1.92	0.50
1:B:832:ILE:HD11	1:B:838:TYR:HA	1.93	0.50
1:A:393:LYS:H	1:A:395:ASN:CB	2.21	0.50
1:A:403:ILE:CD1	1:A:403:ILE:N	2.73	0.50
1:A:714:TYR:HE1	1:A:718:ILE:HD11	1.75	0.50
1:A:1024:TYR:HB2	1:A:1067:ILE:CD1	2.41	0.50
1:A:1382:ILE:O	1:A:1382:ILE:HG23	2.12	0.50
1:A:535:ARG:HH11	1:A:535:ARG:HG2	1.76	0.50
1:A:937:ILE:HD11	1:A:995:VAL:HG22	1.91	0.50
1:B:1291:PHE:CE1	1:B:1381:LYS:HB3	2.47	0.50
1:B:767:ASN:OD1	1:B:767:ASN:N	2.44	0.50
1:B:778:ILE:O	1:B:782:ILE:HG12	2.12	0.50
1:A:1147:LYS:O	1:A:1148:ASN:C	2.50	0.50
1:A:973:SER:HB3	1:A:975:ILE:N	2.26	0.50
1:B:1203:VAL:HG11	1:B:1241:TYR:CD2	2.46	0.50
1:B:987:ASN:O	1:B:991:LEU:N	2.31	0.50
1:B:1027:GLU:HG2	1:B:1076:TYR:HE2	1.76	0.50
1:B:616:ASP:HA	1:B:619:LYS:HB2	1.94	0.50
1:A:683:LEU:CD2	1:A:793:PHE:HD2	2.21	0.50
1:B:616:ASP:O	1:B:620:VAL:CB	2.60	0.50
1:A:1024:TYR:CD1	1:A:1024:TYR:C	2.85	0.50
1:A:1054:ASN:N	1:A:1055:GLU:CB	2.75	0.50
1:A:886:THR:O	1:A:890:GLU:HB2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1058:ILE:CG1	1:B:1059:TYR:CE2	2.94	0.50
1:B:1265:GLU:CA	1:B:1266:ASN:CB	2.90	0.50
1:A:662:GLU:CG	1:A:663:ASN:H	2.25	0.50
1:B:436:LYS:HB3	1:B:436:LYS:HZ3	1.76	0.50
1:B:491:ARG:NE	1:B:1207:ARG:HH21	1.96	0.49
1:B:1366:TYR:CE1	1:B:1367:ASN:CG	2.85	0.49
1:B:425:LYS:O	1:B:428:TYR:N	2.45	0.49
1:A:389:LYS:O	1:A:390:GLU:HB2	2.11	0.49
1:A:535:ARG:HH11	1:A:535:ARG:CB	2.24	0.49
1:A:493:ASN:OD1	1:A:603:ALA:HB1	2.12	0.49
1:B:403:ILE:O	1:B:407:HIS:N	2.41	0.49
1:B:897:ASN:ND2	1:B:897:ASN:N	2.60	0.49
1:A:920:GLN:NE2	1:A:1006:ILE:HD13	2.27	0.49
1:A:493:ASN:OD1	1:A:603:ALA:HB2	2.11	0.49
1:B:431:ILE:HG23	1:B:472:ILE:HD12	1.94	0.49
1:B:505:PHE:O	1:B:508:LEU:N	2.46	0.49
1:B:516:LEU:HD11	1:B:1194:ARG:HD3	1.93	0.49
1:A:369:GLU:HG3	1:A:373:LYS:HE3	1.92	0.49
1:A:714:TYR:CE1	1:A:718:ILE:HD11	2.48	0.49
1:A:760:ILE:O	1:A:764:LYS:HG2	2.12	0.49
1:B:1200:HIS:CE1	1:B:1224:ALA:HB2	2.48	0.49
1:B:684:TYR:HB3	1:B:685:ARG:CA	2.42	0.49
1:A:1024:TYR:HB2	1:A:1067:ILE:HD11	1.94	0.49
1:A:1105:SER:O	1:A:1109:ALA:HB2	2.12	0.49
1:A:1226:PRO:HD2	1:A:1249:TYR:HE1	1.78	0.49
1:A:1277:ILE:HD11	1:A:1281:ILE:CD1	2.37	0.49
1:A:400:ILE:CD1	1:A:400:ILE:N	2.73	0.49
1:B:1079:ILE:HG22	1:B:1083:ILE:CD1	2.43	0.49
1:B:1163:LYS:HE2	1:B:1366:TYR:CE2	2.47	0.49
1:B:1208:GLU:OE2	1:B:1208:GLU:HA	2.13	0.49
1:B:433:ARG:O	1:B:436:LYS:HG2	2.13	0.49
1:B:616:ASP:HB3	1:B:620:VAL:HG13	1.94	0.49
1:B:666:ASP:O	1:B:667:ILE:HG23	2.13	0.49
1:B:1046:ILE:C	1:B:1047:TYR:CD1	2.85	0.49
1:B:1058:ILE:HD12	1:B:1059:TYR:CZ	2.47	0.49
1:B:439:ILE:HA	1:B:442:ILE:HB	1.93	0.49
1:B:851:VAL:HA	1:B:854:LYS:HG3	1.95	0.49
1:A:1177:ILE:HD11	1:A:1374:LEU:CD1	2.35	0.49
1:A:1269:ILE:O	1:A:1278:ARG:NH2	2.46	0.49
1:B:1049:PRO:O	1:B:1050:LYS:HB2	2.13	0.49
1:A:1148:ASN:ND2	1:A:1151:SER:CB	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1251:LYS:O	1:B:1255:ILE:HG12	2.13	0.49
1:B:412:PHE:CB	1:B:413:ASP:CA	2.87	0.49
1:B:434:TYR:CE2	1:B:468:LEU:HD21	2.47	0.49
1:B:614:GLN:C	1:B:615:ASP:O	2.49	0.49
1:B:823:VAL:HG12	1:B:824:LYS:N	2.28	0.49
1:A:735:GLU:HB3	1:A:784:TYR:CE2	2.48	0.49
1:B:1249:TYR:CE1	1:B:1253:GLU:HB2	2.48	0.49
1:A:1366:TYR:CD1	1:A:1366:TYR:C	2.85	0.49
1:A:403:ILE:O	1:A:406:LYS:CB	2.61	0.49
1:A:608:ARG:HH21	1:A:836:PHE:HB2	1.75	0.49
1:B:1265:GLU:HA	1:B:1266:ASN:HB2	1.94	0.49
1:B:570:ARG:HA	1:B:575:ILE:HG22	1.94	0.49
1:B:900:LEU:HD13	1:B:1056:LEU:CG	2.37	0.49
1:A:1105:SER:O	1:A:1109:ALA:CB	2.61	0.48
1:B:1099:ILE:HG22	1:B:1104:ILE:HG13	1.94	0.48
1:A:973:SER:N	1:A:974:ASN:HA	2.29	0.48
1:B:431:ILE:HG22	1:B:435:LEU:HD11	1.94	0.48
1:B:669:TYR:CB	1:B:755:TYR:OH	2.62	0.48
1:A:1048:TYR:C	1:A:1048:TYR:CD1	2.86	0.48
1:B:1043:PHE:O	1:B:1046:ILE:HD11	2.13	0.48
1:B:1051:GLU:HB2	1:B:1055:GLU:N	2.28	0.48
1:A:1055:GLU:HG3	1:A:1057:TYR:CZ	2.49	0.48
1:A:418:SER:HB2	1:A:419:LYS:CA	2.18	0.48
1:B:1069:ASN:ND2	1:B:1178:GLU:OE2	2.46	0.48
1:B:624:ILE:O	1:B:628:LYS:HG2	2.14	0.48
1:B:711:LYS:O	1:B:715:LYS:HG3	2.13	0.48
1:B:1044:GLN:CA	1:B:1048:TYR:HE2	2.11	0.48
1:B:457:ILE:O	1:B:457:ILE:CG2	2.49	0.48
1:A:1118:LEU:HB2	1:A:1125:TYR:CZ	2.32	0.48
1:A:462:ILE:CG2	1:A:463:LEU:H	2.24	0.48
1:A:659:ILE:CG2	1:A:719:LEU:O	2.61	0.48
1:A:899:ASN:OD1	1:A:1059:TYR:HD1	1.95	0.48
