Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 04:41 pm BST

PDB ID	:	5L5L
Title	:	Plexin A4 full extracellular region, domains 1 to 8 modeled, data to 8 angstrom, spacegroup P2(1)
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Deposited on	:	2016-05-28
Resolution	:	8.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

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

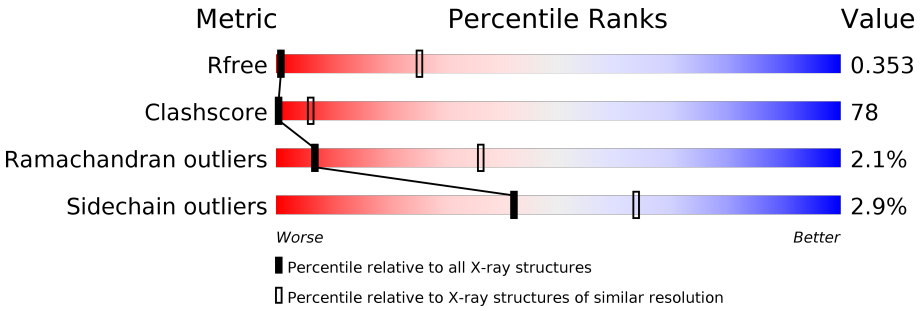
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 8.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1005 (11.50-3.90)
Clashscore	141614	1070 (11.50-3.90)
Ramachandran outliers	138981	1003 (11.50-3.90)
Sidechain outliers	138945	1003 (11.50-3.86)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	1207	27% 52% · 17%
1	B	1207	25% 47% · 24%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 15030 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 Plexin-A4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1000	Total	C	N	O	S	0	0	0
			7841	4938	1356	1482	65			
1	B	915	Total	C	N	O	S	0	0	0
			7189	4533	1239	1357	60			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	GLU	-	expression tag	UNP Q80UG2
A	34	THR	-	expression tag	UNP Q80UG2
A	35	GLY	-	expression tag	UNP Q80UG2
A	1230	GLY	-	expression tag	UNP Q80UG2
A	1231	ARG	-	expression tag	UNP Q80UG2
A	1232	THR	-	expression tag	UNP Q80UG2
A	1233	LYS	-	expression tag	UNP Q80UG2
A	1234	HIS	-	expression tag	UNP Q80UG2
A	1235	HIS	-	expression tag	UNP Q80UG2
A	1236	HIS	-	expression tag	UNP Q80UG2
A	1237	HIS	-	expression tag	UNP Q80UG2
A	1238	HIS	-	expression tag	UNP Q80UG2
A	1239	HIS	-	expression tag	UNP Q80UG2
B	33	GLU	-	expression tag	UNP Q80UG2
B	34	THR	-	expression tag	UNP Q80UG2
B	35	GLY	-	expression tag	UNP Q80UG2
B	1230	GLY	-	expression tag	UNP Q80UG2
B	1231	ARG	-	expression tag	UNP Q80UG2
B	1232	THR	-	expression tag	UNP Q80UG2
B	1233	LYS	-	expression tag	UNP Q80UG2
B	1234	HIS	-	expression tag	UNP Q80UG2
B	1235	HIS	-	expression tag	UNP Q80UG2
B	1236	HIS	-	expression tag	UNP Q80UG2
B	1237	HIS	-	expression tag	UNP Q80UG2
B	1238	HIS	-	expression tag	UNP Q80UG2

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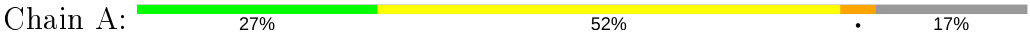
Chain	Residue	Modelled	Actual	Comment	Reference
B	1239	HIS	-	expression tag	UNP Q80UG2

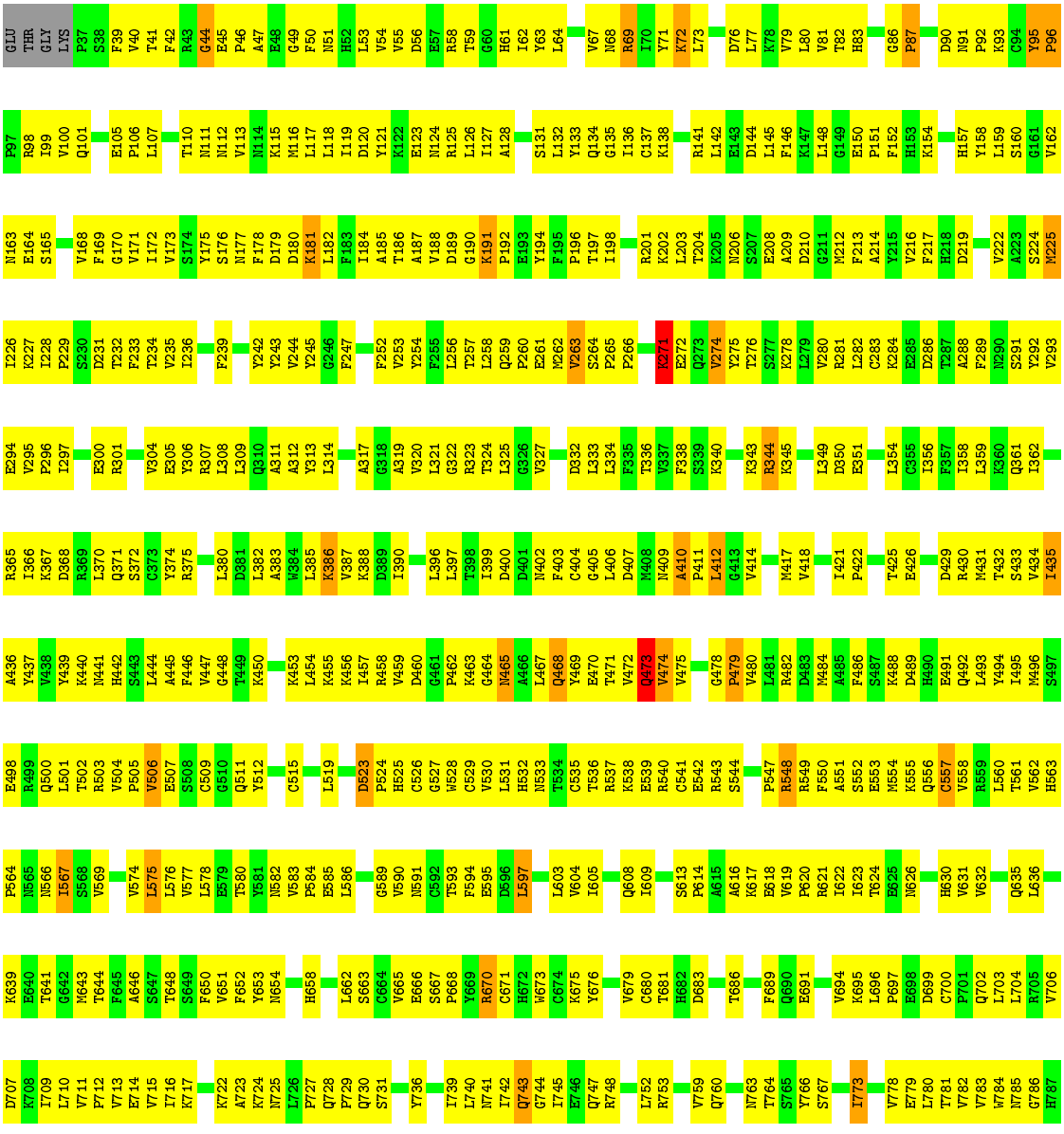
3 Residue-property plots (i)

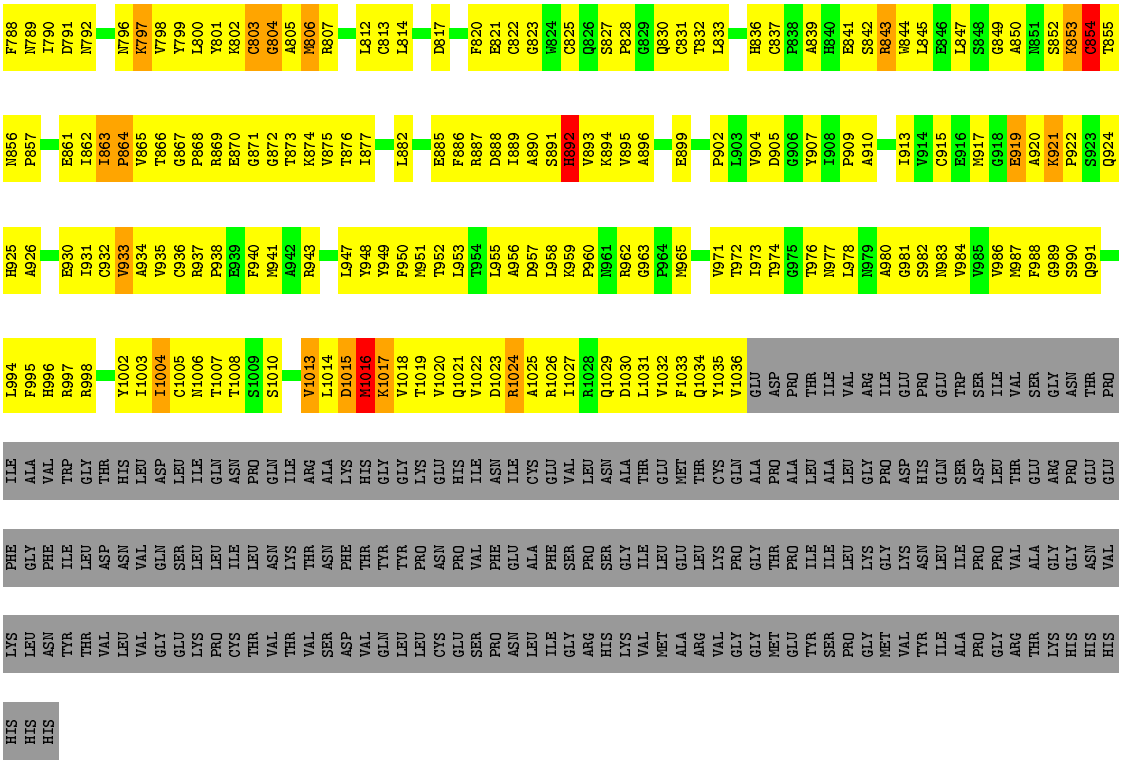
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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: Plexin-A4

Chain A:

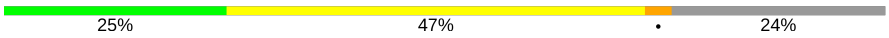


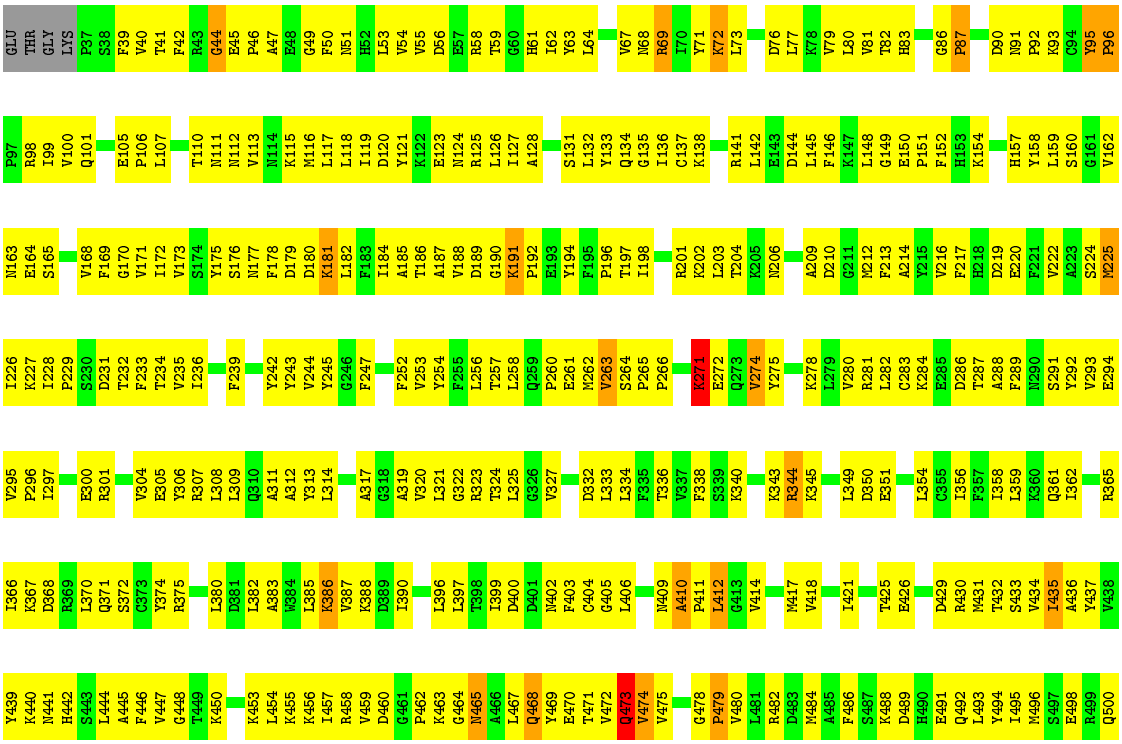




• Molecule 1: Plexin-A4

Chain B:





L501 T502 R503 V504 P505 V506 E507 S508 C509 G510 Q511 Y512 C515 L519 G520 S521 G522 D523 P524 H525 C526 G527 W528 C529 V530 L531 H532 N533 T534 C535 T536 R537 K538 E539 R540 C541 E542 R543 S544 P547 R548 R549 F550 A551 S552 E553 M554 K555 Q556 C557 V558 R559 L560 T561 V562 H563 P564

N565 N566 I567 S568 V569 V574 L575 L576 V577 L578 E579 T580 V583 P584 E585 L586 G589 V590 N591 C592 T593 F594 E595 D596 L597 L603 V604 I605 Q608 I609 S613 P614 A615 A616 K617 E618 V619 P620 R621 I622 I623 T624 E625 N626 H629 H630 V631 V632 Q635 L636 K639

E640 T641 T644 F645 A646 S647 T648 S649 F650 V651 F652 Y653 N654 H658 N659 S660 C661 L662 S663 C664 V665 E666 S667 P668 Y669 R670 C671 H672 W673 C674 K675 Y676 V679 C680 T681 H682 D683 P684 N685 T686 F689 Q690 E691 V694 K695 L696 P697 E698 D699 C700 P701 Q702 L703 L704 R705

V706 D707 K708 I709 L710 V711 P712 V713 E714 V715 I716 K717 K722 A723 K724 N725 L726 P727 Q728 P729 Q730 S731 Y736 I739 L740 N741 I742 Q743 G744 I745 E746 Q747 R748 R753 V759 Q760 N763 T764 S765 Y766 S767 I773 V778 E779 L780 T781 V782 V783 W784 N785 G786 H787

F788 N789 I790 D791 N792 N796 K797 V798 Y799 L800 Y801 K802 C803 G804 A805 M806 R807 E808 S809 L812 C813 L814 D817 F820 E821 C822 G823 W824 C825 Q826 S827 P828 G829 Q830 C831 T832 L833 H836 C837 P838 A839 H840 E841 S842 R843 W844 L845 E846 L847 S848 G849 A850 N851 S852 K853

C854 T855 N856 P857 E861 I862 I863 P864 V865 T866 G867 P868 R869 T873 K874 V875 T876 I877 N881 L882 G883 L884 E885 F886 R887 D888 I889 A890 S891 H892 V893 K894 V895 A896 E899 C900 S901 P902 L903 V904 D905 G906 Y907 I908 P909 A910 I913 V914 C915 E916 M917 G918 E919 A920 K921

P922 S923 Q924 H925 A926 E930 I931 C932 V933 A934 V935 C936 R937 P938 E939 F940 M941 A942 R943 L947 Y948 Y949 F950 M951 THR LEU THR LEU ALA ASP LEU LYS PRO ASN ARG GLY PRO MET SER GLY GLY THR GLN VAL THR ILE THR GLY THR ASN LEU ASN ALA GLY SER ASN VAL VAL

VAL MET PHE GLY SER GLN PRO CYS LEU PHE HIS ARG ARG SER PRO SER TYR ILE ILE CYS ASN THR THR SER SER GLU GLU VAL LEU ASP MET LYS VAL THR VAL GLN VAL ASP ARG ALA ARG ILE ARG GLN ASP LEU VAL PHE GLN TYR VAL GLU ASP PRO THR ILE VAL ARG ILE GLU

PRO GLU TRP SER ILE VAL SER GLY ASN THR PRO ILE ALA VAL TRP GLY THR HIS LEU ASP LEU ILE GLN ASN PRO GLN ILE ARG ALA LYS HIS GLY GLY LYS GLU HIS ILE ASN ILE CYS GLU VAL LEU ASN ALA THR GLU MET THR CYS GLN ALA PRO ALA LEU ALA LEU GLY PRO ASP

HIS GLN SER ASP LEU THR GLU ARG PRO GLU GLU PHE GLY PHE ILE LEU ASP ASN VAL GLN SER LEU LEU ILE LEU ASN LYS THR ASN PHE THR TYR TYR PRO ASN PRO VAL PHE GLU ALA PHE SER PRO SER GLY ILE LEU GLU LEU LYS PRO GLY THR PRO ILE ILE LEU LYS GLY LYS

ASN LEU ILE PRO PRO VAL ALA GLY GLY ASN VAL LYS LEU ASN TYR THR VAL LEU VAL GLY GLU LYS PRO CYS THR VAL THR VAL SER ASP VAL GLN LEU LEU CYS GLU SER PRO ASN LEU ILE GLY ARG HIS LYS VAL MET ALA ARG VAL GLY GLY MET GLU TYR SER PRO GLY MET VAL

TYR ILE ALA PRO GLY ARG THR LYS HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	142.18Å 241.00Å 144.07Å 90.00° 99.83° 90.00°	Depositor
Resolution (Å)	47.74 – 8.00 47.74 – 8.00	Depositor EDS
% Data completeness (in resolution range)	99.1 (47.74-8.00) 99.5 (47.74-8.00)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.18 (at 8.32Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.349 , 0.349 0.348 , 0.353	Depositor DCC
R_{free} test set	488 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å^2)	450.9	Xtriage
Anisotropy	0.543	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 550.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.043 for l,-k,h	Xtriage
F_o,F_c correlation	0.70	EDS
Total number of atoms	15030	wwPDB-VP
Average B, all atoms (Å^2)	264.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.04% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.01	5/8007 (0.1%)	1.36	27/10846 (0.2%)
1	B	1.00	5/7344 (0.1%)	1.32	24/9943 (0.2%)
All	All	1.01	10/15351 (0.1%)	1.34	51/20789 (0.2%)

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	3
1	B	0	4
All	All	0	7

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	506	VAL	C-N	23.13	1.87	1.34
1	B	506	VAL	C-N	21.10	1.82	1.34
1	A	557	CYS	C-N	-20.82	0.86	1.34
1	B	557	CYS	C-N	-17.13	0.94	1.34
1	A	700	CYS	C-N	-15.63	1.04	1.34
1	B	700	CYS	C-N	15.54	1.63	1.34
1	B	49	GLY	CA-C	6.43	1.62	1.51
1	A	49	GLY	CA-C	6.42	1.62	1.51
1	A	49	GLY	C-N	5.06	1.45	1.34
1	B	49	GLY	C-N	5.05	1.45	1.34

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	747	GLN	CG-CD-OE1	-38.83	43.94	121.60
1	A	747	GLN	CG-CD-OE1	-38.81	43.98	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	653	TYR	O-C-N	-33.42	69.23	122.70
1	B	557	CYS	O-C-N	-31.89	71.68	122.70
1	A	653	TYR	CA-C-N	23.37	168.61	117.20
1	A	854	CYS	O-C-N	-23.21	85.56	122.70
1	A	557	CYS	O-C-N	18.53	152.35	122.70
1	B	557	CYS	CA-C-N	17.95	156.70	117.20
1	B	700	CYS	C-N-CD	-17.94	81.14	120.60
1	A	557	CYS	CA-C-N	-17.52	78.65	117.20
1	B	506	VAL	O-C-N	17.20	150.23	122.70
1	A	854	CYS	C-N-CA	16.73	163.51	121.70
1	A	653	TYR	C-N-CA	16.67	163.37	121.70
1	B	506	VAL	CA-C-N	-16.51	80.87	117.20
1	B	506	VAL	C-N-CA	-14.85	84.57	121.70
1	A	506	VAL	O-C-N	-14.82	98.98	122.70
1	A	854	CYS	CA-C-N	13.98	147.96	117.20
1	A	557	CYS	C-N-CA	-13.97	86.77	121.70
1	B	557	CYS	C-N-CA	11.36	150.09	121.70
1	B	747	GLN	CG-CD-NE2	-9.58	93.70	116.70
1	A	747	GLN	CG-CD-NE2	-9.56	93.76	116.70
1	A	700	CYS	O-C-N	-8.60	104.76	121.10
1	A	479	PRO	N-CA-C	8.18	133.37	112.10
1	B	479	PRO	N-CA-C	8.16	133.31	112.10
1	A	843	ARG	C-N-CA	7.76	141.10	121.70
1	B	843	ARG	C-N-CA	7.75	141.07	121.70
1	A	747	GLN	OE1-CD-NE2	6.89	137.74	121.90
1	A	478	GLY	CA-C-O	-6.87	108.23	120.60
1	B	478	GLY	CA-C-O	-6.85	108.27	120.60
1	B	747	GLN	OE1-CD-NE2	6.84	137.63	121.90
1	B	473	GLN	C-N-CA	-6.70	104.95	121.70
1	A	473	GLN	C-N-CA	-6.69	104.97	121.70
1	B	892	HIS	CA-CB-CG	6.59	124.81	113.60
1	A	892	HIS	CA-CB-CG	6.57	124.77	113.60
1	B	700	CYS	CA-C-N	-6.33	99.38	117.10
1	A	225	MET	CG-SD-CE	-5.72	91.05	100.20
1	B	225	MET	CG-SD-CE	-5.71	91.06	100.20
1	A	409	ASN	C-N-CA	5.67	135.87	121.70
1	B	409	ASN	C-N-CA	5.66	135.85	121.70
1	A	49	GLY	C-N-CA	5.62	135.74	121.70
1	B	49	GLY	C-N-CA	5.57	135.63	121.70
1	B	700	CYS	O-C-N	-5.55	110.55	121.10
1	A	700	CYS	CA-C-N	5.48	132.43	117.10
1	B	274	VAL	CG1-CB-CG2	5.47	119.65	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	274	VAL	CG1-CB-CG2	5.45	119.61	110.90
1	B	919	GLU	C-N-CA	5.27	134.88	121.70
1	A	919	GLU	C-N-CA	5.24	134.81	121.70
1	B	676	TYR	CA-CB-CG	-5.12	103.67	113.40
1	A	676	TYR	CA-CB-CG	-5.11	103.70	113.40
1	A	803	CYS	C-N-CA	5.09	132.98	122.30
1	B	803	CYS	C-N-CA	5.08	132.96	122.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	854	CYS	Mainchain
1	A	863	ILE	Peptide
1	A	95	TYR	Peptide
1	B	557	CYS	Mainchain
1	B	700	CYS	Mainchain
1	B	863	ILE	Peptide
1	B	95	TYR	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7841	0	7710	1244	34
1	B	7189	0	7050	1075	67
All	All	15030	0	14760	2319	69

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 78.

