Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:34 AM GMT

PDB ID	:	2DHH
Title	:	Crystal structure of a multidrug transporter reveal a functionally rotating mechanism
Authors	:	Murakami, S.; Nakashima, R.; Yamashita, E.; Matsumoto, T.
Deposited on	:	2006-03-23
Resolution	:	2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

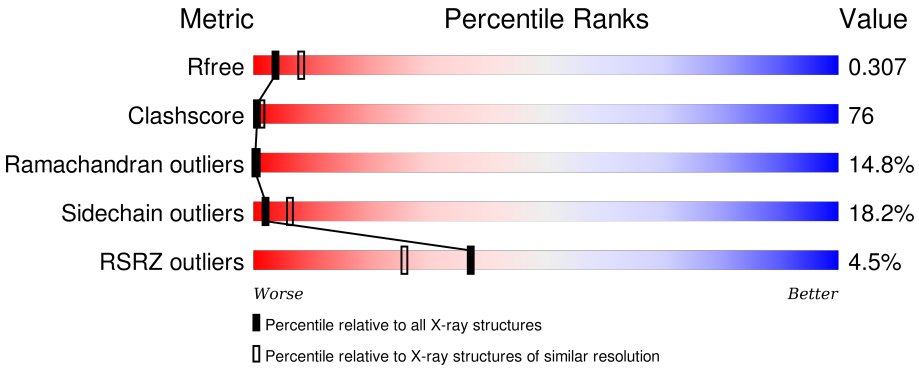
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	1053	4% 23% 49% 20% 5%
1	B	1053	5% 19% 55% 21%
1	C	1053	5% 18% 53% 22% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23378 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 ACRB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1022	Total	C	N	O	S	0	0	0
			7774	5003	1283	1444	44			
1	B	1022	Total	C	N	O	S	0	0	0
			7774	5003	1283	1444	44			
1	C	1022	Total	C	N	O	S	0	0	0
			7774	5003	1283	1444	44			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1050	HIS	-	EXPRESSION TAG	UNP P31224
A	1051	HIS	-	EXPRESSION TAG	UNP P31224
A	1052	HIS	-	EXPRESSION TAG	UNP P31224
A	1053	HIS	-	EXPRESSION TAG	UNP P31224
B	1050	HIS	-	EXPRESSION TAG	UNP P31224
B	1051	HIS	-	EXPRESSION TAG	UNP P31224
B	1052	HIS	-	EXPRESSION TAG	UNP P31224
B	1053	HIS	-	EXPRESSION TAG	UNP P31224
C	1050	HIS	-	EXPRESSION TAG	UNP P31224
C	1051	HIS	-	EXPRESSION TAG	UNP P31224
C	1052	HIS	-	EXPRESSION TAG	UNP P31224
C	1053	HIS	-	EXPRESSION TAG	UNP P31224

- Molecule 2 is water.

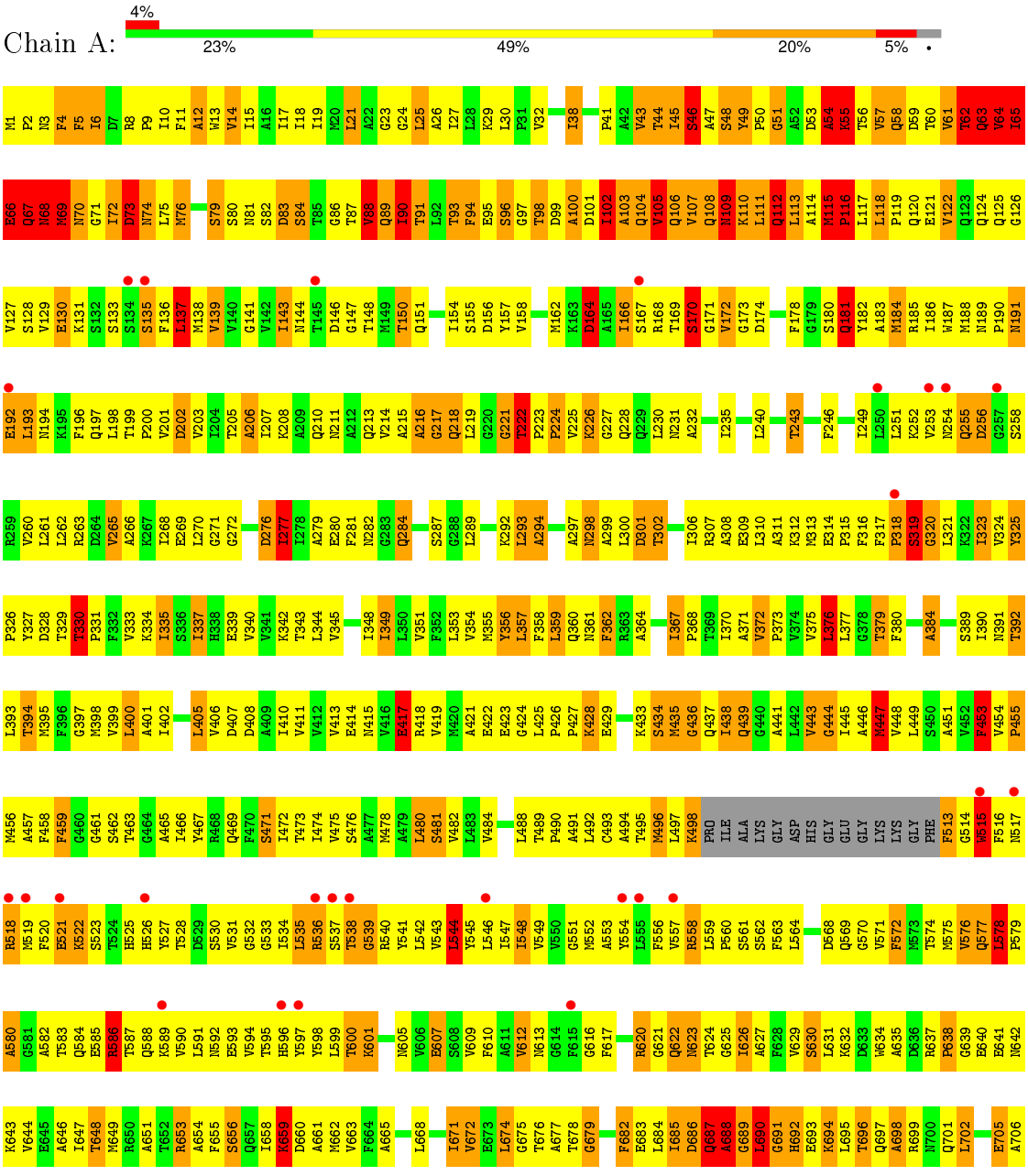
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	22	Total	O	0	0
			22	22		
2	B	8	Total	O	0	0
			8	8		
2	C	26	Total	O	0	0
			26	26		

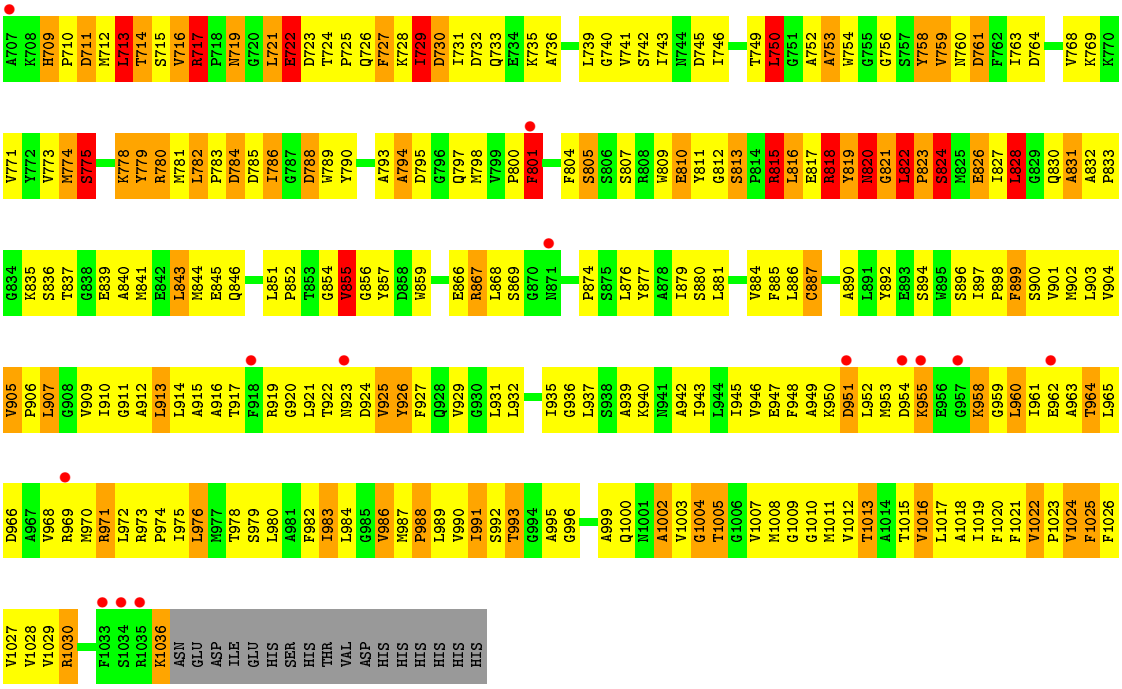
3 Residue-property plots (i)

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: ACRB

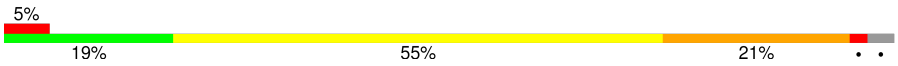
Chain A:

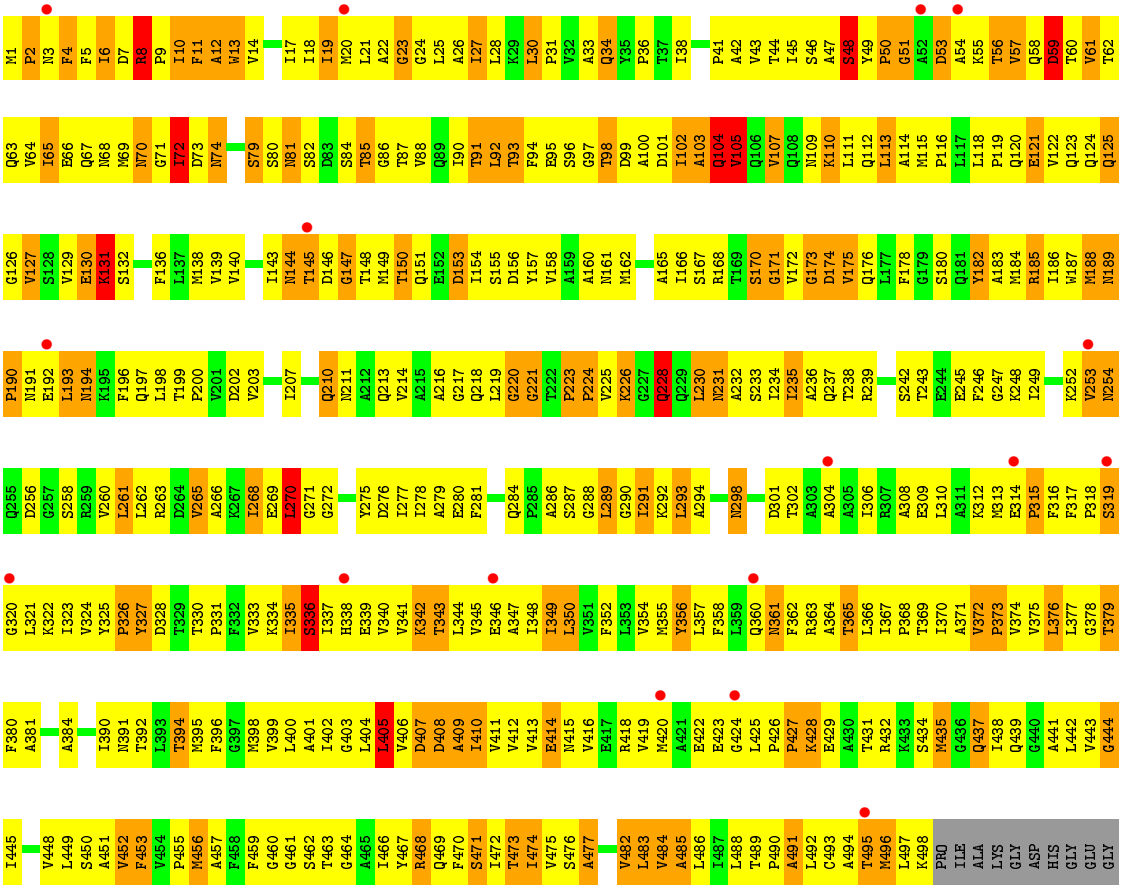


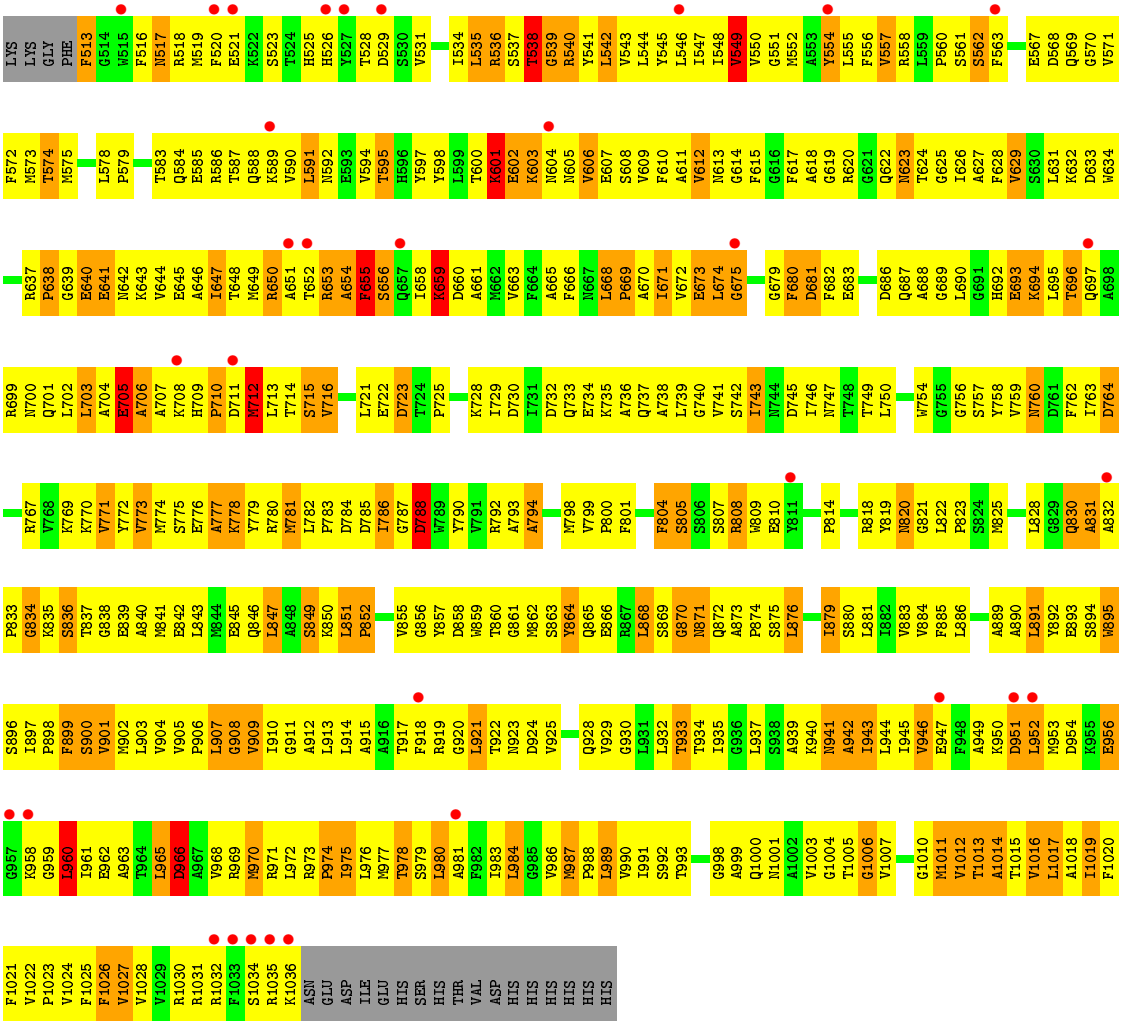


- Molecule 1: ACRB

Chain B:

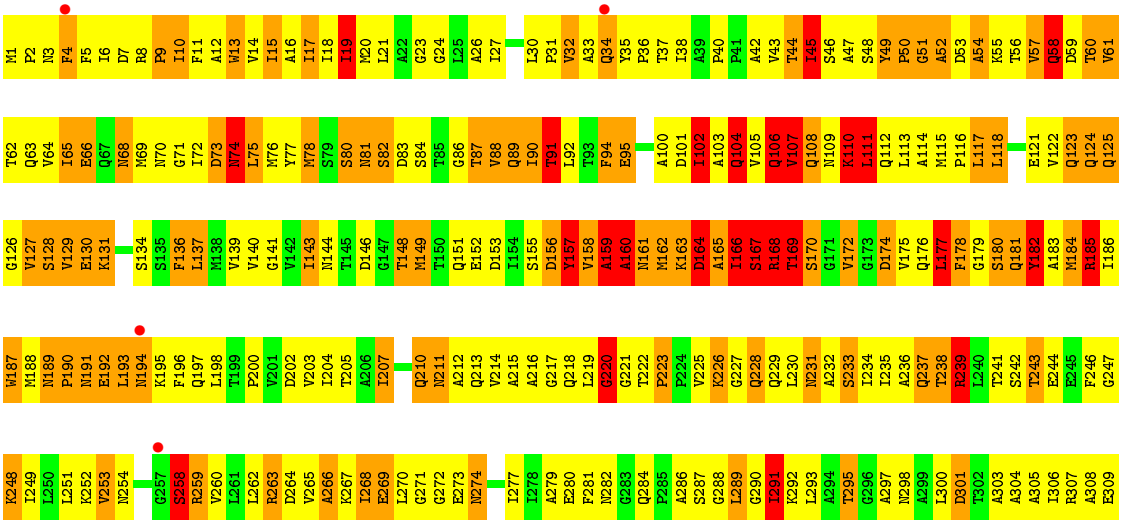


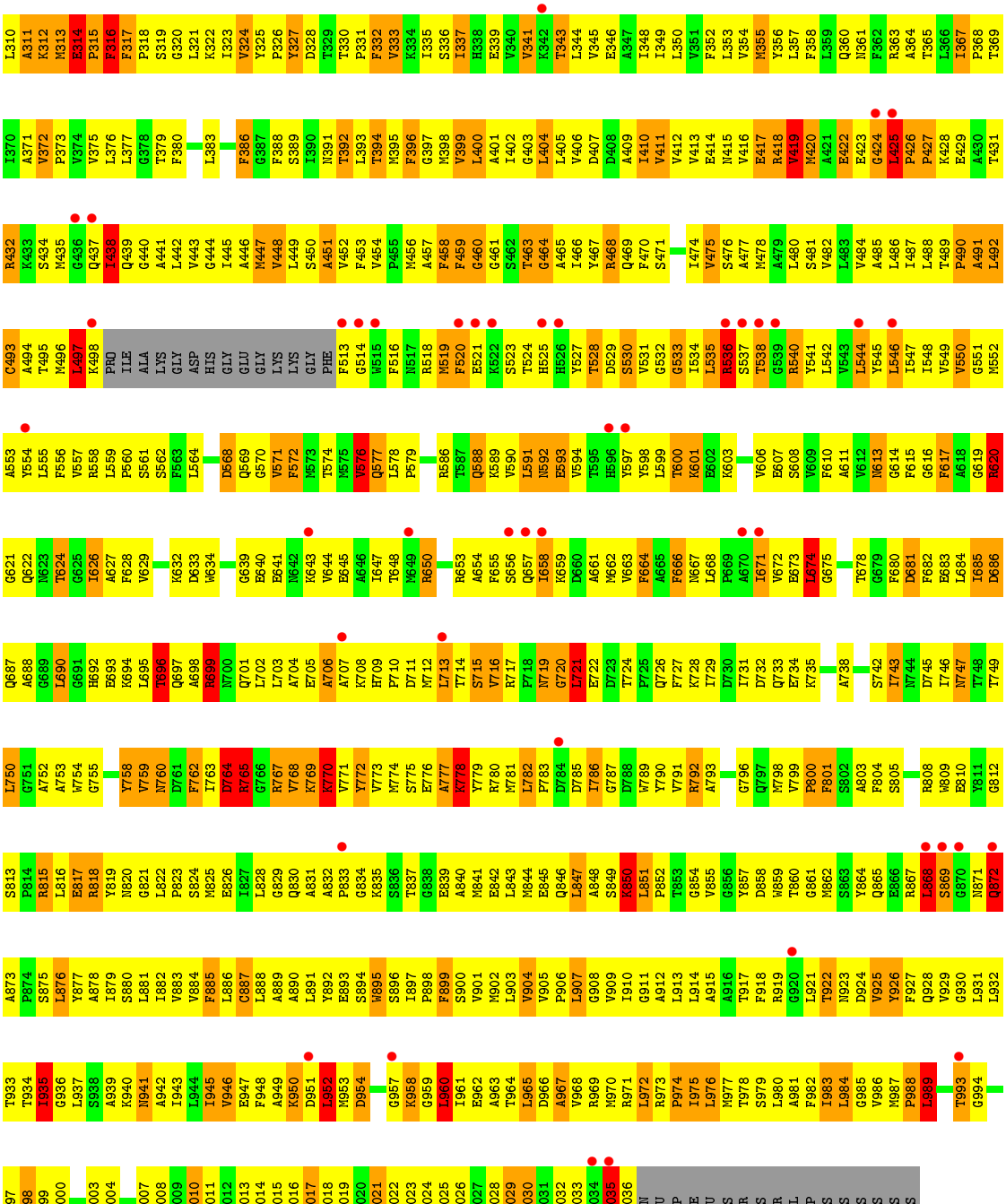




• Molecule 1: ACRB

Chain C:




L310 A311 K312 M313 E314 P315 F316 F317 P318 S319 G320 L321 K322 I323 V324 Y325 P326 Y327 D328 T329 T330 P331 F332 V333 K334 I335 S336 I337 H338 E339 V340 V341 K342 T343 L344 V345 E346 A347 T348 I349 L350 V351 F352 L353 V354 M355 Y356 L357 F358 L359 Q360 N361 F362 R363 A364 T365 L366 I367 P368 T369
I370 A371 V372 P373 V374 V375 L376 L377 G378 T379 F380 L383 F386 G387 F388 S389 I390 N391 T392 L393 T394 N395 F396 G397 N398 V399 L400 A401 I402 G403 L404 L405 V406 D407 D408 A409 I410 V411 V412 V413 E414 N415 V416 E417 R418 V419 M420 A421 E422 E423 G424 L425 P426 P427 K428 E429 A430 T431
R432 K433 S434 M435 G436 Q437 I438 Q439 G440 A441 L442 V443 G444 I445 A446 M447 V448 L449 S450 A451 V452 F453 V454 P455 M456 A457 F458 F459 G460 G461 S462 T463 G464 A465 I466 Y467 R468 Q469 F470 S471 I474 V475 S476 A477 M478 A479 L480 S481 V482 L483 V484 A485 L486 I487 L488 T489 P490 A491 L492
C493 A494 T495 M496 L497 K498 PRO ILE ALA LYS GLY ASP HIS GLY GLU GLY LYS LYS GLY PHE F513 G514 W515 F516 N517 R518 M519 F520 E521 K522 S523 T524 H525 H526 Y527 T528 D529 S530 V531 G532 G533 I534 L535 R536 S537 T538 G539 R540 Y541 L542 V543 L544 Y545 L546 I547 L548 T549 V550 G551 M552
A553 Y554 L555 F556 V557 R558 L559 P560 S561 S562 F563 L564 D568 Q569 G570 V571 F572 M573 T574 M575 V576 Q577 L578 P579 R586 T587 Q588 K589 V590 L591 N592 E593 V594 T595 H596 Y597 Y598 L599 T600 K601 E602 K603 V606 E607 S608 V609 F610 A611 V612 N613 G614 F615 G616 F617 A618 G619 R620
G621 Q622 N623 T624 G625 I626 A627 F628 V629 K632 D633 W634 G639 E640 E641 N642 K643 V644 E645 A646 I647 T648 M649 R650 R653 A654 F655 S656 Q657 I658 K659 D660 A661 M662 V663 F664 A665 F666 N667 L668 P669 A670 I671 V672 E673 L674 G675 T678 G679 F680 D681 F682 E683 L684 I685 D686
Q687 A688 G689 L690 G691 H692 E693 K694 L695 T696 Q697 A698 R699 N700 Q701 L702 L703 A704 E705 A706 A707 K708 H709 P710 D711 M712 L713 T714 S715 V716 R717 F718 N719 G720 L721 E722 D723 T724 F725 Q726 F727 K728 I729 D730 I731 D732 Q733 E734 K735 A738 S742 I743 N744 D745 I746 N747 I748 T749
L750 G751 A752 A753 W754 G755 Y758 V759 N760 D761 F762 I763 D764 R765 G766 R767 V768 K769 K770 V771 Y772 V773 M774 S775 E776 A777 R778 Y779 R780 M781 L782 P783 D784 D785 I786 G787 D788 W789 Y790 V791 R792 A793 G796 Q797 M798 V799 P800 F801 S802 A803 F804 S805 R808 W809 E810 Y811 G812
S813 P814 R815 L816 E817 R818 Y819 N820 G821 L822 P823 S824 M825 E826 I827 L828 G829 Q830 A831 A832 P833 G834 K835 S836 T837 G838 E839 A840 M841 E842 L843 M844 E845 Q846 L847 A848 S849 K850 L851 P852 T853 G854 V855 G856 Y857 D858 W859 T860 G861 M862 S863 Y864 Q865 E866 R867 L868 S869 G870 N871 Q872
A873 P874 S875 L876 Y877 A878 I879 S880 L881 I882 V883 V884 F885 L886 G887 L888 A889 A890 L891 Y892 E893 S894 W895 S896 I897 P898 F899 S900 V901 M902 L903 V904 V905 P906 L907 G908 V909 I910 G911 A912 L913 L914 A915 A916 T917 F918 R919 G920 L921 T922 N923 D924 V925 Y926 F927 Q928 V929 G930 L931 L932
T933 T934 I935 G936 L937 S938 A939 K940 N941 A942 I943 L944 I945 V946 E947 F948 A949 K950 D951 L952 M953 D954 G957 K958 G959 L960 I961 E962 A963 T964 L965 D966 A967 V968 R969 M970 R971 L972 R973 P974 I975 L976 M977 T978 S979 L980 A981 F982 I983 L984 G985 V986 M987 P988 L989 T993 G994
S997 G998 A999 Q1000 V1003 G1004 V1007 M1008 G1009 G1010 M1011 V1012 T1013 A1014 T1015 V1016 L1017 A1018 I1019 F1020 F1021 V1022 P1023 V1024 F1025 F1026 V1027 V1028 V1029 R1030 R1031 R1032 F1033 S1034 R1035 K1036 ASN GLU ASP ILE GLU HIS SER HIS THR VAL ASP HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	225.87Å 134.42Å 163.19Å 90.00° 97.71° 90.00°	Depositor
Resolution (Å)	10.00 – 2.80 10.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.0 (10.00-2.80) 99.0 (10.00-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.40 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.268 , 0.307 0.262 , 0.307	Depositor DCC
R_{free} test set	5752 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	73.4	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 103.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 115025 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	23378	wwPDB-VP
Average B, all atoms (Å^2)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	1.50	104/7920 (1.3%)	1.28	74/10756 (0.7%)
1	B	1.02	6/7920 (0.1%)	1.05	18/10756 (0.2%)
1	C	1.54	94/7920 (1.2%)	1.33	82/10756 (0.8%)
All	All	1.37	204/23760 (0.9%)	1.23	174/32268 (0.5%)

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	4
1	B	0	2
1	C	0	6
All	All	0	12

All (204) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	67	GLN	CB-CG	23.76	2.16	1.52
1	C	129	VAL	CB-CG2	21.03	1.97	1.52
1	C	167	SER	N-CA	20.35	1.87	1.46
1	A	818	ARG	CG-CD	20.25	2.02	1.51
1	C	166	ILE	CA-CB	20.11	2.01	1.54
1	A	68	ASN	CA-CB	16.05	1.94	1.53
1	C	164	ASP	C-O	15.81	1.53	1.23
1	C	161	ASN	N-CA	14.93	1.76	1.46
1	A	54	ALA	CA-CB	-14.74	1.21	1.52
1	C	45	ILE	CA-CB	14.56	1.88	1.54
1	C	128	SER	CA-CB	14.17	1.74	1.52
1	C	166	ILE	CA-C	-12.56	1.20	1.52
1	C	169	THR	CA-CB	12.51	1.85	1.53
1	C	160	ALA	CA-CB	-12.39	1.26	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	108	GLN	CB-CG	12.39	1.85	1.52
1	A	823	PRO	C-O	12.22	1.47	1.23
1	A	68	ASN	N-CA	12.03	1.70	1.46
1	A	819	TYR	CG-CD1	12.02	1.54	1.39
1	A	63	GLN	N-CA	-11.79	1.22	1.46
1	C	158	VAL	CB-CG2	11.70	1.77	1.52
1	C	157	TYR	C-O	11.57	1.45	1.23
1	A	69	MET	C-O	11.39	1.45	1.23
1	C	767	ARG	CZ-NH2	-11.12	1.18	1.33
1	C	46	SER	CA-CB	10.61	1.68	1.52
1	A	823	PRO	N-CA	-10.60	1.29	1.47
1	A	45	ILE	CA-CB	-10.55	1.30	1.54
1	C	164	ASP	CG-OD2	10.47	1.49	1.25
1	C	42	ALA	CA-CB	-10.25	1.30	1.52
1	C	157	TYR	CE2-CZ	-10.24	1.25	1.38
1	A	65	ILE	C-O	10.17	1.42	1.23
1	C	181	GLN	CD-OE1	10.08	1.46	1.24
1	A	65	ILE	CA-C	10.05	1.79	1.52
1	C	127	VAL	CA-CB	9.97	1.75	1.54
1	C	91	THR	CA-CB	9.49	1.78	1.53
1	A	43	VAL	CB-CG1	-9.27	1.33	1.52
1	A	67	GLN	CA-C	-8.97	1.29	1.52
1	C	161	ASN	CA-CB	-8.83	1.30	1.53
1	A	55	LYS	CD-CE	8.80	1.73	1.51
1	C	289	LEU	N-CA	-8.73	1.28	1.46
1	A	819	TYR	CE2-CZ	8.63	1.49	1.38
1	A	813	SER	CA-CB	8.50	1.65	1.52
1	C	157	TYR	CE1-CZ	-8.49	1.27	1.38
1	A	107	VAL	C-N	8.34	1.53	1.34
1	A	110	LYS	N-CA	-8.34	1.29	1.46
1	C	316	PHE	CG-CD1	-8.30	1.26	1.38
1	C	58	GLN	CB-CG	8.28	1.75	1.52
1	A	105	VAL	C-O	8.19	1.39	1.23
1	A	108	GLN	CA-C	-8.16	1.31	1.52
1	A	66	GLU	CA-C	8.09	1.74	1.52
1	A	819	TYR	CE1-CZ	8.08	1.49	1.38
1	A	61	VAL	CA-CB	7.84	1.71	1.54
1	A	819	TYR	CA-CB	-7.84	1.36	1.53
1	C	316	PHE	CG-CD2	-7.84	1.26	1.38
1	A	70	ASN	CA-C	7.80	1.73	1.52
1	C	104	GLN	CA-CB	7.79	1.71	1.53
1	A	46	SER	CA-CB	-7.77	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	104	GLN	CG-CD	7.74	1.68	1.51
1	A	688	ALA	CA-CB	7.72	1.68	1.52
1	A	73	ASP	CB-CG	7.69	1.68	1.51
1	A	66	GLU	CD-OE1	7.57	1.33	1.25
1	A	811	TYR	CE2-CZ	-7.53	1.28	1.38
1	C	165	ALA	C-O	7.52	1.37	1.23
1	C	772	TYR	CE2-CZ	-7.51	1.28	1.38
1	C	164	ASP	CG-OD1	7.43	1.42	1.25
1	C	166	ILE	N-CA	-7.41	1.31	1.46
1	B	107	VAL	CB-CG1	7.39	1.68	1.52
1	A	819	TYR	C-O	7.38	1.37	1.23
1	A	722	GLU	CB-CG	7.37	1.66	1.52
1	C	127	VAL	CB-CG1	7.32	1.68	1.52
1	A	855	VAL	CB-CG2	-7.29	1.37	1.52
1	C	164	ASP	CB-CG	7.27	1.67	1.51
1	A	69	MET	CB-CG	7.26	1.74	1.51
1	A	818	ARG	C-N	7.24	1.50	1.34
1	C	104	GLN	CG-CD	-7.21	1.34	1.51
1	A	816	LEU	N-CA	-7.19	1.31	1.46
1	C	94	PHE	CD2-CE2	-7.15	1.25	1.39
1	C	94	PHE	CD1-CE1	-7.14	1.25	1.39
1	C	297	ALA	CA-CB	-7.14	1.37	1.52
1	A	107	VAL	CA-C	-7.12	1.34	1.52
1	C	769	LYS	CA-C	7.00	1.71	1.52
1	A	70	ASN	CB-CG	-6.96	1.35	1.51
1	A	122	VAL	CB-CG2	-6.91	1.38	1.52
1	A	111	LEU	N-CA	6.89	1.60	1.46
1	C	128	SER	CB-OG	6.86	1.51	1.42
1	A	819	TYR	CB-CG	6.82	1.61	1.51
1	A	109	ASN	CB-CG	6.80	1.66	1.51
1	A	64	VAL	C-N	6.78	1.49	1.34
1	A	685	ILE	C-O	-6.78	1.10	1.23
1	A	821	GLY	N-CA	6.72	1.56	1.46
1	A	94	PHE	CG-CD1	6.71	1.48	1.38
1	A	79	SER	C-O	6.69	1.36	1.23
1	A	822	LEU	CA-CB	6.68	1.69	1.53
1	C	157	TYR	CD1-CE1	6.66	1.49	1.39
1	C	106	GLN	C-O	6.60	1.35	1.23
1	C	130	GLU	CG-CD	6.59	1.61	1.51
1	C	758	TYR	CE2-CZ	6.59	1.47	1.38
1	C	131	LYS	CE-NZ	6.57	1.65	1.49
1	A	57	VAL	CA-CB	-6.55	1.41	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	130	GLU	CD-OE2	6.55	1.32	1.25
1	C	169	THR	C-O	6.49	1.35	1.23
1	C	770	LYS	CD-CE	6.43	1.67	1.51
1	C	316	PHE	CB-CG	6.40	1.62	1.51
1	C	160	ALA	CA-C	-6.38	1.36	1.52
1	A	88	VAL	CB-CG1	6.30	1.66	1.52
1	A	66	GLU	C-O	-6.28	1.11	1.23
1	B	105	VAL	CA-CB	6.27	1.68	1.54
1	A	682	PHE	CE2-CZ	6.18	1.49	1.37
1	C	46	SER	CB-OG	6.18	1.50	1.42
1	C	168	ARG	CZ-NH2	6.17	1.41	1.33
1	A	696	THR	CA-CB	6.11	1.69	1.53
1	C	167	SER	CB-OG	6.10	1.50	1.42
1	A	65	ILE	CA-CB	-6.10	1.40	1.54
1	A	105	VAL	CA-CB	-6.09	1.42	1.54
1	C	139	VAL	CB-CG1	-6.09	1.40	1.52
1	C	767	ARG	C-O	6.08	1.34	1.23
1	A	698	ALA	CA-CB	-6.08	1.39	1.52
1	C	182	TYR	CE1-CZ	6.08	1.46	1.38
1	C	770	LYS	CG-CD	6.06	1.73	1.52
1	A	801	PHE	CB-CG	6.05	1.61	1.51
1	A	116	PRO	CA-C	-6.04	1.40	1.52
1	A	129	VAL	N-CA	-6.04	1.34	1.46
1	A	820	ASN	C-N	6.00	1.43	1.33
1	A	88	VAL	CB-CG2	-5.99	1.40	1.52
1	C	269	GLU	CD-OE1	5.99	1.32	1.25
1	C	182	TYR	CD2-CE2	5.97	1.48	1.39
1	A	725	PRO	C-O	5.95	1.35	1.23
1	A	66	GLU	CA-CB	5.92	1.67	1.53
1	A	67	GLN	C-O	5.87	1.34	1.23
1	A	55	LYS	CB-CG	5.86	1.68	1.52
1	B	773	VAL	CB-CG2	-5.82	1.40	1.52
1	C	44	THR	C-O	5.79	1.34	1.23
1	C	127	VAL	CB-CG2	-5.79	1.40	1.52
1	A	103	ALA	CA-CB	5.79	1.64	1.52
1	A	61	VAL	CA-C	5.78	1.68	1.52
1	C	764	ASP	N-CA	5.78	1.57	1.46
1	C	174	ASP	N-CA	5.76	1.57	1.46
1	C	324	VAL	CB-CG2	-5.75	1.40	1.52
1	C	772	TYR	CG-CD2	-5.75	1.31	1.39
1	C	212	ALA	CA-CB	5.75	1.64	1.52
1	C	180	SER	CB-OG	5.73	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	45	ILE	C-O	5.70	1.34	1.23
1	B	459	PHE	CB-CG	5.69	1.61	1.51
1	C	817	GLU	CB-CG	5.66	1.62	1.52
1	A	61	VAL	CB-CG1	5.64	1.64	1.52
1	A	94	PHE	CE1-CZ	5.64	1.48	1.37
1	A	817	GLU	CD-OE2	5.63	1.31	1.25
1	A	48	SER	CA-CB	-5.61	1.44	1.52
1	C	772	TYR	CD2-CE2	-5.58	1.30	1.39
1	A	41	PRO	CG-CD	5.56	1.69	1.50
1	C	136	PHE	CD2-CE2	-5.53	1.28	1.39
1	A	682	PHE	CD1-CE1	5.51	1.50	1.39
1	A	62	THR	N-CA	5.50	1.57	1.46
1	A	44	THR	C-O	5.47	1.33	1.23
1	A	45	ILE	N-CA	-5.45	1.35	1.46
1	A	69	MET	CG-SD	5.45	1.95	1.81
1	B	110	LYS	N-CA	5.45	1.57	1.46
1	C	178	PHE	CD1-CE1	5.44	1.50	1.39
1	A	72	ILE	C-O	5.43	1.33	1.23
1	C	107	VAL	CA-CB	5.43	1.66	1.54
1	A	100	ALA	CA-CB	-5.40	1.41	1.52
1	C	157	TYR	CG-CD1	-5.40	1.32	1.39
1	C	57	VAL	CB-CG1	-5.39	1.41	1.52
1	C	617	PHE	CE2-CZ	5.38	1.47	1.37
1	A	811	TYR	CA-CB	-5.35	1.42	1.53
1	C	273	GLU	CB-CG	-5.35	1.42	1.52
1	C	162	MET	CA-CB	5.35	1.65	1.53
1	A	106	GLN	N-CA	5.33	1.57	1.46
1	C	172	VAL	CB-CG1	5.33	1.64	1.52
1	A	826	GLU	CG-CD	5.31	1.59	1.51
1	C	887	CYS	CB-SG	-5.30	1.73	1.81
1	C	102	ILE	CA-CB	-5.29	1.42	1.54
1	A	94	PHE	CE2-CZ	5.29	1.47	1.37
1	C	266	ALA	CA-CB	-5.29	1.41	1.52
1	A	81	ASN	C-O	5.27	1.33	1.23
1	A	113	LEU	CG-CD1	5.26	1.71	1.51
1	A	111	LEU	CG-CD1	5.26	1.71	1.51
1	C	78	MET	CB-CG	5.25	1.68	1.51
1	A	93	THR	C-O	5.22	1.33	1.23
1	A	94	PHE	CD1-CE1	5.21	1.49	1.39
1	C	157	TYR	CG-CD2	-5.20	1.32	1.39
1	C	238	THR	CB-CG2	5.16	1.69	1.52
1	C	839	GLU	CG-CD	5.15	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	314	GLU	N-CA	5.14	1.56	1.46
1	C	156	ASP	CB-CG	5.13	1.62	1.51
1	A	815	ARG	NE-CZ	5.13	1.39	1.33
1	A	727	PHE	CA-C	-5.12	1.39	1.52
1	A	687	GLN	CA-CB	5.11	1.65	1.53
1	C	74	ASN	C-O	-5.09	1.13	1.23
1	A	112	GLN	N-CA	-5.09	1.36	1.46
1	A	688	ALA	N-CA	5.09	1.56	1.46
1	A	67	GLN	N-CA	-5.08	1.36	1.46
1	C	88	VAL	CB-CG2	-5.08	1.42	1.52
1	B	130	GLU	CB-CG	-5.07	1.42	1.52
1	C	572	PHE	CE1-CZ	5.07	1.47	1.37
1	C	291	ILE	CA-CB	-5.07	1.43	1.54
1	A	104	GLN	N-CA	5.04	1.56	1.46
1	C	273	GLU	C-O	-5.04	1.13	1.23
1	A	45	ILE	C-N	5.03	1.45	1.34
1	A	63	GLN	CD-NE2	5.03	1.45	1.32
1	C	220	GLY	C-O	-5.02	1.15	1.23
1	A	691	GLY	C-O	5.02	1.31	1.23
1	C	683	GLU	CG-CD	-5.01	1.44	1.51
1	A	55	LYS	CG-CD	5.01	1.69	1.52
1	C	158	VAL	CB-CG1	-5.00	1.42	1.52