1:A:997:GLN:O	1:A:1000:LYS:HB2	2.13	0.48
1:B:490:LEU:O	1:B:493:ASN:O	2.32	0.48
1:B:568:ILE:HD13	1:B:845:LEU:O	2.14	0.48
1:B:899:ASN:HA	1:B:900:LEU:HA	1.58	0.48
1:A:1349:LEU:O	1:A:1349:LEU:HD12	2.14	0.48
1:A:758:ALA:O	1:A:762:ALA:N	2.37	0.48
1:B:647:LYS:CB	1:B:648:LYS:CG	2.85	0.48
1:B:792:LEU:HD23	1:B:792:LEU:O	2.13	0.48
1:B:893:THR:O	1:B:897:ASN:ND2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:LYS:HG2	1:A:1211:ILE:HD11	1.96	0.48
1:A:538:ILE:O	1:A:538:ILE:HG13	2.13	0.48
1:A:613:THR:HG23	1:A:614:GLN:CA	2.31	0.48
1:A:614:GLN:CB	1:A:618:ASN:CB	2.90	0.48
1:B:486:TYR:O	1:B:490:LEU:HG	2.14	0.48
1:B:671:PRO:HB2	1:B:675:LYS:HD3	1.96	0.48
1:A:1134:LYS:HG3	1:A:1135:GLU:HG2	1.94	0.48
1:A:473:LEU:CD2	1:A:477:LYS:HE3	2.44	0.48
1:B:1262:ASP:O	1:B:1263:LEU:HD12	2.14	0.48
1:B:746:ILE:O	1:B:747:ASP:HB2	2.14	0.48
1:B:920:GLN:O	1:B:925:ILE:CD1	2.62	0.48
1:A:1227:LYS:HG3	1:A:1270:ASN:ND2	2.29	0.48
1:A:374:ILE:HG23	1:A:428:TYR:CE2	2.49	0.48
1:A:501:ASN:HB3	1:A:504:ASP:H	1.79	0.48
1:A:738:LYS:CA	1:A:746:ILE:HG12	2.44	0.48
1:B:1164:LYS:HD3	1:B:1367:ASN:H	1.79	0.48
1:B:507:ARG:O	1:B:866:LEU:HD21	2.14	0.48
1:A:1026:LYS:HG3	1:A:1027:GLU:N	2.29	0.47
1:A:1330:ASN:HD22	1:A:1357:LYS:HG2	1.79	0.47
1:B:1366:TYR:CD1	1:B:1367:ASN:CG	2.87	0.47
1:B:873:ASN:HD22	1:B:873:ASN:C	2.17	0.47
1:B:1142:LYS:CG	1:B:1144:ILE:N	2.77	0.47
1:A:500:VAL:O	1:A:500:VAL:HG13	2.14	0.47
1:A:673:PHE:O	1:A:674:SER:C	2.53	0.47
1:B:1063:LEU:HD12	1:B:1171:PHE:CE1	2.49	0.47
1:B:1072:PHE:HA	1:B:1075:ILE:HB	1.96	0.47
1:B:1084:LYS:HB3	1:B:1084:LYS:NZ	2.30	0.47
1:B:1352:LEU:HD13	1:B:1352:LEU:H	1.78	0.47
1:B:461:LYS:HG3	1:B:462:ILE:CB	2.45	0.47
1:A:1111:LEU:CD2	1:A:1359:SER:OG	2.61	0.47
1:A:802:ILE:C	1:A:805:ILE:CB	2.82	0.47
1:A:806:LYS:HA	1:A:809:ILE:HD13	1.97	0.47
1:B:1223:ARG:HB3	1:B:1223:ARG:NH1	2.29	0.47
1:B:907:MSE:O	1:B:911:GLU:CG	2.62	0.47
1:A:802:ILE:O	1:A:805:ILE:CA	2.63	0.47
1:B:1130:ILE:O	1:B:1130:ILE:CG2	2.63	0.47
1:A:1133:LEU:CD2	1:A:1149:TYR:CE2	2.98	0.47
1:A:1199:MSE:O	1:A:1203:VAL:HG23	2.14	0.47
1:A:1346:ASN:ND2	1:A:1349:LEU:HD22	2.25	0.47
1:A:368:LYS:CA	1:A:371:ILE:CG2	2.90	0.47
1:B:376:ALA:CA	1:B:379:LYS:CB	2.92	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:LYS:O	1:B:388:GLU:N	2.45	0.47
1:B:609:ASP:O	1:B:610:LEU:CB	2.59	0.47
1:B:620:VAL:HA	1:B:623:ILE:HD12	1.96	0.47
1:B:807:LYS:HE3	1:B:807:LYS:HB3	1.62	0.47
1:B:582:THR:CA	1:B:583:ASN:CG	2.78	0.47
1:B:656:ASP:N	1:B:656:ASP:OD1	2.47	0.47
1:B:627:LEU:HD21	1:B:829:THR:HA	1.95	0.47
1:B:842:ILE:O	1:B:846:LEU:HD13	2.14	0.47
1:A:1215:SER:OG	1:A:1242:LYS:HB3	2.10	0.47
1:A:431:ILE:O	1:A:435:LEU:HG	2.15	0.47
1:A:643:VAL:C	1:A:645:LYS:N	2.63	0.47
1:A:684:TYR:OH	1:A:693:PHE:CE2	2.68	0.47
1:B:900:LEU:CD1	1:B:1056:LEU:HD13	2.44	0.47
1:B:1177:ILE:HD11	1:B:1374:LEU:HD21	1.96	0.47
1:A:1047:TYR:HE1	1:A:1171:PHE:HE2	1.61	0.47
1:B:684:TYR:C	1:B:684:TYR:CD1	2.85	0.47
1:B:398:THR:HG22	1:B:398:THR:O	2.15	0.46
1:B:439:ILE:CA	1:B:442:ILE:HB	2.45	0.46
1:B:772:LYS:O	1:B:776:LYS:HG3	2.15	0.46
1:B:920:GLN:O	1:B:925:ILE:HD11	2.16	0.46
1:B:925:ILE:HD13	1:B:1003:ASP:OD1	2.14	0.46
1:A:1096:GLY:O	1:A:1099:ILE:N	2.48	0.46
1:A:1277:ILE:HG23	1:A:1278:ARG:N	2.30	0.46
1:A:1375:ILE:O	1:A:1379:LEU:HG	2.15	0.46
1:A:485:MSE:HE1	1:A:1309:TYR:CE1	2.50	0.46
1:A:578:LYS:O	1:A:579:ASN:HB2	2.15	0.46
1:A:702:VAL:HG11	1:A:795:PHE:HE2	1.81	0.46
1:A:986:ILE:O	1:A:987:ASN:ND2	2.48	0.46
1:B:671:PRO:HG3	1:B:774:GLN:CD	2.27	0.46
1:A:1046:ILE:HG21	1:A:1169:VAL:HG11	1.97	0.46
1:A:1322:PHE:CE2	1:A:1352:LEU:HD12	2.50	0.46
1:A:368:LYS:HA	1:A:371:ILE:HG21	1.95	0.46
1:A:802:ILE:C	1:A:805:ILE:H	2.19	0.46
1:B:665:ASN:N	1:B:665:ASN:HD22	2.13	0.46
1:B:713:LEU:HG	1:B:717:LEU:HD11	1.98	0.46
1:B:930:TYR:CE2	1:B:954:LYS:HG2	2.50	0.46
1:A:464:ASN:ND2	1:A:467:ILE:CG1	2.73	0.46
1:A:566:ILE:HA	1:A:569:ILE:HG22	1.96	0.46
1:B:462:ILE:HD13	1:B:464:ASN:ND2	2.31	0.46
1:B:613:THR:HA	1:B:614:GLN:HA	1.72	0.46
1:B:671:PRO:HG3	1:B:774:GLN:HE21	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:880:GLU:O	1:B:884:LEU:HG	2.14	0.46
1:A:748:GLU:HG3	1:A:749:ASN:N	2.30	0.46
1:A:756:LYS:O	1:A:759:GLN:HG2	2.16	0.46
1:B:1028:ILE:O	1:B:1032:ILE:HG12	2.16	0.46