All (2319) 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:A:868:PRO:HD2	1:A:981:GLY:CA	1.32	1.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:868:PRO:CD	1:A:981:GLY:CA	1.87	1.50
1:A:873:THR:CA	1:A:982:SER:HB2	1.46	1.43
1:A:873:THR:HA	1:A:982:SER:CB	1.48	1.40
1:B:506:VAL:HG22	1:B:525:HIS:NE2	1.33	1.38
1:B:629:HIS:CE1	1:B:669:TYR:OH	1.76	1.37
1:B:629:HIS:ND1	1:B:669:TYR:OH	1.56	1.34
1:A:870:GLU:CD	1:A:1025:ALA:HB2	1.46	1.33
1:A:868:PRO:HD3	1:A:981:GLY:N	1.06	1.33
1:B:506:VAL:N	1:B:507:GLU:N	1.77	1.29
1:B:506:VAL:C	1:B:507:GLU:N	1.82	1.28
1:A:868:PRO:CD	1:A:981:GLY:N	1.88	1.27
1:A:506:VAL:C	1:A:507:GLU:N	1.87	1.26
1:B:700:CYS:O	1:B:725:ASN:HB2	1.38	1.23
1:A:870:GLU:HB3	1:A:1024:ARG:CG	1.70	1.22
1:B:809:SER:CB	1:B:881:ASN:OD1	1.89	1.19
1:B:809:SER:HB2	1:B:881:ASN:CG	1.62	1.18
1:A:569:VAL:CG2	1:A:654:ASN:HB2	1.71	1.18
1:A:867:GLY:HA2	1:A:981:GLY:N	1.59	1.17
1:A:359:LEU:HD12	1:A:362:ILE:HD11	1.24	1.17
1:B:118:LEU:HD12	1:B:172:ILE:HD12	1.17	1.17
1:B:456:LYS:HD2	1:B:523:ASP:OD2	1.44	1.17
1:A:868:PRO:HD3	1:A:980:ALA:C	1.63	1.17
1:B:676:TYR:CE1	1:B:730:GLN:HG2	1.80	1.15
1:B:295:VAL:HG12	1:B:414:VAL:HG11	1.27	1.14
1:B:802:LYS:C	1:B:803:CYS:N	2.01	1.14
1:A:453:LYS:HG2	1:A:472:VAL:HG22	1.25	1.14
1:B:359:LEU:HD12	1:B:362:ILE:HD11	1.24	1.14
1:B:506:VAL:CG2	1:B:525:HIS:NE2	2.11	1.14
1:A:324:THR:HB	1:A:462:PRO:HB3	1.27	1.13
1:A:458:ARG:HD2	1:A:524:PRO:HB3	1.31	1.12
1:A:118:LEU:HD12	1:A:172:ILE:HD12	1.17	1.12
1:A:435:ILE:HG22	1:A:446:PHE:HB2	1.22	1.12
1:A:295:VAL:HG12	1:A:414:VAL:HG11	1.27	1.12
1:B:453:LYS:HG2	1:B:472:VAL:HG22	1.25	1.12
1:B:809:SER:HB2	1:B:881:ASN:OD1	0.95	1.11
1:B:435:ILE:HG22	1:B:446:PHE:HB2	1.22	1.11
1:A:533:ASN:ND2	1:A:644:THR:O	1.83	1.11
1:A:595:GLU:HB2	1:A:597:LEU:HD23	1.32	1.11
1:B:676:TYR:CD1	1:B:730:GLN:CG	2.33	1.11
1:B:469:TYR:HB2	1:B:523:ASP:OD1	1.50	1.10
1:B:595:GLU:HB2	1:B:597:LEU:HD23	1.32	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:806:MET:H	1:A:806:MET:HE3	1.14	1.10
1:B:324:THR:HB	1:B:462:PRO:HB3	1.27	1.09
1:B:806:MET:HE3	1:B:806:MET:H	1.14	1.09
1:A:868:PRO:CD	1:A:981:GLY:HA3	1.61	1.09
1:A:871:GLY:O	1:A:1023:ASP:CB	2.00	1.09
1:B:444:LEU:HD23	1:B:524:PRO:CG	1.83	1.08
1:A:1017:LYS:HE2	1:A:1017:LYS:H	1.18	1.08
1:B:676:TYR:CE1	1:B:730:GLN:CG	2.37	1.08
1:A:868:PRO:HD2	1:A:981:GLY:HA2	1.17	1.08
1:A:474:VAL:HG12	1:A:475:VAL:HG23	1.33	1.08
1:B:468:GLN:HG3	1:B:523:ASP:HA	1.16	1.07
1:B:469:TYR:CB	1:B:523:ASP:OD1	2.02	1.07
1:B:506:VAL:C	1:B:507:GLU:CA	2.21	1.07
1:A:870:GLU:CB	1:A:1024:ARG:HG2	1.84	1.07
1:B:474:VAL:HG12	1:B:475:VAL:HG23	1.33	1.07
1:A:549:ARG:HD3	1:A:584:PRO:CB	1.84	1.06
1:A:440:LYS:HB2	1:A:538:LYS:NZ	1.68	1.06
1:A:439:TYR:CE2	1:A:538:LYS:NZ	2.23	1.05
1:B:506:VAL:CA	1:B:507:GLU:N	2.17	1.05
1:B:676:TYR:CD1	1:B:730:GLN:HG3	1.91	1.05
1:A:569:VAL:HG21	1:A:654:ASN:HB2	1.32	1.04
1:B:506:VAL:HG22	1:B:525:HIS:CE1	1.92	1.04
1:B:444:LEU:HD23	1:B:524:PRO:HG3	1.37	1.03
1:B:494:TYR:HB3	1:B:501:LEU:HD21	1.40	1.03
1:B:301:ARG:HD2	1:B:425:THR:HG21	1.37	1.03
1:B:620:PRO:HA	1:B:623:ILE:HG13	1.41	1.03
1:A:46:PRO:HG2	1:A:69:ARG:HG3	1.41	1.02
1:A:301:ARG:HD2	1:A:425:THR:HG21	1.37	1.02
1:A:560:LEU:HD23	1:A:648:THR:HG23	1.37	1.02
1:A:440:LYS:HD2	1:A:538:LYS:HD3	1.37	1.02
1:A:871:GLY:O	1:A:1023:ASP:CG	1.98	1.01
1:A:620:PRO:HA	1:A:623:ILE:HG13	1.41	1.01
1:A:867:GLY:CA	1:A:981:GLY:H	1.72	1.01
1:A:494:TYR:HB3	1:A:501:LEU:HD21	1.40	1.01
1:B:676:TYR:CD1	1:B:730:GLN:HG2	1.94	1.00
1:B:560:LEU:HD23	1:B:648:THR:HG23	1.37	1.00
1:B:46:PRO:HG2	1:B:69:ARG:HG3	1.41	1.00
1:A:873:THR:OG1	1:A:981:GLY:HA2	1.60	0.99
1:B:117:LEU:HD11	1:B:126:LEU:HD21	1.45	0.99
1:A:117:LEU:HD11	1:A:126:LEU:HD21	1.45	0.99
1:A:870:GLU:CB	1:A:1024:ARG:CG	2.40	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:623:ILE:HA	1:B:626:ASN:HD21	1.28	0.99
1:A:870:GLU:HB3	1:A:1024:ARG:HG2	1.01	0.99
1:A:868:PRO:HD3	1:A:981:GLY:CA	1.73	0.99
1:A:458:ARG:HD2	1:A:524:PRO:CB	1.92	0.98
1:B:548:ARG:HG3	1:B:583:VAL:C	1.84	0.98
1:B:444:LEU:HD12	1:B:446:PHE:CE1	1.98	0.98
1:B:862:ILE:HG22	1:B:877:ILE:HA	1.46	0.98
1:A:870:GLU:CD	1:A:1025:ALA:CB	2.33	0.97
1:A:444:LEU:HD12	1:A:446:PHE:CE1	1.98	0.97
1:A:870:GLU:OE1	1:A:1025:ALA:HB2	1.62	0.97
1:A:563:HIS:HB3	1:A:564:PRO:HD3	1.44	0.97
1:B:563:HIS:HB3	1:B:564:PRO:HD3	1.44	0.97
1:A:623:ILE:HA	1:A:626:ASN:HD21	1.28	0.96
1:A:862:ILE:HG22	1:A:877:ILE:HA	1.46	0.96
1:B:662:LEU:HD23	1:B:791:ASP:OD2	1.65	0.96
1:B:566:ASN:HA	1:B:651:VAL:HG23	1.49	0.95
1:B:458:ARG:HD2	1:B:524:PRO:HB3	1.45	0.95
1:B:629:HIS:CG	1:B:669:TYR:OH	2.15	0.95
1:A:566:ASN:HA	1:A:651:VAL:HG23	1.49	0.95
1:B:506:VAL:C	1:B:507:GLU:HA	1.84	0.95
1:A:440:LYS:HB2	1:A:538:LYS:HZ2	1.27	0.94
1:B:505:PRO:C	1:B:507:GLU:N	2.19	0.94
1:A:42:PHE:HE1	1:A:79:VAL:HG22	1.31	0.94
1:A:870:GLU:OE2	1:A:1025:ALA:HB2	1.65	0.94
1:A:868:PRO:HD2	1:A:981:GLY:HA3	1.16	0.94
1:A:994:LEU:HD11	1:A:1006:ASN:HD22	1.31	0.94
1:A:72:LYS:HE3	1:A:80:LEU:HD13	1.49	0.94
1:A:871:GLY:O	1:A:1023:ASP:HB3	1.68	0.93
1:B:62:ILE:CG1	1:B:73:LEU:HB2	1.98	0.93
1:B:42:PHE:HE1	1:B:79:VAL:HG22	1.31	0.93
1:A:297:ILE:HG22	1:A:418:VAL:CG1	1.97	0.93
1:A:870:GLU:CG	1:A:1024:ARG:HG3	1.97	0.93
1:B:456:LYS:CD	1:B:523:ASP:OD2	2.15	0.93
1:B:297:ILE:HG22	1:B:418:VAL:HG12	1.49	0.93
1:B:804:GLY:HA2	1:B:806:MET:SD	2.09	0.93
1:A:62:ILE:CG1	1:A:73:LEU:HB2	1.98	0.93
1:A:440:LYS:HD2	1:A:538:LYS:CD	1.98	0.93
1:A:804:GLY:HA2	1:A:806:MET:SD	2.09	0.93
1:B:297:ILE:HG22	1:B:418:VAL:CG1	1.97	0.93
1:B:865:VAL:HG13	1:B:866:THR:HG23	1.50	0.93
1:A:297:ILE:HG22	1:A:418:VAL:HG12	1.49	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:863:ILE:HG22	1:B:876:THR:HB	1.48	0.92
1:A:863:ILE:HG22	1:A:876:THR:HB	1.48	0.92
1:A:39:PHE:CE2	1:A:473:GLN:HG3	2.05	0.92
1:B:72:LYS:HE3	1:B:80:LEU:HD13	1.49	0.92
1:B:271:LYS:HG3	1:B:272:GLU:H	1.34	0.92
1:A:435:ILE:HD13	1:A:436:ALA:H	1.34	0.92
1:B:527:GLY:HA3	1:B:550:PHE:CZ	2.04	0.92
1:A:239:PHE:HA	1:A:260:PRO:HG2	1.51	0.92
1:A:865:VAL:HG13	1:A:866:THR:HG23	1.50	0.92
1:B:39:PHE:CE2	1:B:473:GLN:HG3	2.05	0.92
1:A:933:VAL:HG23	1:A:934:ALA:H	1.35	0.91
1:B:239:PHE:HA	1:B:260:PRO:HG2	1.51	0.91
1:A:870:GLU:HG2	1:A:1024:ARG:C	1.91	0.91
1:B:806:MET:SD	1:B:807:ARG:HG3	2.11	0.91
1:B:435:ILE:HD13	1:B:436:ALA:H	1.34	0.91
1:A:806:MET:SD	1:A:807:ARG:HG3	2.11	0.91
1:A:527:GLY:HA3	1:A:550:PHE:CZ	2.05	0.90
1:A:447:VAL:HG22	1:A:455:LYS:HB2	1.53	0.90
1:A:549:ARG:HD3	1:A:584:PRO:HB2	1.53	0.90
1:B:933:VAL:HG23	1:B:934:ALA:H	1.36	0.90
1:A:271:LYS:HG3	1:A:272:GLU:H	1.34	0.90
1:A:359:LEU:CD1	1:A:362:ILE:HD11	2.02	0.89
1:A:447:VAL:CG2	1:A:455:LYS:HB2	2.03	0.89
1:A:972:THR:HG23	1:A:1002:TYR:CE1	2.07	0.89
1:A:873:THR:C	1:A:982:SER:HB2	1.91	0.89
1:B:653:TYR:HE2	1:B:682:HIS:ND1	1.69	0.89
1:A:453:LYS:CG	1:A:472:VAL:HG22	2.03	0.88
1:B:447:VAL:CG2	1:B:455:LYS:HB2	2.03	0.88
1:B:453:LYS:CG	1:B:472:VAL:HG22	2.03	0.88
1:B:95:TYR:CD2	1:B:96:PRO:HD3	2.08	0.88
1:B:447:VAL:HG22	1:B:455:LYS:HB2	1.53	0.88
1:B:802:LYS:O	1:B:803:CYS:N	2.06	0.88
1:B:181:LYS:CD	1:B:202:LYS:HA	2.04	0.88
1:A:870:GLU:OE2	1:A:1025:ALA:CB	2.22	0.88
1:B:359:LEU:CD1	1:B:362:ILE:HD11	2.02	0.88
1:A:863:ILE:HG23	1:A:864:PRO:HD2	1.55	0.88
1:B:892:HIS:HB2	1:B:932:CYS:O	1.74	0.88
1:A:446:PHE:HD2	1:A:454:LEU:HD21	1.38	0.87
1:B:847:LEU:HG	1:B:850:ALA:H	1.39	0.87
1:B:486:PHE:CD1	1:B:493:LEU:HD13	2.09	0.87
1:A:532:HIS:HA	1:A:641:THR:OG1	1.73	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:892:HIS:HB2	1:A:932:CYS:O	1.73	0.87
1:A:95:TYR:CD2	1:A:96:PRO:HD3	2.08	0.87
1:A:867:GLY:HA2	1:A:981:GLY:H	0.77	0.87
1:A:486:PHE:CD1	1:A:493:LEU:HD13	2.09	0.87
1:B:468:GLN:HG3	1:B:523:ASP:CA	2.03	0.87
1:B:863:ILE:HG23	1:B:864:PRO:HD2	1.56	0.86
1:B:110:THR:CG2	1:B:132:LEU:HD21	2.05	0.86
1:B:439:TYR:CE2	1:B:538:LYS:NZ	2.42	0.86
1:A:39:PHE:CE1	1:A:505:PRO:HD2	2.10	0.86
1:A:959:LYS:HB2	1:A:972:THR:HB	1.57	0.86
1:A:110:THR:CG2	1:A:132:LEU:HD21	2.05	0.86
1:A:181:LYS:CD	1:A:202:LYS:HA	2.04	0.86
1:A:833:LEU:HB2	1:A:836:HIS:HD2	1.39	0.86
1:B:446:PHE:HD2	1:B:454:LEU:HD21	1.38	0.86
1:B:603:LEU:HD23	1:B:604:VAL:N	1.90	0.86
1:B:699:ASP:HA	1:B:725:ASN:OD1	1.74	0.86
1:A:370:LEU:CD1	1:A:399:ILE:HD12	2.06	0.86
1:B:256:LEU:HB3	1:B:309:LEU:HD22	1.56	0.86
1:B:435:ILE:CG2	1:B:446:PHE:HB2	2.06	0.86
1:B:833:LEU:HB2	1:B:836:HIS:HD2	1.39	0.86
1:B:295:VAL:HA	1:B:414:VAL:CG2	2.05	0.86
1:A:118:LEU:HD13	1:A:119:ILE:N	1.91	0.86
1:A:295:VAL:HA	1:A:414:VAL:CG2	2.05	0.86
1:B:100:VAL:HG12	1:B:101:GLN:HG3	1.58	0.86
1:B:473:GLN:CG	1:B:504:VAL:HG22	2.06	0.86
1:B:700:CYS:HB3	1:B:701:PRO:CD	1.92	0.86
1:B:847:LEU:HD12	1:B:852:SER:HB3	1.58	0.86
1:A:603:LEU:HD23	1:A:604:VAL:N	1.90	0.85
1:B:370:LEU:CD1	1:B:399:ILE:HD12	2.05	0.85
1:B:531:LEU:O	1:B:641:THR:OG1	1.94	0.85
1:B:847:LEU:HD11	1:B:850:ALA:HA	1.58	0.85
1:A:100:VAL:HG12	1:A:101:GLN:HG3	1.58	0.85
1:B:676:TYR:HE1	1:B:730:GLN:HG2	1.41	0.85
1:B:133:TYR:CG	1:B:136:ILE:HG12	2.12	0.85
1:A:882:LEU:HB2	1:A:910:ALA:HA	1.58	0.85
1:A:847:LEU:HD12	1:A:852:SER:HB3	1.58	0.85
1:A:133:TYR:CG	1:A:136:ILE:HG12	2.12	0.85
1:A:706:VAL:HG22	1:A:707:ASP:H	1.42	0.85
1:A:473:GLN:CG	1:A:504:VAL:HG22	2.06	0.85
1:A:42:PHE:CZ	1:A:45:GLU:HB2	2.12	0.84
1:A:847:LEU:HG	1:A:850:ALA:H	1.39	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:LEU:HD13	1:B:119:ILE:N	1.91	0.84
1:B:39:PHE:CE1	1:B:505:PRO:HD2	2.11	0.84
1:A:256:LEU:HB3	1:A:309:LEU:HD22	1.56	0.84
1:B:548:ARG:HG3	1:B:583:VAL:O	1.77	0.84
1:A:989:GLY:HA2	1:A:1017:LYS:HE3	1.57	0.84
1:B:42:PHE:CZ	1:B:45:GLU:HB2	2.12	0.84
1:B:356:ILE:CG2	1:B:421:ILE:HB	2.07	0.84
1:B:295:VAL:CG1	1:B:414:VAL:HG11	2.07	0.84
1:B:50:PHE:HB2	1:B:498:GLU:O	1.78	0.84
1:B:40:VAL:CG1	1:B:503:ARG:HB3	2.08	0.84
1:B:653:TYR:C	1:B:654:ASN:N	2.31	0.83
1:A:40:VAL:CG1	1:A:503:ARG:HB3	2.08	0.83
1:B:295:VAL:HA	1:B:414:VAL:HG22	1.60	0.83
1:A:229:PRO:O	1:A:232:THR:HG22	1.79	0.83
1:A:356:ILE:CG2	1:A:421:ILE:HB	2.07	0.83
1:A:336:THR:O	1:A:354:LEU:HD12	1.78	0.83
1:A:863:ILE:CG2	1:A:876:THR:HB	2.07	0.83
1:A:971:VAL:HG22	1:A:1005:CYS:O	1.78	0.83
1:B:706:VAL:HG22	1:B:707:ASP:H	1.42	0.83
1:A:118:LEU:HD12	1:A:172:ILE:CD1	2.05	0.83
1:B:830:GLN:HG2	1:B:831:CYS:H	1.43	0.83
1:B:474:VAL:HG22	1:B:495:ILE:HG21	1.61	0.83
1:B:118:LEU:HD12	1:B:172:ILE:CD1	2.05	0.83
1:B:336:THR:O	1:B:354:LEU:HD12	1.78	0.83
1:B:358:ILE:HG23	1:B:361:GLN:H	1.44	0.83
1:A:397:LEU:HD23	1:A:399:ILE:HD13	1.61	0.83
1:A:42:PHE:CE1	1:A:79:VAL:HG22	2.14	0.83
1:A:847:LEU:HD11	1:A:850:ALA:HA	1.58	0.83
1:A:996:HIS:HB3	1:A:1004:ILE:HG23	1.59	0.83
1:B:229:PRO:O	1:B:232:THR:HG22	1.79	0.83
1:A:295:VAL:CG1	1:A:414:VAL:HG11	2.07	0.83
1:B:133:TYR:CB	1:B:136:ILE:HG12	2.09	0.83
1:A:440:LYS:CD	1:A:538:LYS:HD3	2.08	0.82
1:A:474:VAL:HG22	1:A:495:ILE:HG21	1.61	0.82
1:B:397:LEU:HD23	1:B:399:ILE:HD13	1.61	0.82
1:B:53:LEU:HD23	1:B:54:VAL:N	1.94	0.82
1:A:358:ILE:HG23	1:A:361:GLN:H	1.44	0.82
1:A:951:MET:C	1:A:952:THR:N	2.32	0.82
1:B:295:VAL:HG12	1:B:414:VAL:CG1	2.09	0.82
1:A:435:ILE:CG2	1:A:446:PHE:HB2	2.06	0.82
1:A:548:ARG:HG3	1:A:583:VAL:O	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:785:ASN:HB3	1:B:788:PHE:CD2	2.14	0.82
1:B:863:ILE:CG2	1:B:876:THR:HB	2.07	0.82
1:A:987:MET:HB2	1:A:1019:THR:CG2	2.09	0.82
1:A:44:GLY:HA2	1:A:50:PHE:CE2	2.15	0.82
1:A:53:LEU:HD23	1:A:54:VAL:N	1.94	0.82
1:A:44:GLY:HA2	1:A:50:PHE:HE2	1.44	0.82
1:B:44:GLY:HA2	1:B:50:PHE:CE2	2.15	0.82
1:A:133:TYR:CB	1:A:136:ILE:HG12	2.09	0.82
1:A:785:ASN:HB3	1:A:788:PHE:CD2	2.14	0.82
1:A:295:VAL:HA	1:A:414:VAL:HG22	1.60	0.82
1:A:50:PHE:HB2	1:A:498:GLU:O	1.78	0.82
1:A:991:GLN:CG	1:A:1008:THR:HG21	2.10	0.82
1:A:439:TYR:CE2	1:A:538:LYS:CE	2.63	0.82
1:B:185:ALA:HB1	1:B:243:TYR:CE1	2.15	0.82
1:A:397:LEU:HD23	1:A:399:ILE:CD1	2.10	0.81
1:B:882:LEU:HB2	1:B:910:ALA:HA	1.58	0.81
1:A:225:MET:HE1	1:A:227:LYS:HG3	1.63	0.81
1:A:994:LEU:HD11	1:A:1006:ASN:HB2	1.63	0.81
1:B:356:ILE:HG22	1:B:421:ILE:HB	1.61	0.81
1:B:62:ILE:HG13	1:B:73:LEU:HB2	1.62	0.81
1:A:889:ILE:HG23	1:A:892:HIS:CE1	2.16	0.81
1:B:154:LYS:HD3	1:B:210:ASP:OD1	1.81	0.81
1:B:397:LEU:HD23	1:B:399:ILE:CD1	2.11	0.81
1:B:863:ILE:HG13	1:B:864:PRO:HD3	1.62	0.81
1:A:458:ARG:HD2	1:A:524:PRO:CG	2.10	0.81
1:B:42:PHE:CE1	1:B:79:VAL:HG22	2.14	0.81
1:A:440:LYS:CB	1:A:538:LYS:NZ	2.44	0.81
1:A:154:LYS:HD3	1:A:210:ASP:OD1	1.81	0.80
1:B:154:LYS:HB2	1:B:157:HIS:CD2	2.16	0.80
1:B:324:THR:HB	1:B:462:PRO:CB	2.10	0.80
1:A:185:ALA:HB1	1:A:243:TYR:CE1	2.15	0.80
1:A:623:ILE:HD12	1:A:624:THR:N	1.96	0.80
1:B:486:PHE:CE1	1:B:493:LEU:HD13	2.16	0.80
1:B:889:ILE:HG23	1:B:892:HIS:CE1	2.16	0.80
1:A:830:GLN:HG2	1:A:831:CYS:H	1.43	0.80
1:A:356:ILE:HG22	1:A:421:ILE:HB	1.61	0.80
1:A:486:PHE:CE1	1:A:493:LEU:HD13	2.16	0.80
1:B:444:LEU:HD13	1:B:445:ALA:N	1.97	0.80
1:B:623:ILE:HD12	1:B:624:THR:N	1.96	0.80
1:A:620:PRO:HA	1:A:623:ILE:CG1	2.12	0.80
1:B:314:LEU:HD11	1:B:332:ASP:HB3	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:PRO:HB3	1:B:233:PHE:CE1	2.17	0.80
1:B:653:TYR:HE2	1:B:682:HIS:HD1	1.27	0.80
1:A:994:LEU:CD1	1:A:1006:ASN:HB2	2.12	0.79
1:B:620:PRO:HA	1:B:623:ILE:CG1	2.12	0.79
1:A:192:PRO:HB3	1:A:233:PHE:CE1	2.17	0.79
1:B:239:PHE:CE1	1:B:260:PRO:HD2	2.17	0.79
1:B:317:ALA:HB1	1:B:321:LEU:HB3	1.64	0.79
1:B:380:LEU:HD12	1:B:386:LYS:HE3	1.64	0.79
1:A:321:LEU:HD12	1:A:462:PRO:HG2	1.64	0.79
1:A:591:ASN:OD1	1:A:639:LYS:HE2	1.83	0.79
1:A:926:ALA:HB1	1:A:947:LEU:HD12	1.63	0.79
1:B:699:ASP:CA	1:B:725:ASN:OD1	2.29	0.79
1:A:154:LYS:HB2	1:A:157:HIS:CD2	2.16	0.79
1:A:370:LEU:HD12	1:A:399:ILE:HD12	1.64	0.79
1:A:951:MET:HG2	1:A:977:ASN:CG	2.03	0.79
1:B:370:LEU:HD12	1:B:399:ILE:HD12	1.63	0.79
1:A:239:PHE:CE1	1:A:260:PRO:HD2	2.17	0.79
1:A:244:VAL:HG13	1:A:482:ARG:NH1	1.98	0.79
1:B:244:VAL:HG13	1:B:482:ARG:NH1	1.98	0.79
1:A:324:THR:HB	1:A:462:PRO:CB	2.10	0.79
1:A:444:LEU:HD13	1:A:445:ALA:N	1.97	0.79
1:A:863:ILE:HG13	1:A:864:PRO:HD3	1.62	0.79
1:B:591:ASN:OD1	1:B:639:LYS:HE2	1.83	0.79
1:A:62:ILE:HG13	1:A:73:LEU:HB2	1.62	0.79
1:B:319:ALA:H	1:B:441:ASN:HD22	1.31	0.79
1:B:44:GLY:HA2	1:B:50:PHE:HE2	1.44	0.79
1:B:926:ALA:HB1	1:B:947:LEU:HD12	1.63	0.79
1:A:715:VAL:HG21	1:A:717:LYS:HD2	1.65	0.78
1:B:453:LYS:HE3	1:B:472:VAL:CG2	2.13	0.78
1:B:715:VAL:HG21	1:B:717:LYS:HD2	1.65	0.78
1:A:319:ALA:H	1:A:441:ASN:HD22	1.31	0.78
1:A:440:LYS:CB	1:A:538:LYS:HZ3	1.96	0.78
1:A:231:ASP:O	1:A:234:THR:HG22	1.84	0.78
1:A:295:VAL:HG12	1:A:414:VAL:CG1	2.09	0.78
1:A:847:LEU:CG	1:A:850:ALA:HA	2.13	0.78
1:B:320:VAL:HG21	1:B:442:HIS:CD2	2.19	0.78
1:A:453:LYS:HE3	1:A:472:VAL:CG2	2.13	0.78
1:A:320:VAL:HG21	1:A:442:HIS:CD2	2.19	0.78
1:A:742:ILE:HB	1:A:745:ILE:O	1.84	0.78
1:A:873:THR:HA	1:A:982:SER:HB2	0.82	0.78
1:B:469:TYR:HB3	1:B:523:ASP:OD1	1.81	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:742:ILE:HB	1:B:745:ILE:O	1.84	0.78
1:A:380:LEU:HD12	1:A:386:LYS:HE3	1.64	0.78
1:A:868:PRO:CG	1:A:981:GLY:HA3	2.12	0.78
1:B:56:ASP:OD2	1:B:142:LEU:HD11	1.83	0.78
1:B:321:LEU:HD12	1:B:462:PRO:HG2	1.64	0.78
1:A:972:THR:HA	1:A:1002:TYR:HE1	1.47	0.78
1:A:181:LYS:NZ	1:A:216:VAL:HG23	1.98	0.78
1:A:327:VAL:HG12	1:A:358:ILE:HD11	1.66	0.78
1:B:439:TYR:OH	1:B:538:LYS:HE3	1.83	0.78
1:A:439:TYR:CZ	1:A:538:LYS:CE	2.67	0.78
1:A:870:GLU:HG2	1:A:1025:ALA:N	1.98	0.78
1:A:51:ASN:HD21	1:A:67:VAL:HG23	1.49	0.78
1:A:994:LEU:O	1:A:994:LEU:HD12	1.84	0.78
1:B:847:LEU:CG	1:B:850:ALA:HA	2.13	0.78
1:A:314:LEU:HD11	1:A:332:ASP:HB3	1.64	0.77
1:A:710:LEU:HD12	1:A:710:LEU:O	1.84	0.77
1:A:284:LYS:HD3	1:A:284:LYS:O	1.84	0.77
1:B:168:VAL:HG23	1:B:185:ALA:O	1.84	0.77
1:B:51:ASN:HD21	1:B:67:VAL:HG23	1.50	0.77
1:A:1014:LEU:H	1:A:1014:LEU:HD22	1.48	0.77
1:A:1016:MET:HG2	1:A:1035:TYR:CE2	2.19	0.77
1:A:327:VAL:CG1	1:A:358:ILE:HD11	2.14	0.77
1:B:327:VAL:CG1	1:B:358:ILE:HD11	2.14	0.77
1:A:56:ASP:OD2	1:A:142:LEU:HD11	1.83	0.77
1:B:710:LEU:O	1:B:710:LEU:HD12	1.84	0.77
1:B:595:GLU:CB	1:B:597:LEU:HD23	2.14	0.77
1:B:231:ASP:O	1:B:234:THR:HG22	1.84	0.77
1:B:327:VAL:HG12	1:B:358:ILE:HD11	1.65	0.77
1:B:567:ILE:HD13	1:B:567:ILE:H	1.50	0.77
1:A:168:VAL:HG23	1:A:185:ALA:O	1.84	0.77
1:B:662:LEU:HD11	1:B:702:GLN:NE2	1.99	0.77
1:A:317:ALA:HB1	1:A:321:LEU:HB3	1.64	0.77
1:A:547:PRO:O	1:A:548:ARG:HG2	1.84	0.77
1:A:870:GLU:HG3	1:A:1024:ARG:HG3	1.64	0.77
1:B:204:THR:HG21	1:B:209:ALA:HB3	1.66	0.77
1:B:181:LYS:NZ	1:B:216:VAL:HG23	1.98	0.77
1:B:359:LEU:HD12	1:B:362:ILE:CD1	2.10	0.77
1:A:1021:GLN:HG2	1:A:1026:ARG:HG3	1.67	0.77
1:B:403:PHE:CE1	1:B:406:LEU:HD23	2.20	0.77
1:A:567:ILE:H	1:A:567:ILE:HD13	1.50	0.76
1:A:549:ARG:HD3	1:A:584:PRO:HB3	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:LYS:O	1:B:284:LYS:HD3	1.84	0.76
1:A:120:ASP:OD2	1:A:123:GLU:HG3	1.86	0.76
1:A:403:PHE:CE1	1:A:406:LEU:HD23	2.20	0.76
1:A:439:TYR:OH	1:A:538:LYS:HE3	1.84	0.76
1:A:460:ASP:HB3	1:A:464:GLY:N	2.00	0.76
1:B:780:LEU:O	1:B:780:LEU:HD12	1.86	0.76
1:B:847:LEU:CD1	1:B:850:ALA:HA	2.16	0.76
1:A:873:THR:HA	1:A:982:SER:CA	2.15	0.76
1:B:172:ILE:HG12	1:B:182:LEU:HD13	1.68	0.76
1:B:616:ALA:O	1:B:620:PRO:HD2	1.85	0.76
1:A:359:LEU:HD12	1:A:362:ILE:CD1	2.09	0.76
1:A:616:ALA:O	1:A:620:PRO:HD2	1.85	0.76
1:A:780:LEU:HD12	1:A:780:LEU:O	1.86	0.76
1:B:120:ASP:OD2	1:B:123:GLU:HG3	1.86	0.76
1:B:460:ASP:HB3	1:B:464:GLY:N	2.00	0.76
1:B:64:LEU:HD12	1:B:496:MET:CE	2.16	0.76
1:A:873:THR:OG1	1:A:981:GLY:CA	2.34	0.76
1:A:1010:SER:HB2	1:A:1035:TYR:CE2	2.20	0.75
1:A:256:LEU:CB	1:A:309:LEU:HD22	2.16	0.75
1:A:42:PHE:HZ	1:A:45:GLU:HB2	1.50	0.75
1:A:869:ARG:O	1:A:920:ALA:HB3	1.86	0.75
1:A:868:PRO:HG2	1:A:1022:VAL:HG22	1.65	0.75
1:A:172:ILE:HG12	1:A:182:LEU:HD13	1.68	0.75
1:A:458:ARG:CD	1:A:524:PRO:HB3	2.12	0.75
1:A:919:GLU:HB3	1:A:1024:ARG:HH11	1.51	0.75
1:B:278:LYS:HE3	1:B:296:PRO:HG3	1.67	0.75
1:B:547:PRO:O	1:B:548:ARG:HG2	1.84	0.75
1:B:806:MET:HE3	1:B:806:MET:N	1.99	0.75
1:B:847:LEU:HD12	1:B:852:SER:CB	2.16	0.75
1:A:874:LYS:N	1:A:982:SER:HB2	2.02	0.75
1:B:506:VAL:HG22	1:B:525:HIS:CD2	2.21	0.75
1:B:785:ASN:HB3	1:B:788:PHE:HD2	1.48	0.75
1:B:873:THR:HB	1:B:917:MET:CE	2.17	0.75
1:A:204:THR:HG21	1:A:209:ALA:HB3	1.66	0.75
1:A:847:LEU:CD1	1:A:850:ALA:HA	2.16	0.75
1:A:278:LYS:HE3	1:A:296:PRO:HG3	1.67	0.75
1:A:473:GLN:CB	1:A:504:VAL:HG22	2.17	0.75
1:B:323:ARG:HG3	1:B:324:THR:N	2.02	0.75
1:B:473:GLN:CB	1:B:504:VAL:HG22	2.17	0.75
1:B:784:TRP:HD1	1:B:790:ILE:HD11	1.51	0.75
1:B:806:MET:H	1:B:806:MET:CE	1.97	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:PHE:HB3	1:B:454:LEU:HD11	1.69	0.75
1:B:448:GLY:HA3	1:B:480:VAL:HG21	1.68	0.75
1:A:188:VAL:HG22	1:A:191:LYS:H	1.52	0.75
1:A:278:LYS:HG2	1:A:296:PRO:HA	1.69	0.75
1:A:64:LEU:HD12	1:A:496:MET:CE	2.16	0.75
1:A:739:ILE:CD1	1:A:748:ARG:HG2	2.17	0.75
1:A:847:LEU:HD12	1:A:852:SER:CB	2.16	0.75
1:B:699:ASP:C	1:B:725:ASN:OD1	2.26	0.75
1:B:700:CYS:CB	1:B:701:PRO:CD	2.50	0.75
1:A:323:ARG:HG3	1:A:324:THR:N	2.02	0.74
1:A:623:ILE:HA	1:A:626:ASN:ND2	2.01	0.74
1:A:683:ASP:O	1:A:686:THR:HG22	1.87	0.74
1:A:873:THR:HB	1:A:917:MET:CE	2.17	0.74
1:B:196:PRO:HB3	1:B:225:MET:HE1	1.68	0.74
1:A:321:LEU:CD1	1:A:462:PRO:HG2	2.17	0.74
1:B:202:LYS:HD3	1:B:214:ALA:HB3	1.69	0.74
1:B:256:LEU:CB	1:B:309:LEU:HD22	2.16	0.74
1:B:42:PHE:HZ	1:B:45:GLU:HB2	1.50	0.74
1:B:321:LEU:CD1	1:B:462:PRO:HG2	2.17	0.74
1:B:869:ARG:O	1:B:920:ALA:HB3	1.86	0.74
1:A:99:ILE:HD11	1:A:152:PHE:HB2	1.69	0.74
1:A:785:ASN:HB3	1:A:788:PHE:HD2	1.48	0.74
1:A:151:PRO:HB2	1:A:157:HIS:ND1	2.02	0.74
1:B:623:ILE:HA	1:B:626:ASN:ND2	2.01	0.74
1:A:868:PRO:HG2	1:A:1022:VAL:CG2	2.17	0.74
1:A:448:GLY:HA3	1:A:480:VAL:HG21	1.68	0.74
1:B:151:PRO:HB2	1:B:157:HIS:ND1	2.03	0.74
1:B:188:VAL:HG22	1:B:191:LYS:H	1.52	0.74
1:A:1010:SER:HB2	1:A:1035:TYR:CZ	2.23	0.74
1:B:814:LEU:HB3	1:B:847:LEU:HB2	1.70	0.74
1:A:567:ILE:HD12	1:A:650:PHE:CZ	2.22	0.74
1:B:185:ALA:HB1	1:B:243:TYR:CZ	2.23	0.74
1:B:548:ARG:CG	1:B:584:PRO:HA	2.16	0.74
1:A:324:THR:HG21	1:A:462:PRO:HA	1.70	0.73
1:B:278:LYS:HG2	1:B:296:PRO:HA	1.68	0.73
1:B:739:ILE:CD1	1:B:748:ARG:HG2	2.17	0.73
1:A:185:ALA:HB1	1:A:243:TYR:CZ	2.23	0.73
1:A:569:VAL:CB	1:A:654:ASN:HB2	2.17	0.73
1:B:548:ARG:HG3	1:B:584:PRO:N	2.03	0.73
1:B:562:VAL:HG22	1:B:578:LEU:CD2	2.18	0.73
1:A:562:VAL:HG22	1:A:578:LEU:CD2	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:814:LEU:HB3	1:A:847:LEU:HB2	1.70	0.73
1:B:324:THR:HG21	1:B:462:PRO:HA	1.70	0.73
1:A:435:ILE:HD13	1:A:436:ALA:N	2.03	0.73
1:A:446:PHE:HB3	1:A:454:LEU:HD11	1.69	0.73
1:A:704:LEU:HD11	1:A:724:LYS:HE3	1.69	0.73
1:B:439:TYR:OH	1:B:538:LYS:CE	2.37	0.73
1:A:154:LYS:H	1:A:157:HIS:HD2	1.36	0.73
1:A:958:LEU:HD22	1:A:960:PRO:O	1.87	0.73
1:B:683:ASP:O	1:B:686:THR:HG22	1.88	0.73
1:A:225:MET:CE	1:A:227:LYS:HG3	2.19	0.73
1:B:468:GLN:CG	1:B:523:ASP:HA	2.08	0.73
1:B:225:MET:CE	1:B:227:LYS:HG3	2.19	0.73
1:A:446:PHE:CD2	1:A:454:LEU:HD21	2.24	0.73
1:B:225:MET:HE1	1:B:227:LYS:HG3	1.70	0.73
1:B:435:ILE:HD13	1:B:436:ALA:N	2.03	0.73
1:B:46:PRO:HG2	1:B:69:ARG:CG	2.17	0.73
1:A:548:ARG:O	1:A:584:PRO:HD3	1.88	0.73
1:B:39:PHE:CD2	1:B:473:GLN:HG3	2.23	0.73
1:B:567:ILE:HD12	1:B:650:PHE:CZ	2.22	0.73
1:B:704:LEU:HD11	1:B:724:LYS:HE3	1.69	0.73
1:A:670:ARG:HA	1:A:670:ARG:HE	1.54	0.72
1:A:46:PRO:HG2	1:A:69:ARG:CG	2.17	0.72
1:B:184:ILE:O	1:B:184:ILE:HD12	1.89	0.72
1:A:1030:ASP:O	1:A:1032:VAL:HG23	1.89	0.72
1:A:181:LYS:HZ3	1:A:216:VAL:HG23	1.54	0.72
1:A:184:ILE:HD12	1:A:184:ILE:O	1.89	0.72
1:A:784:TRP:HD1	1:A:790:ILE:HD11	1.51	0.72
1:A:73:LEU:HD22	1:A:79:VAL:HA	1.72	0.72
1:B:99:ILE:HD11	1:B:152:PHE:HB2	1.69	0.72
1:B:670:ARG:HA	1:B:670:ARG:HE	1.55	0.72
1:A:822:CYS:HA	1:A:833:LEU:HD23	1.70	0.72
1:A:994:LEU:HD11	1:A:1006:ASN:ND2	2.05	0.72
1:B:181:LYS:HD2	1:B:202:LYS:HA	1.71	0.72
1:B:822:CYS:HA	1:B:833:LEU:HD23	1.70	0.72
1:A:558:VAL:HG11	1:A:646:ALA:HB2	1.71	0.72
1:B:261:GLU:HA	1:B:264:SER:O	1.89	0.72
1:A:202:LYS:HD3	1:A:214:ALA:HB3	1.69	0.72
1:B:115:LYS:HB3	1:B:168:VAL:HG11	1.71	0.72
1:A:39:PHE:CD2	1:A:473:GLN:HG3	2.23	0.72
1:A:619:VAL:HB	1:A:620:PRO:HD3	1.72	0.72
1:A:832:THR:CG2	1:A:836:HIS:HB2	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:458:ARG:HG3	1:B:468:GLN:OE1	1.90	0.72
1:B:704:LEU:HB2	1:B:722:LYS:HG3	1.72	0.72
1:A:261:GLU:HA	1:A:264:SER:O	1.89	0.71
1:A:595:GLU:CB	1:A:597:LEU:HD23	2.14	0.71
1:A:937:ARG:CG	1:A:938:PRO:HD2	2.20	0.71
1:B:93:LYS:HD2	1:B:105:GLU:OE1	1.90	0.71
1:B:446:PHE:HZ	1:B:506:VAL:HG23	1.55	0.71
1:B:595:GLU:HG2	1:B:632:VAL:HG13	1.72	0.71
1:A:519:LEU:HD12	1:A:552:SER:O	1.90	0.71
1:A:806:MET:H	1:A:806:MET:CE	1.97	0.71
1:B:380:LEU:HB2	1:B:386:LYS:CE	2.20	0.71
1:B:471:THR:HG23	1:B:473:GLN:HE22	1.55	0.71
1:A:1017:LYS:H	1:A:1017:LYS:CE	2.01	0.71
1:A:321:LEU:HG	1:A:325:LEU:CD1	2.20	0.71
1:B:832:THR:CG2	1:B:836:HIS:HB2	2.20	0.71
1:A:595:GLU:HG2	1:A:632:VAL:HG13	1.72	0.71
1:A:847:LEU:CD1	1:A:852:SER:HB3	2.20	0.71
1:B:937:ARG:CG	1:B:938:PRO:HD2	2.20	0.71
1:A:989:GLY:HA2	1:A:1017:LYS:CE	2.20	0.71
1:A:370:LEU:HD21	1:A:374:TYR:HE1	1.55	0.71
1:B:563:HIS:HB2	1:B:577:VAL:CG1	2.21	0.71
1:B:619:VAL:HB	1:B:620:PRO:HD3	1.72	0.71
1:B:847:LEU:CD1	1:B:852:SER:HB3	2.20	0.71
1:A:321:LEU:HG	1:A:325:LEU:HD11	1.71	0.71
1:B:188:VAL:HG13	1:B:190:GLY:H	1.56	0.71
1:B:321:LEU:HG	1:B:325:LEU:CD1	2.20	0.71
1:A:1016:MET:O	1:A:1032:VAL:HG13	1.91	0.71
1:A:304:VAL:HG11	1:A:351:GLU:OE2	1.91	0.71
1:A:40:VAL:HG12	1:A:503:ARG:HB3	1.73	0.71
1:B:450:LYS:HA	1:B:479:PRO:HB3	1.73	0.71
1:A:1004:ILE:HD13	1:A:1005:CYS:N	2.06	0.71
1:A:380:LEU:HB2	1:A:386:LYS:CE	2.20	0.71
1:A:474:VAL:HG21	1:A:495:ILE:HD13	1.72	0.71
1:A:515:CYS:O	1:A:519:LEU:HD23	1.91	0.71
1:A:704:LEU:HB2	1:A:722:LYS:HG3	1.71	0.71
1:A:806:MET:HE3	1:A:806:MET:N	1.99	0.71
1:B:474:VAL:HG21	1:B:495:ILE:HD13	1.72	0.71
1:B:575:LEU:HD22	1:B:575:LEU:H	1.56	0.71
1:A:962:ARG:HB3	1:A:1034:GLN:HG3	1.73	0.70
1:B:154:LYS:H	1:B:157:HIS:HD2	1.36	0.70
1:B:72:LYS:HE3	1:B:80:LEU:CD1	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:ARG:HG3	1:A:468:GLN:OE1	1.90	0.70
1:B:321:LEU:HG	1:B:325:LEU:HD11	1.71	0.70
1:A:115:LYS:HB3	1:A:168:VAL:HG11	1.71	0.70
1:A:446:PHE:HZ	1:A:506:VAL:HG23	1.55	0.70
1:A:480:VAL:HB	1:A:484:MET:CE	2.21	0.70
1:A:507:GLU:HG3	1:A:537:ARG:HG3	1.74	0.70
1:A:556:GLN:O	1:A:582:ASN:HB3	1.91	0.70
1:B:281:ARG:HB3	1:B:293:VAL:CG1	2.22	0.70
1:B:304:VAL:HG11	1:B:351:GLU:OE2	1.91	0.70
1:A:281:ARG:HB3	1:A:293:VAL:CG1	2.22	0.70
1:A:563:HIS:HB2	1:A:577:VAL:CG1	2.21	0.70
1:B:519:LEU:HD12	1:B:552:SER:O	1.90	0.70
1:A:471:THR:HG23	1:A:473:GLN:HE22	1.55	0.70
1:B:370:LEU:HD21	1:B:374:TYR:HE1	1.55	0.70
1:A:63:TYR:C	1:A:64:LEU:HD22	2.12	0.70
1:A:39:PHE:HE1	1:A:505:PRO:HD2	1.56	0.70
1:A:93:LYS:HD2	1:A:105:GLU:OE1	1.91	0.70
1:A:1016:MET:HE3	1:A:1017:LYS:C	2.12	0.70
1:A:181:LYS:HD2	1:A:202:LYS:HA	1.71	0.70
1:B:847:LEU:HD21	1:B:850:ALA:HA	1.73	0.70
1:A:42:PHE:HE1	1:A:79:VAL:CG2	2.05	0.70
1:B:216:VAL:HG12	1:B:224:SER:OG	1.92	0.70
1:B:480:VAL:HB	1:B:484:MET:CE	2.21	0.70
1:A:873:THR:HG23	1:A:981:GLY:C	2.11	0.70
1:B:551:ALA:HA	1:B:556:GLN:OE1	1.92	0.70
1:A:367:LYS:HE2	1:A:399:ILE:O	1.91	0.69
1:A:474:VAL:CG1	1:A:475:VAL:HG23	2.18	0.69
1:A:450:LYS:HA	1:A:479:PRO:HB3	1.73	0.69
1:A:551:ALA:HA	1:A:556:GLN:OE1	1.92	0.69
1:B:558:VAL:HG11	1:B:646:ALA:HB2	1.71	0.69
1:B:73:LEU:HD22	1:B:79:VAL:HA	1.72	0.69
1:A:72:LYS:HE3	1:A:80:LEU:CD1	2.22	0.69
1:A:739:ILE:HB	1:A:781:THR:CG2	2.22	0.69
1:B:110:THR:HG22	1:B:132:LEU:HD21	1.73	0.69
1:B:63:TYR:C	1:B:64:LEU:HD22	2.12	0.69
1:B:367:LYS:HE2	1:B:399:ILE:O	1.91	0.69
1:B:515:CYS:O	1:B:519:LEU:HD23	1.91	0.69
1:A:847:LEU:HD21	1:A:850:ALA:HA	1.73	0.69
1:B:40:VAL:HG12	1:B:503:ARG:HB3	1.73	0.69
1:A:1016:MET:HG2	1:A:1035:TYR:HE2	1.57	0.69
