



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:25 AM GMT

PDB ID : 3AQP
Title : Crystal structure of SecDF, a translocon-associated membrane protein, from *Thermus thermophilus*
Authors : Tsukazaki, T.; Mori, H.; Echizen, Y.; Ishitani, R.; Fukai, S.; Tanaka, T.; Perederina, A.; Vassylyev, D.G.; Kohno, T.; Ito, K.; Nureki, O.
Deposited on : 2010-11-16
Resolution : 3.30 Å(reported)

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

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

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

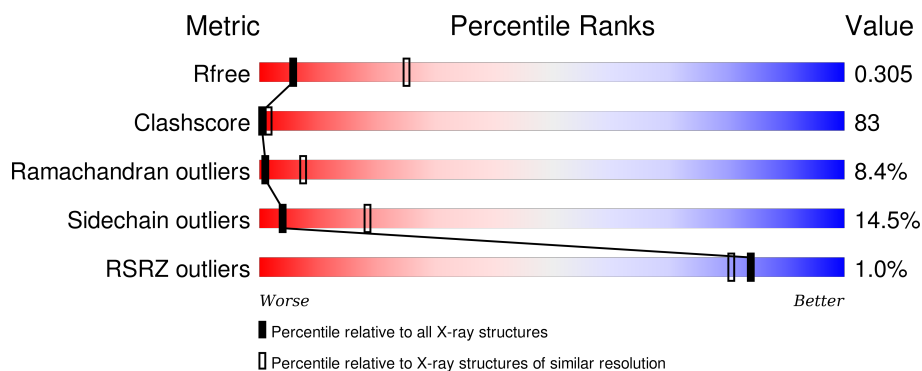
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	741	<div> <div></div> <div> <div></div> <div>18%</div> <div>63%</div> <div>16%</div> <div>• •</div> </div> </div>
1	B	741	<div> <div></div> <div> <div></div> <div>18%</div> <div>63%</div> <div>16%</div> <div>• •</div> </div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11028 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 Probable SecDF protein-export membrane protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	719	Total	C	N	O	S	0	0	0
			5514	3571	947	990	6			
1	B	719	Total	C	N	O	S	0	0	0
			5514	3571	947	990	6			

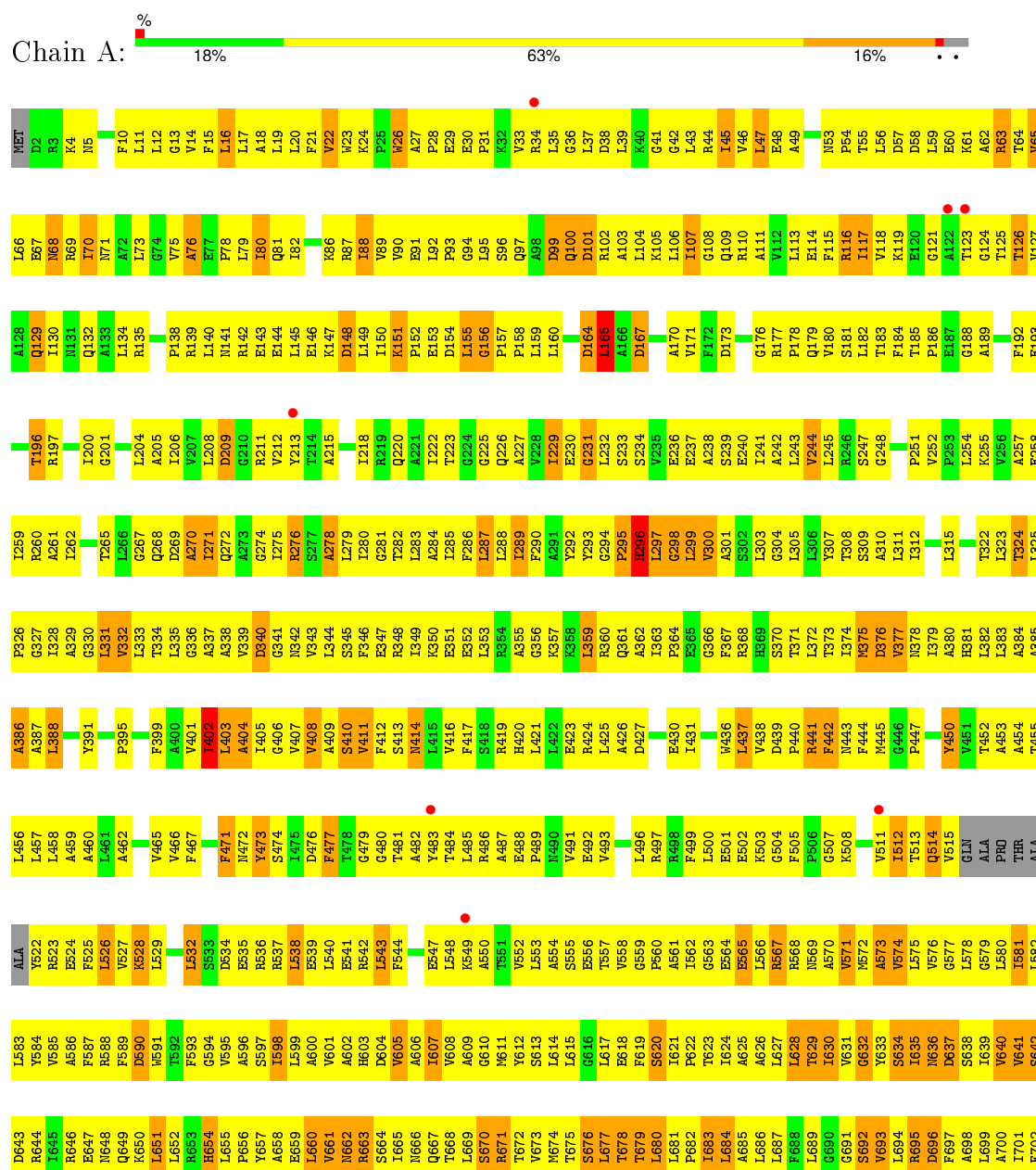
There are 14 discrepancies between the modelled and reference sequences:

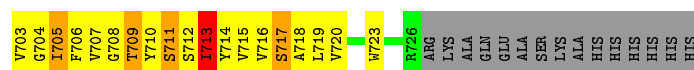
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ASP	ASN	ENGINEERED MUTATION	UNP Q5SKE6
A	736	HIS	-	EXPRESSION TAG	UNP Q5SKE6
A	737	HIS	-	EXPRESSION TAG	UNP Q5SKE6
A	738	HIS	-	EXPRESSION TAG	UNP Q5SKE6
A	739	HIS	-	EXPRESSION TAG	UNP Q5SKE6
A	740	HIS	-	EXPRESSION TAG	UNP Q5SKE6
A	741	HIS	-	EXPRESSION TAG	UNP Q5SKE6
B	2	ASP	ASN	ENGINEERED MUTATION	UNP Q5SKE6
B	736	HIS	-	EXPRESSION TAG	UNP Q5SKE6
B	737	HIS	-	EXPRESSION TAG	UNP Q5SKE6
B	738	HIS	-	EXPRESSION TAG	UNP Q5SKE6
B	739	HIS	-	EXPRESSION TAG	UNP Q5SKE6
B	740	HIS	-	EXPRESSION TAG	UNP Q5SKE6
B	741	HIS	-	EXPRESSION TAG	UNP Q5SKE6

3 Residue-property plots

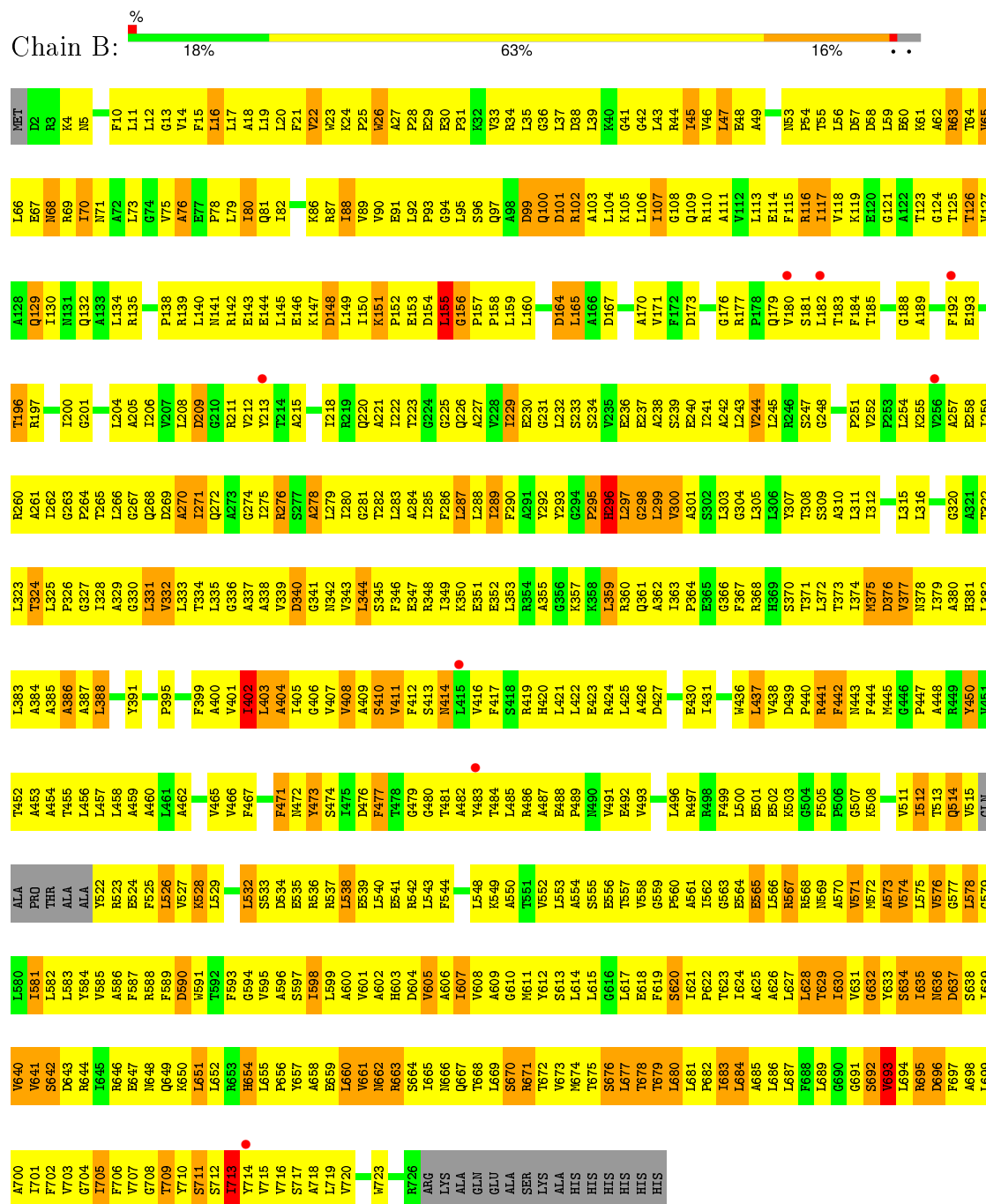
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

- Molecule 1: Probable SecDF protein-export membrane protein





• Molecule 1: Probable SecDF protein-export membrane protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	140.64Å 140.64Å 160.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.88 – 3.30 46.88 – 3.30	Depositor EDS
% Data completeness (in resolution range)	89.0 (46.88-3.30) 89.0 (46.88-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 3.32Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6 _289)	Depositor
R, R_{free}	0.298 , 0.319 0.285 , 0.305	Depositor DCC
R_{free} test set	2122 reflections (5.08%)	DCC
Wilson B-factor (Å ²)	106.4	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 352.2	EDS
Estimated twinning fraction	0.501 for h,-k,-l 0.407 for h,-k,-l	Xtriage
Reported twinning fraction	0.501 for h,-k,-l	Depositor
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Outliers	0 of 41834 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11028	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.44	0/5608	0.67	1/7622 (0.0%)
1	B	0.44	0/5608	0.67	1/7622 (0.0%)
All	All	0.44	0/11216	0.67	2/15244 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	165	LEU	CA-CB-CG	5.09	127.02	115.30
1	B	155	LEU	CA-CB-CG	5.05	126.91	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5514	0	5787	939	0
1	B	5514	0	5787	944	0
All	All	11028	0	11574	1880	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 83.