All (174) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	164	ASP	CB-CG-OD1	-17.91	102.18	118.30
1	C	767	ARG	CD-NE-CZ	-16.19	100.94	123.60
1	C	168	ARG	N-CA-C	10.95	140.57	111.00
1	A	818	ARG	NE-CZ-NH2	9.96	125.28	120.30
1	A	111	LEU	CB-CA-C	-9.93	91.33	110.20
1	A	717	ARG	NE-CZ-NH2	-9.81	115.39	120.30
1	C	126	GLY	N-CA-C	-9.77	88.68	113.10
1	C	131	LYS	CD-CE-NZ	-9.68	89.43	111.70
1	A	818	ARG	CA-CB-CG	-9.66	92.14	113.40
1	A	68	ASN	N-CA-CB	-9.62	93.28	110.60
1	A	62	THR	CA-CB-CG2	-9.41	99.22	112.40
1	C	815	ARG	NE-CZ-NH2	-9.40	115.60	120.30
1	A	828	LEU	CB-CG-CD1	-9.39	95.03	111.00
1	A	70	ASN	N-CA-C	-9.26	85.99	111.00
1	C	166	ILE	O-C-N	9.18	137.39	122.70
1	A	818	ARG	CD-NE-CZ	-9.04	110.95	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	164	ASP	CB-CG-OD2	8.98	126.38	118.30
1	C	157	TYR	CA-CB-CG	-8.97	96.36	113.40
1	A	812	GLY	N-CA-C	-8.93	90.78	113.10
1	B	30	LEU	CA-CB-CG	8.58	135.04	115.30
1	C	767	ARG	NE-CZ-NH2	-8.35	116.12	120.30
1	B	230	LEU	CA-CB-CG	8.31	134.41	115.30
1	A	717	ARG	NE-CZ-NH1	8.28	124.44	120.30
1	C	168	ARG	CB-CA-C	-8.16	94.09	110.40
1	A	721	LEU	CB-CG-CD2	-8.04	97.33	111.00
1	C	239	ARG	NE-CZ-NH2	-7.99	116.30	120.30
1	C	425	LEU	CA-CB-CG	7.67	132.95	115.30
1	A	118	LEU	CB-CG-CD1	7.61	123.94	111.00
1	A	686	ASP	CB-CG-OD2	7.52	125.07	118.30
1	A	818	ARG	N-CA-CB	7.51	124.11	110.60
1	A	578	LEU	CA-CB-CG	7.50	132.54	115.30
1	A	65	ILE	CB-CG1-CD1	-7.36	93.29	113.90
1	B	989	LEU	CA-CB-CG	7.32	132.14	115.30
1	B	705	GLU	N-CA-C	-7.31	91.25	111.00
1	A	817	GLU	OE1-CD-OE2	7.26	132.01	123.30
1	C	167	SER	C-N-CA	-7.20	103.69	121.70
1	B	468	ARG	NE-CZ-NH1	-7.17	116.71	120.30
1	A	723	ASP	CB-CG-OD2	-7.16	111.86	118.30
1	C	73	ASP	CB-CG-OD1	-7.07	111.93	118.30
1	C	185	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	C	166	ILE	CB-CG1-CD1	-6.99	94.32	113.90
1	A	696	THR	N-CA-C	-6.96	92.20	111.00
1	B	289	LEU	CA-CB-CG	6.96	131.31	115.30
1	C	620	ARG	NE-CZ-NH1	-6.93	116.83	120.30
1	A	108	GLN	CB-CA-C	-6.88	96.65	110.40
1	A	723	ASP	CB-CG-OD1	6.83	124.45	118.30
1	C	239	ARG	NE-CZ-NH1	6.83	123.71	120.30
1	C	166	ILE	N-CA-CB	6.79	126.42	110.80
1	C	172	VAL	CA-CB-CG1	6.78	121.07	110.90
1	A	544	LEU	CA-CB-CG	6.78	130.88	115.30
1	B	4	PHE	N-CA-C	-6.76	92.75	111.00
1	C	66	GLU	OE1-CD-OE2	-6.74	115.21	123.30
1	B	952	LEU	CA-CB-CG	6.73	130.79	115.30
1	A	761	ASP	CB-CG-OD2	-6.67	112.29	118.30
1	C	127	VAL	CG1-CB-CG2	-6.53	100.46	110.90
1	C	160	ALA	N-CA-C	6.51	128.59	111.00
1	A	750	LEU	CA-CB-CG	6.48	130.21	115.30
1	A	44	THR	CA-CB-CG2	6.46	121.45	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	818	ARG	NH1-CZ-NH2	-6.45	112.31	119.40
1	A	57	VAL	CB-CA-C	-6.44	99.17	111.40
1	C	686	ASP	CB-CG-OD2	6.43	124.09	118.30
1	C	818	ARG	NE-CZ-NH2	6.38	123.49	120.30
1	C	68	ASN	N-CA-C	6.36	128.17	111.00
1	B	73	ASP	CB-CG-OD2	6.35	124.02	118.30
1	C	163	LYS	CD-CE-NZ	-6.34	97.12	111.70
1	C	131	LYS	CG-CD-CE	-6.33	92.91	111.90
1	C	45	ILE	CB-CA-C	-6.33	98.94	111.60
1	C	168	ARG	NE-CZ-NH1	-6.32	117.14	120.30
1	A	118	LEU	CA-CB-CG	-6.31	100.78	115.30
1	A	61	VAL	N-CA-C	6.30	128.00	111.00
1	A	67	GLN	N-CA-C	6.29	127.98	111.00
1	A	729	ILE	CG1-CB-CG2	-6.27	97.61	111.40
1	C	162	MET	CB-CG-SD	-6.26	93.62	112.40
1	A	724	THR	OG1-CB-CG2	-6.25	95.62	110.00
1	A	66	GLU	N-CA-CB	6.25	121.85	110.60
1	A	164	ASP	CB-CG-OD1	-6.15	112.76	118.30
1	C	620	ARG	NE-CZ-NH2	6.13	123.36	120.30
1	A	823	PRO	CA-N-CD	6.13	120.28	111.70
1	A	181	GLN	N-CA-C	-6.12	94.48	111.00
1	A	55	LYS	CD-CE-NZ	6.11	125.76	111.70
1	A	586	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	A	63	GLN	CA-CB-CG	6.09	126.80	113.40
1	B	220	GLY	N-CA-C	-6.00	98.10	113.10
1	A	115	MET	N-CA-CB	5.99	121.38	110.60
1	C	159	ALA	N-CA-CB	-5.99	101.72	110.10
1	C	166	ILE	CB-CA-C	5.99	123.57	111.60
1	A	821	GLY	N-CA-C	-5.92	98.31	113.10
1	A	276	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	A	69	MET	CG-SD-CE	5.91	109.65	100.20
1	A	819	TYR	CB-CA-C	5.88	122.17	110.40
1	C	792	ARG	NE-CZ-NH1	-5.87	117.36	120.30
1	C	239	ARG	CG-CD-NE	-5.87	99.47	111.80
1	C	127	VAL	N-CA-C	-5.86	95.18	111.00
1	A	674	LEU	CA-CB-CG	5.85	128.76	115.30
1	C	159	ALA	C-N-CA	-5.85	107.08	121.70
1	C	732	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	C	755	GLY	N-CA-C	-5.81	98.57	113.10
1	C	177	LEU	CB-CG-CD2	5.81	120.88	111.00
1	C	90	ILE	CB-CA-C	-5.80	100.00	111.60
1	C	157	TYR	CG-CD2-CE2	5.80	125.94	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	825	MET	CG-SD-CE	5.79	109.46	100.20
1	A	81	ASN	CB-CA-C	-5.78	98.84	110.40
1	A	118	LEU	CB-CG-CD2	-5.76	101.20	111.00
1	C	357	LEU	CA-CB-CG	5.76	128.55	115.30
1	C	87	THR	N-CA-C	5.76	126.55	111.00
1	C	164	ASP	N-CA-CB	-5.73	100.29	110.60
1	A	90	ILE	N-CA-C	-5.70	95.60	111.00
1	A	113	LEU	CB-CG-CD1	5.70	120.68	111.00
1	C	168	ARG	CG-CD-NE	-5.68	99.87	111.80
1	A	822	LEU	C-N-CD	-5.68	108.10	120.60
1	A	107	VAL	N-CA-C	-5.67	95.70	111.00
1	C	767	ARG	CG-CD-NE	-5.66	99.91	111.80
1	C	66	GLU	N-CA-CB	5.63	120.74	110.60
1	A	93	THR	O-C-N	5.60	131.66	122.70
1	A	62	THR	CA-C-N	-5.59	104.89	117.20
1	A	89	GLN	N-CA-C	-5.59	95.91	111.00
1	C	818	ARG	NE-CZ-NH1	-5.54	117.53	120.30
1	A	913	LEU	CA-CB-CG	5.52	128.00	115.30
1	C	156	ASP	CB-CG-OD1	5.51	123.25	118.30
1	C	681	ASP	CB-CG-OD2	5.51	123.26	118.30
1	C	972	LEU	CA-CB-CG	5.48	127.91	115.30
1	C	773	VAL	N-CA-C	-5.48	96.21	111.00
1	C	699	ARG	NE-CZ-NH1	-5.45	117.57	120.30
1	B	113	LEU	CB-CG-CD1	5.44	120.25	111.00
1	C	721	LEU	CA-CB-CG	5.44	127.81	115.30
1	A	68	ASN	N-CA-C	-5.44	96.32	111.00
1	C	166	ILE	CA-CB-CG1	-5.43	100.68	111.00
1	C	248	LYS	CD-CE-NZ	-5.43	99.22	111.70
1	A	109	ASN	CB-CA-C	-5.41	99.57	110.40
1	C	165	ALA	N-CA-CB	5.40	117.66	110.10
1	C	576	VAL	CB-CA-C	-5.40	101.14	111.40
1	A	818	ARG	CB-CG-CD	-5.39	97.58	111.60
1	B	350	LEU	CB-CG-CD1	-5.37	101.86	111.00
1	C	989	LEU	CA-CB-CG	5.36	127.63	115.30
1	A	788	ASP	CB-CG-OD1	-5.35	113.48	118.30
1	A	63	GLN	CA-C-N	-5.34	105.46	117.20
1	C	868	LEU	CA-CB-CG	5.34	127.57	115.30
1	A	64	VAL	C-N-CA	-5.33	108.36	121.70
1	B	650	ARG	NE-CZ-NH2	5.33	122.97	120.30
1	C	960	LEU	CA-CB-CG	5.32	127.54	115.30
1	C	822	LEU	CA-CB-CG	-5.30	103.11	115.30
1	C	772	TYR	CB-CG-CD1	5.29	124.17	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	66	GLU	CB-CA-C	-5.28	99.84	110.40
1	C	157	TYR	CA-C-N	-5.28	105.58	117.20
1	C	686	ASP	CB-CG-OD1	-5.28	113.55	118.30
1	A	867	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	B	72	ILE	CG1-CB-CG2	-5.26	99.83	111.40
1	B	998	GLY	N-CA-C	-5.25	99.98	113.10
1	C	125	GLN	CB-CA-C	5.25	120.89	110.40
1	A	816	LEU	N-CA-C	-5.23	96.87	111.00
1	C	129	VAL	CA-CB-CG1	-5.22	103.07	110.90
1	B	980	LEU	CA-CB-CG	5.20	127.27	115.30
1	C	720	GLY	N-CA-C	5.18	126.06	113.10
1	C	952	LEU	CA-CB-CG	5.17	127.20	115.30
1	A	721	LEU	CA-CB-CG	5.17	127.20	115.30
1	A	71	GLY	N-CA-C	-5.17	100.18	113.10
1	A	222	THR	N-CA-C	-5.17	97.05	111.00
1	C	104	GLN	CA-CB-CG	-5.17	102.04	113.40
1	B	376	LEU	CB-CG-CD1	-5.15	102.24	111.00
1	A	820	ASN	CB-CA-C	-5.14	100.11	110.40
1	C	765	ARG	CB-CA-C	-5.13	100.13	110.40
1	C	165	ALA	CA-C-N	-5.10	105.98	117.20
1	A	102	ILE	O-C-N	-5.10	114.54	122.70
1	C	157	TYR	CG-CD1-CE1	-5.09	117.23	121.30
1	C	123	GLN	N-CA-C	-5.08	97.29	111.00
1	C	172	VAL	N-CA-C	-5.07	97.32	111.00
1	C	815	ARG	CG-CD-NE	-5.06	101.17	111.80
1	A	67	GLN	CA-C-N	5.05	128.32	117.20
1	C	88	VAL	CB-CA-C	-5.05	101.81	111.40
1	C	167	SER	N-CA-C	-5.04	97.39	111.00
1	A	478	MET	CG-SD-CE	5.04	108.26	100.20
1	C	772	TYR	OH-CZ-CE2	-5.03	106.53	120.10
1	A	107	VAL	CB-CA-C	-5.01	101.87	111.40
1	A	824	SER	N-CA-C	5.00	124.51	111.00

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	62	THR	Mainchain
1	A	65	ILE	Mainchain
1	A	66	GLU	Peptide
1	A	818	ARG	Mainchain
1	B	102	ILE	Peptide

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Mol	Chain	Res	Type	Group
1	B	706	ALA	Peptide
1	C	104	GLN	Mainchain
1	C	160	ALA	Mainchain,Peptide
1	C	166	ILE	Peptide
1	C	168	ARG	Mainchain
1	C	45	ILE	Mainchain

5.2 Too-close contacts

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	7774	0	7931	1178	0
1	B	7774	0	7931	1189	0
1	C	7774	0	7931	1304	0
2	A	22	0	0	30	0
2	B	8	0	0	6	0
2	C	26	0	0	35	0
All	All	23378	0	23793	3559	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 76.