1:A:216:VAL:HG12	1:A:224:SER:OG	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:LEU:HB2	1:A:386:LYS:HE3	1.74	0.69
1:A:439:TYR:CZ	1:A:538:LYS:HE3	2.28	0.69
1:A:560:LEU:CD2	1:A:648:THR:HG23	2.19	0.69
1:A:188:VAL:HG13	1:A:190:GLY:H	1.56	0.69
1:A:473:GLN:OE1	1:A:504:VAL:HG13	1.93	0.69
1:A:435:ILE:HD12	1:A:486:PHE:CD1	2.27	0.69
1:A:802:LYS:C	1:A:803:CYS:N	2.46	0.69
1:A:873:THR:HG23	1:A:982:SER:N	2.07	0.69
1:B:473:GLN:OE1	1:B:504:VAL:HG13	1.93	0.69
1:A:595:GLU:CG	1:A:632:VAL:HG13	2.22	0.69
1:A:959:LYS:CB	1:A:972:THR:HB	2.21	0.69
1:A:988:PHE:HB3	1:A:1016:MET:SD	2.33	0.69
1:B:453:LYS:HE3	1:B:472:VAL:HG21	1.73	0.69
1:A:958:LEU:HD23	1:A:959:LYS:N	2.08	0.69
1:B:380:LEU:HB2	1:B:386:LYS:HE3	1.74	0.69
1:A:133:TYR:CD2	1:A:136:ILE:HG12	2.28	0.69
1:A:133:TYR:HB2	1:A:136:ILE:HG12	1.75	0.69
1:B:133:TYR:CD2	1:B:136:ILE:HG12	2.28	0.69
1:A:196:PRO:HB3	1:A:225:MET:HE1	1.73	0.68
1:B:446:PHE:CD2	1:B:454:LEU:HD21	2.24	0.68
1:B:507:GLU:HG3	1:B:537:ARG:HG3	1.74	0.68
1:A:453:LYS:HE3	1:A:472:VAL:HG21	1.73	0.68
1:B:46:PRO:HG3	1:B:69:ARG:HD2	1.75	0.68
1:A:972:THR:HG23	1:A:1002:TYR:CD1	2.28	0.68
1:B:739:ILE:HB	1:B:781:THR:CG2	2.23	0.68
1:B:412:LEU:H	1:B:412:LEU:HD13	1.59	0.68
1:A:773:ILE:HD13	1:A:773:ILE:H	1.59	0.68
1:B:474:VAL:CG1	1:B:475:VAL:HG23	2.18	0.68
1:B:773:ILE:HD13	1:B:773:ILE:H	1.59	0.68
1:A:110:THR:HG22	1:A:132:LEU:HD21	1.74	0.68
1:A:323:ARG:HG3	1:A:324:THR:H	1.58	0.68
1:A:689:PHE:CD1	1:A:691:GLU:HG2	2.28	0.68
1:A:703:LEU:HD13	1:A:723:ALA:HB2	1.76	0.68
1:B:435:ILE:HD12	1:B:486:PHE:CD1	2.27	0.68
1:A:594:PHE:O	1:A:595:GLU:HG2	1.94	0.68
1:A:867:GLY:HA3	1:A:948:TYR:OH	1.94	0.68
1:B:190:GLY:HA2	1:B:233:PHE:CE2	2.29	0.68
1:B:548:ARG:NE	1:B:583:VAL:O	2.26	0.68
1:B:595:GLU:CG	1:B:632:VAL:HG13	2.22	0.68
1:A:53:LEU:HB2	1:A:496:MET:HE1	1.76	0.68
1:B:594:PHE:O	1:B:595:GLU:HG2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:700:CYS:O	1:B:725:ASN:CB	2.30	0.68
1:A:190:GLY:HA2	1:A:233:PHE:CE2	2.29	0.68
1:A:40:VAL:HG11	1:A:503:ARG:NE	2.09	0.68
1:A:555:LYS:HG3	1:A:556:GLN:N	2.09	0.68
1:A:830:GLN:HG2	1:A:831:CYS:N	2.09	0.68
1:B:98:ARG:HE	1:B:107:LEU:CD1	2.07	0.68
1:B:689:PHE:CD1	1:B:691:GLU:HG2	2.28	0.68
1:B:830:GLN:HG2	1:B:831:CYS:N	2.09	0.68
1:A:575:LEU:HD22	1:A:575:LEU:H	1.56	0.68
1:A:73:LEU:CD2	1:A:79:VAL:HA	2.23	0.68
1:B:323:ARG:HG3	1:B:324:THR:H	1.58	0.68
1:B:62:ILE:HD11	1:B:73:LEU:HD12	1.76	0.68
1:B:62:ILE:O	1:B:62:ILE:HG13	1.94	0.68
1:A:867:GLY:C	1:A:980:ALA:HB1	2.14	0.67
1:A:962:ARG:HB3	1:A:1034:GLN:CG	2.23	0.67
1:B:548:ARG:HG3	1:B:584:PRO:CA	2.25	0.67
1:A:1013:VAL:HG22	1:A:1014:LEU:H	1.60	0.67
1:A:532:HIS:O	1:A:641:THR:HG21	1.94	0.67
1:B:42:PHE:HE1	1:B:79:VAL:CG2	2.05	0.67
1:B:560:LEU:CD2	1:B:648:THR:HG23	2.19	0.67
1:B:863:ILE:HG23	1:B:864:PRO:CD	2.23	0.67
1:A:46:PRO:HG3	1:A:69:ARG:HD2	1.75	0.67
1:B:460:ASP:HB3	1:B:463:LYS:HB3	1.77	0.67
1:B:867:GLY:HA3	1:B:948:TYR:OH	1.94	0.67
1:A:531:LEU:HG	1:A:584:PRO:HG2	1.77	0.67
1:A:951:MET:HG3	1:A:952:THR:N	2.09	0.67
1:A:98:ARG:HE	1:A:107:LEU:HD11	1.60	0.67
1:B:98:ARG:HE	1:B:107:LEU:HD11	1.60	0.67
1:A:137:CYS:HB2	1:A:213:PHE:CZ	2.30	0.67
1:A:321:LEU:O	1:A:325:LEU:HG	1.95	0.67
1:A:460:ASP:HB3	1:A:463:LYS:HB3	1.77	0.67
1:B:555:LYS:HG3	1:B:556:GLN:N	2.09	0.67
1:A:994:LEU:CD1	1:A:1006:ASN:HD22	2.07	0.67
1:A:863:ILE:HG23	1:A:864:PRO:CD	2.23	0.67
1:B:321:LEU:O	1:B:325:LEU:HG	1.95	0.67
1:B:595:GLU:HG2	1:B:632:VAL:CG1	2.25	0.67
1:B:62:ILE:HD12	1:B:64:LEU:HD21	1.75	0.67
1:B:73:LEU:CD2	1:B:79:VAL:HA	2.24	0.67
1:A:62:ILE:HD11	1:A:73:LEU:HD12	1.76	0.67
1:B:53:LEU:HB2	1:B:496:MET:HE1	1.77	0.67
1:A:62:ILE:HD12	1:A:64:LEU:HD21	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:LEU:CD1	1:B:333:LEU:HD11	2.25	0.66
1:A:98:ARG:HE	1:A:107:LEU:CD1	2.07	0.66
1:A:595:GLU:HG2	1:A:632:VAL:CG1	2.25	0.66
1:A:847:LEU:HG	1:A:850:ALA:N	2.10	0.66
1:B:703:LEU:HD13	1:B:723:ALA:HB2	1.76	0.66
1:B:847:LEU:HG	1:B:850:ALA:N	2.10	0.66
1:A:532:HIS:HA	1:A:641:THR:CG2	2.25	0.66
1:A:873:THR:HG1	1:A:981:GLY:HA2	1.61	0.66
1:B:133:TYR:HB2	1:B:136:ILE:HG12	1.75	0.66
1:B:863:ILE:HG13	1:B:864:PRO:CD	2.25	0.66
1:B:40:VAL:HG11	1:B:503:ARG:NE	2.09	0.66
1:B:98:ARG:HH21	1:B:107:LEU:HD12	1.60	0.66
1:A:98:ARG:HH21	1:A:107:LEU:HD12	1.59	0.66
1:A:239:PHE:CD1	1:A:260:PRO:HD2	2.30	0.66
1:A:566:ASN:HA	1:A:651:VAL:CG2	2.25	0.66
1:A:955:LEU:HG	1:A:973:ILE:CG2	2.24	0.66
1:B:133:TYR:HB2	1:B:136:ILE:H	1.61	0.66
1:A:446:PHE:CZ	1:A:486:PHE:HZ	2.13	0.66
1:B:739:ILE:HD12	1:B:748:ARG:HG2	1.76	0.66
1:B:854:CYS:C	1:B:855:THR:N	2.49	0.66
1:B:809:SER:CB	1:B:881:ASN:CG	2.47	0.66
1:A:325:LEU:CD1	1:A:333:LEU:HD11	2.25	0.66
1:A:739:ILE:HD12	1:A:748:ARG:HG2	1.76	0.66
1:A:863:ILE:HG13	1:A:864:PRO:CD	2.25	0.66
1:A:567:ILE:HD13	1:A:651:VAL:O	1.96	0.66
1:B:181:LYS:HD3	1:B:202:LYS:HA	1.78	0.66
1:B:137:CYS:HB2	1:B:213:PHE:CZ	2.30	0.66
1:B:410:ALA:HB1	1:B:411:PRO:HD2	1.78	0.66
1:B:548:ARG:HG3	1:B:584:PRO:HA	1.78	0.66
1:A:1016:MET:CE	1:A:1033:PHE:HB3	2.25	0.66
1:A:892:HIS:NE2	1:A:931:ILE:HB	2.11	0.66
1:B:110:THR:HB	1:B:132:LEU:CD2	2.26	0.66
1:B:629:HIS:CE1	1:B:669:TYR:CZ	2.69	0.66
1:A:261:GLU:HG2	1:A:264:SER:C	2.17	0.65
1:A:296:PRO:HD2	1:A:414:VAL:CG2	2.27	0.65
1:B:261:GLU:HG2	1:B:264:SER:C	2.17	0.65
1:A:216:VAL:HG12	1:A:224:SER:CB	2.26	0.65
1:A:412:LEU:HD13	1:A:412:LEU:H	1.59	0.65
1:A:474:VAL:HG12	1:A:475:VAL:CG2	2.21	0.65
1:A:782:VAL:HG23	1:A:790:ILE:HB	1.78	0.65
1:A:797:LYS:HD2	1:A:797:LYS:N	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:870:GLU:CB	1:A:1024:ARG:HG3	2.17	0.65
1:B:239:PHE:CD1	1:B:260:PRO:HD2	2.30	0.65
1:B:782:VAL:HG23	1:B:790:ILE:HB	1.78	0.65
1:A:133:TYR:HB2	1:A:136:ILE:H	1.61	0.65
1:A:62:ILE:HG13	1:A:62:ILE:O	1.94	0.65
1:A:432:THR:OG1	1:A:480:VAL:HG23	1.96	0.65
1:A:473:GLN:HG2	1:A:504:VAL:HG22	1.79	0.65
1:B:676:TYR:HD1	1:B:730:GLN:CG	2.08	0.65
1:B:847:LEU:CD2	1:B:850:ALA:HA	2.27	0.65
1:A:181:LYS:HD3	1:A:202:LYS:HA	1.78	0.65
1:A:154:LYS:H	1:A:157:HIS:CD2	2.15	0.65
1:B:265:PRO:HD3	1:B:274:VAL:CG2	2.27	0.65
1:B:446:PHE:CZ	1:B:486:PHE:HZ	2.14	0.65
1:B:675:LYS:HE3	1:B:694:VAL:HG22	1.79	0.65
1:A:110:THR:HB	1:A:132:LEU:CD2	2.26	0.65
1:A:453:LYS:HG2	1:A:472:VAL:CG2	2.16	0.65
1:A:706:VAL:HG13	1:A:707:ASP:O	1.96	0.65
1:B:216:VAL:HG12	1:B:224:SER:CB	2.26	0.65
1:A:872:GLY:HA3	1:A:1023:ASP:OD1	1.97	0.65
1:A:807:ARG:HD3	1:A:812:LEU:C	2.18	0.65
1:B:653:TYR:OH	1:B:682:HIS:CE1	2.50	0.65
1:B:807:ARG:HD3	1:B:812:LEU:C	2.17	0.65
1:A:368:ASP:O	1:A:371:GLN:HG2	1.97	0.64
1:A:675:LYS:HE3	1:A:694:VAL:HG22	1.79	0.64
1:B:432:THR:OG1	1:B:480:VAL:HG23	1.96	0.64
1:A:405:GLY:O	1:A:406:LEU:HD22	1.98	0.64
1:A:410:ALA:HB1	1:A:411:PRO:HD2	1.78	0.64
1:B:39:PHE:HE1	1:B:505:PRO:HD2	1.57	0.64
1:B:405:GLY:O	1:B:406:LEU:HD22	1.98	0.64
1:A:105:GLU:HB3	1:A:106:PRO:HD2	1.80	0.64
1:A:265:PRO:HD3	1:A:274:VAL:CG2	2.27	0.64
1:A:309:LEU:HD11	1:A:311:ALA:O	1.98	0.64
1:A:926:ALA:HB1	1:A:947:LEU:CD1	2.27	0.64
1:B:186:THR:HG22	1:B:187:ALA:N	2.12	0.64
1:B:320:VAL:O	1:B:323:ARG:HG2	1.98	0.64
1:B:474:VAL:HG12	1:B:475:VAL:CG2	2.21	0.64
1:B:53:LEU:HB2	1:B:496:MET:CE	2.28	0.64
1:B:567:ILE:HD13	1:B:651:VAL:O	1.96	0.64
1:A:186:THR:HG22	1:A:187:ALA:N	2.12	0.64
1:A:53:LEU:HB2	1:A:496:MET:CE	2.28	0.64
1:A:620:PRO:CA	1:A:623:ILE:HG13	2.23	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:LEU:HG	1:A:64:LEU:CD1	2.28	0.64
1:B:797:LYS:N	1:B:797:LYS:HD2	2.11	0.64
1:B:926:ALA:HB1	1:B:947:LEU:CD1	2.27	0.64
1:A:175:TYR:HD2	1:A:179:ASP:HB3	1.63	0.64
1:A:460:ASP:CB	1:A:463:LYS:HB3	2.28	0.64
1:B:473:GLN:HG2	1:B:504:VAL:HG22	1.79	0.64
1:B:469:TYR:HB3	1:B:523:ASP:CG	2.18	0.64
1:B:175:TYR:HD2	1:B:179:ASP:HB3	1.63	0.64
1:B:296:PRO:HD2	1:B:414:VAL:CG2	2.27	0.64
1:B:460:ASP:CB	1:B:463:LYS:HB3	2.28	0.64
1:B:505:PRO:CB	1:B:507:GLU:O	2.46	0.64
1:A:566:ASN:HB3	1:A:651:VAL:HG21	1.80	0.64
1:A:847:LEU:CD2	1:A:850:ALA:HA	2.27	0.64
1:B:56:ASP:OD1	1:B:119:ILE:HD12	1.98	0.64
1:A:741:ASN:O	1:A:778:VAL:HG13	1.98	0.64
1:B:105:GLU:HB3	1:B:106:PRO:HD2	1.80	0.64
1:B:473:GLN:HB2	1:B:504:VAL:HG22	1.80	0.64
1:B:566:ASN:HA	1:B:651:VAL:CG2	2.25	0.64
1:A:56:ASP:OD1	1:A:119:ILE:HD12	1.98	0.64
1:B:118:LEU:HG	1:B:172:ILE:HG13	1.80	0.64
1:B:154:LYS:H	1:B:157:HIS:CD2	2.15	0.64
1:B:309:LEU:HD11	1:B:311:ALA:O	1.98	0.64
1:B:53:LEU:HG	1:B:64:LEU:CD1	2.28	0.64
1:B:706:VAL:HG13	1:B:707:ASP:O	1.96	0.64
1:B:713:VAL:HG12	1:B:714:GLU:HG3	1.79	0.64
1:B:806:MET:HG2	1:B:807:ARG:HG3	1.80	0.64
1:A:405:GLY:C	1:A:406:LEU:HD22	2.19	0.63
1:B:185:ALA:HB1	1:B:243:TYR:CD1	2.33	0.63
1:B:653:TYR:CE2	1:B:682:HIS:ND1	2.60	0.63
1:B:892:HIS:NE2	1:B:931:ILE:HB	2.11	0.63
1:B:368:ASP:O	1:B:371:GLN:HG2	1.97	0.63
1:B:405:GLY:C	1:B:406:LEU:HD22	2.19	0.63
1:B:446:PHE:CE1	1:B:486:PHE:HZ	2.16	0.63
1:B:480:VAL:HG11	1:B:495:ILE:HD11	1.81	0.63
1:B:653:TYR:CE2	1:B:682:HIS:CE1	2.87	0.63
1:B:894:LYS:HD3	1:B:899:GLU:HA	1.81	0.63
1:A:320:VAL:O	1:A:323:ARG:HG2	1.98	0.63
1:B:181:LYS:HE2	1:B:202:LYS:HG2	1.80	0.63
1:A:1002:TYR:CZ	1:A:1004:ILE:HB	2.32	0.63
1:A:118:LEU:HG	1:A:172:ILE:HG13	1.80	0.63
1:A:713:VAL:HG12	1:A:714:GLU:HG3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:978:LEU:O	1:A:998:ARG:HD2	1.98	0.63
1:B:620:PRO:CA	1:B:623:ILE:HG13	2.23	0.63
1:A:806:MET:HG2	1:A:807:ARG:HG3	1.80	0.63
1:B:386:LYS:HG3	1:B:386:LYS:O	1.99	0.63
1:B:41:THR:HG22	1:B:502:THR:HA	1.81	0.63
1:B:446:PHE:CZ	1:B:506:VAL:HG23	2.33	0.63
1:B:566:ASN:HB3	1:B:651:VAL:HG21	1.79	0.63
1:A:933:VAL:HG23	1:A:934:ALA:N	2.10	0.63
1:A:1014:LEU:HD22	1:A:1014:LEU:N	2.14	0.63
1:A:295:VAL:HA	1:A:414:VAL:HG21	1.81	0.63
1:A:446:PHE:CE1	1:A:486:PHE:HZ	2.16	0.63
1:A:894:LYS:HD3	1:A:899:GLU:HA	1.80	0.63
1:A:40:VAL:HG11	1:A:503:ARG:CZ	2.29	0.63
1:B:448:GLY:CA	1:B:480:VAL:HG21	2.29	0.63
1:B:575:LEU:N	1:B:575:LEU:HD22	2.14	0.63
1:A:1015:ASP:O	1:A:1016:MET:HB3	1.98	0.62
1:A:197:THR:HG21	1:A:228:ILE:HD11	1.81	0.62
1:B:741:ASN:O	1:B:778:VAL:HG13	1.98	0.62
1:B:949:TYR:HE2	1:B:951:MET:CE	2.12	0.62
1:A:180:ASP:O	1:A:181:LYS:HG2	1.99	0.62
1:A:185:ALA:HB1	1:A:243:TYR:CD1	2.33	0.62
1:A:372:SER:O	1:A:375:ARG:HB2	1.99	0.62
1:B:180:ASP:O	1:B:181:LYS:HG2	1.99	0.62
1:B:295:VAL:HA	1:B:414:VAL:HG21	1.81	0.62
1:B:474:VAL:CG2	1:B:495:ILE:HD13	2.29	0.62
1:A:949:TYR:HE2	1:A:951:MET:CE	2.12	0.62
1:B:458:ARG:HG3	1:B:468:GLN:CD	2.20	0.62
1:A:382:LEU:HD23	1:A:385:LEU:HB3	1.81	0.62
1:A:439:TYR:OH	1:A:538:LYS:CE	2.47	0.62
1:A:492:GLN:HG2	1:A:503:ARG:CG	2.29	0.62
1:B:469:TYR:HE2	1:B:471:THR:HB	1.65	0.62
1:B:432:THR:HG1	1:B:480:VAL:HG23	1.65	0.62
1:A:458:ARG:HG3	1:A:468:GLN:CD	2.20	0.62
1:A:448:GLY:CA	1:A:480:VAL:HG21	2.28	0.62
1:A:446:PHE:CZ	1:A:506:VAL:HG23	2.33	0.62
1:B:320:VAL:HG21	1:B:442:HIS:HD2	1.64	0.62
1:A:575:LEU:HD22	1:A:575:LEU:N	2.14	0.62
1:B:933:VAL:HG23	1:B:934:ALA:N	2.10	0.62
1:B:296:PRO:HB2	1:B:417:MET:SD	2.39	0.62
1:B:40:VAL:HG11	1:B:503:ARG:CZ	2.29	0.62
1:A:386:LYS:O	1:A:386:LYS:HG3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:696:LEU:N	1:B:696:LEU:HD12	2.15	0.62
1:B:806:MET:CG	1:B:807:ARG:HG3	2.30	0.62
1:B:474:VAL:HG22	1:B:495:ILE:CG2	2.29	0.62
1:B:492:GLN:HG2	1:B:503:ARG:CG	2.29	0.62
1:B:855:THR:HG23	1:B:856:ASN:OD1	2.00	0.62
1:A:182:LEU:HG	1:A:184:ILE:HG23	1.82	0.61
1:A:473:GLN:HB2	1:A:504:VAL:HG22	1.80	0.61
1:A:72:LYS:CD	1:A:80:LEU:HD12	2.30	0.61
1:B:382:LEU:HD23	1:B:385:LEU:HB3	1.81	0.61
1:B:715:VAL:CG2	1:B:717:LYS:HD2	2.30	0.61
1:A:855:THR:HG23	1:A:856:ASN:OD1	1.99	0.61
1:B:372:SER:O	1:B:375:ARG:HB2	1.99	0.61
1:A:110:THR:HG22	1:A:111:ASN:N	2.14	0.61
1:B:204:THR:HG22	1:B:212:MET:SD	2.40	0.61
1:A:181:LYS:HE2	1:A:202:LYS:HG2	1.80	0.61
1:A:296:PRO:HB2	1:A:417:MET:SD	2.39	0.61
1:A:1016:MET:HE2	1:A:1033:PHE:HB3	1.82	0.61
1:A:41:THR:HG22	1:A:502:THR:HA	1.81	0.61
1:A:873:THR:HG23	1:A:982:SER:CA	2.30	0.61
1:B:110:THR:HG22	1:B:111:ASN:N	2.14	0.61
1:B:706:VAL:HG22	1:B:707:ASP:N	2.12	0.61
1:A:175:TYR:CD2	1:A:179:ASP:HB3	2.36	0.61
1:A:204:THR:HG22	1:A:212:MET:SD	2.40	0.61
1:A:410:ALA:HB1	1:A:411:PRO:CD	2.30	0.61
1:A:474:VAL:CG2	1:A:495:ILE:HD13	2.29	0.61
1:A:488:LYS:HG3	1:A:489:ASP:N	2.14	0.61
1:A:480:VAL:HG11	1:A:495:ILE:HD11	1.81	0.61
1:A:712:PRO:HG3	1:A:801:TYR:OH	2.01	0.61
1:A:806:MET:CG	1:A:807:ARG:HG3	2.30	0.61
1:B:833:LEU:HB2	1:B:836:HIS:CD2	2.29	0.61
1:A:119:ILE:HD13	1:A:121:TYR:CZ	2.36	0.61
1:A:532:HIS:HA	1:A:641:THR:HG21	1.82	0.61
1:B:410:ALA:HB1	1:B:411:PRO:CD	2.30	0.61
1:B:41:THR:HG22	1:B:502:THR:HG23	1.83	0.61
1:A:257:THR:C	1:A:258:LEU:HD12	2.21	0.61
1:A:696:LEU:N	1:A:696:LEU:HD12	2.15	0.61
1:B:175:TYR:CD2	1:B:179:ASP:HB3	2.36	0.61
1:B:181:LYS:HZ3	1:B:216:VAL:HG23	1.66	0.61
1:B:333:LEU:CD2	1:B:358:ILE:HG13	2.31	0.61
1:B:46:PRO:HD2	1:B:71:TYR:CE1	2.35	0.61
1:B:847:LEU:HD11	1:B:850:ALA:CA	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:VAL:HG22	1:A:495:ILE:CG2	2.29	0.60
1:A:569:VAL:HB	1:A:654:ASN:HB2	1.83	0.60
1:A:665:VAL:HG12	1:A:697:PRO:HG3	1.83	0.60
1:A:706:VAL:HG22	1:A:707:ASP:N	2.12	0.60
1:B:488:LYS:HG3	1:B:489:ASP:N	2.14	0.60
1:A:313:TYR:CE1	1:A:435:ILE:HG12	2.37	0.60
1:A:469:TYR:HE2	1:A:471:THR:HB	1.65	0.60
1:A:870:GLU:CG	1:A:1025:ALA:N	2.64	0.60
1:B:444:LEU:CD2	1:B:524:PRO:HG3	2.23	0.60
1:B:548:ARG:HG2	1:B:584:PRO:HA	1.83	0.60
1:B:95:TYR:CG	1:B:96:PRO:HD3	2.36	0.60
1:A:715:VAL:CG2	1:A:717:LYS:HD2	2.30	0.60
1:B:99:ILE:HG13	1:B:100:VAL:N	2.16	0.60
1:B:257:THR:C	1:B:258:LEU:HD12	2.21	0.60
1:A:314:LEU:HD12	1:A:333:LEU:O	2.01	0.60
1:B:773:ILE:HD13	1:B:773:ILE:N	2.17	0.60
1:A:963:GLY:O	1:A:1036:VAL:HG22	2.01	0.60
1:A:919:GLU:HB3	1:A:1024:ARG:NH1	2.16	0.60
1:B:314:LEU:HD12	1:B:333:LEU:O	2.01	0.60
1:B:313:TYR:CE1	1:B:435:ILE:HG12	2.37	0.60
1:B:712:PRO:HG3	1:B:801:TYR:OH	2.01	0.60
1:A:333:LEU:CD2	1:A:358:ILE:HG13	2.31	0.60
1:A:46:PRO:HD2	1:A:71:TYR:CE1	2.35	0.60
1:A:773:ILE:HD13	1:A:773:ILE:N	2.17	0.60
1:B:46:PRO:HD2	1:B:71:TYR:CZ	2.36	0.60
1:A:403:PHE:CZ	1:A:406:LEU:HD23	2.37	0.60
1:A:320:VAL:HG21	1:A:442:HIS:HD2	1.64	0.60
1:A:62:ILE:HD13	1:A:77:LEU:CD2	2.32	0.60
1:A:630:HIS:HD2	1:A:632:VAL:CG2	2.15	0.60
1:B:181:LYS:HZ2	1:B:216:VAL:HG23	1.64	0.60
1:B:495:ILE:CG2	1:B:502:THR:HB	2.32	0.60
1:B:182:LEU:HG	1:B:184:ILE:HG23	1.82	0.60
1:B:323:ARG:HH21	1:B:463:LYS:HD2	1.67	0.60
1:B:119:ILE:HD13	1:B:121:TYR:CZ	2.36	0.60
1:B:171:VAL:O	1:B:182:LEU:HD12	2.02	0.60
1:B:403:PHE:CZ	1:B:406:LEU:HD23	2.37	0.60
1:B:469:TYR:CE2	1:B:471:THR:HB	2.36	0.60
1:B:665:VAL:HG12	1:B:697:PRO:HG3	1.83	0.60
1:B:662:LEU:HD11	1:B:702:GLN:HE22	1.65	0.60
1:B:72:LYS:CD	1:B:80:LEU:HD12	2.30	0.60
1:A:1029:GLN:HG2	1:A:1030:ASP:H	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:VAL:HG13	1:B:388:LYS:HG3	1.83	0.60
1:A:1002:TYR:CE2	1:A:1004:ILE:HB	2.37	0.59
1:A:991:GLN:HG3	1:A:1008:THR:HG21	1.84	0.59
1:B:154:LYS:N	1:B:157:HIS:HD2	2.00	0.59
1:A:387:VAL:HG13	1:A:388:LYS:HG3	1.83	0.59
1:A:469:TYR:CE2	1:A:471:THR:HB	2.36	0.59
1:A:566:ASN:CA	1:A:651:VAL:HG23	2.28	0.59
1:A:95:TYR:CG	1:A:96:PRO:HD3	2.36	0.59
1:A:99:ILE:HG13	1:A:100:VAL:N	2.16	0.59
1:B:243:TYR:CD2	1:B:257:THR:HG22	2.37	0.59
1:B:873:THR:HB	1:B:917:MET:HE2	1.84	0.59
1:A:271:LYS:HG3	1:A:272:GLU:N	2.13	0.59
1:A:432:THR:HG1	1:A:480:VAL:HG23	1.65	0.59
1:A:457:ILE:HG12	1:A:467:LEU:HD13	1.84	0.59
1:A:560:LEU:HD23	1:A:648:THR:CG2	2.25	0.59
1:A:847:LEU:HD11	1:A:850:ALA:CA	2.29	0.59
1:B:197:THR:HG21	1:B:228:ILE:HD11	1.82	0.59
1:B:239:PHE:CA	1:B:260:PRO:HG2	2.30	0.59
1:B:387:VAL:HG13	1:B:388:LYS:N	2.18	0.59
1:B:665:VAL:HG11	1:B:697:PRO:HD3	1.84	0.59
1:A:243:TYR:CD2	1:A:257:THR:HG22	2.37	0.59
1:A:46:PRO:HD2	1:A:71:TYR:CZ	2.37	0.59
1:A:904:VAL:HG13	1:A:905:ASP:N	2.18	0.59
1:A:931:ILE:O	1:A:931:ILE:HG13	2.02	0.59
1:A:40:VAL:HG13	1:A:503:ARG:HB3	1.85	0.59
1:A:41:THR:HG22	1:A:502:THR:HG23	1.82	0.59
1:A:62:ILE:HD12	1:A:501:LEU:CD1	2.33	0.59
1:A:833:LEU:HB2	1:A:836:HIS:CD2	2.28	0.59
1:A:987:MET:HB2	1:A:1019:THR:HG23	1.83	0.59
1:A:994:LEU:CG	1:A:1006:ASN:HB2	2.31	0.59
1:B:453:LYS:HG2	1:B:472:VAL:CG2	2.16	0.59
1:B:548:ARG:CG	1:B:583:VAL:O	2.50	0.59
1:B:904:VAL:HG13	1:B:905:ASP:N	2.18	0.59
1:A:196:PRO:HB3	1:A:225:MET:CE	2.33	0.59
1:A:889:ILE:HD12	1:A:907:TYR:CZ	2.38	0.59
1:B:473:GLN:H	1:B:473:GLN:NE2	2.01	0.59
1:B:630:HIS:HD2	1:B:632:VAL:CG2	2.15	0.59
1:B:931:ILE:HG13	1:B:931:ILE:O	2.02	0.59
1:A:972:THR:HA	1:A:1002:TYR:CE1	2.32	0.59
1:B:62:ILE:HD13	1:B:77:LEU:CD2	2.32	0.59
1:A:439:TYR:CZ	1:A:538:LYS:NZ	2.70	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:ARG:HH21	1:A:463:LYS:HD2	1.67	0.59
1:A:563:HIS:HB3	1:A:564:PRO:CD	2.28	0.59
1:B:349:LEU:HD22	1:B:349:LEU:N	2.18	0.59
1:B:578:LEU:HD13	1:B:636:LEU:HD21	1.85	0.59
1:A:814:LEU:HD22	1:A:847:LEU:N	2.18	0.59
1:A:959:LYS:CG	1:A:972:THR:HB	2.33	0.59
1:B:40:VAL:HG13	1:B:503:ARG:HB3	1.85	0.59
1:B:937:ARG:HG2	1:B:938:PRO:HD2	1.85	0.59
1:A:171:VAL:O	1:A:182:LEU:HD12	2.02	0.58
1:A:495:ILE:CG2	1:A:502:THR:HB	2.32	0.58
1:A:530:VAL:HG11	1:A:584:PRO:HD2	1.84	0.58
1:A:759:VAL:HG12	1:A:760:GLN:N	2.18	0.58
1:A:955:LEU:CD1	1:A:973:ILE:HG23	2.33	0.58
1:B:457:ILE:HG12	1:B:467:LEU:HD13	1.84	0.58
1:B:814:LEU:HD22	1:B:847:LEU:N	2.18	0.58
1:A:387:VAL:HG13	1:A:388:LYS:N	2.18	0.58
1:A:62:ILE:HG12	1:A:73:LEU:HB2	1.84	0.58
1:A:870:GLU:CG	1:A:1024:ARG:CG	2.69	0.58
1:B:271:LYS:HG3	1:B:272:GLU:N	2.13	0.58
1:A:349:LEU:N	1:A:349:LEU:HD22	2.18	0.58
1:A:665:VAL:HG11	1:A:697:PRO:HD3	1.84	0.58
1:B:560:LEU:HD23	1:B:648:THR:CG2	2.25	0.58
1:A:110:THR:HB	1:A:132:LEU:HD23	1.85	0.58
1:A:506:VAL:HG22	1:A:525:HIS:NE2	2.18	0.58
1:B:263:VAL:O	1:B:263:VAL:HG12	2.04	0.58
1:B:426:GLU:HA	1:B:426:GLU:OE1	2.04	0.58
1:B:198:ILE:HB	1:B:226:ILE:CG2	2.34	0.58
1:A:350:ASP:HA	1:A:430:ARG:HB2	1.86	0.58
1:A:473:GLN:H	1:A:473:GLN:NE2	2.01	0.58
1:A:949:TYR:CE2	1:A:951:MET:HE1	2.38	0.58
1:B:188:VAL:HG22	1:B:191:LYS:N	2.18	0.58
1:B:653:TYR:HE2	1:B:682:HIS:CE1	2.21	0.58
1:B:832:THR:HG23	1:B:836:HIS:HB2	1.85	0.58
1:B:889:ILE:HD12	1:B:907:TYR:CZ	2.38	0.58
1:A:426:GLU:OE1	1:A:426:GLU:HA	2.04	0.58
1:A:430:ARG:HH21	1:A:432:THR:HG22	1.68	0.58
1:A:578:LEU:HD13	1:A:636:LEU:HD21	1.85	0.58
1:A:814:LEU:HD22	1:A:847:LEU:H	1.68	0.58
1:A:873:THR:HA	1:A:982:SER:N	2.17	0.58
1:B:110:THR:HB	1:B:132:LEU:HD23	1.85	0.58
1:B:196:PRO:HB3	1:B:225:MET:CE	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:ASN:HD21	1:B:67:VAL:CG2	2.15	0.58
1:B:759:VAL:HG12	1:B:760:GLN:N	2.18	0.58
1:A:1021:GLN:CG	1:A:1026:ARG:HG3	2.34	0.58
1:A:456:LYS:O	1:A:468:GLN:HG2	2.04	0.58
1:A:585:GLU:OE1	1:A:585:GLU:HA	2.04	0.58
1:A:873:THR:HG23	1:A:982:SER:HA	1.86	0.58
1:B:254:TYR:CZ	1:B:281:ARG:HD2	2.39	0.58
1:B:430:ARG:HH21	1:B:432:THR:HG22	1.68	0.58
1:B:62:ILE:HD12	1:B:501:LEU:CD1	2.33	0.58
1:A:972:THR:CA	1:A:1002:TYR:HE1	2.15	0.58
1:B:456:LYS:O	1:B:468:GLN:HG2	2.04	0.58
1:B:566:ASN:CA	1:B:651:VAL:HG23	2.28	0.58
1:A:254:TYR:CZ	1:A:281:ARG:HD2	2.39	0.57
1:A:703:LEU:HD21	1:A:782:VAL:HG21	1.86	0.57
1:B:505:PRO:HB2	1:B:507:GLU:O	2.03	0.57
1:A:937:ARG:HG2	1:A:938:PRO:HD2	1.85	0.57
1:A:458:ARG:HD2	1:A:524:PRO:HG3	1.86	0.57
1:A:994:LEU:HG	1:A:1006:ASN:HB2	1.87	0.57
1:A:1018:VAL:HG13	1:A:1018:VAL:O	2.04	0.57
1:A:892:HIS:CE1	1:A:931:ILE:HB	2.40	0.57
1:A:874:LYS:N	1:A:982:SER:CB	2.66	0.57
1:B:350:ASP:HA	1:B:430:ARG:HB2	1.86	0.57
1:A:154:LYS:N	1:A:157:HIS:HD2	2.00	0.57
1:A:265:PRO:HD3	1:A:274:VAL:HG21	1.87	0.57
1:B:370:LEU:HD21	1:B:374:TYR:CE1	2.39	0.57
1:A:198:ILE:HB	1:A:226:ILE:CG2	2.34	0.57
1:A:262:MET:HG3	1:A:262:MET:O	2.05	0.57
1:A:532:HIS:HA	1:A:641:THR:CB	2.35	0.57
1:A:188:VAL:HG22	1:A:191:LYS:N	2.18	0.57
1:A:263:VAL:O	1:A:263:VAL:HG12	2.04	0.57
1:A:370:LEU:HD21	1:A:374:TYR:CE1	2.39	0.57
1:A:324:THR:CG2	1:A:462:PRO:HA	2.34	0.57
1:A:458:ARG:CG	1:A:524:PRO:HG3	2.34	0.57
1:A:51:ASN:HD21	1:A:67:VAL:CG2	2.15	0.57
1:A:832:THR:HG23	1:A:836:HIS:HB2	1.85	0.57
1:B:265:PRO:HD3	1:B:274:VAL:HG21	1.87	0.57
1:B:433:SER:HB3	1:B:484:MET:SD	2.45	0.57
1:B:42:PHE:CE2	1:B:50:PHE:HZ	2.23	0.57
1:A:239:PHE:CA	1:A:260:PRO:HG2	2.30	0.57
1:A:459:VAL:O	1:A:459:VAL:HG23	2.05	0.57
1:A:45:GLU:HB3	1:A:46:PRO:CD	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:434:VAL:HG22	1:B:435:ILE:N	2.20	0.57
1:B:459:VAL:HG23	1:B:459:VAL:O	2.05	0.57
1:A:446:PHE:CE1	1:A:486:PHE:CZ	2.93	0.57
1:B:262:MET:O	1:B:262:MET:HG3	2.05	0.57
1:A:1013:VAL:HG22	1:A:1014:LEU:N	2.19	0.56
1:A:926:ALA:CB	1:A:947:LEU:HD12	2.35	0.56
1:B:665:VAL:CG1	1:B:697:PRO:HD3	2.35	0.56
1:A:435:ILE:CG2	1:A:486:PHE:HE1	2.19	0.56
1:A:501:LEU:HD23	1:A:502:THR:H	1.70	0.56
1:A:820:PHE:O	1:A:821:GLU:HB3	2.05	0.56
1:B:444:LEU:HD23	1:B:524:PRO:CD	2.35	0.56
1:A:305:GLU:O	1:A:340:LYS:HG3	2.06	0.56
1:A:434:VAL:HG22	1:A:435:ILE:N	2.20	0.56
1:B:53:LEU:HG	1:B:64:LEU:HD13	1.87	0.56
1:B:882:LEU:N	1:B:882:LEU:HD12	2.21	0.56
1:A:882:LEU:HD12	1:A:882:LEU:N	2.21	0.56
1:B:116:MET:HG3	1:B:117:LEU:N	2.20	0.56
1:B:41:THR:CG2	1:B:502:THR:HG23	2.36	0.56
1:A:42:PHE:CE2	1:A:50:PHE:HZ	2.23	0.56
1:A:955:LEU:HG	1:A:973:ILE:HG23	1.86	0.56
1:B:305:GLU:O	1:B:340:LYS:HG3	2.06	0.56
1:B:45:GLU:HB3	1:B:46:PRO:CD	2.35	0.56
1:B:785:ASN:HD22	1:B:788:PHE:HE2	1.54	0.56
1:B:885:GLU:HG3	1:B:887:ARG:H	1.70	0.56
1:A:665:VAL:CG1	1:A:697:PRO:HD3	2.35	0.56
1:B:585:GLU:OE1	1:B:585:GLU:HA	2.04	0.56
1:B:700:CYS:HB3	1:B:701:PRO:HD2	1.81	0.56
1:B:710:LEU:HB2	1:B:801:TYR:HE1	1.70	0.56
1:B:814:LEU:HD22	1:B:847:LEU:H	1.69	0.56
1:A:865:VAL:HG13	1:A:866:THR:N	2.21	0.56
1:B:892:HIS:CE1	1:B:931:ILE:HB	2.40	0.56
1:A:474:VAL:CG2	1:A:495:ILE:HG21	2.35	0.56
1:A:785:ASN:ND2	1:A:788:PHE:HE2	2.03	0.56
1:B:446:PHE:CE1	1:B:486:PHE:CZ	2.93	0.56
1:B:324:THR:CG2	1:B:462:PRO:HA	2.34	0.56
1:B:526:CYS:HB3	1:B:535:CYS:SG	2.46	0.56
1:B:804:GLY:HA2	1:B:806:MET:CE	2.36	0.56
1:A:226:ILE:O	1:A:226:ILE:HG23	2.06	0.56
1:A:321:LEU:HD12	1:A:462:PRO:CG	2.34	0.56
1:A:41:THR:CG2	1:A:502:THR:HG23	2.35	0.56
1:A:549:ARG:HA	1:A:584:PRO:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:569:VAL:HB	1:A:654:ASN:CB	2.36	0.56
1:A:885:GLU:HG3	1:A:887:ARG:H	1.70	0.56
1:B:118:LEU:HB3	1:B:127:ILE:CG2	2.36	0.56
1:B:435:ILE:CG2	1:B:486:PHE:HE1	2.19	0.56
1:B:567:ILE:N	1:B:567:ILE:HD13	2.20	0.56
1:B:569:VAL:HG21	1:B:654:ASN:HB2	1.87	0.56
1:A:118:LEU:HB3	1:A:127:ILE:CG2	2.36	0.56
1:A:42:PHE:HE2	1:A:50:PHE:HZ	1.54	0.56
1:A:526:CYS:HB3	1:A:535:CYS:SG	2.46	0.56
1:A:567:ILE:HD13	1:A:567:ILE:N	2.20	0.56
1:A:983:ASN:O	1:A:1022:VAL:HG23	2.06	0.56
1:A:447:VAL:HG23	1:A:447:VAL:O	2.06	0.56
1:A:53:LEU:HG	1:A:64:LEU:HD13	1.87	0.56
1:A:46:PRO:CG	1:A:69:ARG:HD2	2.36	0.56
1:B:505:PRO:HB3	1:B:507:GLU:O	2.04	0.56
1:B:785:ASN:ND2	1:B:788:PHE:HE2	2.03	0.56
1:B:865:VAL:HG13	1:B:866:THR:N	2.21	0.56
1:A:1022:VAL:HG13	1:A:1022:VAL:O	2.06	0.55
1:A:433:SER:HB3	1:A:484:MET:SD	2.45	0.55
1:A:710:LEU:HB2	1:A:801:TYR:HE1	1.70	0.55
1:A:704:LEU:HD11	1:A:724:LYS:CE	2.35	0.55
1:A:460:ASP:OD2	1:A:463:LYS:HB3	2.06	0.55
1:A:873:THR:HB	1:A:917:MET:HE2	1.86	0.55
1:A:949:TYR:HE2	1:A:951:MET:HE1	1.71	0.55
1:B:46:PRO:CG	1:B:69:ARG:HD2	2.36	0.55
1:A:474:VAL:HG12	1:A:475:VAL:N	2.21	0.55
1:A:435:ILE:HD12	1:A:486:PHE:HD1	1.70	0.55
1:A:548:ARG:HG3	1:A:583:VAL:C	2.26	0.55
1:A:619:VAL:CB	1:A:620:PRO:HD3	2.36	0.55
1:A:845:LEU:HD13	1:A:845:LEU:C	2.26	0.55
1:B:412:LEU:N	1:B:412:LEU:HD13	2.21	0.55
1:B:501:LEU:HD23	1:B:502:THR:H	1.70	0.55
1:B:62:ILE:HG12	1:B:73:LEU:HB2	1.84	0.55
1:B:807:ARG:HD3	1:B:812:LEU:O	2.07	0.55
1:A:382:LEU:HD23	1:A:385:LEU:CB	2.36	0.55
1:B:110:THR:HG22	1:B:111:ASN:H	1.72	0.55
1:B:190:GLY:O	1:B:192:PRO:HD3	2.07	0.55
1:B:359:LEU:HA	1:B:362:ILE:HG12	1.89	0.55
1:B:447:VAL:O	1:B:447:VAL:HG23	2.06	0.55
1:B:474:VAL:CG2	1:B:495:ILE:HG21	2.34	0.55
1:B:713:VAL:HG13	1:B:766:TYR:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:703:LEU:HD21	1:B:782:VAL:HG21	1.86	0.55
1:A:448:GLY:HA3	1:A:480:VAL:CG2	2.37	0.55
1:B:51:ASN:ND2	1:B:67:VAL:HG23	2.20	0.55
1:B:710:LEU:HB2	1:B:801:TYR:CE1	2.42	0.55
1:B:820:PHE:O	1:B:821:GLU:HB3	2.06	0.55
1:B:845:LEU:C	1:B:845:LEU:HD13	2.26	0.55
1:B:91:ASN:CG	1:B:92:PRO:HD2	2.27	0.55
1:B:949:TYR:HE2	1:B:951:MET:HE2	1.71	0.55
1:A:1014:LEU:H	1:A:1014:LEU:CD2	2.17	0.55
1:A:713:VAL:HG13	1:A:766:TYR:O	2.06	0.55
1:A:825:CYS:HB3	1:A:828:PRO:HG2	1.89	0.55
1:A:861:GLU:HG3	1:A:862:ILE:N	2.21	0.55
1:A:91:ASN:CG	1:A:92:PRO:HD2	2.27	0.55
1:B:280:VAL:HG12	1:B:281:ARG:N	2.22	0.55
1:B:72:LYS:HD2	1:B:80:LEU:HB2	1.87	0.55
1:A:168:VAL:HG22	1:A:169:PHE:N	2.22	0.55
1:A:190:GLY:O	1:A:192:PRO:HD3	2.07	0.55
1:A:280:VAL:HG12	1:A:281:ARG:N	2.22	0.55
1:A:509:CYS:HB3	1:A:535:CYS:SG	2.47	0.55
1:B:226:ILE:O	1:B:226:ILE:HG23	2.06	0.55
1:B:380:LEU:HB2	1:B:386:LYS:HE2	1.87	0.55
1:B:42:PHE:HE2	1:B:50:PHE:HZ	1.54	0.55
1:A:116:MET:HG3	1:A:117:LEU:N	2.21	0.55
1:B:242:TYR:CD1	1:B:345:LYS:HE2	2.41	0.55
1:B:619:VAL:CB	1:B:620:PRO:HD3	2.36	0.55
1:B:937:ARG:HG3	1:B:938:PRO:HD2	1.89	0.55
1:A:988:PHE:HD2	1:A:1016:MET:SD	2.30	0.55
1:A:242:TYR:CD1	1:A:345:LYS:HE2	2.41	0.55
1:A:380:LEU:HB2	1:A:386:LYS:HE2	1.87	0.55
1:B:380:LEU:CD1	1:B:386:LYS:HE3	2.37	0.55
1:B:501:LEU:HD23	1:B:502:THR:N	2.22	0.55
1:A:239:PHE:HA	1:A:260:PRO:CG	2.32	0.55
1:A:370:LEU:HD13	1:A:370:LEU:O	2.07	0.55
1:A:501:LEU:HD23	1:A:502:THR:N	2.22	0.55
1:A:72:LYS:HD2	1:A:80:LEU:HB2	1.87	0.55
1:A:804:GLY:HA2	1:A:806:MET:CE	2.36	0.55
1:A:1016:MET:HE3	1:A:1017:LYS:CA	2.38	0.54
1:A:597:LEU:HD22	1:A:597:LEU:N	2.21	0.54
1:B:168:VAL:HG22	1:B:169:PHE:N	2.22	0.54
1:B:370:LEU:HD13	1:B:370:LEU:O	2.07	0.54
1:B:597:LEU:N	1:B:597:LEU:HD22	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:704:LEU:HD11	1:B:724:LYS:CE	2.35	0.54
1:A:785:ASN:HD22	1:A:788:PHE:HE2	1.54	0.54
1:A:797:LYS:HD2	1:A:797:LYS:H	1.72	0.54
1:B:382:LEU:HD23	1:B:385:LEU:CB	2.37	0.54
1:B:435:ILE:HD12	1:B:486:PHE:HD1	1.71	0.54