1:B:1048:TYR:O	1:B:1049:PRO:C	2.53	0.46
1:B:671:PRO:CB	1:B:675:LYS:NZ	2.78	0.46
1:B:1367:ASN:C	1:B:1367:ASN:HD22	2.18	0.46
1:B:756:LYS:O	1:B:759:GLN:HG2	2.16	0.46
1:A:528:GLU:OE1	1:A:565:LYS:HD3	2.15	0.46
1:A:569:ILE:O	1:A:574:PHE:HB2	2.16	0.46
1:A:901:GLU:H	1:A:1056:LEU:HD23	1.79	0.46
1:A:946:ASN:O	1:A:950:VAL:HG23	2.16	0.46
1:B:485:MSE:HG3	1:B:1202:ILE:HD11	1.97	0.46
1:B:350:LYS:O	1:B:351:LYS:HB3	2.16	0.46
1:B:539:ASN:ND2	1:B:551:ARG:HH12	2.14	0.46
1:B:578:LYS:O	1:B:579:ASN:CB	2.63	0.46
1:A:405:LYS:O	1:A:409:LYS:N	2.40	0.46
1:A:718:ILE:HA	1:A:733:LEU:HD21	1.98	0.46
1:A:825:THR:C	1:A:826:SER:O	2.48	0.46
1:A:994:LYS:HD2	1:A:994:LYS:HA	1.82	0.46
1:B:562:LEU:HD13	1:B:565:LYS:CE	2.45	0.46
1:B:675:LYS:O	1:B:678:PRO:HD2	2.15	0.46
1:A:900:LEU:HG	1:A:1056:LEU:HD22	1.97	0.46
1:A:397:ASP:O	1:A:400:ILE:HG12	2.16	0.46
1:A:547:PHE:N	1:A:547:PHE:HD1	2.14	0.46
1:A:608:ARG:HA	1:A:608:ARG:HD3	1.70	0.46
1:B:1119:ASN:HA	1:B:1120:GLY:HA2	1.69	0.46
1:B:685:ARG:HB3	1:B:686:ASN:H	1.59	0.46
1:A:1072:PHE:CD2	1:A:1076:TYR:HB2	2.51	0.46
1:A:370:LYS:HB2	1:A:370:LYS:HE3	1.76	0.46
1:A:576:ASP:OD2	1:A:580:ASN:O	2.34	0.46
1:A:759:GLN:O	1:A:763:SER:N	2.46	0.46
1:B:900:LEU:CD1	1:B:1056:LEU:CB	2.55	0.46
1:B:439:ILE:HA	1:B:442:ILE:HD12	1.97	0.46
1:B:539:ASN:HD21	1:B:551:ARG:HH12	1.63	0.46
1:A:1096:GLY:O	1:A:1099:ILE:HB	2.16	0.45
1:B:644:PHE:HE2	1:B:651:ILE:CG1	2.29	0.45
1:B:804:GLU:O	1:B:807:LYS:HG2	2.16	0.45
1:B:969:ILE:CB	1:B:970:ASP:CB	2.88	0.45
1:B:1048:TYR:O	1:B:1048:TYR:CD2	2.70	0.45
1:A:1215:SER:HG	1:A:1242:LYS:CB	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:696:ILE:CB	1:A:700:LYS:H	2.30	0.45
1:A:806:LYS:N	1:A:809:ILE:HD13	2.32	0.45
1:A:930:TYR:OH	1:A:954:LYS:HG2	2.15	0.45
1:B:1048:TYR:O	1:B:1048:TYR:CG	2.69	0.45
1:B:434:TYR:CE2	1:B:468:LEU:CG	2.96	0.45
1:B:735:GLU:O	1:B:739:THR:HG23	2.17	0.45
1:A:399:GLU:CG	1:A:400:ILE:CD1	2.90	0.45
1:A:537:ASN:C	1:A:537:ASN:HD22	2.15	0.45
1:A:762:ALA:CB	1:A:770:ILE:CG1	2.80	0.45
1:A:766:ASN:OD1	1:A:769:ALA:HB2	2.16	0.45
1:B:1084:LYS:HB3	1:B:1084:LYS:HZ3	1.80	0.45
1:B:1265:GLU:CB	1:B:1266:ASN:C	2.84	0.45
1:B:467:ILE:C	1:B:467:ILE:HD12	2.35	0.45
1:B:559:LYS:HB3	1:B:560:LYS:H	1.47	0.45
1:B:631:ASP:OD2	1:B:888:ARG:HG2	2.16	0.45
1:A:670:LEU:HD22	1:A:670:LEU:C	2.37	0.45
1:A:930:TYR:OH	1:A:954:LYS:N	2.49	0.45
1:B:1269:ILE:CA	1:B:1270:ASN:CB	2.95	0.45
1:B:355:VAL:O	1:B:359:VAL:HG23	2.16	0.45
1:B:732:PHE:HB2	1:B:784:TYR:CE2	2.51	0.45
1:A:1078:LEU:HD12	1:A:1177:ILE:HD13	1.99	0.45
1:A:1367:ASN:OD1	1:A:1371:ILE:CD1	2.64	0.45
1:A:576:ASP:C	1:A:578:LYS:H	2.15	0.45
1:B:900:LEU:CG	1:B:1056:LEU:HD12	2.42	0.45
1:B:900:LEU:HD21	1:B:1056:LEU:HD12	1.84	0.45
1:B:1062:ASN:HB2	1:B:1170:GLU:O	2.17	0.45
1:B:675:LYS:NZ	1:B:774:GLN:OE1	2.50	0.45
1:A:554:ASN:H	1:A:555:TYR:HA	1.82	0.45
1:B:515:ASP:O	1:B:519:ILE:HG12	2.17	0.45
1:B:771:LYS:NZ	1:B:869:SER:HB2	2.32	0.45
1:B:833:ASN:OD1	1:B:834:ASP:N	2.46	0.45
1:B:521:PHE:CD2	1:B:855:ILE:HD12	2.52	0.45
1:A:1006:ILE:HG22	1:A:1006:ILE:O	2.16	0.45
1:A:682:ASN:O	1:A:686:ASN:N	2.44	0.45
1:B:531:LYS:HB3	1:B:562:LEU:CD1	2.14	0.45
1:B:626:ASN:O	1:B:629:ILE:HG12	2.17	0.45
1:B:695:THR:OG1	1:B:698:THR:HG23	2.17	0.45
1:A:1112:LYS:O	1:A:1115:ASN:N	2.49	0.45
1:A:1152:PHE:O	1:A:1155:ASP:N	2.50	0.45
1:A:383:LEU:CD2	1:A:383:LEU:C	2.86	0.45
1:A:934:LYS:O	1:A:938:LEU:HG	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:601:LEU:O	1:B:602:HIS:HB2	2.17	0.45
1:B:753:ASN:O	1:B:757:ASN:OD1	2.34	0.45
1:A:1229:ASN:HB3	1:A:1238:THR:HG21	1.99	0.45
1:A:1244:PHE:CD2	1:A:1245:ASP:OD2	2.70	0.45
1:A:411:ASN:CB	1:A:414:SER:N	2.79	0.45
1:B:461:LYS:HA	1:B:462:ILE:HA	1.77	0.45
1:B:464:ASN:H	1:B:467:ILE:HG21	1.82	0.45
1:B:500:VAL:O	1:B:505:PHE:CE1	2.70	0.45
1:B:794:ASP:C	1:B:795:PHE:CD1	2.90	0.45
1:A:1048:TYR:CD1	1:A:1048:TYR:O	2.70	0.44
1:A:1053:LYS:O	1:A:1055:GLU:CB	2.31	0.44
1:A:1094:ILE:HG22	1:A:1094:ILE:O	2.18	0.44
1:A:868:THR:CG2	1:A:869:SER:N	2.79	0.44
1:A:973:SER:CB	1:A:974:ASN:HA	2.37	0.44
1:A:980:GLN:O	1:A:984:SER:N	2.50	0.44
1:B:1113:ASN:O	1:B:1117:LYS:N	2.47	0.44
1:B:494:ASP:O	1:B:495:ILE:CD1	2.58	0.44
1:B:575:ILE:HG12	1:B:579:ASN:HA	1.98	0.44
1:B:792:LEU:CD2	1:B:792:LEU:C	2.85	0.44