All (1880) 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:41:GLY:O	1:A:94:GLY:HA2	1.32	1.27
1:B:41:GLY:O	1:B:94:GLY:HA2	1.31	1.24
1:B:683:ILE:HD11	1:B:702:PHE:HB2	1.23	1.20
1:B:541:GLU:HA	1:B:544:PHE:CD1	1.79	1.17
1:A:541:GLU:HA	1:A:544:PHE:CD1	1.80	1.16
1:A:485:LEU:HA	1:A:553:LEU:HG	1.26	1.15
1:A:116:ARG:HB2	1:A:158:PRO:HA	1.18	1.15
1:B:116:ARG:HB2	1:B:158:PRO:HA	1.20	1.15
1:B:621:ILE:HG13	1:B:622:PRO:HD3	1.16	1.15
1:A:683:ILE:HD11	1:A:702:PHE:HB2	1.22	1.15
1:A:621:ILE:HG13	1:A:622:PRO:HD3	1.17	1.12
1:A:541:GLU:HA	1:A:544:PHE:HD1	1.02	1.11
1:A:716:VAL:HA	1:A:719:LEU:HD12	1.30	1.10
1:A:485:LEU:HB2	1:A:552:VAL:HA	1.35	1.09
1:B:324:THR:HB	1:B:326:PRO:HD2	1.32	1.09
1:A:324:THR:HB	1:A:326:PRO:HD2	1.33	1.08
1:B:541:GLU:HA	1:B:544:PHE:HD1	1.01	1.08
1:B:485:LEU:HA	1:B:553:LEU:HG	1.28	1.08
1:A:116:ARG:CB	1:A:158:PRO:HA	1.83	1.08
1:B:716:VAL:HA	1:B:719:LEU:HD12	1.31	1.08
1:A:117:ILE:HG13	1:A:159:LEU:HD21	1.34	1.07
1:A:156:GLY:O	1:A:158:PRO:HD3	1.54	1.07
1:B:116:ARG:CB	1:B:158:PRO:HA	1.84	1.07
1:B:117:ILE:HG13	1:B:159:LEU:HD21	1.36	1.06
1:B:485:LEU:HB2	1:B:552:VAL:HA	1.35	1.06
1:B:156:GLY:O	1:B:158:PRO:HD3	1.56	1.03
1:A:118:VAL:HG11	1:A:152:PRO:HB2	1.39	1.01
1:A:182:LEU:O	1:A:226:GLN:HA	1.60	1.00
1:B:182:LEU:O	1:B:226:GLN:HA	1.60	0.99
1:B:118:VAL:HG11	1:B:152:PRO:HB2	1.39	0.99
1:B:664:SER:HA	1:B:667:GLN:HE21	1.28	0.98
1:A:620:SER:HB2	1:A:622:PRO:HD2	1.43	0.98
1:B:347:GLU:HB3	1:B:671:ARG:HH11	1.29	0.98
1:A:630:ILE:HD11	1:A:704:GLY:HA3	1.46	0.98
1:A:377:VAL:HG13	1:A:636:ASN:HB2	1.43	0.98
1:B:377:VAL:HG13	1:B:636:ASN:HB2	1.45	0.97
1:B:620:SER:HB2	1:B:622:PRO:HD2	1.43	0.97
1:B:630:ILE:HD11	1:B:704:GLY:HA3	1.46	0.97
1:A:664:SER:HA	1:A:667:GLN:HE21	1.27	0.96
1:B:621:ILE:HG13	1:B:622:PRO:CD	1.95	0.96
1:B:505:PHE:HD2	1:B:536:ARG:HH21	1.14	0.95
1:B:346:PHE:HA	1:B:349:ILE:HD12	1.47	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:621:ILE:HG13	1:A:622:PRO:CD	1.95	0.95
1:A:117:ILE:O	1:A:157:PRO:HG2	1.68	0.94
1:B:479:GLY:HA2	1:B:558:VAL:HB	1.50	0.94
1:B:45:ILE:HG13	1:B:90:VAL:HB	1.49	0.94
1:A:285:ILE:HG12	1:A:681:LEU:HD12	1.48	0.94
1:A:479:GLY:HA2	1:A:558:VAL:HB	1.50	0.93
1:B:489:PRO:HA	1:B:523:ARG:HB2	1.49	0.93
1:A:45:ILE:HG13	1:A:90:VAL:HB	1.49	0.93
1:B:326:PRO:HG2	1:B:395:PRO:HB2	1.50	0.93
1:A:347:GLU:HB3	1:A:671:ARG:HH11	1.30	0.93
1:A:346:PHE:HA	1:A:349:ILE:HD12	1.51	0.93
1:B:165:LEU:HB2	1:B:183:THR:O	1.68	0.92
1:B:285:ILE:HG12	1:B:681:LEU:HD12	1.49	0.92
1:A:326:PRO:HG2	1:A:395:PRO:HB2	1.49	0.92
1:B:378:ASN:HA	1:B:381:HIS:CD2	2.05	0.92
1:B:117:ILE:O	1:B:157:PRO:HG2	1.68	0.92
1:A:165:LEU:HB2	1:A:183:THR:O	1.69	0.92
1:A:489:PRO:HA	1:A:523:ARG:HB2	1.49	0.92
1:A:505:PHE:HD2	1:A:536:ARG:HH21	1.13	0.91
1:B:118:VAL:HG11	1:B:152:PRO:CB	2.01	0.91
1:B:116:ARG:HH11	1:B:157:PRO:HD2	1.36	0.90
1:A:118:VAL:HG11	1:A:152:PRO:CB	2.01	0.90
1:A:323:LEU:HD11	1:A:328:ILE:N	1.86	0.90
1:B:297:LEU:H	1:B:297:LEU:HD22	1.37	0.90
1:A:378:ASN:HA	1:A:381:HIS:CD2	2.06	0.90
1:B:119:LYS:HB3	1:B:153:GLU:HB2	1.52	0.90
1:B:241:ILE:O	1:B:244:VAL:HG22	1.72	0.90
1:A:116:ARG:NH1	1:A:157:PRO:HD2	1.87	0.89
1:B:657:TYR:O	1:B:660:LEU:HB3	1.71	0.89
1:B:116:ARG:NH1	1:B:157:PRO:HD2	1.86	0.89
1:A:683:ILE:HD11	1:A:702:PHE:CB	2.03	0.89
1:B:323:LEU:HD11	1:B:328:ILE:N	1.86	0.89
1:A:119:LYS:HB3	1:A:153:GLU:HB2	1.53	0.88
1:A:241:ILE:O	1:A:244:VAL:HG22	1.72	0.88
1:B:267:GLY:O	1:B:271:ILE:HG22	1.73	0.88
1:A:288:LEU:HD13	1:A:681:LEU:HD11	1.56	0.88
1:B:173:ASP:HB3	1:B:177:ARG:HB2	1.56	0.88
1:A:204:LEU:O	1:A:215:ALA:HA	1.73	0.88
1:B:68:ASN:HB2	1:B:211:ARG:NH1	1.89	0.87
1:A:267:GLY:O	1:A:271:ILE:HG22	1.74	0.87
1:B:204:LEU:O	1:B:215:ALA:HA	1.73	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:ARG:HH11	1:A:157:PRO:HD2	1.37	0.87
1:A:297:LEU:HD22	1:A:297:LEU:H	1.37	0.87
1:B:683:ILE:HD11	1:B:702:PHE:CB	2.04	0.86
1:B:687:LEU:HD21	1:B:699:LEU:HD12	1.55	0.86
1:A:687:LEU:HD21	1:A:699:LEU:HD12	1.55	0.86
1:B:359:LEU:HD23	1:B:426:ALA:HA	1.58	0.86
1:B:315:LEU:HB3	1:B:405:ILE:HD11	1.58	0.86
1:B:258:GLU:HB2	1:B:557:THR:O	1.75	0.86
1:B:487:ALA:HA	1:B:550:ALA:HB3	1.57	0.85
1:B:288:LEU:HD13	1:B:681:LEU:HD11	1.58	0.85
1:A:359:LEU:HD23	1:A:426:ALA:HA	1.59	0.85
1:A:657:TYR:O	1:A:660:LEU:HB3	1.75	0.85
1:A:487:ALA:HA	1:A:550:ALA:HB3	1.57	0.85
1:A:258:GLU:HB2	1:A:557:THR:O	1.76	0.85
1:A:82:ILE:HG13	1:A:88:ILE:HG23	1.59	0.85
1:A:68:ASN:HB2	1:A:211:ARG:NH1	1.91	0.84
1:B:64:THR:O	1:B:67:GLU:HB3	1.75	0.84
1:A:315:LEU:HB3	1:A:405:ILE:HD11	1.57	0.84
1:A:636:ASN:HA	1:A:639:ILE:HD12	1.59	0.84
1:A:64:THR:O	1:A:67:GLU:HB3	1.77	0.84
1:B:693:VAL:O	1:B:696:ASP:HB2	1.78	0.84
1:A:324:THR:HG21	1:A:395:PRO:HA	1.59	0.84
1:A:116:ARG:HH12	1:A:155:LEU:HA	1.43	0.84
1:B:564:GLU:O	1:B:568:ARG:HG2	1.78	0.84
1:A:173:ASP:HB3	1:A:177:ARG:HB2	1.57	0.84
1:B:62:ALA:HB1	1:B:254:LEU:HD11	1.59	0.84
1:B:636:ASN:HA	1:B:639:ILE:HD12	1.59	0.83
1:A:462:ALA:HB1	1:A:610:GLY:HA3	1.58	0.83
1:A:591:TRP:O	1:A:595:VAL:HG23	1.77	0.83
1:A:564:GLU:O	1:A:568:ARG:HG2	1.78	0.83
1:A:62:ALA:HB1	1:A:254:LEU:HD11	1.61	0.83
1:A:716:VAL:O	1:A:719:LEU:HB2	1.79	0.83
1:A:485:LEU:CB	1:A:552:VAL:HA	2.08	0.83
1:A:608:VAL:HA	1:A:611:MET:HB3	1.61	0.82
1:B:462:ALA:HB1	1:B:610:GLY:HA3	1.59	0.82
1:B:343:VAL:O	1:B:347:GLU:N	2.12	0.82
1:B:82:ILE:HG13	1:B:88:ILE:HG23	1.60	0.82
1:B:324:THR:HG21	1:B:395:PRO:HA	1.59	0.82
1:A:693:VAL:O	1:A:696:ASP:HB2	1.78	0.82
1:A:116:ARG:HB2	1:A:158:PRO:CA	2.06	0.82
1:B:116:ARG:HB2	1:B:158:PRO:CA	2.08	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:THR:O	1:B:455:THR:HG22	1.80	0.82
1:B:591:TRP:O	1:B:595:VAL:HG23	1.79	0.82
1:A:452:THR:O	1:A:455:THR:HG22	1.80	0.82
1:B:372:LEU:O	1:B:375:MET:HB2	1.80	0.82
1:B:608:VAL:HA	1:B:611:MET:HB3	1.61	0.81
1:B:541:GLU:CA	1:B:544:PHE:HD1	1.90	0.81
1:A:513:THR:HG22	1:A:526:LEU:HB3	1.63	0.81
1:B:707:VAL:HA	1:B:710:TYR:CE2	2.16	0.81
1:B:439:ASP:O	1:B:441:ARG:HD3	1.81	0.81
1:B:127:VAL:HA	1:B:130:ILE:HD12	1.61	0.81
1:B:485:LEU:CB	1:B:552:VAL:HA	2.09	0.80
1:B:60:GLU:HB3	1:B:243:LEU:HD11	1.61	0.80
1:A:116:ARG:HA	1:A:159:LEU:HG	1.64	0.80
1:A:117:ILE:HG22	1:A:117:ILE:O	1.81	0.80
1:A:541:GLU:CA	1:A:544:PHE:HD1	1.91	0.80
1:A:707:VAL:HA	1:A:710:TYR:CE2	2.16	0.80
1:A:538:LEU:O	1:A:542:ARG:HG3	1.80	0.80
1:B:117:ILE:O	1:B:117:ILE:HG22	1.82	0.80
1:B:68:ASN:O	1:B:71:ASN:HB2	1.81	0.80
1:A:60:GLU:HB3	1:A:243:LEU:HD11	1.61	0.80
1:B:116:ARG:HH12	1:B:155:LEU:HA	1.45	0.80
1:B:513:THR:HG22	1:B:526:LEU:HB3	1.64	0.80
1:A:375:MET:O	1:A:379:ILE:HG12	1.82	0.79
1:A:658:ALA:O	1:A:661:VAL:HB	1.82	0.79
1:A:68:ASN:O	1:A:71:ASN:HB2	1.81	0.79
1:B:538:LEU:O	1:B:542:ARG:HG3	1.83	0.79