1:B:930:GLU:OE2	1:B:941:MET:HG3	2.07	0.54
1:A:471:THR:CG2	1:A:473:GLN:HE22	2.20	0.54
1:A:46:PRO:CG	1:A:69:ARG:HG3	2.27	0.54
1:A:709:ILE:O	1:A:799:TYR:HD1	1.91	0.54
1:A:72:LYS:HD2	1:A:80:LEU:HD12	1.90	0.54
1:A:710:LEU:HB2	1:A:801:TYR:CE1	2.41	0.54
1:A:874:LYS:H	1:A:982:SER:CB	2.20	0.54
1:B:236:ILE:O	1:B:236:ILE:HG23	2.07	0.54
1:B:370:LEU:C	1:B:370:LEU:HD13	2.27	0.54
1:B:440:LYS:HB2	1:B:538:LYS:NZ	2.22	0.54
1:B:72:LYS:HD2	1:B:80:LEU:HD12	1.90	0.54
1:A:301:ARG:CD	1:A:425:THR:HG21	2.26	0.54
1:A:556:GLN:O	1:A:582:ASN:CB	2.56	0.54
1:A:947:LEU:CD2	1:A:947:LEU:H	2.21	0.54
1:B:460:ASP:OD2	1:B:463:LYS:HB3	2.06	0.54
1:A:151:PRO:O	1:A:157:HIS:HB3	2.07	0.54
1:A:359:LEU:HA	1:A:362:ILE:HG12	1.89	0.54
1:A:63:TYR:CE2	1:A:72:LYS:HG2	2.43	0.54
1:B:474:VAL:HG12	1:B:475:VAL:N	2.21	0.54
1:B:509:CYS:HB3	1:B:535:CYS:SG	2.47	0.54
1:A:412:LEU:C	1:A:412:LEU:HD22	2.28	0.54
1:A:994:LEU:HD11	1:A:1006:ASN:CB	2.37	0.54
1:B:412:LEU:HD22	1:B:412:LEU:C	2.28	0.54
1:B:426:GLU:HG2	1:B:429:ASP:O	2.08	0.54
1:A:495:ILE:O	1:A:495:ILE:HG23	2.08	0.54
1:A:699:ASP:HA	1:A:725:ASN:OD1	2.07	0.54
1:A:739:ILE:HB	1:A:781:THR:HG22	1.90	0.54
1:B:154:LYS:HB2	1:B:157:HIS:HD2	1.70	0.54
1:B:151:PRO:O	1:B:157:HIS:HB3	2.08	0.54
1:B:471:THR:CG2	1:B:473:GLN:HE22	2.20	0.54
1:A:236:ILE:O	1:A:236:ILE:HG23	2.07	0.54
1:A:370:LEU:HD13	1:A:370:LEU:C	2.27	0.54
1:A:429:ASP:OD1	1:A:450:LYS:HB3	2.08	0.54
1:A:930:GLU:OE2	1:A:941:MET:HG3	2.07	0.54
1:B:370:LEU:HD11	1:B:399:ILE:HD12	1.88	0.54
1:B:797:LYS:HD2	1:B:797:LYS:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:GLY:O	1:A:159:LEU:HD13	2.08	0.54
1:A:175:TYR:HB3	1:A:179:ASP:HB3	1.89	0.54
1:A:412:LEU:HD13	1:A:412:LEU:N	2.21	0.54
1:A:531:LEU:O	1:A:641:THR:OG1	2.25	0.54
1:A:662:LEU:HD23	1:A:791:ASP:OD2	2.08	0.54
1:A:780:LEU:HD12	1:A:780:LEU:C	2.27	0.54
1:B:861:GLU:HG3	1:B:862:ILE:N	2.21	0.54
1:A:370:LEU:HD11	1:A:399:ILE:HD12	1.88	0.54
1:A:51:ASN:ND2	1:A:67:VAL:HG23	2.20	0.54
1:B:175:TYR:HB3	1:B:179:ASP:HB3	1.89	0.54
1:B:716:ILE:HG12	1:B:763:ASN:HB3	1.90	0.54
1:B:780:LEU:C	1:B:780:LEU:HD12	2.27	0.54
1:B:825:CYS:HB3	1:B:828:PRO:HG2	1.89	0.54
1:B:301:ARG:CD	1:B:425:THR:HG21	2.26	0.53
1:B:921:LYS:N	1:B:922:PRO:HD2	2.23	0.53
1:B:947:LEU:CD2	1:B:947:LEU:H	2.21	0.53
1:A:110:THR:HG22	1:A:111:ASN:H	1.72	0.53
1:A:225:MET:HE1	1:A:227:LYS:CG	2.37	0.53
1:A:957:ASP:O	1:A:974:THR:HG22	2.08	0.53
1:A:955:LEU:CG	1:A:973:ILE:HG23	2.38	0.53
1:B:63:TYR:CE2	1:B:72:LYS:HG2	2.43	0.53
1:B:926:ALA:CB	1:B:947:LEU:HD12	2.35	0.53
1:B:925:HIS:O	1:B:950:PHE:HD2	1.91	0.53
1:A:739:ILE:HB	1:A:781:THR:HG23	1.90	0.53
1:A:921:LYS:N	1:A:922:PRO:HD2	2.23	0.53
1:A:924:GLN:O	1:A:925:HIS:HB2	2.09	0.53
1:A:426:GLU:HG2	1:A:429:ASP:O	2.08	0.53
1:A:589:GLY:HA3	1:A:639:LYS:HG3	1.90	0.53
1:A:807:ARG:HD3	1:A:812:LEU:O	2.07	0.53
1:A:867:GLY:CA	1:A:981:GLY:N	2.49	0.53
1:B:429:ASP:OD1	1:B:450:LYS:HB3	2.08	0.53
1:B:623:ILE:C	1:B:623:ILE:HD12	2.28	0.53
1:B:924:GLN:O	1:B:925:HIS:HB2	2.09	0.53
1:A:321:LEU:CD2	1:A:325:LEU:HD11	2.39	0.53
1:A:533:ASN:HD22	1:A:643:MET:HB3	1.73	0.53
1:A:827:SER:HB2	1:A:828:PRO:HD3	1.91	0.53
1:B:181:LYS:CE	1:B:202:LYS:HG2	2.39	0.53
1:B:371:GLN:O	1:B:375:ARG:HG3	2.09	0.53
1:B:385:LEU:HD13	1:B:385:LEU:C	2.29	0.53
1:B:578:LEU:HB2	1:B:609:ILE:HB	1.91	0.53
1:B:709:ILE:O	1:B:799:TYR:HD1	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ALA:HB3	1:A:243:TYR:CG	2.44	0.53
1:A:509:CYS:HB2	1:A:536:THR:HA	1.91	0.53
1:A:623:ILE:HD12	1:A:623:ILE:C	2.29	0.53
1:A:679:VAL:HG12	1:A:680:CYS:N	2.23	0.53
1:A:716:ILE:HG12	1:A:763:ASN:HB3	1.90	0.53
1:B:278:LYS:HG2	1:B:296:PRO:CA	2.38	0.53
1:B:321:LEU:CD2	1:B:325:LEU:HD11	2.39	0.53
1:B:563:HIS:HB3	1:B:564:PRO:CD	2.28	0.53
1:A:190:GLY:HA2	1:A:233:PHE:HE2	1.73	0.53
1:A:549:ARG:CD	1:A:584:PRO:HB2	2.33	0.53
1:A:805:ALA:H	1:A:806:MET:CE	2.22	0.53
1:B:356:ILE:HG22	1:B:421:ILE:O	2.09	0.53
1:B:448:GLY:HA3	1:B:480:VAL:CG2	2.37	0.53
1:B:39:PHE:CD1	1:B:505:PRO:HD2	2.44	0.53
1:B:739:ILE:HB	1:B:781:THR:HG22	1.90	0.53
1:B:947:LEU:HD23	1:B:947:LEU:O	2.09	0.53
1:A:997:ARG:H	1:A:1004:ILE:CG2	2.22	0.53
1:A:119:ILE:O	1:A:119:ILE:HG23	2.09	0.53
1:A:356:ILE:HG22	1:A:421:ILE:O	2.09	0.53
1:A:385:LEU:HD13	1:A:385:LEU:C	2.29	0.53
1:A:925:HIS:O	1:A:950:PHE:HD2	1.91	0.53
1:A:958:LEU:HD23	1:A:959:LYS:H	1.73	0.53
1:A:963:GLY:C	1:A:1036:VAL:HG22	2.29	0.53
1:B:198:ILE:HB	1:B:226:ILE:HG22	1.91	0.53
1:B:308:LEU:O	1:B:338:PHE:HA	2.09	0.53
1:B:716:ILE:HG23	1:B:716:ILE:O	2.09	0.53
1:A:575:LEU:H	1:A:575:LEU:CD2	2.22	0.53
1:A:937:ARG:HG3	1:A:938:PRO:HD2	1.89	0.53
1:A:1032:VAL:HG12	1:A:1033:PHE:N	2.23	0.53
1:A:308:LEU:O	1:A:338:PHE:HA	2.09	0.53
1:A:40:VAL:HG11	1:A:503:ARG:NH2	2.24	0.53
1:A:578:LEU:HB2	1:A:609:ILE:HB	1.91	0.53
1:A:805:ALA:N	1:A:806:MET:HE3	2.24	0.53
1:A:807:ARG:HD2	1:A:813:CYS:HA	1.90	0.53
1:B:882:LEU:HD13	1:B:910:ALA:O	2.09	0.53
1:A:181:LYS:CE	1:A:202:LYS:HG2	2.39	0.52
1:A:580:THR:HG21	1:A:583:VAL:HG11	1.91	0.52
1:A:806:MET:HG2	1:A:807:ARG:CG	2.39	0.52
1:A:875:VAL:HG22	1:A:915:CYS:O	2.09	0.52
1:A:933:VAL:HG22	1:A:940:PHE:HB3	1.91	0.52
1:B:40:VAL:HG11	1:B:503:ARG:NH2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1019:THR:HG23	1:A:1019:THR:O	2.10	0.52
1:A:716:ILE:HG23	1:A:716:ILE:O	2.09	0.52
1:A:947:LEU:O	1:A:947:LEU:HD23	2.09	0.52
1:A:952:THR:HG23	1:A:952:THR:O	2.08	0.52
1:A:959:LYS:HG2	1:A:972:THR:CG2	2.39	0.52
1:B:439:TYR:CZ	1:B:538:LYS:CE	2.92	0.52
1:B:495:ILE:HG23	1:B:495:ILE:O	2.08	0.52
1:B:64:LEU:N	1:B:64:LEU:HD22	2.24	0.52
1:B:783:VAL:HG12	1:B:784:TRP:N	2.25	0.52
1:B:807:ARG:HD2	1:B:813:CYS:HA	1.90	0.52
1:A:1004:ILE:HG23	1:A:1004:ILE:O	2.08	0.52
1:A:281:ARG:O	1:A:282:LEU:HD23	2.09	0.52
1:A:827:SER:HB2	1:A:828:PRO:CD	2.39	0.52
1:B:135:GLY:O	1:B:159:LEU:HD13	2.08	0.52
1:B:321:LEU:HD12	1:B:462:PRO:CG	2.34	0.52
1:B:679:VAL:HG12	1:B:680:CYS:N	2.23	0.52
1:B:185:ALA:HB3	1:B:243:TYR:CG	2.44	0.52
1:B:589:GLY:HA3	1:B:639:LYS:HG3	1.90	0.52
1:B:739:ILE:HB	1:B:781:THR:HG23	1.90	0.52
1:B:827:SER:HB2	1:B:828:PRO:CD	2.40	0.52
1:A:42:PHE:HZ	1:A:45:GLU:CB	2.22	0.52
1:B:127:ILE:O	1:B:127:ILE:HG23	2.09	0.52
1:B:281:ARG:O	1:B:282:LEU:HD23	2.09	0.52
1:A:296:PRO:HD2	1:A:414:VAL:HG22	1.92	0.52
1:A:371:GLN:O	1:A:375:ARG:HG3	2.09	0.52
1:A:868:PRO:CG	1:A:1022:VAL:HG21	2.40	0.52
1:A:882:LEU:HD13	1:A:910:ALA:O	2.09	0.52
1:B:630:HIS:HD2	1:B:632:VAL:HG23	1.73	0.52
1:B:875:VAL:HG22	1:B:915:CYS:O	2.09	0.52
1:A:560:LEU:HG	1:A:648:THR:HG21	1.92	0.52
1:B:396:LEU:C	1:B:396:LEU:HD13	2.30	0.52
1:B:439:TYR:CZ	1:B:538:LYS:NZ	2.75	0.52
1:A:593:THR:HG23	1:A:593:THR:O	2.10	0.52
1:A:64:LEU:N	1:A:64:LEU:HD22	2.24	0.52
1:A:566:ASN:HB3	1:A:651:VAL:CG2	2.40	0.52
1:B:228:ILE:HG22	1:B:233:PHE:CE1	2.45	0.52
1:B:472:VAL:HG12	1:B:472:VAL:O	2.09	0.52
1:B:575:LEU:CD2	1:B:575:LEU:H	2.22	0.52
1:B:59:THR:HB	1:B:61:HIS:CE1	2.45	0.52
1:A:198:ILE:HB	1:A:226:ILE:HG22	1.91	0.52
1:A:472:VAL:O	1:A:472:VAL:HG12	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:PHE:CD1	1:A:505:PRO:HD2	2.44	0.52
1:A:553:GLU:HG3	1:A:554:MET:N	2.24	0.52
1:B:322:GLY:CA	1:B:327:VAL:HG22	2.40	0.52
1:B:560:LEU:HG	1:B:648:THR:HG21	1.92	0.52
1:B:806:MET:HG2	1:B:807:ARG:CG	2.39	0.52
1:A:322:GLY:CA	1:A:327:VAL:HG22	2.40	0.52
1:A:712:PRO:O	1:A:715:VAL:HG22	2.09	0.52
1:A:873:THR:CG2	1:A:981:GLY:C	2.78	0.52
1:A:956:ALA:O	1:A:1031:LEU:HD11	2.10	0.52
1:B:171:VAL:HG12	1:B:172:ILE:N	2.25	0.52
1:B:64:LEU:HD11	1:B:501:LEU:HD12	1.92	0.52
1:B:509:CYS:HB2	1:B:536:THR:HA	1.91	0.52
1:B:580:THR:HG21	1:B:583:VAL:HG11	1.92	0.52
1:B:827:SER:HB2	1:B:828:PRO:HD3	1.91	0.52
1:A:870:GLU:CD	1:A:1025:ALA:CA	2.78	0.51
1:A:171:VAL:HG12	1:A:172:ILE:N	2.26	0.51
1:A:473:GLN:CD	1:A:504:VAL:HG13	2.31	0.51
1:A:54:VAL:HG22	1:A:55:VAL:N	2.25	0.51
1:A:64:LEU:HD11	1:A:501:LEU:HD12	1.92	0.51
1:A:716:ILE:CG1	1:A:763:ASN:HB3	2.41	0.51
1:A:986:VAL:HG12	1:A:988:PHE:CE1	2.45	0.51
1:B:444:LEU:HD12	1:B:446:PHE:CZ	2.44	0.51
1:A:127:ILE:O	1:A:127:ILE:HG23	2.09	0.51
1:A:154:LYS:HB2	1:A:157:HIS:HD2	1.71	0.51
1:A:185:ALA:CB	1:A:243:TYR:CG	2.94	0.51
1:A:228:ILE:HG22	1:A:233:PHE:CE1	2.45	0.51
1:B:712:PRO:O	1:B:715:VAL:HG22	2.09	0.51
1:B:805:ALA:H	1:B:806:MET:CE	2.22	0.51
1:A:93:LYS:HD3	1:A:105:GLU:OE2	2.10	0.51
1:A:712:PRO:HG3	1:A:801:TYR:CZ	2.45	0.51
1:B:119:ILE:HG23	1:B:119:ILE:O	2.09	0.51
1:B:553:GLU:HG3	1:B:554:MET:N	2.24	0.51
1:B:567:ILE:CD1	1:B:650:PHE:CE2	2.94	0.51
1:A:468:GLN:HG3	1:A:523:ASP:HA	1.92	0.51
1:B:418:VAL:O	1:B:418:VAL:HG13	2.11	0.51
1:B:468:GLN:HB2	1:B:522:GLY:C	2.30	0.51
1:B:519:LEU:N	1:B:519:LEU:HD22	2.26	0.51
1:B:695:LYS:CB	1:B:696:LEU:HD12	2.41	0.51
1:B:727:PRO:O	1:B:729:PRO:HD3	2.10	0.51
1:A:216:VAL:HG13	1:A:217:PHE:N	2.26	0.51
1:A:53:LEU:HG	1:A:64:LEU:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:LYS:CB	1:A:696:LEU:HD12	2.41	0.51
1:A:984:VAL:HG11	1:A:998:ARG:HD3	1.91	0.51
1:B:265:PRO:HD3	1:B:274:VAL:HG22	1.92	0.51
1:B:541:CYS:SG	1:B:550:PHE:HD2	2.33	0.51
1:B:712:PRO:HG3	1:B:801:TYR:CZ	2.45	0.51
1:B:716:ILE:CG1	1:B:763:ASN:HB3	2.40	0.51
1:B:933:VAL:HG22	1:B:940:PHE:HB3	1.91	0.51
1:A:805:ALA:H	1:A:806:MET:HE3	1.75	0.51
1:B:184:ILE:C	1:B:184:ILE:HD12	2.31	0.51
1:B:53:LEU:HD23	1:B:53:LEU:C	2.31	0.51
1:B:54:VAL:HG22	1:B:55:VAL:N	2.25	0.51
1:A:997:ARG:H	1:A:1004:ILE:HG23	1.75	0.51
1:A:278:LYS:HG2	1:A:296:PRO:CA	2.39	0.51
1:A:370:LEU:HD11	1:A:374:TYR:CE1	2.46	0.51
1:A:790:ILE:HD12	1:A:790:ILE:N	2.25	0.51
1:A:889:ILE:CD1	1:A:907:TYR:CE1	2.94	0.51
1:B:426:GLU:HG3	1:B:429:ASP:H	1.75	0.51
1:B:548:ARG:O	1:B:584:PRO:HD3	2.11	0.51
1:B:823:GLY:HA3	1:B:844:TRP:CZ2	2.46	0.51
1:B:930:GLU:HG3	1:B:941:MET:SD	2.51	0.51
1:A:133:TYR:O	1:A:134:GLN:HB2	2.11	0.51
1:A:396:LEU:C	1:A:396:LEU:HD13	2.30	0.51
1:A:473:GLN:HB2	1:A:504:VAL:CG2	2.40	0.51
1:B:239:PHE:HA	1:B:260:PRO:CG	2.33	0.51
1:B:284:LYS:HD3	1:B:284:LYS:C	2.31	0.51
1:B:370:LEU:HD11	1:B:374:TYR:CE1	2.46	0.51
1:A:418:VAL:O	1:A:418:VAL:HG13	2.10	0.51
1:A:519:LEU:N	1:A:519:LEU:HD22	2.26	0.51
1:A:59:THR:HB	1:A:61:HIS:CE1	2.45	0.51
1:A:630:HIS:HD2	1:A:632:VAL:HG23	1.73	0.51
1:A:567:ILE:CD1	1:A:650:PHE:CE2	2.94	0.51
1:A:727:PRO:O	1:A:729:PRO:HD3	2.10	0.51
1:A:76:ASP:O	1:A:77:LEU:HB2	2.11	0.51
1:A:847:LEU:HG	1:A:850:ALA:HA	1.91	0.51
1:B:296:PRO:HD2	1:B:414:VAL:HG22	1.92	0.51
1:B:527:GLY:HA3	1:B:550:PHE:CE1	2.45	0.51
1:B:53:LEU:HG	1:B:64:LEU:HD11	1.92	0.51
1:B:703:LEU:N	1:B:703:LEU:HD22	2.26	0.51
1:B:847:LEU:HG	1:B:850:ALA:HA	1.91	0.51
1:A:507:GLU:HG3	1:A:537:ARG:CG	2.41	0.51
1:A:807:ARG:HD3	1:A:812:LEU:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:ALA:CB	1:B:243:TYR:CG	2.94	0.51
1:B:93:LYS:HD3	1:B:105:GLU:OE2	2.10	0.51
1:A:358:ILE:CG2	1:A:361:GLN:HB2	2.41	0.50
1:A:541:CYS:SG	1:A:550:PHE:HD2	2.33	0.50
1:A:823:GLY:HA3	1:A:844:TRP:CZ2	2.46	0.50
1:A:870:GLU:OE2	1:A:1025:ALA:CA	2.58	0.50
1:A:987:MET:HB2	1:A:1019:THR:HG22	1.91	0.50
1:B:204:THR:HG23	1:B:206:ASN:O	2.11	0.50
1:B:228:ILE:CG2	1:B:233:PHE:CE1	2.94	0.50
1:B:566:ASN:HB3	1:B:651:VAL:CG2	2.40	0.50
1:B:689:PHE:CE1	1:B:691:GLU:CG	2.94	0.50
1:B:790:ILE:HD12	1:B:790:ILE:N	2.25	0.50
1:B:807:ARG:HD3	1:B:812:LEU:HB3	1.93	0.50
1:B:895:VAL:O	1:B:896:ALA:HB3	2.11	0.50
1:A:204:THR:HG23	1:A:206:ASN:O	2.11	0.50
1:A:469:TYR:HB2	1:A:523:ASP:OD2	2.11	0.50
1:A:783:VAL:HG12	1:A:784:TRP:N	2.25	0.50
1:A:798:VAL:O	1:A:798:VAL:HG13	2.10	0.50
1:A:930:GLU:HG3	1:A:941:MET:SD	2.51	0.50
1:B:119:ILE:CG2	1:B:121:TYR:CE1	2.95	0.50
1:B:300:GLU:HG2	1:B:305:GLU:HA	1.93	0.50
1:B:400:ASP:HB2	1:B:402:ASN:OD1	2.11	0.50
1:A:1004:ILE:HD13	1:A:1004:ILE:C	2.32	0.50
1:A:1029:GLN:HG2	1:A:1030:ASP:N	2.26	0.50
1:A:228:ILE:CG2	1:A:233:PHE:CE1	2.94	0.50
1:A:265:PRO:HD3	1:A:274:VAL:HG22	1.92	0.50
1:A:284:LYS:HD3	1:A:284:LYS:C	2.31	0.50
1:A:703:LEU:HD22	1:A:703:LEU:N	2.26	0.50
1:A:785:ASN:HB3	1:A:788:PHE:CE2	2.46	0.50
1:B:370:LEU:CD1	1:B:374:TYR:CD1	2.95	0.50
1:B:370:LEU:HD13	1:B:374:TYR:CD1	2.46	0.50
1:B:473:GLN:HB2	1:B:504:VAL:CG2	2.40	0.50
1:A:185:ALA:CB	1:A:243:TYR:CD2	2.94	0.50
1:A:261:GLU:HG2	1:A:265:PRO:N	2.25	0.50
1:A:53:LEU:HD23	1:A:53:LEU:C	2.31	0.50
1:A:689:PHE:CE1	1:A:691:GLU:CG	2.94	0.50
1:A:782:VAL:CG2	1:A:790:ILE:HB	2.41	0.50
1:A:894:LYS:CD	1:A:899:GLU:HA	2.41	0.50
1:B:295:VAL:O	1:B:295:VAL:HG23	2.12	0.50
1:B:785:ASN:HB3	1:B:788:PHE:CE2	2.46	0.50
1:B:853:LYS:H	1:B:853:LYS:HD2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:ILE:HD12	1:A:184:ILE:C	2.31	0.50
1:A:370:LEU:CD1	1:A:374:TYR:CD1	2.95	0.50
1:A:439:TYR:CE2	1:A:538:LYS:HE2	2.43	0.50
1:B:412:LEU:HD22	1:B:412:LEU:O	2.11	0.50
1:B:541:CYS:CB	1:B:544:SER:HB3	2.42	0.50
1:B:76:ASP:O	1:B:77:LEU:HB2	2.11	0.50
1:A:1029:GLN:CG	1:A:1030:ASP:H	2.24	0.50
1:A:662:LEU:CD2	1:A:791:ASP:OD2	2.60	0.50
1:A:895:VAL:O	1:A:896:ALA:HB3	2.11	0.50
1:A:868:PRO:CD	1:A:980:ALA:C	2.54	0.50
1:B:133:TYR:O	1:B:134:GLN:HB2	2.11	0.50
1:B:185:ALA:CB	1:B:243:TYR:CD2	2.94	0.50
1:B:261:GLU:HG2	1:B:265:PRO:N	2.25	0.50
1:B:403:PHE:CE1	1:B:406:LEU:CD2	2.94	0.50
1:B:473:GLN:CD	1:B:504:VAL:HG13	2.31	0.50
1:B:491:GLU:O	1:B:506:VAL:HG12	2.11	0.50
1:B:64:LEU:HB2	1:B:71:TYR:HD2	1.77	0.50
1:A:110:THR:CB	1:A:132:LEU:HD21	2.42	0.50
1:A:185:ALA:HB1	1:A:243:TYR:CE2	2.47	0.50
1:A:39:PHE:CD2	1:A:473:GLN:CG	2.95	0.50
1:A:491:GLU:O	1:A:506:VAL:HG12	2.11	0.50
1:A:527:GLY:HA3	1:A:550:PHE:CE1	2.45	0.50
1:A:673:TRP:HB3	1:A:694:VAL:HB	1.94	0.50
1:A:81:VAL:HG12	1:A:82:THR:N	2.26	0.50
1:B:358:ILE:CG2	1:B:361:GLN:HB2	2.41	0.50
1:B:457:ILE:HG12	1:B:467:LEU:CD1	2.42	0.50
1:B:798:VAL:HG13	1:B:798:VAL:O	2.10	0.50
1:A:320:VAL:HG23	1:A:441:ASN:HB3	1.94	0.50
1:A:40:VAL:HG21	1:A:76:ASP:O	2.12	0.50
1:A:736:TYR:CD2	1:A:784:TRP:HB3	2.47	0.50
1:B:889:ILE:CD1	1:B:907:TYR:CE1	2.94	0.50
1:A:119:ILE:CG2	1:A:121:TYR:CE1	2.95	0.50
1:A:300:GLU:HG2	1:A:305:GLU:HA	1.93	0.50
1:A:370:LEU:HD13	1:A:374:TYR:CD1	2.46	0.50
1:A:433:SER:HB3	1:A:484:MET:HE3	1.93	0.50
1:A:892:HIS:HD2	1:A:893:VAL:N	2.10	0.50
1:A:986:VAL:CG1	1:A:988:PHE:CE1	2.94	0.50
1:B:593:THR:O	1:B:593:THR:HG23	2.10	0.50
1:B:736:TYR:CD2	1:B:784:TRP:HB3	2.47	0.50
1:B:81:VAL:HG12	1:B:82:THR:N	2.26	0.50
1:B:841:GLU:HG3	1:B:842:SER:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:LEU:CD1	1:A:386:LYS:HE3	2.37	0.49
1:A:457:ILE:HG12	1:A:467:LEU:CD1	2.42	0.49
1:A:597:LEU:HD22	1:A:597:LEU:H	1.78	0.49
1:B:278:LYS:CE	1:B:296:PRO:HG3	2.41	0.49
1:B:882:LEU:HD23	1:B:913:ILE:HD11	1.94	0.49
1:A:265:PRO:CD	1:A:274:VAL:HG22	2.42	0.49
1:A:426:GLU:HG3	1:A:429:ASP:H	1.75	0.49
1:A:444:LEU:HD12	1:A:446:PHE:CZ	2.44	0.49
1:A:623:ILE:HD12	1:A:624:THR:CA	2.42	0.49
1:A:976:THR:HG22	1:A:977:ASN:N	2.27	0.49
1:B:623:ILE:HD12	1:B:624:THR:CA	2.42	0.49
1:B:790:ILE:H	1:B:790:ILE:HD12	1.77	0.49
1:B:856:ASN:N	1:B:857:PRO:HD3	2.27	0.49
1:B:892:HIS:HD2	1:B:893:VAL:N	2.10	0.49
1:A:105:GLU:CB	1:A:106:PRO:HD2	2.42	0.49
1:A:234:THR:HG23	1:A:235:VAL:N	2.26	0.49
1:A:400:ASP:HB2	1:A:402:ASN:OD1	2.11	0.49
1:B:234:THR:HG23	1:B:235:VAL:N	2.27	0.49
1:B:333:LEU:HD21	1:B:358:ILE:HG13	1.94	0.49
1:B:597:LEU:H	1:B:597:LEU:CD2	2.26	0.49
1:B:59:THR:HB	1:B:61:HIS:ND1	2.27	0.49
1:B:792:ASN:HD21	1:B:796:ASN:N	2.10	0.49
1:B:894:LYS:CD	1:B:899:GLU:HA	2.41	0.49
1:A:333:LEU:HD21	1:A:358:ILE:HG13	1.94	0.49
1:A:792:ASN:HD21	1:A:796:ASN:N	2.10	0.49
1:B:185:ALA:HB1	1:B:243:TYR:CE2	2.47	0.49
1:B:265:PRO:HB2	1:B:266:PRO:HD2	1.94	0.49
1:B:713:VAL:HG13	1:B:767:SER:HA	1.94	0.49
1:A:412:LEU:O	1:A:412:LEU:HD22	2.11	0.49
1:A:790:ILE:H	1:A:790:ILE:HD12	1.77	0.49
1:A:955:LEU:HD11	1:A:973:ILE:HG23	1.94	0.49
1:B:312:ALA:HB1	1:B:334:LEU:HD11	1.94	0.49
1:B:475:VAL:HG22	1:B:500:GLN:OE1	2.13	0.49
1:B:40:VAL:HG21	1:B:76:ASP:O	2.12	0.49
1:A:132:LEU:HD11	1:A:163:ASN:HD22	1.77	0.49
1:A:185:ALA:HA	1:A:197:THR:O	2.13	0.49
1:A:475:VAL:HG22	1:A:500:GLN:OE1	2.13	0.49
1:A:597:LEU:CD2	1:A:597:LEU:H	2.26	0.49
1:A:532:HIS:CA	1:A:641:THR:HG21	2.43	0.49
1:A:782:VAL:HG23	1:A:782:VAL:O	2.12	0.49
1:B:110:THR:CB	1:B:132:LEU:HD21	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:TYR:HB3	1:B:136:ILE:HG23	1.94	0.49
1:B:265:PRO:CD	1:B:274:VAL:HG22	2.42	0.49
1:B:374:TYR:CE2	1:B:397:LEU:HD22	2.48	0.49
1:B:782:VAL:HG23	1:B:782:VAL:O	2.12	0.49
1:A:1002:TYR:OH	1:A:1004:ILE:HB	2.12	0.49
1:A:1021:GLN:HG2	1:A:1026:ARG:CG	2.41	0.49
1:A:254:TYR:CE2	1:A:281:ARG:HD2	2.48	0.49
1:A:295:VAL:O	1:A:295:VAL:HG23	2.12	0.49
1:A:374:TYR:CE2	1:A:397:LEU:HD22	2.48	0.49
1:A:995:PHE:HZ	1:A:998:ARG:HB2	1.77	0.49
1:B:444:LEU:CD2	1:B:524:PRO:CD	2.91	0.49
1:B:548:ARG:CD	1:B:583:VAL:O	2.60	0.49
1:A:541:CYS:CB	1:A:544:SER:HB3	2.42	0.49
1:A:841:GLU:HG3	1:A:842:SER:H	1.78	0.49
1:A:889:ILE:O	1:A:892:HIS:HB3	2.13	0.49
1:B:132:LEU:HD11	1:B:163:ASN:HD22	1.77	0.49
1:B:190:GLY:C	1:B:192:PRO:HD3	2.33	0.49
1:B:216:VAL:HG13	1:B:217:PHE:N	2.26	0.49
1:B:433:SER:HB3	1:B:484:MET:HE3	1.95	0.49
1:B:889:ILE:O	1:B:892:HIS:HB3	2.13	0.49
1:A:265:PRO:HB2	1:A:266:PRO:HD2	1.94	0.49
1:A:991:GLN:CB	1:A:1008:THR:HG21	2.42	0.49
1:B:473:GLN:HB3	1:B:502:THR:HG21	1.94	0.49
1:B:590:VAL:HG12	1:B:591:ASN:N	2.27	0.49
1:B:847:LEU:HG	1:B:850:ALA:CA	2.42	0.49
1:A:133:TYR:HB3	1:A:136:ILE:HG23	1.94	0.49
1:A:853:LYS:HD2	1:A:853:LYS:H	1.76	0.49
1:A:868:PRO:HG2	1:A:981:GLY:HA3	1.91	0.49
1:B:182:LEU:HD21	1:B:184:ILE:HG21	1.94	0.49
1:B:190:GLY:HA2	1:B:233:PHE:HE2	1.73	0.49
1:B:662:LEU:HD23	1:B:791:ASP:CG	2.32	0.49
1:B:809:SER:CB	1:B:881:ASN:ND2	2.75	0.49
1:A:603:LEU:C	1:A:603:LEU:HD23	2.33	0.48
1:A:856:ASN:N	1:A:857:PRO:HD3	2.27	0.48
1:A:863:ILE:HG13	1:A:864:PRO:N	2.28	0.48
1:A:99:ILE:HD11	1:A:152:PHE:CB	2.41	0.48
1:B:39:PHE:CD2	1:B:473:GLN:CG	2.95	0.48
1:B:506:VAL:O	1:B:525:HIS:CE1	2.66	0.48
1:B:541:CYS:SG	1:B:550:PHE:CD2	3.06	0.48
1:B:863:ILE:HG13	1:B:864:PRO:N	2.28	0.48
1:B:907:TYR:CZ	1:B:909:PRO:HA	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:868:PRO:CG	1:A:1022:VAL:CG2	2.88	0.48
1:A:473:GLN:CD	1:A:504:VAL:HG22	2.33	0.48
1:A:59:THR:HB	1:A:61:HIS:ND1	2.27	0.48
1:A:790:ILE:HG22	1:A:791:ASP:N	2.29	0.48
1:A:847:LEU:HG	1:A:850:ALA:CA	2.42	0.48
1:B:160:SER:OG	1:B:162:VAL:HG23	2.13	0.48
1:B:949:TYR:CE2	1:B:951:MET:CE	2.95	0.48
1:A:1020:VAL:HG13	1:A:1020:VAL:O	2.13	0.48
1:A:590:VAL:HG12	1:A:591:ASN:N	2.27	0.48
1:A:713:VAL:HG13	1:A:767:SER:HA	1.94	0.48
1:A:882:LEU:HD23	1:A:913:ILE:HD11	1.94	0.48
1:B:185:ALA:HA	1:B:197:THR:O	2.13	0.48
1:B:435:ILE:HG21	1:B:486:PHE:CE1	2.48	0.48
1:B:603:LEU:HD23	1:B:603:LEU:C	2.33	0.48
1:B:673:TRP:HB3	1:B:694:VAL:HB	1.94	0.48
1:A:239:PHE:CD1	1:A:260:PRO:HG2	2.48	0.48
1:A:321:LEU:CG	1:A:325:LEU:HD11	2.40	0.48
1:A:991:GLN:HB3	1:A:1008:THR:HG21	1.96	0.48
1:B:254:TYR:CE2	1:B:281:ARG:HD2	2.48	0.48
1:B:239:PHE:CD1	1:B:260:PRO:HG2	2.48	0.48
1:B:320:VAL:HG23	1:B:441:ASN:HB3	1.94	0.48
1:B:781:THR:HG23	1:B:781:THR:O	2.12	0.48
1:B:807:ARG:HB3	1:B:812:LEU:HB2	1.95	0.48
1:A:435:ILE:HG21	1:A:486:PHE:CE1	2.48	0.48
1:A:473:GLN:HB3	1:A:502:THR:HG21	1.94	0.48
1:A:681:THR:HG21	1:A:686:THR:HG21	1.94	0.48
1:A:740:LEU:HD12	1:A:740:LEU:N	2.29	0.48
1:A:716:ILE:HD11	1:A:763:ASN:HB3	1.95	0.48
1:A:781:THR:O	1:A:781:THR:HG23	2.12	0.48
1:B:258:LEU:HD12	1:B:258:LEU:N	2.29	0.48
1:B:453:LYS:HE3	1:B:472:VAL:HG22	1.94	0.48
1:B:715:VAL:HG23	1:B:715:VAL:O	2.13	0.48
1:A:182:LEU:HD21	1:A:184:ILE:HG21	1.94	0.48
1:A:567:ILE:HD12	1:A:650:PHE:CE2	2.49	0.48
1:B:716:ILE:HD11	1:B:763:ASN:HB3	1.95	0.48
1:B:935:VAL:HG12	1:B:936:CYS:N	2.28	0.48
1:A:190:GLY:C	1:A:192:PRO:HD3	2.33	0.48
1:A:312:ALA:HB1	1:A:334:LEU:HD11	1.94	0.48
1:A:144:ASP:O	1:A:145:LEU:HB2	2.13	0.48
1:A:543:ARG:HH11	1:A:549:ARG:HH22	1.62	0.48
1:A:626:ASN:ND2	1:A:630:HIS:HB2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:LEU:HB2	1:A:71:TYR:HD2	1.77	0.48
1:A:807:ARG:HB3	1:A:812:LEU:HB2	1.95	0.48
1:A:935:VAL:HG12	1:A:936:CYS:N	2.28	0.48
1:B:144:ASP:O	1:B:145:LEU:HB2	2.13	0.48
1:B:42:PHE:HZ	1:B:45:GLU:CB	2.22	0.48
1:B:626:ASN:ND2	1:B:630:HIS:HB2	2.29	0.48
1:B:782:VAL:CG2	1:B:790:ILE:HB	2.41	0.48
1:B:783:VAL:HG13	1:B:788:PHE:O	2.13	0.48
1:B:471:THR:HG23	1:B:473:GLN:NE2	2.27	0.48
1:A:710:LEU:HD13	1:A:801:TYR:OH	2.13	0.48
1:A:1010:SER:HB2	1:A:1035:TYR:CD2	2.49	0.47
1:A:361:GLN:HE21	1:A:365:ARG:HH21	1.61	0.47
1:A:469:TYR:CB	1:A:523:ASP:OD2	2.62	0.47
1:A:704:LEU:H	1:A:723:ALA:HA	1.79	0.47
1:A:987:MET:HE3	1:A:990:SER:HA	1.95	0.47
1:B:440:LYS:O	1:B:440:LYS:HG2	2.14	0.47
1:B:561:THR:HG22	1:B:562:VAL:N	2.29	0.47
1:B:681:THR:HG21	1:B:686:THR:HG21	1.95	0.47
1:B:710:LEU:HD13	1:B:801:TYR:OH	2.13	0.47
1:A:124:ASN:OD1	1:A:142:LEU:HB3	2.14	0.47
1:A:258:LEU:HD12	1:A:258:LEU:N	2.28	0.47
1:A:440:LYS:HG2	1:A:440:LYS:O	2.14	0.47
1:A:541:CYS:SG	1:A:550:PHE:CD2	3.07	0.47
1:A:862:ILE:CG2	1:A:877:ILE:HG23	2.44	0.47
1:A:907:TYR:CZ	1:A:909:PRO:HA	2.48	0.47
1:A:991:GLN:HA	1:A:991:GLN:OE1	2.13	0.47
1:B:124:ASN:OD1	1:B:142:LEU:HB3	2.15	0.47
1:B:430:ARG:HG2	1:B:431:MET:O	2.14	0.47
1:B:814:LEU:HD11	1:B:845:LEU:CD1	2.44	0.47
1:A:468:GLN:HB3	1:A:468:GLN:HE21	1.47	0.47
1:A:695:LYS:HB2	1:A:696:LEU:HD12	1.97	0.47
1:A:728:GLN:HA	1:A:753:ARG:NH2	2.30	0.47
1:A:953:LEU:HB3	1:A:977:ASN:O	2.14	0.47
1:B:113:VAL:HG11	1:B:165:SER:HB3	1.97	0.47
1:B:361:GLN:HE21	1:B:365:ARG:HH21	1.61	0.47
1:B:473:GLN:CD	1:B:504:VAL:HG22	2.34	0.47
1:B:507:GLU:HG3	1:B:537:ARG:CG	2.40	0.47
1:B:698:GLU:O	1:B:725:ASN:OD1	2.32	0.47
1:B:728:GLN:HA	1:B:753:ARG:NH2	2.29	0.47
1:A:991:GLN:HG2	1:A:1008:THR:HG21	1.96	0.47
1:A:783:VAL:HG13	1:A:788:PHE:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:984:VAL:HG23	1:A:984:VAL:O	2.14	0.47
1:A:997:ARG:HG2	1:A:998:ARG:N	2.30	0.47
1:B:98:ARG:NH2	1:B:107:LEU:HD12	2.29	0.47
1:B:175:TYR:CG	1:B:176:SER:N	2.82	0.47
1:B:543:ARG:HH11	1:B:549:ARG:HH22	1.62	0.47
1:A:264:SER:HA	1:A:265:PRO:HA	1.53	0.47
1:A:40:VAL:HG11	1:A:503:ARG:HE	1.79	0.47
1:A:458:ARG:CD	1:A:524:PRO:HG3	2.44	0.47
1:A:702:GLN:O	1:A:723:ALA:HB1	2.14	0.47
1:A:715:VAL:HG23	1:A:715:VAL:O	2.13	0.47
1:A:863:ILE:CG1	1:A:864:PRO:HD3	2.39	0.47
1:A:175:TYR:CG	1:A:176:SER:N	2.82	0.47
1:A:430:ARG:HG2	1:A:431:MET:O	2.14	0.47
1:A:77:LEU:HD22	1:A:501:LEU:HD13	1.96	0.47
1:A:68:ASN:ND2	1:A:87:PRO:HD3	2.29	0.47
1:B:118:LEU:HD13	1:B:118:LEU:C	2.34	0.47
1:B:380:LEU:HD12	1:B:390:ILE:CG2	2.45	0.47
1:B:469:TYR:HB3	1:B:523:ASP:OD2	2.15	0.47
1:B:480:VAL:HB	1:B:484:MET:HE1	1.94	0.47
1:B:597:LEU:H	1:B:597:LEU:HD22	1.78	0.47
1:B:699:ASP:O	1:B:725:ASN:CB	2.63	0.47
1:B:745:ILE:O	1:B:745:ILE:HG23	2.14	0.47
1:A:333:LEU:CD2	1:A:358:ILE:HA	2.45	0.47
1:A:569:VAL:HG23	1:A:654:ASN:HB2	1.80	0.47
1:A:72:LYS:O	1:A:80:LEU:HB2	2.15	0.47
1:A:745:ILE:O	1:A:745:ILE:HG23	2.15	0.47
1:A:814:LEU:HD11	1:A:845:LEU:CD1	2.44	0.47
1:A:987:MET:CE	1:A:990:SER:HA	2.45	0.47
1:B:372:SER:HA	1:B:375:ARG:NE	2.29	0.47
1:B:704:LEU:H	1:B:723:ALA:HA	1.79	0.47
1:B:702:GLN:O	1:B:723:ALA:HB1	2.14	0.47
1:B:884:LEU:HD23	1:B:884:LEU:HA	1.75	0.47
1:B:262:MET:O	1:B:263:VAL:HB	2.14	0.47
1:B:569:VAL:CG1	1:B:620:PRO:HG3	2.45	0.47
1:B:947:LEU:HD23	1:B:947:LEU:H	1.80	0.47
1:A:253:VAL:O	1:A:253:VAL:HG23	2.15	0.47
1:A:453:LYS:HE3	1:A:472:VAL:HG22	1.94	0.47
1:A:843:ARG:NH1	1:A:843:ARG:HB2	2.30	0.47
1:A:892:HIS:CD2	1:A:893:VAL:CG2	2.98	0.47
1:A:958:LEU:HD13	1:A:1033:PHE:HD1	1.79	0.47
1:B:253:VAL:O	1:B:253:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:PHE:HE1	1:B:406:LEU:HD23	1.75	0.47
1:B:45:GLU:HB3	1:B:46:PRO:HD3	1.97	0.47
1:B:740:LEU:HD12	1:B:740:LEU:N	2.29	0.47
1:B:790:ILE:HG22	1:B:791:ASP:N	2.28	0.47
1:A:245:TYR:CE2	1:A:247:PHE:HD2	2.33	0.47
1:A:569:VAL:CG1	1:A:620:PRO:HG3	2.45	0.47
1:A:873:THR:CG2	1:A:982:SER:N	2.78	0.47
1:B:68:ASN:ND2	1:B:87:PRO:HD3	2.30	0.47
1:A:1020:VAL:HG13	1:A:1027:ILE:HG12	1.96	0.47
1:A:160:SER:OG	1:A:162:VAL:HG23	2.14	0.47
1:A:495:ILE:HG22	1:A:502:THR:HB	1.96	0.47
1:A:561:THR:HG22	1:A:562:VAL:N	2.28	0.47
1:A:947:LEU:N	1:A:947:LEU:HD23	2.30	0.47
1:B:105:GLU:CB	1:B:106:PRO:HD2	2.42	0.47
1:B:333:LEU:CD2	1:B:358:ILE:HA	2.45	0.47
1:B:343:LYS:HG2	1:B:344:ARG:HG2	1.97	0.47
1:B:82:THR:O	1:B:82:THR:HG23	2.14	0.47
1:A:118:LEU:C	1:A:118:LEU:HD13	2.34	0.46
1:A:372:SER:HA	1:A:375:ARG:NE	2.30	0.46
1:B:244:VAL:HB	1:B:309:LEU:HD23	1.97	0.46
1:B:783:VAL:HG11	1:B:786:GLY:O	2.15	0.46
1:B:843:ARG:HB2	1:B:843:ARG:NH1	2.30	0.46
1:B:862:ILE:CG2	1:B:877:ILE:HG23	2.44	0.46
1:B:863:ILE:CG1	1:B:864:PRO:HD3	2.39	0.46
1:A:181:LYS:HZ2	1:A:216:VAL:HG23	1.77	0.46
1:A:403:PHE:HE1	1:A:406:LEU:HD23	1.75	0.46
1:A:68:ASN:HB3	1:A:86:GLY:HA3	1.97	0.46
1:A:949:TYR:CE2	1:A:951:MET:CE	2.95	0.46
1:A:873:THR:HG23	1:A:981:GLY:O	2.14	0.46
1:B:567:ILE:HD12	1:B:650:PHE:CE2	2.49	0.46
1:B:72:LYS:O	1:B:80:LEU:HB2	2.15	0.46
1:A:244:VAL:HB	1:A:309:LEU:HD23	1.97	0.46
1:B:286:ASP:OD1	1:B:288:ALA:HB3	2.15	0.46
1:B:380:LEU:CB	1:B:386:LYS:HE3	2.44	0.46
1:B:505:PRO:HB2	1:B:507:GLU:C	2.35	0.46
1:A:1007:THR:HG22	1:A:1008:THR:O	2.15	0.46
1:A:532:HIS:CA	1:A:641:THR:OG1	2.57	0.46
1:A:82:THR:O	1:A:82:THR:HG23	2.14	0.46
1:B:321:LEU:CG	1:B:325:LEU:HD11	2.40	0.46
1:A:252:PHE:CD1	1:A:283:CYS:HA	2.50	0.46
1:A:503:ARG:O	1:A:505:PRO:HD3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:ARG:CD	1:A:584:PRO:CB	2.76	0.46
1:A:549:ARG:HA	1:A:584:PRO:HG3	1.97	0.46
1:A:862:ILE:HG22	1:A:877:ILE:CA	2.32	0.46
1:A:873:THR:HG22	1:A:874:LYS:N	2.31	0.46
1:B:159:LEU:HG	1:B:201:ARG:HH12	1.81	0.46
1:B:245:TYR:CD2	1:B:312:ALA:HB3	2.51	0.46
1:B:296:PRO:CD	1:B:414:VAL:HG22	2.45	0.46
1:B:468:GLN:O	1:B:521:SER:O	2.34	0.46
1:B:68:ASN:HB3	1:B:86:GLY:HA3	1.97	0.46
1:B:660:SER:HB2	1:B:791:ASP:OD1	2.16	0.46
1:B:892:HIS:CD2	1:B:893:VAL:CG2	2.98	0.46
1:A:1015:ASP:H	1:A:1035:TYR:H	1.63	0.46
1:A:265:PRO:CB	1:A:266:PRO:HD2	2.45	0.46
1:A:296:PRO:CD	1:A:414:VAL:HG22	2.46	0.46