1:B:917:PHE:O	1:B:917:PHE:CD1	2.70	0.44
1:A:1017:ASN:HD22	1:A:1020:PHE:HD1	1.65	0.44
1:A:1027:GLU:OE2	1:A:1027:GLU:HA	2.17	0.44
1:A:1048:TYR:CD1	1:A:1049:PRO:O	2.66	0.44
1:A:1075:ILE:HD11	1:A:1181:LEU:HD11	1.99	0.44
1:A:546:PHE:C	1:A:547:PHE:CD1	2.90	0.44
1:A:755:TYR:O	1:A:755:TYR:CD1	2.70	0.44
1:A:767:ASN:HB2	1:A:867:ASN:CG	2.37	0.44
1:B:531:LYS:HB2	1:B:562:LEU:CD1	2.44	0.44
1:B:856:ARG:CD	1:B:875:ILE:HG23	2.48	0.44
1:A:499:THR:O	1:A:499:THR:OG1	2.34	0.44
1:B:1046:ILE:O	1:B:1047:TYR:HD1	2.00	0.44
1:B:793:PHE:O	1:B:795:PHE:CD1	2.70	0.44
1:A:1148:ASN:HD21	1:A:1151:SER:HB3	1.82	0.44
1:A:1278:ARG:HE	1:A:1278:ARG:HB3	1.63	0.44
1:A:375:LEU:CB	1:A:380:ILE:HD11	2.46	0.44
1:A:557:LEU:HD11	1:A:566:ILE:HD11	2.00	0.44
1:A:738:LYS:CD	1:A:746:ILE:HD11	2.47	0.44
1:A:799:LYS:O	1:A:804:GLU:HB3	2.17	0.44
1:A:899:ASN:HD22	1:A:899:ASN:HA	1.60	0.44
1:B:1265:GLU:HA	1:B:1266:ASN:CB	2.47	0.44
1:B:1365:SER:O	1:B:1366:TYR:CD2	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:ILE:CG2	1:B:358:PHE:HE2	2.30	0.44
1:A:979:GLU:OE2	1:A:982:LYS:CB	2.66	0.44
1:B:1366:TYR:CE1	1:B:1367:ASN:OD1	2.71	0.44
1:A:1209:LEU:HB2	1:A:1211:ILE:HG13	2.00	0.44
1:A:1230:GLY:HA2	1:A:1231:SER:HA	1.52	0.44
1:A:395:ASN:CG	1:A:396:CYS:H	2.13	0.44
1:A:588:LYS:HZ3	1:A:618:ASN:HD21	1.66	0.44
1:A:638:LEU:C	1:A:638:LEU:CD2	2.85	0.44
1:A:920:GLN:NE2	1:A:1006:ILE:HD12	2.31	0.44
1:B:605:SER:CB	1:B:1219:THR:OG1	2.65	0.44
1:B:1293:ASP:O	1:B:1294:TYR:CD2	2.70	0.44
1:B:358:PHE:CE1	1:B:427:LEU:HG	2.52	0.44
1:B:355:VAL:HG21	1:B:483:HIS:CD2	2.51	0.44
1:B:644:PHE:HD1	1:B:644:PHE:HA	1.71	0.44
1:A:384:ILE:HD13	1:A:463:LEU:HD12	2.00	0.44
1:A:665:ASN:ND2	1:A:669:TYR:CE2	2.72	0.44
1:A:740:LEU:HD13	1:A:754:TYR:CD2	2.53	0.44
1:A:1291:PHE:CD1	1:A:1291:PHE:N	2.85	0.44
1:A:378:PHE:N	1:A:379:LYS:HA	2.32	0.44
1:B:424:GLU:CA	1:B:427:LEU:HD13	2.44	0.44
1:B:495:ILE:HG22	1:B:496:ASP:N	2.33	0.44
1:A:416:LYS:O	1:A:417:PHE:C	2.56	0.44
1:B:1365:SER:O	1:B:1366:TYR:CG	2.70	0.44
1:B:569:ILE:CG2	1:B:575:ILE:HB	2.47	0.44
1:A:377:GLU:HG2	1:A:377:GLU:O	2.17	0.43
1:A:462:ILE:HG22	1:A:463:LEU:C	2.37	0.43
1:B:432:TYR:O	1:B:432:TYR:HD1	2.01	0.43
1:B:636:LYS:O	1:B:641:ASP:HB2	2.17	0.43
1:B:681:LEU:O	1:B:685:ARG:NH1	2.50	0.43
1:A:405:LYS:HE3	1:A:405:LYS:HB3	1.66	0.43
1:A:1026:LYS:HZ2	1:A:1026:LYS:HB2	1.81	0.43
1:A:546:PHE:O	1:A:547:PHE:CG	2.72	0.43
1:A:659:ILE:HG21	1:A:719:LEU:C	2.39	0.43
1:A:775:LYS:CB	1:A:775:LYS:NZ	2.73	0.43
1:B:1147:LYS:N	1:B:1148:ASN:CA	2.76	0.43
1:B:1366:TYR:HE1	1:B:1367:ASN:OD1	2.00	0.43
1:B:614:GLN:CB	1:B:618:ASN:CB	2.96	0.43
1:B:629:ILE:HB	1:B:888:ARG:HG3	1.99	0.43
1:B:830:ILE:HG21	1:B:877:ILE:CD1	2.49	0.43
1:B:946:ASN:O	1:B:950:VAL:HG23	2.18	0.43
1:A:1060:LYS:HZ1	1:A:1170:GLU:CD	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1133:LEU:HD22	1:A:1149:TYR:CE2	2.53	0.43
1:A:599:ARG:HG3	1:A:604:ILE:HB	2.00	0.43
1:A:683:LEU:C	1:A:683:LEU:CD2	2.85	0.43
1:A:707:ILE:H	1:A:707:ILE:HG12	1.66	0.43
1:A:979:GLU:CD	1:A:982:LYS:CB	2.87	0.43
1:B:711:LYS:HE3	1:B:711:LYS:HB3	1.84	0.43
1:A:1049:PRO:HG2	1:A:1056:LEU:HB2	2.01	0.43
1:A:1262:ASP:OD1	1:A:1262:ASP:N	2.48	0.43
1:A:1325:PHE:HB3	1:A:1375:ILE:HD13	2.00	0.43
1:A:1354:LYS:NZ	1:A:1354:LYS:CB	2.73	0.43
1:A:401:PHE:HB3	1:A:404:PHE:CE1	2.51	0.43
1:A:557:LEU:CD2	1:A:558:ASP:N	2.73	0.43
1:A:738:LYS:CG	1:A:746:ILE:HD11	2.48	0.43
1:A:684:TYR:HB2	1:A:793:PHE:CD2	2.53	0.43
1:A:510:ALA:HB2	1:A:865:TRP:CD2	2.54	0.43
1:A:900:LEU:HD23	1:A:1056:LEU:HD13	2.01	0.43
1:B:1029:ASP:OD1	1:B:1056:LEU:HD21	2.18	0.43
1:B:380:ILE:O	1:B:384:ILE:N	2.51	0.43
1:B:511:LYS:HG2	1:B:866:LEU:HD11	2.00	0.43
1:B:641:ASP:C	1:B:643:VAL:H	2.21	0.43
1:A:1089:LYS:C	1:A:1089:LYS:CD	2.85	0.43
1:A:1156:TYR:O	1:A:1159:VAL:HG12	2.18	0.43
1:A:778:ILE:O	1:A:782:ILE:HG12	2.19	0.43
1:B:1047:TYR:O	1:B:1048:TYR:CD2	2.70	0.43
1:B:1102:ASN:O	1:B:1106:GLU:N	2.49	0.43
1:B:430:ILE:HD11	1:B:431:ILE:HD13	2.01	0.43
1:B:569:ILE:HG22	1:B:575:ILE:H	1.83	0.43
1:A:920:GLN:HE22	1:A:1006:ILE:CD1	2.30	0.43
1:A:1354:LYS:HZ3	1:A:1354:LYS:HB2	1.82	0.43
1:A:1111:LEU:CD2	1:A:1359:SER:CB	2.97	0.43
1:A:411:ASN:N	1:A:413:ASP:N	2.60	0.43
1:B:467:ILE:HG13	1:B:468:LEU:HD12	2.00	0.43