All (3559) 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:C:127:VAL:CB	1:C:127:VAL:CA	1.75	1.63
1:C:158:VAL:CB	1:C:158:VAL:CG2	1.77	1.60
1:A:69:MET:CG	1:A:69:MET:CB	1.74	1.60
1:C:58:GLN:CG	1:C:58:GLN:CB	1.74	1.55
1:A:68:ASN:CA	1:A:68:ASN:N	1.70	1.55
1:A:108:GLN:CB	1:A:108:GLN:CG	1.86	1.53
1:C:91:THR:CB	1:C:91:THR:CA	1.78	1.53
1:A:65:ILE:CA	1:A:65:ILE:C	1.79	1.51
1:C:169:THR:CB	1:C:169:THR:CA	1.85	1.50
1:C:45:ILE:CA	1:C:45:ILE:CB	1.88	1.49
1:C:161:ASN:N	1:C:161:ASN:CA	1.76	1.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:VAL:O	1:A:65:ILE:CG2	1.66	1.43
1:C:129:VAL:CB	1:C:129:VAL:CG2	1.97	1.43
1:A:68:ASN:CA	1:A:68:ASN:CB	1.94	1.42
1:C:167:SER:N	1:C:167:SER:CA	1.87	1.38
1:C:166:ILE:CA	1:C:166:ILE:CB	2.01	1.36
1:A:818:ARG:CD	1:A:818:ARG:CG	2.02	1.35
1:B:247:GLY:HA2	1:B:268:ILE:CD1	1.63	1.28
1:B:247:GLY:CA	1:B:268:ILE:HD13	1.67	1.23
1:A:67:GLN:CB	1:A:67:GLN:CG	2.16	1.22
1:A:61:VAL:O	1:A:65:ILE:HG22	1.09	1.22
1:C:115:MET:CE	1:C:118:LEU:HD22	1.70	1.22
1:C:159:ALA:HA	2:C:1078:HOH:O	1.05	1.21
1:C:950:LYS:NZ	1:C:1030:ARG:HD3	1.56	1.21
1:C:44:THR:HG22	1:C:91:THR:CB	1.70	1.20
1:A:66:GLU:HG2	2:A:1058:HOH:O	1.40	1.19
1:C:274:ASN:HB2	2:C:1060:HOH:O	1.43	1.19
1:A:686:ASP:HB3	2:A:1059:HOH:O	1.37	1.18
1:A:108:GLN:HG3	1:B:112:GLN:OE1	1.38	1.18
1:C:291:ILE:HD13	1:C:306:ILE:HD13	1.23	1.18
1:C:44:THR:CG2	1:C:91:THR:HB	1.74	1.17
1:B:456:MET:HG3	1:B:467:TYR:HB3	1.21	1.17
1:C:110:LYS:HA	1:C:113:LEU:HD12	1.28	1.16
1:C:82:SER:HB3	1:C:88:VAL:HA	1.26	1.15
1:C:58:GLN:HB3	2:C:1079:HOH:O	1.45	1.15
1:B:1:MET:HB2	1:B:2:PRO:HD2	1.25	1.15
1:A:344:LEU:HD23	1:A:402:ILE:HD13	1.15	1.15
1:B:544:LEU:HA	1:B:547:ILE:HD12	1.30	1.14
1:C:713:LEU:HG	1:C:832:ALA:O	1.47	1.14
1:C:166:ILE:HA	1:C:166:ILE:HD13	1.20	1.14
1:C:54:ALA:HB2	1:C:84:SER:HB2	1.30	1.14
1:B:1022:VAL:O	1:B:1024:VAL:O	1.66	1.14
1:A:690:LEU:HD11	1:A:854:GLY:HA3	1.27	1.13
1:A:531:VAL:HA	1:A:534:ILE:HD11	1.24	1.13
1:B:445:ILE:HG23	1:B:940:LYS:HG3	1.27	1.13
1:C:190:PRO:HD3	1:C:779:TYR:HD1	1.13	1.12
1:C:432:ARG:HG3	1:C:432:ARG:HH11	1.14	1.12
1:C:69:MET:CE	1:C:92:LEU:HD21	1.78	1.11
1:B:990:VAL:HG13	1:B:1005:THR:OG1	1.48	1.11
1:C:220:GLY:HA3	1:C:231:ASN:ND2	1.65	1.11
1:C:699:ARG:HG2	1:C:699:ARG:HH11	1.16	1.11
1:A:261:LEU:HD12	1:A:263:ARG:HH22	1.08	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:894:SER:HB3	1:B:897:ILE:HG12	1.33	1.10
1:C:358:PHE:HB3	1:C:977:MET:HE2	1.33	1.10
1:A:400:LEU:HD13	1:A:1003:VAL:HG13	1.27	1.10
1:A:686:ASP:O	1:A:688:ALA:N	1.84	1.09
1:C:770:LYS:HG3	2:C:1070:HOH:O	1.48	1.09
1:B:441:ALA:HB2	1:B:947:GLU:HG2	1.18	1.09
1:A:713:LEU:HD22	1:A:714:THR:H	1.15	1.09
1:C:699:ARG:CG	1:C:699:ARG:HH11	1.66	1.09
1:A:729:ILE:HG22	1:A:730:ASP:H	1.14	1.09
1:B:42:ALA:HB2	1:B:93:THR:HG22	1.34	1.08
1:C:847:LEU:HA	1:C:850:LYS:HD3	1.30	1.08
1:C:747:ASN:HA	2:C:1066:HOH:O	1.54	1.08
1:A:443:VAL:HG12	1:A:444:GLY:H	1.19	1.07
1:C:427:PRO:HA	1:C:498:LYS:HE3	1.22	1.07
1:A:945:ILE:HG12	1:A:971:ARG:HG2	1.32	1.07
1:A:66:GLU:HA	2:A:1056:HOH:O	1.54	1.06
1:C:1:MET:HB2	1:C:2:PRO:HD2	1.32	1.06
1:C:166:ILE:HA	1:C:166:ILE:CD1	1.85	1.06
1:C:69:MET:HE2	1:C:92:LEU:CD2	1.86	1.06
1:B:843:LEU:HD23	1:B:847:LEU:HD21	1.07	1.06
1:A:112:GLN:HA	1:A:112:GLN:HE21	1.15	1.05
1:A:713:LEU:HG	1:A:833:PRO:HD3	1.34	1.05
1:A:649:MET:HB3	1:A:653:ARG:HH21	1.22	1.05
1:C:167:SER:OG	1:C:168:ARG:N	1.85	1.05
1:C:163:LYS:O	1:C:166:ILE:N	1.89	1.04
1:A:54:ALA:HB1	1:A:816:LEU:HG	1.38	1.04
1:A:344:LEU:CD2	1:A:402:ILE:HD13	1.88	1.03
1:C:420:MET:SD	1:C:498:LYS:CE	2.46	1.03
1:C:115:MET:HE2	1:C:118:LEU:HD22	1.08	1.03
1:A:400:LEU:CD1	1:A:1003:VAL:HG13	1.87	1.03
1:C:162:MET:HB3	1:C:313:MET:HE1	1.41	1.03
1:B:904:VAL:HG13	1:B:907:LEU:HD12	1.35	1.03
1:C:1022:VAL:HA	1:C:1025:PHE:HD2	1.22	1.03
1:B:574:THR:HG23	1:B:665:ALA:HB2	1.39	1.03
1:C:713:LEU:HD11	1:C:834:GLY:HA3	1.35	1.03
1:B:431:THR:HG21	1:B:493:CYS:HB3	1.37	1.02
1:A:713:LEU:HB3	1:A:832:ALA:HA	1.37	1.02
1:A:959:GLY:HA3	1:A:962:GLU:HB2	1.41	1.02
1:C:712:MET:HB2	1:C:835:LYS:HG3	1.41	1.02
1:A:205:THR:O	1:A:205:THR:HG22	1.54	1.01
1:B:226:LYS:HA	1:B:226:LYS:HE3	1.40	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:415:ASN:ND2	1:C:434:SER:HB2	1.74	1.01
1:C:238:THR:HG22	1:C:239:ARG:O	1.59	1.01
1:B:876:LEU:HD13	1:B:932:LEU:HD11	1.43	1.00
1:C:901:VAL:O	1:C:904:VAL:HG23	1.59	1.00
1:A:713:LEU:CB	1:A:832:ALA:HA	1.91	1.00
1:A:713:LEU:O	1:A:714:THR:HG23	1.61	1.00
1:A:559:LEU:HD12	1:A:560:PRO:HD2	1.41	1.00
1:A:435:MET:HG2	1:A:490:PRO:HB3	1.44	0.99
1:C:115:MET:CE	1:C:118:LEU:CD2	2.40	0.99
1:A:536:ARG:HG2	1:A:537:SER:H	1.22	0.99
1:C:887:CYS:O	1:C:890:ALA:HB3	1.62	0.99
1:C:166:ILE:HA	1:C:166:ILE:CB	1.84	0.99
1:A:328:ASP:OD1	1:A:330:THR:HB	1.62	0.99
1:C:159:ALA:O	1:C:161:ASN:N	1.94	0.99
1:B:49:TYR:CD2	1:B:122:VAL:HA	1.98	0.99
1:B:144:ASN:HB2	1:B:320:GLY:O	1.62	0.99
1:C:143:ILE:HG23	1:C:284:GLN:NE2	1.77	0.98
1:A:819:TYR:H	1:A:824:SER:HB3	1.27	0.98
1:B:523:SER:HA	1:B:526:HIS:HD2	1.29	0.98
1:B:687:GLN:NE2	1:B:856:GLY:HA3	1.79	0.98
1:B:549:VAL:HG22	1:B:550:VAL:N	1.79	0.97
1:C:162:MET:HG2	1:C:313:MET:CE	1.94	0.97
1:A:818:ARG:HD3	1:A:821:GLY:O	1.64	0.97
1:C:729:ILE:HD11	1:C:786:ILE:HD13	1.46	0.97
1:A:687:GLN:NE2	1:A:856:GLY:HA3	1.78	0.97
1:A:251:LEU:HD11	1:A:262:LEU:HA	1.46	0.97
1:A:690:LEU:HD11	1:A:854:GLY:CA	1.96	0.96
1:C:588:GLN:HG2	1:C:613:ASN:HD22	1.25	0.96
1:C:111:LEU:HB3	2:C:1056:HOH:O	1.64	0.96
1:C:674:LEU:HD11	1:C:862:MET:HA	1.46	0.96
1:B:704:ALA:O	1:B:705:GLU:HG3	1.66	0.96
1:C:684:LEU:HG	1:C:684:LEU:O	1.64	0.96
1:B:361:ASN:O	1:B:365:THR:HB	1.64	0.96
1:C:164:ASP:O	1:C:167:SER:OG	1.84	0.95
1:A:105:VAL:O	1:A:109:ASN:N	1.99	0.95
1:C:372:VAL:HG13	1:C:373:PRO:HD3	1.48	0.95
1:B:843:LEU:CD2	1:B:847:LEU:HD21	1.96	0.95
1:B:742:SER:HB3	1:B:745:ASP:OD2	1.66	0.95
1:B:537:SER:HB2	1:B:540:ARG:HG2	1.47	0.95
1:B:714:THR:HG21	1:B:833:PRO:HD2	1.49	0.95
1:B:712:MET:HB3	1:B:713:LEU:HD12	1.46	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:790:TYR:HE1	1:A:800:PRO:HG3	1.30	0.95
1:A:389:SER:O	1:A:394:THR:HG21	1.67	0.95
1:A:108:GLN:HG3	1:B:112:GLN:CD	1.86	0.95
1:A:214:VAL:HG12	1:A:215:ALA:N	1.79	0.95
1:A:979:SER:OG	1:A:1015:THR:HG21	1.66	0.95
1:B:172:VAL:HG12	1:B:172:VAL:O	1.64	0.94
1:B:1022:VAL:HG23	1:B:1023:PRO:HD3	1.48	0.94
1:C:420:MET:SD	1:C:498:LYS:HE2	2.06	0.94
1:A:76:MET:HG2	1:A:95:GLU:OE2	1.66	0.94
1:C:162:MET:CB	1:C:313:MET:CE	2.45	0.94
1:C:162:MET:HB3	1:C:313:MET:CE	1.96	0.94
1:B:431:THR:HG21	1:B:493:CYS:CB	1.96	0.94
1:B:988:PRO:O	1:B:989:LEU:HB3	1.65	0.94
1:A:66:GLU:CG	2:A:1058:HOH:O	2.02	0.94
1:A:818:ARG:HD3	1:A:821:GLY:C	1.88	0.94
1:C:69:MET:HE2	1:C:92:LEU:HD21	0.94	0.94
1:B:930:GLY:O	1:B:934:THR:HG23	1.68	0.94
1:B:807:SER:O	1:B:808:ARG:HG3	1.68	0.94
1:A:742:SER:OG	1:A:745:ASP:HB2	1.68	0.94
1:C:535:LEU:HB2	2:C:1076:HOH:O	1.68	0.94
1:A:418:ARG:HD3	1:A:970:MET:HG3	1.46	0.94
1:C:190:PRO:HD3	1:C:779:TYR:CD1	2.02	0.93
1:C:58:GLN:HG3	1:C:62:THR:OG1	1.67	0.93
1:A:578:LEU:CD2	1:A:587:THR:HG23	1.98	0.93
1:B:987:MET:HE3	1:B:987:MET:HA	1.49	0.93
1:B:225:VAL:HG22	1:C:781:MET:CE	1.98	0.93
1:C:548:ILE:HD12	1:C:549:VAL:N	1.84	0.93
1:B:962:GLU:O	1:B:966:ASP:HB2	1.69	0.93
1:C:979:SER:O	1:C:983:ILE:HG13	1.68	0.93
1:A:560:PRO:HB2	1:A:922:THR:HG22	1.50	0.92
1:C:222:THR:HB	1:C:223:PRO:HD3	1.50	0.92
1:C:115:MET:HE2	1:C:118:LEU:CD2	1.96	0.92
1:C:162:MET:CG	1:C:313:MET:CE	2.48	0.92
1:C:3:ASN:HD21	1:C:432:ARG:HD3	1.35	0.92
1:A:965:LEU:O	1:A:969:ARG:HG3	1.69	0.92
1:A:919:ARG:HG3	1:A:920:GLY:H	1.33	0.92
1:A:57:VAL:HG12	1:A:58:GLN:N	1.84	0.92
1:B:406:VAL:O	1:B:408:ASP:O	1.88	0.92
1:C:950:LYS:H	1:C:953:MET:HE2	1.35	0.92
1:B:549:VAL:HG22	1:B:550:VAL:H	1.33	0.92
1:A:214:VAL:HG12	1:A:215:ALA:H	1.32	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:PHE:HB3	1:C:8:ARG:HH22	1.34	0.91
1:C:143:ILE:HG23	1:C:284:GLN:HE22	1.35	0.91
1:C:1022:VAL:HA	1:C:1025:PHE:CD2	2.05	0.91
1:A:919:ARG:CG	1:A:920:GLY:H	1.82	0.91
1:A:443:VAL:O	1:A:445:ILE:N	2.03	0.91
1:C:1025:PHE:O	1:C:1029:VAL:HG23	1.71	0.91
1:A:495:THR:O	1:A:496:MET:HB2	1.71	0.91
1:A:901:VAL:O	1:A:904:VAL:HG23	1.70	0.91
1:A:5:PHE:CD1	1:A:12:ALA:HB2	2.05	0.91
1:B:81:ASN:O	1:B:81:ASN:ND2	2.02	0.91
1:A:781:MET:HB3	1:C:228:GLN:OE1	1.70	0.91
1:A:585:GLU:OE2	1:C:227:GLY:HA2	1.71	0.91
1:A:128:SER:HB2	1:B:113:LEU:CD2	2.01	0.91
1:A:571:VAL:HG12	1:A:630:SER:HA	1.53	0.91
1:C:459:PHE:HD2	1:C:459:PHE:H	1.13	0.91
1:C:417:GLU:HA	1:C:417:GLU:OE2	1.70	0.91
1:C:431:THR:HG21	1:C:494:ALA:HB2	1.51	0.90
1:C:188:MET:CE	1:C:200:PRO:HB3	2.01	0.90
1:B:115:MET:HE1	1:B:127:VAL:HG21	1.53	0.90
1:A:968:VAL:CG2	1:A:1023:PRO:HB3	2.00	0.90
1:A:578:LEU:HD21	1:A:587:THR:HA	1.52	0.90
1:C:314:GLU:HB2	1:C:315:PRO:HD3	1.54	0.90
1:C:185:ARG:HG3	1:C:271:GLY:HA3	1.54	0.90
1:B:911:GLY:HA3	1:B:1013:THR:HG21	1.51	0.90
1:A:552:MET:HE1	1:A:906:PRO:HA	1.51	0.90
1:B:51:GLY:O	1:B:53:ASP:OD2	1.90	0.90
1:A:418:ARG:HG2	1:A:970:MET:HE3	1.53	0.90
1:C:44:THR:HG22	1:C:91:THR:HB	0.91	0.89
1:A:277:ILE:O	1:A:277:ILE:HG23	1.70	0.89
1:B:441:ALA:O	1:B:445:ILE:HG13	1.72	0.89
1:C:418:ARG:O	1:C:420:MET:N	2.04	0.89
1:C:214:VAL:HG12	1:C:215:ALA:N	1.88	0.89
1:B:49:TYR:CE1	1:B:122:VAL:HG13	2.06	0.89
1:A:139:VAL:CG1	1:A:327:TYR:HB3	2.02	0.89
1:C:950:LYS:HZ1	1:C:1030:ARG:HD3	1.30	0.89
1:B:1:MET:CB	1:B:2:PRO:HD2	2.01	0.89
1:A:968:VAL:HG21	1:A:1023:PRO:HB3	1.52	0.89
1:B:184:MET:HG3	1:B:184:MET:O	1.71	0.89
1:A:190:PRO:HG3	1:A:789:TRP:CE2	2.08	0.89
1:A:909:VAL:HG12	1:A:913:LEU:HD21	1.55	0.89
1:B:456:MET:HG3	1:B:467:TYR:CB	2.02	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:423:GLU:HB3	1:C:426:PRO:HG3	1.54	0.89
1:B:225:VAL:H	1:C:781:MET:HE2	1.34	0.88
1:B:242:SER:HB2	1:B:245:GLU:OE2	1.72	0.88
1:B:171:GLY:HA3	1:B:302:THR:CG2	2.03	0.88
1:A:818:ARG:HD2	2:A:1054:HOH:O	1.72	0.88
1:C:131:LYS:O	1:C:295:THR:HG22	1.72	0.88
1:A:1024:VAL:HG12	1:A:1025:PHE:H	1.37	0.88
1:C:291:ILE:HD13	1:C:306:ILE:CD1	2.03	0.88
1:B:247:GLY:HA2	1:B:268:ILE:HD13	0.88	0.88
1:C:1017:LEU:O	1:C:1017:LEU:HD23	1.73	0.88
1:B:47:ALA:HB3	1:B:88:VAL:HB	1.56	0.88
1:A:64:VAL:O	1:A:65:ILE:C	2.12	0.88
1:C:444:GLY:O	1:C:448:VAL:HG23	1.74	0.88
1:B:103:ALA:O	1:B:107:VAL:HG23	1.73	0.88
1:B:171:GLY:HA3	1:B:302:THR:HG22	1.56	0.87
1:B:14:VAL:HG11	1:C:890:ALA:HB2	1.54	0.87
1:C:950:LYS:NZ	1:C:1030:ARG:CD	2.36	0.87
1:A:355:MET:CE	1:A:410:ILE:HG12	2.03	0.87
1:A:909:VAL:HG12	1:A:913:LEU:CD2	2.03	0.87
1:A:105:VAL:O	1:A:108:GLN:HB3	1.75	0.87
1:A:228:GLN:HG2	1:B:781:MET:HG2	1.54	0.87
1:C:452:VAL:O	1:C:932:LEU:HD13	1.73	0.87
1:A:214:VAL:CG1	1:A:215:ALA:H	1.87	0.87
1:C:396:PHE:O	1:C:400:LEU:HD23	1.73	0.87
1:A:1009:GLY:O	1:A:1011:MET:N	2.08	0.87
1:C:141:GLY:HA3	1:C:324:VAL:HG22	1.56	0.86
1:C:162:MET:HG2	1:C:313:MET:HE2	1.57	0.86
1:C:291:ILE:CD1	1:C:306:ILE:HD13	2.04	0.86
1:B:3:ASN:H	1:B:6:ILE:HG12	1.39	0.86
1:A:528:THR:HG21	1:A:969:ARG:HE	1.38	0.86
1:B:590:VAL:O	1:B:594:VAL:HG23	1.75	0.86
1:A:819:TYR:N	1:A:824:SER:HB3	1.89	0.86
1:B:919:ARG:HG3	1:B:1005:THR:CG2	2.05	0.86
1:B:42:ALA:CB	1:B:93:THR:HG22	2.05	0.86
1:A:261:LEU:HD12	1:A:263:ARG:NH2	1.89	0.86
1:B:49:TYR:CD1	1:B:122:VAL:HG22	2.10	0.86
1:C:513:PHE:HA	1:C:516:PHE:HB3	1.57	0.86
1:A:32:VAL:HG22	1:A:390:ILE:HB	1.57	0.86
1:C:950:LYS:HZ3	1:C:1030:ARG:HD3	1.34	0.86
1:B:714:THR:HG22	1:B:831:ALA:HA	1.57	0.86
1:B:729:ILE:HG13	1:B:730:ASP:N	1.90	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:804:PHE:HD1	1:B:804:PHE:O	1.58	0.86
1:C:181:GLN:OE1	1:C:767:ARG:NE	2.08	0.86
1:B:226:LYS:CE	1:B:226:LYS:HA	2.06	0.86
1:C:743:ILE:HD12	1:C:743:ILE:H	1.38	0.86
1:B:517:ASN:HB3	1:B:521:GLU:OE1	1.75	0.86
1:B:225:VAL:HG22	1:C:781:MET:HE3	1.54	0.86
1:C:872:GLN:HB2	1:C:875:SER:HB3	1.55	0.86
1:C:686:ASP:OD1	1:C:690:LEU:HB2	1.76	0.85
1:A:756:GLY:HA2	1:A:774:MET:HB2	1.56	0.85
1:A:809:TRP:O	1:A:810:GLU:HB3	1.73	0.85
1:A:355:MET:HE1	1:A:410:ILE:HG12	1.58	0.85
1:A:729:ILE:HG22	1:A:730:ASP:N	1.88	0.85
1:B:690:LEU:HB2	1:B:694:LYS:HB2	1.57	0.85
1:C:314:GLU:HB2	1:C:315:PRO:CD	2.06	0.85
1:A:139:VAL:HG13	1:A:327:TYR:HB3	1.58	0.85
1:C:927:PHE:O	1:C:931:LEU:HB2	1.74	0.85
1:C:43:VAL:HA	1:C:130:GLU:O	1.74	0.85
1:A:911:GLY:HA3	1:A:1013:THR:HG21	1.56	0.85
1:A:513:PHE:HD1	1:A:517:ASN:ND2	1.73	0.85
1:C:432:ARG:HG3	1:C:432:ARG:NH1	1.79	0.85
1:A:113:LEU:HD21	1:C:128:SER:HA	1.56	0.85
1:C:62:THR:HG23	1:C:90:ILE:HD11	1.56	0.85
1:A:520:PHE:H	1:A:522:LYS:HE3	1.42	0.84
1:B:431:THR:CG2	1:B:493:CYS:HB3	2.06	0.84
1:B:552:MET:SD	1:B:909:VAL:HG23	2.17	0.84
1:A:632:LYS:O	1:A:637:ARG:HD3	1.76	0.84
1:B:605:ASN:HD21	1:B:642:ASN:ND2	1.75	0.84
1:A:10:ILE:HD11	1:B:895:TRP:HB2	1.58	0.84
1:A:103:ALA:O	1:A:107:VAL:HG23	1.76	0.84
1:A:687:GLN:HG2	1:C:316:PHE:CG	2.13	0.84
1:C:951:ASP:C	1:C:953:MET:H	1.79	0.84
1:B:150:THR:H	1:B:153:ASP:HB3	1.41	0.84
1:A:454:VAL:O	1:A:456:MET:O	1.95	0.84
1:C:162:MET:CG	1:C:313:MET:HE3	2.06	0.84
1:C:685:ILE:HD11	1:C:687:GLN:HA	1.59	0.84
1:B:659:LYS:HD3	1:B:660:ASP:N	1.92	0.84
1:B:190:PRO:HG2	1:B:779:TYR:CD1	2.12	0.84
1:B:49:TYR:CG	1:B:122:VAL:HA	2.12	0.84
1:A:186:ILE:HB	1:A:773:VAL:HG23	1.60	0.84
1:C:759:VAL:O	1:C:760:ASN:HB3	1.78	0.84
1:A:441:ALA:O	1:A:445:ILE:HG23	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:PRO:HD2	1:B:749:THR:HG22	1.58	0.84
1:A:1024:VAL:O	1:A:1026:PHE:N	2.11	0.84
1:C:72:ILE:HG22	1:C:94:PHE:CE2	2.13	0.84
1:B:26:ALA:O	1:B:30:LEU:HD22	1.78	0.84
1:A:1029:VAL:HG12	1:A:1030:ARG:H	1.43	0.83
1:A:154:ILE:HG22	1:A:287:SER:HB3	1.60	0.83
1:B:831:ALA:CB	1:B:840:ALA:HB2	2.08	0.83
1:A:406:VAL:HG13	1:A:407:ASP:N	1.92	0.83
1:A:1020:PHE:O	1:A:1024:VAL:HG23	1.77	0.83
1:B:555:LEU:HB2	1:B:913:LEU:HD23	1.59	0.83
1:A:46:SER:O	1:A:127:VAL:HG13	1.78	0.83
1:A:63:GLN:O	1:A:66:GLU:N	2.10	0.83
1:B:945:ILE:HD12	1:B:1026:PHE:HE2	1.42	0.83
1:C:247:GLY:HA2	1:C:268:ILE:HD13	1.59	0.83
1:C:713:LEU:HD11	1:C:834:GLY:CA	2.07	0.83
1:C:699:ARG:HD2	1:C:703:LEU:HD11	1.60	0.83
1:C:190:PRO:CD	1:C:779:TYR:HD1	1.89	0.83
1:C:4:PHE:CB	1:C:8:ARG:HH22	1.92	0.83
1:A:649:MET:HB3	1:A:653:ARG:NH2	1.93	0.83
1:B:158:VAL:HA	1:B:162:MET:HG2	1.58	0.83
1:B:187:TRP:CZ3	1:B:774:MET:HE3	2.13	0.83
1:C:420:MET:SD	1:C:498:LYS:NZ	2.52	0.83
1:C:568:ASP:OD1	1:C:634:TRP:NE1	2.10	0.83
1:B:528:THR:O	1:B:531:VAL:HG12	1.79	0.83
1:A:902:MET:O	1:A:905:VAL:HG23	1.79	0.83
1:B:894:SER:CB	1:B:897:ILE:HG12	2.07	0.83
1:C:164:ASP:O	1:C:168:ARG:HG2	1.78	0.83
1:C:418:ARG:C	1:C:420:MET:H	1.81	0.83
1:B:563:PHE:O	1:B:925:VAL:HG12	1.78	0.83
1:C:164:ASP:CG	2:C:1058:HOH:O	2.15	0.82
1:C:165:ALA:HA	1:C:168:ARG:HG3	1.59	0.82
1:C:950:LYS:HZ1	1:C:1030:ARG:CD	1.92	0.82
1:B:493:CYS:O	1:B:494:ALA:HB3	1.79	0.82
1:B:892:TYR:CB	1:B:897:ILE:HD11	2.09	0.82
1:B:713:LEU:H	1:B:713:LEU:HD12	1.44	0.82
1:B:613:ASN:HD22	1:B:614:GLY:N	1.75	0.82
1:A:106:GLN:O	1:A:107:VAL:O	1.97	0.82
1:B:104:GLN:HG3	1:B:105:VAL:N	1.93	0.82
1:A:405:LEU:HD22	1:A:406:VAL:N	1.93	0.82
1:C:699:ARG:HG2	1:C:699:ARG:NH1	1.93	0.82
1:B:987:MET:CE	1:B:987:MET:HA	2.09	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:ALA:H	1:C:57:VAL:HG23	1.44	0.82
1:C:562:SER:O	1:C:924:ASP:HA	1.79	0.82
1:C:686:ASP:HB3	1:C:823:PRO:HG2	1.61	0.82
1:B:45:ILE:HD12	1:B:90:ILE:HB	1.61	0.82
1:C:55:LYS:HE2	1:C:59:ASP:OD1	1.79	0.82
1:A:820:ASN:O	1:C:168:ARG:NH2	2.13	0.82
1:A:342:LYS:HG3	1:A:343:THR:H	1.43	0.82
1:C:962:GLU:O	1:C:965:LEU:HB3	1.79	0.82
1:C:144:ASN:HB3	2:C:1077:HOH:O	1.80	0.82
1:B:245:GLU:HA	1:B:248:LYS:HG2	1.62	0.82
1:A:115:MET:HE3	1:A:115:MET:HA	1.60	0.82
1:C:115:MET:HA	1:C:115:MET:CE	2.10	0.82
1:C:166:ILE:CD1	2:C:1075:HOH:O	2.27	0.82
1:A:443:VAL:HG12	1:A:444:GLY:N	1.95	0.82
1:A:69:MET:HG2	2:A:1056:HOH:O	1.77	0.82
1:A:498:LYS:O	1:A:498:LYS:NZ	2.11	0.82
1:B:1:MET:HB2	1:B:2:PRO:CD	2.09	0.82
1:A:545:TYR:HB2	1:A:1021:PHE:CE1	2.14	0.82
1:A:722:GLU:HG3	2:A:1060:HOH:O	1.78	0.82
1:A:713:LEU:CD2	1:A:714:THR:H	1.92	0.81
1:B:104:GLN:CG	1:B:105:VAL:N	2.42	0.81
1:A:276:ASP:HB3	1:C:222:THR:HG23	1.62	0.81
1:B:276:ASP:O	1:B:614:GLY:HA3	1.81	0.81
1:A:419:VAL:O	1:A:424:GLY:HA3	1.81	0.81
1:B:880:SER:O	1:B:884:VAL:HG23	1.81	0.81
1:B:213:GLN:HE21	1:B:239:ARG:HD2	1.45	0.81
1:A:45:ILE:HG22	1:A:45:ILE:O	1.81	0.81
1:A:223:PRO:HD3	1:B:275:TYR:CD2	2.16	0.81
1:C:164:ASP:O	1:C:168:ARG:CG	2.28	0.81
1:C:888:LEU:HB3	1:C:898:PRO:HB3	1.62	0.81
1:C:644:VAL:HG11	1:C:667:ASN:HD22	1.45	0.81
1:B:92:LEU:N	1:B:92:LEU:HD22	1.94	0.81
1:B:674:LEU:HD23	1:B:675:GLY:N	1.94	0.81
1:B:859:TRP:HB3	1:B:863:SER:HB2	1.61	0.81
1:C:38:ILE:HG21	1:C:466:ILE:HD11	1.61	0.81
1:A:536:ARG:HG2	1:A:537:SER:N	1.95	0.81
1:A:214:VAL:CG1	1:A:215:ALA:N	2.44	0.81
1:B:405:LEU:HD12	1:B:406:VAL:N	1.96	0.81
1:A:314:GLU:HA	2:A:1061:HOH:O	1.79	0.81
1:B:399:VAL:O	1:B:402:ILE:HG22	1.81	0.81
1:A:713:LEU:HB3	1:A:832:ALA:CA	2.11	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:THR:O	1:A:205:THR:CG2	2.27	0.81
1:A:413:VAL:HG23	1:A:493:CYS:HB2	1.63	0.81
1:B:70:ASN:ND2	1:B:70:ASN:O	2.14	0.81
1:B:314:GLU:H	1:B:315:PRO:HD2	1.44	0.81
1:B:623:ASN:C	1:B:623:ASN:HD22	1.82	0.81
1:A:467:TYR:CE1	1:A:925:VAL:HG22	2.16	0.80
1:A:253:VAL:HG23	1:A:258:SER:O	1.80	0.80
1:B:350:LEU:HB3	1:B:984:LEU:HD12	1.61	0.80
1:C:713:LEU:HD21	1:C:835:LYS:H	1.46	0.80
1:C:350:LEU:HD13	1:C:984:LEU:CD2	2.11	0.80
1:B:456:MET:CG	1:B:467:TYR:HB3	2.09	0.80
1:B:416:VAL:HG11	1:B:431:THR:HG22	1.64	0.80
1:B:100:ALA:O	1:B:103:ALA:HB3	1.81	0.80
1:A:634:TRP:CE3	1:A:995:ALA:HB1	2.16	0.80
1:A:605:ASN:OD1	1:A:637:ARG:HG2	1.82	0.80
1:C:702:LEU:HB2	1:C:851:LEU:HD21	1.62	0.80
1:C:184:MET:HE3	1:C:184:MET:HA	1.62	0.80
1:B:879:ILE:O	1:B:883:VAL:HG23	1.82	0.80
1:A:951:ASP:O	1:A:955:LYS:HB2	1.81	0.80
1:A:801:PHE:CD2	1:A:805:SER:OG	2.34	0.80
1:B:157:TYR:HA	1:B:161:ASN:ND2	1.97	0.80
1:B:849:SER:O	1:B:850:LYS:HD3	1.81	0.80
1:B:646:ALA:O	1:B:648:THR:N	2.13	0.80
1:A:298:ASN:HD22	1:A:298:ASN:C	1.84	0.80
1:B:11:PHE:O	1:B:14:VAL:HB	1.81	0.80
1:B:945:ILE:HD11	1:B:1022:VAL:HB	1.64	0.80
1:A:949:ALA:HB1	1:A:1026:PHE:CE2	2.17	0.80
1:C:346:GLU:OE1	1:C:988:PRO:HG3	1.82	0.80
1:C:188:MET:HE1	1:C:200:PRO:HB3	1.62	0.80
1:A:372:VAL:HB	1:A:373:PRO:HD3	1.62	0.80
1:C:190:PRO:CD	1:C:779:TYR:CD1	2.64	0.80
1:A:406:VAL:HG13	1:A:407:ASP:H	1.45	0.79
1:C:536:ARG:HH11	1:C:961:ILE:HD11	1.47	0.79
1:B:568:ASP:OD1	1:B:644:VAL:HG22	1.82	0.79
1:A:66:GLU:OE2	2:A:1058:HOH:O	1.99	0.79
1:C:169:THR:HB	1:C:172:VAL:HG21	1.63	0.79
1:B:912:ALA:HB2	1:B:1010:GLY:HA3	1.65	0.79
1:B:830:GLN:H	1:B:830:GLN:HE21	1.30	0.79
1:B:230:LEU:HD21	1:C:809:TRP:CH2	2.16	0.79
1:A:105:VAL:O	1:A:108:GLN:CB	2.30	0.79
1:A:685:ILE:HG22	1:A:687:GLN:H	1.48	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:MET:HG2	1:C:313:MET:HE3	1.63	0.79
1:A:986:VAL:C	1:A:988:PRO:HD2	2.02	0.79
1:C:350:LEU:HD12	1:C:985:GLY:HA2	1.64	0.79
1:A:112:GLN:HE21	1:A:112:GLN:CA	1.95	0.79
1:A:61:VAL:O	1:A:65:ILE:HG23	1.77	0.79
1:B:2:PRO:HD3	1:B:486:LEU:HD12	1.65	0.79
1:B:972:LEU:HD13	1:B:976:LEU:HD23	1.64	0.79
1:A:590:VAL:O	1:A:594:VAL:HG23	1.83	0.79
1:C:423:GLU:HB3	1:C:426:PRO:CG	2.12	0.79
1:C:728:LYS:HG3	1:C:729:ILE:N	1.97	0.79
1:C:427:PRO:CA	1:C:498:LYS:HE3	2.09	0.79
1:C:183:ALA:O	1:C:185:ARG:HG2	1.82	0.79
1:A:568:ASP:OD2	1:A:637:ARG:NH1	2.16	0.79
1:C:158:VAL:O	1:C:162:MET:N	2.15	0.79
1:B:358:PHE:HZ	1:B:976:LEU:HD12	1.47	0.79
1:C:778:LYS:HD2	1:C:779:TYR:HE2	1.48	0.79
1:A:255:GLN:CD	1:A:255:GLN:H	1.85	0.79
1:B:452:VAL:O	1:B:453:PHE:HB2	1.82	0.78
1:C:685:ILE:HG12	1:C:687:GLN:OE1	1.82	0.78
1:A:584:GLN:H	1:A:622:GLN:HB3	1.48	0.78
1:C:911:GLY:HA3	1:C:1013:THR:HG21	1.63	0.78
1:A:60:THR:HG21	1:A:119:PRO:HG3	1.65	0.78
1:C:61:VAL:HG12	2:C:1064:HOH:O	1.81	0.78
1:B:531:VAL:HG13	1:B:965:LEU:HD21	1.64	0.78
1:A:781:MET:HE1	1:C:225:VAL:H	1.49	0.78
1:C:252:LYS:O	1:C:260:VAL:HG12	1.82	0.78
1:C:352:PHE:HA	1:C:369:THR:HG21	1.65	0.78
1:B:538:THR:N	1:B:540:ARG:HH21	1.81	0.78
1:B:729:ILE:HG13	1:B:730:ASP:H	1.46	0.78
1:A:61:VAL:HG13	1:A:118:LEU:HD22	1.64	0.78
1:B:525:HIS:HA	1:B:528:THR:HG22	1.64	0.78
1:A:298:ASN:ND2	1:A:300:LEU:H	1.80	0.78
1:A:210:GLN:HG3	1:A:249:ILE:HG23	1.63	0.78
1:A:400:LEU:HD13	1:A:1003:VAL:CG1	2.11	0.78
1:B:587:THR:O	1:B:591:LEU:HB2	1.83	0.78
1:A:886:LEU:HD21	1:C:17:ILE:HG21	1.63	0.78
1:A:578:LEU:HD23	1:A:587:THR:HG23	1.66	0.78
1:C:463:THR:O	1:C:465:ALA:N	2.17	0.78
1:B:157:TYR:HA	1:B:161:ASN:HD22	1.49	0.78
1:A:836:SER:OG	1:A:839:GLU:HG2	1.84	0.78
1:A:166:ILE:HD13	1:A:166:ILE:N	1.96	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:410:ILE:HG22	1:C:411:VAL:N	1.98	0.78
1:A:520:PHE:N	1:A:522:LYS:HE3	1.99	0.78
1:A:783:PRO:HD3	1:C:219:LEU:HD13	1.65	0.78
1:B:602:GLU:OE2	1:B:650:ARG:HD2	1.82	0.78
1:A:467:TYR:HE1	1:A:925:VAL:HG22	1.46	0.78
1:A:314:GLU:N	1:A:315:PRO:CD	2.47	0.78
1:A:719:ASN:HD22	1:A:719:ASN:C	1.85	0.78
1:B:562:SER:O	1:B:924:ASP:HA	1.84	0.78
1:C:115:MET:N	1:C:116:PRO:CD	2.47	0.77
1:B:448:VAL:O	1:B:452:VAL:HG22	1.84	0.77
1:C:143:ILE:HD11	1:C:286:ALA:HB2	1.67	0.77
1:C:578:LEU:HB3	1:C:579:PRO:HD2	1.65	0.77
1:B:6:ILE:HD12	1:B:490:PRO:HB2	1.64	0.77
1:A:909:VAL:O	1:A:912:ALA:HB3	1.84	0.77
1:B:699:ARG:HG2	1:B:700:ASN:H	1.49	0.77
1:A:168:ARG:HG3	1:A:168:ARG:O	1.84	0.77
1:A:843:LEU:HA	1:A:846:GLN:NE2	1.98	0.77
1:A:54:ALA:CB	1:A:816:LEU:HG	2.15	0.77
1:A:108:GLN:CG	1:B:112:GLN:OE1	2.28	0.77
1:B:346:GLU:OE1	1:B:988:PRO:HB3	1.84	0.77
1:A:495:THR:O	1:A:495:THR:HG22	1.83	0.77
1:B:983:ILE:HD13	1:B:1012:VAL:HG12	1.66	0.77
1:C:754:TRP:CZ2	1:C:786:ILE:HG13	2.20	0.77
1:B:345:VAL:HA	1:B:348:ILE:HD12	1.67	0.77
1:C:220:GLY:CA	1:C:231:ASN:ND2	2.46	0.77
1:A:1018:ALA:O	1:A:1022:VAL:HG13	1.85	0.77
1:A:522:LYS:N	1:A:522:LYS:HE2	2.00	0.77
1:B:674:LEU:HD13	1:B:860:THR:HG21	1.66	0.77
1:A:57:VAL:HG13	1:A:57:VAL:O	1.81	0.77
1:A:687:GLN:HE21	1:A:856:GLY:HA3	1.47	0.77
1:A:596:HIS:O	1:A:598:TYR:N	2.18	0.77
1:C:127:VAL:CG2	1:C:127:VAL:CA	2.60	0.77
1:B:714:THR:HG21	1:B:833:PRO:CD	2.14	0.77
1:A:514:GLY:O	1:A:518:ARG:HB2	1.84	0.77
1:C:62:THR:CA	2:C:1064:HOH:O	2.33	0.76
1:B:945:ILE:CD1	1:B:1026:PHE:HE2	1.98	0.76
1:A:728:LYS:NZ	1:C:235:ILE:HG22	2.00	0.76
1:C:717:ARG:HH12	1:C:829:GLY:HA2	1.50	0.76
1:C:162:MET:CB	1:C:313:MET:HE1	2.11	0.76
1:B:411:VAL:O	1:B:438:ILE:HG12	1.86	0.76
1:A:543:VAL:O	1:A:544:LEU:HB3	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:975:ILE:HG21	1:C:1019:ILE:HD13	1.65	0.76
1:A:885:PHE:HD2	1:A:886:LEU:HD12	1.50	0.76
1:B:707:ALA:O	1:B:708:LYS:HB3	1.83	0.76
1:C:72:ILE:HG22	1:C:94:PHE:HE2	1.49	0.76
1:A:48:SER:HA	1:A:86:GLY:O	1.85	0.76
1:C:82:SER:HB3	1:C:88:VAL:CA	2.13	0.76
1:C:972:LEU:H	1:C:974:PRO:HD2	1.49	0.76
1:B:517:ASN:O	1:B:521:GLU:HG3	1.85	0.76
1:B:520:PHE:HA	1:B:523:SER:OG	1.85	0.76
1:A:539:GLY:HA2	1:A:542:LEU:HB2	1.67	0.76
1:C:190:PRO:O	1:C:191:ASN:C	2.23	0.76
1:B:418:ARG:HG3	1:B:970:MET:CE	2.16	0.76
1:C:407:ASP:OD2	1:C:940:LYS:NZ	2.17	0.76
1:A:522:LYS:H	1:A:522:LYS:HE2	1.50	0.76
1:C:259:ARG:HB2	1:C:259:ARG:HH11	1.46	0.76
1:C:391:ASN:H	1:C:394:THR:CG2	1.97	0.76
1:C:527:TYR:OH	1:C:968:VAL:HG12	1.86	0.76
1:B:420:MET:HE2	1:B:425:LEU:HD23	1.68	0.76
1:B:136:PHE:HE1	1:B:617:PHE:CZ	2.04	0.76
1:A:818:ARG:HA	1:A:824:SER:H	1.49	0.76
1:B:894:SER:HB3	1:B:897:ILE:CG1	2.15	0.76
1:B:690:LEU:HB2	1:B:694:LYS:CB	2.14	0.76
1:A:60:THR:HG22	1:A:119:PRO:HD3	1.68	0.76
1:C:713:LEU:H	1:C:713:LEU:HD22	1.51	0.76
1:A:472:ILE:N	1:A:472:ILE:HD12	1.98	0.76
1:B:221:GLY:HA3	1:C:780:ARG:NH1	2.02	0.75
1:B:234:ILE:O	1:B:234:ILE:HG22	1.87	0.75
1:B:269:GLU:O	1:B:270:LEU:HB2	1.86	0.75
1:B:418:ARG:HG3	1:B:970:MET:HE1	1.66	0.75
1:A:472:ILE:H	1:A:472:ILE:HD12	1.48	0.75
1:A:1:MET:N	1:A:2:PRO:HD2	2.01	0.75
1:C:156:ASP:O	1:C:157:TYR:C	2.22	0.75
1:A:282:ASN:HD21	1:A:609:VAL:H	1.31	0.75
1:A:515:TRP:HA	1:A:519:MET:SD	2.26	0.75
1:A:227:GLY:HA2	1:B:585:GLU:OE1	1.87	0.75
1:B:328:ASP:HB2	2:B:1059:HOH:O	1.86	0.75
1:A:890:ALA:HB1	1:C:11:PHE:CD1	2.22	0.75
1:B:804:PHE:CD1	1:B:804:PHE:O	2.39	0.75
1:B:610:PHE:O	1:B:627:ALA:HB1	1.86	0.75
1:A:818:ARG:HE	1:A:818:ARG:CB	1.98	0.75
1:A:713:LEU:HD22	1:A:714:THR:N	1.97	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:790:TYR:CE1	1:A:800:PRO:HG3	2.20	0.75
1:C:459:PHE:CD2	1:C:459:PHE:N	2.48	0.75
1:A:61:VAL:HG13	1:A:118:LEU:CD2	2.16	0.75
1:B:1022:VAL:HG23	1:B:1023:PRO:CD	2.16	0.75
1:B:549:VAL:CG2	1:B:550:VAL:N	2.49	0.75
1:A:534:ILE:HB	1:A:540:ARG:NH1	2.01	0.75
1:A:661:ALA:O	1:A:663:VAL:HG23	1.87	0.75
1:A:112:GLN:HA	1:A:112:GLN:NE2	1.97	0.74
1:B:560:PRO:HB2	1:B:836:SER:HB3	1.69	0.74
1:A:73:ASP:HB3	1:A:106:GLN:HE22	1.51	0.74
1:C:489:THR:O	1:C:493:CYS:HB3	1.88	0.74
1:A:781:MET:HE1	1:C:225:VAL:N	2.02	0.74
1:A:1023:PRO:O	1:A:1027:VAL:HG23	1.87	0.74
1:C:975:ILE:HG22	1:C:976:LEU:N	2.00	0.74
1:A:599:LEU:O	1:A:600:THR:HB	1.86	0.74
1:C:32:VAL:HG12	1:C:32:VAL:O	1.87	0.74
1:C:457:ALA:HB1	1:C:468:ARG:HA	1.67	0.74
1:C:73:ASP:O	1:C:74:ASN:O	2.06	0.74
1:C:643:LYS:O	1:C:647:ILE:HG13	1.87	0.74
1:C:424:GLY:HA2	2:C:1073:HOH:O	1.86	0.74
1:C:577:GLN:HB3	1:C:624:THR:HG22	1.69	0.74
1:C:158:VAL:CG1	1:C:158:VAL:CG2	2.62	0.74
1:B:946:VAL:HG22	1:B:1026:PHE:CZ	2.23	0.74
1:A:559:LEU:HD12	1:A:560:PRO:CD	2.15	0.74
1:A:578:LEU:HD21	1:A:587:THR:HG23	1.69	0.74
1:C:655:PHE:C	1:C:657:GLN:H	1.91	0.74
1:C:166:ILE:HG12	2:C:1075:HOH:O	1.88	0.74
1:B:262:LEU:HB3	1:B:268:ILE:HD11	1.69	0.74
1:C:588:GLN:HG2	1:C:613:ASN:ND2	2.03	0.74
1:C:513:PHE:HA	1:C:516:PHE:CB	2.18	0.74
1:C:643:LYS:HG2	1:C:645:GLU:H	1.52	0.74
1:C:655:PHE:HA	1:C:659:LYS:HD3	1.70	0.74
1:A:68:ASN:C	1:A:68:ASN:N	2.41	0.74
1:B:973:ARG:HG2	1:B:974:PRO:HD3	1.70	0.74
1:A:44:THR:O	1:A:45:ILE:CG1	2.36	0.74
1:A:44:THR:O	1:A:45:ILE:HG13	1.88	0.74
1:A:701:GLN:OE1	1:A:852:PRO:HD3	1.87	0.74
1:B:686:ASP:HB3	1:B:823:PRO:O	1.87	0.74
1:A:568:ASP:HB3	1:A:634:TRP:HZ3	1.53	0.74
1:C:592:ASN:HD22	1:C:592:ASN:N	1.84	0.74
1:A:919:ARG:HG3	1:A:920:GLY:N	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:184:MET:HG2	1:C:246:PHE:CD1	2.23	0.73
1:C:69:MET:CE	1:C:92:LEU:CD2	2.54	0.73
1:C:950:LYS:O	1:C:954:ASP:HB2	1.88	0.73
1:B:704:ALA:O	1:B:705:GLU:CG	2.35	0.73
1:A:749:THR:O	1:A:753:ALA:HB2	1.88	0.73
1:A:578:LEU:O	1:A:623:ASN:ND2	2.20	0.73
1:C:879:ILE:O	1:C:883:VAL:HG23	1.88	0.73
1:A:69:MET:C	1:A:70:ASN:HD22	1.91	0.73
1:C:62:THR:HA	2:C:1064:HOH:O	1.86	0.73
1:B:945:ILE:CD1	1:B:1026:PHE:CE2	2.72	0.73
1:A:993:THR:HG21	1:A:1000:GLN:OE1	1.87	0.73
1:A:736:ALA:O	1:A:741:VAL:HG13	1.88	0.73
1:C:87:THR:CG2	1:C:88:VAL:N	2.51	0.73
1:A:832:ALA:HB3	1:A:835:LYS:HB2	1.70	0.73
1:C:144:ASN:ND2	1:C:149:MET:H	1.86	0.73
1:B:291:ILE:HG21	1:B:306:ILE:HD11	1.69	0.73
1:A:947:GLU:O	1:A:951:ASP:HB2	1.88	0.73
1:A:426:PRO:HG2	1:A:429:GLU:OE2	1.88	0.73
1:A:773:VAL:HG13	1:A:773:VAL:O	1.87	0.73
1:B:350:LEU:HB3	1:B:984:LEU:CD1	2.17	0.73
1:B:790:TYR:HE1	1:B:800:PRO:HB3	1.53	0.73
1:A:190:PRO:HG3	1:A:789:TRP:CD2	2.23	0.73
1:C:922:THR:HG22	1:C:923:ASN:H	1.53	0.73
1:B:423:GLU:OE1	1:B:427:PRO:CD	2.37	0.73
1:B:1018:ALA:O	1:B:1022:VAL:HG22	1.88	0.73
1:C:1:MET:HB2	1:C:2:PRO:CD	2.16	0.73
1:C:726:GLN:CD	1:C:812:GLY:HA3	2.08	0.73
1:C:45:ILE:C	1:C:45:ILE:CB	2.56	0.73
1:A:428:LYS:HG3	1:A:429:GLU:H	1.52	0.73
1:A:540:ARG:HG3	1:A:541:TYR:H	1.53	0.73
1:A:919:ARG:CG	1:A:920:GLY:N	2.52	0.73
1:B:759:VAL:HG12	1:B:760:ASN:HB2	1.70	0.73
1:B:439:GLN:HA	1:B:442:LEU:HD12	1.71	0.73
1:A:461:GLY:O	1:A:463:THR:O	2.06	0.73
1:B:7:ASP:O	1:B:8:ARG:HB2	1.89	0.73
1:C:144:ASN:HD21	1:C:149:MET:H	1.33	0.73
1:C:365:THR:O	1:C:368:PRO:HD2	1.88	0.73
1:A:102:ILE:HA	1:A:105:VAL:CG2	2.18	0.72
1:A:115:MET:C	1:A:117:LEU:H	1.92	0.72
1:B:42:ALA:HB2	1:B:93:THR:CG2	2.16	0.72
1:A:801:PHE:HD2	1:A:805:SER:OG	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:822:LEU:HB3	1:A:823:PRO:HD2	1.69	0.72
1:B:412:VAL:HG13	1:B:435:MET:HE1	1.71	0.72
1:A:90:ILE:O	1:A:90:ILE:HG22	1.85	0.72
1:B:136:PHE:HD2	1:B:290:GLY:O	1.72	0.72
1:B:845:GLU:CG	1:B:857:TYR:OH	2.37	0.72
1:B:65:ILE:O	1:B:69:MET:HG2	1.89	0.72
1:B:750:LEU:C	1:B:750:LEU:HD13	2.10	0.72
1:C:108:GLN:C	2:C:1056:HOH:O	2.28	0.72
1:A:10:ILE:HG12	1:B:893:GLU:O	1.90	0.72
1:B:740:GLY:O	1:B:794:ALA:N	2.22	0.72
1:C:450:SER:O	1:C:451:ALA:CB	2.35	0.72
1:C:84:SER:C	1:C:86:GLY:H	1.92	0.72
1:C:729:ILE:CD1	1:C:786:ILE:HD13	2.18	0.72
1:B:713:LEU:CD1	1:B:843:LEU:HD13	2.19	0.72
1:B:642:ASN:H	1:B:650:ARG:HH12	1.38	0.72
1:A:418:ARG:HG2	1:A:970:MET:CE	2.19	0.72
1:B:412:VAL:HG13	1:B:435:MET:CE	2.20	0.72
1:B:489:THR:O	1:B:492:LEU:HB2	1.89	0.72
1:C:592:ASN:H	1:C:592:ASN:ND2	1.87	0.72
1:C:519:MET:HG3	1:C:520:PHE:N	2.03	0.72
1:C:946:VAL:HG12	1:C:946:VAL:O	1.90	0.72
1:C:104:GLN:HG3	1:C:131:LYS:HG2	1.72	0.72
1:B:944:LEU:O	1:B:971:ARG:HD2	1.89	0.72
1:B:48:SER:OG	1:B:48:SER:O	2.00	0.72
1:B:172:VAL:O	1:B:173:GLY:O	2.06	0.72
1:A:225:VAL:HG22	1:B:778:LYS:NZ	2.04	0.72
1:B:30:LEU:HD23	1:B:390:ILE:HD11	1.72	0.72
1:A:415:ASN:HB3	1:A:434:SER:OG	1.90	0.72
1:A:67:GLN:C	1:A:68:ASN:CA	2.57	0.72
1:A:69:MET:O	1:A:70:ASN:ND2	2.19	0.72
2:B:1060:HOH:O	1:C:110:LYS:HD3	1.90	0.72
1:B:970:MET:HE2	1:B:970:MET:HA	1.72	0.72
1:C:536:ARG:NH1	1:C:961:ILE:HD11	2.05	0.72
1:A:733:GLN:OE1	1:A:743:ILE:HG12	1.90	0.72
1:A:311:ALA:O	1:A:312:LYS:HB2	1.89	0.72
1:A:314:GLU:N	1:A:315:PRO:HD3	2.04	0.71
1:B:136:PHE:HE1	1:B:617:PHE:HZ	1.38	0.71
1:B:235:ILE:HD13	1:B:235:ILE:H	1.55	0.71
1:A:447:MET:HB3	1:A:887:CYS:SG	2.30	0.71
1:B:314:GLU:H	1:B:315:PRO:CD	2.03	0.71
1:A:782:LEU:O	1:A:784:ASP:O	2.07	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:LEU:N	1:B:92:LEU:CD2	2.53	0.71
1:A:359:LEU:HD12	1:A:417:GLU:HG2	1.72	0.71
1:C:108:GLN:HA	2:C:1056:HOH:O	1.89	0.71
1:A:406:VAL:CG1	1:A:407:ASP:H	2.02	0.71
1:B:892:TYR:HB3	1:B:897:ILE:HD11	1.71	0.71
1:A:729:ILE:CG2	1:A:730:ASP:H	1.99	0.71
1:B:714:THR:HG22	1:B:831:ALA:CA	2.20	0.71
1:A:436:GLY:HA2	1:A:439:GLN:HB2	1.73	0.71
1:C:327:TYR:HB3	1:C:628:PHE:HB3	1.70	0.71
1:C:764:ASP:OD2	1:C:765:ARG:HD2	1.90	0.71
1:C:695:LEU:HD22	1:C:825:MET:HG3	1.73	0.71
1:C:713:LEU:CD1	1:C:834:GLY:HA3	2.16	0.71
1:A:904:VAL:HG21	1:A:942:ALA:HB2	1.72	0.71
1:A:896:SER:O	1:A:899:PHE:HB2	1.90	0.71
1:C:542:LEU:HD23	1:C:542:LEU:O	1.89	0.71
1:B:115:MET:O	1:B:123:GLN:NE2	2.23	0.71
1:A:11:PHE:CD1	1:B:890:ALA:HB1	2.26	0.71
1:A:644:VAL:O	1:A:648:THR:HG23	1.90	0.71
1:C:105:VAL:O	1:C:108:GLN:N	2.23	0.71
1:B:116:PRO:HA	1:B:123:GLN:NE2	2.06	0.71
1:C:568:ASP:OD2	1:C:644:VAL:HG23	1.88	0.71
1:B:790:TYR:CE1	1:B:800:PRO:HB3	2.25	0.71
1:C:166:ILE:CG1	2:C:1075:HOH:O	2.38	0.71
1:C:169:THR:HG22	1:C:172:VAL:HG23	1.72	0.71
1:A:1027:VAL:O	1:A:1029:VAL:O	2.07	0.71
1:A:894:SER:OG	1:A:897:ILE:HB	1.90	0.71
1:C:777:ALA:O	1:C:779:TYR:N	2.24	0.71
1:B:987:MET:HE2	1:B:987:MET:O	1.90	0.71
1:C:945:ILE:O	1:C:946:VAL:HG23	1.90	0.71
1:B:623:ASN:HD22	1:B:624:THR:N	1.88	0.71
1:B:219:LEU:HD12	1:B:234:ILE:HG12	1.71	0.71
1:C:290:GLY:O	1:C:291:ILE:HG13	1.91	0.71
1:C:317:PHE:HB2	1:C:318:PRO:HD2	1.71	0.71
1:C:418:ARG:HG3	1:C:419:VAL:HG13	1.73	0.71
1:B:518:ARG:HA	1:B:521:GLU:HB2	1.73	0.71
1:B:228:GLN:HG2	1:C:781:MET:HE1	1.73	0.71
1:C:463:THR:HG22	1:C:464:GLY:N	2.05	0.71
1:B:231:ASN:C	1:B:231:ASN:ND2	2.43	0.71
1:A:65:ILE:O	1:A:68:ASN:HB2	1.91	0.71
1:C:350:LEU:HD13	1:C:984:LEU:HD23	1.73	0.71
1:C:552:MET:O	1:C:553:ALA:HB3	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:818:ARG:NE	1:A:818:ARG:CB	2.54	0.70
1:A:687:GLN:HG2	1:C:316:PHE:CD1	2.25	0.70
1:A:328:ASP:O	1:A:331:PRO:HD2	1.91	0.70
1:A:189:ASN:HD21	1:A:192:GLU:CB	2.04	0.70
1:C:158:VAL:CG2	1:C:158:VAL:CA	2.69	0.70
1:A:551:GLY:O	1:A:554:TYR:HB3	1.91	0.70
1:C:399:VAL:HA	1:C:402:ILE:CD1	2.21	0.70
1:B:188:MET:SD	1:B:200:PRO:HB3	2.31	0.70
1:C:144:ASN:ND2	1:C:149:MET:HG3	2.07	0.70
1:B:291:ILE:HG21	1:B:306:ILE:CD1	2.22	0.70
1:A:9:PRO:HB3	1:A:491:ALA:HB1	1.73	0.70
1:C:959:GLY:H	1:C:962:GLU:HB2	1.56	0.70
1:B:556:PHE:N	1:B:913:LEU:HD21	2.06	0.70
1:B:537:SER:HB2	1:B:540:ARG:CG	2.21	0.70
1:B:1005:THR:O	1:B:1005:THR:HG22	1.89	0.70
1:C:12:ALA:HB1	1:C:487:ILE:HG22	1.73	0.70
1:A:228:GLN:HG2	1:B:781:MET:CG	2.22	0.70
1:B:279:ALA:HA	1:B:611:ALA:O	1.91	0.70
1:C:166:ILE:C	1:C:172:VAL:HG11	2.11	0.70
1:B:987:MET:O	1:B:990:VAL:HB	1.92	0.70
1:C:192:GLU:O	1:C:195:LYS:N	2.25	0.70
1:B:523:SER:HA	1:B:526:HIS:CD2	2.18	0.70
1:C:785:ASP:C	1:C:787:GLY:H	1.93	0.70
1:B:705:GLU:O	1:B:707:ALA:N	2.23	0.70
1:A:634:TRP:HE3	1:A:995:ALA:HB1	1.54	0.70
1:A:1013:THR:O	1:A:1017:LEU:HB3	1.91	0.70
1:A:73:ASP:CB	1:A:106:GLN:HE22	2.05	0.70
1:C:945:ILE:HB	1:C:971:ARG:HG3	1.72	0.70
1:A:155:SER:HA	1:A:287:SER:OG	1.92	0.70
1:C:1035:ARG:HA	1:C:1035:ARG:HE	1.57	0.70
1:A:68:ASN:O	1:A:70:ASN:N	2.25	0.69
1:C:166:ILE:CA	1:C:166:ILE:CG1	2.70	0.69
1:B:542:LEU:HD11	1:B:1028:VAL:HG11	1.74	0.69
1:A:936:GLY:O	1:A:940:LYS:HB2	1.91	0.69
1:C:146:ASP:HB2	1:C:148:THR:OG1	1.92	0.69
1:A:64:VAL:C	1:A:65:ILE:C	2.50	0.69
1:C:915:ALA:HA	1:C:918:PHE:HB3	1.73	0.69
1:B:713:LEU:H	1:B:713:LEU:CD1	2.05	0.69
1:C:450:SER:O	1:C:451:ALA:HB2	1.92	0.69
1:A:11:PHE:CE1	1:B:890:ALA:HB1	2.27	0.69
1:A:114:ALA:O	1:A:117:LEU:HB2	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:VAL:HA	1:A:534:ILE:CD1	2.14	0.69
1:B:118:LEU:HD23	1:B:122:VAL:HG11	1.74	0.69
1:B:13:TRP:O	1:B:17:ILE:HG12	1.92	0.69
1:B:1024:VAL:HG12	1:B:1025:PHE:H	1.56	0.69
1:C:7:ASP:O	1:C:9:PRO:HD3	1.92	0.69
1:B:225:VAL:HG22	1:C:781:MET:HE2	1.72	0.69
1:C:247:GLY:CA	1:C:268:ILE:HD13	2.23	0.69
1:A:901:VAL:HG11	1:A:943:ILE:HG12	1.74	0.69
1:B:986:VAL:O	1:B:990:VAL:HG23	1.92	0.69
1:B:851:LEU:N	1:B:852:PRO:HD3	2.08	0.69
1:B:49:TYR:CG	1:B:122:VAL:HG22	2.27	0.69
1:B:157:TYR:CA	1:B:161:ASN:HD22	2.05	0.69
1:C:159:ALA:O	1:C:160:ALA:C	2.17	0.69
1:C:163:LYS:HG2	1:C:175:VAL:HG11	1.74	0.69
1:C:131:LYS:C	1:C:295:THR:HG22	2.12	0.69
1:C:402:ILE:O	1:C:406:VAL:HG23	1.92	0.69
1:C:415:ASN:HD21	1:C:434:SER:HB2	1.57	0.69
1:C:556:PHE:HB2	1:C:913:LEU:CD1	2.22	0.69
1:A:340:VAL:HG13	1:A:399:VAL:CG2	2.23	0.69
1:A:115:MET:O	1:A:117:LEU:N	2.25	0.69
1:B:943:ILE:O	1:B:947:GLU:HB3	1.92	0.69
1:B:773:VAL:O	1:B:773:VAL:HG13	1.92	0.69
1:A:822:LEU:N	1:A:822:LEU:HD22	2.08	0.69
1:B:973:ARG:HG2	1:B:974:PRO:CD	2.22	0.69
1:A:653:ARG:O	1:A:656:SER:N	2.24	0.69
1:B:572:PHE:CZ	1:B:629:VAL:HG21	2.27	0.69
1:C:184:MET:CE	1:C:184:MET:HA	2.23	0.69
1:B:845:GLU:HG3	1:B:857:TYR:OH	1.93	0.69
1:A:731:ILE:HD12	1:A:731:ILE:N	2.07	0.69
1:A:108:GLN:CG	1:B:112:GLN:CD	2.62	0.69
1:C:157:TYR:O	1:C:161:ASN:HB2	1.93	0.69
1:C:82:SER:OG	1:C:88:VAL:HG13	1.93	0.69
1:B:929:VAL:O	1:B:933:THR:OG1	2.11	0.69
1:C:358:PHE:HB3	1:C:977:MET:CE	2.19	0.69
1:C:214:VAL:CG1	1:C:215:ALA:N	2.56	0.69
1:B:211:ASN:ND2	1:B:246:PHE:HZ	1.91	0.69
1:A:659:LYS:O	1:A:661:ALA:N	2.26	0.69
1:A:200:PRO:HG2	1:A:749:THR:HA	1.73	0.69
1:A:124:GLN:HG2	1:A:758:TYR:CE2	2.28	0.69
1:B:1012:VAL:HG23	1:B:1013:THR:N	2.08	0.68
1:B:151:GLN:HE22	1:B:279:ALA:H	1.39	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:LEU:HB3	1:B:498:LYS:O	1.93	0.68
1:A:279:ALA:HA	1:A:612:VAL:HG12	1.74	0.68
1:A:406:VAL:CG1	1:A:407:ASP:N	2.56	0.68
1:A:572:PHE:CE1	1:A:629:VAL:HG13	2.29	0.68
1:B:771:VAL:O	1:B:771:VAL:HG12	1.92	0.68
1:B:281:PHE:HE1	1:B:608:SER:HG	1.39	0.68
1:C:33:ALA:HB2	1:C:298:ASN:ND2	2.08	0.68
1:A:813:SER:HB3	1:A:816:LEU:HD21	1.73	0.68
1:A:950:LYS:O	1:A:951:ASP:HB3	1.93	0.68
1:B:214:VAL:HG21	1:C:747:ASN:HD21	1.58	0.68
1:B:207:ILE:CG2	1:B:759:VAL:HG11	2.22	0.68
1:C:590:VAL:O	1:C:594:VAL:HG23	1.92	0.68
1:C:592:ASN:O	1:C:593:GLU:CB	2.42	0.68
1:B:109:ASN:HD22	1:B:112:GLN:HE22	1.41	0.68
1:C:939:ALA:O	1:C:943:ILE:CD1	2.42	0.68
1:B:922:THR:OG1	1:B:923:ASN:N	2.26	0.68
1:A:73:ASP:HB3	2:C:1054:HOH:O	1.93	0.68
1:A:413:VAL:HG23	1:A:493:CYS:CB	2.23	0.68
1:A:596:HIS:C	1:A:598:TYR:H	1.95	0.68
1:A:199:THR:HB	1:A:200:PRO:HD2	1.76	0.68
1:B:584:GLN:HB2	1:B:622:GLN:HE21	1.58	0.68
1:A:372:VAL:O	1:A:375:VAL:N	2.26	0.68
1:A:106:GLN:O	1:A:107:VAL:C	2.26	0.68
1:C:713:LEU:HD12	1:C:833:PRO:O	1.91	0.68
1:B:327:TYR:CD2	1:B:628:PHE:HB3	2.28	0.68
1:A:521:GLU:HB3	1:A:522:LYS:NZ	2.08	0.68
1:C:1016:VAL:O	1:C:1018:ALA:N	2.22	0.68
1:B:659:LYS:NZ	1:B:659:LYS:HA	2.08	0.68
1:B:356:TYR:C	1:B:358:PHE:H	1.95	0.68
1:A:552:MET:HE1	1:A:906:PRO:CA	2.24	0.68
1:B:919:ARG:HG3	1:B:1005:THR:HG21	1.76	0.68
1:B:420:MET:CE	1:B:425:LEU:HD23	2.23	0.68
1:B:138:MET:HE3	1:B:306:ILE:HD13	1.76	0.68
1:B:739:LEU:O	1:B:793:ALA:HB1	1.94	0.68
1:C:420:MET:SD	1:C:498:LYS:CD	2.81	0.68
1:A:773:VAL:O	1:A:773:VAL:CG1	2.42	0.68
1:C:576:VAL:HG12	1:C:663:VAL:HG22	1.74	0.68
1:B:129:VAL:HG12	1:B:129:VAL:O	1.94	0.68
1:A:819:TYR:O	1:A:822:LEU:N	2.18	0.68
1:A:822:LEU:HB3	2:A:1059:HOH:O	1.94	0.68
1:C:713:LEU:N	1:C:713:LEU:HD22	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:713:LEU:HB2	1:C:832:ALA:HB3	1.75	0.68
1:B:418:ARG:HE	1:B:970:MET:HE3	1.58	0.68
1:B:591:LEU:O	1:B:595:THR:HG22	1.92	0.68
1:A:855:VAL:HG23	1:A:855:VAL:O	1.94	0.68
1:A:104:GLN:O	1:A:108:GLN:HB2	1.94	0.67
1:B:120:GLN:HG2	1:B:124:GLN:HG2	1.76	0.67
1:C:110:LYS:O	1:C:112:GLN:N	2.27	0.67
1:B:358:PHE:CZ	1:B:976:LEU:HD12	2.27	0.67
1:B:404:LEU:HD13	1:B:449:LEU:HD13	1.75	0.67
1:A:901:VAL:O	1:A:904:VAL:CG2	2.41	0.67
1:A:909:VAL:CG1	1:A:913:LEU:HD21	2.22	0.67
1:B:119:PRO:HG2	1:B:122:VAL:CG2	2.24	0.67
1:B:116:PRO:HA	1:B:123:GLN:HE22	1.59	0.67
1:C:727:PHE:CZ	1:C:783:PRO:HB3	2.29	0.67
1:C:658:ILE:HD12	1:C:658:ILE:H	1.60	0.67
1:C:58:GLN:OE1	1:C:82:SER:CA	2.43	0.67
1:C:58:GLN:OE1	1:C:82:SER:N	2.26	0.67
1:B:525:HIS:HA	1:B:528:THR:CG2	2.25	0.67
1:A:435:MET:HA	1:A:438:ILE:HD11	1.76	0.67
1:B:190:PRO:HG2	1:B:779:TYR:CG	2.30	0.67
1:A:342:LYS:HG3	1:A:343:THR:N	2.10	0.67
1:C:159:ALA:C	1:C:161:ASN:H	1.98	0.67
1:B:416:VAL:CG2	1:B:431:THR:HA	2.25	0.67
1:B:537:SER:O	1:B:540:ARG:HB2	1.94	0.67
1:C:778:LYS:O	1:C:779:TYR:HD2	1.77	0.67
1:C:905:VAL:HB	1:C:906:PRO:HD3	1.75	0.67
1:B:150:THR:H	1:B:153:ASP:CB	2.08	0.67
1:A:173:GLY:HA3	1:A:294:ALA:HA	1.76	0.67
1:A:815:ARG:CZ	2:A:1071:HOH:O	2.41	0.67
1:A:818:ARG:HA	1:A:824:SER:N	2.10	0.67
1:B:347:ALA:HB1	1:B:402:ILE:HG21	1.76	0.67
1:C:5:PHE:HE2	1:C:11:PHE:HD2	1.40	0.67
1:A:571:VAL:HG12	1:A:630:SER:CA	2.24	0.67
1:C:457:ALA:CB	1:C:468:ARG:HA	2.23	0.67
1:A:818:ARG:HB2	1:A:818:ARG:HE	1.57	0.67
1:C:426:PRO:HB2	1:C:429:GLU:HB2	1.77	0.67
1:A:742:SER:HG	1:A:745:ASP:HB2	1.57	0.67
1:A:201:VAL:HG21	1:A:745:ASP:OD2	1.95	0.67
1:C:166:ILE:HA	1:C:166:ILE:CG1	2.24	0.67
1:C:613:ASN:C	1:C:613:ASN:OD1	2.32	0.67
1:B:94:PHE:HB2	1:B:98:THR:HG21	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:ILE:HA	1:B:491:ALA:HA	1.77	0.67
1:A:536:ARG:HD2	1:A:536:ARG:H	1.60	0.67
1:C:225:VAL:O	1:C:226:LYS:C	2.32	0.67
1:B:298:ASN:O	1:B:302:THR:HG23	1.94	0.67
1:B:178:PHE:HE1	1:B:615:PHE:CE2	2.13	0.67
1:B:175:VAL:O	1:B:175:VAL:HG12	1.94	0.67
1:B:940:LYS:O	1:B:941:ASN:C	2.32	0.67
1:C:103:ALA:O	1:C:104:GLN:C	2.32	0.67
1:A:1018:ALA:HB1	1:A:1022:VAL:CG1	2.24	0.67
1:C:190:PRO:HG3	1:C:789:TRP:CH2	2.30	0.67
1:B:172:VAL:CG1	1:B:172:VAL:O	2.39	0.67
1:A:69:MET:C	1:A:70:ASN:ND2	2.48	0.66
1:C:953:MET:HE1	1:C:1030:ARG:HH22	1.61	0.66
1:C:389:SER:OG	1:C:391:ASN:ND2	2.28	0.66
1:A:583:THR:HG22	1:A:585:GLU:H	1.58	0.66
1:B:30:LEU:HD23	1:B:390:ILE:CG1	2.24	0.66
1:B:860:THR:HG22	1:B:861:GLY:N	2.10	0.66
1:A:376:LEU:O	1:A:377:LEU:C	2.34	0.66
1:C:713:LEU:O	1:C:831:ALA:HA	1.95	0.66
1:B:641:GLU:HA	1:B:650:ARG:NH1	2.11	0.66
1:B:124:GLN:O	1:B:125:GLN:HB2	1.95	0.66
1:B:125:GLN:HG2	1:B:125:GLN:O	1.94	0.66
1:C:457:ALA:N	1:C:459:PHE:CE2	2.61	0.66
1:A:987:MET:N	1:A:988:PRO:HD2	2.10	0.66
1:A:521:GLU:HB3	1:A:522:LYS:HZ3	1.60	0.66
1:B:330:THR:N	1:B:331:PRO:HD2	2.11	0.66
1:A:674:LEU:HD22	1:A:675:GLY:H	1.61	0.66
1:B:74:ASN:O	1:B:94:PHE:HB3	1.95	0.66
1:C:1024:VAL:O	1:C:1028:VAL:HG23	1.95	0.66
1:C:476:SER:C	1:C:478:MET:H	1.98	0.66
1:A:736:ALA:O	1:A:741:VAL:CG1	2.43	0.66
1:B:671:ILE:O	1:B:673:GLU:HB2	1.95	0.66
1:C:586:ARG:O	1:C:589:LYS:HB2	1.95	0.66
1:C:688:ALA:O	1:C:690:LEU:N	2.25	0.66
1:C:143:ILE:CD1	1:C:286:ALA:HB2	2.25	0.66
1:A:55:LYS:HD3	1:A:816:LEU:HD11	1.77	0.66
1:C:317:PHE:HB2	1:C:318:PRO:CD	2.26	0.66
1:B:990:VAL:CG1	1:B:1005:THR:OG1	2.38	0.66
1:A:243:THR:HG22	1:A:268:ILE:HG22	1.78	0.66
1:C:997:SER:O	1:C:998:GLY:C	2.31	0.66
1:A:119:PRO:HG2	1:A:122:VAL:HG23	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ASN:HD21	1:A:192:GLU:HB3	1.61	0.66
1:A:759:VAL:HG12	1:A:760:ASN:N	2.09	0.66
1:C:1026:PHE:O	1:C:1029:VAL:HB	1.96	0.66
1:C:35:TYR:CD1	1:C:671:ILE:HG12	2.31	0.66
1:C:380:PHE:CE1	1:C:398:MET:SD	2.88	0.66
1:A:693:GLU:O	1:A:696:THR:N	2.23	0.66
1:C:592:ASN:HD22	1:C:592:ASN:H	1.40	0.66
1:C:713:LEU:HG	1:C:832:ALA:C	2.17	0.66
1:A:540:ARG:HD2	1:A:541:TYR:CD2	2.30	0.66
1:C:189:ASN:CG	1:C:779:TYR:HE1	1.98	0.66
1:C:372:VAL:HG21	1:C:402:ILE:HG23	1.78	0.66
1:C:416:VAL:HG12	1:C:434:SER:OG	1.96	0.66
1:C:801:PHE:HA	1:C:804:PHE:CZ	2.31	0.66
1:C:714:THR:HG22	1:C:715:SER:H	1.60	0.66
1:C:163:LYS:HD2	1:C:177:LEU:HB2	1.76	0.66
1:C:181:GLN:HG2	1:C:769:LYS:HE3	1.78	0.66
1:B:238:THR:OG1	1:B:239:ARG:N	2.29	0.66
1:B:940:LYS:NZ	1:B:978:THR:HG23	2.10	0.66
1:C:474:ILE:O	1:C:476:SER:O	2.14	0.66
1:C:367:ILE:HG23	1:C:368:PRO:HD3	1.78	0.66
1:A:719:ASN:HB2	1:A:828:LEU:HD23	1.78	0.66
1:B:95:GLU:O	1:B:98:THR:HB	1.96	0.66
1:C:843:LEU:O	1:C:846:GLN:HB2	1.96	0.66
1:A:111:LEU:O	1:A:113:LEU:N	2.29	0.66
1:B:1026:PHE:O	1:B:1030:ARG:HG3	1.95	0.66
1:A:344:LEU:CD2	1:A:402:ILE:CD1	2.68	0.66
1:C:901:VAL:HG11	1:C:943:ILE:HD13	1.76	0.66
1:C:166:ILE:CA	1:C:166:ILE:HD13	2.12	0.65
1:C:423:GLU:O	1:C:426:PRO:HD3	1.97	0.65
1:B:199:THR:N	1:B:202:ASP:OD2	2.27	0.65
1:C:102:ILE:O	1:C:103:ALA:C	2.31	0.65
1:B:30:LEU:HD23	1:B:390:ILE:CD1	2.26	0.65
1:C:633:ASP:O	1:C:634:TRP:HB2	1.95	0.65
1:A:44:THR:HA	1:A:91:THR:HA	1.79	0.65
1:A:706:ALA:HB3	1:A:716:VAL:HG21	1.77	0.65
1:B:902:MET:O	1:B:905:VAL:HG12	1.97	0.65
1:C:939:ALA:O	1:C:943:ILE:HD11	1.95	0.65
1:A:330:THR:HG23	1:A:334:LYS:HE2	1.78	0.65
1:C:188:MET:HA	1:C:266:ALA:HB1	1.78	0.65
1:B:644:VAL:HG23	1:B:645:GLU:H	1.61	0.65
1:C:115:MET:HE1	1:C:118:LEU:CD2	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:775:SER:HB3	1:B:780:ARG:CG	2.27	0.65
1:B:984:LEU:O	1:B:984:LEU:HD13	1.96	0.65
1:B:495:THR:O	1:B:498:LYS:HE3	1.97	0.65
1:A:108:GLN:CA	1:A:108:GLN:CG	2.74	0.65
1:A:128:SER:HB2	1:B:113:LEU:HD21	1.77	0.65
1:A:100:ALA:CB	1:A:131:LYS:HE3	2.27	0.65
1:B:405:LEU:HD12	1:B:406:VAL:H	1.60	0.65
1:C:713:LEU:CG	1:C:832:ALA:O	2.36	0.65
1:C:524:THR:O	1:C:527:TYR:HB3	1.97	0.65
1:B:328:ASP:C	1:B:328:ASP:OD2	2.35	0.65
1:B:773:VAL:CG1	1:B:773:VAL:O	2.45	0.65
1:A:83:ASP:HB3	2:A:1068:HOH:O	1.96	0.65
1:A:76:MET:CG	1:A:95:GLU:OE2	2.42	0.65
1:A:128:SER:CB	1:B:113:LEU:CD2	2.75	0.65
1:C:324:VAL:HG23	1:C:326:PRO:HD3	1.79	0.65
1:C:45:ILE:CA	1:C:45:ILE:CG2	2.71	0.65
1:B:1024:VAL:CG1	1:B:1028:VAL:HG21	2.27	0.65
1:A:527:TYR:O	1:A:530:SER:OG	2.11	0.65
1:C:14:VAL:HG13	1:C:15:ILE:N	2.12	0.65
1:B:45:ILE:HG22	1:B:46:SER:N	2.12	0.65
1:B:293:LEU:HD22	1:B:294:ALA:O	1.97	0.65
1:C:74:ASN:HB3	1:C:95:GLU:HB2	1.78	0.65
1:B:330:THR:N	1:B:331:PRO:CD	2.59	0.65
1:C:197:GLN:HB3	1:C:798:MET:HE2	1.79	0.65
1:B:655:PHE:HA	1:B:658:ILE:HG21	1.79	0.65
1:A:133:SER:HG	1:A:136:PHE:HE1	1.43	0.65
1:C:169:THR:C	1:C:169:THR:CB	2.64	0.65
1:B:6:ILE:CD1	1:B:490:PRO:HB2	2.26	0.65
1:A:263:ARG:HB3	1:A:263:ARG:HH21	1.62	0.65
1:A:521:GLU:HG3	2:A:1075:HOH:O	1.97	0.65
1:B:601:LYS:O	1:B:603:LYS:N	2.30	0.65
1:A:100:ALA:HB1	1:A:131:LYS:HE3	1.79	0.65
1:C:54:ALA:N	1:C:57:VAL:HG23	2.12	0.65
1:C:728:LYS:HG3	1:C:729:ILE:H	1.60	0.65
1:C:431:THR:O	1:C:435:MET:HG2	1.96	0.65
1:B:646:ALA:C	1:B:648:THR:N	2.46	0.65
1:B:572:PHE:HB2	1:B:666:PHE:O	1.97	0.65
1:B:49:TYR:CE2	1:B:125:GLN:HB3	2.31	0.65
1:B:578:LEU:HB2	1:B:623:ASN:HB2	1.79	0.65
1:A:222:THR:HG22	1:A:223:PRO:HD2	1.79	0.65
1:A:60:THR:CG2	1:A:119:PRO:HD3	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:592:ASN:O	1:C:593:GLU:HB3	1.97	0.65
1:B:598:TYR:HB3	1:B:606:VAL:HG11	1.78	0.65
1:B:160:ALA:HB1	1:B:767:ARG:HD3	1.76	0.65
1:C:60:THR:CG2	1:C:61:VAL:HG23	2.26	0.65
1:C:786:ILE:O	1:C:786:ILE:HG22	1.97	0.65
1:B:699:ARG:HB3	1:B:699:ARG:HH11	1.62	0.65
1:B:835:LYS:HB2	1:B:839:GLU:OE2	1.96	0.65
1:B:561:SER:HB2	1:B:838:GLY:HA3	1.78	0.65
1:C:520:PHE:O	1:C:523:SER:N	2.29	0.65
1:C:1024:VAL:HG12	1:C:1028:VAL:HG21	1.78	0.65
1:A:56:THR:HG23	1:C:213:GLN:HG3	1.79	0.65
1:C:110:LYS:O	1:C:111:LEU:C	2.35	0.64
1:B:1012:VAL:CG2	1:B:1013:THR:N	2.61	0.64
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.78	0.64
1:C:844:MET:HA	1:C:847:LEU:HD21	1.78	0.64
1:C:395:MET:O	1:C:398:MET:N	2.30	0.64
1:C:545:TYR:OH	1:C:1021:PHE:CG	2.49	0.64
1:C:657:GLN:O	1:C:659:LYS:N	2.30	0.64
1:A:95:GLU:O	1:A:98:THR:HG23	1.97	0.64
1:C:64:VAL:HG12	1:C:65:ILE:N	2.11	0.64
1:B:468:ARG:O	1:B:469:GLN:C	2.34	0.64
1:B:537:SER:C	1:B:540:ARG:HE	2.00	0.64
1:B:544:LEU:CA	1:B:547:ILE:HD12	2.19	0.64
1:B:960:LEU:HD12	1:B:961:ILE:HG13	1.79	0.64
1:A:885:PHE:CD2	1:A:886:LEU:HD12	2.32	0.64
1:C:244:GLU:HA	1:C:263:ARG:HH22	1.61	0.64
1:B:972:LEU:CD1	1:B:976:LEU:HD23	2.28	0.64
1:A:355:MET:HE3	1:A:410:ILE:HG12	1.78	0.64
1:C:545:TYR:OH	1:C:1021:PHE:CB	2.45	0.64
1:C:222:THR:HB	1:C:223:PRO:CD	2.24	0.64
1:A:418:ARG:CD	1:A:970:MET:HG3	2.25	0.64
1:B:139:VAL:O	1:B:139:VAL:HG12	1.96	0.64
1:A:476:SER:O	1:A:480:LEU:HB2	1.96	0.64
1:C:62:THR:CB	2:C:1064:HOH:O	2.45	0.64
1:A:534:ILE:HD12	1:A:540:ARG:NH2	2.13	0.64
1:A:727:PHE:O	1:C:234:ILE:HA	1.97	0.64
1:C:418:ARG:HG3	1:C:419:VAL:CG1	2.28	0.64
1:B:654:ALA:O	1:B:656:SER:N	2.31	0.64
1:A:574:THR:HG21	1:A:598:TYR:HE1	1.63	0.64
1:B:659:LYS:HA	1:B:659:LYS:HZ3	1.62	0.64
1:A:298:ASN:HD22	1:A:300:LEU:N	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:715:SER:HB2	1:B:830:GLN:NE2	2.12	0.64
1:C:899:PHE:CD1	1:C:899:PHE:N	2.65	0.64
1:A:59:ASP:HB3	1:C:763:ILE:HD11	1.78	0.64
1:B:314:GLU:N	1:B:315:PRO:HD2	2.12	0.64
1:C:710:PRO:O	1:C:712:MET:O	2.16	0.64
1:A:540:ARG:HG2	2:A:1064:HOH:O	1.96	0.64
1:C:1:MET:CE	1:C:439:GLN:HE22	2.11	0.64
1:A:785:ASP:O	1:A:788:ASP:N	2.30	0.64
1:B:1012:VAL:CG2	1:B:1013:THR:H	2.10	0.64
1:B:2:PRO:CD	1:B:486:LEU:HD12	2.28	0.64
1:A:911:GLY:H	1:A:914:LEU:HD13	1.63	0.64
1:C:404:LEU:O	1:C:405:LEU:HD23	1.98	0.64
1:C:114:ALA:O	1:C:118:LEU:HD13	1.98	0.64
1:C:115:MET:SD	1:C:123:GLN:NE2	2.71	0.64
1:C:344:LEU:CD2	1:C:402:ILE:HD11	2.28	0.64
1:B:68:ASN:O	1:B:70:ASN:ND2	2.31	0.64
1:B:184:MET:O	1:B:184:MET:CG	2.46	0.64
1:B:136:PHE:CE1	1:B:617:PHE:HZ	2.16	0.64
1:C:26:ALA:O	1:C:30:LEU:HG	1.98	0.64
1:A:949:ALA:HB1	1:A:1026:PHE:CZ	2.33	0.64
1:C:850:LYS:O	1:C:851:LEU:O	2.16	0.64
1:C:371:ALA:O	1:C:375:VAL:HG23	1.98	0.64
1:B:328:ASP:OD2	1:B:330:THR:N	2.31	0.64
1:B:335:ILE:C	1:B:337:ILE:H	2.00	0.64
1:C:672:VAL:HG12	1:C:672:VAL:O	1.98	0.64
1:C:167:SER:C	1:C:167:SER:N	2.51	0.64
1:B:187:TRP:HZ3	1:B:774:MET:HE3	1.61	0.64
1:B:9:PRO:O	1:B:12:ALA:HB3	1.97	0.64
1:C:894:SER:C	1:C:896:SER:H	2.01	0.64
1:B:356:TYR:C	1:B:358:PHE:N	2.50	0.64
1:A:728:LYS:HZ3	1:C:235:ILE:HG22	1.60	0.64
1:C:545:TYR:HA	1:C:548:ILE:HG13	1.80	0.64
1:A:601:LYS:O	1:A:601:LYS:HG3	1.98	0.64
1:B:463:THR:HG21	1:B:869:SER:HB2	1.80	0.64
1:A:692:HIS:O	1:A:696:THR:OG1	2.13	0.64
1:A:44:THR:HG22	1:A:89:GLN:HG3	1.80	0.64
1:A:255:GLN:O	1:A:256:ASP:OD1	2.16	0.64
1:C:176:GLN:NE2	1:C:620:ARG:HH11	1.96	0.64
1:B:437:GLN:HA	1:B:437:GLN:HE21	1.63	0.64
1:B:410:ILE:HG23	1:B:414:GLU:OE2	1.98	0.63
1:C:687:GLN:HB2	1:C:854:GLY:O	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:750:LEU:HD13	1:B:750:LEU:O	1.98	0.63
1:A:225:VAL:HG12	1:A:226:LYS:N	2.12	0.63
1:A:46:SER:HA	1:A:88:VAL:O	1.99	0.63
1:A:935:ILE:O	1:A:935:ILE:HG22	1.97	0.63
1:C:60:THR:HG23	1:C:61:VAL:HG23	1.80	0.63
1:C:391:ASN:H	1:C:394:THR:HG23	1.63	0.63
1:A:649:MET:CB	1:A:653:ARG:HH21	2.04	0.63
1:A:367:ILE:HG12	1:A:413:VAL:HG21	1.80	0.63
1:B:371:ALA:O	1:B:375:VAL:HG23	1.98	0.63
1:C:361:ASN:HB2	1:C:364:ALA:HB3	1.80	0.63
1:B:953:MET:O	1:B:953:MET:HG2	1.98	0.63
1:A:818:ARG:CD	1:A:818:ARG:CB	2.76	0.63
1:B:416:VAL:HG21	1:B:431:THR:HA	1.80	0.63
1:B:314:GLU:N	1:B:315:PRO:CD	2.61	0.63
1:C:644:VAL:HG11	1:C:667:ASN:ND2	2.11	0.63
1:A:298:ASN:HD22	1:A:300:LEU:H	1.44	0.63
1:A:102:ILE:HA	1:A:105:VAL:HG23	1.80	0.63
1:C:159:ALA:CA	2:C:1078:HOH:O	1.89	0.63
1:A:348:ILE:HA	1:A:351:VAL:HG23	1.80	0.63
1:A:443:VAL:CG1	1:A:444:GLY:H	1.98	0.63
1:B:228:GLN:CG	1:C:781:MET:HE1	2.29	0.63
1:C:465:ALA:O	1:C:469:GLN:HG2	1.99	0.63
1:C:615:PHE:O	1:C:615:PHE:CD2	2.51	0.63
1:B:452:VAL:O	1:B:453:PHE:CB	2.46	0.63
1:C:924:ASP:C	1:C:925:VAL:O	2.31	0.63
1:B:235:ILE:N	1:B:235:ILE:HD13	2.13	0.63
1:C:598:TYR:CD2	1:C:606:VAL:HG21	2.33	0.63
1:A:688:ALA:O	1:A:689:GLY:C	2.36	0.63
1:C:950:LYS:HZ3	1:C:1030:ARG:CD	2.06	0.63
1:A:983:ILE:HG13	1:A:984:LEU:N	2.14	0.63
1:A:968:VAL:HG21	1:A:1023:PRO:CB	2.29	0.63
1:A:989:LEU:HG	1:A:993:THR:HG23	1.81	0.63
1:A:516:PHE:C	1:A:518:ARG:H	2.00	0.63
1:B:674:LEU:HD13	1:B:860:THR:CG2	2.28	0.63
1:B:859:TRP:HB3	1:B:863:SER:CB	2.28	0.63
1:C:177:LEU:HD13	1:C:179:GLY:C	2.18	0.63
1:A:1024:VAL:HG12	1:A:1025:PHE:N	2.13	0.63
1:C:346:GLU:O	1:C:349:ILE:HB	1.99	0.63
1:B:613:ASN:ND2	1:B:614:GLY:N	2.46	0.63
1:A:255:GLN:CD	1:A:255:GLN:N	2.52	0.63
1:B:10:ILE:HG13	1:C:893:GLU:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:391:ASN:N	1:C:394:THR:CG2	2.62	0.63
1:B:360:GLN:O	1:B:361:ASN:HB2	1.99	0.63
1:C:114:ALA:O	1:C:115:MET:C	2.35	0.63
1:B:545:TYR:OH	1:B:906:PRO:HG3	1.99	0.63
1:B:713:LEU:N	1:B:713:LEU:HD12	2.14	0.63
1:C:221:GLY:O	1:C:222:THR:C	2.37	0.63
1:A:54:ALA:O	1:A:58:GLN:N	2.29	0.62
1:A:73:ASP:CG	1:A:106:GLN:NE2	2.53	0.62
1:B:136:PHE:HA	1:B:292:LYS:HG3	1.81	0.62
1:C:274:ASN:CB	2:C:1060:HOH:O	2.20	0.62
1:B:538:THR:HG23	1:B:540:ARG:NH2	2.14	0.62
1:B:945:ILE:HD12	1:B:1026:PHE:CE2	2.31	0.62
1:A:154:ILE:O	1:A:158:VAL:HG23	1.99	0.62
1:A:574:THR:OG1	1:A:627:ALA:HB3	1.99	0.62
1:C:204:ILE:HG12	1:C:759:VAL:CG1	2.29	0.62
1:B:775:SER:HB3	1:B:780:ARG:HG3	1.80	0.62
1:A:64:VAL:O	1:A:65:ILE:O	2.17	0.62
1:A:756:GLY:CA	1:A:774:MET:HB2	2.29	0.62
1:A:5:PHE:CE1	1:A:12:ALA:HB2	2.33	0.62
1:C:457:ALA:H	1:C:459:PHE:HE2	1.42	0.62
1:A:106:GLN:O	1:A:110:LYS:HB2	1.98	0.62
1:C:190:PRO:HG3	1:C:789:TRP:CZ2	2.34	0.62
1:C:379:THR:HB	1:C:398:MET:HE3	1.81	0.62
1:B:831:ALA:HB3	1:B:840:ALA:HB2	1.80	0.62
1:A:298:ASN:C	1:A:298:ASN:ND2	2.52	0.62
1:B:252:LYS:HB3	1:B:260:VAL:CG1	2.30	0.62
1:C:189:ASN:HD22	1:C:190:PRO:N	1.98	0.62
1:B:723:ASP:HA	1:B:814:PRO:HD3	1.81	0.62
1:B:589:LYS:O	1:B:592:ASN:HB2	2.00	0.62
1:C:785:ASP:C	1:C:787:GLY:N	2.51	0.62
1:B:148:THR:O	1:B:148:THR:HG22	2.00	0.62
1:C:999:ALA:O	1:C:1003:VAL:HG23	1.99	0.62
1:C:463:THR:HA	1:C:466:ILE:HD13	1.80	0.62
1:A:750:LEU:HD11	1:C:216:ALA:HB2	1.82	0.62
1:C:104:GLN:NE2	1:C:131:LYS:HE2	2.15	0.62
1:C:830:GLN:OE1	1:C:832:ALA:HA	2.00	0.62
1:C:554:TYR:O	1:C:555:LEU:HB2	1.99	0.62
1:B:699:ARG:HG2	1:B:700:ASN:N	2.14	0.62
1:B:831:ALA:HB2	1:B:840:ALA:HB2	1.82	0.62
1:C:925:VAL:C	1:C:927:PHE:H	2.03	0.62
1:A:184:MET:HB3	1:A:771:VAL:HG13	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:534:ILE:HG23	1:B:541:TYR:CZ	2.35	0.62
1:C:778:LYS:C	1:C:779:TYR:HD2	2.03	0.62
1:A:728:LYS:HG3	1:A:729:ILE:O	2.00	0.62
1:B:852:PRO:HA	1:B:855:VAL:HB	1.80	0.62
1:C:644:VAL:CG1	1:C:667:ASN:HB2	2.30	0.62
1:A:1:MET:H2	1:A:2:PRO:HD2	1.65	0.62
1:C:92:LEU:HD22	1:C:107:VAL:HG22	1.82	0.62
1:B:407:ASP:C	1:B:408:ASP:O	2.37	0.62
1:A:228:GLN:CG	1:B:781:MET:HG2	2.30	0.62
1:A:719:ASN:HB2	1:A:828:LEU:CD2	2.29	0.62
1:C:657:GLN:HB3	1:C:658:ILE:HD12	1.82	0.62
1:C:899:PHE:HD1	1:C:899:PHE:N	1.96	0.62
1:C:530:SER:O	1:C:534:ILE:HG23	1.99	0.62
1:A:113:LEU:CD2	1:C:128:SER:HA	2.27	0.62
1:C:703:LEU:O	1:C:706:ALA:HB3	2.00	0.62
1:B:921:LEU:CD2	1:B:1005:THR:HG22	2.30	0.62
1:A:713:LEU:HB3	1:A:831:ALA:O	1.99	0.62
1:C:143:ILE:CG2	1:C:284:GLN:HE22	2.08	0.62