1:A:492:GLN:HG2	1:A:503:ARG:HG2	1.98	0.46
1:B:46:PRO:CG	1:B:69:ARG:HG3	2.27	0.46
1:B:77:LEU:HD22	1:B:501:LEU:HD13	1.96	0.46
1:B:902:PRO:HA	1:B:915:CYS:HA	1.97	0.46
1:B:99:ILE:HD11	1:B:152:PHE:CB	2.41	0.46
1:A:113:VAL:HG11	1:A:165:SER:HB3	1.96	0.46
1:A:226:ILE:HD11	1:A:385:LEU:CD2	2.46	0.46
1:A:444:LEU:HD13	1:A:445:ALA:H	1.79	0.46
1:A:62:ILE:CD1	1:A:77:LEU:CD2	2.94	0.46
1:A:62:ILE:HD11	1:A:73:LEU:CD1	2.45	0.46
1:A:873:THR:OG1	1:A:982:SER:N	2.48	0.46
1:B:295:VAL:CA	1:B:414:VAL:HG21	2.45	0.46
1:A:262:MET:O	1:A:263:VAL:HB	2.14	0.46
1:A:274:VAL:HG23	1:A:275:TYR:N	2.30	0.46
1:A:295:VAL:CA	1:A:414:VAL:HG21	2.45	0.46
1:A:343:LYS:HG2	1:A:344:ARG:HG2	1.97	0.46
1:A:947:LEU:H	1:A:947:LEU:HD23	1.80	0.46
1:B:495:ILE:HG22	1:B:502:THR:HB	1.96	0.46
1:B:594:PHE:CZ	1:B:614:PRO:HD3	2.51	0.46
1:A:403:PHE:CE1	1:A:406:LEU:CD2	2.94	0.46
1:A:437:TYR:CE2	1:A:439:TYR:HB2	2.51	0.46
1:B:245:TYR:CE2	1:B:247:PHE:HD2	2.34	0.46
1:B:278:LYS:HD3	1:B:294:GLU:HG2	1.98	0.46
1:B:46:PRO:HD2	1:B:71:TYR:OH	2.16	0.46
1:B:91:ASN:OD1	1:B:92:PRO:HD2	2.16	0.46
1:A:870:GLU:CA	1:A:1024:ARG:HG2	2.43	0.46
1:A:286:ASP:OD1	1:A:288:ALA:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:LEU:HD12	1:A:390:ILE:CG2	2.45	0.46
1:A:902:PRO:HA	1:A:915:CYS:HA	1.98	0.46
1:B:118:LEU:CD1	1:B:172:ILE:HD12	2.12	0.46
1:B:225:MET:HE1	1:B:227:LYS:CG	2.45	0.46
1:B:361:GLN:O	1:B:365:ARG:HG2	2.16	0.46
1:A:327:VAL:HG11	1:A:358:ILE:HD11	1.97	0.45
1:A:624:THR:O	1:A:624:THR:HG23	2.15	0.45
1:A:828:PRO:HG3	1:A:837:CYS:SG	2.56	0.45
1:A:892:HIS:CD2	1:A:893:VAL:HG22	2.51	0.45
1:B:252:PHE:CD1	1:B:283:CYS:HA	2.50	0.45
1:B:435:ILE:HG23	1:B:486:PHE:HE1	1.81	0.45
1:B:439:TYR:CE2	1:B:538:LYS:CE	2.99	0.45
1:B:689:PHE:CE1	1:B:691:GLU:HG2	2.50	0.45
1:B:62:ILE:CD1	1:B:73:LEU:HB2	2.47	0.45
1:B:743:GLN:HG2	1:B:744:GLY:N	2.31	0.45
1:A:110:THR:CB	1:A:132:LEU:CD2	2.95	0.45
1:A:435:ILE:HG23	1:A:486:PHE:HE1	1.81	0.45
1:A:480:VAL:HB	1:A:484:MET:HE1	1.97	0.45
1:A:563:HIS:CB	1:A:577:VAL:HG12	2.46	0.45
1:A:532:HIS:C	1:A:641:THR:HG21	2.36	0.45
1:A:870:GLU:OE2	1:A:1025:ALA:HA	2.16	0.45
1:A:890:ALA:O	1:A:891:SER:HB2	2.17	0.45
1:B:265:PRO:CB	1:B:266:PRO:HD2	2.45	0.45
1:A:1020:VAL:CG1	1:A:1027:ILE:CG1	2.95	0.45
1:A:380:LEU:CB	1:A:386:LYS:HE3	2.43	0.45
1:A:45:GLU:HB3	1:A:46:PRO:HD3	1.97	0.45
1:B:118:LEU:HB3	1:B:127:ILE:HG22	1.98	0.45
1:B:663:SER:O	1:B:667:SER:HB2	2.17	0.45
1:B:695:LYS:HB2	1:B:696:LEU:HD12	1.96	0.45
1:A:361:GLN:O	1:A:365:ARG:HG2	2.16	0.45
1:A:458:ARG:HG3	1:A:468:GLN:NE2	2.32	0.45
1:A:469:TYR:CG	1:A:470:GLU:N	2.84	0.45
1:A:689:PHE:CE1	1:A:691:GLU:HG2	2.50	0.45
1:A:783:VAL:HG11	1:A:786:GLY:O	2.16	0.45
1:B:256:LEU:HD22	1:B:256:LEU:N	2.31	0.45
1:B:435:ILE:HG21	1:B:486:PHE:HE1	1.81	0.45
1:B:58:ARG:HG2	1:B:58:ARG:NH1	2.31	0.45
1:B:62:ILE:HD11	1:B:73:LEU:CD1	2.45	0.45
1:B:828:PRO:HG3	1:B:837:CYS:SG	2.56	0.45
1:B:892:HIS:CD2	1:B:893:VAL:N	2.85	0.45
1:A:159:LEU:HG	1:A:201:ARG:HH12	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:LEU:HD22	1:A:256:LEU:N	2.31	0.45
1:A:288:ALA:O	1:A:289:PHE:HB2	2.17	0.45
1:A:322:GLY:HA2	1:A:327:VAL:HG22	1.99	0.45
1:A:511:GLN:HG3	1:A:512:TYR:CD2	2.51	0.45
1:A:743:GLN:HG2	1:A:744:GLY:N	2.31	0.45
1:B:563:HIS:CB	1:B:577:VAL:HG12	2.46	0.45
1:B:624:THR:O	1:B:624:THR:HG23	2.15	0.45
1:B:62:ILE:CD1	1:B:77:LEU:CD2	2.94	0.45
1:B:805:ALA:N	1:B:806:MET:HE3	2.31	0.45
1:A:1014:LEU:HD12	1:A:1035:TYR:O	2.16	0.45
1:A:118:LEU:HB3	1:A:127:ILE:HG22	1.98	0.45
1:A:278:LYS:CE	1:A:296:PRO:HG3	2.41	0.45
1:A:245:TYR:CD2	1:A:312:ALA:HB3	2.51	0.45
1:A:506:VAL:O	1:A:507:GLU:N	2.39	0.45
1:A:695:LYS:C	1:A:696:LEU:HD12	2.37	0.45
1:B:442:HIS:CD2	1:B:458:ARG:HH21	2.35	0.45
1:B:503:ARG:O	1:B:505:PRO:HD3	2.15	0.45
1:B:671:CYS:HB3	1:B:680:CYS:SG	2.57	0.45
1:B:873:THR:HG22	1:B:874:LYS:N	2.31	0.45
1:B:892:HIS:CD2	1:B:893:VAL:HG22	2.51	0.45
1:B:947:LEU:HD23	1:B:947:LEU:N	2.30	0.45
1:A:358:ILE:CG2	1:A:361:GLN:CB	2.95	0.45
1:A:53:LEU:HD12	1:A:501:LEU:HG	1.99	0.45
1:A:539:GLU:HG3	1:A:540:ARG:N	2.31	0.45
1:A:594:PHE:CZ	1:A:614:PRO:HD3	2.51	0.45
1:A:46:PRO:HD2	1:A:71:TYR:OH	2.16	0.45
1:B:118:LEU:O	1:B:127:ILE:HG22	2.17	0.45
1:B:226:ILE:HD11	1:B:385:LEU:CD2	2.46	0.45
1:B:40:VAL:HG11	1:B:503:ARG:HE	1.80	0.45
1:B:62:ILE:CD1	1:B:501:LEU:CD1	2.95	0.45
1:B:635:GLN:HB3	1:B:644:THR:HB	1.99	0.45
1:B:890:ALA:O	1:B:891:SER:HB2	2.17	0.45
1:A:182:LEU:HB2	1:A:203:LEU:HD11	1.99	0.45
1:A:62:ILE:CD1	1:A:501:LEU:CD1	2.95	0.45
1:A:663:SER:O	1:A:667:SER:HB2	2.16	0.45
1:A:715:VAL:HG21	1:A:717:LYS:CD	2.44	0.45
1:A:841:GLU:HG3	1:A:842:SER:N	2.32	0.45
1:A:955:LEU:CD1	1:A:973:ILE:CG2	2.94	0.45
1:B:133:TYR:CG	1:B:136:ILE:CG1	2.94	0.45
1:B:464:GLY:O	1:B:465:ASN:HB3	2.17	0.45
1:A:492:GLN:HG2	1:A:503:ARG:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:873:THR:CB	1:A:982:SER:N	2.80	0.45
1:B:192:PRO:HB3	1:B:233:PHE:CZ	2.51	0.45
1:B:288:ALA:O	1:B:289:PHE:HB2	2.17	0.45
1:B:492:GLN:HG2	1:B:503:ARG:HG2	1.98	0.45
1:B:511:GLN:HG3	1:B:512:TYR:CD2	2.51	0.45
1:B:539:GLU:HG3	1:B:540:ARG:N	2.31	0.45
1:B:814:LEU:HB2	1:B:884:LEU:HD11	1.98	0.45
1:A:118:LEU:CD1	1:A:172:ILE:HD12	2.12	0.45
1:A:531:LEU:HG	1:A:584:PRO:CG	2.46	0.45
1:A:91:ASN:OD1	1:A:92:PRO:HD2	2.16	0.45
1:B:327:VAL:HG11	1:B:358:ILE:HD11	1.97	0.45
1:B:468:GLN:HB3	1:B:468:GLN:HE21	1.47	0.45
1:B:862:ILE:HG22	1:B:877:ILE:CA	2.32	0.45
1:A:464:GLY:O	1:A:465:ASN:HB3	2.17	0.44
1:A:703:LEU:CD2	1:A:790:ILE:CG2	2.95	0.44
1:A:778:VAL:O	1:A:797:LYS:HB2	2.17	0.44
1:B:295:VAL:CB	1:B:414:VAL:HG21	2.48	0.44
1:B:469:TYR:CG	1:B:470:GLU:N	2.84	0.44
1:B:586:LEU:HD13	1:B:590:VAL:HG21	1.99	0.44
1:B:703:LEU:CD2	1:B:790:ILE:CG2	2.95	0.44
1:B:832:THR:HG21	1:B:836:HIS:CB	2.48	0.44
1:A:151:PRO:HB2	1:A:157:HIS:CE1	2.52	0.44
1:A:247:PHE:CD1	1:A:314:LEU:HD22	2.52	0.44
1:A:278:LYS:HD3	1:A:294:GLU:HG2	1.98	0.44
1:A:252:PHE:HD1	1:A:283:CYS:HA	1.82	0.44
1:A:471:THR:HG23	1:A:473:GLN:NE2	2.27	0.44
1:A:564:PRO:HB2	1:A:576:LEU:CD2	2.48	0.44
1:A:567:ILE:HD11	1:A:652:PHE:CD1	2.53	0.44
1:A:892:HIS:CD2	1:A:893:VAL:N	2.85	0.44
1:B:162:VAL:HG21	1:B:187:ALA:HB3	1.99	0.44
1:B:252:PHE:HD1	1:B:283:CYS:HA	1.82	0.44
1:B:305:GLU:HG2	1:B:307:ARG:HG2	1.99	0.44
1:B:291:SER:HB3	1:B:404:CYS:O	2.18	0.44
1:B:458:ARG:HG3	1:B:468:GLN:NE2	2.32	0.44
1:B:53:LEU:HD12	1:B:501:LEU:HG	1.99	0.44
1:B:492:GLN:HG2	1:B:503:ARG:HD2	1.98	0.44
1:B:566:ASN:CB	1:B:651:VAL:CG2	2.95	0.44
1:A:189:ASP:HB3	1:A:191:LYS:HD3	1.99	0.44
1:B:597:LEU:HG	1:B:622:ILE:HG12	1.99	0.44
1:A:291:SER:HB3	1:A:404:CYS:O	2.18	0.44
1:A:566:ASN:CB	1:A:651:VAL:CG2	2.94	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:868:PRO:HG2	1:A:1022:VAL:HG21	1.94	0.44
1:A:995:PHE:CZ	1:A:998:ARG:HB2	2.52	0.44
1:B:182:LEU:HB2	1:B:203:LEU:HD11	1.99	0.44
1:B:247:PHE:CD1	1:B:314:LEU:HD22	2.52	0.44
1:B:264:SER:HA	1:B:265:PRO:HA	1.53	0.44
1:B:370:LEU:CD2	1:B:374:TYR:HE1	2.27	0.44
1:B:437:TYR:CE2	1:B:439:TYR:HB2	2.51	0.44
1:B:567:ILE:HD11	1:B:652:PHE:CD1	2.53	0.44
1:B:695:LYS:C	1:B:696:LEU:HD12	2.37	0.44
1:B:805:ALA:H	1:B:806:MET:HE3	1.82	0.44
1:A:116:MET:SD	1:A:169:PHE:HA	2.57	0.44
1:A:262:MET:SD	1:A:383:ALA:HB3	2.57	0.44
1:A:541:CYS:HB3	1:A:544:SER:HB3	1.99	0.44
1:A:58:ARG:HG2	1:A:58:ARG:NH1	2.31	0.44
1:A:53:LEU:CG	1:A:64:LEU:CD1	2.96	0.44
1:A:889:ILE:CD1	1:A:907:TYR:CZ	3.01	0.44
1:A:958:LEU:HD13	1:A:1033:PHE:CD1	2.53	0.44
1:B:116:MET:SD	1:B:169:PHE:HA	2.57	0.44
1:A:281:ARG:NH1	1:A:366:ILE:HG21	2.33	0.44
1:A:306:TYR:HE1	1:A:351:GLU:HG2	1.83	0.44
1:A:635:GLN:HB3	1:A:644:THR:HB	1.99	0.44
1:A:671:CYS:HB3	1:A:680:CYS:SG	2.57	0.44
1:A:951:MET:HG2	1:A:977:ASN:OD1	2.17	0.44
1:B:179:ASP:O	1:B:180:ASP:HB3	2.17	0.44
1:B:185:ALA:CB	1:B:243:TYR:CD1	3.00	0.44
1:B:262:MET:SD	1:B:383:ALA:HB3	2.58	0.44
1:A:98:ARG:NH2	1:A:107:LEU:HD12	2.29	0.44
1:A:179:ASP:O	1:A:180:ASP:HB3	2.17	0.44
1:A:40:VAL:HG13	1:A:40:VAL:O	2.17	0.44
1:A:421:ILE:HA	1:A:422:PRO:HD2	1.84	0.44
1:A:586:LEU:HD13	1:A:590:VAL:HG21	1.99	0.44
1:A:597:LEU:HG	1:A:622:ILE:HG12	1.99	0.44
1:A:72:LYS:CE	1:A:80:LEU:CD1	2.95	0.44
1:B:117:LEU:HD11	1:B:126:LEU:CD2	2.31	0.44
1:B:119:ILE:HG23	1:B:121:TYR:CE1	2.53	0.44
1:B:173:VAL:O	1:B:173:VAL:HG23	2.18	0.44
1:B:256:LEU:CB	1:B:309:LEU:CD2	2.94	0.44
1:B:281:ARG:NH1	1:B:366:ILE:HG21	2.33	0.44
1:B:676:TYR:CE1	1:B:730:GLN:CD	2.90	0.44
1:B:699:ASP:O	1:B:725:ASN:HB3	2.18	0.44
1:B:62:ILE:CD1	1:B:73:LEU:HD12	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:LEU:O	1:A:127:ILE:HG22	2.17	0.44
1:A:133:TYR:CG	1:A:136:ILE:CG1	2.94	0.44
1:A:162:VAL:HG21	1:A:187:ALA:HB3	1.99	0.44
1:A:217:PHE:CE2	1:A:219:ASP:HB2	2.53	0.44
1:A:889:ILE:HA	1:A:892:HIS:ND1	2.33	0.44
1:B:110:THR:CB	1:B:132:LEU:CD2	2.95	0.44
1:B:274:VAL:HG23	1:B:275:TYR:N	2.30	0.44
1:B:322:GLY:HA2	1:B:327:VAL:HG22	1.99	0.44
1:B:332:ASP:O	1:B:333:LEU:HD23	2.18	0.44
1:B:42:PHE:CZ	1:B:45:GLU:CB	2.95	0.44
1:B:564:PRO:HB2	1:B:576:LEU:CD2	2.48	0.44
1:B:55:VAL:HG22	1:B:62:ILE:HG22	2.00	0.44
1:A:442:HIS:CD2	1:A:458:ARG:HH21	2.35	0.44
1:A:528:TRP:HZ2	1:A:533:ASN:OD1	2.01	0.44
1:A:569:VAL:CG2	1:A:654:ASN:CB	2.65	0.44
1:A:574:VAL:HG22	1:A:613:SER:OG	2.17	0.44
1:A:713:VAL:O	1:A:714:GLU:HB2	2.18	0.44
1:B:358:ILE:CG2	1:B:361:GLN:CB	2.95	0.44
1:B:743:GLN:H	1:B:743:GLN:CD	2.21	0.44
1:B:778:VAL:O	1:B:797:LYS:HB2	2.17	0.44
1:B:863:ILE:HG22	1:B:876:THR:CB	2.35	0.44
1:B:889:ILE:CD1	1:B:907:TYR:CZ	3.01	0.44
1:A:332:ASP:O	1:A:333:LEU:HD23	2.18	0.43
1:A:53:LEU:HD11	1:A:501:LEU:HD11	2.00	0.43
1:A:567:ILE:HD11	1:A:650:PHE:CE2	2.53	0.43
1:A:574:VAL:CG2	1:A:613:SER:HB3	2.48	0.43
1:A:62:ILE:CD1	1:A:73:LEU:HD12	2.45	0.43
1:A:764:THR:CG2	1:A:766:TYR:CZ	3.01	0.43
1:A:874:LYS:H	1:A:982:SER:HB2	1.80	0.43
1:B:189:ASP:HB3	1:B:191:LYS:HD3	1.99	0.43
1:B:306:TYR:HE1	1:B:351:GLU:HG2	1.83	0.43
1:B:53:LEU:HD11	1:B:501:LEU:HD11	2.00	0.43
1:B:711:VAL:HG21	1:B:798:VAL:CG2	2.48	0.43
1:B:841:GLU:HG3	1:B:842:SER:N	2.32	0.43
1:A:711:VAL:HG21	1:A:798:VAL:CG2	2.48	0.43
1:A:832:THR:HG21	1:A:836:HIS:CB	2.48	0.43
1:B:541:CYS:HB3	1:B:544:SER:HB3	1.99	0.43
1:A:119:ILE:HG23	1:A:121:TYR:CE1	2.53	0.43
1:A:333:LEU:HD23	1:A:358:ILE:HG13	2.00	0.43
1:A:589:GLY:C	1:A:639:LYS:HG2	2.39	0.43
1:B:151:PRO:HB2	1:B:157:HIS:CE1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:THR:HG22	1:B:324:THR:O	2.18	0.43
1:B:555:LYS:NZ	1:B:556:GLN:HG2	2.33	0.43
1:B:574:VAL:HG22	1:B:613:SER:OG	2.17	0.43
1:B:764:THR:CG2	1:B:766:TYR:CZ	3.01	0.43
1:B:889:ILE:HA	1:B:892:HIS:ND1	2.33	0.43
1:A:1016:MET:HE2	1:A:1033:PHE:H	1.84	0.43
1:A:1031:LEU:HD22	1:A:1031:LEU:N	2.34	0.43
1:A:1014:LEU:HA	1:A:1035:TYR:HB2	2.00	0.43
1:A:435:ILE:CD1	1:A:486:PHE:HD1	2.31	0.43
1:A:590:VAL:CG1	1:A:591:ASN:N	2.82	0.43
1:A:62:ILE:CD1	1:A:501:LEU:HD13	2.49	0.43
1:A:531:LEU:C	1:A:641:THR:HG1	2.19	0.43
1:A:743:GLN:CD	1:A:743:GLN:H	2.22	0.43
1:A:839:ALA:HB1	1:A:841:GLU:O	2.18	0.43
1:B:296:PRO:HB2	1:B:417:MET:CE	2.48	0.43
1:B:370:LEU:HD12	1:B:399:ILE:HG23	2.00	0.43
1:B:456:LYS:HD3	1:B:523:ASP:OD2	2.10	0.43
1:B:527:GLY:HA3	1:B:550:PHE:HZ	1.72	0.43
1:B:528:TRP:HZ2	1:B:533:ASN:OD1	2.01	0.43
1:B:563:HIS:CB	1:B:577:VAL:CG1	2.95	0.43
1:B:589:GLY:C	1:B:639:LYS:HG2	2.39	0.43
1:A:173:VAL:HG23	1:A:173:VAL:O	2.18	0.43
1:A:224:SER:HA	1:A:289:PHE:CD1	2.54	0.43
1:A:501:LEU:CD2	1:A:502:THR:N	2.81	0.43
1:A:832:THR:CG2	1:A:836:HIS:CB	2.95	0.43
1:B:333:LEU:HD23	1:B:358:ILE:HG13	2.00	0.43
1:B:458:ARG:HB2	1:B:468:GLN:HE22	1.83	0.43
1:B:574:VAL:CG2	1:B:613:SER:HB3	2.48	0.43
1:B:839:ALA:HB1	1:B:841:GLU:O	2.18	0.43
1:A:978:LEU:HD13	1:A:1003:ILE:HG13	2.01	0.43
1:A:100:VAL:HG21	1:A:158:TYR:OH	2.19	0.43
1:A:962:ARG:HD3	1:A:1034:GLN:HE21	1.83	0.43
1:A:128:ALA:O	1:A:138:LYS:HG2	2.19	0.43
1:A:162:VAL:HG12	1:A:164:GLU:H	1.84	0.43
1:A:295:VAL:CB	1:A:414:VAL:HG21	2.48	0.43
1:A:296:PRO:HB2	1:A:417:MET:CE	2.48	0.43
1:A:470:GLU:HG2	1:A:471:THR:N	2.34	0.43
1:A:716:ILE:CD1	1:A:763:ASN:HB3	2.49	0.43
1:B:117:LEU:HG	1:B:126:LEU:HD11	2.01	0.43
1:B:217:PHE:CE2	1:B:219:ASP:HB2	2.53	0.43
1:B:281:ARG:HB3	1:B:293:VAL:HG11	1.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:VAL:O	1:B:40:VAL:HG13	2.17	0.43
1:B:435:ILE:CD1	1:B:486:PHE:HD1	2.31	0.43
1:B:440:LYS:HB2	1:B:538:LYS:HZ2	1.84	0.43
1:B:764:THR:HG23	1:B:766:TYR:CZ	2.54	0.43
1:B:95:TYR:HA	1:B:95:TYR:HD1	1.70	0.43
1:A:965:MET:HG3	1:A:1010:SER:O	2.18	0.43
1:A:962:ARG:CB	1:A:1034:GLN:HG3	2.45	0.43
1:A:185:ALA:CB	1:A:243:TYR:CE2	3.02	0.43
1:A:305:GLU:HG2	1:A:307:ARG:HG2	1.99	0.43
1:A:764:THR:HG23	1:A:766:TYR:CZ	2.54	0.43
1:B:119:ILE:HG21	1:B:121:TYR:CE1	2.54	0.43
1:B:460:ASP:CG	1:B:463:LYS:HB3	2.39	0.43
1:B:542:GLU:HG2	1:B:543:ARG:HG3	2.01	0.43
1:B:549:ARG:HD3	1:B:584:PRO:CB	2.48	0.43
1:A:1010:SER:HB2	1:A:1035:TYR:CE1	2.52	0.43
1:A:1016:MET:CE	1:A:1033:PHE:CB	2.94	0.43
1:A:555:LYS:NZ	1:A:556:GLN:HG2	2.33	0.43
1:A:562:VAL:HG22	1:A:578:LEU:HD22	1.98	0.43
1:A:620:PRO:O	1:A:623:ILE:HG13	2.18	0.43
1:A:72:LYS:CD	1:A:80:LEU:CD1	2.97	0.43
1:B:506:VAL:CG2	1:B:525:HIS:CE1	2.81	0.43
1:A:333:LEU:HD23	1:A:358:ILE:HA	2.01	0.43
1:A:62:ILE:CD1	1:A:64:LEU:HD21	2.46	0.43
1:A:789:ASN:HD22	1:A:790:ILE:N	2.17	0.43
1:B:100:VAL:HG21	1:B:158:TYR:OH	2.19	0.43
1:B:234:THR:CG2	1:B:235:VAL:N	2.82	0.43
1:B:358:ILE:HG23	1:B:358:ILE:O	2.18	0.43
1:B:506:VAL:HG21	1:B:525:HIS:NE2	2.22	0.43
1:B:620:PRO:O	1:B:623:ILE:HG13	2.18	0.43
1:B:949:TYR:CE2	1:B:951:MET:HE2	2.53	0.43
1:A:112:ASN:ND2	1:A:133:TYR:HE2	2.17	0.43
1:A:117:LEU:HG	1:A:126:LEU:HD11	2.01	0.43
1:A:186:THR:CG2	1:A:187:ALA:N	2.81	0.43
1:A:281:ARG:HB3	1:A:293:VAL:HG11	1.97	0.43
1:A:617:LYS:HG3	1:A:618:GLU:N	2.34	0.43
1:A:55:VAL:HG22	1:A:62:ILE:HG22	2.00	0.43
1:A:805:ALA:N	1:A:806:MET:CE	2.82	0.43
1:A:885:GLU:HG3	1:A:886:PHE:N	2.34	0.43
1:B:123:GLU:HB2	1:B:125:ARG:HG2	2.01	0.43
1:B:470:GLU:HG2	1:B:471:THR:N	2.34	0.43
1:B:501:LEU:CD2	1:B:502:THR:N	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:617:LYS:HG3	1:B:618:GLU:N	2.34	0.43
1:B:789:ASN:HD22	1:B:790:ILE:N	2.17	0.43
1:A:665:VAL:HG11	1:A:697:PRO:CD	2.48	0.42
1:A:98:ARG:HE	1:A:107:LEU:HD12	1.83	0.42
1:B:90:ASP:C	1:B:107:LEU:HD22	2.39	0.42
1:B:128:ALA:O	1:B:138:LYS:HG2	2.19	0.42
1:B:62:ILE:CD1	1:B:501:LEU:HD13	2.49	0.42
1:B:713:VAL:O	1:B:714:GLU:HB2	2.18	0.42
1:A:192:PRO:HB3	1:A:233:PHE:CZ	2.51	0.42
1:A:90:ASP:C	1:A:107:LEU:HD22	2.39	0.42
1:A:972:THR:HG23	1:A:1002:TYR:HE1	1.72	0.42
1:B:133:TYR:CB	1:B:136:ILE:HG23	2.49	0.42
1:B:178:PHE:O	1:B:178:PHE:HD1	2.02	0.42
1:B:543:ARG:HB2	1:B:549:ARG:NH1	2.34	0.42
1:B:567:ILE:HD11	1:B:650:PHE:CE2	2.53	0.42
1:B:665:VAL:HG11	1:B:697:PRO:CD	2.48	0.42
1:A:1032:VAL:CG1	1:A:1033:PHE:N	2.82	0.42
1:A:110:THR:HG21	1:A:132:LEU:HD21	1.97	0.42
1:A:458:ARG:HB2	1:A:468:GLN:HE22	1.83	0.42
1:A:541:CYS:HB2	1:A:544:SER:HB3	2.01	0.42
1:A:630:HIS:CD2	1:A:632:VAL:CG2	3.00	0.42
1:A:889:ILE:HG23	1:A:892:HIS:NE2	2.33	0.42
1:B:185:ALA:CB	1:B:243:TYR:CE2	3.02	0.42
1:B:358:ILE:HG23	1:B:361:GLN:N	2.24	0.42
1:B:605:ILE:O	1:B:608:GLN:HG2	2.20	0.42
1:B:689:PHE:HD1	1:B:691:GLU:HG2	1.80	0.42
1:A:1029:GLN:CG	1:A:1030:ASP:N	2.83	0.42
1:A:119:ILE:HG21	1:A:121:TYR:CE1	2.54	0.42
1:A:225:MET:CE	1:A:227:LYS:CG	2.94	0.42
1:A:370:LEU:HD12	1:A:399:ILE:HG23	2.00	0.42
1:A:471:THR:HG21	1:A:473:GLN:OE1	2.19	0.42
1:A:567:ILE:CD1	1:A:567:ILE:N	2.82	0.42
1:A:710:LEU:HD12	1:A:710:LEU:C	2.40	0.42
1:A:865:VAL:CG1	1:A:866:THR:N	2.82	0.42
1:A:953:LEU:HD12	1:A:978:LEU:HD23	2.01	0.42
1:A:868:PRO:CD	1:A:981:GLY:HA2	1.99	0.42
1:B:224:SER:HA	1:B:289:PHE:CD1	2.54	0.42
1:B:662:LEU:HD23	1:B:791:ASP:CB	2.48	0.42
1:A:962:ARG:HD3	1:A:1034:GLN:NE2	2.34	0.42
1:A:169:PHE:CD2	1:A:170:GLY:N	2.84	0.42
1:A:178:PHE:O	1:A:178:PHE:HD1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:ILE:HG23	1:A:361:GLN:N	2.24	0.42
1:A:358:ILE:HG23	1:A:358:ILE:O	2.18	0.42
1:A:955:LEU:CG	1:A:973:ILE:CG2	2.95	0.42
1:B:216:VAL:CG1	1:B:217:PHE:N	2.82	0.42
1:B:333:LEU:HD23	1:B:358:ILE:HA	2.01	0.42
1:B:567:ILE:N	1:B:567:ILE:CD1	2.82	0.42
1:B:590:VAL:CG1	1:B:591:ASN:N	2.82	0.42
1:B:759:VAL:CG1	1:B:760:GLN:N	2.81	0.42
1:B:885:GLU:HG3	1:B:886:PHE:N	2.34	0.42
1:B:889:ILE:HG23	1:B:892:HIS:NE2	2.33	0.42
1:A:1007:THR:HG22	1:A:1008:THR:N	2.33	0.42
1:A:123:GLU:HB2	1:A:125:ARG:HG2	2.01	0.42
1:A:460:ASP:CG	1:A:463:LYS:HB3	2.39	0.42
1:A:435:ILE:HG21	1:A:486:PHE:HE1	1.81	0.42
1:A:543:ARG:HB2	1:A:549:ARG:NH1	2.34	0.42
1:A:959:LYS:HG2	1:A:972:THR:HG21	2.01	0.42
1:B:112:ASN:ND2	1:B:133:TYR:HE2	2.17	0.42
1:B:186:THR:CG2	1:B:187:ALA:N	2.81	0.42
1:B:471:THR:HG21	1:B:473:GLN:OE1	2.19	0.42
1:B:68:ASN:CB	1:B:86:GLY:HA3	2.50	0.42
1:A:256:LEU:CB	1:A:309:LEU:CD2	2.94	0.42
1:A:549:ARG:CD	1:A:584:PRO:HB3	2.42	0.42
1:A:830:GLN:CG	1:A:831:CYS:H	2.24	0.42
1:B:321:LEU:HD23	1:B:333:LEU:CD1	2.50	0.42
1:A:542:GLU:HG2	1:A:543:ARG:HG3	2.00	0.42
1:A:845:LEU:HD11	1:A:852:SER:OG	2.20	0.42
1:B:458:ARG:HD2	1:B:524:PRO:CB	2.31	0.42
1:B:437:TYR:HH	1:B:525:HIS:CD2	2.37	0.42
1:B:653:TYR:CZ	1:B:682:HIS:CE1	3.07	0.42
1:B:700:CYS:HA	1:B:701:PRO:HD3	1.45	0.42
1:A:234:THR:CG2	1:A:235:VAL:N	2.82	0.42
1:A:324:THR:HG22	1:A:324:THR:O	2.18	0.42
1:A:370:LEU:CD2	1:A:374:TYR:HE1	2.28	0.42
1:A:562:VAL:HG22	1:A:578:LEU:HD23	1.99	0.42
1:A:566:ASN:CA	1:A:651:VAL:CG2	2.95	0.42
1:A:783:VAL:CG1	1:A:784:TRP:N	2.83	0.42
1:B:446:PHE:CB	1:B:454:LEU:HD11	2.43	0.42
1:B:562:VAL:HG22	1:B:578:LEU:HD23	1.99	0.42
1:B:563:HIS:HB2	1:B:577:VAL:HG13	2.01	0.42
1:A:380:LEU:HD22	1:A:412:LEU:HB3	2.02	0.42
1:A:662:LEU:O	1:A:666:GLU:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ILE:CD1	1:A:73:LEU:HB2	2.47	0.42
1:A:888:ASP:OD1	1:A:889:ILE:HG13	2.20	0.42
1:A:920:ALA:C	1:A:922:PRO:HD2	2.41	0.42
1:B:39:PHE:CZ	1:B:473:GLN:HG3	2.53	0.42
1:B:528:TRP:CZ2	1:B:533:ASN:OD1	2.73	0.42
1:B:783:VAL:CG1	1:B:784:TRP:N	2.83	0.42
1:B:926:ALA:HB2	1:B:949:TYR:CD1	2.55	0.42
1:A:412:LEU:CD1	1:A:412:LEU:N	2.83	0.41
1:A:440:LYS:HD2	1:A:538:LYS:HD2	1.93	0.41
1:A:605:ILE:O	1:A:608:GLN:HG2	2.19	0.41
1:A:67:VAL:CG1	1:A:111:ASN:HB3	2.50	0.41
1:B:162:VAL:HG12	1:B:164:GLU:H	1.84	0.41
1:B:177:ASN:O	1:B:178:PHE:CG	2.73	0.41
1:B:256:LEU:HD12	1:B:297:ILE:HD11	2.02	0.41
1:B:575:LEU:N	1:B:575:LEU:CD2	2.83	0.41
1:B:623:ILE:HD12	1:B:624:THR:HA	2.02	0.41
1:B:64:LEU:HD12	1:B:496:MET:HE3	1.98	0.41
1:B:817:ASP:OD1	1:B:820:PHE:CD2	2.73	0.41
1:A:216:VAL:CG1	1:A:217:PHE:N	2.82	0.41
1:A:44:GLY:O	1:A:47:ALA:HA	2.20	0.41
1:A:440:LYS:HB3	1:A:538:LYS:HZ3	1.79	0.41
1:A:817:ASP:OD1	1:A:820:PHE:CD2	2.73	0.41
1:A:68:ASN:CB	1:A:86:GLY:HA3	2.50	0.41
1:A:959:LYS:CG	1:A:972:THR:CB	2.97	0.41
1:B:159:LEU:HG	1:B:201:ARG:NH1	2.35	0.41
1:B:403:PHE:CE2	1:B:405:GLY:HA2	2.55	0.41
1:B:492:GLN:HB3	1:B:503:ARG:HG3	2.02	0.41
1:B:728:GLN:HG3	1:B:753:ARG:NH2	2.35	0.41
1:B:716:ILE:CD1	1:B:763:ASN:HB3	2.49	0.41
1:B:72:LYS:CE	1:B:80:LEU:CD1	2.95	0.41
1:A:1016:MET:HE2	1:A:1033:PHE:CB	2.49	0.41
1:A:177:ASN:O	1:A:178:PHE:CG	2.73	0.41
1:A:387:VAL:CG1	1:A:388:LYS:N	2.82	0.41
1:A:446:PHE:CD1	1:A:446:PHE:N	2.88	0.41
1:A:569:VAL:HB	1:A:654:ASN:CG	2.41	0.41
1:A:728:GLN:HG3	1:A:753:ARG:NH2	2.35	0.41
1:B:412:LEU:N	1:B:412:LEU:CD1	2.83	0.41
1:B:444:LEU:HD23	1:B:524:PRO:HG2	1.91	0.41
1:B:619:VAL:HB	1:B:620:PRO:CD	2.47	0.41
1:B:865:VAL:CG1	1:B:866:THR:N	2.82	0.41
1:A:111:ASN:O	1:A:132:LEU:HD13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:VAL:HG22	1:A:188:VAL:O	2.21	0.41
1:A:307:ARG:HA	1:A:307:ARG:HD3	1.88	0.41
1:A:349:LEU:CD2	1:A:349:LEU:N	2.84	0.41
1:A:403:PHE:CE2	1:A:405:GLY:HA2	2.55	0.41
1:A:563:HIS:HB2	1:A:577:VAL:HG13	2.01	0.41
1:A:631:VAL:HG13	1:A:631:VAL:O	2.19	0.41
1:A:711:VAL:HB	1:A:800:LEU:HD23	2.02	0.41
1:A:926:ALA:HB2	1:A:949:TYR:CD1	2.55	0.41
1:A:978:LEU:HA	1:A:978:LEU:HD23	1.93	0.41
1:B:110:THR:HG21	1:B:132:LEU:HD21	1.97	0.41
1:B:225:MET:CE	1:B:227:LYS:CG	2.94	0.41
1:B:446:PHE:CD1	1:B:446:PHE:N	2.89	0.41
1:B:562:VAL:HG22	1:B:578:LEU:HD22	1.98	0.41
1:B:679:VAL:CG1	1:B:680:CYS:N	2.82	0.41
1:B:862:ILE:HG21	1:B:877:ILE:HG12	2.03	0.41
1:B:920:ALA:C	1:B:922:PRO:HD2	2.40	0.41
1:A:988:PHE:CB	1:A:1016:MET:SD	3.06	0.41
1:A:1031:LEU:H	1:A:1031:LEU:HD22	1.84	0.41
1:A:133:TYR:CB	1:A:136:ILE:HG23	2.49	0.41
1:A:159:LEU:HG	1:A:201:ARG:NH1	2.36	0.41
1:A:226:ILE:HD11	1:A:385:LEU:HD23	2.03	0.41
1:A:531:LEU:HA	1:A:531:LEU:HD23	1.91	0.41
1:B:137:CYS:SG	1:B:159:LEU:CD1	3.09	0.41
1:B:280:VAL:CG1	1:B:281:ARG:N	2.83	0.41
1:B:380:LEU:HD22	1:B:412:LEU:HB3	2.02	0.41
1:B:631:VAL:HG13	1:B:631:VAL:O	2.19	0.41
1:B:803:CYS:SG	1:B:832:THR:HA	2.61	0.41
1:B:949:TYR:CE2	1:B:951:MET:HE1	2.55	0.41
1:A:446:PHE:CB	1:A:454:LEU:HD11	2.43	0.41
1:A:703:LEU:HD13	1:A:723:ALA:CB	2.47	0.41
1:A:862:ILE:HG21	1:A:877:ILE:HG12	2.03	0.41
1:A:958:LEU:HD22	1:A:960:PRO:N	2.35	0.41
1:A:959:LYS:CG	1:A:972:THR:HG21	2.51	0.41
1:B:185:ALA:HB3	1:B:243:TYR:CD2	2.56	0.41
1:B:444:LEU:HD12	1:B:446:PHE:CD1	2.51	0.41
1:B:444:LEU:HD13	1:B:445:ALA:H	1.79	0.41
1:B:453:LYS:CE	1:B:472:VAL:HG22	2.51	0.41
1:B:506:VAL:CG1	1:B:507:GLU:N	2.84	0.41
1:B:541:CYS:HB2	1:B:544:SER:HB3	2.01	0.41
1:B:551:ALA:HB1	1:B:556:GLN:HB2	2.03	0.41
1:B:778:VAL:HG12	1:B:779:GLU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:805:ALA:N	1:B:806:MET:CE	2.82	0.41
1:B:888:ASP:OD1	1:B:889:ILE:HG13	2.20	0.41
1:A:380:LEU:CB	1:A:386:LYS:CE	2.95	0.41
1:A:492:GLN:HB3	1:A:503:ARG:HG3	2.02	0.41
1:A:679:VAL:CG1	1:A:680:CYS:N	2.82	0.41
1:A:759:VAL:CG1	1:A:760:GLN:N	2.81	0.41
1:A:95:TYR:CG	1:A:96:PRO:CD	3.03	0.41
1:B:137:CYS:O	1:B:150:GLU:HG3	2.20	0.41
1:B:387:VAL:CG1	1:B:388:LYS:N	2.82	0.41
1:B:44:GLY:O	1:B:47:ALA:HA	2.20	0.41
1:B:658:HIS:ND1	1:B:663:SER:HB3	2.36	0.41
1:B:67:VAL:CG1	1:B:111:ASN:HB3	2.50	0.41
1:A:972:THR:CG2	1:A:1002:TYR:CE1	2.93	0.41
1:A:988:PHE:CD2	1:A:1016:MET:SD	3.12	0.41
1:A:137:CYS:O	1:A:150:GLU:HG3	2.20	0.41
1:A:185:ALA:HB3	1:A:243:TYR:CD2	2.56	0.41
1:A:188:VAL:CG2	1:A:191:LYS:HB2	2.51	0.41
1:A:280:VAL:CG1	1:A:281:ARG:N	2.83	0.41
1:B:492:GLN:CG	1:B:503:ARG:HD2	2.51	0.41
1:B:95:TYR:CG	1:B:96:PRO:CD	3.03	0.41
1:A:137:CYS:SG	1:A:159:LEU:CD1	3.09	0.41
1:A:236:ILE:CG2	1:A:239:PHE:HB2	2.51	0.41
1:A:480:VAL:HB	1:A:484:MET:HE2	2.01	0.41
1:A:492:GLN:CG	1:A:503:ARG:HD2	2.51	0.41
1:A:528:TRP:CZ2	1:A:533:ASN:OD1	2.73	0.41
1:B:188:VAL:CG2	1:B:191:LYS:HB2	2.51	0.41
1:B:226:ILE:HD11	1:B:385:LEU:HD23	2.03	0.41
1:B:239:PHE:CD1	1:B:260:PRO:CD	3.03	0.41
1:B:696:LEU:HA	1:B:697:PRO:HD3	1.87	0.41
1:B:710:LEU:C	1:B:710:LEU:HD12	2.40	0.41
1:B:832:THR:HG21	1:B:836:HIS:HB2	1.99	0.41
1:B:843:ARG:CZ	1:B:843:ARG:CB	2.99	0.41
1:A:117:LEU:HD11	1:A:126:LEU:CD2	2.31	0.41
1:A:619:VAL:HB	1:A:620:PRO:CD	2.47	0.41
1:A:623:ILE:HD12	1:A:624:THR:HA	2.01	0.41
1:A:953:LEU:HA	1:A:977:ASN:HB2	2.02	0.41
1:A:959:LYS:HG2	1:A:972:THR:HB	2.02	0.41
1:B:111:ASN:O	1:B:132:LEU:HD13	2.20	0.41
1:B:236:ILE:CG2	1:B:239:PHE:HB2	2.51	0.41
1:B:349:LEU:CD2	1:B:349:LEU:N	2.84	0.41
1:B:560:LEU:CG	1:B:648:THR:CG2	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:683:ASP:HA	1:B:684:PRO:HD3	1.83	0.41
1:B:703:LEU:HD13	1:B:723:ALA:CB	2.47	0.41
1:B:901:SER:HA	1:B:902:PRO:HD2	1.89	0.41
1:A:111:ASN:O	1:A:132:LEU:HD22	2.21	0.41
1:A:95:TYR:CE2	1:A:194:TYR:CD1	3.09	0.41
1:A:252:PHE:HE1	1:A:283:CYS:SG	2.44	0.41
1:A:256:LEU:HD12	1:A:297:ILE:HD11	2.01	0.41
1:A:321:LEU:HD23	1:A:333:LEU:CD1	2.50	0.41
1:A:551:ALA:HB1	1:A:556:GLN:HB2	2.03	0.41
1:A:560:LEU:CG	1:A:648:THR:CG2	2.98	0.41
1:A:658:HIS:ND1	1:A:663:SER:HB3	2.36	0.41
1:A:778:VAL:HG12	1:A:779:GLU:O	2.20	0.41
1:A:832:THR:HG21	1:A:836:HIS:HB2	1.99	0.41
1:B:469:TYR:CZ	1:B:470:GLU:O	2.74	0.41
1:B:560:LEU:HB3	1:B:648:THR:CG2	2.51	0.41
1:B:711:VAL:HB	1:B:800:LEU:HD23	2.02	0.41
1:A:313:TYR:CZ	1:A:435:ILE:CD1	3.05	0.40
1:B:141:ARG:HB3	1:B:144:ASP:OD1	2.21	0.40
1:B:188:VAL:HG22	1:B:188:VAL:O	2.21	0.40
1:B:667:SER:HB3	1:B:668:PRO:CD	2.51	0.40
1:B:832:THR:CG2	1:B:836:HIS:CB	2.95	0.40
1:A:185:ALA:CB	1:A:243:TYR:CD1	3.00	0.40
1:A:45:GLU:CB	1:A:46:PRO:CD	3.00	0.40
1:A:469:TYR:CZ	1:A:470:GLU:O	2.74	0.40
1:A:667:SER:HB3	1:A:668:PRO:CD	2.51	0.40
1:A:873:THR:OG1	1:A:981:GLY:C	2.59	0.40
1:A:955:LEU:HD23	1:A:957:ASP:N	2.37	0.40
1:B:169:PHE:CD2	1:B:170:GLY:N	2.84	0.40
1:B:219:ASP:HB3	1:B:222:VAL:H	1.86	0.40
1:B:242:TYR:CE1	1:B:345:LYS:HE2	2.56	0.40
1:B:44:GLY:CA	1:B:50:PHE:HE2	2.23	0.40
1:A:131:SER:O	1:A:133:TYR:CD2	2.74	0.40
1:A:453:LYS:CE	1:A:472:VAL:HG22	2.51	0.40
1:A:527:GLY:HA3	1:A:550:PHE:HZ	1.72	0.40
1:B:172:ILE:CG1	1:B:182:LEU:HD13	2.46	0.40
1:B:95:TYR:CE2	1:B:194:TYR:CD1	3.09	0.40
1:B:282:LEU:HD23	1:B:292:TYR:HA	2.03	0.40
1:B:450:LYS:CA	1:B:479:PRO:HB3	2.49	0.40
1:B:62:ILE:CD1	1:B:64:LEU:HD21	2.46	0.40
1:B:662:LEU:O	1:B:666:GLU:HB3	2.20	0.40
1:A:188:VAL:HG13	1:A:189:ASP:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:ASP:HB3	1:A:222:VAL:H	1.86	0.40
1:A:259:GLN:HA	1:A:260:PRO:HD3	1.82	0.40
1:A:276:THR:HB	1:A:278:LYS:HZ2	1.86	0.40
1:A:455:LYS:HB3	1:A:467:LEU:CD1	2.52	0.40
1:A:773:ILE:N	1:A:773:ILE:CD1	2.82	0.40
1:A:803:CYS:SG	1:A:832:THR:HA	2.61	0.40
1:A:904:VAL:CG1	1:A:905:ASP:N	2.82	0.40
1:A:896:ALA:HB1	1:A:924:GLN:OE1	2.22	0.40
1:B:313:TYR:CZ	1:B:435:ILE:CD1	3.04	0.40
1:B:410:ALA:CB	1:B:411:PRO:CD	2.98	0.40
1:B:660:SER:HB2	1:B:791:ASP:OD2	2.22	0.40
1:B:904:VAL:CG1	1:B:905:ASP:N	2.82	0.40
1:A:282:LEU:HD23	1:A:292:TYR:HA	2.03	0.40
1:A:242:TYR:CE1	1:A:345:LYS:HE2	2.56	0.40
1:A:847:LEU:CD1	1:A:850:ALA:CA	2.94	0.40
1:A:943:ARG:HB2	1:A:943:ARG:CZ	2.51	0.40
1:B:131:SER:O	1:B:133:TYR:CD2	2.74	0.40
1:B:53:LEU:CG	1:B:64:LEU:CD1	2.96	0.40
1:B:681:THR:OG1	1:B:686:THR:HG21	2.21	0.40
1:B:81:VAL:CG1	1:B:82:THR:N	2.85	0.40
1:B:889:ILE:HD12	1:B:907:TYR:CE1	2.56	0.40
1:B:943:ARG:CZ	1:B:943:ARG:HB2	2.51	0.40