1:A:119:LYS:HB2	1:A:154:ASP:H	1.46	0.79
1:B:716:VAL:O	1:B:719:LEU:HB2	1.81	0.79
1:A:439:ASP:O	1:A:441:ARG:HD3	1.82	0.79
1:B:80:ILE:HG23	1:B:90:VAL:HG22	1.64	0.79
1:B:119:LYS:HB2	1:B:154:ASP:H	1.45	0.79
1:A:680:LEU:HD13	1:A:705:ILE:HD13	1.65	0.79
1:A:442:PHE:HE1	1:A:445:MET:HB2	1.47	0.79
1:A:372:LEU:O	1:A:375:MET:HB2	1.81	0.79
1:B:347:GLU:CG	1:B:671:ARG:HD2	2.13	0.79
1:B:326:PRO:CG	1:B:395:PRO:HB2	2.13	0.79
1:B:45:ILE:HD11	1:B:92:LEU:CD1	2.13	0.79
1:A:258:GLU:HB3	1:A:562:ILE:HD12	1.65	0.79
1:A:45:ILE:HD11	1:A:92:LEU:CD1	2.13	0.78
1:A:343:VAL:O	1:A:347:GLU:N	2.11	0.78
1:B:441:ARG:N	1:B:441:ARG:HE	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:VAL:HA	1:A:130:ILE:HD12	1.65	0.78
1:B:442:PHE:HE1	1:B:445:MET:HB2	1.49	0.78
1:A:101:ASP:HA	1:A:104:LEU:HD12	1.66	0.78
1:A:325:LEU:O	1:A:328:ILE:HG13	1.83	0.78
1:A:347:GLU:CG	1:A:671:ARG:HD2	2.14	0.78
1:B:325:LEU:O	1:B:328:ILE:HG13	1.83	0.77
1:B:375:MET:O	1:B:379:ILE:HG12	1.83	0.77
1:B:116:ARG:HA	1:B:159:LEU:HG	1.66	0.77
1:A:308:THR:HA	1:A:311:LEU:HB2	1.66	0.77
1:B:101:ASP:HA	1:B:104:LEU:HD12	1.67	0.77
1:B:699:LEU:O	1:B:702:PHE:HB3	1.84	0.77
1:A:41:GLY:O	1:A:94:GLY:CA	2.26	0.77
1:B:675:THR:O	1:B:678:THR:HB	1.83	0.77
1:A:649:GLN:HG3	1:A:650:LYS:N	1.99	0.77
1:B:701:ILE:O	1:B:705:ILE:HG22	1.85	0.77
1:B:439:ASP:HB3	1:B:440:PRO:HD3	1.67	0.77
1:A:441:ARG:N	1:A:441:ARG:HE	1.83	0.77
1:B:308:THR:HA	1:B:311:LEU:HB2	1.67	0.77
1:A:117:ILE:CG1	1:A:159:LEU:HD21	2.13	0.77
1:A:326:PRO:CG	1:A:395:PRO:HB2	2.13	0.77
1:B:189:ALA:HB1	1:B:225:GLY:HA2	1.67	0.77
1:B:104:LEU:O	1:B:107:ILE:HG23	1.85	0.77
1:B:489:PRO:HG3	1:B:522:TYR:HA	1.67	0.76
1:A:80:ILE:HG23	1:A:90:VAL:HG22	1.66	0.76
1:B:258:GLU:HB3	1:B:562:ILE:HD12	1.66	0.76
1:B:680:LEU:O	1:B:683:ILE:HG23	1.85	0.76
1:B:16:LEU:HD23	1:B:17:LEU:N	2.01	0.76
1:B:680:LEU:HD13	1:B:705:ILE:HD13	1.66	0.76
1:A:675:THR:O	1:A:678:THR:HB	1.84	0.76
1:A:537:ARG:O	1:A:540:LEU:HB3	1.86	0.76
1:B:437:LEU:H	1:B:437:LEU:HD23	1.51	0.76
1:A:437:LEU:HD23	1:A:437:LEU:H	1.50	0.76
1:A:407:VAL:O	1:A:410:SER:HB3	1.85	0.76
1:A:439:ASP:HB3	1:A:440:PRO:HD3	1.66	0.76
1:A:116:ARG:NH1	1:A:156:GLY:H	1.83	0.75
1:A:412:PHE:O	1:A:416:VAL:HG23	1.86	0.75
1:B:289:ILE:HD11	1:B:298:GLY:HA2	1.67	0.75
1:B:658:ALA:O	1:B:661:VAL:HB	1.84	0.75
1:B:541:GLU:CA	1:B:544:PHE:CD1	2.67	0.75
1:B:119:LYS:CB	1:B:153:GLU:HB2	2.16	0.75
1:B:649:GLN:HG3	1:B:650:LYS:N	2.00	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:699:LEU:O	1:A:702:PHE:HB3	1.86	0.75
1:B:548:LEU:HD23	1:B:550:ALA:H	1.51	0.75
1:B:24:LYS:HD3	1:B:26:TRP:HE1	1.52	0.75
1:B:116:ARG:NH1	1:B:156:GLY:H	1.84	0.75
1:B:165:LEU:HD22	1:B:183:THR:N	2.02	0.75
1:A:489:PRO:HG3	1:A:522:TYR:HA	1.66	0.75
1:A:289:ILE:HD11	1:A:298:GLY:HA2	1.68	0.75
1:A:325:LEU:HB3	1:A:326:PRO:HD3	1.69	0.75
1:A:165:LEU:HD22	1:A:183:THR:N	2.01	0.75
1:B:165:LEU:HB2	1:B:183:THR:C	2.07	0.75
1:B:571:VAL:O	1:B:574:VAL:HB	1.86	0.75
1:A:24:LYS:HD3	1:A:26:TRP:HE1	1.52	0.75
1:B:234:SER:HB3	1:B:237:GLU:HB2	1.67	0.75
1:B:485:LEU:HA	1:B:553:LEU:H	1.52	0.75
1:A:16:LEU:HD23	1:A:17:LEU:N	2.01	0.75
1:A:119:LYS:CB	1:A:153:GLU:HB2	2.17	0.74
1:A:664:SER:HA	1:A:667:GLN:NE2	2.01	0.74
1:B:117:ILE:CG1	1:B:159:LEU:HD21	2.14	0.74
1:A:165:LEU:HD22	1:A:183:THR:H	1.51	0.74
1:A:189:ALA:HB1	1:A:225:GLY:HA2	1.67	0.74
1:B:165:LEU:HD22	1:B:183:THR:H	1.52	0.74
1:B:512:ILE:HG23	1:B:527:VAL:HG22	1.68	0.74
1:A:293:TYR:CE2	1:A:346:PHE:HB3	2.22	0.74
1:A:548:LEU:HD23	1:A:550:ALA:H	1.51	0.74
1:B:41:GLY:O	1:B:94:GLY:CA	2.25	0.74
1:B:407:VAL:O	1:B:410:SER:HB3	1.86	0.74
1:B:441:ARG:HE	1:B:441:ARG:H	1.35	0.74
1:B:412:PHE:O	1:B:416:VAL:HG23	1.87	0.74
1:A:165:LEU:HB2	1:A:183:THR:C	2.07	0.74
1:B:66:LEU:O	1:B:70:ILE:HG22	1.88	0.74
1:B:141:ASN:O	1:B:145:LEU:HG	1.88	0.74
1:B:537:ARG:O	1:B:540:LEU:HB3	1.88	0.74
1:A:701:ILE:O	1:A:705:ILE:HG22	1.87	0.74
1:A:141:ASN:O	1:A:145:LEU:HG	1.86	0.74
1:A:441:ARG:H	1:A:441:ARG:HE	1.36	0.74
1:B:44:ARG:HH11	1:B:260:ARG:HH22	1.36	0.74
1:B:391:TYR:HB2	1:B:573:ALA:HB2	1.70	0.74
1:A:104:LEU:O	1:A:107:ILE:HG23	1.87	0.74
1:A:44:ARG:HH11	1:A:260:ARG:HH22	1.35	0.74
1:A:44:ARG:HH11	1:A:260:ARG:NH2	1.85	0.74
1:A:473:TYR:CD1	1:A:618:GLU:HA	2.23	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:ILE:HG23	1:B:290:PHE:H	1.53	0.73
1:A:493:VAL:HA	1:A:496:LEU:HD12	1.69	0.73
1:B:363:ILE:HD11	1:B:426:ALA:CB	2.17	0.73
1:B:619:PHE:HB2	1:B:623:THR:HG21	1.70	0.73
1:A:680:LEU:O	1:A:683:ILE:HG23	1.86	0.73
1:A:540:LEU:HG	1:A:544:PHE:CE1	2.23	0.73
1:A:571:VAL:O	1:A:574:VAL:HB	1.88	0.73
1:B:116:ARG:HD3	1:B:158:PRO:CA	2.18	0.73
1:A:391:TYR:HB2	1:A:573:ALA:HB2	1.70	0.73
1:B:44:ARG:HH11	1:B:260:ARG:NH2	1.85	0.73
1:B:452:THR:O	1:B:456:LEU:HG	1.88	0.73
1:A:485:LEU:HA	1:A:553:LEU:H	1.53	0.73
1:B:493:VAL:HA	1:B:496:LEU:HD12	1.69	0.73
1:A:116:ARG:HD3	1:A:158:PRO:CA	2.19	0.73
1:B:657:TYR:O	1:B:661:VAL:HG23	1.88	0.73
1:B:473:TYR:CD1	1:B:618:GLU:HA	2.23	0.73
1:B:636:ASN:O	1:B:639:ILE:HB	1.87	0.73
1:A:619:PHE:HB2	1:A:623:THR:HG21	1.69	0.73
1:A:234:SER:HB3	1:A:237:GLU:HB2	1.69	0.73
1:A:657:TYR:O	1:A:661:VAL:HG23	1.88	0.73
1:B:540:LEU:HG	1:B:544:PHE:CE1	2.22	0.73
1:B:116:ARG:NH1	1:B:118:VAL:HG22	2.04	0.73
1:B:590:ASP:HB2	1:B:646:ARG:NH2	2.03	0.73
1:B:55:THR:HG22	1:B:58:ASP:H	1.53	0.73
1:B:664:SER:HA	1:B:667:GLN:NE2	2.01	0.73
1:A:626:ALA:HB2	1:A:697:PHE:CD1	2.24	0.73
1:A:66:LEU:O	1:A:70:ILE:HG22	1.88	0.72
1:A:590:ASP:HB2	1:A:646:ARG:NH2	2.04	0.72
1:B:325:LEU:HB3	1:B:326:PRO:HD3	1.70	0.72
1:A:119:LYS:HB3	1:A:153:GLU:CB	2.19	0.72
1:A:46:VAL:HB	1:A:258:GLU:O	1.89	0.72
1:B:119:LYS:HB3	1:B:153:GLU:CB	2.18	0.72
1:B:659:GLU:HA	1:B:662:ASN:HD22	1.54	0.72
1:B:363:ILE:HD11	1:B:426:ALA:HB2	1.71	0.72
1:B:285:ILE:O	1:B:289:ILE:HG22	1.89	0.72
1:B:293:TYR:CE2	1:B:346:PHE:HB3	2.24	0.72
1:B:402:ILE:O	1:B:405:ILE:HG22	1.90	0.72
1:A:452:THR:O	1:A:456:LEU:HG	1.88	0.72
1:A:512:ILE:HG23	1:A:527:VAL:HG22	1.71	0.72
1:B:687:LEU:HA	1:B:698:ALA:CB	2.20	0.72
1:A:402:ILE:O	1:A:405:ILE:HG22	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:600:ALA:O	1:A:603:HIS:HB3	1.90	0.72
1:A:285:ILE:O	1:A:289:ILE:HG22	1.90	0.71
1:A:135:ARG:HD2	1:A:237:GLU:CD	2.10	0.71
1:A:512:ILE:HA	1:A:526:LEU:O	1.90	0.71
1:B:347:GLU:HG2	1:B:671:ARG:HD2	1.73	0.71
1:B:359:LEU:HD22	1:B:430:GLU:HA	1.72	0.71
1:A:55:THR:HG22	1:A:58:ASP:H	1.54	0.71
1:A:713:ILE:HG12	1:A:714:TYR:N	2.05	0.71
1:B:323:LEU:HD11	1:B:328:ILE:H	1.53	0.71
1:B:681:LEU:HB2	1:B:682:PRO:HD3	1.71	0.71
1:B:135:ARG:HD2	1:B:237:GLU:CD	2.11	0.71
1:A:363:ILE:HD11	1:A:426:ALA:CB	2.19	0.71
1:B:489:PRO:HA	1:B:523:ARG:CB	2.21	0.71
1:B:713:ILE:HG12	1:B:714:TYR:N	2.06	0.71