1:B:856:ARG:HB3	1:B:882:MSE:HE1	2.01	0.43
1:A:398:THR:O	1:A:399:GLU:C	2.57	0.43
1:A:468:LEU:HA	1:A:468:LEU:HD12	1.80	0.43
1:A:575:ILE:HG22	1:A:577:ASN:OD1	2.18	0.43
1:A:696:ILE:HA	1:A:698:THR:H	1.82	0.43
1:B:1046:ILE:C	1:B:1047:TYR:HD1	2.21	0.43
1:B:899:ASN:HD22	1:B:1058:ILE:HG23	1.83	0.43
1:B:1079:ILE:H	1:B:1079:ILE:CD1	2.28	0.43
1:B:1161:GLU:O	1:B:1165:ILE:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:GLY:HA2	1:B:395:ASN:HB3	2.00	0.43
1:B:533:PHE:CD1	1:B:555:TYR:CB	3.01	0.43
1:B:746:ILE:HG22	1:B:747:ASP:OD1	2.18	0.43
1:A:408:TYR:C	1:A:411:ASN:N	2.73	0.43
1:A:549:GLY:HA2	1:A:594:THR:CG2	2.49	0.43
1:A:791:GLU:O	1:A:794:ASP:HB3	2.18	0.43
1:B:1347:ASP:O	1:B:1348:ILE:HB	2.19	0.43
1:B:1367:ASN:C	1:B:1367:ASN:ND2	2.72	0.43
1:A:1118:LEU:N	1:A:1125:TYR:CZ	2.87	0.43
1:A:1235:TYR:HD1	1:A:1236:THR:HG1	1.65	0.43
1:A:1111:LEU:CD2	1:A:1363:LEU:HD12	2.43	0.43
1:B:1048:TYR:CB	1:B:1052:ARG:HA	2.43	0.43
1:B:1099:ILE:CG2	1:B:1103:LYS:CB	2.94	0.43
1:B:561:ILE:HG22	1:B:562:LEU:HG	2.01	0.43
1:B:538:ILE:O	1:B:538:ILE:HG12	2.19	0.42
1:B:578:LYS:O	1:B:579:ASN:HB3	2.19	0.42
1:B:659:ILE:CB	1:B:719:LEU:CB	2.96	0.42
1:A:1191:GLN:HB3	1:A:1307:LEU:HD11	2.00	0.42
1:A:401:PHE:CB	1:A:402:GLY:HA2	2.47	0.42
1:A:575:ILE:CA	1:A:582:THR:HG23	2.49	0.42
1:A:806:LYS:CA	1:A:809:ILE:HD13	2.49	0.42
1:B:1050:LYS:HA	1:B:1050:LYS:HD3	1.84	0.42
1:B:1049:PRO:O	1:B:1050:LYS:HE2	2.19	0.42
1:B:1031:LEU:HD13	1:B:1084:LYS:HD3	2.00	0.42
1:B:1195:PHE:CG	1:B:1306:LEU:HD21	2.53	0.42
1:B:427:LEU:H	1:B:427:LEU:CD1	2.23	0.42
1:B:809:ILE:C	1:B:811:ASP:N	2.72	0.42
1:B:934:LYS:O	1:B:938:LEU:HG	2.19	0.42
1:B:930:TYR:CZ	1:B:954:LYS:HG2	2.54	0.42
1:B:930:TYR:OH	1:B:954:LYS:N	2.52	0.42
1:A:691:GLU:CB	1:A:692:PRO:HD2	2.49	0.42
1:A:780:CYS:O	1:A:784:TYR:N	2.42	0.42
1:A:792:LEU:C	1:A:792:LEU:CD1	2.85	0.42
1:B:557:LEU:CD2	1:B:575:ILE:HD13	2.43	0.42
1:A:1111:LEU:CD2	1:A:1363:LEU:CD1	2.77	0.42
1:A:404:PHE:O	1:A:407:HIS:N	2.53	0.42
1:A:738:LYS:HZ1	1:A:743:ILE:HA	1.84	0.42
1:A:983:LEU:O	1:A:986:ILE:HD12	2.18	0.42
1:B:900:LEU:CD1	1:B:1056:LEU:HD12	2.48	0.42
1:B:657:ILE:CD1	1:B:657:ILE:N	2.73	0.42
1:B:634:VAL:HG23	1:B:891:CYS:SG	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:942:LYS:HB2	1:B:942:LYS:HE3	1.82	0.42
1:A:1032:ILE:CD1	1:A:1048:TYR:HD2	2.32	0.42
1:A:1063:LEU:HD12	1:A:1171:PHE:CE2	2.55	0.42
1:A:463:LEU:N	1:A:463:LEU:CD1	2.76	0.42
1:B:1352:LEU:N	1:B:1352:LEU:CD1	2.82	0.42
1:B:589:PHE:CE1	1:B:842:ILE:HG21	2.54	0.42
1:B:591:LYS:HD3	1:B:591:LYS:HA	1.76	0.42
1:B:930:TYR:OH	1:B:954:LYS:HG2	2.20	0.42
1:A:1063:LEU:O	1:A:1067:ILE:HG13	2.19	0.42
1:A:461:LYS:NZ	1:A:461:LYS:C	2.73	0.42
1:A:643:VAL:O	1:A:643:VAL:HG12	2.18	0.42
1:B:384:ILE:CG2	1:B:385:LYS:N	2.82	0.42
1:B:614:GLN:O	1:B:615:ASP:C	2.56	0.42
1:B:568:ILE:HG23	1:B:625:GLN:NE2	2.34	0.42
1:A:1240:TYR:HD2	1:A:1241:TYR:CE1	2.38	0.42
1:A:997:GLN:O	1:A:1000:LYS:N	2.52	0.42
1:B:1034:ASP:OD1	1:B:1040:GLU:HB2	2.18	0.42
1:B:588:LYS:O	1:B:592:ILE:HG13	2.20	0.42
1:B:670:LEU:HA	1:B:670:LEU:HD12	1.76	0.42
1:B:716:LYS:HE2	1:B:716:LYS:HA	2.01	0.42
1:B:733:LEU:O	1:B:737:LYS:HG3	2.19	0.42
1:A:1148:ASN:ND2	1:A:1151:SER:OG	2.53	0.42
1:A:1046:ILE:CG2	1:A:1169:VAL:HG11	2.49	0.42
1:A:384:ILE:CD1	1:A:463:LEU:HD12	2.48	0.42
1:A:995:VAL:O	1:A:996:ASP:C	2.58	0.42
1:B:1043:PHE:CA	1:B:1046:ILE:HD11	2.49	0.42
1:B:1133:LEU:HA	1:B:1136:ASN:HB2	2.02	0.42
1:B:675:LYS:HZ2	1:B:774:GLN:HE22	1.68	0.42
1:A:575:ILE:C	1:A:582:THR:HG23	2.40	0.42
1:A:775:LYS:HB2	1:A:775:LYS:HZ2	1.82	0.42
1:A:801:ASN:O	1:A:802:ILE:HB	2.20	0.42
1:A:893:THR:HB	1:A:1059:TYR:OH	2.20	0.42
1:B:1055:GLU:O	1:B:1056:LEU:C	2.58	0.42
1:B:1202:ILE:O	1:B:1202:ILE:HG22	2.19	0.42
1:B:1357:LYS:CB	1:B:1362:GLU:OE1	2.68	0.42
1:B:616:ASP:O	1:B:620:VAL:N	2.43	0.42
1:B:670:LEU:HG	1:B:671:PRO:HD2	2.02	0.42
1:B:713:LEU:O	1:B:716:LYS:N	2.51	0.42
1:A:1117:LYS:HA	1:A:1117:LYS:HD3	1.81	0.42
1:A:1340:PHE:CD1	1:A:1349:LEU:HD21	2.55	0.42
1:A:409:LYS:O	1:A:413:ASP:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:710:ASN:HA	1:A:713:LEU:HB3	2.01	0.42
1:B:1091:LEU:O	1:B:1162:TYR:CE1	2.69	0.42
1:B:478:GLN:HA	1:B:481:LEU:HB3	2.02	0.42
1:B:639:ASN:HA	1:B:640:LEU:HA	1.71	0.42
1:A:514:LEU:HD12	1:A:514:LEU:C	2.34	0.41