All (69) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:PHE:CE1	1:B:730:GLN:CD[1_655]	0.64	1.56
1:B:287:THR:OG1	1:B:840:HIS:CG[1_655]	0.67	1.53
1:A:146:PHE:CE1	1:B:730:GLN:OE1[1_655]	0.77	1.43
1:A:146:PHE:CD1	1:B:730:GLN:OE1[1_655]	0.78	1.42
1:B:287:THR:CA	1:B:840:HIS:NE2[1_655]	0.79	1.41
1:B:287:THR:CB	1:B:840:HIS:CG[1_655]	0.85	1.35
1:B:287:THR:CB	1:B:840:HIS:CD2[1_655]	0.93	1.27
1:B:287:THR:CA	1:B:840:HIS:CD2[1_655]	1.03	1.17
1:A:731:SER:OG	1:B:83:HIS:CE1[2_646]	1.19	1.01
1:A:146:PHE:CZ	1:B:730:GLN:NE2[1_655]	1.20	1.00
1:A:146:PHE:CZ	1:B:730:GLN:CD[1_655]	1.29	0.91
1:A:730:GLN:OE1	1:B:146:PHE:CD1[2_646]	1.43	0.77
1:B:219:ASP:OD1	1:B:826:GLN:CD[1_655]	1.50	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:THR:OG1	1:B:840:HIS:ND1[1_655]	1.52	0.68
1:A:730:GLN:NE2	1:B:146:PHE:CE1[2_646]	1.52	0.68
1:B:287:THR:C	1:B:840:HIS:NE2[1_655]	1.55	0.65
1:A:407:ASP:OD2	1:A:926:ALA:O[1_554]	1.55	0.65
1:B:220:GLU:OE2	1:B:939:GLU:OE1[1_655]	1.56	0.64
1:A:148:LEU:O	1:B:728:GLN:OE1[1_655]	1.56	0.64
1:A:730:GLN:CD	1:B:146:PHE:CE1[2_646]	1.57	0.63
1:B:287:THR:OG1	1:B:840:HIS:CB[1_655]	1.58	0.62
1:B:287:THR:C	1:B:840:HIS:CD2[1_655]	1.60	0.60
1:B:287:THR:OG1	1:B:840:HIS:CD2[1_655]	1.61	0.59
1:A:83:HIS:CE1	1:B:731:SER:OG[1_655]	1.62	0.58
1:B:219:ASP:OD1	1:B:826:GLN:OE1[1_655]	1.68	0.52
1:B:288:ALA:CB	1:B:841:GLU:OE1[1_655]	1.71	0.49
1:B:287:THR:CA	1:B:840:HIS:CE1[1_655]	1.74	0.46
1:A:146:PHE:CE1	1:B:730:GLN:CG[1_655]	1.75	0.45
1:A:146:PHE:CZ	1:B:730:GLN:OE1[1_655]	1.75	0.45
1:A:146:PHE:CG	1:B:730:GLN:OE1[1_655]	1.75	0.45
1:B:287:THR:CG2	1:B:840:HIS:CD2[1_655]	1.77	0.43
1:B:287:THR:CG2	1:B:840:HIS:C[1_655]	1.78	0.42
1:A:728:GLN:OE1	1:B:148:LEU:O[2_646]	1.83	0.37
1:A:730:GLN:OE1	1:B:146:PHE:CE1[2_646]	1.84	0.36
1:A:731:SER:OG	1:B:83:HIS:ND1[2_646]	1.85	0.35
1:B:219:ASP:OD1	1:B:826:GLN:CG[1_655]	1.86	0.34
1:A:146:PHE:CE1	1:B:730:GLN:NE2[1_655]	1.88	0.32
1:A:728:GLN:NE2	1:B:148:LEU:O[2_646]	1.89	0.31
1:B:217:PHE:CD1	1:B:827:SER:OG[1_655]	1.90	0.30
1:A:752:LEU:CD2	1:B:152:PHE:CE1[2_646]	1.91	0.29
1:B:287:THR:CB	1:B:840:HIS:CB[1_655]	1.91	0.29
1:B:287:THR:CB	1:B:840:HIS:ND1[1_655]	1.92	0.28
1:B:217:PHE:CE1	1:B:827:SER:OG[1_655]	1.93	0.27
1:A:208:GLU:OE2	1:B:728:GLN:NE2[1_655]	1.93	0.27
1:A:146:PHE:CD1	1:B:730:GLN:CD[1_655]	1.94	0.26
1:B:220:GLU:OE2	1:B:939:GLU:CD[1_655]	1.96	0.24
1:B:287:THR:N	1:B:840:HIS:NE2[1_655]	1.98	0.22
1:A:148:LEU:O	1:B:728:GLN:CD[1_655]	1.99	0.21
1:B:220:GLU:OE1	1:B:939:GLU:OE2[1_655]	2.00	0.20
1:B:287:THR:CA	1:B:840:HIS:CG[1_655]	2.01	0.19
1:A:730:GLN:NE2	1:B:146:PHE:CZ[2_646]	2.01	0.19
1:B:219:ASP:OD2	1:B:826:GLN:OE1[1_655]	2.01	0.19
1:B:287:THR:CB	1:B:840:HIS:NE2[1_655]	2.01	0.19
1:B:219:ASP:CG	1:B:826:GLN:OE1[1_655]	2.03	0.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:731:SER:OG	1:B:83:HIS:NE2[2_646]	2.03	0.17
1:B:219:ASP:CG	1:B:826:GLN:CD[1_655]	2.04	0.16
1:B:287:THR:O	1:B:840:HIS:NE2[1_655]	2.05	0.15
1:A:141:ARG:NH2	1:B:691:GLU:OE2[1_655]	2.06	0.14
1:A:208:GLU:OE2	1:B:728:GLN:CD[1_655]	2.08	0.12
1:A:728:GLN:CD	1:B:148:LEU:O[2_646]	2.09	0.11
1:B:287:THR:CG2	1:B:840:HIS:O[1_655]	2.09	0.11
1:A:407:ASP:OD1	1:A:924:GLN:OE1[1_554]	2.11	0.09
1:A:730:GLN:CD	1:B:146:PHE:CD1[2_646]	2.11	0.09
1:B:287:THR:CG2	1:B:840:HIS:CG[1_655]	2.12	0.08
1:B:287:THR:CG2	1:B:841:GLU:N[1_655]	2.13	0.07
1:A:208:GLU:OE1	1:B:753:ARG:NH2[1_655]	2.15	0.05
1:B:219:ASP:OD2	1:B:826:GLN:NE2[1_655]	2.16	0.04
1:A:728:GLN:OE1	1:B:148:LEU:C[2_646]	2.18	0.02
1:A:728:GLN:OE1	1:B:149:GLY:CA[2_646]	2.19	0.01