1:B:626:ALA:HB2	1:B:697:PHE:CD1	2.25	0.71
1:A:636:ASN:O	1:A:639:ILE:HB	1.90	0.71
1:B:45:ILE:HD11	1:B:92:LEU:HD11	1.71	0.71
1:A:323:LEU:HD11	1:A:328:ILE:H	1.54	0.70
1:A:687:LEU:HA	1:A:698:ALA:CB	2.20	0.70
1:B:710:TYR:O	1:B:713:ILE:HG23	1.91	0.70
1:B:388:LEU:HD11	1:B:625:ALA:HA	1.73	0.70
1:A:289:ILE:HG23	1:A:290:PHE:H	1.54	0.70
1:A:503:LYS:C	1:A:505:PHE:H	1.94	0.70
1:A:307:TYR:O	1:A:310:ALA:HB3	1.91	0.70
1:B:11:LEU:HD13	1:B:417:PHE:HD1	1.57	0.70
1:B:27:ALA:HB3	1:B:31:PRO:HG3	1.72	0.70
1:A:117:ILE:HG13	1:A:159:LEU:CD2	2.19	0.70
1:A:681:LEU:HB2	1:A:682:PRO:HD3	1.71	0.70
1:A:629:THR:HG21	1:A:701:ILE:HD12	1.73	0.70
1:B:512:ILE:HA	1:B:526:LEU:O	1.90	0.70
1:A:710:TYR:O	1:A:713:ILE:HG23	1.92	0.70
1:A:181:SER:HA	1:A:227:ALA:O	1.91	0.70
1:B:45:ILE:HG22	1:B:259:ILE:CG2	2.21	0.70
1:B:67:GLU:O	1:B:70:ILE:HG23	1.91	0.70
1:A:659:GLU:HA	1:A:662:ASN:HD22	1.56	0.70
1:B:586:ALA:HB1	1:B:591:TRP:CD1	2.26	0.70
1:A:586:ALA:HB1	1:A:591:TRP:CD1	2.27	0.70
1:B:46:VAL:HB	1:B:258:GLU:O	1.91	0.70
1:A:45:ILE:HG22	1:A:259:ILE:CG2	2.22	0.70
1:B:125:THR:O	1:B:149:LEU:HD12	1.92	0.70
1:A:622:PRO:O	1:A:625:ALA:HB3	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:585:VAL:O	1:B:589:PHE:N	2.23	0.69
1:A:27:ALA:HB3	1:A:31:PRO:HG3	1.72	0.69
1:B:534:ASP:O	1:B:537:ARG:HG3	1.92	0.69
1:A:573:ALA:O	1:A:576:VAL:HB	1.92	0.69
1:A:67:GLU:O	1:A:70:ILE:HG23	1.91	0.69
1:B:252:VAL:HG12	1:B:254:LEU:HD23	1.75	0.69
1:A:11:LEU:HD13	1:A:417:PHE:HD1	1.57	0.69
1:B:477:PHE:HE2	1:B:621:ILE:HG23	1.57	0.69
1:B:622:PRO:O	1:B:625:ALA:HB3	1.91	0.69
1:B:629:THR:HG21	1:B:701:ILE:HD12	1.73	0.69
1:B:629:THR:HG22	1:B:630:ILE:N	2.07	0.69
1:A:347:GLU:HG2	1:A:671:ARG:HD2	1.74	0.69
1:A:388:LEU:HD11	1:A:625:ALA:HA	1.72	0.69
1:A:124:GLY:HA2	1:A:150:ILE:HD11	1.74	0.69
1:B:687:LEU:HD13	1:B:699:LEU:N	2.08	0.69
1:A:489:PRO:HA	1:A:523:ARG:CB	2.21	0.69
1:B:156:GLY:H	1:B:157:PRO:CD	2.05	0.69
1:B:44:ARG:HG3	1:B:91:GLU:HG2	1.74	0.69
1:A:45:ILE:HD11	1:A:92:LEU:HD11	1.72	0.69
1:A:125:THR:HG21	1:A:148:ASP:HB2	1.73	0.69
1:B:328:ILE:O	1:B:331:LEU:HB2	1.93	0.69
1:A:328:ILE:O	1:A:331:LEU:HB2	1.93	0.69
1:A:363:ILE:HD11	1:A:426:ALA:HB2	1.74	0.69
1:A:359:LEU:HA	1:A:362:ALA:HB3	1.75	0.69
1:A:355:ALA:HB3	1:A:357:LYS:HG2	1.74	0.69
1:A:180:VAL:H	1:A:229:ILE:CG2	2.06	0.69
1:B:596:ALA:HB1	1:B:716:VAL:HG13	1.75	0.69
1:B:600:ALA:O	1:B:603:HIS:HB3	1.93	0.69
1:B:305:LEU:O	1:B:308:THR:HG22	1.93	0.69
1:B:36:GLY:HA2	1:B:323:LEU:O	1.93	0.69
1:A:477:PHE:HE2	1:A:621:ILE:HG23	1.57	0.69
1:B:307:TYR:O	1:B:310:ALA:HB3	1.93	0.69
1:B:201:GLY:H	1:B:218:ILE:HB	1.58	0.69
1:B:355:ALA:HB3	1:B:357:LYS:HG2	1.74	0.69
1:B:337:ALA:HA	1:B:340:ASP:OD2	1.93	0.68
1:B:672:THR:O	1:B:675:THR:HG22	1.93	0.68
1:A:687:LEU:HD13	1:A:699:LEU:N	2.08	0.68
1:B:573:ALA:O	1:B:576:VAL:HB	1.93	0.68
1:A:125:THR:O	1:A:149:LEU:HD12	1.93	0.68
1:B:342:ASN:O	1:B:345:SER:OG	2.11	0.68
1:A:337:ALA:HA	1:A:340:ASP:OD2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:TYR:CB	1:A:573:ALA:HB2	2.23	0.68
1:A:683:ILE:O	1:A:686:LEU:HB3	1.94	0.68
1:B:412:PHE:HD2	1:B:413:SER:N	1.91	0.68
1:B:363:ILE:HB	1:B:364:PRO:HD3	1.75	0.68
1:B:345:SER:O	1:B:349:ILE:HG13	1.94	0.68
1:A:116:ARG:NH1	1:A:118:VAL:HG22	2.07	0.68
1:A:359:LEU:HD22	1:A:430:GLU:HA	1.74	0.68
1:A:252:VAL:HG12	1:A:254:LEU:HD23	1.76	0.68
1:A:679:THR:O	1:A:682:PRO:HD2	1.94	0.68
1:B:417:PHE:CZ	1:B:421:LEU:HD11	2.29	0.68
1:A:151:LYS:HG2	1:A:153:GLU:OE2	1.93	0.68
1:A:541:GLU:CA	1:A:544:PHE:CD1	2.68	0.67
1:A:342:ASN:O	1:A:345:SER:OG	2.11	0.67
1:A:672:THR:O	1:A:675:THR:HG22	1.93	0.67
1:B:359:LEU:HB3	1:B:426:ALA:HB1	1.76	0.67
1:A:629:THR:HG22	1:A:630:ILE:N	2.07	0.67
1:A:363:ILE:HB	1:A:364:PRO:HD3	1.75	0.67
1:A:305:LEU:O	1:A:308:THR:HG22	1.93	0.67
1:B:180:VAL:H	1:B:229:ILE:CG2	2.06	0.67
1:B:636:ASN:HA	1:B:639:ILE:CD1	2.24	0.67
1:B:540:LEU:HG	1:B:544:PHE:CZ	2.30	0.67
1:A:596:ALA:HB1	1:A:716:VAL:HG13	1.75	0.67
1:A:201:GLY:H	1:A:218:ILE:HB	1.58	0.67
1:A:345:SER:O	1:A:349:ILE:HG13	1.95	0.67
1:A:608:VAL:CA	1:A:611:MET:HB3	2.24	0.67
1:B:537:ARG:O	1:B:541:GLU:HG3	1.94	0.67
1:B:181:SER:HA	1:B:227:ALA:O	1.94	0.67
1:B:359:LEU:HA	1:B:362:ALA:HB3	1.77	0.67
1:B:462:ALA:O	1:B:465:VAL:HG12	1.94	0.67
1:B:125:THR:HG21	1:B:148:ASP:HB2	1.75	0.67
1:A:156:GLY:H	1:A:157:PRO:CD	2.07	0.67
1:A:36:GLY:HA2	1:A:323:LEU:O	1.95	0.67
1:B:391:TYR:CB	1:B:573:ALA:HB2	2.24	0.67
1:B:683:ILE:O	1:B:686:LEU:HB3	1.95	0.66
1:A:417:PHE:CZ	1:A:421:LEU:HD11	2.30	0.66
1:B:652:LEU:HB3	1:B:654:HIS:CE1	2.29	0.66
1:B:293:TYR:HB3	1:B:297:LEU:HB2	1.76	0.66
1:B:679:THR:O	1:B:682:PRO:HD2	1.96	0.66
1:A:534:ASP:O	1:A:537:ARG:HG3	1.95	0.66
1:A:636:ASN:HA	1:A:639:ILE:CD1	2.24	0.66
1:B:608:VAL:CA	1:B:611:MET:HB3	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:LEU:HG	1:A:544:PHE:CZ	2.30	0.66
1:A:44:ARG:HG3	1:A:91:GLU:HG2	1.76	0.66
1:A:608:VAL:O	1:A:611:MET:HB3	1.95	0.66
1:B:373:THR:HB	1:B:643:ASP:OD2	1.94	0.66
1:A:412:PHE:HD2	1:A:413:SER:N	1.93	0.66
1:A:359:LEU:HB3	1:A:426:ALA:HB1	1.77	0.66
1:A:596:ALA:HA	1:A:719:LEU:HD13	1.76	0.66
1:A:115:PHE:HA	1:A:205:ALA:O	1.95	0.66
1:B:604:ASP:OD1	1:B:708:GLY:HA2	1.96	0.66
1:B:503:LYS:C	1:B:505:PHE:H	1.97	0.66
1:B:49:ALA:HB1	1:B:252:VAL:HG11	1.78	0.66
1:A:537:ARG:O	1:A:541:GLU:HG3	1.96	0.66
1:A:293:TYR:HB3	1:A:297:LEU:HB2	1.78	0.66
1:A:620:SER:O	1:A:623:THR:HB	1.95	0.66
1:B:596:ALA:HA	1:B:719:LEU:HD13	1.76	0.66
1:B:115:PHE:HA	1:B:205:ALA:O	1.96	0.66
1:B:659:GLU:H	1:B:659:GLU:CD	2.00	0.66
1:B:660:LEU:O	1:B:663:ARG:HB2	1.96	0.66
1:A:377:VAL:HA	1:A:639:ILE:HD12	1.78	0.66
1:A:49:ALA:HB1	1:A:252:VAL:HG11	1.79	0.66
1:B:55:THR:O	1:B:58:ASP:HB3	1.96	0.65
1:B:151:LYS:HG2	1:B:153:GLU:OE2	1.95	0.65
1:A:288:LEU:CD1	1:A:681:LEU:HD11	2.25	0.65
1:B:608:VAL:O	1:B:611:MET:HB3	1.95	0.65
1:B:620:SER:O	1:B:623:THR:HB	1.95	0.65
1:B:377:VAL:HA	1:B:639:ILE:HD12	1.79	0.65
1:A:604:ASP:OD1	1:A:708:GLY:HA2	1.96	0.65
1:A:656:PRO:HB2	1:A:659:GLU:OE1	1.97	0.65
1:A:462:ALA:O	1:A:465:VAL:HG12	1.97	0.65
1:B:288:LEU:CD1	1:B:681:LEU:HD11	2.26	0.65
1:B:412:PHE:CD2	1:B:413:SER:N	2.65	0.65
1:A:660:LEU:O	1:A:663:ARG:HB2	1.97	0.65
1:B:117:ILE:HG13	1:B:159:LEU:CD2	2.20	0.65
1:A:185:THR:O	1:A:189:ALA:N	2.30	0.65
1:A:707:VAL:HA	1:A:710:TYR:HE2	1.62	0.65
1:A:124:GLY:H	1:A:150:ILE:HG12	1.60	0.65
1:B:116:ARG:HD3	1:B:158:PRO:HA	1.78	0.65
1:A:283:LEU:O	1:A:286:PHE:HB2	1.97	0.65
1:A:585:VAL:O	1:A:589:PHE:N	2.22	0.64
1:A:173:ASP:HB2	1:A:179:GLN:HG3	1.78	0.64
1:B:19:LEU:O	1:B:22:VAL:HG13	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:THR:HB	1:A:643:ASP:OD2	1.97	0.64
1:A:476:ASP:O	1:A:558:VAL:HG11	1.97	0.64
1:B:283:LEU:O	1:B:286:PHE:HB2	1.97	0.64