1:A:513:PHE:CD1	1:A:517:ASN:ND2	2.63	0.62
1:C:578:LEU:HD22	1:C:661:ALA:CB	2.30	0.62
1:C:259:ARG:CB	1:C:259:ARG:HH11	2.13	0.62
1:C:167:SER:H	1:C:175:VAL:HG21	1.64	0.61
1:C:417:GLU:HB3	1:C:973:ARG:HH12	1.64	0.61
1:C:184:MET:HG2	1:C:246:PHE:CE1	2.35	0.61
1:A:709:HIS:N	1:A:710:PRO:HD3	2.14	0.61
1:C:693:GLU:O	1:C:694:LYS:C	2.38	0.61
1:C:164:ASP:O	1:C:168:ARG:HG3	1.99	0.61
1:B:978:THR:CG2	1:B:979:SER:N	2.62	0.61
1:C:345:VAL:O	1:C:348:ILE:HG12	2.00	0.61
1:C:418:ARG:NE	1:C:970:MET:HE2	2.15	0.61
1:B:49:TYR:HE2	1:B:125:GLN:HB3	1.65	0.61
1:A:61:VAL:HG13	1:A:118:LEU:HD13	1.81	0.61
1:B:109:ASN:HD22	1:B:112:GLN:NE2	1.98	0.61
1:C:54:ALA:HB2	1:C:84:SER:CB	2.20	0.61
1:A:950:LYS:O	1:A:951:ASP:CB	2.47	0.61
1:C:344:LEU:HD22	1:C:402:ILE:HD11	1.82	0.61
1:B:184:MET:HB3	1:B:771:VAL:HG22	1.82	0.61
1:B:280:GLU:CB	1:B:284:GLN:O	2.48	0.61
1:A:340:VAL:HG13	1:A:399:VAL:HG21	1.83	0.61
1:B:585:GLU:O	1:B:588:GLN:N	2.32	0.61
1:C:410:ILE:HG22	1:C:411:VAL:H	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:673:GLU:HA	1:B:673:GLU:OE1	2.00	0.61
1:C:607:GLU:O	1:C:607:GLU:HG3	2.00	0.61
1:C:305:ALA:O	1:C:309:GLU:N	2.33	0.61
1:C:310:LEU:O	1:C:313:MET:N	2.31	0.61
1:C:62:THR:HG23	1:C:90:ILE:CD1	2.28	0.61
1:C:115:MET:HE2	1:C:115:MET:HA	1.83	0.61
1:C:705:GLU:O	1:C:707:ALA:N	2.33	0.61
1:A:909:VAL:HG12	1:A:913:LEU:HD23	1.81	0.61
1:A:950:LYS:HA	1:A:953:MET:HB3	1.80	0.61
1:B:697:GLN:O	1:B:699:ARG:O	2.18	0.61
1:B:703:LEU:HA	1:B:706:ALA:HB3	1.82	0.61
1:A:367:ILE:HG13	1:A:368:PRO:HD3	1.83	0.61
1:B:280:GLU:HB2	1:B:284:GLN:O	2.01	0.61
1:A:44:THR:CG2	1:A:89:GLN:HG3	2.31	0.61
1:C:600:THR:OG1	1:C:601:LYS:N	2.34	0.61
1:A:481:SER:O	1:A:484:VAL:N	2.32	0.61
1:C:131:LYS:HB2	1:C:295:THR:CG2	2.30	0.61
1:C:57:VAL:CG1	1:C:88:VAL:CG2	2.79	0.61
1:A:554:TYR:CE1	1:A:558:ARG:HD3	2.36	0.61
1:C:431:THR:HG21	1:C:494:ALA:CB	2.28	0.61
1:A:563:PHE:O	1:A:564:LEU:HD12	2.00	0.61
1:B:115:MET:HA	1:B:115:MET:CE	2.30	0.61
1:A:48:SER:HB2	1:A:125:GLN:HG3	1.83	0.61
1:A:544:LEU:O	1:A:547:ILE:HB	2.01	0.61
1:A:897:ILE:N	1:A:898:PRO:HD2	2.15	0.61
1:A:154:ILE:CG2	1:A:287:SER:HB3	2.27	0.61
1:B:975:ILE:H	1:B:975:ILE:HD12	1.65	0.61
1:B:646:ALA:O	1:B:647:ILE:C	2.38	0.61
1:C:161:ASN:N	1:C:164:ASP:OD2	2.34	0.61
1:B:187:TRP:O	1:B:266:ALA:HA	2.01	0.61
1:B:7:ASP:C	1:B:8:ARG:HD2	2.21	0.61
1:C:911:GLY:CA	1:C:1013:THR:HG21	2.31	0.61
1:C:160:ALA:C	1:C:164:ASP:OD2	2.39	0.61
1:B:310:LEU:O	1:B:314:GLU:HG3	2.01	0.61
1:A:324:VAL:HG12	1:A:325:TYR:N	2.15	0.61
1:B:517:ASN:C	1:B:521:GLU:HG3	2.22	0.61
1:C:453:PHE:O	1:C:456:MET:HG2	2.00	0.61
1:B:775:SER:HB3	1:B:780:ARG:CD	2.30	0.61
1:B:143:ILE:HD12	1:B:322:LYS:HB3	1.83	0.61
1:B:709:HIS:N	1:B:710:PRO:HD3	2.15	0.61
1:C:688:ALA:C	1:C:690:LEU:H	2.04	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:699:ARG:HG2	1:C:825:MET:HE1	1.82	0.60
1:C:851:LEU:HD12	1:C:851:LEU:N	2.16	0.60
1:C:908:GLY:HA2	1:C:1014:ALA:HB2	1.81	0.60
1:C:554:TYR:HD1	1:C:558:ARG:HH21	1.42	0.60
1:A:418:ARG:HH12	1:A:973:ARG:HB3	1.65	0.60
1:A:171:GLY:O	1:A:172:VAL:C	2.39	0.60
1:C:368:PRO:HG3	1:C:413:VAL:HG11	1.82	0.60
1:B:235:ILE:CD1	1:B:235:ILE:N	2.64	0.60
1:C:254:ASN:OD1	1:C:258:SER:O	2.19	0.60
1:B:543:VAL:O	1:B:547:ILE:CD1	2.49	0.60
1:B:314:GLU:HB2	1:B:315:PRO:HD3	1.82	0.60
1:A:713:LEU:O	1:A:714:THR:CG2	2.44	0.60
1:C:2:PRO:O	1:C:6:ILE:HG13	2.00	0.60
1:A:323:ILE:HG12	1:A:325:TYR:HE1	1.65	0.60
1:B:157:TYR:C	1:B:161:ASN:HD22	2.04	0.60
1:B:219:LEU:CD2	1:C:783:PRO:HG3	2.31	0.60
1:B:143:ILE:HG23	1:B:286:ALA:HB2	1.84	0.60
1:A:58:GLN:HG3	1:A:63:GLN:HE22	1.66	0.60
1:A:391:ASN:H	1:A:394:THR:HG22	1.65	0.60
1:C:657:GLN:C	1:C:659:LYS:H	2.04	0.60
1:C:615:PHE:HD2	1:C:615:PHE:O	1.84	0.60
1:A:857:TYR:CD1	1:A:857:TYR:C	2.73	0.60
1:C:57:VAL:HG12	1:C:88:VAL:CG2	2.31	0.60
1:C:942:ALA:HA	1:C:945:ILE:HG22	1.84	0.60
1:C:576:VAL:HG21	1:C:591:LEU:HD22	1.83	0.60
1:C:266:ALA:O	1:C:267:LYS:C	2.40	0.60
1:A:51:GLY:O	1:C:215:ALA:HB1	2.01	0.60
1:A:719:ASN:C	1:A:719:ASN:ND2	2.49	0.60
1:A:643:LYS:O	1:A:647:ILE:HG13	2.01	0.60
1:A:108:GLN:CB	1:A:108:GLN:CD	2.66	0.60
1:B:591:LEU:CD1	1:B:611:ALA:HB1	2.31	0.60
1:C:552:MET:CE	1:C:909:VAL:HG21	2.31	0.60
1:C:291:ILE:HG22	1:C:291:ILE:O	1.99	0.60
1:C:897:ILE:HG12	1:C:950:LYS:HE3	1.82	0.60
1:A:905:VAL:O	1:A:909:VAL:HG23	2.00	0.60
1:C:560:PRO:O	1:C:922:THR:HG22	2.01	0.60
1:A:246:PHE:O	1:A:249:ILE:CD1	2.49	0.60
1:C:10:ILE:O	1:C:10:ILE:HG22	2.00	0.60
1:A:425:LEU:HB3	1:A:426:PRO:HD2	1.82	0.60
1:C:663:VAL:O	1:C:664:PHE:HB3	2.02	0.60
1:A:10:ILE:HD11	1:B:895:TRP:CB	2.29	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1024:VAL:HG12	1:C:1028:VAL:CG2	2.32	0.60
1:C:933:THR:O	1:C:937:LEU:HB2	2.02	0.60
1:C:485:ALA:O	1:C:490:PRO:HD3	2.02	0.60
1:B:574:THR:HG23	1:B:665:ALA:CB	2.22	0.60
1:B:808:ARG:CB	1:B:808:ARG:HH21	2.15	0.60
1:A:758:TYR:CG	1:A:758:TYR:O	2.55	0.60
1:C:308:ALA:O	1:C:311:ALA:HB3	2.02	0.60
1:C:758:TYR:HB3	1:C:772:TYR:CE2	2.36	0.60
1:A:540:ARG:HD2	1:A:541:TYR:CE2	2.37	0.60
1:A:952:LEU:HD12	1:A:953:MET:N	2.17	0.60
1:A:728:LYS:HD2	1:C:235:ILE:HG22	1.84	0.60
1:A:583:THR:HG22	1:A:585:GLU:N	2.17	0.60
1:A:171:GLY:O	1:A:294:ALA:HB2	2.02	0.60
1:A:827:ILE:N	1:A:827:ILE:HD12	2.16	0.60
1:C:236:ALA:O	1:C:237:GLN:C	2.40	0.60
1:C:790:TYR:CD1	1:C:800:PRO:HB3	2.37	0.60
1:A:54:ALA:HB1	1:A:816:LEU:CG	2.24	0.60
1:B:3:ASN:N	1:B:6:ILE:HG12	2.13	0.60
1:C:684:LEU:HD11	1:C:855:VAL:CG1	2.32	0.60
1:B:418:ARG:HH21	1:B:970:MET:CG	2.14	0.60
1:B:207:ILE:HG21	1:B:759:VAL:HG11	1.82	0.60
1:A:699:ARG:NH2	1:A:722:GLU:OE1	2.35	0.60
1:A:17:ILE:HG22	1:A:21:LEU:CD2	2.31	0.60
1:C:166:ILE:O	1:C:172:VAL:HG11	2.02	0.59
1:A:528:THR:CG2	1:A:969:ARG:HE	2.10	0.59
1:B:214:VAL:HG21	1:C:747:ASN:ND2	2.16	0.59
1:B:623:ASN:C	1:B:623:ASN:ND2	2.53	0.59
1:C:590:VAL:O	1:C:592:ASN:O	2.20	0.59
1:A:196:PHE:O	1:A:197:GLN:HB2	2.03	0.59
1:A:68:ASN:CB	1:A:68:ASN:N	2.65	0.59
1:C:886:LEU:O	1:C:890:ALA:HB2	2.02	0.59
1:B:431:THR:HG21	1:B:493:CYS:HB2	1.84	0.59
1:B:346:GLU:OE1	1:B:988:PRO:CB	2.48	0.59
1:C:911:GLY:HA3	1:C:1013:THR:CG2	2.32	0.59
1:C:912:ALA:C	1:C:914:LEU:H	2.04	0.59
1:C:140:VAL:O	1:C:288:GLY:HA3	2.02	0.59
1:C:200:PRO:HG2	1:C:749:THR:HA	1.83	0.59
1:B:776:GLU:HG2	1:B:777:ALA:N	2.17	0.59
1:C:540:ARG:HE	1:C:541:TYR:HE1	1.47	0.59
1:B:560:PRO:CB	1:B:836:SER:HB3	2.32	0.59
1:C:211:ASN:C	1:C:211:ASN:HD22	2.05	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:952:LEU:HA	1:B:956:GLU:OE2	2.02	0.59
1:B:907:LEU:O	1:B:909:VAL:N	2.35	0.59
1:B:975:ILE:HD12	1:B:975:ILE:N	2.17	0.59
1:C:847:LEU:O	1:C:850:LYS:HG2	2.03	0.59
1:B:692:HIS:O	1:B:693:GLU:HG3	2.02	0.59
1:A:26:ALA:O	1:A:30:LEU:HG	2.02	0.59
1:A:795:ASP:OD1	1:A:797:GLN:HG2	2.03	0.59
1:C:84:SER:C	1:C:86:GLY:N	2.56	0.59
1:A:548:ILE:CG2	1:A:910:ILE:HG12	2.32	0.59
1:A:571:VAL:CG1	1:A:630:SER:HA	2.30	0.59
1:B:281:PHE:CE2	1:B:324:VAL:HG11	2.37	0.59
1:A:10:ILE:CD1	1:B:895:TRP:HB2	2.29	0.59
1:C:262:LEU:CD2	1:C:268:ILE:HD11	2.33	0.59
1:A:321:LEU:CD1	2:A:1061:HOH:O	2.49	0.59
1:C:352:PHE:HA	1:C:369:THR:CG2	2.33	0.59
1:B:330:THR:H	1:B:331:PRO:CD	2.14	0.59
1:A:269:GLU:HG3	1:A:270:LEU:O	2.03	0.59
1:A:115:MET:C	1:A:117:LEU:N	2.56	0.59
1:C:951:ASP:C	1:C:953:MET:N	2.48	0.59
1:C:14:VAL:HG13	1:C:15:ILE:H	1.66	0.59
1:A:435:MET:HA	1:A:438:ILE:CD1	2.32	0.59
1:B:754:TRP:CZ2	1:B:786:ILE:HG12	2.37	0.59
1:C:72:ILE:CG2	1:C:94:PHE:CE2	2.83	0.59
1:A:223:PRO:HD3	1:B:275:TYR:HB2	1.84	0.59
1:B:568:ASP:O	1:B:634:TRP:CH2	2.55	0.59
1:A:166:ILE:O	1:A:168:ARG:N	2.36	0.59
1:A:687:GLN:HB3	1:A:854:GLY:O	2.03	0.59
1:B:1024:VAL:HG12	1:B:1028:VAL:HG21	1.84	0.59
1:B:980:LEU:HD23	1:B:983:ILE:HD12	1.83	0.59
1:B:371:ALA:HA	1:B:374:VAL:HG12	1.84	0.59
1:C:185:ARG:HD3	1:C:272:GLY:O	2.01	0.59
1:A:576:VAL:HG11	1:A:591:LEU:HD23	1.84	0.59
1:B:563:PHE:HB2	1:B:866:GLU:HG2	1.85	0.59
1:A:644:VAL:C	1:A:646:ALA:H	2.06	0.59
1:B:99:ASP:C	1:B:99:ASP:OD2	2.39	0.59
1:B:1024:VAL:O	1:B:1025:PHE:HB2	2.03	0.59
1:A:534:ILE:HD12	1:A:540:ARG:HH22	1.68	0.59
1:C:414:GLU:OE2	1:C:977:MET:SD	2.61	0.59
1:A:886:LEU:HD21	1:C:17:ILE:CG2	2.31	0.59
1:A:282:ASN:ND2	1:A:609:VAL:H	2.00	0.59
1:C:94:PHE:O	1:C:95:GLU:O	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ILE:O	1:A:169:THR:HG23	2.03	0.59
1:B:196:PHE:O	1:B:197:GLN:HB2	2.03	0.59
1:A:49:TYR:HE2	1:A:121:GLU:HG2	1.68	0.59
1:B:6:ILE:HD12	1:B:491:ALA:N	2.17	0.59
1:B:652:THR:O	1:B:656:SER:HB3	2.02	0.59
1:A:467:TYR:HE1	1:A:925:VAL:CG2	2.15	0.59
1:B:860:THR:CG2	1:B:861:GLY:N	2.66	0.59
1:A:90:ILE:O	1:A:90:ILE:CG2	2.50	0.59
1:B:606:VAL:HA	1:B:631:LEU:HD23	1.84	0.59
1:A:857:TYR:CD1	1:A:857:TYR:O	2.55	0.59
1:A:30:LEU:HD21	1:A:384:ALA:HB2	1.85	0.59
1:C:60:THR:HG23	1:C:60:THR:O	2.00	0.59
1:C:547:ILE:O	1:C:550:VAL:HG12	2.03	0.59
1:C:972:LEU:N	1:C:974:PRO:HD2	2.17	0.59
1:C:459:PHE:O	1:C:460:GLY:O	2.19	0.59
1:C:925:VAL:O	1:C:927:PHE:N	2.35	0.59
1:B:231:ASN:C	1:B:231:ASN:HD22	2.06	0.59
1:A:709:HIS:H	1:A:710:PRO:HD3	1.68	0.59
1:A:193:LEU:HD12	1:A:265:VAL:CG1	2.32	0.59
1:B:876:LEU:CD1	1:B:932:LEU:HD11	2.27	0.58
1:A:961:ILE:O	1:A:965:LEU:HD23	2.02	0.58
1:B:986:VAL:HG12	1:B:990:VAL:HG23	1.85	0.58
1:C:545:TYR:HH	1:C:1021:PHE:CB	2.16	0.58
1:C:907:LEU:O	1:C:910:ILE:HG22	2.03	0.58
1:C:919:ARG:HB3	1:C:921:LEU:HD23	1.83	0.58
1:C:987:MET:HB3	1:C:988:PRO:CD	2.33	0.58
1:A:5:PHE:HD1	1:A:12:ALA:HB2	1.64	0.58
1:A:702:LEU:HD11	1:A:844:MET:CE	2.32	0.58
1:C:553:ALA:O	1:C:557:VAL:HG23	2.03	0.58
1:A:855:VAL:CG2	1:A:855:VAL:O	2.51	0.58
1:B:921:LEU:HD23	1:B:1005:THR:O	2.03	0.58
1:B:851:LEU:N	1:B:852:PRO:CD	2.65	0.58
1:A:185:ARG:O	1:A:186:ILE:HG13	2.02	0.58
1:A:277:ILE:O	1:A:277:ILE:CG2	2.43	0.58
1:C:162:MET:CG	1:C:313:MET:HE2	2.24	0.58
1:C:91:THR:CB	1:C:91:THR:C	2.68	0.58
1:C:15:ILE:O	1:C:16:ALA:C	2.41	0.58
1:B:48:SER:N	1:B:49:TYR:CE1	2.62	0.58
1:B:80:SER:HB2	1:B:90:ILE:HG23	1.84	0.58
1:A:375:VAL:O	1:A:379:THR:HG23	2.02	0.58
1:C:726:GLN:NE2	1:C:812:GLY:HA3	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:GLN:OE1	1:C:767:ARG:NH2	2.37	0.58
1:B:13:TRP:HA	1:B:13:TRP:CE3	2.37	0.58
1:A:190:PRO:HG3	1:A:789:TRP:CZ2	2.38	0.58
1:B:200:PRO:CD	1:B:749:THR:HG22	2.30	0.58
1:A:13:TRP:O	1:A:17:ILE:HG13	2.03	0.58
1:A:124:GLN:HG2	1:A:758:TYR:HE2	1.67	0.58
1:B:472:ILE:HG23	1:B:473:THR:H	1.68	0.58
1:A:685:ILE:HG22	1:A:687:GLN:N	2.18	0.58
1:C:327:TYR:CB	1:C:628:PHE:HB3	2.33	0.58
1:B:456:MET:HA	1:B:876:LEU:HD21	1.86	0.58
1:C:786:ILE:O	1:C:786:ILE:CG2	2.51	0.58
1:C:847:LEU:H	1:C:847:LEU:HD22	1.69	0.58
1:B:842:GLU:O	1:B:846:GLN:HG3	2.04	0.58
1:C:414:GLU:OE1	1:C:977:MET:HE1	2.03	0.58
1:B:646:ALA:C	1:B:648:THR:H	2.05	0.58
1:A:60:THR:HG22	1:A:119:PRO:CD	2.33	0.58
1:A:1:MET:N	1:A:2:PRO:CD	2.66	0.58
1:B:328:ASP:CB	2:B:1059:HOH:O	2.48	0.58
1:A:135:SER:O	1:A:136:PHE:CD2	2.56	0.58
1:A:69:MET:HA	1:A:69:MET:HE2	1.84	0.58
1:C:844:MET:HA	1:C:847:LEU:CD2	2.34	0.58
1:A:780:ARG:HG2	1:A:780:ARG:HH11	1.68	0.58
1:B:30:LEU:HD23	1:B:390:ILE:HG13	1.85	0.58
1:B:230:LEU:HD21	1:C:809:TRP:HH2	1.64	0.58
1:B:601:LYS:C	1:B:603:LYS:H	2.07	0.58
1:B:309:GLU:O	1:B:312:LYS:N	2.36	0.58
1:A:528:THR:O	1:A:532:GLY:N	2.35	0.58
1:B:602:GLU:C	1:B:604:ASN:H	2.06	0.58
1:A:588:GLN:HG2	1:A:613:ASN:ND2	2.19	0.58
1:C:762:PHE:H	1:C:771:VAL:CG2	2.17	0.58
1:C:102:ILE:HG22	1:C:103:ALA:N	2.13	0.58
1:C:928:GLN:OE1	1:C:928:GLN:N	2.37	0.58
1:B:420:MET:HE2	1:B:425:LEU:HA	1.86	0.58
1:B:219:LEU:CD1	1:B:234:ILE:HG12	2.33	0.58
1:A:463:THR:O	1:A:465:ALA:N	2.36	0.58
1:C:169:THR:O	1:C:170:SER:C	2.42	0.58
1:B:975:ILE:H	1:B:975:ILE:CD1	2.17	0.58
1:C:686:ASP:CG	1:C:690:LEU:HB2	2.23	0.58
1:C:497:LEU:CD1	1:C:498:LYS:H	2.17	0.58
1:B:850:LYS:C	1:B:852:PRO:HD3	2.24	0.58
1:B:419:VAL:O	1:B:426:PRO:HG3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:LEU:O	1:A:492:LEU:HB2	2.04	0.58
1:C:1028:VAL:HG12	1:C:1032:ARG:NH1	2.18	0.58
1:A:292:LYS:O	1:A:293:LEU:O	2.22	0.58
1:B:911:GLY:CA	1:B:1013:THR:HG21	2.30	0.57
1:B:403:GLY:O	1:B:404:LEU:HD23	2.04	0.57
1:B:531:VAL:CG1	1:B:965:LEU:HD21	2.34	0.57
1:C:489:THR:N	1:C:490:PRO:HD2	2.18	0.57
1:B:369:THR:O	1:B:373:PRO:HD3	2.04	0.57
1:C:185:ARG:HG3	1:C:271:GLY:CA	2.32	0.57
1:B:644:VAL:HG23	1:B:645:GLU:N	2.18	0.57
1:C:885:PHE:CD1	1:C:886:LEU:N	2.72	0.57
1:C:832:ALA:HB1	1:C:833:PRO:HD2	1.85	0.57
1:A:1021:PHE:O	1:A:1024:VAL:HB	2.04	0.57
1:C:220:GLY:CA	1:C:231:ASN:HD22	2.15	0.57
1:A:401:ALA:HB2	1:A:474:ILE:HG12	1.86	0.57
1:C:277:ILE:HD11	1:C:620:ARG:NH2	2.18	0.57
1:B:472:ILE:HG23	1:B:473:THR:N	2.20	0.57
1:B:24:GLY:HA2	1:B:27:ILE:HG23	1.85	0.57
1:C:719:ASN:N	1:C:719:ASN:OD1	2.37	0.57
1:A:164:ASP:OD1	1:A:164:ASP:N	2.35	0.57
1:C:314:GLU:O	1:C:317:PHE:CE2	2.57	0.57
1:B:485:ALA:HA	1:B:489:THR:HB	1.86	0.57
1:C:685:ILE:HD11	1:C:687:GLN:CA	2.33	0.57
1:C:399:VAL:HA	1:C:402:ILE:HD11	1.84	0.57
1:C:721:LEU:HD12	1:C:815:ARG:O	2.04	0.57
1:C:66:GLU:OE2	1:C:818:ARG:HD3	2.05	0.57
1:A:600:THR:O	1:A:601:LYS:HB2	2.05	0.57
1:B:115:MET:CE	1:B:127:VAL:HG21	2.32	0.57
1:A:139:VAL:O	1:A:139:VAL:HG22	2.04	0.57
1:A:843:LEU:HA	1:A:846:GLN:HE21	1.66	0.57
1:C:57:VAL:O	1:C:61:VAL:HB	2.03	0.57
1:B:531:VAL:HA	1:B:534:ILE:HG12	1.86	0.57
1:C:831:ALA:HB2	1:C:840:ALA:HB2	1.85	0.57
1:B:640:GLU:OE2	1:B:640:GLU:N	2.38	0.57
1:B:65:ILE:HD11	1:B:118:LEU:HD21	1.87	0.57
1:A:194:ASN:ND2	1:A:790:TYR:CD2	2.72	0.57
1:B:211:ASN:ND2	1:B:246:PHE:CZ	2.71	0.57
1:A:182:TYR:HB3	1:A:270:LEU:HD12	1.85	0.57
1:B:873:ALA:O	1:B:875:SER:N	2.36	0.57
1:B:873:ALA:C	1:B:875:SER:H	2.08	0.57
1:C:124:GLN:HB3	1:C:758:TYR:HE2	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:655:PHE:C	1:A:656:SER:O	2.41	0.57
1:B:49:TYR:CE2	1:B:122:VAL:HA	2.40	0.57
1:B:663:VAL:O	1:B:663:VAL:HG12	2.05	0.57
1:A:644:VAL:C	1:A:646:ALA:N	2.58	0.57
1:A:318:PRO:O	1:A:319:SER:C	2.42	0.57
1:A:822:LEU:CB	1:A:823:PRO:HD2	2.22	0.57
1:C:105:VAL:HG12	1:C:106:GLN:N	2.18	0.57
1:B:940:LYS:HZ1	1:B:978:THR:HG23	1.69	0.57
1:A:911:GLY:N	1:A:914:LEU:HD13	2.19	0.57
1:C:548:ILE:HD12	1:C:549:VAL:H	1.67	0.57
1:C:214:VAL:HG12	1:C:215:ALA:H	1.67	0.57
1:B:622:GLN:O	1:B:622:GLN:CG	2.53	0.57
1:A:345:VAL:O	1:A:349:ILE:HD13	2.05	0.57
1:C:50:PRO:HD3	1:C:125:GLN:HG3	1.86	0.57
1:C:92:LEU:HD12	1:C:92:LEU:N	2.19	0.57
1:B:1013:THR:HG23	1:B:1013:THR:O	2.05	0.57
1:B:910:ILE:O	1:B:914:LEU:HG	2.05	0.57
1:A:983:ILE:HD12	1:A:983:ILE:C	2.24	0.57
1:B:847:LEU:H	1:B:847:LEU:HD23	1.69	0.57
1:A:228:GLN:HG2	1:B:781:MET:SD	2.45	0.57
1:A:188:MET:HA	1:A:266:ALA:HB2	1.86	0.57
1:B:1015:THR:O	1:B:1018:ALA:HB3	2.05	0.57
1:B:945:ILE:HD11	1:B:1026:PHE:CE2	2.39	0.57
1:B:431:THR:CG2	1:B:493:CYS:CB	2.74	0.57
1:C:699:ARG:CD	1:C:703:LEU:HD11	2.32	0.57
1:A:907:LEU:O	1:A:910:ILE:HG13	2.05	0.57
1:C:549:VAL:C	1:C:551:GLY:N	2.56	0.57
1:A:927:PHE:CE2	1:A:931:LEU:HD22	2.39	0.57
1:B:966:ASP:O	1:B:970:MET:HB2	2.04	0.57
1:A:583:THR:O	1:A:584:GLN:C	2.43	0.57
1:C:644:VAL:HG11	1:C:667:ASN:HB2	1.87	0.57
1:A:45:ILE:HB	1:A:90:ILE:HB	1.86	0.57
1:B:439:GLN:HA	1:B:442:LEU:CD1	2.34	0.57
1:B:57:VAL:HG23	1:B:58:GLN:H	1.68	0.57
1:C:699:ARG:CG	1:C:699:ARG:NH1	2.42	0.56
1:C:189:ASN:HD22	1:C:189:ASN:C	2.08	0.56
1:A:649:MET:O	1:A:653:ARG:NE	2.37	0.56
1:A:325:TYR:CD1	1:A:325:TYR:N	2.70	0.56
1:C:229:GLN:O	1:C:230:LEU:HB3	2.05	0.56
1:A:170:SER:OG	1:A:170:SER:O	2.23	0.56
1:B:845:GLU:HG2	1:B:857:TYR:OH	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:GLN:HG3	1:B:249:ILE:HG23	1.86	0.56
1:B:193:LEU:HD22	1:B:198:LEU:O	2.05	0.56
1:C:897:ILE:N	1:C:898:PRO:HD2	2.20	0.56
1:A:282:ASN:ND2	1:A:599:LEU:HD11	2.20	0.56
1:B:785:ASP:O	1:B:787:GLY:N	2.38	0.56
1:B:651:ALA:O	1:B:655:PHE:CE2	2.58	0.56
1:A:926:TYR:CE1	1:A:999:ALA:HB2	2.39	0.56
1:C:123:GLN:O	1:C:125:GLN:N	2.37	0.56
1:C:311:ALA:O	1:C:313:MET:N	2.39	0.56
1:C:58:GLN:OE1	1:C:82:SER:CB	2.54	0.56
1:B:941:ASN:HD22	1:B:1015:THR:HA	1.70	0.56
1:B:221:GLY:HA3	1:C:780:ARG:HH11	1.71	0.56
1:A:400:LEU:HG	1:A:929:VAL:HG12	1.87	0.56
1:C:418:ARG:C	1:C:420:MET:N	2.50	0.56
1:C:527:TYR:OH	1:C:1019:ILE:HG13	2.05	0.56
1:A:162:MET:CE	1:A:310:LEU:HD22	2.36	0.56
1:C:988:PRO:O	1:C:989:LEU:C	2.43	0.56
1:A:516:PHE:CD1	1:A:517:ASN:N	2.73	0.56
1:B:585:GLU:O	1:B:586:ARG:C	2.42	0.56
1:B:913:LEU:O	1:B:917:THR:OG1	2.19	0.56
1:A:11:PHE:O	1:A:14:VAL:N	2.38	0.56
1:A:191:ASN:C	1:A:193:LEU:H	2.07	0.56
1:A:191:ASN:O	1:A:193:LEU:N	2.39	0.56
1:A:252:LYS:HB3	1:A:260:VAL:HG21	1.87	0.56
1:C:274:ASN:ND2	2:C:1057:HOH:O	2.26	0.56
1:C:379:THR:CG2	1:C:477:ALA:HB2	2.36	0.56
1:C:912:ALA:C	1:C:914:LEU:N	2.59	0.56
1:B:639:GLY:HA2	1:B:643:LYS:NZ	2.20	0.56
1:A:394:THR:HG23	1:A:395:MET:HE2	1.88	0.56
1:A:726:GLN:N	1:A:810:GLU:O	2.38	0.56
1:A:298:ASN:HB3	1:A:301:ASP:OD1	2.05	0.56
1:C:601:LYS:O	1:C:603:LYS:N	2.37	0.56
1:C:953:MET:HE1	1:C:1030:ARG:NH2	2.21	0.56
1:A:911:GLY:HA2	1:A:914:LEU:HD13	1.86	0.56
1:A:400:LEU:HD11	1:A:1003:VAL:HG13	1.80	0.56
1:C:391:ASN:O	1:C:392:THR:C	2.44	0.56
1:B:571:VAL:O	1:B:572:PHE:HB3	2.05	0.56
1:A:428:LYS:HG3	1:A:429:GLU:N	2.20	0.56
1:A:456:MET:O	1:A:457:ALA:HB3	2.05	0.56
1:A:223:PRO:HD3	1:B:275:TYR:CG	2.39	0.56
1:A:60:THR:CG2	1:A:119:PRO:HG3	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:764:ASP:OD2	1:C:765:ARG:CD	2.53	0.56
1:C:306:ILE:O	1:C:309:GLU:N	2.38	0.56
1:C:56:THR:O	1:C:60:THR:HB	2.06	0.56
1:C:91:THR:CA	1:C:91:THR:CG2	2.76	0.56
1:C:697:GLN:O	1:C:698:ALA:C	2.41	0.56
1:A:530:SER:O	1:A:534:ILE:HG12	2.06	0.56
1:A:263:ARG:HB3	1:A:263:ARG:NH2	2.20	0.56
1:C:5:PHE:CE2	1:C:11:PHE:HD2	2.22	0.56
1:C:5:PHE:CD2	1:C:12:ALA:HB2	2.41	0.56
1:C:868:LEU:O	1:C:869:SER:HB3	2.06	0.56
1:B:47:ALA:HB3	1:B:88:VAL:CB	2.31	0.56
1:A:717:ARG:NH1	1:A:830:GLN:HE22	2.02	0.56
1:C:764:ASP:CG	1:C:765:ARG:HD2	2.24	0.56
1:A:268:ILE:N	1:A:268:ILE:HD12	2.20	0.56
1:A:102:ILE:O	1:A:102:ILE:HG23	2.01	0.56
1:C:62:THR:HG21	1:C:80:SER:HB3	1.88	0.56
1:A:897:ILE:O	1:A:900:SER:OG	2.20	0.56
1:C:427:PRO:O	1:C:431:THR:HG22	2.06	0.56
1:B:48:SER:HA	1:B:87:THR:HA	1.86	0.56
1:A:199:THR:HB	1:A:200:PRO:CD	2.35	0.56
1:B:370:ILE:O	1:B:370:ILE:HG22	2.05	0.56
1:A:169:THR:O	1:A:172:VAL:HG22	2.06	0.56
1:C:409:ALA:O	1:C:413:VAL:HG12	2.04	0.56
1:A:690:LEU:HD11	1:A:854:GLY:C	2.26	0.56
1:A:687:GLN:HE22	1:A:856:GLY:HA3	1.70	0.56
1:B:104:GLN:CG	1:B:105:VAL:H	2.18	0.56
1:B:1026:PHE:HB3	1:B:1030:ARG:NH2	2.21	0.56
1:B:942:ALA:HA	1:B:1022:VAL:HG11	1.88	0.56
1:B:441:ALA:CB	1:B:947:GLU:HG2	2.13	0.56
1:A:911:GLY:HA3	1:A:1013:THR:CG2	2.32	0.56
1:A:901:VAL:HG13	1:A:942:ALA:HB3	1.87	0.56
1:B:701:GLN:HA	1:B:704:ALA:HB3	1.88	0.56
1:A:594:VAL:HA	1:A:655:PHE:CE2	2.41	0.56
1:B:110:LYS:O	1:B:111:LEU:C	2.40	0.56
1:B:591:LEU:HD12	1:B:611:ALA:HB1	1.87	0.56
1:B:681:ASP:O	1:B:859:TRP:HE3	1.88	0.56
1:B:25:LEU:C	1:B:27:ILE:H	2.09	0.56
1:C:102:ILE:HG22	1:C:106:GLN:HG3	1.88	0.56
1:B:186:ILE:HD13	1:B:262:LEU:HD13	1.88	0.56
1:B:1024:VAL:HG12	1:B:1025:PHE:N	2.21	0.56
1:B:905:VAL:N	1:B:906:PRO:HD2	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:GLN:O	1:A:256:ASP:CG	2.43	0.56
1:A:731:ILE:CD1	1:A:731:ILE:N	2.69	0.56
1:C:169:THR:CG2	1:C:169:THR:CA	2.79	0.56
1:C:894:SER:O	1:C:896:SER:N	2.39	0.56
1:C:950:LYS:H	1:C:953:MET:CE	2.13	0.56
1:C:3:ASN:HD21	1:C:432:ARG:CD	2.15	0.56
1:B:987:MET:CE	1:B:987:MET:CA	2.82	0.56
1:A:418:ARG:HH12	1:A:973:ARG:CB	2.18	0.56
1:B:278:ILE:HD11	1:B:584:GLN:NE2	2.20	0.56
1:A:188:MET:HA	1:A:266:ALA:CB	2.36	0.56
1:B:71:GLY:O	1:B:72:ILE:O	2.24	0.56
1:A:99:ASP:OD1	1:A:101:ASP:HB2	2.06	0.55
1:A:818:ARG:CG	2:A:1062:HOH:O	2.54	0.55
1:B:899:PHE:O	1:B:903:LEU:HG	2.06	0.55
1:C:847:LEU:CA	1:C:850:LYS:HD3	2.20	0.55
1:A:945:ILE:CG1	1:A:971:ARG:HG2	2.22	0.55
1:C:615:PHE:C	1:C:615:PHE:CD2	2.79	0.55
1:B:216:ALA:HB2	1:B:236:ALA:HB2	1.88	0.55
1:B:535:LEU:O	1:B:536:ARG:C	2.45	0.55
1:B:632:LYS:O	1:B:637:ARG:HD2	2.05	0.55
1:B:557:VAL:O	1:B:557:VAL:HG12	2.06	0.55
1:A:686:ASP:C	1:A:688:ALA:H	2.08	0.55
1:B:1027:VAL:O	1:B:1030:ARG:O	2.24	0.55
1:C:415:ASN:HA	1:C:418:ARG:NH1	2.21	0.55
1:C:525:HIS:O	1:C:529:ASP:N	2.38	0.55
1:B:699:ARG:O	1:B:701:GLN:N	2.38	0.55
1:A:699:ARG:NH1	1:A:722:GLU:OE1	2.36	0.55
1:A:298:ASN:ND2	1:A:300:LEU:N	2.49	0.55
1:B:419:VAL:HG12	1:B:419:VAL:O	2.06	0.55
1:B:146:ASP:O	1:B:148:THR:N	2.39	0.55
1:B:737:GLN:HG2	1:B:737:GLN:O	2.06	0.55
1:C:169:THR:N	1:C:169:THR:CB	2.62	0.55
1:A:961:ILE:O	1:A:965:LEU:CD2	2.54	0.55
1:C:192:GLU:O	1:C:194:ASN:N	2.39	0.55
1:C:910:ILE:HG23	1:C:911:GLY:N	2.22	0.55
1:C:457:ALA:HB1	1:C:468:ARG:CA	2.35	0.55
1:B:325:TYR:O	1:B:326:PRO:O	2.25	0.55
1:A:169:THR:O	1:A:170:SER:C	2.43	0.55
1:B:71:GLY:O	1:B:72:ILE:C	2.44	0.55
1:B:544:LEU:HD22	1:B:1021:PHE:HZ	1.72	0.55
1:B:485:ALA:HA	1:B:489:THR:CB	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:975:ILE:O	1:B:979:SER:HB2	2.07	0.55
1:A:367:ILE:HG13	1:A:368:PRO:CD	2.37	0.55
1:A:200:PRO:CD	1:A:749:THR:HG23	2.37	0.55
1:B:743:ILE:HA	1:B:746:ILE:HD12	1.88	0.55
1:B:941:ASN:ND2	1:B:1015:THR:HA	2.21	0.55
1:B:2:PRO:C	1:B:4:PHE:H	2.08	0.55
1:A:400:LEU:HG	1:A:929:VAL:CG1	2.36	0.55
1:B:713:LEU:HD13	1:B:843:LEU:HD13	1.88	0.55
1:A:325:TYR:HD1	1:A:325:TYR:N	2.04	0.55
1:A:29:LYS:HG2	1:A:29:LYS:O	2.07	0.55
1:B:356:TYR:O	1:B:358:PHE:N	2.39	0.55
1:B:545:TYR:O	1:B:547:ILE:N	2.40	0.55
1:C:824:SER:O	1:C:825:MET:HG2	2.06	0.55
1:A:548:ILE:HG23	1:A:910:ILE:HG12	1.87	0.55
1:A:901:VAL:HG13	1:A:942:ALA:CB	2.37	0.55
1:C:190:PRO:O	1:C:192:GLU:N	2.39	0.55
1:B:986:VAL:O	1:B:988:PRO:O	2.24	0.55
1:C:742:SER:O	1:C:746:ILE:HG13	2.07	0.55
1:B:807:SER:C	1:B:808:ARG:HG3	2.27	0.55
1:B:785:ASP:O	1:B:786:ILE:C	2.44	0.55
1:A:47:ALA:HB2	1:A:127:VAL:HG22	1.88	0.55
1:B:335:ILE:HG22	1:B:336:SER:N	2.20	0.55
1:C:598:TYR:HB3	1:C:606:VAL:HG11	1.88	0.55
1:C:819:TYR:O	1:C:820:ASN:HB2	2.05	0.55
1:B:165:ALA:O	1:B:166:ILE:C	2.45	0.55
1:C:767:ARG:O	1:C:769:LYS:HG2	2.07	0.55
1:B:493:CYS:O	1:B:494:ALA:CB	2.46	0.55
1:B:898:PRO:O	1:B:900:SER:N	2.40	0.55
1:A:1009:GLY:C	1:A:1011:MET:H	2.07	0.55
1:A:513:PHE:HD1	1:A:517:ASN:HD21	1.55	0.55
1:B:674:LEU:HD22	1:B:681:ASP:OD2	2.06	0.55
1:A:717:ARG:NH2	1:A:828:LEU:HG	2.22	0.55
1:A:68:ASN:N	1:A:69:MET:N	2.54	0.55
1:C:570:GLY:O	1:C:571:VAL:HG13	2.07	0.55
1:C:1030:ARG:HA	1:C:1033:PHE:HD2	1.72	0.55
1:B:947:GLU:O	1:B:951:ASP:HB2	2.06	0.55
1:C:383:LEU:HD11	1:C:394:THR:OG1	2.07	0.55
1:B:707:ALA:O	1:B:708:LYS:CB	2.51	0.55
1:C:533:GLY:O	1:C:536:ARG:HB2	2.07	0.55
1:A:815:ARG:HD2	2:A:1068:HOH:O	2.06	0.55
1:C:156:ASP:O	1:C:159:ALA:HB3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:960:LEU:C	1:B:960:LEU:CD1	2.76	0.55
1:C:549:VAL:O	1:C:551:GLY:N	2.40	0.55
1:C:946:VAL:O	1:C:946:VAL:CG1	2.54	0.55
1:B:639:GLY:HA2	1:B:643:LYS:HZ3	1.70	0.55
1:A:916:ALA:O	1:A:919:ARG:O	2.25	0.55
1:C:456:MET:O	1:C:457:ALA:HB3	2.07	0.55
1:A:988:PRO:O	1:A:990:VAL:O	2.25	0.55
1:A:225:VAL:CG1	1:A:226:LYS:N	2.69	0.55
1:A:11:PHE:O	1:A:14:VAL:HG23	2.06	0.55
1:C:136:PHE:CE2	1:C:292:LYS:HE2	2.41	0.55
1:C:328:ASP:OD1	1:C:330:THR:HB	2.06	0.55
1:A:54:ALA:HB2	1:A:82:SER:O	2.07	0.55
1:C:87:THR:HG22	1:C:88:VAL:N	2.18	0.55
1:A:354:VAL:O	1:A:355:MET:HB3	2.08	0.55
1:C:778:LYS:C	1:C:779:TYR:CD2	2.80	0.55
1:C:778:LYS:HD2	1:C:779:TYR:CE2	2.38	0.55
1:A:10:ILE:HG21	1:B:893:GLU:HB2	1.88	0.55
1:C:210:GLN:OE1	1:C:249:ILE:HG23	2.06	0.55
1:B:570:GLY:N	1:B:634:TRP:CH2	2.75	0.55
1:A:14:VAL:HG11	1:B:886:LEU:O	2.06	0.55
1:B:59:ASP:HA	1:B:63:GLN:HB2	1.89	0.55
1:A:62:THR:O	1:A:63:GLN:O	2.24	0.54
1:A:689:GLY:O	1:A:690:LEU:O	2.25	0.54
1:B:534:ILE:HA	1:B:541:TYR:CE1	2.42	0.54
1:C:707:ALA:O	1:C:710:PRO:HD3	2.06	0.54
1:B:1001:ASN:O	1:B:1005:THR:HB	2.06	0.54
1:B:344:LEU:O	1:B:345:VAL:C	2.45	0.54
1:B:641:GLU:HA	1:B:650:ARG:HH12	1.72	0.54
1:B:362:PHE:O	1:B:364:ALA:N	2.40	0.54
1:B:228:GLN:HA	1:B:228:GLN:NE2	2.23	0.54
1:A:987:MET:N	1:A:988:PRO:CD	2.69	0.54
1:C:251:LEU:HB2	1:C:260:VAL:O	2.08	0.54
1:B:952:LEU:HD12	1:B:956:GLU:OE2	2.07	0.54
1:B:2:PRO:HG3	1:B:435:MET:HG2	1.87	0.54
1:C:190:PRO:HD2	1:C:779:TYR:CD1	2.42	0.54
1:B:897:ILE:HG13	1:B:898:PRO:HD3	1.89	0.54
1:C:847:LEU:O	1:C:851:LEU:HD11	2.07	0.54
1:A:310:LEU:HD12	1:A:325:TYR:OH	2.07	0.54
1:A:186:ILE:CB	1:A:773:VAL:HG23	2.34	0.54
1:B:372:VAL:HG22	1:B:373:PRO:CD	2.38	0.54
1:C:645:GLU:O	1:C:648:THR:HG22	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:860:THR:HG23	1:C:860:THR:O	2.07	0.54
1:A:740:GLY:O	1:A:793:ALA:HB1	2.08	0.54
1:B:7:ASP:O	1:B:8:ARG:CB	2.54	0.54
1:B:540:ARG:O	1:B:541:TYR:CD1	2.60	0.54
1:B:891:LEU:HD12	1:B:892:TYR:CE1	2.42	0.54
1:C:398:MET:O	1:C:402:ILE:HG13	2.07	0.54
1:C:475:VAL:CG1	1:C:476:SER:N	2.70	0.54
1:B:245:GLU:O	1:B:246:PHE:C	2.44	0.54
1:C:913:LEU:HD23	1:C:927:PHE:HZ	1.72	0.54
1:A:329:THR:O	1:A:329:THR:HG23	2.06	0.54
1:C:317:PHE:N	1:C:317:PHE:CD2	2.71	0.54
1:B:448:VAL:O	1:B:452:VAL:CG2	2.53	0.54
1:B:945:ILE:HD11	1:B:1026:PHE:CZ	2.42	0.54
1:B:399:VAL:HG11	1:B:989:LEU:HG	1.89	0.54
1:C:903:LEU:O	1:C:906:PRO:HD2	2.08	0.54
1:A:780:ARG:HG2	1:A:780:ARG:NH1	2.23	0.54
1:B:418:ARG:HE	1:B:970:MET:CE	2.21	0.54
1:B:131:LYS:O	1:B:132:SER:HB3	2.06	0.54
1:C:268:ILE:HG22	1:C:268:ILE:O	2.06	0.54
1:B:156:ASP:OD2	1:B:182:TYR:HB2	2.07	0.54
1:A:818:ARG:NE	1:A:818:ARG:HB2	2.19	0.54
1:A:104:GLN:NE2	1:B:109:ASN:HB3	2.22	0.54
1:B:940:LYS:O	1:B:943:ILE:N	2.41	0.54
1:B:979:SER:CB	1:B:1011:MET:HE3	2.38	0.54
1:C:851:LEU:HD12	1:C:851:LEU:H	1.73	0.54
1:C:477:ALA:H	1:C:480:LEU:HD23	1.72	0.54
1:B:706:ALA:HA	1:B:713:LEU:HD22	1.90	0.54
1:B:49:TYR:CE2	1:B:122:VAL:O	2.61	0.54
1:C:633:ASP:CG	1:C:633:ASP:O	2.45	0.54
1:C:144:ASN:HD21	1:C:149:MET:N	2.05	0.54
1:C:144:ASN:OD1	1:C:320:GLY:O	2.25	0.54
1:A:231:ASN:OD1	1:B:622:GLN:OE1	2.26	0.54
1:B:136:PHE:CE1	1:B:617:PHE:CZ	2.90	0.54
1:C:951:ASP:O	1:C:953:MET:N	2.38	0.54
1:B:1010:GLY:HA2	1:B:1013:THR:CG2	2.38	0.54
1:B:483:LEU:O	1:B:485:ALA:O	2.26	0.54
1:B:971:ARG:O	1:B:975:ILE:HD13	2.08	0.54
1:B:42:ALA:CB	1:B:93:THR:CG2	2.82	0.54
1:B:640:GLU:O	1:B:643:LYS:HB2	2.07	0.54
1:C:801:PHE:HA	1:C:804:PHE:CE1	2.42	0.54
1:C:731:ILE:HD13	1:C:805:SER:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:GLU:OE1	1:C:110:LYS:HE2	2.08	0.54
1:B:431:THR:OG1	1:B:494:ALA:HB2	2.07	0.54
1:C:713:LEU:HD21	1:C:835:LYS:N	2.19	0.54
1:A:203:VAL:HG13	1:A:262:LEU:CD1	2.37	0.54
1:C:461:GLY:HA3	1:C:869:SER:OG	2.07	0.54
1:B:750:LEU:HB2	1:B:801:PHE:CE1	2.42	0.54
1:A:843:LEU:O	1:A:846:GLN:N	2.40	0.54
1:A:736:ALA:HA	1:A:741:VAL:CG1	2.38	0.54
1:A:99:ASP:HB3	1:A:102:ILE:HG22	1.90	0.54
1:A:58:GLN:HG3	1:A:63:GLN:NE2	2.22	0.54
1:B:367:ILE:HG12	1:B:492:LEU:HD13	1.89	0.54
1:B:941:ASN:OD1	1:B:979:SER:OG	2.26	0.54
1:C:778:LYS:HG3	1:C:779:TYR:CE2	2.43	0.54
1:B:70:ASN:H	1:B:70:ASN:HD22	1.55	0.54
1:C:188:MET:CE	1:C:200:PRO:CB	2.82	0.54
1:A:172:VAL:HG23	1:A:172:VAL:O	2.08	0.54
1:C:578:LEU:HD21	1:C:590:VAL:HG21	1.90	0.54
1:C:861:GLY:H	1:C:864:TYR:HB2	1.73	0.54
1:C:241:THR:OG1	1:C:241:THR:O	2.25	0.54
1:C:137:LEU:HG	1:C:293:LEU:HB2	1.90	0.54
1:C:87:THR:HG23	1:C:88:VAL:N	2.22	0.54
1:A:1021:PHE:HB3	1:A:1025:PHE:CE1	2.43	0.54
1:B:885:PHE:CE2	1:B:898:PRO:HB2	2.42	0.54
1:B:372:VAL:HG22	1:B:373:PRO:HD3	1.90	0.54
1:B:740:GLY:HA3	1:B:794:ALA:HB2	1.90	0.54
1:A:65:ILE:O	1:A:68:ASN:OD1	2.26	0.54
1:C:115:MET:SD	1:C:127:VAL:HG11	2.48	0.54
1:A:966:ASP:O	1:A:969:ARG:HB2	2.08	0.54
1:C:682:PHE:HE2	1:C:702:LEU:HD11	1.73	0.54
1:C:924:ASP:O	1:C:925:VAL:O	2.25	0.54
1:C:966:ASP:HA	1:C:969:ARG:HB2	1.90	0.54
1:A:210:GLN:HG3	1:A:249:ILE:CG2	2.34	0.54
1:A:38:ILE:O	1:A:462:SER:HA	2.08	0.54
1:B:143:ILE:CD1	1:B:322:LYS:HB3	2.37	0.54
1:C:666:PHE:O	1:C:666:PHE:CD2	2.61	0.54
1:A:687:GLN:HA	2:A:1055:HOH:O	2.08	0.53
1:B:233:SER:OG	1:C:53:ASP:OD1	2.25	0.53
1:B:416:VAL:HG11	1:B:431:THR:CG2	2.36	0.53
1:B:537:SER:CA	1:B:540:ARG:HE	2.21	0.53
1:C:705:GLU:O	1:C:706:ALA:C	2.47	0.53
1:A:939:ALA:O	1:A:943:ILE:HG13	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:713:LEU:HB2	1:A:833:PRO:HD2	1.89	0.53
1:C:484:VAL:HG12	1:C:489:THR:HG23	1.90	0.53
1:B:119:PRO:HG2	1:B:122:VAL:HG23	1.90	0.53
1:B:832:ALA:N	1:B:833:PRO:HD2	2.22	0.53
1:B:925:VAL:HA	1:B:928:GLN:OE1	2.08	0.53
1:A:472:ILE:H	1:A:472:ILE:CD1	2.19	0.53
1:B:178:PHE:HA	1:B:277:ILE:HG21	1.88	0.53
1:A:138:MET:HE3	1:A:306:ILE:HB	1.89	0.53
1:A:43:VAL:HG11	1:A:107:VAL:HG21	1.91	0.53
1:A:58:GLN:NE2	1:A:816:LEU:HD13	2.23	0.53
1:A:68:ASN:CB	1:A:68:ASN:C	2.72	0.53
1:C:947:GLU:O	1:C:949:ALA:O	2.26	0.53
1:C:476:SER:O	1:C:477:ALA:HB3	2.08	0.53
1:A:575:MET:O	1:A:663:VAL:HA	2.08	0.53
1:C:186:ILE:O	1:C:188:MET:N	2.41	0.53
1:B:184:MET:HB2	1:B:762:PHE:CE2	2.44	0.53
1:C:410:ILE:O	1:C:412:VAL:N	2.40	0.53
1:C:714:THR:HG22	1:C:715:SER:N	2.22	0.53
1:B:146:ASP:O	1:B:147:GLY:C	2.44	0.53
1:A:764:ASP:HB3	1:A:769:LYS:HD2	1.90	0.53
1:A:116:PRO:HB3	1:C:123:GLN:HG3	1.91	0.53
1:B:525:HIS:CA	1:B:528:THR:HG22	2.38	0.53
1:A:344:LEU:HD22	1:A:376:LEU:HD11	1.89	0.53
1:C:753:ALA:HB1	1:C:789:TRP:CZ2	2.43	0.53
1:C:776:GLU:O	1:C:777:ALA:C	2.46	0.53
1:C:778:LYS:CD	1:C:779:TYR:HE2	2.19	0.53
1:C:35:TYR:CG	1:C:671:ILE:HG12	2.43	0.53
1:C:673:GLU:O	1:C:674:LEU:HB3	2.07	0.53
1:A:568:ASP:O	1:A:634:TRP:HH2	1.91	0.53
1:C:246:PHE:HZ	1:C:762:PHE:HB2	1.72	0.53
1:A:342:LYS:O	1:A:343:THR:C	2.46	0.53
1:A:694:LYS:O	1:A:698:ALA:HB2	2.08	0.53
1:A:638:PRO:HG2	1:A:639:GLY:H	1.73	0.53
1:C:616:GLY:HA3	1:C:619:GLY:O	2.08	0.53
1:A:818:ARG:HD3	1:A:822:LEU:N	2.23	0.53
1:C:103:ALA:O	1:C:105:VAL:N	2.41	0.53
1:C:949:ALA:C	1:C:951:ASP:H	2.11	0.53
1:B:989:LEU:HA	1:B:992:SER:HB2	1.90	0.53
1:C:915:ALA:O	1:C:919:ARG:N	2.40	0.53
1:A:752:ALA:O	1:A:774:MET:HG3	2.08	0.53
1:C:204:ILE:HG12	1:C:759:VAL:HG13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:562:SER:HB3	1:B:922:THR:HG21	1.90	0.53
1:A:2:PRO:O	1:A:6:ILE:HG23	2.09	0.53
1:B:261:LEU:HD13	1:B:261:LEU:N	2.23	0.53
1:C:80:SER:O	1:C:81:ASN:HB3	2.08	0.53
1:A:402:ILE:O	1:A:405:LEU:HD13	2.08	0.53
1:B:395:MET:O	1:B:396:PHE:C	2.44	0.53
1:C:901:VAL:HG12	1:C:942:ALA:HB1	1.90	0.53
1:A:575:MET:SD	1:A:626:ILE:HG13	2.49	0.53
1:C:743:ILE:CD1	1:C:743:ILE:H	2.04	0.53
1:A:399:VAL:C	1:A:401:ALA:H	2.12	0.53
1:B:613:ASN:ND2	1:B:613:ASN:C	2.62	0.53
1:C:965:LEU:O	1:C:969:ARG:HB2	2.09	0.53
1:B:291:ILE:CG2	1:B:306:ILE:HD11	2.38	0.53
1:B:25:LEU:O	1:B:27:ILE:N	2.41	0.53
1:B:443:VAL:O	1:B:444:GLY:C	2.44	0.53
1:C:175:VAL:O	1:C:175:VAL:HG12	2.08	0.53
1:C:157:TYR:CE1	1:C:318:PRO:HD3	2.43	0.53
1:B:937:LEU:O	1:B:940:LYS:HB3	2.08	0.53
1:A:897:ILE:HG21	1:A:950:LYS:HE2	1.89	0.53
1:B:668:LEU:HD23	1:B:668:LEU:N	2.24	0.53
1:B:962:GLU:O	1:B:966:ASP:CB	2.48	0.53
1:B:58:GLN:HA	1:B:62:THR:HB	1.90	0.53
1:A:393:LEU:HD11	1:A:466:ILE:HG12	1.91	0.53
1:B:525:HIS:O	1:B:529:ASP:OD2	2.27	0.53
1:B:6:ILE:N	1:B:6:ILE:HD13	2.24	0.53
1:B:944:LEU:CB	1:B:975:ILE:HD11	2.39	0.53
1:A:1021:PHE:HB3	1:A:1025:PHE:CZ	2.44	0.53
1:A:901:VAL:HG11	1:A:943:ILE:CG1	2.38	0.53
1:A:443:VAL:CG1	1:A:444:GLY:N	2.65	0.53
1:C:914:LEU:O	1:C:915:ALA:HB3	2.09	0.53
1:C:17:ILE:CD1	1:C:17:ILE:N	2.71	0.53
1:A:780:ARG:NH2	1:C:223:PRO:HG2	2.24	0.53
1:C:674:LEU:HD11	1:C:862:MET:CA	2.31	0.53
1:A:472:ILE:CD1	1:A:472:ILE:N	2.72	0.53
1:A:911:GLY:H	1:A:914:LEU:CD1	2.20	0.53
1:A:884:VAL:HG12	1:A:902:MET:HE3	1.91	0.53
1:B:987:MET:N	1:B:988:PRO:CD	2.70	0.53
1:C:389:SER:HG	1:C:391:ASN:HD22	1.52	0.53
1:C:4:PHE:O	1:C:8:ARG:HG2	2.09	0.53
1:A:141:GLY:N	1:A:324:VAL:O	2.38	0.53
1:A:774:MET:O	1:A:775:SER:O	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:492:LEU:HA	1:C:495:THR:HB	1.91	0.53
1:A:444:GLY:O	1:A:448:VAL:HG23	2.09	0.53
1:C:564:LEU:CD2	1:C:671:ILE:HD12	2.39	0.53
1:A:143:ILE:HG21	1:A:281:PHE:CD2	2.44	0.53
1:C:868:LEU:O	1:C:869:SER:CB	2.57	0.53
1:B:586:ARG:HH22	1:B:660:ASP:HB2	1.74	0.53
1:C:155:SER:HB3	1:C:180:SER:H	1.74	0.53
1:A:64:VAL:O	1:A:68:ASN:OD1	2.27	0.52
1:B:401:ALA:O	1:B:404:LEU:N	2.41	0.52
1:C:699:ARG:HH11	1:C:699:ARG:HG3	1.67	0.52
1:A:649:MET:HE2	1:A:653:ARG:NH2	2.24	0.52
1:A:600:THR:O	1:A:600:THR:HG22	2.10	0.52
1:C:578:LEU:HB3	1:C:579:PRO:CD	2.35	0.52
1:B:541:TYR:C	1:B:543:VAL:H	2.12	0.52
1:C:404:LEU:CD2	1:C:937:LEU:HD13	2.40	0.52
1:C:997:SER:O	1:C:1000:GLN:N	2.42	0.52
1:B:613:ASN:HD22	1:B:614:GLY:CA	2.22	0.52
1:C:443:VAL:O	1:C:447:MET:HB2	2.09	0.52
1:A:739:LEU:HD22	1:A:739:LEU:H	1.74	0.52
1:A:61:VAL:HG22	1:A:118:LEU:HD22	1.90	0.52
1:C:177:LEU:HD13	1:C:179:GLY:O	2.09	0.52
1:A:1007:VAL:O	1:A:1011:MET:HB2	2.08	0.52
1:A:986:VAL:O	1:A:991:ILE:HD12	2.09	0.52
1:C:410:ILE:CG2	1:C:411:VAL:N	2.69	0.52
1:C:520:PHE:O	1:C:523:SER:OG	2.27	0.52
1:C:552:MET:O	1:C:553:ALA:CB	2.56	0.52
1:C:841:MET:O	1:C:845:GLU:HG3	2.10	0.52
1:B:961:ILE:O	1:B:965:LEU:HB2	2.09	0.52
1:A:902:MET:O	1:A:904:VAL:N	2.43	0.52
1:C:6:ILE:HA	1:C:491:ALA:HB2	1.90	0.52
1:B:777:ALA:O	1:B:780:ARG:HB2	2.09	0.52
1:A:189:ASN:HD21	1:A:192:GLU:HB2	1.72	0.52
1:B:952:LEU:O	1:B:963:ALA:HB2	2.09	0.52
1:A:999:ALA:O	1:A:1002:ALA:HB3	2.10	0.52
1:A:107:VAL:O	1:A:110:LYS:CB	2.58	0.52
1:C:110:LYS:CA	1:C:113:LEU:HD12	2.20	0.52
1:C:161:ASN:N	1:C:161:ASN:CB	2.59	0.52
1:A:406:VAL:O	1:A:407:ASP:C	2.45	0.52
1:A:572:PHE:CD1	1:A:572:PHE:N	2.78	0.52
1:C:459:PHE:HD2	1:C:459:PHE:N	1.89	0.52
1:A:399:VAL:O	1:A:401:ALA:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:MET:HB2	1:B:313:MET:SD	2.50	0.52
1:B:41:PRO:HG2	1:B:98:THR:HG22	1.90	0.52
1:C:211:ASN:C	1:C:211:ASN:ND2	2.61	0.52
1:A:616:GLY:HA3	1:A:624:THR:OG1	2.09	0.52
1:B:551:GLY:O	1:B:554:TYR:HB2	2.09	0.52
1:A:128:SER:HB2	1:B:113:LEU:HD22	1.90	0.52
1:C:324:VAL:CG2	1:C:326:PRO:HD3	2.39	0.52
1:A:407:ASP:O	1:A:408:ASP:C	2.48	0.52
1:C:432:ARG:CG	1:C:432:ARG:HH11	2.02	0.52
1:C:419:VAL:HA	1:C:422:GLU:HB3	1.91	0.52
1:B:649:MET:O	1:B:653:ARG:HB2	2.10	0.52
1:B:87:THR:HG21	1:B:620:ARG:NH1	2.25	0.52
1:A:644:VAL:O	1:A:646:ALA:N	2.43	0.52
1:A:133:SER:OG	1:A:136:PHE:HE1	1.91	0.52
1:B:960:LEU:HD11	1:B:1027:VAL:CG1	2.39	0.52
1:C:394:THR:O	1:C:395:MET:HE2	2.08	0.52
1:C:939:ALA:O	1:C:943:ILE:HG12	2.10	0.52
1:B:365:THR:O	1:B:368:PRO:HD2	2.10	0.52
1:C:352:PHE:CA	1:C:369:THR:HG21	2.37	0.52
1:A:246:PHE:O	1:A:249:ILE:HD12	2.09	0.52
1:B:740:GLY:HA3	1:B:794:ALA:CB	2.39	0.52
1:B:34:GLN:HB2	1:B:333:VAL:HG22	1.92	0.52
1:A:113:LEU:CD2	1:C:127:VAL:O	2.58	0.52
1:A:58:GLN:HG2	1:A:59:ASP:OD1	2.09	0.52
1:A:59:ASP:CB	1:C:763:ILE:HD11	2.38	0.52
1:A:67:GLN:NE2	2:A:1063:HOH:O	2.12	0.52
1:B:973:ARG:CG	1:B:974:PRO:HD3	2.37	0.52
1:C:752:ALA:O	1:C:774:MET:HA	2.10	0.52
1:B:518:ARG:HA	1:B:521:GLU:CB	2.40	0.52
1:B:784:ASP:O	1:B:785:ASP:C	2.46	0.52
1:B:763:ILE:HD11	1:C:59:ASP:HB3	1.91	0.52
1:B:570:GLY:N	1:B:634:TRP:HH2	2.07	0.52
1:A:246:PHE:O	1:A:249:ILE:HD13	2.10	0.52
1:A:717:ARG:HH11	1:A:830:GLN:HE22	1.55	0.52
1:C:877:TYR:O	1:C:880:SER:HB3	2.09	0.52
1:A:686:ASP:C	1:A:688:ALA:N	2.62	0.52
1:C:314:GLU:CB	1:C:315:PRO:CD	2.79	0.52
1:B:4:PHE:O	1:B:5:PHE:HB2	2.10	0.52
1:B:358:PHE:HB3	1:B:977:MET:CE	2.39	0.52
1:C:442:LEU:O	1:C:445:ILE:HG13	2.10	0.52
1:B:572:PHE:CE2	1:B:629:VAL:HG21	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:287:SER:OG	1:C:288:GLY:N	2.43	0.52
1:A:183:ALA:N	1:A:271:GLY:O	2.43	0.52
1:C:519:MET:O	1:C:523:SER:OG	2.24	0.52
1:C:1024:VAL:CG1	1:C:1028:VAL:CG2	2.88	0.52
1:B:335:ILE:O	1:B:337:ILE:N	2.43	0.52
1:C:599:LEU:O	1:C:603:LYS:HB2	2.10	0.52
1:A:761:ASP:N	1:A:761:ASP:OD2	2.42	0.52
1:C:572:PHE:CZ	1:C:629:VAL:HG11	2.45	0.52
1:B:304:ALA:O	1:B:308:ALA:HB2	2.10	0.52
1:B:168:ARG:HD3	1:C:69:MET:O	2.10	0.52
1:B:545:TYR:C	1:B:547:ILE:N	2.62	0.52
1:B:968:VAL:O	1:B:972:LEU:HB2	2.09	0.52
1:C:945:ILE:CB	1:C:971:ARG:HG3	2.40	0.52
1:A:102:ILE:HA	1:A:105:VAL:HG21	1.92	0.51
1:C:159:ALA:C	2:C:1078:HOH:O	2.32	0.51
1:B:399:VAL:O	1:B:400:LEU:C	2.47	0.51
1:B:360:GLN:O	1:B:361:ASN:CB	2.58	0.51
1:A:1004:GLY:O	1:A:1007:VAL:N	2.43	0.51
1:C:248:LYS:O	1:C:249:ILE:C	2.48	0.51
1:C:655:PHE:C	1:C:657:GLN:N	2.58	0.51
1:A:100:ALA:HB1	1:A:131:LYS:CE	2.39	0.51
1:A:68:ASN:H	1:A:69:MET:N	2.08	0.51
1:B:6:ILE:HD12	1:B:490:PRO:CB	2.39	0.51
1:A:354:VAL:HG13	1:A:980:LEU:HD23	1.92	0.51
1:A:911:GLY:CA	1:A:914:LEU:HD13	2.38	0.51
1:A:904:VAL:O	1:A:905:VAL:C	2.49	0.51
1:A:578:LEU:HD21	1:A:587:THR:CA	2.34	0.51
1:B:659:LYS:HD3	1:B:660:ASP:H	1.72	0.51
1:C:1035:ARG:HA	1:C:1035:ARG:NE	2.25	0.51
1:B:25:LEU:O	1:B:28:LEU:HG	2.10	0.51
1:B:55:LYS:O	1:B:57:VAL:N	2.43	0.51
1:A:65:ILE:N	1:A:65:ILE:C	2.61	0.51
1:A:819:TYR:O	1:A:820:ASN:C	2.48	0.51
1:B:358:PHE:HB3	1:B:977:MET:HE1	1.92	0.51
1:B:978:THR:HG22	1:B:979:SER:H	1.76	0.51
1:A:783:PRO:C	1:A:784:ASP:O	2.48	0.51
1:C:682:PHE:CE2	1:C:702:LEU:HD11	2.46	0.51
1:B:712:MET:HB3	1:B:713:LEU:CD1	2.29	0.51
1:C:214:VAL:CG1	1:C:215:ALA:H	2.23	0.51
1:B:729:ILE:CG1	1:B:730:ASP:N	2.70	0.51
1:B:556:PHE:HA	1:B:913:LEU:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:641:GLU:O	1:C:650:ARG:NH1	2.41	0.51
1:C:121:GLU:O	1:C:758:TYR:OH	2.27	0.51
1:C:695:LEU:HD22	1:C:825:MET:HE2	1.92	0.51
1:A:902:MET:C	1:A:904:VAL:H	2.13	0.51
1:B:594:VAL:HG22	1:B:663:VAL:HG11	1.91	0.51
1:C:263:ARG:HG3	1:C:263:ARG:O	2.08	0.51
1:A:826:GLU:C	1:A:827:ILE:HD12	2.31	0.51
1:A:116:PRO:HA	2:A:1072:HOH:O	2.10	0.51
1:B:105:VAL:O	1:B:109:ASN:N	2.35	0.51
1:B:1022:VAL:CG2	1:B:1023:PRO:CD	2.86	0.51
1:B:1026:PHE:HB3	1:B:1030:ARG:NE	2.25	0.51
1:C:341:VAL:O	1:C:345:VAL:HG23	2.11	0.51
1:A:314:GLU:H	1:A:315:PRO:HD3	1.74	0.51
1:A:311:ALA:O	1:A:312:LYS:CB	2.53	0.51
1:A:148:THR:HG21	1:A:319:SER:OG	2.10	0.51
1:B:736:ALA:C	1:B:738:ALA:H	2.12	0.51
1:B:104:GLN:HG2	1:B:105:VAL:H	1.74	0.51
1:B:1027:VAL:O	1:B:1031:ARG:HB3	2.10	0.51
1:A:543:VAL:O	1:A:544:LEU:CB	2.55	0.51
1:A:621:GLY:O	1:A:623:ASN:N	2.43	0.51
1:C:978:THR:O	1:C:979:SER:C	2.46	0.51
1:B:583:THR:HG22	1:B:586:ARG:HG3	1.93	0.51
1:C:760:ASN:C	1:C:760:ASN:OD1	2.49	0.51
1:B:420:MET:HA	1:B:423:GLU:O	2.09	0.51
1:B:330:THR:O	1:B:334:LYS:HG3	2.09	0.51
1:A:11:PHE:CD1	1:B:890:ALA:CB	2.94	0.51
1:A:191:ASN:C	1:A:193:LEU:N	2.63	0.51
1:A:280:GLU:HB2	1:A:284:GLN:O	2.09	0.51
1:A:63:GLN:O	1:A:65:ILE:C	2.49	0.51
1:A:687:GLN:O	1:A:688:ALA:HB2	2.09	0.51
1:C:115:MET:N	1:C:116:PRO:HD3	2.23	0.51
1:C:708:LYS:C	1:C:710:PRO:HD3	2.31	0.51
1:A:831:ALA:HB2	1:A:837:THR:HA	1.93	0.51
1:C:399:VAL:C	1:C:401:ALA:H	2.14	0.51
1:A:651:ALA:O	1:A:655:PHE:HD1	1.93	0.51
1:A:158:VAL:HA	1:A:162:MET:HG2	1.92	0.51
1:C:792:ARG:HG2	1:C:793:ALA:O	2.11	0.51
1:A:69:MET:CG	1:A:69:MET:CA	2.80	0.51
1:C:129:VAL:CA	1:C:129:VAL:CG2	2.84	0.51
1:B:186:ILE:HG23	1:B:266:ALA:HB1	1.91	0.51
1:B:1024:VAL:HG13	1:B:1028:VAL:HG21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:974:PRO:O	1:B:976:LEU:N	2.44	0.51
1:A:1016:VAL:HG12	1:A:1016:VAL:O	2.10	0.51
1:B:986:VAL:HG12	1:B:990:VAL:CG2	2.40	0.51
1:B:778:LYS:O	1:B:779:TYR:HB2	2.11	0.51
1:A:166:ILE:N	1:A:166:ILE:CD1	2.67	0.51
1:A:488:LEU:HG	1:A:492:LEU:HD22	1.93	0.51
1:B:476:SER:O	1:B:477:ALA:C	2.49	0.51
1:C:326:PRO:O	1:C:327:TYR:C	2.50	0.51
1:C:181:GLN:CD	1:C:769:LYS:HD2	2.31	0.51
1:B:552:MET:SD	1:B:909:VAL:CG2	2.96	0.51
1:C:701:GLN:O	1:C:704:ALA:N	2.44	0.51
1:C:1016:VAL:O	1:C:1019:ILE:HG22	2.11	0.51
1:C:392:THR:O	1:C:395:MET:N	2.42	0.51
1:C:549:VAL:HG12	1:C:550:VAL:N	2.25	0.51
1:B:863:SER:O	1:B:866:GLU:N	2.44	0.51
1:A:14:VAL:CG1	1:B:886:LEU:HB3	2.41	0.51
1:C:482:VAL:O	1:C:486:LEU:HG	2.11	0.51
1:A:112:GLN:NE2	1:A:112:GLN:CA	2.65	0.51
1:A:818:ARG:NH1	1:A:821:GLY:O	2.43	0.51
1:C:50:PRO:CD	1:C:125:GLN:HG3	2.41	0.51
1:B:168:ARG:HH11	1:C:69:MET:HB2	1.75	0.51
1:C:713:LEU:CD1	1:C:833:PRO:O	2.59	0.51
1:C:754:TRP:CH2	1:C:780:ARG:HA	2.46	0.51
1:B:898:PRO:C	1:B:900:SER:N	2.63	0.51
1:C:911:GLY:O	1:C:914:LEU:O	2.29	0.51
1:C:16:ALA:O	1:C:20:MET:HG3	2.10	0.51
1:C:280:GLU:HB3	1:C:284:GLN:O	2.11	0.51
1:A:584:GLN:N	1:A:622:GLN:HB3	2.23	0.51
1:A:691:GLY:O	1:A:692:HIS:C	2.50	0.51
1:B:91:THR:C	1:B:92:LEU:HD22	2.31	0.51
1:C:785:ASP:O	1:C:787:GLY:N	2.44	0.51
1:A:750:LEU:HD11	1:C:216:ALA:CB	2.41	0.51
1:A:579:PRO:O	1:A:580:ALA:C	2.49	0.51
1:C:734:GLU:O	1:C:738:ALA:N	2.44	0.51
1:A:65:ILE:HG13	1:A:66:GLU:N	2.26	0.50
1:B:946:VAL:HG22	1:B:1026:PHE:CE1	2.45	0.50
1:C:907:LEU:HG	1:C:1017:LEU:HD23	1.93	0.50
1:C:418:ARG:CD	1:C:970:MET:HE2	2.40	0.50
1:C:425:LEU:N	1:C:426:PRO:HD3	2.26	0.50
1:A:583:THR:HB	1:A:586:ARG:HG3	1.93	0.50
1:C:655:PHE:O	1:C:657:GLN:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:732:ASP:HB3	1:A:735:LYS:HB2	1.93	0.50
1:A:107:VAL:O	1:A:110:LYS:HB3	2.11	0.50
1:B:316:PHE:CZ	1:C:687:GLN:HG3	2.46	0.50
1:A:533:GLY:O	1:A:534:ILE:C	2.49	0.50
1:B:987:MET:N	1:B:988:PRO:HD2	2.26	0.50
1:A:658:ILE:O	1:A:659:LYS:O	2.27	0.50
1:B:149:MET:SD	1:B:154:ILE:HG22	2.51	0.50
1:B:595:THR:HB	1:B:609:VAL:HG11	1.93	0.50
1:A:116:PRO:C	1:A:117:LEU:HD22	2.32	0.50
1:A:527:TYR:CD2	1:A:972:LEU:HG	2.47	0.50
1:A:599:LEU:O	1:A:600:THR:CB	2.59	0.50
1:A:418:ARG:NH1	1:A:973:ARG:HB3	2.26	0.50
1:C:188:MET:HA	1:C:266:ALA:CB	2.40	0.50
1:C:556:PHE:HB2	1:C:913:LEU:HD11	1.93	0.50
1:A:399:VAL:C	1:A:401:ALA:N	2.65	0.50
1:C:247:GLY:HA2	1:C:268:ILE:CD1	2.38	0.50
1:B:462:SER:OG	1:B:865:GLN:NE2	2.44	0.50
1:C:666:PHE:CD2	1:C:666:PHE:N	2.79	0.50
1:A:76:MET:SD	1:A:95:GLU:OE2	2.70	0.50
1:C:102:ILE:O	1:C:105:VAL:HB	2.12	0.50
1:B:960:LEU:C	1:B:960:LEU:HD13	2.31	0.50
1:C:490:PRO:C	1:C:491:ALA:O	2.47	0.50
1:A:276:ASP:CB	1:C:222:THR:HG23	2.35	0.50
1:B:228:GLN:HA	1:B:228:GLN:HE21	1.76	0.50
1:C:188:MET:HE2	1:C:200:PRO:HB3	1.92	0.50
1:B:679:GLY:HA2	1:B:830:GLN:HB3	1.94	0.50
1:B:25:LEU:O	1:B:28:LEU:N	2.36	0.50
1:A:73:ASP:CG	1:A:106:GLN:HE22	2.15	0.50
1:A:952:LEU:C	1:A:952:LEU:HD12	2.32	0.50
1:A:428:LYS:CG	1:A:429:GLU:H	2.22	0.50
1:A:421:ALA:O	1:A:423:GLU:N	2.44	0.50
1:C:226:LYS:HA	2:C:1072:HOH:O	2.11	0.50
1:A:635:ALA:C	1:A:637:ARG:H	2.14	0.50
1:B:578:LEU:HD12	1:B:586:ARG:NH2	2.26	0.50
1:C:467:TYR:C	1:C:469:GLN:H	2.15	0.50
1:A:254:ASN:O	1:A:258:SER:OG	2.20	0.50
1:C:726:GLN:N	1:C:810:GLU:O	2.38	0.50
1:C:169:THR:CB	1:C:172:VAL:HG21	2.38	0.50
1:C:758:TYR:H	1:C:758:TYR:HD1	1.55	0.50
1:C:949:ALA:C	1:C:951:ASP:N	2.64	0.50
1:B:317:PHE:CD1	1:B:321:LEU:HD23	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:695:LEU:CD2	1:C:825:MET:HG3	2.41	0.50
1:A:552:MET:SD	1:A:909:VAL:HG11	2.52	0.50
1:C:191:ASN:O	1:C:194:ASN:HB2	2.11	0.50
1:B:49:TYR:CD1	1:B:122:VAL:HG13	2.46	0.50
1:C:674:LEU:HD12	1:C:865:GLN:OE1	2.12	0.50
1:C:643:LYS:C	1:C:647:ILE:HG13	2.32	0.50
1:C:644:VAL:O	1:C:648:THR:HG22	2.12	0.50
1:C:536:ARG:NH1	1:C:961:ILE:CD1	2.75	0.50
1:B:728:LYS:HD3	1:B:810:GLU:OE1	2.12	0.50
1:A:75:LEU:HD12	1:A:76:MET:N	2.26	0.50
1:B:10:ILE:O	1:B:11:PHE:C	2.48	0.50
1:A:534:ILE:HD12	1:A:540:ARG:NH1	2.26	0.50
1:C:428:LYS:O	1:C:432:ARG:HB2	2.12	0.50
1:C:422:GLU:OE2	1:C:423:GLU:HG3	2.12	0.50
1:B:833:PRO:HG2	1:B:834:GLY:H	1.77	0.50
1:A:588:GLN:O	1:A:591:LEU:N	2.43	0.50
1:B:324:VAL:C	1:B:326:PRO:HD2	2.32	0.50
1:C:243:THR:OG1	1:C:244:GLU:N	2.45	0.50
1:A:371:ALA:O	1:A:372:VAL:O	2.30	0.50
1:A:709:HIS:N	1:A:710:PRO:CD	2.74	0.50
1:A:193:LEU:HA	1:A:265:VAL:HG13	1.94	0.50
1:C:735:LYS:O	1:C:738:ALA:HB3	2.11	0.50
1:A:235:ILE:O	1:A:235:ILE:HG22	2.11	0.50
1:C:311:ALA:O	1:C:312:LYS:C	2.49	0.50
1:B:8:ARG:H	1:B:9:PRO:HD3	1.76	0.50
1:B:1019:ILE:O	1:B:1023:PRO:HG3	2.11	0.50
1:C:192:GLU:C	1:C:194:ASN:N	2.64	0.50
1:C:393:LEU:O	1:C:395:MET:N	2.45	0.50
1:C:559:LEU:HD13	1:C:917:THR:HG23	1.94	0.50
1:B:572:PHE:HA	1:B:668:LEU:HD21	1.93	0.50
1:A:186:ILE:HD12	1:A:207:ILE:HD13	1.94	0.50
1:A:200:PRO:HG2	1:A:749:THR:HG23	1.93	0.50
1:A:578:LEU:H	1:A:578:LEU:HD22	1.76	0.50
1:C:997:SER:O	1:C:999:ALA:N	2.45	0.50
1:C:463:THR:HG22	1:C:464:GLY:H	1.73	0.50
1:C:540:ARG:HG3	1:C:541:TYR:CD1	2.46	0.50
1:A:689:GLY:O	1:A:690:LEU:C	2.51	0.50
1:C:127:VAL:C	1:C:127:VAL:CB	2.73	0.50
1:B:693:GLU:C	1:B:695:LEU:H	2.15	0.50
1:B:703:LEU:O	1:B:704:ALA:C	2.50	0.50
1:C:934:THR:O	1:C:936:GLY:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:830:GLN:H	1:B:830:GLN:NE2	2.04	0.50
1:B:129:VAL:H	1:C:109:ASN:HD21	1.58	0.50
1:A:133:SER:HB3	1:A:136:PHE:CD1	2.46	0.50
1:B:1016:VAL:C	1:B:1018:ALA:H	2.16	0.49
1:B:1017:LEU:O	1:B:1021:PHE:HB2	2.12	0.49
1:B:1022:VAL:CG2	1:B:1023:PRO:HD3	2.33	0.49
1:B:401:ALA:HA	1:B:404:LEU:HB2	1.93	0.49
1:B:547:ILE:O	1:B:550:VAL:O	2.30	0.49
1:C:1010:GLY:C	1:C:1013:THR:HG22	2.32	0.49
1:C:376:LEU:HD22	1:C:398:MET:HE1	1.93	0.49
1:B:712:MET:HA	1:B:712:MET:CE	2.42	0.49
1:B:115:MET:HA	1:B:118:LEU:HD13	1.94	0.49
1:A:395:MET:HA	1:A:395:MET:CE	2.41	0.49
1:A:218:GLN:HB3	1:A:231:ASN:HD21	1.77	0.49
1:C:260:VAL:O	1:C:260:VAL:HG13	2.11	0.49
1:C:1032:ARG:O	1:C:1032:ARG:HG2	2.11	0.49
1:B:600:THR:OG1	1:B:601:LYS:HE2	2.13	0.49
1:B:25:LEU:C	1:B:27:ILE:N	2.64	0.49
1:C:88:VAL:HG11	2:C:1064:HOH:O	2.12	0.49
1:B:1012:VAL:C	1:B:1014:ALA:H	2.15	0.49
1:B:542:LEU:HD11	1:B:1028:VAL:CG1	2.40	0.49
1:B:973:ARG:N	1:B:974:PRO:HD2	2.27	0.49
1:C:966:ASP:HA	1:C:969:ARG:CB	2.42	0.49
1:C:519:MET:CG	1:C:520:PHE:N	2.75	0.49
1:B:413:VAL:HG13	1:B:414:GLU:N	2.27	0.49
1:A:728:LYS:HZ3	1:C:235:ILE:CG2	2.23	0.49
1:C:847:LEU:N	1:C:847:LEU:HD22	2.28	0.49
1:C:847:LEU:HD23	1:C:847:LEU:C	2.33	0.49
1:A:790:TYR:HE1	1:A:800:PRO:CG	2.14	0.49
1:B:100:ALA:HB1	1:B:131:LYS:HD2	1.94	0.49
1:A:455:PRO:HB2	1:A:877:TYR:CE1	2.48	0.49
1:C:100:ALA:O	1:C:101:ASP:C	2.50	0.49
1:C:219:LEU:O	1:C:220:GLY:O	2.30	0.49
1:C:333:VAL:O	1:C:337:ILE:HD12	2.12	0.49
1:B:119:PRO:HG2	1:B:122:VAL:HG21	1.95	0.49
1:A:613:ASN:HA	1:A:625:GLY:HA3	1.95	0.49
1:B:690:LEU:HB2	1:B:694:LYS:HB3	1.94	0.49
1:C:561:SER:HA	1:C:923:ASN:CB	2.43	0.49
1:A:516:PHE:C	1:A:518:ARG:N	2.66	0.49
1:A:568:ASP:HB3	1:A:634:TRP:CZ3	2.41	0.49
1:C:184:MET:HB3	1:C:771:VAL:HG13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ILE:HD11	1:A:671:ILE:HG21	1.94	0.49
1:A:359:LEU:CD1	1:A:417:GLU:HG2	2.41	0.49
1:A:682:PHE:CZ	1:A:857:TYR:HB2	2.48	0.49
1:C:166:ILE:CA	1:C:166:ILE:CD1	2.75	0.49
1:A:1024:VAL:HG12	1:A:1028:VAL:HG23	1.94	0.49
1:A:552:MET:C	1:A:554:TYR:H	2.16	0.49
1:C:1022:VAL:N	1:C:1023:PRO:CD	2.75	0.49
1:C:1025:PHE:C	1:C:1029:VAL:HG23	2.33	0.49
1:C:389:SER:O	1:C:394:THR:HG21	2.12	0.49
1:B:602:GLU:C	1:B:604:ASN:N	2.65	0.49
1:C:461:GLY:CA	1:C:869:SER:OG	2.61	0.49
1:C:454:VAL:O	1:C:456:MET:O	2.31	0.49
1:B:158:VAL:HA	1:B:162:MET:CG	2.36	0.49
1:A:719:ASN:N	1:A:826:GLU:O	2.46	0.49
1:A:843:LEU:HD23	1:A:846:GLN:NE2	2.27	0.49
1:C:23:GLY:O	1:C:27:ILE:HG13	2.13	0.49
1:C:166:ILE:CG2	1:C:166:ILE:CA	2.85	0.49
1:C:314:GLU:HA	1:C:317:PHE:CZ	2.47	0.49
1:B:1026:PHE:HB3	1:B:1030:ARG:CZ	2.42	0.49
1:B:410:ILE:C	1:B:412:VAL:H	2.15	0.49
1:A:533:GLY:O	1:A:535:LEU:HB2	2.12	0.49
1:B:343:THR:O	1:B:347:ALA:N	2.39	0.49
1:C:545:TYR:CZ	1:C:1021:PHE:CD2	3.01	0.49
1:C:399:VAL:HA	1:C:402:ILE:HD12	1.92	0.49
1:C:8:ARG:HG2	1:C:8:ARG:HH21	1.78	0.49
1:B:701:GLN:HB3	1:B:851:LEU:HD13	1.95	0.49
1:A:330:THR:H	1:A:331:PRO:HD2	1.78	0.49
1:A:574:THR:HG21	1:A:598:TYR:CE1	2.44	0.49
1:A:754:TRP:CZ2	1:A:786:ILE:HG12	2.48	0.49
1:C:781:MET:O	1:C:782:LEU:HD23	2.13	0.49
1:A:693:GLU:C	1:A:695:LEU:N	2.65	0.49
1:C:492:LEU:O	1:C:496:MET:HG2	2.13	0.49
1:A:68:ASN:H	1:A:69:MET:H	1.61	0.49
1:C:912:ALA:O	1:C:914:LEU:N	2.46	0.49
1:A:219:LEU:HD23	1:B:754:TRP:HZ3	1.78	0.49
1:C:513:PHE:CA	1:C:516:PHE:HB3	2.33	0.49
1:C:562:SER:OG	1:C:922:THR:HG21	2.12	0.49
1:A:372:VAL:HB	1:A:373:PRO:CD	2.37	0.49
1:A:999:ALA:HA	1:A:1002:ALA:CB	2.43	0.49
1:B:380:PHE:CZ	1:B:398:MET:HE2	2.48	0.49
1:B:619:GLY:H	1:B:721:LEU:CD1	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:818:ARG:HG3	2:A:1062:HOH:O	2.11	0.49
1:C:80:SER:O	1:C:89:GLN:O	2.31	0.49
1:B:471:SER:O	1:B:475:VAL:HB	2.13	0.49
1:B:404:LEU:HD13	1:B:449:LEU:CD1	2.42	0.49
1:C:685:ILE:HD12	1:C:686:ASP:N	2.28	0.49
1:C:705:GLU:O	1:C:708:LYS:N	2.45	0.49
1:A:963:ALA:O	1:A:965:LEU:N	2.46	0.49
1:C:476:SER:C	1:C:478:MET:N	2.66	0.49
1:B:20:MET:HG3	1:B:374:VAL:HG23	1.94	0.49
1:C:568:ASP:OD1	1:C:634:TRP:CD1	2.65	0.49
1:C:650:ARG:O	1:C:653:ARG:HG2	2.12	0.49
1:A:631:LEU:HD11	1:A:644:VAL:HG22	1.94	0.49
1:C:102:ILE:O	1:C:105:VAL:N	2.46	0.49
1:B:490:PRO:O	1:B:493:CYS:O	2.30	0.49
1:C:192:GLU:O	1:C:193:LEU:C	2.51	0.49
1:B:642:ASN:N	1:B:650:ARG:HH12	2.05	0.49
1:B:125:GLN:CG	1:B:125:GLN:O	2.59	0.49
1:C:987:MET:HB3	1:C:988:PRO:HD3	1.94	0.49
1:C:188:MET:HE2	1:C:200:PRO:HA	1.95	0.49
1:A:521:GLU:CG	2:A:1075:HOH:O	2.57	0.49
1:B:183:ALA:H	1:B:272:GLY:HA2	1.78	0.49
1:B:453:PHE:HA	1:B:456:MET:SD	2.52	0.49
1:B:485:ALA:HA	1:B:489:THR:OG1	2.13	0.49
1:B:905:VAL:N	1:B:906:PRO:CD	2.76	0.49
1:A:832:ALA:CB	1:A:835:LYS:HB2	2.40	0.49
1:C:396:PHE:HA	1:C:399:VAL:HB	1.94	0.49
1:C:4:PHE:HB3	1:C:8:ARG:NH2	2.16	0.49
1:B:362:PHE:HA	1:B:365:THR:HG22	1.95	0.49
1:B:583:THR:HG23	1:B:585:GLU:H	1.78	0.49
1:A:171:GLY:O	1:A:173:GLY:N	2.45	0.49
1:A:736:ALA:CA	1:A:741:VAL:HG13	2.42	0.49
1:C:574:THR:O	1:C:626:ILE:HD13	2.12	0.49
1:A:63:GLN:O	1:A:64:VAL:C	2.50	0.48
1:A:67:GLN:CB	2:A:1057:HOH:O	2.60	0.48
1:B:7:ASP:CG	1:B:8:ARG:HH21	2.16	0.48
1:B:942:ALA:O	1:B:945:ILE:HG12	2.13	0.48
1:B:900:SER:O	1:B:903:LEU:N	2.39	0.48
1:B:638:PRO:HG2	1:B:639:GLY:H	1.78	0.48
1:B:355:MET:O	1:B:365:THR:OG1	2.30	0.48
1:B:369:THR:O	1:B:372:VAL:HG13	2.13	0.48
1:B:578:LEU:HD12	1:B:586:ARG:CZ	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:586:ARG:NH2	1:B:660:ASP:HB2	2.26	0.48
1:A:193:LEU:HB2	1:A:265:VAL:HG13	1.95	0.48
1:B:969:ARG:HH11	1:B:969:ARG:HG2	1.78	0.48
1:A:64:VAL:HG12	1:A:65:ILE:N	2.27	0.48
1:C:324:VAL:HG23	1:C:325:TYR:N	2.27	0.48
1:C:65:ILE:O	1:C:66:GLU:C	2.48	0.48
1:C:893:GLU:HG3	1:C:893:GLU:O	2.13	0.48
1:A:534:ILE:HD12	1:A:540:ARG:CZ	2.43	0.48
1:A:554:TYR:HE1	1:A:558:ARG:HD3	1.76	0.48
1:C:753:ALA:HB1	1:C:775:SER:HB2	1.95	0.48
1:C:576:VAL:HG21	1:C:591:LEU:CD2	2.43	0.48
1:C:449:LEU:O	1:C:452:VAL:N	2.26	0.48
1:A:449:LEU:O	1:A:453:PHE:HD1	1.96	0.48
1:B:218:GLN:HA	1:B:234:ILE:HG13	1.95	0.48
1:B:956:GLU:CD	1:B:956:GLU:H	2.17	0.48
1:B:261:LEU:CD2	1:B:263:ARG:HB2	2.43	0.48
1:B:261:LEU:HD13	1:B:261:LEU:H	1.78	0.48
1:B:743:ILE:H	1:B:743:ILE:HD12	1.78	0.48
1:A:72:ILE:HG22	1:A:72:ILE:O	2.13	0.48
1:C:110:LYS:HA	1:C:113:LEU:CD1	2.20	0.48
1:C:127:VAL:CA	1:C:127:VAL:CG1	2.83	0.48
1:B:4:PHE:O	1:B:6:ILE:N	2.44	0.48
1:B:341:VAL:CG1	1:B:342:LYS:N	2.76	0.48
1:C:545:TYR:OH	1:C:1021:PHE:HB3	2.13	0.48
1:C:435:MET:HA	1:C:438:ILE:HG22	1.95	0.48
1:C:252:LYS:O	1:C:260:VAL:CG1	2.57	0.48
1:A:671:ILE:O	1:A:672:VAL:C	2.51	0.48
1:A:819:TYR:N	1:A:822:LEU:O	2.45	0.48
1:C:163:LYS:O	1:C:165:ALA:N	2.46	0.48
1:B:220:GLY:O	1:B:221:GLY:O	2.30	0.48
1:C:4:PHE:CB	1:C:8:ARG:NH2	2.68	0.48
1:A:281:PHE:O	1:A:282:ASN:C	2.51	0.48
1:B:418:ARG:HG3	1:B:970:MET:HE3	1.92	0.48
1:A:190:PRO:HG2	1:A:788:ASP:HB3	1.95	0.48
1:B:423:GLU:OE1	1:B:427:PRO:HD3	2.10	0.48
1:B:610:PHE:O	1:B:627:ALA:CB	2.59	0.48
1:B:174:ASP:CG	1:B:175:VAL:H	2.16	0.48
1:B:197:GLN:O	1:B:792:ARG:NH2	2.45	0.48
1:A:686:ASP:O	1:A:687:GLN:C	2.50	0.48
1:B:912:ALA:HB1	1:B:1006:GLY:O	2.13	0.48
1:A:531:VAL:CA	1:A:534:ILE:HD11	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:417:GLU:HB3	1:C:973:ARG:NH1	2.28	0.48
1:A:924:ASP:O	1:A:925:VAL:C	2.50	0.48
1:A:600:THR:O	1:A:601:LYS:CB	2.61	0.48
1:C:925:VAL:O	1:C:926:TYR:HB2	2.14	0.48
1:B:26:ALA:O	1:B:30:LEU:HB2	2.14	0.48
1:C:466:ILE:N	1:C:466:ILE:HD12	2.28	0.48
1:A:60:THR:CG2	1:A:119:PRO:CD	2.90	0.48
1:A:309:GLU:O	1:A:311:ALA:O	2.32	0.48
1:A:189:ASN:ND2	1:A:192:GLU:HB3	2.27	0.48
1:B:709:HIS:N	1:B:710:PRO:CD	2.76	0.48
1:C:964:THR:O	1:C:967:ALA:HB3	2.13	0.48
1:A:289:LEU:HD23	1:A:289:LEU:C	2.33	0.48
1:C:386:PHE:O	1:C:388:PHE:HD1	1.96	0.48
1:A:818:ARG:CD	1:A:821:GLY:O	2.51	0.48
1:A:105:VAL:HA	1:B:109:ASN:HD21	1.79	0.48
1:B:892:TYR:C	1:B:894:SER:H	2.16	0.48
1:C:1018:ALA:HA	1:C:1021:PHE:HB2	1.94	0.48
1:B:648:THR:HG21	1:B:666:PHE:HA	1.95	0.48
1:B:742:SER:CB	1:B:745:ASP:OD2	2.52	0.48
1:C:997:SER:HA	1:C:1000:GLN:OE1	2.12	0.48
1:B:327:TYR:HD2	1:B:628:PHE:HB3	1.75	0.48
1:A:255:GLN:N	1:A:255:GLN:OE1	2.46	0.48