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	994/1207 (82%)	923 (93%)	51 (5%)	20 (2%)	7 38
1	B	907/1207 (75%)	845 (93%)	43 (5%)	19 (2%)	7 36
All	All	1901/2414 (79%)	1768 (93%)	94 (5%)	39 (2%)	7 36

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	PRO
1	A	181	LYS
1	A	191	LYS
1	A	410	ALA
1	A	465	ASN

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Mol	Chain	Res	Type
1	A	804	GLY
1	A	864	PRO
1	B	96	PRO
1	B	181	LYS
1	B	191	LYS
1	B	410	ALA
1	B	465	ASN
1	B	557	CYS
1	B	700	CYS
1	B	701	PRO
1	B	804	GLY
1	B	864	PRO
1	A	87	PRO
1	B	87	PRO
1	A	271	LYS
1	A	474	VAL
1	A	557	CYS
1	A	849	GLY
1	A	1015	ASP
1	A	1016	MET
1	B	271	LYS
1	B	474	VAL
1	B	849	GLY
1	A	263	VAL
1	B	263	VAL
1	A	344	ARG
1	B	344	ARG
1	A	933	VAL
1	A	1013	VAL
1	B	933	VAL
1	A	44	GLY
1	A	921	LYS
1	B	921	LYS
1	B	44	GLY