1:B:626:ALA:O	1:B:629:THR:HG22	1.98	0.64
1:A:485:LEU:CA	1:A:553:LEU:HG	2.17	0.64
1:A:466:VAL:HA	1:A:613:SER:OG	1.98	0.64
1:A:326:PRO:O	1:A:329:ALA:HB3	1.96	0.64
1:A:45:ILE:HD11	1:A:92:LEU:HD13	1.80	0.64
1:A:412:PHE:CD2	1:A:413:SER:N	2.66	0.64
1:B:55:THR:HB	1:B:58:ASP:HB3	1.79	0.64
1:A:296:HIS:CE1	1:A:431:ILE:HG21	2.33	0.64
1:B:326:PRO:O	1:B:329:ALA:HB3	1.97	0.64
1:A:55:THR:HB	1:A:58:ASP:HB3	1.78	0.64
1:B:607:ILE:O	1:B:611:MET:N	2.28	0.64
1:A:652:LEU:HB3	1:A:654:HIS:CE1	2.32	0.64
1:B:124:GLY:HA2	1:B:150:ILE:HD11	1.78	0.64
1:A:620:SER:CB	1:A:622:PRO:HD2	2.26	0.64
1:A:55:THR:O	1:A:58:ASP:HB3	1.98	0.64
1:A:471:PHE:HD1	1:A:472:ASN:N	1.96	0.64
1:B:347:GLU:HB3	1:B:671:ARG:NH1	2.09	0.63
1:B:477:PHE:N	1:B:477:PHE:CD2	2.65	0.63
1:B:185:THR:O	1:B:189:ALA:N	2.31	0.63
1:A:19:LEU:O	1:A:22:VAL:HG13	1.97	0.63
1:B:119:LYS:HD3	1:B:153:GLU:HB2	1.81	0.63
1:A:456:LEU:O	1:A:459:ALA:HB3	1.98	0.63
1:B:107:ILE:HD13	1:B:108:GLY:N	2.13	0.63
1:B:620:SER:HB2	1:B:622:PRO:CD	2.25	0.63
1:B:656:PRO:HB2	1:B:659:GLU:OE1	1.98	0.63
1:A:173:ASP:CB	1:A:177:ARG:HB2	2.28	0.63
1:B:707:VAL:HA	1:B:710:TYR:HE2	1.61	0.63
1:B:275:ILE:O	1:B:278:ALA:HB3	1.97	0.63
1:A:702:PHE:O	1:A:705:ILE:HG23	1.99	0.63
1:A:107:ILE:HD13	1:A:108:GLY:N	2.13	0.63
1:B:702:PHE:O	1:B:705:ILE:HG23	1.98	0.63
1:A:636:ASN:OD1	1:A:637:ASP:N	2.32	0.63
1:A:353:LEU:HD21	1:A:362:ALA:HB2	1.80	0.63
1:B:17:LEU:O	1:B:20:LEU:HB3	1.99	0.63
1:B:441:ARG:NE	1:B:441:ARG:N	2.47	0.63
1:A:39:LEU:HD21	1:A:325:LEU:HA	1.81	0.63
1:A:370:SER:O	1:A:373:THR:HG22	1.99	0.63
1:B:173:ASP:HB2	1:B:179:GLN:HG3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:ARG:O	1:B:200:ILE:HG12	1.99	0.63
1:B:534:ASP:HA	1:B:537:ARG:HD3	1.81	0.63
1:B:466:VAL:HA	1:B:613:SER:OG	1.99	0.63
1:B:471:PHE:HD1	1:B:472:ASN:N	1.96	0.63
1:A:116:ARG:HD3	1:A:158:PRO:HA	1.79	0.62
1:A:315:LEU:CB	1:A:405:ILE:HD11	2.27	0.62
1:B:486:ARG:HG2	1:B:522:TYR:CD2	2.34	0.62
1:B:173:ASP:CB	1:B:177:ARG:HB2	2.27	0.62
1:B:353:LEU:HD21	1:B:362:ALA:HB2	1.80	0.62
1:B:636:ASN:OD1	1:B:637:ASP:N	2.32	0.62
1:B:476:ASP:O	1:B:558:VAL:HG11	1.99	0.62
1:A:68:ASN:OD1	1:A:69:ARG:N	2.32	0.62
1:B:637:ASP:O	1:B:640:VAL:HG23	1.99	0.62
1:B:296:HIS:CE1	1:B:431:ILE:HG21	2.34	0.62
1:B:45:ILE:HD11	1:B:92:LEU:HD13	1.80	0.62
1:B:260:ARG:HG2	1:B:556:GLU:HB3	1.81	0.62
1:B:323:LEU:HD21	1:B:328:ILE:HG12	1.82	0.62
1:A:170:ALA:HB3	1:A:242:ALA:HB2	1.81	0.62
1:B:63:ARG:HG2	1:B:64:THR:N	2.14	0.62
1:B:68:ASN:OD1	1:B:69:ARG:N	2.32	0.62
1:B:315:LEU:CB	1:B:405:ILE:HD11	2.28	0.62
1:A:477:PHE:N	1:A:477:PHE:CD2	2.65	0.62
1:B:476:ASP:O	1:B:566:LEU:HD12	1.99	0.62
1:A:497:ARG:NH2	1:A:508:LYS:HA	2.15	0.62
1:B:124:GLY:H	1:B:150:ILE:HG12	1.64	0.62
1:A:441:ARG:N	1:A:441:ARG:NE	2.48	0.62
1:B:88:ILE:N	1:B:88:ILE:HD12	2.15	0.62
1:B:193:GLU:O	1:B:196:THR:HG23	1.98	0.62
1:A:275:ILE:O	1:A:278:ALA:HB3	1.99	0.62
1:A:659:GLU:H	1:A:659:GLU:CD	2.03	0.62
1:B:497:ARG:NH2	1:B:508:LYS:HA	2.15	0.62
1:A:63:ARG:HG2	1:A:64:THR:N	2.15	0.62
1:B:595:VAL:O	1:B:598:ILE:HG23	1.99	0.62
1:B:127:VAL:O	1:B:130:ILE:HB	2.00	0.62
1:A:127:VAL:O	1:A:130:ILE:HB	2.00	0.62
1:A:631:VAL:O	1:A:633:TYR:N	2.33	0.61
1:A:473:TYR:CE1	1:A:618:GLU:HB3	2.34	0.61
1:B:456:LEU:O	1:B:459:ALA:HB3	1.99	0.61
1:A:119:LYS:HD3	1:A:153:GLU:HB2	1.81	0.61
1:B:473:TYR:CE1	1:B:618:GLU:HB3	2.35	0.61
1:A:626:ALA:HB2	1:A:697:PHE:CE1	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ASP:O	1:A:61:LYS:HG3	1.99	0.61
1:A:486:ARG:HG2	1:A:522:TYR:CD2	2.36	0.61
1:B:165:LEU:CB	1:B:184:PHE:HA	2.31	0.61
1:B:57:ASP:O	1:B:61:LYS:HG3	2.00	0.61
1:B:97:GLN:HA	1:B:100:GLN:HB3	1.82	0.61
1:A:534:ASP:HA	1:A:537:ARG:HD3	1.81	0.61
1:A:326:PRO:HB2	1:A:399:PHE:HB2	1.83	0.61
1:A:401:VAL:O	1:A:404:ALA:HB3	2.00	0.61
1:A:165:LEU:HD13	1:A:167:ASP:O	2.01	0.61
1:A:17:LEU:O	1:A:20:LEU:HB3	2.01	0.61
1:A:582:LEU:HD11	1:A:598:ILE:HD12	1.83	0.61
1:A:595:VAL:O	1:A:598:ILE:HG23	2.01	0.61
1:A:11:LEU:HD13	1:A:417:PHE:CD1	2.35	0.61
1:B:11:LEU:HD13	1:B:417:PHE:CD1	2.35	0.61
1:A:197:ARG:O	1:A:200:ILE:HG12	2.01	0.61
1:B:170:ALA:HB3	1:B:242:ALA:HB2	1.83	0.61
1:A:165:LEU:CB	1:A:184:PHE:HA	2.30	0.61
1:B:359:LEU:CD2	1:B:430:GLU:HA	2.31	0.61
1:B:575:LEU:O	1:B:578:LEU:HB2	2.01	0.61
1:B:96:SER:HB2	1:B:99:ASP:HB2	1.83	0.61
1:A:30:GLU:HG3	1:A:31:PRO:HD3	1.83	0.61
1:B:30:GLU:HG3	1:B:31:PRO:HD3	1.83	0.61
1:B:687:LEU:HA	1:B:698:ALA:HB1	1.82	0.60
1:B:626:ALA:HB2	1:B:697:PHE:CE1	2.36	0.60
1:A:236:GLU:O	1:A:239:SER:HB2	2.01	0.60
1:A:593:PHE:CE2	1:A:642:SER:HB3	2.35	0.60
1:A:193:GLU:O	1:A:196:THR:HG23	2.01	0.60
1:B:193:GLU:HG3	1:B:223:THR:HB	1.83	0.60
1:B:39:LEU:HD21	1:B:325:LEU:HA	1.82	0.60
1:A:514:GLN:HG2	1:A:525:PHE:CE2	2.37	0.60
1:B:268:GLN:O	1:B:271:ILE:HG23	2.02	0.60
1:A:42:GLY:O	1:A:261:ALA:HA	2.01	0.60
1:B:42:GLY:O	1:B:261:ALA:HA	2.01	0.60
1:B:293:TYR:O	1:B:297:LEU:HD23	2.01	0.60
1:A:88:ILE:N	1:A:88:ILE:HD12	2.15	0.60
1:A:620:SER:HB2	1:A:622:PRO:CD	2.25	0.60
1:B:514:GLN:HG2	1:B:525:PHE:CE2	2.37	0.60
1:A:503:LYS:C	1:A:505:PHE:N	2.55	0.60
1:A:423:GLU:O	1:A:426:ALA:HB3	2.01	0.60
1:A:193:GLU:HG3	1:A:223:THR:HB	1.84	0.60
1:B:39:LEU:HD21	1:B:325:LEU:CA	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:LEU:HD12	1:A:164:ASP:OD2	2.01	0.60
1:B:160:LEU:HD12	1:B:164:ASP:OD2	2.01	0.60
1:B:593:PHE:CE2	1:B:642:SER:HB3	2.37	0.60
1:B:236:GLU:O	1:B:239:SER:HB2	2.01	0.60
1:A:483:TYR:OH	1:A:537:ARG:HB3	2.01	0.60
1:A:485:LEU:HA	1:A:553:LEU:CG	2.18	0.60
1:A:293:TYR:O	1:A:297:LEU:HD23	2.02	0.60
1:A:391:TYR:CE2	1:A:572:MET:HG2	2.37	0.60
1:A:687:LEU:HA	1:A:698:ALA:HB1	1.83	0.60
1:B:82:ILE:HA	1:B:88:ILE:HA	1.84	0.60
1:B:326:PRO:HB2	1:B:399:PHE:HB2	1.82	0.60
1:B:119:LYS:HB2	1:B:154:ASP:N	2.17	0.60
1:A:323:LEU:HD21	1:A:328:ILE:HG12	1.83	0.60
1:A:575:LEU:O	1:A:578:LEU:HB2	2.00	0.60
1:A:241:ILE:HA	1:A:244:VAL:HG13	1.83	0.60
1:A:268:GLN:O	1:A:271:ILE:HG23	2.02	0.60
1:A:96:SER:HB2	1:A:99:ASP:HB2	1.84	0.60
1:B:420:HIS:CD2	1:B:421:LEU:HD23	2.37	0.60
1:B:370:SER:O	1:B:373:THR:HG22	2.01	0.60
1:B:675:THR:HG23	1:B:676:SER:H	1.65	0.60
1:A:260:ARG:HG2	1:A:556:GLU:HB3	1.81	0.60
1:B:374:ILE:O	1:B:375:MET:C	2.40	0.59
1:A:473:TYR:CD1	1:A:618:GLU:CA	2.85	0.59
1:B:377:VAL:O	1:B:380:ALA:HB3	2.02	0.59
1:A:279:LEU:O	1:A:282:THR:HB	2.03	0.59
1:B:241:ILE:HA	1:B:244:VAL:HG13	1.82	0.59
1:B:500:LEU:HB2	1:B:507:GLY:HA3	1.84	0.59
1:B:126:THR:O	1:B:130:ILE:HG13	2.02	0.59
1:B:652:LEU:HB3	1:B:654:HIS:HE1	1.67	0.59
1:B:631:VAL:O	1:B:633:TYR:N	2.35	0.59
1:A:476:ASP:O	1:A:566:LEU:HD12	2.02	0.59
1:B:483:TYR:OH	1:B:537:ARG:HB3	2.02	0.59
1:A:39:LEU:HD21	1:A:325:LEU:CA	2.32	0.59
1:B:601:VAL:O	1:B:602:ALA:C	2.41	0.59
1:B:97:GLN:O	1:B:100:GLN:HG2	2.02	0.59