1:A:56:THR:HG22	1:A:56:THR:O	2.12	0.48
1:B:335:ILE:C	1:B:337:ILE:N	2.66	0.48
1:C:758:TYR:CD2	1:C:770:LYS:HE2	2.49	0.48
1:B:932:LEU:HA	1:B:935:ILE:HD12	1.95	0.48
1:B:407:ASP:O	1:B:410:ILE:HG22	2.13	0.48
1:B:416:VAL:HG22	1:B:431:THR:HA	1.94	0.48
1:C:528:THR:O	1:C:531:VAL:HG22	2.14	0.48
1:C:910:ILE:CG2	1:C:911:GLY:N	2.77	0.48
1:C:1:MET:HE3	1:C:439:GLN:HE22	1.75	0.48
1:A:189:ASN:O	1:A:189:ASN:CG	2.52	0.48
1:C:846:GLN:O	1:C:849:SER:OG	2.29	0.48
1:C:958:LYS:N	1:C:958:LYS:HD2	2.29	0.48
1:A:99:ASP:O	1:A:102:ILE:HG22	2.13	0.48
1:C:165:ALA:C	2:C:1075:HOH:O	2.52	0.48
1:B:485:ALA:O	1:B:486:LEU:HB3	2.14	0.48
1:C:545:TYR:OH	1:C:1021:PHE:CD2	2.51	0.48
1:A:158:VAL:O	1:A:158:VAL:HG12	2.13	0.48
1:B:20:MET:HE2	1:B:373:PRO:O	2.13	0.48
1:A:578:LEU:HD21	1:A:587:THR:CG2	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:913:LEU:HD23	1:C:927:PHE:CZ	2.49	0.48
1:C:350:LEU:HD12	1:C:985:GLY:CA	2.39	0.48
1:A:702:LEU:HA	1:A:705:GLU:HB2	1.96	0.48
1:B:252:LYS:HB3	1:B:260:VAL:HG11	1.95	0.48
1:B:101:ASP:O	1:B:105:VAL:HG23	2.14	0.48
1:C:950:LYS:HZ3	1:C:1030:ARG:NH1	2.11	0.48
1:B:409:ALA:HB2	1:B:485:ALA:HB2	1.94	0.48
1:C:974:PRO:O	1:C:975:ILE:C	2.52	0.48
1:A:307:ARG:NH1	1:A:325:TYR:CD2	2.82	0.48
1:B:362:PHE:C	1:B:364:ALA:H	2.16	0.48
1:A:391:ASN:O	1:A:392:THR:C	2.51	0.48
1:B:298:ASN:HB2	1:B:301:ASP:OD1	2.14	0.48
1:C:644:VAL:HG12	1:C:667:ASN:HB2	1.95	0.48
1:A:498:LYS:HA	1:A:498:LYS:HE2	1.95	0.48
1:A:218:GLN:OE1	1:A:221:GLY:HA3	2.14	0.48
1:A:841:MET:O	1:A:844:MET:HB3	2.14	0.48
1:A:108:GLN:CD	1:B:112:GLN:CD	2.72	0.48
1:C:104:GLN:HG3	1:C:131:LYS:CG	2.42	0.48
1:C:115:MET:HE1	1:C:118:LEU:HD23	1.96	0.48
1:C:121:GLU:OE2	1:C:121:GLU:N	2.44	0.48
1:B:438:ILE:CD1	1:B:971:ARG:NH1	2.77	0.48
1:B:341:VAL:HG13	1:B:342:LYS:N	2.29	0.48
1:C:420:MET:SD	1:C:498:LYS:HD3	2.53	0.48
1:B:833:PRO:O	1:B:834:GLY:O	2.31	0.48
1:B:324:VAL:O	1:B:326:PRO:HD2	2.13	0.48
1:C:246:PHE:HZ	1:C:762:PHE:CB	2.27	0.48
1:C:262:LEU:HD23	1:C:268:ILE:HD11	1.95	0.48
1:C:536:ARG:HH21	1:C:536:ARG:HG2	1.79	0.48
1:B:830:GLN:N	1:B:830:GLN:HE21	2.06	0.48
1:B:423:GLU:OE1	1:B:427:PRO:CG	2.60	0.48
1:B:219:LEU:HD12	1:B:219:LEU:H	1.79	0.48
1:C:115:MET:HB2	1:C:116:PRO:HD3	1.95	0.47
1:C:181:GLN:OE1	1:C:767:ARG:CZ	2.62	0.47
1:B:525:HIS:O	1:B:529:ASP:HB2	2.14	0.47
1:A:978:THR:C	1:A:980:LEU:H	2.16	0.47
1:C:945:ILE:HD12	1:C:945:ILE:C	2.34	0.47
1:B:665:ALA:O	1:B:666:PHE:CG	2.67	0.47
1:A:251:LEU:CD1	1:A:262:LEU:HA	2.29	0.47
1:B:366:LEU:O	1:B:369:THR:N	2.41	0.47
1:A:1004:GLY:O	1:A:1005:THR:C	2.52	0.47
1:B:626:ILE:HD11	1:B:628:PHE:CZ	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:GLU:O	1:C:263:ARG:NH2	2.47	0.47
1:B:562:SER:HA	1:B:837:THR:OG1	2.14	0.47
1:C:653:ARG:O	1:C:655:PHE:O	2.32	0.47
1:B:391:ASN:H	1:B:394:THR:HG1	1.57	0.47
1:A:54:ALA:O	1:A:55:LYS:C	2.50	0.47
1:C:131:LYS:HB2	1:C:295:THR:HG21	1.96	0.47
1:B:247:GLY:HA2	1:B:268:ILE:HD11	1.78	0.47
1:C:950:LYS:HE2	1:C:1030:ARG:CZ	2.45	0.47
1:B:339:GLU:HB3	1:B:1000:GLN:HE22	1.79	0.47
1:A:729:ILE:O	1:A:730:ASP:HB2	2.13	0.47
1:A:574:THR:HG22	1:A:665:ALA:HB2	1.96	0.47
1:A:418:ARG:HH21	1:A:970:MET:HA	1.78	0.47
1:B:280:GLU:CA	1:B:284:GLN:O	2.62	0.47
1:B:573:MET:HE2	1:B:626:ILE:HD12	1.96	0.47
1:B:575:MET:O	1:B:663:VAL:HA	2.14	0.47
1:B:984:LEU:O	1:B:984:LEU:CD1	2.60	0.47
1:C:1024:VAL:CG1	1:C:1028:VAL:HG21	2.44	0.47
1:B:58:GLN:HB2	1:B:82:SER:CB	2.44	0.47
1:B:249:ILE:O	1:B:261:LEU:HB2	2.14	0.47
1:A:639:GLY:O	1:A:642:ASN:N	2.37	0.47
1:A:964:THR:O	1:A:964:THR:HG22	2.12	0.47
1:A:102:ILE:CA	1:A:105:VAL:HG23	2.44	0.47
1:A:111:LEU:O	1:A:112:GLN:C	2.47	0.47
1:C:57:VAL:CG1	1:C:88:VAL:HG23	2.45	0.47
1:B:1024:VAL:O	1:B:1025:PHE:CB	2.62	0.47
1:B:415:ASN:ND2	1:B:438:ILE:HD13	2.29	0.47
1:B:489:THR:N	1:B:490:PRO:HD2	2.29	0.47
1:A:538:THR:C	1:A:540:ARG:H	2.17	0.47
1:B:988:PRO:O	1:B:989:LEU:CB	2.45	0.47
1:B:889:ALA:O	1:B:892:TYR:O	2.33	0.47
1:C:13:TRP:O	1:C:17:ILE:HD13	2.14	0.47
1:A:920:GLY:O	1:A:921:LEU:HD23	2.14	0.47
1:A:568:ASP:CG	1:A:637:ARG:HH12	2.16	0.47
1:B:560:PRO:O	1:B:922:THR:OG1	2.32	0.47
1:B:330:THR:H	1:B:331:PRO:HD2	1.74	0.47
1:A:779:TYR:CD1	1:A:779:TYR:N	2.82	0.47
1:A:999:ALA:HA	1:A:1002:ALA:HB3	1.97	0.47
1:C:300:LEU:O	1:C:303:ALA:N	2.48	0.47
1:A:592:ASN:O	1:A:595:THR:HB	2.14	0.47
1:A:113:LEU:HD23	1:C:127:VAL:O	2.14	0.47
1:B:548:ILE:HD13	1:B:1017:LEU:HD23	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:972:LEU:CD1	1:B:976:LEU:CD2	2.92	0.47
1:A:1019:ILE:O	1:A:1023:PRO:HG3	2.14	0.47
1:C:358:PHE:CB	1:C:977:MET:HE2	2.25	0.47
1:B:20:MET:O	1:B:23:GLY:O	2.32	0.47
1:B:418:ARG:NE	1:B:970:MET:SD	2.87	0.47
1:C:978:THR:O	1:C:981:ALA:N	2.47	0.47
1:B:281:PHE:O	1:B:284:GLN:HB3	2.15	0.47
1:A:455:PRO:HB2	1:A:877:TYR:HE1	1.79	0.47
1:C:71:GLY:C	1:C:72:ILE:HG13	2.33	0.47
1:B:953:MET:HA	1:B:958:LYS:HA	1.96	0.47
1:A:481:SER:OG	1:A:482:VAL:N	2.46	0.47
1:C:66:GLU:HB3	1:C:78:MET:CE	2.45	0.47
1:C:438:ILE:O	1:C:441:ALA:HB3	2.14	0.47
1:A:438:ILE:H	1:A:438:ILE:HD13	1.79	0.47
1:A:277:ILE:HA	1:A:613:ASN:O	2.13	0.47
1:A:877:TYR:OH	1:A:932:LEU:HD11	2.15	0.47
1:A:736:ALA:HA	1:A:741:VAL:HG13	1.95	0.47
1:B:600:THR:O	1:B:603:LYS:HG2	2.15	0.47
1:B:450:SER:O	1:B:451:ALA:C	2.50	0.47
1:B:185:ARG:NH2	2:B:1054:HOH:O	2.47	0.47
1:A:96:SER:OG	1:A:97:GLY:N	2.44	0.47
1:C:767:ARG:HG2	1:C:769:LYS:HD3	1.96	0.47
1:B:944:LEU:HB2	1:B:975:ILE:HD11	1.96	0.47
1:B:892:TYR:HB2	1:B:897:ILE:HD11	1.95	0.47
1:C:474:ILE:O	1:C:478:MET:HB2	2.15	0.47
1:C:1:MET:HE1	1:C:439:GLN:HE22	1.80	0.47
1:C:140:VAL:HG12	1:C:140:VAL:O	2.13	0.47
1:B:355:MET:SD	1:B:368:PRO:HB2	2.54	0.47
1:B:729:ILE:CG1	1:B:730:ASP:H	2.24	0.47
1:B:750:LEU:C	1:B:750:LEU:CD1	2.82	0.47
1:B:158:VAL:CA	1:B:162:MET:HG2	2.36	0.47
1:B:864:TYR:O	1:B:868:LEU:HB2	2.14	0.47
1:B:568:ASP:HA	1:B:644:VAL:HG21	1.96	0.47
1:A:65:ILE:HD12	1:A:65:ILE:C	2.34	0.47
1:C:327:TYR:HD1	1:C:571:VAL:HB	1.80	0.47
1:A:114:ALA:O	1:A:115:MET:C	2.53	0.47
1:A:130:GLU:HG2	1:B:113:LEU:HD11	1.97	0.47
1:A:65:ILE:CA	1:A:66:GLU:N	2.66	0.47
1:A:69:MET:HA	1:A:69:MET:CE	2.44	0.47
1:A:95:GLU:O	1:A:98:THR:CG2	2.62	0.47
1:C:66:GLU:HB3	1:C:78:MET:HE1	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:THR:O	1:C:66:GLU:HG3	2.15	0.47
1:B:467:TYR:O	1:B:470:PHE:HB2	2.14	0.47
1:B:908:GLY:C	1:B:910:ILE:H	2.17	0.47
1:B:978:THR:HG23	1:B:979:SER:N	2.30	0.47
1:A:1015:THR:C	1:A:1017:LEU:H	2.18	0.47
1:A:344:LEU:HD22	1:A:402:ILE:CD1	2.45	0.47
1:B:314:GLU:HA	1:B:317:PHE:CD2	2.50	0.47
1:A:1026:PHE:O	1:A:1030:ARG:HB2	2.14	0.47
1:C:415:ASN:HD21	1:C:434:SER:CB	2.27	0.47
1:C:417:GLU:CA	1:C:417:GLU:OE2	2.55	0.47
1:C:1:MET:CB	1:C:2:PRO:HD2	2.21	0.47
1:B:85:THR:HG23	1:B:87:THR:HB	1.95	0.47
1:B:144:ASN:OD1	1:B:149:MET:HG3	2.15	0.47
1:A:185:ARG:NH2	1:A:774:MET:HE2	2.29	0.47
1:A:200:PRO:CG	1:A:749:THR:HG23	2.45	0.47
1:B:612:VAL:HG23	1:B:626:ILE:O	2.15	0.47
1:C:925:VAL:C	1:C:927:PHE:N	2.68	0.47
1:C:934:THR:O	1:C:935:ILE:C	2.52	0.47
1:A:674:LEU:HD13	1:A:675:GLY:N	2.30	0.47
1:C:607:GLU:HB2	1:C:632:LYS:HD3	1.97	0.47
1:B:166:ILE:HG22	1:B:167:SER:N	2.30	0.47
1:C:300:LEU:O	1:C:301:ASP:C	2.53	0.47
1:B:17:ILE:HG21	1:C:886:LEU:HD21	1.97	0.47
1:B:354:VAL:HG21	1:B:981:ALA:HA	1.96	0.47
1:B:904:VAL:HG13	1:B:907:LEU:CD1	2.25	0.47
1:B:945:ILE:HG13	1:B:946:VAL:N	2.30	0.47
1:B:314:GLU:O	1:B:316:PHE:N	2.47	0.47
1:A:711:ASP:C	1:A:713:LEU:H	2.18	0.47
1:B:418:ARG:HH21	1:B:970:MET:HG2	1.80	0.47
1:A:221:GLY:C	1:A:222:THR:O	2.50	0.47
1:B:425:LEU:HA	1:B:426:PRO:HD3	1.70	0.47
1:C:688:ALA:C	1:C:690:LEU:N	2.66	0.47
1:C:695:LEU:O	1:C:696:THR:C	2.54	0.47
1:B:343:THR:HG21	1:B:1000:GLN:OE1	2.15	0.47
1:C:355:MET:CE	1:C:355:MET:HA	2.45	0.47
1:A:831:ALA:HA	1:A:840:ALA:CB	2.45	0.47
1:B:692:HIS:CE1	1:B:723:ASP:OD1	2.68	0.47
1:A:426:PRO:CB	1:A:427:PRO:HD2	2.45	0.47
1:B:588:GLN:HA	1:B:588:GLN:OE1	2.14	0.47
1:A:695:LEU:HG	1:A:695:LEU:O	2.14	0.47
1:A:223:PRO:HD3	1:B:275:TYR:CB	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:ASN:HB3	1:A:301:ASP:HB2	1.97	0.47
1:C:32:VAL:CG1	1:C:32:VAL:O	2.56	0.47
1:A:150:THR:O	1:A:151:GLN:C	2.54	0.47
1:A:8:ARG:HG3	1:A:8:ARG:O	2.15	0.47
1:A:118:LEU:HA	1:A:118:LEU:HD23	1.50	0.47
1:B:262:LEU:HD22	1:B:266:ALA:HB3	1.96	0.47
1:C:705:GLU:C	1:C:707:ALA:N	2.67	0.47
1:C:393:LEU:C	1:C:395:MET:H	2.18	0.47
1:C:184:MET:HE3	1:C:270:LEU:HA	1.97	0.47
1:B:790:TYR:HD1	1:B:800:PRO:N	2.13	0.47
1:B:792:ARG:HB2	1:B:798:MET:HE1	1.97	0.47
1:C:721:LEU:HD23	1:C:721:LEU:O	2.15	0.47
1:B:57:VAL:HG11	1:B:86:GLY:HA2	1.97	0.47
1:B:428:LYS:O	1:B:432:ARG:HB2	2.15	0.47
1:A:58:GLN:HE21	1:A:816:LEU:CD1	2.28	0.46
1:C:315:PRO:HB2	1:C:316:PHE:CD1	2.50	0.46
1:B:538:THR:H	1:B:540:ARG:HH21	1.61	0.46
1:B:979:SER:HB3	1:B:1011:MET:HE3	1.97	0.46
1:C:713:LEU:CD2	1:C:835:LYS:H	2.24	0.46
1:C:729:ILE:HD11	1:C:786:ILE:CD1	2.33	0.46
1:A:713:LEU:HB2	1:A:833:PRO:CD	2.45	0.46
1:A:922:THR:C	1:A:924:ASP:H	2.18	0.46
1:B:115:MET:HE1	1:B:127:VAL:CG2	2.36	0.46
1:C:872:GLN:HB2	1:C:875:SER:CB	2.37	0.46
1:B:556:PHE:CA	1:B:913:LEU:HD21	2.46	0.46
1:C:578:LEU:CD2	1:C:590:VAL:HG21	2.45	0.46
1:C:332:PHE:CE1	1:C:569:GLN:HG2	2.50	0.46
1:C:169:THR:CG2	1:C:172:VAL:CG2	2.93	0.46
1:C:52:ALA:O	1:C:53:ASP:CG	2.53	0.46
1:B:538:THR:HG23	1:B:540:ARG:HH22	1.77	0.46
1:B:546:LEU:O	1:B:550:VAL:HB	2.15	0.46
1:B:217:GLY:HA3	1:C:754:TRP:O	2.16	0.46
1:C:399:VAL:O	1:C:401:ALA:N	2.49	0.46
1:C:445:ILE:HD13	1:C:940:LYS:HE3	1.97	0.46
1:B:375:VAL:HG22	1:B:484:VAL:HG21	1.97	0.46
1:C:228:GLN:HG3	1:C:228:GLN:O	2.15	0.46
1:B:690:LEU:HD22	1:B:694:LYS:HB2	1.97	0.46
1:C:259:ARG:CB	1:C:259:ARG:NH1	2.77	0.46
1:B:174:ASP:CG	1:B:175:VAL:N	2.69	0.46
1:C:719:ASN:N	2:C:1063:HOH:O	2.26	0.46
1:B:743:ILE:O	1:B:747:ASN:ND2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:279:ALA:HA	1:C:611:ALA:O	2.16	0.46
1:A:335:ILE:HD12	1:A:335:ILE:C	2.36	0.46
1:A:822:LEU:O	1:A:823:PRO:C	2.52	0.46
1:A:113:LEU:HD13	1:C:108:GLN:HE22	1.80	0.46
1:A:909:VAL:O	1:A:912:ALA:CB	2.59	0.46
1:B:345:VAL:HG12	1:B:349:ILE:CD1	2.45	0.46
1:B:898:PRO:O	1:B:899:PHE:C	2.53	0.46
1:A:728:LYS:HZ2	1:C:235:ILE:HG22	1.78	0.46
1:B:42:ALA:HA	1:B:93:THR:HA	1.97	0.46
1:C:559:LEU:HD13	1:C:917:THR:CG2	2.45	0.46
1:C:16:ALA:HB2	1:C:488:LEU:HD22	1.97	0.46
1:C:674:LEU:HD21	1:C:862:MET:N	2.29	0.46
1:B:355:MET:CE	1:B:369:THR:HG22	2.46	0.46
1:B:366:LEU:O	1:B:370:ILE:HG13	2.15	0.46
1:C:989:LEU:HD12	1:C:1000:GLN:HA	1.96	0.46
1:A:572:PHE:CD1	1:A:629:VAL:HG13	2.50	0.46
1:B:804:PHE:O	1:B:805:SER:CB	2.63	0.46
1:B:189:ASN:HB3	1:B:192:GLU:HB3	1.98	0.46
1:C:26:ALA:O	1:C:30:LEU:CG	2.64	0.46
1:A:822:LEU:HG	2:A:1055:HOH:O	2.15	0.46
1:C:169:THR:HG22	1:C:172:VAL:CG2	2.41	0.46
1:B:11:PHE:O	1:B:14:VAL:N	2.48	0.46
1:C:897:ILE:HD13	1:C:950:LYS:HG3	1.98	0.46
1:B:316:PHE:CE2	1:C:687:GLN:HG3	2.50	0.46
1:C:1022:VAL:O	1:C:1023:PRO:C	2.50	0.46
1:B:693:GLU:C	1:B:695:LEU:N	2.68	0.46
1:A:316:PHE:O	1:A:321:LEU:HD11	2.15	0.46
1:A:741:VAL:HG22	1:A:746:ILE:HD11	1.97	0.46
1:A:135:SER:O	1:A:136:PHE:CG	2.69	0.46
1:C:470:PHE:CD2	1:C:929:VAL:HG11	2.50	0.46
1:B:104:GLN:HG2	1:B:105:VAL:N	2.27	0.46
2:B:1060:HOH:O	1:C:110:LYS:CD	2.59	0.46
1:C:60:THR:HG22	1:C:61:VAL:HG23	1.97	0.46
1:B:1020:PHE:O	1:B:1023:PRO:HG2	2.15	0.46
1:A:1015:THR:OG1	1:A:1016:VAL:N	2.48	0.46
1:C:696:THR:O	1:C:697:GLN:C	2.52	0.46
1:A:713:LEU:CG	1:A:832:ALA:HA	2.46	0.46
1:A:729:ILE:HD13	1:C:234:ILE:HG23	1.97	0.46
1:B:518:ARG:O	1:B:520:PHE:N	2.48	0.46
1:B:518:ARG:HA	1:B:521:GLU:CG	2.46	0.46
1:A:203:VAL:HG13	1:A:262:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:PRO:HG2	1:B:98:THR:CG2	2.46	0.46
1:B:287:SER:OG	1:B:288:GLY:N	2.49	0.46
1:C:321:LEU:C	1:C:321:LEU:HD13	2.36	0.46
1:A:109:ASN:CG	1:C:108:GLN:OE1	2.53	0.46
1:A:820:ASN:HB3	1:C:168:ARG:NH2	2.31	0.46
1:C:58:GLN:C	2:C:1079:HOH:O	2.54	0.46
1:A:552:MET:HB2	1:A:910:ILE:HG23	1.96	0.46
1:C:355:MET:CE	1:C:977:MET:HG2	2.45	0.46
1:C:418:ARG:NH2	1:C:948:PHE:HZ	2.14	0.46
1:B:693:GLU:O	1:B:695:LEU:N	2.49	0.46
1:A:572:PHE:CE1	1:A:629:VAL:CG1	2.99	0.46
1:B:613:ASN:O	1:B:625:GLY:HA2	2.16	0.46
1:A:166:ILE:HG22	1:A:172:VAL:HG11	1.98	0.46
1:B:174:ASP:OD1	1:B:175:VAL:N	2.49	0.46
1:A:252:LYS:HB3	1:A:260:VAL:CG2	2.45	0.46
1:C:666:PHE:HD2	1:C:666:PHE:N	2.13	0.46
1:C:895:TRP:HA	1:C:895:TRP:CE3	2.51	0.46
1:A:58:GLN:NE2	1:A:816:LEU:CD1	2.78	0.46
1:B:213:GLN:CG	1:C:56:THR:HG23	2.45	0.46
1:B:470:PHE:O	1:B:471:SER:C	2.52	0.46
1:B:920:GLY:O	1:B:921:LEU:O	2.34	0.46
1:C:400:LEU:HD12	1:C:930:GLY:HA2	1.98	0.46
1:C:663:VAL:HG12	1:C:664:PHE:N	2.30	0.46
1:B:819:TYR:O	1:B:820:ASN:C	2.54	0.46
1:B:252:LYS:HG2	1:B:253:VAL:H	1.80	0.46
1:A:349:ILE:CD1	1:A:349:ILE:N	2.79	0.46
1:A:639:GLY:O	1:A:640:GLU:C	2.54	0.46
1:B:973:ARG:CG	1:B:974:PRO:CD	2.92	0.46
1:B:344:LEU:O	1:B:347:ALA:HB3	2.16	0.46
1:B:897:ILE:HG13	1:B:898:PRO:CD	2.46	0.46
1:C:356:TYR:C	1:C:358:PHE:H	2.18	0.46
1:A:443:VAL:O	1:A:444:GLY:C	2.54	0.46
1:A:187:TRP:HH2	1:C:223:PRO:HG3	1.79	0.46
1:A:572:PHE:N	1:A:572:PHE:HD1	2.13	0.46
1:A:576:VAL:HG11	1:A:591:LEU:CD2	2.45	0.46
1:B:716:VAL:HA	1:B:828:LEU:O	2.16	0.46
1:B:219:LEU:HD21	1:C:783:PRO:HG3	1.97	0.46
1:B:231:ASN:O	1:B:231:ASN:CG	2.52	0.46
1:B:671:ILE:HB	1:B:672:VAL:H	1.50	0.46
1:A:66:GLU:OE2	1:A:818:ARG:HD2	2.16	0.46
1:C:165:ALA:O	1:C:166:ILE:O	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:307:ARG:HA	1:C:310:LEU:HD12	1.98	0.46
1:C:49:TYR:HB3	1:C:52:ALA:HB3	1.98	0.46
1:C:66:GLU:O	1:C:69:MET:N	2.49	0.46
1:B:396:PHE:CD2	1:B:1003:VAL:HG21	2.50	0.46
1:C:545:TYR:CZ	1:C:1025:PHE:CZ	3.04	0.46
1:B:20:MET:HE2	1:B:377:LEU:HD12	1.98	0.46
1:A:988:PRO:O	1:A:989:LEU:C	2.54	0.46
1:B:575:MET:HA	1:B:626:ILE:HG22	1.96	0.46
1:B:778:LYS:O	1:B:779:TYR:CB	2.64	0.46
1:A:44:THR:C	1:A:45:ILE:HG13	2.35	0.46
1:B:429:GLU:HA	1:B:432:ARG:HB3	1.97	0.46
1:A:23:GLY:O	1:A:27:ILE:HG12	2.16	0.46
1:C:514:GLY:O	1:C:518:ARG:HG3	2.16	0.46
1:C:818:ARG:NH2	1:C:821:GLY:O	2.47	0.46
1:C:711:ASP:CG	1:C:712:MET:N	2.70	0.46
1:A:543:VAL:HG22	1:A:544:LEU:H	1.80	0.46
1:C:549:VAL:C	1:C:551:GLY:H	2.18	0.46
1:C:945:ILE:CG2	1:C:1022:VAL:HG11	2.46	0.46
1:A:428:LYS:HE3	1:A:429:GLU:OE2	2.15	0.46
1:C:228:GLN:NE2	1:C:230:LEU:O	2.49	0.46
1:C:446:ALA:C	1:C:448:VAL:H	2.20	0.46
1:A:521:GLU:N	1:A:522:LYS:HE2	2.31	0.46
1:C:759:VAL:O	1:C:760:ASN:CB	2.47	0.46
1:A:371:ALA:O	1:A:372:VAL:C	2.54	0.46
1:A:171:GLY:O	1:A:294:ALA:CB	2.64	0.46
1:C:367:ILE:HG13	1:C:368:PRO:N	2.30	0.46
1:B:686:ASP:CB	1:B:823:PRO:O	2.62	0.46
1:B:112:GLN:HB2	2:B:1055:HOH:O	2.16	0.45
1:C:114:ALA:HA	1:C:117:LEU:HD12	1.97	0.45
1:C:88:VAL:HG12	1:C:89:GLN:N	2.32	0.45
1:C:44:THR:O	1:C:45:ILE:C	2.54	0.45
1:B:907:LEU:O	1:B:910:ILE:HG22	2.16	0.45
1:B:939:ALA:O	1:B:943:ILE:HB	2.15	0.45
1:B:975:ILE:N	1:B:975:ILE:CD1	2.78	0.45
1:C:695:LEU:HD22	1:C:825:MET:CE	2.46	0.45
1:B:1005:THR:CG2	1:B:1005:THR:O	2.60	0.45
1:B:987:MET:HE2	1:B:991:ILE:HG23	1.98	0.45
1:C:939:ALA:O	1:C:943:ILE:CG1	2.64	0.45
1:C:491:ALA:O	1:C:493:CYS:N	2.38	0.45
1:B:597:TYR:CE1	1:B:654:ALA:CB	2.99	0.45
1:B:602:GLU:CD	1:B:650:ARG:HH21	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:PRO:HG3	1:A:497:LEU:O	2.16	0.45
1:B:45:ILE:CG2	1:B:46:SER:N	2.79	0.45
1:C:143:ILE:CG2	1:C:284:GLN:NE2	2.64	0.45
1:B:714:THR:HG22	1:B:831:ALA:N	2.30	0.45
1:B:170:SER:C	1:B:172:VAL:H	2.19	0.45
1:B:579:PRO:HD3	1:B:660:ASP:O	2.16	0.45
1:B:189:ASN:HD22	1:B:190:PRO:HD2	1.81	0.45
1:C:246:PHE:O	1:C:249:ILE:HG13	2.17	0.45
1:B:162:MET:CB	1:B:313:MET:SD	3.04	0.45
1:C:350:LEU:HD13	1:C:984:LEU:HD22	1.93	0.45
1:B:157:TYR:O	1:B:161:ASN:ND2	2.45	0.45
1:B:74:ASN:O	1:B:94:PHE:CB	2.62	0.45
1:B:193:LEU:HD23	1:B:265:VAL:HG21	1.98	0.45
1:C:111:LEU:HD13	1:C:111:LEU:C	2.35	0.45
1:C:162:MET:O	1:C:166:ILE:HG12	2.16	0.45
1:B:539:GLY:C	1:B:541:TYR:H	2.20	0.45
1:B:545:TYR:C	1:B:547:ILE:H	2.20	0.45
1:A:1018:ALA:HB1	1:A:1022:VAL:HG13	1.95	0.45
1:A:552:MET:C	1:A:554:TYR:N	2.69	0.45
1:C:1017:LEU:CD2	1:C:1017:LEU:O	2.56	0.45
1:C:907:LEU:HD23	1:C:1018:ALA:HA	1.99	0.45
1:C:343:THR:O	1:C:344:LEU:C	2.55	0.45
1:C:399:VAL:C	1:C:401:ALA:N	2.70	0.45
1:C:547:ILE:HA	1:C:550:VAL:HG12	1.98	0.45
1:B:633:ASP:CG	1:B:634:TRP:N	2.68	0.45
1:A:189:ASN:HB2	1:A:779:TYR:CZ	2.51	0.45
1:A:243:THR:HG22	1:A:268:ILE:CG2	2.46	0.45
1:C:626:ILE:HD13	1:C:627:ALA:H	1.80	0.45
1:A:569:GLN:O	1:A:570:GLY:C	2.55	0.45
1:B:513:PHE:N	1:B:513:PHE:CD1	2.83	0.45
1:C:159:ALA:HB1	1:C:181:GLN:HG3	1.98	0.45
1:A:913:LEU:C	1:A:915:ALA:H	2.20	0.45
1:C:535:LEU:HG	1:C:535:LEU:O	2.16	0.45
1:B:970:MET:HE2	1:B:970:MET:CA	2.45	0.45
1:A:696:THR:O	1:A:699:ARG:N	2.49	0.45
1:C:363:ARG:O	1:C:367:ILE:HG22	2.15	0.45
1:C:108:GLN:HG3	1:C:129:VAL:HG21	1.97	0.45
1:C:160:ALA:HA	1:C:767:ARG:CZ	2.47	0.45
1:B:972:LEU:HD13	1:B:976:LEU:CD2	2.41	0.45
1:A:1022:VAL:N	1:A:1023:PRO:HD2	2.31	0.45
1:A:552:MET:O	1:A:554:TYR:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:693:GLU:O	1:B:696:THR:OG1	2.26	0.45
1:B:705:GLU:C	1:B:707:ALA:N	2.70	0.45
1:B:602:GLU:O	1:B:604:ASN:N	2.50	0.45
1:B:97:GLY:O	1:B:98:THR:O	2.34	0.45
1:C:858:ASP:OD1	1:C:859:TRP:N	2.50	0.45
1:C:614:GLY:HA2	1:C:621:GLY:O	2.17	0.45
1:C:897:ILE:HG12	1:C:950:LYS:CE	2.47	0.45
1:C:685:ILE:CG1	1:C:687:GLN:OE1	2.61	0.45
1:C:140:VAL:HB	1:C:289:LEU:HB2	1.99	0.45
1:B:659:LYS:HD3	1:B:659:LYS:C	2.36	0.45
1:B:776:GLU:CG	1:B:777:ALA:N	2.79	0.45
1:A:294:ALA:HB3	1:A:297:ALA:HB3	1.97	0.45
1:A:740:GLY:O	1:A:794:ALA:N	2.43	0.45
1:C:218:GLN:HG2	1:C:232:ALA:O	2.17	0.45
1:C:114:ALA:O	1:C:115:MET:O	2.34	0.45
1:C:758:TYR:O	1:C:758:TYR:CG	2.70	0.45
1:C:1016:VAL:C	1:C:1018:ALA:H	2.16	0.45
1:C:940:LYS:HA	1:C:943:ILE:HG12	1.99	0.45
1:C:937:LEU:O	1:C:940:LYS:HB3	2.16	0.45
1:B:847:LEU:HD23	1:B:847:LEU:N	2.29	0.45
1:A:281:PHE:CZ	1:A:324:VAL:HG11	2.52	0.45
1:B:65:ILE:HG23	1:B:111:LEU:HD13	1.98	0.45
1:A:583:THR:HG22	1:A:584:GLN:N	2.31	0.45
1:B:188:MET:HE1	1:B:203:VAL:HG11	1.97	0.45
1:B:26:ALA:HB1	1:B:384:ALA:HB2	1.98	0.45
1:C:577:GLN:HB3	1:C:624:THR:CG2	2.42	0.45
1:A:11:PHE:C	1:A:13:TRP:H	2.18	0.45
1:A:607:GLU:HB2	1:A:631:LEU:O	2.17	0.45
1:C:714:THR:CG2	1:C:716:VAL:HG23	2.46	0.45
1:B:709:HIS:O	1:B:711:ASP:N	2.50	0.45
1:C:721:LEU:CD1	1:C:815:ARG:O	2.64	0.45
1:B:725:PRO:HB2	1:B:809:TRP:CZ3	2.51	0.45
1:B:680:PHE:C	1:B:680:PHE:CD1	2.90	0.45
1:B:569:GLN:OE1	1:B:569:GLN:HA	2.16	0.45
1:A:822:LEU:HA	1:A:823:PRO:HD3	1.32	0.45
1:C:162:MET:CB	1:C:313:MET:HE3	2.35	0.45
1:C:950:LYS:NZ	1:C:1030:ARG:NE	2.65	0.45
1:B:1018:ALA:O	1:B:1020:PHE:N	2.50	0.45
1:B:974:PRO:C	1:B:976:LEU:N	2.70	0.45
1:B:987:MET:CE	1:B:990:VAL:HB	2.47	0.45
1:B:418:ARG:NH2	1:B:970:MET:CG	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:987:MET:HA	1:C:1008:MET:HE1	1.99	0.45
1:B:863:SER:O	1:B:864:TYR:C	2.55	0.45
1:B:868:LEU:O	1:B:869:SER:C	2.55	0.45
1:A:1:MET:H3	1:A:2:PRO:HD2	1.75	0.45
1:A:492:LEU:HD12	1:A:492:LEU:HA	1.64	0.45
1:A:684:LEU:HD11	1:A:851:LEU:HD13	1.98	0.45
1:B:376:LEU:O	1:B:379:THR:N	2.49	0.45
1:A:65:ILE:O	1:A:68:ASN:CB	2.63	0.45
1:C:310:LEU:HD22	1:C:323:ILE:HD13	1.99	0.45
1:C:758:TYR:HA	1:C:772:TYR:HA	1.98	0.45
1:B:187:TRP:CZ3	1:B:774:MET:CE	2.94	0.45
1:C:774:MET:HG2	1:C:775:SER:N	2.31	0.45
1:C:779:TYR:CD2	1:C:779:TYR:N	2.83	0.45
1:B:987:MET:CE	1:B:987:MET:O	2.62	0.45
1:C:34:GLN:HA	1:C:333:VAL:CG1	2.47	0.45
1:C:14:VAL:CG1	1:C:15:ILE:N	2.79	0.45
1:B:687:GLN:CD	1:B:856:GLY:HA3	2.34	0.45
1:C:249:ILE:HD13	1:C:249:ILE:HG21	1.61	0.45
1:C:242:SER:O	1:C:243:THR:C	2.55	0.45
1:B:269:GLU:HB3	1:B:270:LEU:H	1.61	0.45
1:B:174:ASP:C	1:B:175:VAL:HG23	2.37	0.45
1:C:176:GLN:HE21	1:C:620:ARG:HH11	1.64	0.45
1:A:73:ASP:O	1:A:75:LEU:N	2.42	0.45
1:A:82:SER:HB2	1:A:816:LEU:HB2	1.99	0.45
1:C:104:GLN:CD	1:C:131:LYS:HE2	2.38	0.45
1:C:163:LYS:HG2	1:C:175:VAL:CG1	2.45	0.45
1:C:753:ALA:O	1:C:775:SER:CB	2.65	0.45
1:B:345:VAL:HG12	1:B:349:ILE:HD13	1.98	0.45
1:C:355:MET:HE1	1:C:977:MET:HG2	1.98	0.45
1:A:400:LEU:HD21	1:A:1003:VAL:HG22	1.98	0.45
1:A:713:LEU:CG	1:A:714:THR:H	2.30	0.45
1:C:395:MET:C	1:C:397:GLY:N	2.69	0.45
1:C:439:GLN:HG3	1:C:440:GLY:N	2.32	0.45
1:A:418:ARG:NH2	1:A:970:MET:HA	2.32	0.45
1:B:690:LEU:CB	1:B:694:LYS:HB2	2.38	0.45
1:B:775:SER:CB	1:B:780:ARG:HG3	2.46	0.45
1:B:271:GLY:HA3	1:B:275:TYR:OH	2.17	0.45
1:C:463:THR:CG2	1:C:464:GLY:H	2.28	0.45
1:A:372:VAL:O	1:A:373:PRO:C	2.55	0.45
1:C:680:PHE:HB2	1:C:859:TRP:HZ3	1.82	0.45
1:A:102:ILE:O	1:A:106:GLN:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:820:ASN:HB3	1:C:168:ARG:CZ	2.46	0.45
1:B:438:ILE:HD12	1:B:971:ARG:NH1	2.32	0.45
1:A:407:ASP:OD2	1:A:978:THR:HG21	2.17	0.45
1:A:897:ILE:HG21	1:A:950:LYS:CE	2.47	0.45
1:C:682:PHE:HE2	1:C:702:LEU:CD1	2.29	0.45
1:C:497:LEU:HD13	1:C:498:LYS:H	1.81	0.45
1:B:640:GLU:H	1:B:643:LYS:HG3	1.82	0.45
1:A:418:ARG:HH11	1:A:973:ARG:NE	2.14	0.45
1:B:762:PHE:HE1	1:B:764:ASP:HB2	1.82	0.45
1:A:219:LEU:HD12	1:A:232:ALA:HB3	1.99	0.45
1:B:819:TYR:CE1	1:B:860:THR:OG1	2.70	0.45
1:A:298:ASN:O	1:A:299:ALA:C	2.55	0.45
1:A:836:SER:OG	1:A:839:GLU:CG	2.62	0.45
1:A:208:LYS:HA	1:A:760:ASN:HD21	1.82	0.45
1:A:102:ILE:C	1:A:105:VAL:HG23	2.37	0.44
1:A:115:MET:N	1:A:116:PRO:CD	2.80	0.44
1:C:166:ILE:HD11	2:C:1075:HOH:O	2.05	0.44
1:B:341:VAL:HG23	1:B:395:MET:CE	2.47	0.44
1:B:640:GLU:N	1:B:643:LYS:HG3	2.32	0.44
1:B:643:LYS:C	1:B:647:ILE:HG13	2.38	0.44
1:A:330:THR:N	1:A:331:PRO:HD2	2.32	0.44
1:B:371:ALA:O	1:B:372:VAL:C	2.55	0.44
1:C:188:MET:HE1	1:C:200:PRO:CB	2.38	0.44
1:B:762:PHE:CE1	1:B:764:ASP:HB2	2.52	0.44
1:C:934:THR:HG22	1:C:1011:MET:SD	2.57	0.44
1:C:130:GLU:OE1	1:C:174:ASP:HB2	2.17	0.44
1:B:592:ASN:HA	1:B:595:THR:HG23	2.00	0.44
1:C:72:ILE:CG2	1:C:94:PHE:CZ	3.00	0.44
1:A:843:LEU:O	1:A:844:MET:C	2.56	0.44
1:A:846:GLN:HB2	1:A:846:GLN:HE21	1.60	0.44
1:A:94:PHE:HZ	1:A:107:VAL:HG22	1.82	0.44
1:C:58:GLN:NE2	1:C:82:SER:O	2.50	0.44
1:B:314:GLU:C	1:B:316:PHE:H	2.20	0.44
1:A:537:SER:O	1:A:538:THR:C	2.55	0.44
1:B:891:LEU:HD12	1:B:892:TYR:CD1	2.52	0.44
1:C:354:VAL:C	1:C:356:TYR:H	2.20	0.44
1:A:713:LEU:HB2	1:A:832:ALA:HA	1.90	0.44
1:C:418:ARG:NH2	1:C:948:PHE:CZ	2.85	0.44
1:A:562:SER:HB3	1:A:924:ASP:HB3	1.99	0.44
1:B:115:MET:HE2	1:B:115:MET:HA	1.98	0.44
1:A:790:TYR:CE1	1:A:800:PRO:CG	2.96	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:VAL:O	1:B:140:VAL:C	2.55	0.44
1:B:778:LYS:HZ2	1:B:778:LYS:HB3	1.82	0.44
1:C:335:ILE:HD13	1:C:634:TRP:CZ3	2.51	0.44
1:B:155:SER:O	1:B:156:ASP:C	2.55	0.44
1:C:657:GLN:C	1:C:659:LYS:N	2.71	0.44
1:A:393:LEU:HD13	1:A:466:ILE:HG23	1.98	0.44
1:C:873:ALA:O	1:C:876:LEU:N	2.50	0.44
1:A:356:TYR:C	1:A:358:PHE:H	2.21	0.44
1:C:323:ILE:HG22	1:C:324:VAL:O	2.17	0.44
1:C:758:TYR:CD1	1:C:758:TYR:N	2.83	0.44
1:A:1029:VAL:HG12	1:A:1030:ARG:N	2.21	0.44
1:A:545:TYR:HE1	1:A:907:LEU:HD11	1.82	0.44
1:C:527:TYR:O	1:C:531:VAL:HG13	2.17	0.44
1:C:912:ALA:O	1:C:914:LEU:O	2.34	0.44
1:C:948:PHE:O	1:C:952:LEU:HB2	2.16	0.44
1:B:696:THR:O	1:B:699:ARG:HB3	2.17	0.44
1:B:703:LEU:O	1:B:705:GLU:HB2	2.17	0.44
1:B:115:MET:HE1	1:B:127:VAL:HG11	2.00	0.44
1:A:207:ILE:HG22	1:A:207:ILE:O	2.17	0.44
1:C:931:LEU:O	1:C:935:ILE:HB	2.17	0.44
1:A:702:LEU:HD11	1:A:844:MET:HE2	1.99	0.44
1:B:740:GLY:O	1:B:794:ALA:HB2	2.17	0.44
1:C:801:PHE:CD1	1:C:804:PHE:HE1	2.36	0.44
1:A:678:THR:O	1:A:679:GLY:O	2.35	0.44
1:A:94:PHE:CZ	1:A:103:ALA:HB1	2.52	0.44
1:B:945:ILE:O	1:B:949:ALA:N	2.32	0.44
1:A:978:THR:C	1:A:980:LEU:N	2.70	0.44
1:C:685:ILE:HD11	1:C:687:GLN:CD	2.38	0.44
1:A:1018:ALA:HB1	1:A:1022:VAL:HG11	1.98	0.44
1:A:540:ARG:O	1:A:543:VAL:HG12	2.18	0.44
1:C:395:MET:O	1:C:397:GLY:N	2.50	0.44
1:B:835:LYS:HD2	1:B:839:GLU:OE1	2.18	0.44
1:B:44:THR:HG22	1:B:45:ILE:O	2.17	0.44
1:C:286:ALA:HB1	1:C:287:SER:H	1.48	0.44
1:B:520:PHE:O	1:B:523:SER:N	2.43	0.44
1:B:362:PHE:O	1:B:365:THR:N	2.43	0.44
1:B:785:ASP:O	1:B:788:ASP:N	2.47	0.44
1:B:804:PHE:O	1:B:805:SER:HB3	2.17	0.44
1:B:150:THR:O	1:B:151:GLN:C	2.55	0.44
1:A:340:VAL:HG13	1:A:399:VAL:HG23	1.96	0.44
1:B:188:MET:HB2	1:B:775:SER:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:682:PHE:HD1	1:B:859:TRP:CZ3	2.36	0.44
1:B:79:SER:OG	1:B:79:SER:O	2.26	0.44
1:A:178:PHE:HD1	1:A:178:PHE:N	2.15	0.44
1:A:130:GLU:HB3	2:A:1074:HOH:O	2.17	0.44
1:A:687:GLN:HG2	1:C:316:PHE:CD2	2.49	0.44
1:A:820:ASN:HB3	1:C:168:ARG:NH1	2.33	0.44
1:C:181:GLN:HG2	1:C:769:LYS:CE	2.46	0.44
1:B:1021:PHE:HB3	1:B:1025:PHE:CE1	2.53	0.44
1:A:407:ASP:OD1	1:A:940:LYS:NZ	2.40	0.44
1:C:434:SER:O	1:C:438:ILE:HB	2.17	0.44
1:B:702:LEU:HD22	1:B:702:LEU:HA	1.78	0.44
1:A:307:ARG:NH1	1:A:325:TYR:CE2	2.86	0.44
1:B:26:ALA:O	1:B:30:LEU:CB	2.65	0.44
1:A:746:ILE:HD13	1:A:804:PHE:CE1	2.52	0.44
1:C:197:GLN:HB3	1:C:197:GLN:HE21	1.57	0.44
1:A:437:GLN:HG2	1:A:948:PHE:CE2	2.52	0.44
1:A:687:GLN:HB2	1:A:687:GLN:HE21	1.18	0.44
1:C:163:LYS:C	1:C:165:ALA:N	2.71	0.44
1:C:686:ASP:HB2	1:C:695:LEU:HD12	1.98	0.44
1:A:1020:PHE:C	1:A:1023:PRO:HD2	2.38	0.44
1:A:729:ILE:CD1	1:A:729:ILE:N	2.78	0.44
1:C:35:TYR:HB3	1:C:36:PRO:HD2	2.00	0.44
1:C:901:VAL:HG12	1:C:942:ALA:CB	2.47	0.44
1:A:971:ARG:C	1:A:974:PRO:HD2	2.38	0.44
1:A:323:ILE:HG12	1:A:325:TYR:CE1	2.49	0.44
1:A:621:GLY:C	1:A:623:ASN:H	2.21	0.44
1:B:53:ASP:HB2	1:B:56:THR:HB	1.99	0.44
1:A:521:GLU:HG2	1:A:521:GLU:O	2.18	0.44
1:C:262:LEU:HG	1:C:268:ILE:HD11	2.00	0.44
1:A:254:ASN:O	1:A:256:ASP:N	2.50	0.44
1:A:83:ASP:C	1:A:83:ASP:OD1	2.56	0.44
1:B:58:GLN:NE2	1:B:818:ARG:HH11	2.15	0.44
1:A:362:PHE:C	1:A:364:ALA:H	2.21	0.44
1:A:87:THR:HG21	1:A:620:ARG:NH2	2.33	0.44
1:A:946:VAL:O	1:A:946:VAL:HG12	2.18	0.44
1:C:169:THR:O	1:C:172:VAL:HG23	2.18	0.44
1:C:888:LEU:O	1:C:891:LEU:HB3	2.17	0.44
1:C:894:SER:C	1:C:896:SER:N	2.66	0.44
1:A:979:SER:O	1:A:983:ILE:HG22	2.17	0.44
1:C:696:THR:O	1:C:699:ARG:N	2.50	0.44
1:B:338:HIS:O	1:B:341:VAL:HG12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:712:MET:SD	1:B:839:GLU:HB3	2.57	0.44
1:B:118:LEU:O	1:B:119:PRO:C	2.56	0.44
1:C:182:TYR:HA	1:C:271:GLY:O	2.18	0.44
1:B:682:PHE:HD1	1:B:859:TRP:CH2	2.35	0.44
1:C:467:TYR:C	1:C:469:GLN:N	2.71	0.44
1:C:538:THR:O	1:C:540:ARG:HG2	2.18	0.44
1:A:3:ASN:O	1:A:6:ILE:HD13	2.18	0.44
1:B:767:ARG:HG2	1:B:769:LYS:HE3	2.00	0.44
1:C:198:LEU:HA	1:C:792:ARG:NH2	2.33	0.44
1:B:378:GLY:O	1:B:381:ALA:HB3	2.18	0.44
1:C:124:GLN:HB3	1:C:758:TYR:CE2	2.50	0.44
1:C:87:THR:HG23	1:C:88:VAL:H	1.82	0.44
1:A:1024:VAL:CG1	1:A:1025:PHE:H	2.09	0.44
1:C:432:ARG:CG	1:C:432:ARG:NH1	2.62	0.44
1:C:1010:GLY:HA2	1:C:1013:THR:CG2	2.48	0.44
1:C:892:TYR:OH	1:C:943:ILE:HG23	2.17	0.44
1:A:649:MET:CE	1:A:653:ARG:NH2	2.80	0.44
1:A:594:VAL:HA	1:A:655:PHE:CZ	2.53	0.44
1:B:38:ILE:O	1:B:462:SER:HB2	2.18	0.44
1:A:313:MET:C	1:A:315:PRO:CD	2.85	0.44
1:A:3:ASN:HA	1:A:6:ILE:HD12	1.99	0.44
1:B:58:GLN:NE2	1:B:818:ARG:NH1	2.66	0.44
1:C:470:PHE:O	1:C:471:SER:C	2.55	0.44
1:C:163:LYS:O	1:C:166:ILE:CA	2.61	0.44
1:B:13:TRP:HA	1:B:13:TRP:HE3	1.80	0.44
1:B:534:ILE:HG23	1:B:541:TYR:CE2	2.53	0.44
1:C:832:ALA:HB1	1:C:833:PRO:CD	2.48	0.44
1:A:540:ARG:NH1	1:A:541:TYR:CZ	2.86	0.44
1:C:941:ASN:O	1:C:945:ILE:HG22	2.18	0.44
1:C:928:GLN:O	1:C:932:LEU:HG	2.18	0.44
1:A:520:PHE:O	1:A:522:LYS:N	2.51	0.44
1:A:339:GLU:HA	1:A:342:LYS:HG2	1.99	0.44
1:A:722:GLU:HA	2:A:1060:HOH:O	2.17	0.44
1:A:256:ASP:HB2	1:A:258:SER:HB3	1.99	0.44
1:A:935:ILE:O	1:A:935:ILE:CG2	2.64	0.44
1:A:525:HIS:O	1:A:526:HIS:C	2.53	0.44
1:B:881:LEU:HD21	1:B:905:VAL:HG21	1.99	0.43
1:A:541:TYR:O	1:A:543:VAL:O	2.36	0.43
1:B:921:LEU:CD2	1:B:1005:THR:CG2	2.96	0.43
1:B:699:ARG:NH2	1:B:722:GLU:OE1	2.51	0.43
1:C:267:LYS:HE3	1:C:267:LYS:HB2	1.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:692:HIS:HE1	1:C:721:LEU:HD21	1.83	0.43
1:A:216:ALA:O	1:A:217:GLY:O	2.36	0.43
1:A:116:PRO:CA	1:A:117:LEU:HD22	2.48	0.43
1:B:1031:ARG:O	1:B:1035:ARG:HB2	2.17	0.43
1:C:711:ASP:CG	1:C:712:MET:H	2.22	0.43
1:C:713:LEU:HD11	1:C:835:LYS:H	1.82	0.43
1:C:191:ASN:HA	1:C:194:ASN:OD1	2.18	0.43
1:B:885:PHE:HE2	1:B:898:PRO:HB2	1.83	0.43
1:C:34:GLN:C	1:C:35:TYR:CG	2.91	0.43
1:C:379:THR:HG23	1:C:477:ALA:HB2	1.99	0.43
1:C:403:GLY:C	1:C:405:LEU:H	2.21	0.43
1:A:958:LYS:HB3	1:A:959:GLY:H	1.64	0.43
1:C:226:LYS:HG2	2:C:1072:HOH:O	2.17	0.43
1:A:583:THR:CG2	1:A:584:GLN:N	2.80	0.43
1:B:612:VAL:HG23	1:B:626:ILE:HG13	2.00	0.43
1:A:455:PRO:O	1:A:876:LEU:HD13	2.18	0.43
1:C:72:ILE:CG2	1:C:94:PHE:HE2	2.23	0.43
1:C:262:LEU:O	1:C:264:ASP:N	2.51	0.43
1:B:818:ARG:HH11	1:B:818:ARG:HG3	1.82	0.43
1:B:732:ASP:HB2	1:B:735:LYS:HG3	2.00	0.43
1:A:72:ILE:O	1:A:73:ASP:O	2.37	0.43
1:C:51:GLY:O	1:C:53:ASP:OD2	2.36	0.43
1:B:453:PHE:CZ	1:B:474:ILE:HD13	2.53	0.43
1:B:408:ASP:C	1:B:410:ILE:H	2.20	0.43
1:B:538:THR:C	1:B:540:ARG:H	2.20	0.43
1:B:538:THR:O	1:B:540:ARG:N	2.51	0.43
1:C:686:ASP:C	1:C:686:ASP:OD1	2.55	0.43
1:A:943:ILE:O	1:A:947:GLU:HB2	2.17	0.43
1:B:999:ALA:O	1:B:1003:VAL:HG23	2.19	0.43
1:B:987:MET:HB3	1:B:988:PRO:HD3	1.99	0.43
1:B:699:ARG:O	1:B:700:ASN:HB2	2.18	0.43
1:B:362:PHE:C	1:B:364:ALA:N	2.72	0.43
1:B:801:PHE:HA	1:B:804:PHE:CE1	2.54	0.43
1:B:922:THR:HG1	1:B:923:ASN:H	1.62	0.43
1:C:764:ASP:OD2	1:C:765:ARG:NE	2.51	0.43
1:B:145:THR:O	1:B:146:ASP:CG	2.56	0.43
1:C:532:GLY:O	1:C:534:ILE:HD12	2.19	0.43
1:C:790:TYR:CE1	1:C:800:PRO:HB3	2.52	0.43
1:C:719:ASN:O	1:C:721:LEU:N	2.52	0.43
1:B:185:ARG:NH1	1:B:772:TYR:HB3	2.33	0.43
1:A:178:PHE:CD1	1:A:178:PHE:N	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:681:ASP:OD2	1:C:828:LEU:HD11	2.18	0.43
1:C:35:TYR:HD2	1:C:392:THR:HG1	1.65	0.43
1:B:110:LYS:HD3	1:B:110:LYS:HA	1.62	0.43
1:C:591:LEU:HA	1:C:591:LEU:HD13	1.67	0.43
1:B:225:VAL:CG2	1:C:781:MET:HE3	2.37	0.43
1:B:183:ALA:N	1:B:271:GLY:O	2.52	0.43
1:C:841:MET:O	1:C:842:GLU:C	2.56	0.43
1:C:881:LEU:O	1:C:882:ILE:C	2.57	0.43
1:A:778:LYS:HE2	1:A:778:LYS:HB2	1.48	0.43
1:A:818:ARG:NH2	1:A:823:PRO:HG3	2.33	0.43
1:B:9:PRO:O	1:B:13:TRP:N	2.42	0.43
1:C:896:SER:C	1:C:898:PRO:HD2	2.39	0.43
1:C:356:TYR:C	1:C:358:PHE:N	2.72	0.43
1:C:850:LYS:O	1:C:851:LEU:C	2.57	0.43
1:A:649:MET:HE3	1:A:653:ARG:CZ	2.46	0.43
1:C:238:THR:CG2	1:C:239:ARG:N	2.82	0.43
1:B:831:ALA:C	1:B:833:PRO:HD2	2.39	0.43
1:A:988:PRO:C	1:A:990:VAL:N	2.67	0.43
1:B:326:PRO:HB2	1:B:327:TYR:H	1.55	0.43
1:B:234:ILE:O	1:B:234:ILE:CG2	2.50	0.43
1:C:764:ASP:CB	1:C:765:ARG:HD2	2.49	0.43
1:A:857:TYR:O	1:A:857:TYR:CG	2.71	0.43
1:B:58:GLN:HA	1:B:62:THR:CB	2.48	0.43
1:B:18:ILE:HG22	1:B:19:ILE:N	2.34	0.43
1:B:109:ASN:ND2	1:B:112:GLN:HE22	2.14	0.43
1:C:82:SER:CB	1:C:88:VAL:HA	2.19	0.43
1:C:44:THR:HG22	1:C:91:THR:CA	2.47	0.43
1:C:91:THR:HB	1:C:91:THR:CA	2.20	0.43
1:B:1030:ARG:C	1:B:1032:ARG:H	2.22	0.43
1:B:904:VAL:C	1:B:906:PRO:HD2	2.39	0.43
1:C:695:LEU:O	1:C:696:THR:O	2.37	0.43
1:A:904:VAL:HG21	1:A:942:ALA:CB	2.45	0.43
1:B:396:PHE:HE2	1:B:999:ALA:HB1	1.82	0.43
1:C:4:PHE:CG	1:C:8:ARG:NH2	2.87	0.43
1:B:115:MET:HA	1:B:115:MET:HE3	2.00	0.43
1:B:207:ILE:HG22	1:B:759:VAL:HG11	1.97	0.43
1:A:454:VAL:N	1:A:455:PRO:HD2	2.33	0.43
1:B:776:GLU:HG2	1:B:777:ALA:H	1.83	0.43
1:B:819:TYR:O	1:B:822:LEU:N	2.51	0.43
1:A:222:THR:HG22	1:A:223:PRO:CD	2.48	0.43
1:B:873:ALA:C	1:B:875:SER:N	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:768:VAL:O	1:C:768:VAL:CG1	2.66	0.43
1:A:113:LEU:C	1:A:116:PRO:HD2	2.39	0.43
1:A:65:ILE:HG13	1:A:66:GLU:H	1.83	0.43
1:A:818:ARG:HG2	2:A:1062:HOH:O	2.16	0.43
1:C:118:LEU:CD1	1:C:118:LEU:N	2.82	0.43
1:B:415:ASN:O	1:B:434:SER:OG	2.28	0.43
1:C:685:ILE:O	1:C:685:ILE:HG13	2.08	0.43
1:C:544:LEU:HD12	1:C:1021:PHE:HZ	1.83	0.43
1:C:17:ILE:HD12	1:C:17:ILE:N	2.34	0.43
1:B:639:GLY:O	1:B:641:GLU:O	2.37	0.43
1:A:574:THR:HA	1:A:665:ALA:HA	2.01	0.43
1:A:418:ARG:O	1:A:421:ALA:HB3	2.19	0.43
1:B:245:GLU:O	1:B:248:LYS:N	2.51	0.43
1:A:809:TRP:O	1:A:810:GLU:CB	2.51	0.43
1:C:578:LEU:HA	1:C:661:ALA:HB1	2.00	0.43
1:A:11:PHE:O	1:A:13:TRP:N	2.52	0.43
1:C:534:ILE:H	1:C:534:ILE:HG13	1.55	0.43
1:C:878:ALA:C	1:C:880:SER:N	2.70	0.43
1:A:43:VAL:HA	1:A:130:GLU:O	2.19	0.43
1:A:66:GLU:CD	2:A:1054:HOH:O	2.56	0.43
1:A:822:LEU:CD2	1:A:822:LEU:N	2.81	0.43
1:B:345:VAL:CA	1:B:348:ILE:HD12	2.43	0.43
1:B:228:GLN:HE21	1:B:228:GLN:CA	2.32	0.43
1:A:2:PRO:O	1:A:6:ILE:N	2.51	0.43
1:A:359:LEU:HA	1:A:359:LEU:HD13	1.81	0.43
1:A:13:TRP:CZ2	1:A:492:LEU:HD11	2.54	0.43
1:B:231:ASN:HD22	1:B:232:ALA:N	2.17	0.43
1:B:1022:VAL:HB	1:B:1026:PHE:CZ	2.54	0.43
1:B:492:LEU:O	1:B:496:MET:HB2	2.18	0.43
1:C:728:LYS:CG	1:C:729:ILE:N	2.76	0.43
1:B:892:TYR:CG	1:B:897:ILE:HD11	2.54	0.43
1:C:529:ASP:O	1:C:531:VAL:O	2.36	0.43
1:C:14:VAL:CG1	1:C:15:ILE:H	2.31	0.43
1:A:367:ILE:HD13	1:A:489:THR:HG23	2.00	0.43
1:B:144:ASN:ND2	1:B:144:ASN:O	2.52	0.43
1:C:591:LEU:HD23	1:C:613:ASN:HB2	1.99	0.43
1:B:327:TYR:HB2	1:B:628:PHE:HB3	1.99	0.43
1:C:184:MET:HE1	1:C:270:LEU:N	2.34	0.43
1:B:556:PHE:C	1:B:558:ARG:H	2.22	0.43
1:A:166:ILE:HD13	1:A:166:ILE:H	1.78	0.43
1:C:653:ARG:HG3	1:C:654:ALA:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:845:GLU:CD	1:A:859:TRP:HE1	2.22	0.43
1:C:158:VAL:HG12	1:C:159:ALA:N	2.29	0.43
1:C:163:LYS:HB2	2:C:1078:HOH:O	2.18	0.43
1:C:166:ILE:HG21	1:C:291:ILE:HD11	2.01	0.43
1:B:411:VAL:HG12	1:B:974:PRO:HB3	2.00	0.43
1:B:489:THR:HB	1:B:490:PRO:CD	2.49	0.43
1:A:1023:PRO:C	1:A:1024:VAL:O	2.58	0.43
1:A:531:VAL:O	1:A:534:ILE:HG13	2.19	0.43
1:C:194:ASN:HB3	2:C:1059:HOH:O	2.19	0.43
1:C:778:LYS:CD	1:C:779:TYR:CE2	3.01	0.43
1:A:394:THR:CG2	1:A:395:MET:HE2	2.48	0.43
1:B:173:GLY:H	1:B:294:ALA:H	1.65	0.43
1:C:247:GLY:O	1:C:263:ARG:HB2	2.19	0.43
1:B:819:TYR:CZ	1:B:860:THR:OG1	2.72	0.43
1:B:328:ASP:OD2	1:B:330:THR:HB	2.19	0.43
1:A:197:GLN:HA	1:A:798:MET:HE2	2.00	0.43
1:A:182:TYR:CB	1:A:270:LEU:HD12	2.49	0.43
1:C:47:ALA:HB1	1:C:122:VAL:CG1	2.49	0.43
1:A:108:GLN:HG3	1:B:112:GLN:NE2	2.30	0.42
1:A:59:ASP:HB3	1:C:763:ILE:CD1	2.47	0.42
1:A:66:GLU:O	1:A:68:ASN:N	2.52	0.42
1:C:169:THR:CG2	1:C:169:THR:C	2.87	0.42
1:C:92:LEU:HD22	1:C:107:VAL:CG2	2.47	0.42
1:C:354:VAL:HG13	1:C:980:LEU:HD23	2.01	0.42
1:C:701:GLN:O	1:C:702:LEU:C	2.58	0.42
1:B:48:SER:C	1:B:49:TYR:CG	2.93	0.42
1:B:760:ASN:O	1:B:771:VAL:HB	2.19	0.42
1:A:449:LEU:O	1:A:451:ALA:O	2.37	0.42
1:B:858:ASP:OD1	1:B:859:TRP:N	2.52	0.42
1:B:330:THR:CG2	1:B:330:THR:O	2.67	0.42
1:A:308:ALA:O	1:A:311:ALA:HB3	2.19	0.42
1:A:83:ASP:OD1	1:A:84:SER:N	2.52	0.42
1:C:532:GLY:O	1:C:534:ILE:N	2.52	0.42
1:B:709:HIS:C	1:B:711:ASP:N	2.72	0.42
1:A:57:VAL:HG12	1:A:58:GLN:CA	2.49	0.42
1:C:159:ALA:CB	1:C:181:GLN:HG3	2.49	0.42
1:C:54:ALA:CB	1:C:84:SER:HB2	2.22	0.42
1:A:351:VAL:HG13	1:A:410:ILE:HD11	2.00	0.42
1:A:978:THR:HG23	1:A:979:SER:N	2.33	0.42
1:B:318:PRO:HD2	1:B:321:LEU:HD22	2.00	0.42
1:A:545:TYR:HB2	1:A:1021:PHE:CZ	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:947:GLU:O	1:A:951:ASP:CB	2.63	0.42
1:C:484:VAL:HG13	1:C:488:LEU:HB3	2.00	0.42
1:B:45:ILE:HD13	1:B:65:ILE:CG2	2.50	0.42
1:B:418:ARG:NH2	1:B:970:MET:HG3	2.35	0.42
1:A:219:LEU:HD22	1:B:781:MET:O	2.18	0.42
1:A:453:PHE:CZ	1:A:474:ILE:HG21	2.53	0.42
1:A:337:ILE:O	1:A:339:GLU:O	2.38	0.42
1:C:409:ALA:O	1:C:410:ILE:O	2.37	0.42
1:A:208:LYS:HA	1:A:760:ASN:ND2	2.34	0.42
1:C:532:GLY:C	1:C:534:ILE:N	2.71	0.42
1:A:156:ASP:O	1:A:157:TYR:C	2.55	0.42
1:A:108:GLN:OE1	1:B:112:GLN:NE2	2.53	0.42
1:C:123:GLN:HB3	1:C:124:GLN:H	1.68	0.42
1:B:404:LEU:O	1:B:406:VAL:N	2.53	0.42
1:A:532:GLY:HA2	1:A:965:LEU:HD11	2.01	0.42
1:C:344:LEU:O	1:C:348:ILE:HG23	2.19	0.42
1:C:524:THR:O	1:C:527:TYR:N	2.50	0.42
1:C:547:ILE:O	1:C:551:GLY:N	2.52	0.42
1:A:593:GLU:O	1:A:594:VAL:C	2.55	0.42
1:A:276:ASP:HB3	1:C:222:THR:CG2	2.42	0.42
1:C:983:ILE:HG23	1:C:1008:MET:HG3	2.01	0.42
1:A:937:LEU:HD12	1:A:1011:MET:SD	2.59	0.42
1:B:863:SER:C	1:B:865:GLN:N	2.71	0.42
1:B:715:SER:O	1:B:716:VAL:C	2.57	0.42
1:A:702:LEU:HD11	1:A:844:MET:HE3	2.01	0.42
1:A:471:SER:O	1:A:472:ILE:C	2.57	0.42
1:A:948:PHE:CD2	1:A:948:PHE:N	2.86	0.42
1:C:21:LEU:O	1:C:24:GLY:N	2.50	0.42
1:B:1004:GLY:O	1:B:1007:VAL:HG12	2.18	0.42
1:C:750:LEU:HA	1:C:750:LEU:HD23	1.53	0.42
1:A:25:LEU:C	1:A:25:LEU:HD13	2.40	0.42
1:C:894:SER:OG	1:C:897:ILE:N	2.33	0.42
1:B:885:PHE:CD2	1:B:898:PRO:HB2	2.55	0.42
1:C:417:GLU:OE2	1:C:420:MET:CE	2.67	0.42
1:C:491:ALA:C	1:C:493:CYS:H	2.22	0.42
1:A:562:SER:OG	1:A:563:PHE:N	2.51	0.42
1:B:114:ALA:O	1:B:115:MET:C	2.58	0.42
1:A:455:PRO:HG3	1:A:880:SER:HB2	2.02	0.42
1:B:778:LYS:HZ2	1:B:778:LYS:H	1.66	0.42
1:C:144:ASN:HA	1:C:320:GLY:O	2.20	0.42
1:B:671:ILE:H	1:B:671:ILE:HG12	1.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:ILE:O	1:C:19:ILE:C	2.56	0.42
1:B:870:GLY:O	1:B:872:GLN:N	2.52	0.42
1:A:116:PRO:HB2	1:A:117:LEU:HD22	2.02	0.42
1:A:407:ASP:O	1:A:411:VAL:HG23	2.20	0.42
1:C:775:SER:HG	1:C:789:TRP:HZ2	1.66	0.42
1:B:396:PHE:O	1:B:399:VAL:N	2.44	0.42
1:C:1021:PHE:N	1:C:1023:PRO:HD2	2.35	0.42
1:A:995:ALA:O	1:A:996:GLY:C	2.57	0.42
1:A:225:VAL:CG2	1:B:778:LYS:NZ	2.80	0.42
1:C:281:PHE:O	1:C:282:ASN:C	2.57	0.42
1:C:305:ALA:O	1:C:306:ILE:C	2.55	0.42
1:C:44:THR:HA	1:C:91:THR:HA	2.01	0.42
1:B:12:ALA:O	1:B:13:TRP:C	2.58	0.42
1:B:413:VAL:C	1:B:415:ASN:H	2.23	0.42
1:B:314:GLU:C	1:B:316:PHE:N	2.72	0.42
1:C:545:TYR:CZ	1:C:1021:PHE:CG	3.08	0.42
1:C:417:GLU:CB	1:C:973:ARG:HH12	2.32	0.42
1:B:712:MET:HE3	1:B:712:MET:HA	2.01	0.42
1:B:126:GLY:C	1:B:127:VAL:HG23	2.39	0.42
1:B:970:MET:HA	1:B:970:MET:CE	2.47	0.42
1:C:457:ALA:CB	1:C:468:ARG:CA	2.93	0.42
1:A:515:TRP:HD1	1:A:516:PHE:HB2	1.84	0.42
1:B:578:LEU:HD13	1:B:661:ALA:HB2	2.00	0.42
1:B:915:ALA:C	1:B:917:THR:H	2.23	0.42
1:A:47:ALA:HB3	1:A:88:VAL:CG2	2.50	0.42
1:C:55:LYS:CE	1:C:59:ASP:OD1	2.60	0.42
1:B:182:TYR:HD1	1:B:271:GLY:O	2.02	0.42
1:A:197:GLN:HA	1:A:798:MET:CE	2.49	0.42
1:B:472:ILE:O	1:B:473:THR:C	2.55	0.42
1:C:685:ILE:HD12	1:C:686:ASP:C	2.39	0.42
1:A:534:ILE:HD12	1:A:540:ARG:HH12	1.85	0.42
1:A:547:ILE:O	1:A:551:GLY:N	2.47	0.42
1:C:702:LEU:HD12	1:C:851:LEU:HD21	2.02	0.42
1:C:910:ILE:HG23	1:C:1013:THR:OG1	2.18	0.42
1:C:12:ALA:C	1:C:14:VAL:H	2.23	0.42
1:A:924:ASP:O	1:A:927:PHE:HB3	2.20	0.42
1:A:596:HIS:C	1:A:598:TYR:N	2.65	0.42
1:B:578:LEU:HB3	1:B:579:PRO:HD2	2.00	0.42
1:B:683:GLU:O	1:B:857:TYR:HA	2.18	0.42
1:C:331:PRO:O	1:C:332:PHE:C	2.56	0.42
1:A:105:VAL:HB	1:A:106:GLN:H	1.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:820:ASN:O	1:A:822:LEU:CD2	2.68	0.42
1:C:123:GLN:C	1:C:125:GLN:N	2.73	0.42
1:B:407:ASP:O	1:B:408:ASP:O	2.38	0.42
1:B:543:VAL:HG12	1:B:543:VAL:O	2.20	0.42
1:C:696:THR:HG22	1:C:699:ARG:HH12	1.85	0.42
1:C:777:ALA:HA	1:C:780:ARG:CZ	2.50	0.42
1:B:898:PRO:C	1:B:900:SER:H	2.23	0.42
1:C:379:THR:HB	1:C:398:MET:CE	2.47	0.42
1:C:489:THR:N	1:C:490:PRO:CD	2.81	0.42
1:A:187:TRP:CH2	1:C:223:PRO:HG3	2.55	0.42
1:A:635:ALA:C	1:A:637:ARG:N	2.73	0.42
1:B:463:THR:HA	1:B:466:ILE:HG13	2.00	0.42
1:C:352:PHE:CD1	1:C:369:THR:HG21	2.55	0.42
1:B:873:ALA:HB3	1:B:874:PRO:CD	2.50	0.42
1:C:666:PHE:CD2	1:C:666:PHE:C	2.92	0.42
1:A:180:SER:O	1:A:181:GLN:HB2	2.20	0.42
1:B:455:PRO:C	1:B:457:ALA:N	2.72	0.42
1:C:857:TYR:C	1:C:857:TYR:CD1	2.92	0.42
1:A:370:ILE:O	1:A:370:ILE:HG22	2.19	0.42
1:A:104:GLN:HB2	1:A:131:LYS:NZ	2.35	0.42
1:A:983:ILE:HD13	1:A:1008:MET:SD	2.60	0.42
1:A:983:ILE:CG1	1:A:984:LEU:N	2.81	0.42
1:C:775:SER:HB3	1:C:780:ARG:HD3	2.02	0.42
1:A:728:LYS:HD2	1:C:235:ILE:CG2	2.49	0.42
1:C:478:MET:O	1:C:481:SER:HB3	2.19	0.42
1:C:549:VAL:O	1:C:550:VAL:C	2.57	0.42
1:C:17:ILE:O	1:C:20:MET:HB2	2.20	0.42
1:B:653:ARG:C	1:B:654:ALA:O	2.55	0.42
1:A:186:ILE:HD13	1:A:262:LEU:HD21	2.02	0.42
1:B:674:LEU:CD1	1:B:860:THR:HG21	2.43	0.42
1:C:536:ARG:C	1:C:538:THR:H	2.22	0.42
1:A:469:GLN:O	1:A:473:THR:OG1	2.31	0.42
1:C:986:VAL:HG12	1:C:986:VAL:O	2.20	0.42
1:C:816:LEU:HA	1:C:816:LEU:HD23	1.83	0.42
1:C:50:PRO:O	1:C:52:ALA:N	2.49	0.42
1:B:470:PHE:CD2	1:B:929:VAL:HG11	2.55	0.42
1:B:1021:PHE:O	1:B:1024:VAL:HB	2.20	0.42
1:A:348:ILE:O	1:A:351:VAL:N	2.53	0.42
1:C:415:ASN:OD1	1:C:418:ARG:CZ	2.67	0.42
1:A:653:ARG:O	1:A:655:PHE:N	2.52	0.42
1:B:68:ASN:HD22	1:B:114:ALA:HB2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:753:ALA:HB3	1:A:754:TRP:H	1.61	0.42
1:A:754:TRP:CZ3	1:A:780:ARG:HA	2.54	0.42
1:C:865:GLN:O	1:C:868:LEU:O	2.38	0.42
1:B:808:ARG:HB3	1:B:808:ARG:HH21	1.85	0.42
1:A:571:VAL:HG12	1:A:629:VAL:O	2.19	0.42
1:C:922:THR:HG22	1:C:923:ASN:N	2.26	0.42
1:A:515:TRP:C	1:A:515:TRP:CD1	2.93	0.42
1:C:246:PHE:O	1:C:249:ILE:N	2.33	0.42
1:B:841:MET:O	1:B:845:GLU:HB2	2.20	0.42
1:A:760:ASN:O	1:A:771:VAL:HB	2.19	0.42
1:B:336:SER:O	1:B:392:THR:HG22	2.20	0.42
1:C:880:SER:O	1:C:884:VAL:HG23	2.20	0.42
1:A:104:GLN:O	1:A:105:VAL:C	2.57	0.41
1:B:474:ILE:O	1:B:475:VAL:C	2.59	0.41
1:B:1021:PHE:HB3	1:B:1025:PHE:HE1	1.84	0.41
1:B:544:LEU:O	1:B:547:ILE:HB	2.19	0.41
1:B:941:ASN:O	1:B:942:ALA:C	2.58	0.41
1:B:972:LEU:HD21	1:B:1019:ILE:HG12	2.02	0.41
1:A:1015:THR:O	1:A:1017:LEU:N	2.53	0.41
1:C:353:LEU:O	1:C:356:TYR:HB3	2.19	0.41
1:C:1015:THR:O	1:C:1019:ILE:HB	2.20	0.41
1:C:904:VAL:O	1:C:905:VAL:C	2.58	0.41
1:A:753:ALA:O	1:A:774:MET:CG	2.68	0.41
1:A:605:ASN:O	1:A:632:LYS:N	2.52	0.41
1:B:462:SER:OG	1:B:865:GLN:CD	2.58	0.41
1:B:644:VAL:O	1:B:645:GLU:C	2.58	0.41
1:A:198:LEU:HD22	1:A:202:ASP:HB3	2.00	0.41
1:A:466:ILE:O	1:A:469:GLN:N	2.50	0.41
1:A:114:ALA:C	1:A:116:PRO:HD2	2.41	0.41
1:B:354:VAL:O	1:B:358:PHE:HB2	2.20	0.41
1:B:544:LEU:HD22	1:B:1021:PHE:CZ	2.54	0.41
1:A:355:MET:HE1	1:A:410:ILE:HA	2.02	0.41
1:C:699:ARG:HB3	1:C:825:MET:HE3	2.01	0.41
1:A:545:TYR:HB2	1:A:1021:PHE:HE1	1.76	0.41
1:A:894:SER:CB	1:A:897:ILE:HD13	2.50	0.41
1:C:375:VAL:HB	1:C:405:LEU:HD13	2.02	0.41
1:C:375:VAL:H	1:C:375:VAL:HG23	1.64	0.41
1:C:417:GLU:O	1:C:420:MET:HB3	2.20	0.41
1:C:527:TYR:O	1:C:529:ASP:N	2.53	0.41
1:B:648:THR:O	1:B:652:THR:N	2.40	0.41
1:A:144:ASN:ND2	1:A:320:GLY:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:THR:CG2	1:A:334:LYS:HE2	2.47	0.41
1:B:352:PHE:HE1	1:B:365:THR:HG23	1.84	0.41
1:A:578:LEU:CD2	1:A:587:THR:HA	2.37	0.41
1:A:621:GLY:C	1:A:623:ASN:N	2.73	0.41
1:B:47:ALA:HB3	1:B:88:VAL:CG2	2.50	0.41
1:B:47:ALA:CB	1:B:61:VAL:HG21	2.50	0.41
1:A:211:ASN:ND2	1:A:760:ASN:OD1	2.53	0.41
1:C:77:TYR:CE1	1:C:860:THR:OG1	2.68	0.41
1:A:61:VAL:HG13	1:A:118:LEU:CD1	2.46	0.41
1:B:410:ILE:O	1:B:413:VAL:HG12	2.20	0.41
1:A:831:ALA:HA	1:A:840:ALA:HB1	2.01	0.41
1:C:973:ARG:N	1:C:974:PRO:CD	2.83	0.41
1:C:485:ALA:HA	1:C:489:THR:OG1	2.21	0.41
1:A:594:VAL:HA	1:A:655:PHE:HE2	1.85	0.41
1:A:596:HIS:O	1:A:599:LEU:O	2.37	0.41
1:B:144:ASN:H	1:B:144:ASN:HD22	1.68	0.41
1:A:185:ARG:HD3	1:A:272:GLY:O	2.20	0.41
1:C:673:GLU:O	1:C:674:LEU:CB	2.67	0.41
1:A:988:PRO:HB2	1:A:989:LEU:H	1.57	0.41
1:B:84:SER:O	1:B:86:GLY:N	2.54	0.41
1:A:879:ILE:HG13	1:A:879:ILE:H	1.64	0.41
1:A:686:ASP:HB2	1:A:823:PRO:HB2	2.02	0.41
1:A:690:LEU:CD1	1:A:854:GLY:HA3	2.20	0.41
1:B:468:ARG:HA	1:B:471:SER:HB2	2.01	0.41
1:B:961:ILE:O	1:B:965:LEU:CB	2.68	0.41
1:A:978:THR:O	1:A:980:LEU:N	2.53	0.41
1:C:914:LEU:HA	1:C:917:THR:OG1	2.20	0.41
1:A:583:THR:O	1:A:586:ARG:N	2.54	0.41
1:B:730:ASP:O	1:B:805:SER:HA	2.20	0.41
1:B:750:LEU:HB2	1:B:801:PHE:HE1	1.82	0.41
1:C:144:ASN:CG	1:C:149:MET:HG3	2.40	0.41
1:C:533:GLY:HA3	2:C:1068:HOH:O	2.20	0.41
1:A:683:GLU:OE1	1:A:826:GLU:HB2	2.20	0.41
1:C:680:PHE:HB2	1:C:859:TRP:CZ3	2.55	0.41
1:B:732:ASP:O	1:B:734:GLU:N	2.53	0.41
1:B:669:PRO:HB2	1:B:670:ALA:H	1.65	0.41
1:A:72:ILE:CG1	1:A:107:VAL:HA	2.51	0.41
1:A:72:ILE:HG13	1:A:106:GLN:HB2	2.02	0.41
1:B:404:LEU:HD21	1:B:937:LEU:HD21	2.02	0.41
1:A:405:LEU:HD13	1:A:405:LEU:H	1.85	0.41
1:C:775:SER:OG	1:C:789:TRP:HZ2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:986:VAL:C	1:B:988:PRO:HD2	2.39	0.41
1:C:544:LEU:HD12	1:C:1021:PHE:CZ	2.56	0.41
1:C:395:MET:O	1:C:396:PHE:C	2.58	0.41
1:A:493:CYS:O	1:A:497:LEU:HB2	2.21	0.41
1:A:307:ARG:NH2	1:A:328:ASP:OD2	2.49	0.41
1:B:788:ASP:N	1:B:788:ASP:OD1	2.52	0.41
1:A:44:THR:C	1:A:45:ILE:CG1	2.89	0.41
1:B:43:VAL:O	1:B:92:LEU:N	2.42	0.41
1:A:294:ALA:HB3	1:A:297:ALA:CB	2.51	0.41
1:C:253:VAL:HG12	1:C:259:ARG:HG3	2.03	0.41
1:C:681:ASP:OD2	1:C:828:LEU:CD1	2.68	0.41
1:A:116:PRO:N	2:A:1072:HOH:O	2.54	0.41
1:C:894:SER:OG	1:C:897:ILE:HG13	2.20	0.41
1:B:482:VAL:HG13	1:B:483:LEU:HD23	2.02	0.41
1:C:193:LEU:HA	1:C:193:LEU:HD23	1.86	0.41
1:B:988:PRO:C	1:B:990:VAL:H	2.24	0.41
1:B:989:LEU:CA	1:B:992:SER:HB2	2.50	0.41
1:C:425:LEU:H	1:C:426:PRO:HD3	1.84	0.41
1:C:528:THR:O	1:C:528:THR:HG22	2.20	0.41
1:A:126:GLY:HA3	1:B:116:PRO:HB3	2.01	0.41
1:C:143:ILE:HA	1:C:143:ILE:HD13	1.26	0.41
1:B:763:ILE:HD11	1:C:59:ASP:CB	2.50	0.41
1:A:298:ASN:O	1:A:302:THR:HG23	2.20	0.41
1:B:498:LYS:HB3	1:B:498:LYS:HE2	1.66	0.41
1:A:206:ALA:C	1:A:208:LYS:N	2.74	0.41
1:C:303:ALA:O	1:C:304:ALA:C	2.58	0.41
1:A:589:LYS:HA	1:A:592:ASN:ND2	2.36	0.41
1:C:40:PRO:CB	1:C:76:MET:HE1	2.51	0.41
1:C:115:MET:CB	1:C:116:PRO:HD3	2.48	0.41
1:B:1014:ALA:O	1:B:1018:ALA:HB2	2.20	0.41
1:B:1026:PHE:HB3	1:B:1030:ARG:HE	1.85	0.41
1:A:902:MET:C	1:A:904:VAL:N	2.74	0.41
1:C:187:TRP:HZ3	1:C:774:MET:CE	2.34	0.41
1:C:372:VAL:HG23	1:C:376:LEU:HG	2.02	0.41
1:C:901:VAL:O	1:C:902:MET:C	2.58	0.41
1:C:4:PHE:HD2	1:C:8:ARG:HH12	1.69	0.41
1:A:661:ALA:O	1:A:662:MET:C	2.58	0.41
1:A:426:PRO:HB2	1:A:427:PRO:HD2	2.03	0.41
1:A:324:VAL:CG1	1:A:325:TYR:N	2.81	0.41
1:C:989:LEU:HB3	1:C:1004:GLY:HA3	2.02	0.41
1:B:836:SER:OG	1:B:838:GLY:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:ILE:CG2	1:A:370:ILE:O	2.68	0.41
1:B:213:GLN:HG3	1:C:56:THR:HG23	2.03	0.41
1:C:1030:ARG:HB3	1:C:1030:ARG:HE	1.21	0.41
1:C:894:SER:HB3	1:C:897:ILE:HD12	2.03	0.41
1:B:470:PHE:CE2	1:B:929:VAL:HG11	2.55	0.41
1:B:1026:PHE:HB3	1:B:1030:ARG:HH21	1.82	0.41
1:B:901:VAL:HG21	1:B:943:ILE:HD13	2.02	0.41
1:A:1022:VAL:N	1:A:1023:PRO:CD	2.83	0.41
1:B:896:SER:O	1:B:899:PHE:HB2	2.20	0.41
1:B:850:LYS:CA	1:B:852:PRO:HD3	2.51	0.41
1:A:453:PHE:O	1:A:454:VAL:C	2.59	0.41
1:C:196:PHE:O	1:C:252:LYS:NZ	2.36	0.41
1:C:552:MET:HE1	1:C:909:VAL:HG21	2.02	0.41
1:B:741:VAL:HG22	1:B:793:ALA:HA	2.03	0.41
1:A:193:LEU:HD12	1:A:265:VAL:HG11	2.02	0.41
1:A:685:ILE:CG2	1:A:687:GLN:H	2.27	0.41
1:C:166:ILE:HG22	1:C:172:VAL:CG1	2.51	0.41
1:C:137:LEU:N	1:C:291:ILE:O	2.53	0.41
1:C:322:LYS:HG2	1:C:323:ILE:N	2.34	0.41
1:C:66:GLU:OE1	1:C:821:GLY:HA2	2.20	0.41
1:B:935:ILE:O	1:B:935:ILE:HG22	2.20	0.41
1:B:945:ILE:HG13	1:B:946:VAL:H	1.86	0.41
1:A:539:GLY:CA	1:A:542:LEU:HB2	2.45	0.41
1:B:340:VAL:O	1:B:341:VAL:C	2.59	0.41
1:C:844:MET:O	1:C:847:LEU:CD2	2.69	0.41
1:C:418:ARG:HD2	1:C:970:MET:CE	2.51	0.41
1:C:1014:ALA:O	1:C:1018:ALA:HB3	2.21	0.41
1:C:344:LEU:O	1:C:345:VAL:C	2.59	0.41
1:C:392:THR:O	1:C:393:LEU:C	2.59	0.41
1:C:9:PRO:C	1:C:11:PHE:H	2.24	0.41
1:B:702:LEU:C	1:B:703:LEU:O	2.58	0.41
1:A:655:PHE:O	1:A:658:ILE:HG12	2.20	0.41
1:A:493:CYS:C	1:A:494:ALA:O	2.59	0.41
1:A:991:ILE:HG13	1:A:1004:GLY:HA3	2.03	0.41
1:B:578:LEU:H	1:B:578:LEU:CD2	2.33	0.41
1:A:223:PRO:HA	1:A:224:PRO:HD3	1.92	0.41
1:A:472:ILE:HA	1:A:475:VAL:HG12	2.01	0.41
1:A:736:ALA:O	1:A:741:VAL:HG12	2.20	0.41
1:C:764:ASP:O	1:C:765:ARG:C	2.59	0.41
1:B:33:ALA:O	1:B:337:ILE:HD11	2.20	0.41
1:A:49:TYR:O	1:A:50:PRO:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:826:GLU:O	2:C:1063:HOH:O	2.22	0.41
1:B:64:VAL:O	1:B:66:GLU:N	2.54	0.41
1:B:66:GLU:OE2	1:B:818:ARG:HD3	2.21	0.41
1:B:216:ALA:CB	1:B:236:ALA:HB2	2.50	0.41
1:B:743:ILE:H	1:B:743:ILE:CD1	2.32	0.41
1:A:137:LEU:O	1:A:329:THR:HG22	2.21	0.41
1:A:24:GLY:O	1:A:27:ILE:HB	2.20	0.41
1:C:218:GLN:HG3	1:C:233:SER:HA	2.03	0.41
1:B:121:GLU:HG2	1:B:121:GLU:H	1.41	0.41
1:A:975:ILE:O	1:A:976:LEU:C	2.59	0.41
1:A:360:GLN:HB3	1:A:360:GLN:HE21	1.58	0.41
1:A:542:LEU:HD23	1:A:1028:VAL:HG21	2.02	0.41
1:A:541:TYR:C	1:A:543:VAL:O	2.59	0.41
1:A:729:ILE:CG2	1:A:730:ASP:N	2.62	0.41
1:A:428:LYS:CG	1:A:429:GLU:N	2.83	0.41
1:A:183:ALA:O	1:A:185:ARG:N	2.54	0.41
1:C:188:MET:CE	1:C:200:PRO:HA	2.51	0.41
1:B:139:VAL:O	1:B:326:PRO:HG2	2.21	0.41
1:A:456:MET:HG2	1:A:459:PHE:HE1	1.86	0.41
1:B:775:SER:OG	1:B:776:GLU:N	2.54	0.41
1:B:38:ILE:HD12	1:B:466:ILE:CD1	2.52	0.41
1:C:593:GLU:O	1:C:597:TYR:N	2.32	0.41
1:C:790:TYR:C	1:C:791:VAL:HG23	2.40	0.41
1:C:75:LEU:HD22	1:C:77:TYR:O	2.21	0.41
1:C:202:ASP:O	1:C:205:THR:N	2.54	0.41
1:C:317:PHE:CB	1:C:318:PRO:CD	2.92	0.40
1:C:889:ALA:O	1:C:890:ALA:C	2.59	0.40
1:C:949:ALA:O	1:C:951:ASP:N	2.55	0.40
1:A:897:ILE:HG21	1:A:950:LYS:NZ	2.36	0.40
1:C:900:SER:HA	1:C:1029:VAL:HG21	2.03	0.40
1:C:919:ARG:HD2	1:C:919:ARG:HA	1.92	0.40
1:A:143:ILE:HG12	1:A:144:ASN:N	2.37	0.40
1:C:663:VAL:CG1	1:C:664:PHE:N	2.84	0.40
1:B:592:ASN:O	1:B:595:THR:HG23	2.21	0.40
1:A:333:VAL:O	1:A:337:ILE:HD13	2.21	0.40
1:A:696:THR:O	1:A:697:GLN:C	2.58	0.40
1:A:44:THR:O	1:A:45:ILE:HG12	2.17	0.40
1:A:815:ARG:NH2	2:A:1071:HOH:O	2.54	0.40
1:A:198:LEU:HD11	1:A:252:LYS:HB2	2.03	0.40
1:C:178:PHE:CD1	1:C:610:PHE:HE2	2.38	0.40
1:A:380:PHE:CZ	1:A:398:MET:HE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:PRO:HB2	1:C:316:PHE:CE1	2.56	0.40
1:C:885:PHE:O	1:C:888:LEU:N	2.53	0.40
1:B:974:PRO:O	1:B:978:THR:HG22	2.21	0.40
1:A:545:TYR:HA	1:A:548:ILE:HG12	2.03	0.40
1:A:952:LEU:HD11	1:A:963:ALA:HB1	2.03	0.40
1:C:337:ILE:N	1:C:337:ILE:HD13	2.36	0.40
1:A:753:ALA:O	1:A:774:MET:HG3	2.21	0.40
1:B:418:ARG:HH21	1:B:970:MET:HG3	1.85	0.40
1:C:760:ASN:O	1:C:771:VAL:HG23	2.21	0.40
1:C:568:ASP:O	1:C:568:ASP:OD1	2.39	0.40
1:C:410:ILE:O	1:C:411:VAL:C	2.59	0.40
1:A:461:GLY:O	1:A:462:SER:C	2.58	0.40
1:B:756:GLY:HA2	1:B:773:VAL:O	2.20	0.40
1:C:30:LEU:HA	1:C:31:PRO:HD3	1.95	0.40
1:A:193:LEU:CB	1:A:265:VAL:HG13	2.50	0.40
1:B:58:GLN:C	1:B:60:THR:H	2.25	0.40
1:A:240:LEU:N	1:A:240:LEU:HD12	2.37	0.40
1:A:4:PHE:HA	1:A:4:PHE:HD2	1.80	0.40
1:C:817:GLU:O	1:C:818:ARG:HG2	2.21	0.40
1:A:405:LEU:O	1:A:406:VAL:C	2.57	0.40
1:C:754:TRP:CE3	1:C:780:ARG:HB2	2.56	0.40
1:C:551:GLY:O	1:C:554:TYR:HB2	2.21	0.40
1:C:400:LEU:O	1:C:933:THR:HG21	2.21	0.40
1:A:971:ARG:O	1:A:974:PRO:HD2	2.20	0.40
1:A:790:TYR:CE1	1:A:800:PRO:HB3	2.56	0.40
1:C:203:VAL:O	1:C:204:ILE:C	2.58	0.40
1:A:693:GLU:O	1:A:694:LYS:C	2.59	0.40
1:A:462:SER:HB2	1:A:674:LEU:CD2	2.52	0.40
1:B:460:GLY:HA2	1:B:872:GLN:OE1	2.21	0.40
1:B:670:ALA:H	1:B:862:MET:HE1	1.85	0.40
1:B:223:PRO:HA	1:B:224:PRO:HD3	1.98	0.40
1:B:317:PHE:CE2	1:B:323:ILE:HD11	2.56	0.40
1:C:713:LEU:HD11	1:C:835:LYS:N	2.36	0.40
1:B:921:LEU:HD22	1:B:1005:THR:HG22	2.02	0.40
1:A:713:LEU:HG	1:A:833:PRO:CD	2.25	0.40
1:C:844:MET:O	1:C:848:ALA:N	2.53	0.40
1:C:475:VAL:HG12	1:C:476:SER:N	2.35	0.40
1:C:4:PHE:CD2	1:C:8:ARG:NH1	2.89	0.40
1:B:641:GLU:CA	1:B:650:ARG:HH12	2.33	0.40
1:A:959:GLY:HA3	1:A:962:GLU:CB	2.30	0.40
1:A:489:THR:HB	1:A:490:PRO:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:ARG:CG	1:A:970:MET:CE	2.96	0.40
1:C:360:GLN:OE1	1:C:516:PHE:HE2	2.04	0.40
1:A:520:PHE:C	1:A:522:LYS:H	2.25	0.40
1:A:243:THR:CG2	1:A:268:ILE:HG22	2.49	0.40
1:B:598:TYR:HD1	1:B:606:VAL:HG21	1.85	0.40
1:C:957:GLY:C	1:C:958:LYS:HD2	2.42	0.40
1:A:1036:LYS:HD2	1:A:1036:LYS:C	2.42	0.40
1:A:114:ALA:O	1:A:117:LEU:CD2	2.70	0.40
1:A:65:ILE:HD13	1:A:111:LEU:HD23	2.02	0.40
1:C:950:LYS:N	1:C:953:MET:HE2	2.18	0.40
1:B:945:ILE:CD1	1:B:1022:VAL:CG2	3.00	0.40
1:B:490:PRO:C	1:B:492:LEU:N	2.75	0.40
1:B:552:MET:HA	1:B:910:ILE:HD12	2.04	0.40
1:A:541:TYR:CD2	1:A:541:TYR:N	2.89	0.40
1:B:345:VAL:O	1:B:348:ILE:HB	2.21	0.40
1:C:746:ILE:O	1:C:747:ASN:C	2.59	0.40
1:C:5:PHE:HA	1:C:8:ARG:O	2.22	0.40
1:B:776:GLU:CG	1:B:777:ALA:H	2.35	0.40
1:A:607:GLU:OE2	1:A:607:GLU:O	2.40	0.40
1:A:151:GLN:NE2	1:A:279:ALA:H	2.19	0.40
1:C:714:THR:HG22	1:C:716:VAL:H	1.85	0.40
1:B:194:ASN:ND2	1:B:194:ASN:O	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1018/1053 (97%)	621 (61%)	243 (24%)	154 (15%)	0	0
1	B	1018/1053 (97%)	611 (60%)	259 (25%)	148 (14%)	0	1
1	C	1018/1053 (97%)	642 (63%)	225 (22%)	151 (15%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3054/3159 (97%)	1874 (61%)	727 (24%)	453 (15%)	0 0