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	888/1067 (83%)	861 (97%)	27 (3%)	41 63
1	B	812/1067 (76%)	789 (97%)	23 (3%)	43 65
All	All	1700/2134 (80%)	1650 (97%)	50 (3%)	42 64

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	ARG
1	A	72	LYS
1	A	271	LYS
1	A	386	LYS
1	A	412	LEU
1	A	435	ILE
1	A	468	GLN
1	A	473	GLN
1	A	523	ASP
1	A	529	CYS
1	A	548	ARG
1	A	567	ILE
1	A	575	LEU
1	A	597	LEU
1	A	621	ARG
1	A	670	ARG
1	A	743	GLN
1	A	773	ILE
1	A	797	LYS
1	A	806	MET
1	A	853	LYS
1	A	854	CYS
1	A	892	HIS
1	A	1004	ILE
1	A	1016	MET
1	A	1017	LYS
1	A	1024	ARG
1	B	69	ARG
1	B	72	LYS
1	B	271	LYS
1	B	386	LYS
1	B	412	LEU
1	B	435	ILE
1	B	468	GLN
1	B	473	GLN

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Mol	Chain	Res	Type
1	B	523	ASP
1	B	529	CYS
1	B	548	ARG
1	B	567	ILE
1	B	575	LEU
1	B	597	LEU
1	B	621	ARG
1	B	670	ARG
1	B	743	GLN
1	B	773	ILE
1	B	797	LYS
1	B	806	MET
1	B	853	LYS
1	B	854	CYS
1	B	892	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	101	GLN
1	A	157	HIS
1	A	163	ASN
1	A	273	GLN
1	A	361	GLN
1	A	441	ASN
1	A	442	HIS
1	A	473	GLN
1	A	500	GLN
1	A	533	ASN
1	A	626	ASN
1	A	630	HIS
1	A	672	HIS
1	A	685	ASN
1	A	690	GLN
1	A	702	GLN
1	A	728	GLN
1	A	747	GLN
1	A	789	ASN
1	A	792	ASN
1	A	826	GLN
1	A	836	HIS

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Mol	Chain	Res	Type
1	A	892	HIS
1	A	970	GLN
1	A	983	ASN
1	A	1006	ASN
1	B	51	ASN
1	B	101	GLN
1	B	157	HIS
1	B	163	ASN
1	B	273	GLN
1	B	361	GLN
1	B	441	ASN
1	B	442	HIS
1	B	473	GLN
1	B	500	GLN
1	B	626	ASN
1	B	629	HIS
1	B	630	HIS
1	B	672	HIS
1	B	682	HIS
1	B	685	ASN
1	B	690	GLN
1	B	702	GLN
1	B	728	GLN
1	B	730	GLN
1	B	747	GLN
1	B	789	ASN
1	B	792	ASN
1	B	826	GLN
1	B	836	HIS
1	B	892	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	6
1	A	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	854:CYS	C	855:THR	N	2.49
1	A	802:LYS	C	803:CYS	N	2.46
1	A	951:MET	C	952:THR	N	2.32
1	B	653:TYR	C	654:ASN	N	2.31
1	B	802:LYS	C	803:CYS	N	2.01
1	A	506:VAL	C	507:GLU	N	1.87
1	B	506:VAL	C	507:GLU	N	1.82
1	B	700:CYS	C	701:PRO	N	1.63
1	A	700:CYS	C	701:PRO	N	1.04
1	B	557:CYS	C	558:VAL	N	0.94
1	A	557:CYS	C	558:VAL	N	0.86

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.