1:A:626:ALA:O	1:A:629:THR:HG22	2.01	0.59
1:B:423:GLU:O	1:B:426:ALA:HB3	2.02	0.59
1:A:607:ILE:O	1:A:611:MET:N	2.28	0.59
1:A:97:GLN:O	1:A:100:GLN:HG2	2.02	0.59
1:A:619:PHE:HB2	1:A:623:THR:CG2	2.33	0.59
1:A:675:THR:HG23	1:A:676:SER:N	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:GLN:CG	1:A:101:ASP:N	2.65	0.59
1:B:629:THR:CG2	1:B:630:ILE:N	2.65	0.59
1:A:497:ARG:HA	1:A:500:LEU:HD12	1.84	0.59
1:B:35:LEU:O	1:B:323:LEU:N	2.35	0.59
1:B:675:THR:HG23	1:B:676:SER:N	2.17	0.59
1:B:391:TYR:CE2	1:B:572:MET:HG2	2.37	0.59
1:B:582:LEU:HD11	1:B:598:ILE:HD12	1.84	0.59
1:B:401:VAL:O	1:B:404:ALA:HB3	2.02	0.59
1:A:374:ILE:O	1:A:375:MET:C	2.40	0.59
1:A:637:ASP:O	1:A:640:VAL:HG23	2.02	0.59
1:B:562:ILE:O	1:B:566:LEU:HG	2.03	0.59
1:A:35:LEU:O	1:A:323:LEU:N	2.35	0.58
1:A:675:THR:HG23	1:A:676:SER:H	1.68	0.58
1:A:97:GLN:HA	1:A:100:GLN:HB3	1.83	0.58
1:B:193:GLU:HA	1:B:196:THR:CG2	2.33	0.58
1:A:601:VAL:O	1:A:602:ALA:C	2.41	0.58
1:B:423:GLU:OE1	1:B:426:ALA:HB3	2.03	0.58
1:B:100:GLN:CG	1:B:101:ASP:N	2.66	0.58
1:A:609:ALA:O	1:A:612:TYR:HB2	2.03	0.58
1:A:702:PHE:O	1:A:705:ILE:CG2	2.51	0.58
1:A:258:GLU:OE2	1:A:562:ILE:HG21	2.03	0.58
1:A:500:LEU:HB2	1:A:507:GLY:HA3	1.85	0.58
1:A:359:LEU:CD2	1:A:430:GLU:HA	2.33	0.58
1:B:621:ILE:CG1	1:B:622:PRO:HD3	2.11	0.58
1:A:126:THR:O	1:A:130:ILE:HG13	2.03	0.58
1:A:119:LYS:HB2	1:A:154:ASP:N	2.18	0.58
1:A:629:THR:CG2	1:A:630:ILE:N	2.66	0.58
1:A:88:ILE:H	1:A:88:ILE:HD12	1.68	0.58
1:A:672:THR:O	1:A:675:THR:CG2	2.51	0.58
1:B:499:PHE:O	1:B:503:LYS:HG2	2.03	0.58
1:B:526:LEU:HD13	1:B:618:GLU:OE1	2.04	0.58
1:B:258:GLU:OE2	1:B:562:ILE:HG21	2.02	0.58
1:A:669:LEU:HD23	1:A:670:SER:N	2.18	0.58
1:B:619:PHE:CD1	1:B:619:PHE:O	2.56	0.58
1:B:492:GLU:O	1:B:496:LEU:HG	2.03	0.58
1:A:562:ILE:O	1:A:566:LEU:HG	2.04	0.58
1:A:526:LEU:HD13	1:A:618:GLU:OE1	2.04	0.58
1:B:638:SER:O	1:B:641:VAL:HG23	2.04	0.58
1:A:619:PHE:CD1	1:A:619:PHE:O	2.57	0.58
1:A:82:ILE:HA	1:A:88:ILE:HA	1.85	0.58
1:B:619:PHE:HB2	1:B:623:THR:CG2	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:LEU:HD23	1:A:549:LYS:N	2.19	0.58
1:B:117:ILE:O	1:B:117:ILE:CG2	2.52	0.58
1:B:473:TYR:CD1	1:B:618:GLU:CA	2.86	0.58
1:B:327:GLY:O	1:B:402:ILE:HD12	2.04	0.58
1:B:622:PRO:O	1:B:623:THR:C	2.42	0.58
1:B:702:PHE:O	1:B:705:ILE:CG2	2.51	0.58
1:B:559:GLY:H	1:B:562:ILE:HD12	1.69	0.58
1:A:193:GLU:HA	1:A:196:THR:CG2	2.34	0.58
1:B:286:PHE:O	1:B:289:ILE:HG23	2.03	0.57
1:A:347:GLU:HB3	1:A:671:ARG:NH1	2.10	0.57
1:A:492:GLU:O	1:A:496:LEU:HG	2.03	0.57
1:B:289:ILE:CD1	1:B:298:GLY:HA2	2.34	0.57
1:B:382:LEU:O	1:B:385:ALA:HB3	2.03	0.57
1:B:620:SER:CB	1:B:622:PRO:HD2	2.25	0.57
1:B:606:ALA:O	1:B:609:ALA:HB3	2.04	0.57
1:B:222:ILE:HG21	1:B:227:ALA:HA	1.86	0.57
1:B:621:ILE:CG1	1:B:622:PRO:CD	2.79	0.57
1:B:672:THR:O	1:B:675:THR:CG2	2.52	0.57
1:B:477:PHE:CE2	1:B:621:ILE:HG23	2.39	0.57
1:A:382:LEU:O	1:A:385:ALA:HB3	2.04	0.57
1:A:420:HIS:CD2	1:A:421:LEU:HD23	2.40	0.57
1:B:279:LEU:O	1:B:282:THR:HB	2.04	0.57
1:A:453:ALA:O	1:A:457:LEU:HG	2.05	0.57
1:B:659:GLU:O	1:B:662:ASN:ND2	2.38	0.57
1:B:497:ARG:HA	1:B:500:LEU:HD12	1.85	0.57
1:A:559:GLY:H	1:A:562:ILE:HD12	1.68	0.57
1:B:116:ARG:HH22	1:B:155:LEU:CB	2.17	0.57
1:A:606:ALA:O	1:A:609:ALA:HB3	2.04	0.57
1:A:608:VAL:HA	1:A:611:MET:CB	2.33	0.57
1:A:38:ASP:HB2	1:A:325:LEU:HB2	1.87	0.57
1:A:377:VAL:O	1:A:380:ALA:HB3	2.04	0.57
1:B:488:GLU:HB3	1:B:491:VAL:HG23	1.87	0.57
1:B:88:ILE:H	1:B:88:ILE:HD12	1.68	0.57
1:B:165:LEU:HB3	1:B:184:PHE:HA	1.86	0.57
1:B:601:VAL:O	1:B:604:ASP:N	2.38	0.57
1:B:33:VAL:O	1:B:33:VAL:HG13	2.05	0.57
1:A:289:ILE:CD1	1:A:298:GLY:HA2	2.35	0.56
1:A:619:PHE:HB2	1:A:623:THR:OG1	2.05	0.56
1:B:473:TYR:CG	1:B:618:GLU:HA	2.40	0.56
1:A:499:PHE:O	1:A:503:LYS:HG2	2.04	0.56
1:B:669:LEU:HD23	1:B:670:SER:N	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:ARG:NH1	1:B:155:LEU:HA	2.19	0.56
1:A:659:GLU:O	1:A:662:ASN:ND2	2.37	0.56
1:B:619:PHE:HB2	1:B:623:THR:OG1	2.05	0.56
1:B:548:LEU:HD23	1:B:549:LYS:N	2.20	0.56
1:A:343:VAL:HG13	1:A:344:LEU:H	1.70	0.56
1:A:601:VAL:O	1:A:604:ASP:N	2.39	0.56
1:A:286:PHE:O	1:A:289:ILE:HG23	2.05	0.56
1:B:165:LEU:HD13	1:B:167:ASP:O	2.06	0.56
1:B:82:ILE:HG23	1:B:87:ARG:O	2.05	0.56
1:B:609:ALA:O	1:B:612:TYR:HB2	2.05	0.56
1:B:38:ASP:HB2	1:B:325:LEU:HB2	1.87	0.56
1:B:630:ILE:CD1	1:B:704:GLY:HA3	2.30	0.56
1:B:116:ARG:CZ	1:B:118:VAL:HG22	2.35	0.56
1:A:541:GLU:HA	1:A:544:PHE:CE1	2.37	0.56
1:A:381:HIS:O	1:A:384:ALA:HB3	2.05	0.56
1:A:165:LEU:HB3	1:A:184:PHE:HA	1.87	0.56
1:B:373:THR:HA	1:B:376:ASP:OD2	2.06	0.56
1:B:156:GLY:N	1:B:157:PRO:CD	2.68	0.56
1:A:222:ILE:HG21	1:A:227:ALA:HA	1.88	0.56
1:B:331:LEU:O	1:B:335:LEU:HG	2.05	0.56
1:A:638:SER:O	1:A:641:VAL:HG23	2.05	0.56
1:A:347:GLU:CB	1:A:671:ARG:HD2	2.36	0.56
1:A:473:TYR:CG	1:A:618:GLU:HA	2.40	0.56
1:B:113:LEU:HD23	1:B:114:GLU:N	2.20	0.56
1:B:375:MET:HA	1:B:375:MET:CE	2.34	0.56
1:A:117:ILE:CG2	1:A:117:ILE:O	2.52	0.56
1:A:327:GLY:O	1:A:402:ILE:HD12	2.05	0.56
1:B:213:TYR:CE2	1:B:244:VAL:HG11	2.41	0.56
1:B:297:LEU:H	1:B:297:LEU:CD2	2.13	0.56
1:B:347:GLU:CB	1:B:671:ARG:HD2	2.36	0.56
1:B:639:ILE:O	1:B:640:VAL:C	2.44	0.56
1:B:503:LYS:C	1:B:505:PHE:N	2.57	0.56
1:A:45:ILE:HG22	1:A:259:ILE:HG21	1.88	0.56
1:B:417:PHE:CE2	1:B:421:LEU:HD11	2.41	0.56
1:A:639:ILE:O	1:A:640:VAL:C	2.44	0.55
1:A:182:LEU:HD21	1:A:245:LEU:HD13	1.88	0.55
1:A:652:LEU:HB3	1:A:654:HIS:HE1	1.71	0.55
1:B:621:ILE:O	1:B:624:ILE:HB	2.07	0.55
1:A:621:ILE:CG1	1:A:622:PRO:CD	2.79	0.55
1:A:621:ILE:CG1	1:A:622:PRO:HD3	2.12	0.55
1:A:46:VAL:HG21	1:A:258:GLU:HG2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:GLU:HG2	1:B:671:ARG:CD	2.37	0.55
1:B:515:VAL:HG12	1:B:692:SER:HA	1.89	0.55
1:A:213:TYR:CE2	1:A:244:VAL:HG11	2.41	0.55
1:A:423:GLU:OE1	1:A:426:ALA:HB3	2.06	0.55
1:B:341:GLY:O	1:B:344:LEU:HB2	2.07	0.55
1:A:375:MET:CE	1:A:375:MET:HA	2.36	0.55
1:A:602:ALA:O	1:A:605:VAL:HB	2.07	0.55
1:A:113:LEU:HD23	1:A:114:GLU:N	2.21	0.55
1:B:501:GLU:C	1:B:503:LYS:H	2.09	0.55
1:A:488:GLU:HB3	1:A:491:VAL:HG23	1.88	0.55
1:B:707:VAL:HA	1:B:710:TYR:CD2	2.41	0.55
1:B:326:PRO:HG2	1:B:395:PRO:CB	2.32	0.55
1:B:668:THR:O	1:B:671:ARG:HG3	2.07	0.55
1:B:680:LEU:HD12	1:B:683:ILE:HD13	1.89	0.55
1:B:116:ARG:HH22	1:B:155:LEU:CA	2.20	0.55
1:B:453:ALA:O	1:B:457:LEU:HG	2.06	0.55
1:B:608:VAL:HA	1:B:611:MET:CB	2.33	0.55
1:B:633:TYR:O	1:B:634:SER:C	2.45	0.55
1:A:116:ARG:CZ	1:A:118:VAL:HG22	2.37	0.55
1:A:156:GLY:N	1:A:157:PRO:CD	2.69	0.55
1:A:457:LEU:O	1:A:460:ALA:HB3	2.07	0.55
1:B:414:ASN:HD22	1:B:414:ASN:N	2.03	0.55
1:A:501:GLU:C	1:A:503:LYS:H	2.09	0.55
1:A:590:ASP:HB2	1:A:646:ARG:HH22	1.72	0.55