All (453) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	ASP
1	A	63	GLN
1	A	64	VAL
1	A	65	ILE
1	A	67	GLN
1	A	69	MET
1	A	73	ASP
1	A	74	ASN
1	A	76	MET
1	A	96	SER
1	A	105	VAL
1	A	112	GLN
1	A	137	LEU
1	A	146	ASP
1	A	167	SER
1	A	172	VAL
1	A	181	GLN
1	A	255	GLN
1	A	277	ILE
1	A	293	LEU
1	A	294	ALA
1	A	318	PRO
1	A	330	THR
1	A	376	LEU
1	A	422	GLU
1	A	439	GLN
1	A	443	VAL
1	A	444	GLY
1	A	521	GLU
1	A	538	THR
1	A	597	TYR
1	A	601	LYS
1	A	638	PRO
1	A	659	LYS
1	A	660	ASP
1	A	672	VAL
1	A	676	THR

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Mol	Chain	Res	Type
1	A	677	ALA
1	A	687	GLN
1	A	690	LEU
1	A	713	LEU
1	A	715	SER
1	A	730	ASP
1	A	759	VAL
1	A	775	SER
1	A	820	ASN
1	A	868	LEU
1	A	925	VAL
1	A	988	PRO
1	A	991	ILE
1	A	1016	VAL
1	A	1024	VAL
1	B	8	ARG
1	B	50	PRO
1	B	51	GLY
1	B	54	ALA
1	B	56	THR
1	B	72	ILE
1	B	85	THR
1	B	98	THR
1	B	104	GLN
1	B	147	GLY
1	B	173	GLY
1	B	175	VAL
1	B	228	GLN
1	B	258	SER
1	B	268	ILE
1	B	270	LEU
1	B	326	PRO
1	B	361	ASN
1	B	363	ARG
1	B	517	ASN
1	B	519	MET
1	B	535	LEU
1	B	536	ARG
1	B	538	THR
1	B	549	VAL
1	B	602	GLU
1	B	606	VAL