1:A:755:TYR:C	1:A:755:TYR:CD1	2.89	0.41
1:B:1011:LEU:HD23	1:B:1011:LEU:HA	1.66	0.41
1:B:354:ILE:HG22	1:B:358:PHE:HE2	1.83	0.41
1:B:378:PHE:CZ	1:B:435:LEU:HD11	2.54	0.41
1:B:533:PHE:CE1	1:B:557:LEU:HD13	2.39	0.41
1:A:1321:VAL:HG12	1:A:1322:PHE:HD1	1.86	0.41
1:A:392:LYS:CB	1:A:395:ASN:ND2	2.83	0.41
1:A:659:ILE:CG2	1:A:720:GLU:N	2.83	0.41
1:A:830:ILE:HG22	1:A:831:VAL:N	2.35	0.41
1:A:979:GLU:HG3	1:A:982:LYS:H	1.86	0.41
1:B:1152:PHE:HA	1:B:1155:ASP:HB2	2.02	0.41
1:B:1277:ILE:CG1	1:B:1278:ARG:N	2.82	0.41
1:B:1300:ILE:HD13	1:B:1321:VAL:HG11	2.02	0.41
1:B:681:LEU:O	1:B:685:ARG:HG2	2.19	0.41
1:B:793:PHE:O	1:B:795:PHE:HD1	2.03	0.41
1:A:1091:LEU:N	1:A:1091:LEU:HD12	2.34	0.41
1:A:1094:ILE:CG2	1:A:1094:ILE:O	2.69	0.41
1:A:840:ILE:HG22	1:A:878:LEU:HD11	2.01	0.41
1:B:485:MSE:HG3	1:B:1202:ILE:CD1	2.50	0.41
1:B:473:LEU:O	1:B:476:VAL:N	2.53	0.41
1:B:531:LYS:C	1:B:562:LEU:HD11	2.40	0.41
1:B:637:ALA:HB1	1:B:821:ILE:HG21	2.02	0.41
1:B:697:GLU:O	1:B:701:ILE:CG1	2.67	0.41
1:B:844:ALA:O	1:B:852:ILE:HD11	2.19	0.41
1:A:1059:TYR:HE2	1:A:1061:LYS:HE3	1.85	0.41
1:A:1100:ARG:HA	1:A:1104:ILE:HG23	2.02	0.41
1:A:1118:LEU:HD12	1:A:1121:TYR:CB	2.50	0.41
1:A:992:LYS:O	1:A:992:LYS:HG2	2.20	0.41
1:B:1262:ASP:C	1:B:1263:LEU:CD1	2.89	0.41
1:B:821:ILE:HG22	1:B:822:THR:N	2.35	0.41
1:A:1048:TYR:HA	1:A:1049:PRO:HD3	1.86	0.41
1:B:1102:ASN:O	1:B:1106:GLU:HB2	2.21	0.41
1:B:364:ASN:H	1:B:364:ASN:HD22	1.67	0.41
1:B:432:TYR:CD1	1:B:436:LYS:NZ	2.87	0.41
1:B:615:ASP:C	1:B:617:TYR:H	2.23	0.41
1:A:554:ASN:HB3	1:A:555:TYR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:664:ASN:O	1:A:666:ASP:OD1	2.39	0.41
1:A:733:LEU:O	1:A:737:LYS:CG	2.68	0.41
1:A:906:LYS:O	1:A:910:ILE:HG13	2.21	0.41
1:B:888:ARG:HH11	1:B:1011:LEU:HD11	1.85	0.41
1:B:1198:ASP:OD2	1:B:1309:TYR:OH	2.30	0.41
1:B:1301:ASP:OD2	1:B:1341:LYS:HB2	2.20	0.41
1:B:1332:ASP:HB2	1:B:1354:LYS:CE	2.42	0.41
1:B:476:VAL:O	1:B:479:TYR:N	2.53	0.41
1:B:665:ASN:N	1:B:665:ASN:ND2	2.67	0.41
1:B:882:MSE:O	1:B:886:THR:HG23	2.21	0.41
1:B:943:ASP:O	1:B:946:ASN:ND2	2.53	0.41
1:A:1268:GLU:HG2	1:A:1268:GLU:O	2.21	0.41
1:A:616:ASP:O	1:A:620:VAL:HG23	2.20	0.41
1:A:806:LYS:H	1:A:809:ILE:HD13	1.86	0.41
1:B:1067:ILE:HD13	1:B:1072:PHE:CZ	2.55	0.41
1:B:1166:ARG:O	1:B:1170:GLU:HB2	2.21	0.41
1:B:491:ARG:HG2	1:B:1204:ASN:HD22	1.84	0.41
1:B:747:ASP:N	1:B:747:ASP:OD1	2.53	0.41
1:A:1055:GLU:N	1:A:1055:GLU:CD	2.73	0.41
1:A:556:VAL:HG22	1:A:557:LEU:H	1.86	0.41
1:B:532:ILE:HG22	1:B:562:LEU:CB	2.50	0.41
1:A:1212:ILE:HD13	1:A:1252:PHE:HB2	2.02	0.41
1:A:409:LYS:O	1:A:413:ASP:HA	2.21	0.41
1:A:438:ARG:O	1:A:442:ILE:HG13	2.21	0.41
1:B:1035:MSE:O	1:B:1038:GLU:CD	2.60	0.41
1:B:673:PHE:O	1:B:676:VAL:N	2.53	0.41
1:B:713:LEU:O	1:B:717:LEU:HD12	2.21	0.41
1:B:720:GLU:OE2	1:B:723:LEU:HD13	2.18	0.41
1:B:995:VAL:O	1:B:999:ILE:HG13	2.21	0.41
1:A:379:LYS:O	1:A:407:HIS:NE2	2.53	0.41
1:A:574:PHE:O	1:A:575:ILE:HG13	2.21	0.41
1:A:607:GLU:O	1:A:609:ASP:N	2.54	0.41
1:A:670:LEU:O	1:A:670:LEU:HD22	2.20	0.41
1:A:747:ASP:O	1:A:748:GLU:HG2	2.21	0.41
1:A:798:PHE:CG	1:A:799:LYS:N	2.89	0.41
1:B:1031:LEU:HD13	1:B:1043:PHE:HZ	1.79	0.41
1:B:1043:PHE:O	1:B:1048:TYR:CE2	2.74	0.41
1:B:900:LEU:HD11	1:B:1056:LEU:HD13	2.03	0.41
1:B:595:ASN:OD1	1:B:607:GLU:HG3	2.20	0.41
1:B:812:ILE:O	1:B:816:LYS:N	2.54	0.41
1:A:384:ILE:HD13	1:A:463:LEU:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:796:SER:OG	1:A:797:ASP:O	2.33	0.41
1:B:483:HIS:O	1:B:487:LEU:HD12	2.21	0.41
1:B:644:PHE:CE2	1:B:651:ILE:HG13	2.56	0.41
1:B:899:ASN:N	1:B:899:ASN:OD1	2.54	0.41
1:A:1112:LYS:CA	1:A:1115:ASN:HB2	2.43	0.40
1:A:690:ASN:ND2	1:A:693:PHE:CZ	2.89	0.40
1:A:684:TYR:OH	1:A:693:PHE:CZ	2.74	0.40
1:A:837:GLU:OE1	1:A:873:ASN:ND2	2.54	0.40
1:A:896:TRP:HA	1:A:896:TRP:CE3	2.56	0.40
1:B:900:LEU:HD21	1:B:1056:LEU:CD1	2.46	0.40
1:B:1250:LYS:HB2	1:B:1250:LYS:HE3	1.93	0.40
1:B:512:GLU:OE1	1:B:1197:ARG:NH2	2.54	0.40
1:A:1053:LYS:CG	1:A:1053:LYS:O	2.70	0.40
1:A:781:TYR:O	1:A:785:LEU:N	2.54	0.40
1:B:383:LEU:HG	1:B:383:LEU:O	2.21	0.40
1:B:421:SER:O	1:B:422:ASP:HB2	2.20	0.40
1:B:623:ILE:H	1:B:623:ILE:HG13	1.62	0.40
1:B:641:ASP:OD1	1:B:705:ALA:HB1	2.21	0.40
1:B:899:ASN:CB	1:B:900:LEU:HB2	2.51	0.40