1:A:668:THR:O	1:A:671:ARG:HG3	2.07	0.55
1:B:43:LEU:HD22	1:B:45:ILE:HG23	1.89	0.55
1:B:324:THR:O	1:B:325:LEU:C	2.45	0.55
1:A:621:ILE:O	1:A:624:ILE:HB	2.06	0.55
1:B:46:VAL:HG21	1:B:258:GLU:HG2	1.89	0.55
1:A:43:LEU:HD22	1:A:45:ILE:HG23	1.87	0.55
1:A:304:GLY:O	1:A:307:TYR:HB3	2.07	0.55
1:B:343:VAL:HG13	1:B:344:LEU:H	1.71	0.55
1:A:37:LEU:C	1:A:39:LEU:H	2.10	0.55
1:A:477:PHE:CE2	1:A:621:ILE:HG23	2.40	0.55
1:B:45:ILE:HG22	1:B:259:ILE:HG21	1.88	0.55
1:B:602:ALA:O	1:B:605:VAL:HB	2.07	0.54
1:B:420:HIS:HD2	1:B:421:LEU:HD23	1.72	0.54
1:B:30:GLU:CG	1:B:31:PRO:HD3	2.37	0.54
1:A:324:THR:O	1:A:325:LEU:C	2.44	0.54
1:A:526:LEU:O	1:A:526:LEU:HD23	2.07	0.54
1:A:82:ILE:HG23	1:A:87:ARG:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:VAL:O	1:A:33:VAL:HG13	2.06	0.54
1:A:116:ARG:HH22	1:A:155:LEU:CB	2.19	0.54
1:B:182:LEU:HD21	1:B:245:LEU:HD13	1.89	0.54
1:A:504:GLY:HA3	1:B:431:ILE:HG23	1.90	0.54
1:A:323:LEU:HD11	1:A:328:ILE:HG12	1.90	0.54
1:A:454:ALA:O	1:A:457:LEU:HB2	2.07	0.54
1:B:373:THR:O	1:B:376:ASP:HB2	2.07	0.54
1:A:116:ARG:NH1	1:A:155:LEU:HA	2.18	0.54
1:A:622:PRO:O	1:A:623:THR:C	2.45	0.54
1:B:171:VAL:O	1:B:179:GLN:O	2.25	0.54
1:A:30:GLU:CG	1:A:31:PRO:HD3	2.37	0.54
1:A:414:ASN:HD22	1:A:414:ASN:N	2.03	0.54
1:A:515:VAL:HG12	1:A:692:SER:HA	1.89	0.54
1:A:373:THR:O	1:A:376:ASP:HB2	2.07	0.54
1:B:500:LEU:HB2	1:B:507:GLY:CA	2.38	0.54
1:A:567:ARG:HG2	1:A:568:ARG:N	2.22	0.54
1:B:173:ASP:N	1:B:177:ARG:O	2.40	0.54
1:B:454:ALA:O	1:B:457:LEU:HB2	2.08	0.54
1:B:239:SER:O	1:B:242:ALA:HB3	2.08	0.54
1:A:116:ARG:HB3	1:A:158:PRO:HA	1.82	0.54
1:B:118:VAL:HG13	1:B:154:ASP:O	2.07	0.54
1:B:118:VAL:CG1	1:B:152:PRO:HB2	2.26	0.54
1:A:702:PHE:CD2	1:A:702:PHE:C	2.80	0.54
1:A:707:VAL:HA	1:A:710:TYR:CD2	2.42	0.54
1:A:305:LEU:HA	1:A:308:THR:HG22	1.89	0.54
1:B:590:ASP:HB3	1:B:593:PHE:H	1.73	0.54
1:A:124:GLY:N	1:A:150:ILE:HG12	2.21	0.54
1:B:281:GLY:HA3	1:B:682:PRO:HA	1.90	0.54
1:A:483:TYR:CZ	1:A:540:LEU:HD23	2.43	0.54
1:B:37:LEU:C	1:B:39:LEU:H	2.11	0.54
1:B:483:TYR:CZ	1:B:540:LEU:HD23	2.43	0.54
1:A:341:GLY:O	1:A:344:LEU:HB2	2.08	0.54
1:A:373:THR:HA	1:A:376:ASP:OD2	2.06	0.54
1:A:628:LEU:O	1:A:629:THR:C	2.46	0.54
1:A:633:TYR:O	1:A:634:SER:C	2.44	0.54
1:B:229:ILE:HG12	1:B:230:GLU:H	1.71	0.54
1:B:289:ILE:HG23	1:B:290:PHE:N	2.22	0.54
1:A:382:LEU:HD21	1:A:407:VAL:HG11	1.90	0.54
1:A:171:VAL:O	1:A:179:GLN:O	2.25	0.54
1:A:417:PHE:CE2	1:A:421:LEU:HD11	2.42	0.54
1:B:635:ILE:O	1:B:638:SER:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:LEU:HB2	1:A:507:GLY:CA	2.38	0.53
1:B:635:ILE:HG22	1:B:636:ASN:N	2.22	0.53
1:B:465:VAL:HG22	1:B:613:SER:HB3	1.89	0.53
1:A:590:ASP:HB3	1:A:593:PHE:H	1.73	0.53
1:B:11:LEU:HD11	1:B:417:PHE:HA	1.90	0.53
1:B:305:LEU:HA	1:B:308:THR:HG22	1.89	0.53
1:A:116:ARG:HH22	1:A:155:LEU:CA	2.21	0.53
1:A:625:ALA:O	1:A:629:THR:N	2.23	0.53
1:A:45:ILE:HA	1:A:259:ILE:HG22	1.90	0.53
1:B:124:GLY:N	1:B:150:ILE:HG12	2.23	0.53
1:A:151:LYS:H	1:A:151:LYS:HD2	1.73	0.53
1:A:331:LEU:O	1:A:335:LEU:HG	2.08	0.53
1:B:45:ILE:HG12	1:B:90:VAL:O	2.09	0.53
1:A:139:ARG:O	1:A:140:LEU:HG	2.08	0.53
1:A:239:SER:O	1:A:242:ALA:HB3	2.08	0.53
1:A:243:LEU:O	1:A:245:LEU:N	2.41	0.53
1:B:304:GLY:O	1:B:307:TYR:HB3	2.08	0.53
1:A:326:PRO:HG2	1:A:395:PRO:CB	2.33	0.53
1:A:572:MET:O	1:A:573:ALA:C	2.47	0.53
1:A:631:VAL:C	1:A:633:TYR:H	2.11	0.53
1:A:640:VAL:CG1	1:A:668:THR:HG23	2.38	0.53
1:A:347:GLU:HG2	1:A:671:ARG:CD	2.38	0.53
1:B:457:LEU:O	1:B:460:ALA:HB3	2.08	0.53
1:B:145:LEU:HA	1:B:148:ASP:OD2	2.08	0.53
1:A:11:LEU:HD11	1:A:417:PHE:HA	1.90	0.53
1:B:702:PHE:C	1:B:702:PHE:CD2	2.82	0.53
1:B:541:GLU:HA	1:B:544:PHE:CE1	2.38	0.53
1:B:544:PHE:O	1:B:548:LEU:N	2.42	0.53
1:A:635:ILE:HG22	1:A:636:ASN:N	2.24	0.53
1:A:367:PHE:N	1:A:419:ARG:NH2	2.56	0.53
1:B:82:ILE:HG13	1:B:88:ILE:CG2	2.37	0.53
1:B:347:GLU:HB3	1:B:671:ARG:HD2	1.90	0.53
1:A:405:ILE:HG23	1:A:406:GLY:N	2.24	0.53
1:B:659:GLU:CA	1:B:662:ASN:HD22	2.20	0.53
1:A:82:ILE:HG13	1:A:88:ILE:CG2	2.36	0.53
1:A:71:ASN:CB	1:A:211:ARG:NH2	2.72	0.53
1:A:465:VAL:HG22	1:A:613:SER:HB3	1.91	0.53
1:B:381:HIS:O	1:B:384:ALA:HB3	2.08	0.53
1:A:35:LEU:O	1:A:322:THR:HA	2.09	0.53
1:A:170:ALA:CB	1:A:242:ALA:HB2	2.38	0.53
1:B:71:ASN:HB3	1:B:211:ARG:HH21	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:ARG:HB3	1:B:158:PRO:HA	1.81	0.53
1:A:289:ILE:O	1:A:292:TYR:N	2.40	0.53
1:A:347:GLU:HB3	1:A:671:ARG:HD2	1.90	0.53
1:A:61:LYS:HA	1:A:243:LEU:HD21	1.91	0.53
1:B:476:ASP:O	1:B:563:GLY:HA2	2.09	0.53
1:B:608:VAL:C	1:B:611:MET:HB3	2.30	0.53
1:B:170:ALA:CB	1:B:242:ALA:HB2	2.39	0.53
1:B:293:TYR:HB3	1:B:297:LEU:CB	2.40	0.52
1:B:631:VAL:C	1:B:633:TYR:H	2.12	0.52
1:A:544:PHE:O	1:A:548:LEU:N	2.42	0.52
1:B:119:LYS:HD2	1:B:154:ASP:HB2	1.91	0.52
1:B:473:TYR:OH	1:B:513:THR:HB	2.09	0.52
1:B:196:THR:O	1:B:200:ILE:N	2.42	0.52
1:B:54:PRO:HG3	1:B:86:LYS:HE2	1.90	0.52
1:B:323:LEU:HD11	1:B:328:ILE:HG12	1.90	0.52
1:B:405:ILE:HG23	1:B:406:GLY:N	2.24	0.52
1:B:151:LYS:HD2	1:B:151:LYS:H	1.72	0.52
1:A:297:LEU:H	1:A:297:LEU:CD2	2.14	0.52
1:B:45:ILE:HA	1:B:259:ILE:HG22	1.91	0.52
1:A:71:ASN:HB3	1:A:211:ARG:HH21	1.72	0.52
1:B:471:PHE:HB3	1:B:613:SER:OG	2.08	0.52
1:A:4:LYS:HG3	1:A:5:ASN:H	1.75	0.52
1:A:232:LEU:HD12	1:A:233:SER:N	2.24	0.52
1:B:408:VAL:O	1:B:409:ALA:C	2.47	0.52
1:B:412:PHE:C	1:B:412:PHE:CD2	2.83	0.52
1:B:628:LEU:O	1:B:629:THR:C	2.47	0.52
1:B:629:THR:CG2	1:B:701:ILE:HD12	2.39	0.52
1:A:534:ASP:CG	1:A:535:GLU:N	2.63	0.52
1:B:243:LEU:O	1:B:245:LEU:N	2.42	0.52
1:B:630:ILE:HG22	1:B:631:VAL:N	2.25	0.52
1:A:116:ARG:NH1	1:A:156:GLY:N	2.56	0.52
1:A:635:ILE:O	1:A:638:SER:HB2	2.10	0.52
1:A:437:LEU:O	1:A:440:PRO:HD2	2.09	0.52
1:B:71:ASN:CB	1:B:211:ARG:NH2	2.72	0.52
1:A:608:VAL:C	1:A:611:MET:HB3	2.30	0.52
1:B:572:MET:O	1:B:573:ALA:C	2.48	0.52
1:B:675:THR:O	1:B:679:THR:OG1	2.28	0.52
1:A:412:PHE:C	1:A:412:PHE:CD2	2.83	0.52
1:A:575:LEU:HA	1:A:578:LEU:HD12	1.91	0.52
1:B:575:LEU:HA	1:B:578:LEU:HD12	1.91	0.52
1:A:145:LEU:HA	1:A:148:ASP:OD2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:ASP:CG	1:A:535:GLU:H	2.12	0.52
1:A:118:VAL:HG13	1:A:154:ASP:O	2.10	0.52
1:B:567:ARG:HG2	1:B:568:ARG:N	2.24	0.52
1:B:534:ASP:CG	1:B:535:GLU:H	2.13	0.52
1:A:583:LEU:HD23	1:A:584:TYR:N	2.25	0.52
1:A:675:THR:O	1:A:679:THR:OG1	2.28	0.52
1:B:437:LEU:O	1:B:440:PRO:HD2	2.10	0.52
1:A:473:TYR:OH	1:A:513:THR:HB	2.09	0.52
1:B:466:VAL:HG12	1:B:467:PHE:N	2.25	0.52
1:A:124:GLY:CA	1:A:150:ILE:HD11	2.40	0.52
1:B:197:ARG:HA	1:B:200:ILE:HG23	1.92	0.52
1:B:299:LEU:HD22	1:B:303:LEU:HD11	1.91	0.52
1:B:35:LEU:O	1:B:322:THR:HA	2.09	0.52
1:A:281:GLY:HA3	1:A:682:PRO:HA	1.91	0.52
1:A:237:GLU:HA	1:A:240:GLU:HB3	1.92	0.52