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Mol	Chain	Res	Type
1	B	647	ILE
1	B	654	ALA
1	B	655	PHE
1	B	671	ILE
1	B	688	ALA
1	B	689	GLY
1	B	693	GLU
1	B	703	LEU
1	B	705	GLU
1	B	712	MET
1	B	733	GLN
1	B	820	ASN
1	B	831	ALA
1	B	871	ASN
1	B	891	LEU
1	B	907	LEU
1	B	908	GLY
1	B	921	LEU
1	B	1012	VAL
1	B	1019	ILE
1	B	1034	SER
1	C	52	ALA
1	C	61	VAL
1	C	68	ASN
1	C	95	GLU
1	C	110	LYS
1	C	111	LEU
1	C	157	TYR
1	C	160	ALA
1	C	167	SER
1	C	187	TRP
1	C	226	LYS
1	C	311	ALA
1	C	312	LYS
1	C	314	GLU
1	C	319	SER
1	C	394	THR
1	C	410	ILE
1	C	411	VAL
1	C	419	VAL
1	C	464	GLY
1	C	540	ARG

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Mol	Chain	Res	Type
1	C	601	LYS
1	C	658	ILE
1	C	720	GLY
1	C	778	LYS
1	C	851	LEU
1	C	869	SER
1	C	871	ASN
1	C	895	TRP
1	C	925	VAL
1	C	946	VAL
1	C	960	LEU
1	C	965	LEU
1	C	975	ILE
1	C	989	LEU
1	C	993	THR
1	C	1035	ARG
1	A	12	ALA
1	A	54	ALA
1	A	66	GLU
1	A	90	ILE
1	A	135	SER
1	A	147	GLY
1	A	170	SER
1	A	218	GLN
1	A	221	GLY
1	A	256	ASP
1	A	265	VAL
1	A	400	LEU
1	A	435	MET
1	A	446	ALA
1	A	453	PHE
1	A	455	PRO
1	A	459	PHE
1	A	496	MET
1	A	548	ILE
1	A	553	ALA
1	A	580	ALA
1	A	582	ALA
1	A	600	THR
1	A	622	GLN
1	A	654	ALA
1	A	679	GLY