1:A:1366:TYR:C	1:A:1368:SER:H	2.25	0.40
1:A:365:ASN:O	1:A:368:LYS:HE2	2.20	0.40
1:A:791:GLU:O	1:A:792:LEU:C	2.60	0.40
1:B:614:GLN:CB	1:B:618:ASN:HB2	2.50	0.40
1:A:429:LYS:HB2	1:A:429:LYS:HE3	1.74	0.40
1:B:1093:ASN:HB3	1:B:1096:GLY:H	1.86	0.40
1:B:1155:ASP:O	1:B:1159:VAL:HG23	2.21	0.40
1:B:423:GLU:H	1:B:423:GLU:HG3	1.65	0.40
1:B:640:LEU:HD22	1:B:701:ILE:HG21	2.02	0.40
1:B:908:LYS:HA	1:B:908:LYS:HD2	1.79	0.40
1:B:908:LYS:HA	1:B:911:GLU:HG3	2.04	0.40
1:A:1038:GLU:H	1:A:1038:GLU:HG3	1.56	0.40
1:A:1146:ASN:O	1:A:1147:LYS:CB	2.70	0.40
1:A:1194:ARG:HG3	1:A:1197:ARG:NH2	2.37	0.40
1:A:1299:GLN:O	1:A:1303:VAL:HG23	2.22	0.40
1:A:546:PHE:O	1:A:547:PHE:CB	2.69	0.40
1:B:1036:GLU:O	1:B:1037:SER:CB	2.69	0.40
1:B:1352:LEU:CD1	1:B:1352:LEU:H	2.34	0.40
1:B:504:ASP:HA	1:B:507:ARG:CD	2.43	0.40
1:B:549:GLY:HA2	1:B:594:THR:HG21	2.03	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:426:GLU:OE1	1:B:1037:SER:OG[4_446]	1.51	0.69
1:A:776:LYS:CB	1:A:1348:ILE:CD1[3_655]	1.91	0.29
1:A:398:THR:CB	1:A:907:MSE:CE[3_655]	2.08	0.12
1:A:776:LYS:CD	1:A:1348:ILE:CD1[3_655]	2.10	0.10

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
1	A	1013/1397 (72%)	908 (90%)	79 (8%)	26 (3%)	7 45
1	B	1004/1397 (72%)	888 (88%)	84 (8%)	32 (3%)	5 40
All	All	2017/2794 (72%)	1796 (89%)	163 (8%)	58 (3%)	6 42

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	392	LYS
1	A	410	VAL
1	A	458	GLU
1	A	460	GLU
1	A	461	LYS
1	A	798	PHE
1	A	805	ILE
1	A	806	LYS
1	A	894	GLU
1	A	914	PHE
1	A	969	ILE
1	A	1094	ILE
1	A	1272	PRO
1	B	390	GLU
1	B	615	ASP
1	B	645	LYS
1	B	669	TYR

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Mol	Chain	Res	Type
1	B	685	ARG
1	B	706	LEU
1	B	749	ASN
1	B	805	ILE
1	B	806	LYS
1	B	1042	LYS
1	A	633	GLU
1	A	674	SER
1	A	1014	ILE
1	B	416	LYS
1	B	616	ASP
1	B	810	LYS
1	B	1043	PHE
1	A	730	ASN
1	B	672	SER
1	B	1036	GLU
1	B	1037	SER
1	B	1050	LYS
1	B	1052	ARG
1	B	1267	SER
1	A	421	SER
1	A	747	ASP
1	A	915	ASP
1	A	987	ASN
1	A	996	ASP
1	B	391	LEU
1	B	608	ARG
1	B	766	ASN
1	B	1059	TYR
1	A	390	GLU
1	A	807	LYS
1	A	808	GLN
1	B	611	GLN
1	B	668	LYS
1	B	1144	ILE
1	B	1366	TYR
1	B	667	ILE
1	B	1138	ASP
1	B	832	ILE
1	B	1348	ILE
1	A	1070	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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
1	A	824/1316 (63%)	681 (83%)	143 (17%)	2 14
1	B	822/1316 (62%)	693 (84%)	129 (16%)	3 19
All	All	1646/2632 (62%)	1374 (84%)	272 (16%)	3 16

All (272) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	352	ASP
1	A	363	LYS
1	A	365	ASN
1	A	371	ILE
1	A	372	GLU
1	A	384	ILE
1	A	386	LYS
1	A	396	CYS
1	A	397	ASP
1	A	401	PHE
1	A	403	ILE
1	A	404	PHE
1	A	405	LYS
1	A	422	ASP
1	A	432	TYR
1	A	433	ARG
1	A	459	ILE
1	A	460	GLU
1	A	461	LYS
1	A	463	LEU
1	A	466	SER
1	A	468	LEU
1	A	473	LEU
1	A	475	ARG
1	A	516	LEU
1	A	535	ARG
1	A	537	ASN

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Mol	Chain	Res	Type
1	A	539	ASN
1	A	540	ASN
1	A	542	GLU
1	A	544	ILE
1	A	546	PHE
1	A	547	PHE
1	A	555	TYR
1	A	556	VAL
1	A	557	LEU
1	A	563	ASN
1	A	565	LYS
1	A	572	LEU
1	A	606	LYS
1	A	608	ARG
1	A	611	GLN
1	A	618	ASN
1	A	619	LYS
1	A	625	GLN
1	A	631	ASP
1	A	635	SER
1	A	638	LEU
1	A	642	VAL
1	A	646	ASP
1	A	650	ILE
1	A	653	LYS
1	A	655	ASN
1	A	659	ILE
1	A	666	ASP
1	A	670	LEU
1	A	681	LEU
1	A	683	LEU
1	A	703	LEU
1	A	716	LYS
1	A	728	SER
1	A	729	LYS
1	A	745	GLU
1	A	752	GLU
1	A	761	SER
1	A	775	LYS
1	A	784	TYR
1	A	785	LEU
1	A	793	PHE

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Mol	Chain	Res	Type
1	A	796	SER
1	A	800	MSE
1	A	804	GLU
1	A	817	THR
1	A	820	ARG
1	A	826	SER
1	A	833	ASN
1	A	869	SER
1	A	870	GLU
1	A	888	ARG
1	A	890	GLU
1	A	899	ASN
1	A	916	ASP
1	A	917	PHE
1	A	932	ASP
1	A	970	ASP
1	A	979	GLU
1	A	986	ILE
1	A	987	ASN
1	A	988	LYS
1	A	989	LYS
1	A	994	LYS
1	A	1013	ARG
1	A	1015	ILE
1	A	1021	LEU
1	A	1023	LYS
1	A	1024	TYR
1	A	1025	LYS
1	A	1026	LYS
1	A	1033	GLU
1	A	1035	MSE
1	A	1038	GLU
1	A	1045	GLU
1	A	1050	LYS
1	A	1053	LYS
1	A	1055	GLU
1	A	1072	PHE
1	A	1085	MSE
1	A	1089	LYS
1	A	1095	ASP
1	A	1102	ASN
1	A	1104	ILE

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Mol	Chain	Res	Type
1	A	1106	GLU
1	A	1108	ASP
1	A	1111	LEU
1	A	1112	LYS
1	A	1116	ASP