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Mol	Chain	Res	Type
1	A	688	ALA
1	A	689	GLY
1	A	784	ASP
1	A	866	GLU
1	A	869	SER
1	A	903	LEU
1	A	926	TYR
1	A	951	ASP
1	A	958	LYS
1	A	964	THR
1	A	971	ARG
1	A	1010	GLY
1	A	1012	VAL
1	A	1025	PHE
1	B	22	ALA
1	B	103	ALA
1	B	125	GLN
1	B	221	GLY
1	B	254	ASN
1	B	265	VAL
1	B	291	ILE
1	B	424	GLY
1	B	453	PHE
1	B	471	SER
1	B	539	GLY
1	B	557	VAL
1	B	567	GLU
1	B	603	LYS
1	B	638	PRO
1	B	659	LYS
1	B	669	PRO
1	B	715	SER
1	B	723	ASP
1	B	794	ALA
1	B	805	SER
1	B	834	GLY
1	B	852	PRO
1	B	899	PHE
1	B	901	VAL
1	B	918	PHE
1	B	966	ASP
1	B	975	ILE

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Mol	Chain	Res	Type
1	B	1013	THR
1	C	10	ILE
1	C	34	GLN
1	C	51	GLY
1	C	74	ASN
1	C	164	ASP
1	C	182	TYR
1	C	217	GLY
1	C	220	GLY
1	C	243	THR
1	C	258	SER
1	C	263	ARG
1	C	396	PHE
1	C	404	LEU
1	C	418	ARG
1	C	451	ALA
1	C	460	GLY
1	C	468	ARG
1	C	536	ARG
1	C	576	VAL
1	C	656	SER
1	C	678	THR
1	C	690	LEU
1	C	696	THR
1	C	706	ALA
1	C	715	SER
1	C	803	ALA
1	C	872	GLN
1	C	935	ILE
1	C	998	GLY
1	C	1017	LEU
1	C	1029	VAL
1	A	192	GLU
1	A	206	ALA
1	A	301	ASP
1	A	317	PHE
1	A	319	SER
1	A	320	GLY
1	A	353	LEU
1	A	357	LEU
1	A	372	VAL
1	A	428	LYS

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Mol	Chain	Res	Type
1	A	447	MET
1	A	458	PHE
1	A	515	TRP
1	A	535	LEU
1	A	656	SER
1	A	694	LYS
1	A	753	ALA
1	A	831	ALA
1	A	881	LEU
1	B	2	PRO
1	B	48	SER
1	B	171	GLY
1	B	319	SER
1	B	336	SER
1	B	357	LEU
1	B	405	LEU
1	B	408	ASP
1	B	422	GLU
1	B	491	ALA
1	B	495	THR
1	B	601	LYS
1	B	640	GLU
1	B	675	GLY
1	B	788	ASP
1	B	804	PHE
1	B	1011	MET
1	C	190	PRO
1	C	191	ASN
1	C	193	LEU
1	C	327	TYR
1	C	336	SER
1	C	386	PHE
1	C	422	GLU
1	C	427	PRO
1	C	463	THR
1	C	491	ALA
1	C	497	LEU
1	C	530	SER
1	C	593	GLU
1	C	600	THR
1	C	639	GLY
1	C	671	ILE

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Mol	Chain	Res	Type
1	C	675	GLY
1	C	747	ASN
1	C	760	ASN
1	C	801	PHE
1	C	950	LYS
1	C	952	LEU
1	C	983	ILE
1	C	994	GLY
1	C	1010	GLY
1	A	68	ASN
1	A	116	PRO
1	A	184	MET
1	A	217	GLY
1	A	362	PHE
1	A	384	ALA
1	A	434	SER
1	A	436	GLY
1	A	577	GLN
1	A	712	MET
1	A	810	GLU
1	A	907	LEU
1	A	923	ASN
1	A	960	LEU
1	A	1004	GLY
1	A	1005	THR
1	B	12	ALA
1	B	36	PRO
1	B	59	ASP
1	B	131	LYS
1	B	327	TYR
1	B	407	ASP
1	B	414	GLU
1	B	427	PRO
1	B	461	GLY
1	B	485	ALA
1	B	656	SER
1	B	694	LYS
1	B	870	GLY
1	B	941	ASN
1	B	950	LYS
1	B	959	GLY
1	B	960	LEU

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Mol	Chain	Res	Type
1	B	1014	ALA
1	B	1026	PHE
1	C	54	ALA
1	C	81	ASN
1	C	124	GLN
1	C	159	ALA
1	C	343	THR
1	C	490	PRO
1	C	520	PHE
1	C	620	ARG
1	C	664	PHE
1	C	674	LEU
1	C	777	ALA
1	C	967	ALA
1	C	974	PRO
1	C	976	LEU
1	C	988	PRO
1	A	19	ILE
1	A	174	ASP
1	A	216	ALA
1	A	224	PRO
1	A	392	THR
1	A	417	GLU
1	A	549	VAL
1	A	692	HIS
1	A	714	THR
1	A	818	ARG
1	A	1002	ALA
1	B	10	ILE
1	B	409	ALA
1	B	542	LEU
1	B	618	ALA
1	B	716	VAL
1	B	777	ALA
1	B	849	SER
1	B	851	LEU
1	B	909	VAL
1	B	954	ASP
1	B	1006	GLY
1	B	1017	LEU
1	C	192	GLU
1	C	237	GLN

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Mol	Chain	Res	Type
1	C	332	PHE
1	C	392	THR
1	C	425	LEU
1	C	438	ILE
1	C	458	PHE
1	C	519	MET
1	C	528	THR
1	C	546	LEU
1	C	640	GLU
1	C	716	VAL
1	C	837	THR
1	C	850	LYS
1	C	852	PRO
1	C	963	ALA
1	A	18	ILE
1	A	109	ASN
1	A	191	ASN
1	A	397	GLY
1	A	471	SER
1	A	794	ALA
1	A	892	TYR
1	B	23	GLY
1	B	65	ILE
1	B	105	VAL
1	B	127	VAL
1	B	474	ILE
1	B	477	ALA
1	B	674	LEU
1	B	786	ILE
1	B	942	ALA
1	B	1016	VAL
1	C	80	SER
1	C	106	GLN
1	C	207	ILE
1	C	315	PRO
1	C	333	VAL
1	C	399	VAL
1	C	447	MET
1	C	537	SER
1	C	796	GLY
1	C	926	TYR
1	C	1007	VAL

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Mol	Chain	Res	Type
1	A	709	HIS
1	B	315	PRO
1	B	444	GLY
1	B	484	VAL
1	B	710	PRO
1	B	821	GLY
1	C	19	ILE
1	C	32	VAL
1	C	223	PRO
1	C	426	PRO
1	C	550	VAL
1	A	51	GLY
1	A	539	GLY
1	B	19	ILE
1	B	31	PRO
1	B	190	PRO
1	B	771	VAL
1	C	709	HIS
1	A	729	ILE
1	A	874	PRO
1	B	224	PRO
1	B	974	PRO
1	C	9	PRO
1	C	50	PRO
1	C	291	ILE
1	C	533	GLY
1	A	15	ILE
1	A	716	VAL
1	A	905	VAL
1	B	464	GLY
1	C	15	ILE
1	C	424	GLY
1	C	448	VAL
1	C	571	VAL
1	C	786	ILE
1	C	800	PRO
1	A	326	PRO
1	B	783	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	833/859 (97%)	678 (81%)	155 (19%)	2	6
1	B	833/859 (97%)	688 (83%)	145 (17%)	2	7
1	C	833/859 (97%)	679 (82%)	154 (18%)	2	6
All	All	2499/2577 (97%)	2045 (82%)	454 (18%)	2	6

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

Mol	Chain	Res	Type
1	A	4	PHE
1	A	5	PHE
1	A	6	ILE
1	A	14	VAL
1	A	21	LEU
1	A	25	LEU
1	A	38	ILE
1	A	46	SER
1	A	49	TYR
1	A	55	LYS
1	A	58	GLN
1	A	62	THR
1	A	63	GLN
1	A	65	ILE
1	A	66	GLU
1	A	69	MET
1	A	74	ASN
1	A	79	SER
1	A	80	SER
1	A	83	ASP
1	A	84	SER
1	A	88	VAL
1	A	91	THR
1	A	93	THR
1	A	98	THR
1	A	102	ILE

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Mol	Chain	Res	Type
1	A	105	VAL
1	A	109	ASN
1	A	112	GLN
1	A	115	MET
1	A	120	GLN
1	A	130	GLU
1	A	137	LEU
1	A	139	VAL
1	A	143	ILE
1	A	150	THR
1	A	164	ASP
1	A	166	ILE
1	A	170	SER
1	A	193	LEU
1	A	202	ASP
1	A	213	GLN
1	A	222	THR
1	A	226	LYS
1	A	230	LEU
1	A	243	THR
1	A	277	ILE
1	A	284	GLN
1	A	298	ASN
1	A	302	THR
1	A	319	SER
1	A	323	ILE
1	A	325	TYR
1	A	330	THR
1	A	335	ILE
1	A	337	ILE
1	A	349	ILE
1	A	356	TYR
1	A	357	LEU
1	A	359	LEU
1	A	361	ASN
1	A	367	ILE
1	A	376	LEU
1	A	379	THR
1	A	394	THR
1	A	405	LEU
1	A	414	GLU
1	A	417	GLU

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Mol	Chain	Res	Type
1	A	433	LYS
1	A	438	ILE
1	A	447	MET
1	A	453	PHE
1	A	480	LEU
1	A	481	SER
1	A	498	LYS
1	A	513	PHE
1	A	515	TRP
1	A	518	ARG
1	A	522	LYS
1	A	523	SER
1	A	536	ARG
1	A	544	LEU
1	A	546	LEU
1	A	556	PHE
1	A	557	VAL
1	A	558	ARG
1	A	561	SER
1	A	572	PHE
1	A	576	VAL
1	A	577	GLN
1	A	578	LEU
1	A	586	ARG
1	A	607	GLU
1	A	610	PHE
1	A	612	VAL
1	A	617	PHE
1	A	620	ARG
1	A	623	ASN
1	A	626	ILE
1	A	630	SER
1	A	641	GLU
1	A	648	THR
1	A	653	ARG
1	A	659	LYS
1	A	668	LEU
1	A	671	ILE
1	A	687	GLN
1	A	690	LEU
1	A	702	LEU
1	A	705	GLU

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Mol	Chain	Res	Type
1	A	711	ASP
1	A	713	LEU
1	A	717	ARG
1	A	719	ASN
1	A	721	LEU
1	A	722	GLU
1	A	729	ILE
1	A	750	LEU
1	A	758	TYR
1	A	763	ILE
1	A	768	VAL
1	A	774	MET
1	A	775	SER
1	A	778	LYS
1	A	779	TYR
1	A	780	ARG
1	A	782	LEU
1	A	786	ILE
1	A	801	PHE
1	A	805	SER
1	A	807	SER
1	A	815	ARG
1	A	818	ARG
1	A	822	LEU
1	A	824	SER
1	A	828	LEU
1	A	843	LEU
1	A	855	VAL
1	A	867	ARG
1	A	887	CYS
1	A	899	PHE
1	A	917	THR
1	A	954	ASP
1	A	955	LYS
1	A	960	LEU
1	A	976	LEU
1	A	982	PHE
1	A	983	ILE
1	A	986	VAL
1	A	992	SER
1	A	993	THR
1	A	1013	THR

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Mol	Chain	Res	Type
1	A	1022	VAL
1	A	1030	ARG
1	A	1036	LYS
1	B	6	ILE
1	B	8	ARG
1	B	11	PHE
1	B	13	TRP
1	B	21	LEU
1	B	27	ILE
1	B	34	GLN
1	B	48	SER
1	B	50	PRO
1	B	53	ASP
1	B	57	VAL
1	B	59	ASP
1	B	61	VAL
1	B	67	GLN
1	B	70	ASN
1	B	72	ILE
1	B	74	ASN
1	B	79	SER
1	B	81	ASN
1	B	91	THR
1	B	92	LEU
1	B	93	THR
1	B	96	SER
1	B	102	ILE
1	B	104	GLN
1	B	121	GLU
1	B	131	LYS
1	B	144	ASN
1	B	145	THR
1	B	150	THR
1	B	153	ASP
1	B	170	SER
1	B	174	ASP
1	B	176	GLN
1	B	180	SER
1	B	182	TYR
1	B	185	ARG
1	B	188	MET
1	B	189	ASN

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Mol	Chain	Res	Type
1	B	191	ASN
1	B	193	LEU
1	B	194	ASN
1	B	210	GLN
1	B	223	PRO
1	B	226	LYS
1	B	228	GLN
1	B	231	ASN
1	B	235	ILE
1	B	237	GLN
1	B	243	THR
1	B	253	VAL
1	B	254	ASN
1	B	256	ASP
1	B	261	LEU
1	B	270	LEU
1	B	289	LEU
1	B	293	LEU
1	B	298	ASN
1	B	319	SER
1	B	335	ILE
1	B	336	SER
1	B	342	LYS
1	B	343	THR
1	B	349	ILE
1	B	356	TYR
1	B	365	THR
1	B	372	VAL
1	B	373	PRO
1	B	379	THR
1	B	394	THR
1	B	405	LEU
1	B	410	ILE
1	B	428	LYS
1	B	435	MET
1	B	437	GLN
1	B	452	VAL
1	B	456	MET
1	B	473	THR
1	B	482	VAL
1	B	483	LEU
1	B	488	LEU

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Mol	Chain	Res	Type
1	B	496	MET
1	B	497	LEU
1	B	513	PHE
1	B	516	PHE
1	B	538	THR
1	B	540	ARG
1	B	549	VAL
1	B	554	TYR
1	B	562	SER
1	B	574	THR
1	B	591	LEU
1	B	595	THR
1	B	601	LYS
1	B	607	GLU
1	B	612	VAL
1	B	623	ASN
1	B	629	VAL
1	B	641	GLU
1	B	653	ARG
1	B	655	PHE
1	B	659	LYS
1	B	668	LEU
1	B	673	GLU
1	B	680	PHE
1	B	681	ASP
1	B	696	THR
1	B	712	MET
1	B	743	ILE
1	B	757	SER
1	B	758	TYR
1	B	760	ASN
1	B	764	ASP
1	B	770	LYS
1	B	778	LYS
1	B	781	MET
1	B	782	LEU
1	B	788	ASP
1	B	799	VAL
1	B	808	ARG
1	B	830	GLN
1	B	836	SER
1	B	847	LEU

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Mol	Chain	Res	Type
1	B	864	TYR
1	B	868	LEU
1	B	871	ASN
1	B	876	LEU
1	B	879	ILE
1	B	895	TRP
1	B	900	SER
1	B	933	THR
1	B	943	ILE
1	B	946	VAL
1	B	951	ASP
1	B	956	GLU
1	B	960	LEU
1	B	965	LEU
1	B	966	ASP
1	B	970	MET
1	B	978	THR
1	B	984	LEU
1	B	987	MET
1	B	993	THR
1	B	1027	VAL
1	B	1036	LYS
1	C	4	PHE
1	C	13	TRP
1	C	17	ILE
1	C	19	ILE
1	C	37	THR
1	C	45	ILE
1	C	48	SER
1	C	49	TYR
1	C	58	GLN
1	C	60	THR
1	C	63	GLN
1	C	65	ILE
1	C	70	ASN
1	C	74	ASN
1	C	75	LEU
1	C	82	SER
1	C	83	ASP
1	C	89	GLN
1	C	91	THR
1	C	102	ILE

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Mol	Chain	Res	Type
1	C	104	GLN
1	C	107	VAL
1	C	108	GLN
1	C	110	LYS
1	C	111	LEU
1	C	117	LEU
1	C	118	LEU
1	C	134	SER
1	C	137	LEU
1	C	143	ILE
1	C	148	THR
1	C	149	MET
1	C	151	GLN
1	C	152	GLU
1	C	153	ASP
1	C	168	ARG
1	C	169	THR
1	C	170	SER
1	C	177	LEU
1	C	184	MET
1	C	185	ARG
1	C	189	ASN
1	C	194	ASN
1	C	207	ILE
1	C	210	GLN
1	C	211	ASN
1	C	228	GLN
1	C	231	ASN
1	C	233	SER
1	C	239	ARG
1	C	253	VAL
1	C	258	SER
1	C	259	ARG
1	C	265	VAL
1	C	268	ILE
1	C	269	GLU
1	C	274	ASN
1	C	295	THR
1	C	301	ASP
1	C	313	MET
1	C	316	PHE
1	C	317	PHE

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Mol	Chain	Res	Type
1	C	337	ILE
1	C	339	GLU
1	C	341	VAL
1	C	355	MET
1	C	367	ILE
1	C	372	VAL
1	C	377	LEU
1	C	400	LEU
1	C	417	GLU
1	C	419	VAL
1	C	420	MET
1	C	425	LEU
1	C	432	ARG
1	C	437	GLN
1	C	438	ILE
1	C	458	PHE
1	C	459	PHE
1	C	475	VAL
1	C	492	LEU
1	C	493	CYS
1	C	497	LEU
1	C	521	GLU
1	C	535	LEU
1	C	536	ARG
1	C	538	THR
1	C	544	LEU
1	C	546	LEU
1	C	568	ASP
1	C	576	VAL
1	C	577	GLN
1	C	588	GLN
1	C	591	LEU
1	C	592	ASN
1	C	608	SER
1	C	613	ASN
1	C	617	PHE
1	C	622	GLN
1	C	624	THR
1	C	626	ILE
1	C	650	ARG
1	C	662	MET
1	C	666	PHE

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Mol	Chain	Res	Type
1	C	668	LEU
1	C	674	LEU
1	C	685	ILE
1	C	696	THR
1	C	699	ARG
1	C	713	LEU
1	C	719	ASN
1	C	721	LEU
1	C	722	GLU
1	C	724	THR
1	C	733	GLN
1	C	743	ILE
1	C	745	ASP
1	C	750	LEU
1	C	759	VAL
1	C	762	PHE
1	C	764	ASP
1	C	765	ARG
1	C	768	VAL
1	C	770	LYS
1	C	778	LYS
1	C	782	LEU
1	C	799	VAL
1	C	808	ARG
1	C	813	SER
1	C	847	LEU
1	C	850	LYS
1	C	867	ARG
1	C	868	LEU
1	C	872	GLN
1	C	876	LEU
1	C	885	PHE
1	C	899	PHE
1	C	904	VAL
1	C	907	LEU
1	C	922	THR
1	C	935	ILE
1	C	941	ASN
1	C	945	ILE
1	C	952	LEU
1	C	954	ASP
1	C	958	LYS

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Mol	Chain	Res	Type
1	C	960	LEU
1	C	982	PHE
1	C	984	LEU
1	C	993	THR
1	C	1021	PHE
1	C	1030	ARG
1	C	1035	ARG
1	C	1036	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	63	GLN
1	A	68	ASN
1	A	70	ASN
1	A	89	GLN
1	A	106	GLN
1	A	108	GLN
1	A	109	ASN
1	A	123	GLN
1	A	124	GLN
1	A	181	GLN
1	A	191	ASN
1	A	210	GLN
1	A	231	ASN
1	A	274	ASN
1	A	282	ASN
1	A	284	GLN
1	A	298	ASN
1	A	360	GLN
1	A	361	ASN
1	A	577	GLN
1	A	622	GLN
1	A	623	ASN
1	A	687	GLN
1	A	719	ASN
1	A	830	GLN
1	A	846	GLN
1	A	865	GLN
1	A	871	ASN
1	B	34	GLN

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Mol	Chain	Res	Type
1	B	58	GLN
1	B	68	ASN
1	B	70	ASN
1	B	108	GLN
1	B	109	ASN
1	B	112	GLN
1	B	120	GLN
1	B	125	GLN
1	B	151	GLN
1	B	161	ASN
1	B	189	ASN
1	B	210	GLN
1	B	213	GLN
1	B	218	GLN
1	B	228	GLN
1	B	231	ASN
1	B	237	GLN
1	B	254	ASN
1	B	415	ASN
1	B	437	GLN
1	B	439	GLN
1	B	469	GLN
1	B	517	ASN
1	B	526	HIS
1	B	577	GLN
1	B	584	GLN
1	B	613	ASN
1	B	623	ASN
1	B	642	ASN
1	B	726	GLN
1	B	744	ASN
1	B	760	ASN
1	B	830	GLN
1	B	846	GLN
1	B	865	GLN
1	B	871	ASN
1	C	3	ASN
1	C	63	GLN
1	C	104	GLN
1	C	106	GLN
1	C	120	GLN
1	C	123	GLN

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Mol	Chain	Res	Type
1	C	125	GLN
1	C	144	ASN
1	C	176	GLN
1	C	189	ASN
1	C	197	GLN
1	C	211	ASN
1	C	231	ASN
1	C	237	GLN
1	C	284	GLN
1	C	391	ASN
1	C	439	GLN
1	C	577	GLN
1	C	588	GLN
1	C	592	ASN
1	C	605	ASN
1	C	667	ASN
1	C	747	ASN

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	1022/1053 (97%)	-0.06	41 (4%)	42	30	5, 97, 116, 127	0
1	B	1022/1053 (97%)	0.06	49 (4%)	34	23	49, 102, 116, 127	0
1	C	1022/1053 (97%)	-0.05	48 (4%)	35	24	5, 94, 118, 127	0
All	All	3066/3159 (97%)	-0.02	138 (4%)	37	26	5, 99, 117, 127	0

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1034	SER	11.8
1	C	870	GLY	8.1
1	C	513	PHE	6.8
1	C	538	THR	6.5
1	B	529	ASP	5.9
1	C	514	GLY	5.4
1	A	526	HIS	5.4
1	C	536	ARG	5.3
1	C	515	TRP	5.2
1	C	869	SER	4.8
1	C	539	GLY	4.7
1	C	656	SER	4.6
1	B	526	HIS	4.6
1	C	525	HIS	4.5
1	C	920	GLY	4.4
1	B	957	GLY	4.2
1	B	554	TYR	4.2
1	A	145	THR	4.1
1	A	253	VAL	4.1
1	A	318	PRO	4.1
1	C	1034	SER	4.1
1	B	958	LYS	3.9
1	A	871	ASN	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	596	HIS	3.9
1	B	811	TYR	3.8
1	B	424	GLY	3.8
1	A	801	PHE	3.7
1	A	515	TRP	3.7
1	B	192	GLU	3.6
1	B	832	ALA	3.6
1	C	649	MET	3.5
1	C	521	GLU	3.4
1	B	563	PHE	3.4
1	C	670	ALA	3.4
1	B	420	MET	3.4
1	C	526	HIS	3.3
1	C	554	TYR	3.3
1	A	519	MET	3.2
1	A	536	ARG	3.2
1	B	711	ASP	3.2
1	B	515	TRP	3.2
1	C	957	GLY	3.2
1	A	135	SER	3.2
1	B	1035	ARG	3.1
1	B	1036	LYS	3.1
1	A	955	LYS	3.1
1	C	425	LEU	3.1
1	A	962	GLU	3.0
1	C	671	ILE	3.0
1	A	918	PHE	3.0
1	C	597	TYR	3.0
1	A	957	GLY	2.9
1	A	1034	SER	2.9
1	A	254	ASN	2.9
1	C	520	PHE	2.9
1	C	436	GLY	2.9
1	A	537	SER	2.9
1	C	658	ILE	2.8
1	B	338	HIS	2.8
1	B	320	GLY	2.8
1	B	951	ASP	2.8
1	A	257	GLY	2.8
1	B	145	THR	2.8
1	C	437	GLN	2.8
1	C	872	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	833	PRO	2.8
1	B	52	ALA	2.8
1	B	546	LEU	2.7
1	B	652	THR	2.7
1	A	597	TYR	2.7
1	B	1033	PHE	2.7
1	C	993	THR	2.7
1	C	951	ASP	2.7
1	B	657	GLN	2.7
1	C	34	GLN	2.7
1	A	521	GLU	2.7
1	B	304	ALA	2.7
1	A	250	LEU	2.7
1	A	557	VAL	2.7
1	A	954	ASP	2.6
1	A	1035	ARG	2.6
1	B	708	LYS	2.6
1	A	951	ASP	2.6
1	C	537	SER	2.6
1	B	521	GLU	2.6
1	C	424	GLY	2.6
1	C	1035	ARG	2.5
1	C	522	LYS	2.5
1	B	918	PHE	2.5
1	B	604	ASN	2.5
1	A	192	GLU	2.5
1	C	4	PHE	2.5
1	B	675	GLY	2.5
1	C	546	LEU	2.4
1	C	194	ASN	2.4
1	A	1033	PHE	2.4
1	B	253	VAL	2.4
1	B	981	ALA	2.4
1	B	697	GLN	2.4
1	A	167	SER	2.4
1	B	319	SER	2.4
1	A	134	SER	2.4
1	B	495	THR	2.3
1	A	538	THR	2.3
1	A	615	PHE	2.3
1	A	546	LEU	2.3
1	B	651	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	342	LYS	2.2
1	B	20	MET	2.2
1	C	544	LEU	2.2
1	A	923	ASN	2.2
1	B	346	GLU	2.2
1	A	707	ALA	2.2
1	A	518	ARG	2.1
1	B	952	LEU	2.1
1	A	969	ARG	2.1
1	C	868	LEU	2.1
1	B	3	ASN	2.1
1	B	1032	ARG	2.1
1	A	555	LEU	2.1
1	B	589	LYS	2.1
1	C	707	ALA	2.1
1	A	554	TYR	2.1
1	B	527	TYR	2.1
1	A	589	LYS	2.1
1	C	498	LYS	2.1
1	B	947	GLU	2.0
1	A	517	ASN	2.0
1	C	657	GLN	2.0
1	B	520	PHE	2.0
1	B	360	GLN	2.0
1	C	713	LEU	2.0
1	C	643	LYS	2.0
1	B	314	GLU	2.0
1	A	596	HIS	2.0
1	B	54	ALA	2.0
1	C	257	GLY	2.0
1	C	784	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no 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.