1	A	1117	LYS
1	A	1118	LEU
1	A	1135	GLU
1	A	1149	TYR
1	A	1154	LYS
1	A	1161	GLU
1	A	1163	LYS
1	A	1185	ASN
1	A	1219	THR
1	A	1243	PHE
1	A	1244	PHE
1	A	1254	LYS
1	A	1264	SER
1	A	1265	GLU
1	A	1266	ASN
1	A	1275	GLU
1	A	1276	SER
1	A	1277	ILE
1	A	1293	ASP
1	A	1357	LYS
1	A	1360	VAL
1	A	1361	LEU
1	A	1368	SER
1	A	1370	TYR
1	A	1372	LYS
1	A	1374	LEU
1	A	1378	LEU
1	B	364	ASN
1	B	366	SER
1	B	382	GLU
1	B	389	LYS
1	B	406	LYS
1	B	418	SER
1	B	421	SER
1	B	432	TYR
1	B	436	LYS
1	B	438	ARG

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Mol	Chain	Res	Type
1	B	439	ILE
1	B	461	LYS
1	B	462	ILE
1	B	463	LEU
1	B	464	ASN
1	B	467	ILE
1	B	473	LEU
1	B	486	TYR
1	B	487	LEU
1	B	489	LYS
1	B	492	HIS
1	B	493	ASN
1	B	494	ASP
1	B	499	THR
1	B	502	THR
1	B	503	ASP
1	B	506	SER
1	B	521	PHE
1	B	527	MSE
1	B	532	ILE
1	B	535	ARG
1	B	542	GLU
1	B	550	ASP
1	B	559	LYS
1	B	575	ILE
1	B	591	LYS
1	B	601	LEU
1	B	605	SER
1	B	613	THR
1	B	617	TYR
1	B	640	LEU
1	B	641	ASP
1	B	644	PHE
1	B	656	ASP
1	B	657	ILE
1	B	662	GLU
1	B	663	ASN
1	B	665	ASN
1	B	672	SER
1	B	673	PHE
1	B	675	LYS
1	B	676	VAL

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Mol	Chain	Res	Type
1	B	684	TYR
1	B	685	ARG
1	B	695	THR
1	B	698	THR
1	B	699	GLU
1	B	725	GLU
1	B	726	ASN
1	B	733	LEU
1	B	746	ILE
1	B	747	ASP
1	B	748	GLU
1	B	749	ASN
1	B	759	GLN
1	B	792	LEU
1	B	794	ASP
1	B	807	LYS
1	B	809	ILE
1	B	825	THR
1	B	827	ASP
1	B	828	LYS
1	B	834	ASP
1	B	848	SER
1	B	849	ASN
1	B	873	ASN
1	B	888	ARG
1	B	890	GLU
1	B	896	TRP
1	B	897	ASN
1	B	898	LEU
1	B	911	GLU
1	B	912	LYS
1	B	913	ASP
1	B	915	ASP
1	B	917	PHE
1	B	919	ILE
1	B	930	TYR
1	B	931	GLU
1	B	970	ASP
1	B	980	GLN
1	B	981	ARG
1	B	985	ASN
1	B	1011	LEU

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Mol	Chain	Res	Type
1	B	1026	LYS
1	B	1027	GLU
1	B	1035	MSE
1	B	1043	PHE
1	B	1046	ILE
1	B	1047	TYR
1	B	1048	TYR
1	B	1050	LYS
1	B	1057	TYR
1	B	1058	ILE
1	B	1059	TYR
1	B	1060	LYS
1	B	1072	PHE
1	B	1076	TYR
1	B	1084	LYS
1	B	1089	LYS
1	B	1095	ASP
1	B	1122	SER
1	B	1142	LYS
1	B	1155	ASP
1	B	1185	ASN
1	B	1218	ASN
1	B	1242	LYS
1	B	1244	PHE
1	B	1259	PHE
1	B	1261	ILE
1	B	1263	LEU
1	B	1346	ASN
1	B	1352	LEU
1	B	1353	MSE
1	B	1354	LYS
1	B	1359	SER
1	B	1362	GLU
1	B	1366	TYR
1	B	1367	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	365	ASN
1	A	537	ASN
1	A	618	ASN

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Mol	Chain	Res	Type
1	A	639	ASN
1	A	664	ASN
1	A	899	ASN
1	A	920	GLN
1	A	1066	ASN
1	A	1148	ASN
1	A	1270	ASN
1	A	1346	ASN
1	B	361	ASN
1	B	364	ASN
1	B	464	ASN
1	B	483	HIS
1	B	492	HIS
1	B	501	ASN
1	B	539	ASN
1	B	618	ASN
1	B	625	GLN
1	B	665	ASN
1	B	749	ASN
1	B	788	ASN
1	B	980	GLN
1	B	1062	ASN
1	B	1066	ASN
1	B	1119	ASN
1	B	1175	ASN
1	B	1191	GLN
1	B	1200	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	A	1008/1397 (72%)	-0.36	14 (1%)	78	68	2, 42, 106, 153	0
1	B	1002/1397 (71%)	0.08	48 (4%)	34	27	12, 67, 134, 199	0
All	All	2010/2794 (71%)	-0.14	62 (3%)	52	43	2, 55, 128, 199	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	726	ASN	8.0
1	B	744	ASP	6.9
1	B	728	SER	6.7
1	B	743	ILE	6.7
1	B	727	GLU	6.0
1	B	1138	ASP	5.8
1	B	1345	ASN	5.8
1	B	458	GLU	5.6
1	B	500	VAL	5.4
1	B	742	ASN	4.8
1	B	499	THR	4.5
1	B	1136	ASN	4.4
1	B	390	GLU	4.4
1	B	395	ASN	4.1
1	B	729	LYS	4.1
1	B	1039	ASN	4.0
1	B	396	CYS	3.8
1	B	770	ILE	3.8
1	B	391	LEU	3.8
1	B	457	ILE	3.7
1	A	742	ASN	3.6
1	B	537	ASN	3.5
1	B	1137	ASP	3.4
1	A	744	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	743	ILE	3.2
1	B	407	HIS	3.2
1	B	694	ASP	3.2
1	A	400	ILE	3.1
1	B	666	ASP	3.1
1	B	1347	ASP	3.1
1	B	747	ASP	3.0
1	A	687	ASN	3.0
1	B	398	THR	2.9
1	B	394	GLY	2.9
1	B	749	ASN	2.9
1	B	399	GLU	2.8
1	A	1093	ASN	2.8
1	B	1115	ASN	2.7
1	A	813	ASN	2.6
1	B	1120	GLY	2.6
1	B	505	PHE	2.5
1	B	769	ALA	2.5
1	B	664	ASN	2.5
1	A	728	SER	2.5
1	B	761	SER	2.5
1	A	726	ASN	2.4
1	A	692	PRO	2.3
1	B	751	ILE	2.3
1	A	722	ASP	2.3
1	B	757	ASN	2.3
1	B	690	ASN	2.2
1	B	389	LYS	2.1
1	B	760	ILE	2.1
1	B	695	THR	2.1
1	B	741	GLY	2.1
1	B	1272	PRO	2.1
1	A	789	TYR	2.1
1	B	579	ASN	2.1
1	B	767	ASN	2.1
1	B	745	GLU	2.0
1	A	724	GLU	2.0
1	A	727	GLU	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

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.