1:B:597:SER:O	1:B:600:ALA:HB3	2.09	0.52
1:A:229:ILE:HG12	1:A:230:GLU:H	1.74	0.52
1:A:196:THR:O	1:A:200:ILE:N	2.42	0.52
1:B:4:LYS:HG3	1:B:5:ASN:H	1.74	0.52
1:A:118:VAL:CG1	1:A:152:PRO:HB2	2.26	0.52
1:A:119:LYS:HD2	1:A:154:ASP:HB2	1.92	0.52
1:A:408:VAL:O	1:A:409:ALA:C	2.48	0.52
1:A:705:ILE:O	1:A:706:PHE:C	2.48	0.52
1:B:63:ARG:CG	1:B:64:THR:N	2.73	0.52
1:B:68:ASN:HD21	1:B:209:ASP:HB2	1.75	0.52
1:A:63:ARG:CG	1:A:64:THR:N	2.73	0.52
1:B:481:THR:O	1:B:529:LEU:N	2.35	0.52
1:A:54:PRO:HG3	1:A:86:LYS:HE2	1.91	0.52
1:B:38:ASP:OD1	1:B:324:THR:HG22	2.10	0.52
1:B:640:VAL:CG1	1:B:668:THR:HG23	2.40	0.52
1:B:526:LEU:HD23	1:B:526:LEU:O	2.09	0.52
1:B:655:LEU:HD23	1:B:655:LEU:N	2.24	0.52
1:B:336:GLY:HA3	1:B:679:THR:HA	1.93	0.51
1:A:156:GLY:C	1:A:158:PRO:HD3	2.29	0.51
1:A:289:ILE:HG23	1:A:290:PHE:N	2.23	0.51
1:B:559:GLY:HA3	1:B:562:ILE:HG13	1.92	0.51
1:A:505:PHE:CD2	1:A:536:ARG:NH2	2.73	0.51
1:B:363:ILE:O	1:B:419:ARG:NH1	2.43	0.51
1:B:651:LEU:HB3	1:B:652:LEU:HG	1.93	0.51
1:B:687:LEU:HA	1:B:698:ALA:HB3	1.92	0.51
1:B:659:GLU:CD	1:B:659:GLU:N	2.63	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:ARG:O	1:B:140:LEU:HG	2.10	0.51
1:B:116:ARG:NH1	1:B:156:GLY:N	2.57	0.51
1:A:359:LEU:HD23	1:A:426:ALA:CA	2.38	0.51
1:A:68:ASN:HD21	1:A:209:ASP:HB2	1.76	0.51
1:A:593:PHE:CZ	1:A:642:SER:HB3	2.46	0.51
1:B:232:LEU:HD12	1:B:233:SER:N	2.26	0.51
1:B:382:LEU:HD21	1:B:407:VAL:HG11	1.92	0.51
1:B:628:LEU:O	1:B:631:VAL:HB	2.09	0.51
1:B:636:ASN:CG	1:B:637:ASP:N	2.64	0.51
1:A:680:LEU:HD12	1:A:683:ILE:HD13	1.91	0.51
1:A:476:ASP:O	1:A:563:GLY:HA2	2.10	0.51
1:A:363:ILE:O	1:A:419:ARG:NH1	2.44	0.51
1:A:293:TYR:HB3	1:A:297:LEU:CB	2.41	0.51
1:A:628:LEU:O	1:A:631:VAL:HB	2.10	0.51
1:A:635:ILE:O	1:A:636:ASN:C	2.49	0.51
1:A:559:GLY:HA3	1:A:562:ILE:HG13	1.91	0.51
1:B:646:ARG:HA	1:B:649:GLN:HG2	1.92	0.51
1:B:229:ILE:HG12	1:B:230:GLU:N	2.26	0.51
1:A:325:LEU:CD2	1:A:694:LEU:HD21	2.41	0.51
1:A:598:ILE:O	1:A:601:VAL:HB	2.11	0.51
1:B:234:SER:CB	1:B:237:GLU:HB2	2.40	0.51
1:A:68:ASN:CG	1:A:69:ARG:N	2.63	0.51
1:A:309:SER:O	1:A:310:ALA:C	2.47	0.51
1:A:590:ASP:O	1:A:593:PHE:HB3	2.11	0.51
1:B:590:ASP:HB2	1:B:646:ARG:HH22	1.72	0.51
1:A:355:ALA:HB1	1:A:357:LYS:HE2	1.93	0.51
1:B:711:SER:O	1:B:712:SER:C	2.49	0.51
1:B:703:VAL:O	1:B:704:GLY:C	2.49	0.51
1:B:118:VAL:HG12	1:B:119:LYS:H	1.74	0.51
1:A:630:ILE:HG22	1:A:631:VAL:N	2.25	0.51
1:B:363:ILE:HD13	1:B:423:GLU:HA	1.93	0.51
1:B:309:SER:O	1:B:310:ALA:C	2.49	0.51
1:B:534:ASP:O	1:B:537:ARG:CG	2.59	0.51
1:A:118:VAL:HG12	1:A:119:LYS:H	1.76	0.51
1:A:38:ASP:OD1	1:A:324:THR:HG22	2.11	0.51
1:A:336:GLY:HA3	1:A:679:THR:HA	1.93	0.51
1:A:597:SER:O	1:A:600:ALA:HB3	2.11	0.51
1:A:45:ILE:HG12	1:A:90:VAL:O	2.11	0.51
1:B:289:ILE:O	1:B:292:TYR:N	2.42	0.51
1:A:548:LEU:CD2	1:A:550:ALA:H	2.22	0.51
1:A:687:LEU:HA	1:A:698:ALA:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:LEU:N	1:A:92:LEU:HD12	2.24	0.51
1:B:711:SER:OG	1:B:712:SER:N	2.43	0.51
1:B:614:LEU:O	1:B:614:LEU:HD23	2.11	0.51
1:A:711:SER:OG	1:A:712:SER:N	2.44	0.51
1:B:367:PHE:N	1:B:419:ARG:NH2	2.58	0.50
1:B:583:LEU:HD23	1:B:584:TYR:N	2.25	0.50
1:A:442:PHE:CE1	1:A:445:MET:HB2	2.38	0.50
1:A:127:VAL:HG23	1:A:212:VAL:O	2.11	0.50
1:A:148:ASP:N	1:A:148:ASP:OD1	2.44	0.50
1:B:96:SER:O	1:B:100:GLN:N	2.44	0.50
1:A:651:LEU:HB3	1:A:652:LEU:HG	1.93	0.50
1:A:615:LEU:HB3	1:A:617:LEU:HD13	1.93	0.50
1:B:622:PRO:O	1:B:625:ALA:N	2.45	0.50
1:B:635:ILE:O	1:B:636:ASN:C	2.49	0.50
1:B:534:ASP:CG	1:B:535:GLU:N	2.64	0.50
1:B:485:LEU:CA	1:B:553:LEU:HG	2.19	0.50
1:B:156:GLY:N	1:B:157:PRO:HD3	2.27	0.50
1:A:473:TYR:CD1	1:A:618:GLU:HB3	2.47	0.50
1:B:148:ASP:OD1	1:B:148:ASP:N	2.44	0.50
1:B:4:LYS:HG3	1:B:5:ASN:N	2.26	0.50
1:B:375:MET:O	1:B:376:ASP:C	2.49	0.50
1:B:625:ALA:O	1:B:629:THR:N	2.23	0.50
1:B:61:LYS:HA	1:B:243:LEU:HD21	1.92	0.50
1:B:687:LEU:CA	1:B:698:ALA:HB1	2.42	0.50
1:B:548:LEU:CD2	1:B:550:ALA:H	2.22	0.50
1:A:340:ASP:O	1:A:343:VAL:CG1	2.60	0.50
1:B:68:ASN:CG	1:B:69:ARG:N	2.64	0.50
1:A:363:ILE:HD13	1:A:423:GLU:HA	1.92	0.50
1:A:466:VAL:HG12	1:A:467:PHE:N	2.25	0.50
1:B:593:PHE:CZ	1:B:642:SER:HB3	2.47	0.50
1:A:296:HIS:HB3	1:A:425:LEU:HD21	1.91	0.50
1:B:621:ILE:N	1:B:622:PRO:HD2	2.27	0.50
1:B:621:ILE:O	1:B:622:PRO:C	2.50	0.50
1:B:268:GLN:HA	1:B:271:ILE:CG2	2.42	0.50
1:B:598:ILE:O	1:B:601:VAL:HB	2.12	0.50
1:B:371:THR:O	1:B:374:ILE:HB	2.12	0.50
1:B:36:GLY:HA3	1:B:39:LEU:HD12	1.92	0.50
1:B:325:LEU:CD2	1:B:694:LEU:HD21	2.42	0.50
1:A:331:LEU:O	1:A:332:VAL:C	2.50	0.50
1:A:703:VAL:O	1:A:704:GLY:C	2.50	0.50
1:A:165:LEU:HA	1:A:185:THR:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:441:ARG:HG3	1:B:666:ASN:HD22	1.77	0.50
1:A:96:SER:O	1:A:99:ASP:CB	2.59	0.50
1:B:590:ASP:O	1:B:593:PHE:HB3	2.11	0.50
1:A:4:LYS:HG3	1:A:5:ASN:N	2.27	0.50
1:B:615:LEU:HB3	1:B:617:LEU:HD13	1.94	0.50
1:B:296:HIS:HB3	1:B:425:LEU:HD21	1.93	0.50
1:A:371:THR:O	1:A:374:ILE:HB	2.11	0.50
1:A:36:GLY:HA3	1:A:39:LEU:HD12	1.93	0.50
1:A:577:GLY:O	1:A:581:ILE:HG12	2.11	0.50
1:B:82:ILE:HD12	1:B:82:ILE:N	2.27	0.50
1:B:709:THR:O	1:B:713:ILE:HG22	2.11	0.50
1:A:646:ARG:HA	1:A:649:GLN:HG2	1.92	0.50
1:A:229:ILE:HG12	1:A:230:GLU:N	2.27	0.50
1:B:340:ASP:O	1:B:343:VAL:HG12	2.12	0.50
1:B:402:ILE:HG22	1:B:403:LEU:N	2.27	0.50
1:B:705:ILE:O	1:B:706:PHE:C	2.50	0.50
1:B:115:PHE:CD2	1:B:204:LEU:HD21	2.46	0.50
1:A:655:LEU:N	1:A:655:LEU:HD23	2.26	0.50
1:A:441:ARG:HG3	1:A:666:ASN:HD22	1.76	0.50
1:A:47:LEU:HD23	1:A:88:ILE:O	2.12	0.50
1:A:709:THR:O	1:A:713:ILE:HG22	2.11	0.50
1:A:636:ASN:CG	1:A:637:ASP:N	2.65	0.50
1:B:473:TYR:CD1	1:B:618:GLU:HB3	2.47	0.50
1:A:82:ILE:N	1:A:82:ILE:HD12	2.27	0.50
1:B:626:ALA:O	1:B:630:ILE:N	2.33	0.49
1:A:532:LEU:HD22	1:A:536:ARG:NH1	2.27	0.49
1:A:271:ILE:HG12	1:A:272:GLN:N	2.21	0.49
1:B:340:ASP:O	1:B:343:VAL:CG1	2.60	0.49
1:B:684:LEU:HG	1:B:702:PHE:CE1	2.47	0.49
1:B:485:LEU:HA	1:B:553:LEU:CG	2.20	0.49
1:A:132:GLN:HA	1:A:237:GLU:OE2	2.12	0.49
1:A:364:PRO:O	1:A:367:PHE:HB3	2.12	0.49
1:B:14:VAL:HG12	1:B:15:PHE:N	2.27	0.49
1:B:355:ALA:HB1	1:B:357:LYS:HE2	1.93	0.49
1:A:193:GLU:CG	1:A:223:THR:HB	2.42	0.49
1:A:614:LEU:HD23	1:A:614:LEU:O	2.12	0.49
1:A:299:LEU:HD22	1:A:303:LEU:HD11	1.93	0.49
1:A:687:LEU:O	1:A:695:ARG:HG2	2.12	0.49
1:A:660:LEU:O	1:A:661:VAL:C	2.51	0.49
1:A:46:VAL:CG2	1:A:258:GLU:HG2	2.43	0.49
1:A:566:LEU:O	1:A:567:ARG:C	2.50	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ALA:CB	1:A:252:VAL:HG11	2.41	0.49
1:A:14:VAL:HG12	1:A:15:PHE:N	2.27	0.49
1:A:232:LEU:HD21	1:A:238:ALA:HA	1.94	0.49
1:B:331:LEU:O	1:B:332:VAL:C	2.50	0.49
1:A:340:ASP:O	1:A:343:VAL:HG12	2.12	0.49
1:A:621:ILE:N	1:A:622:PRO:HD2	2.26	0.49
1:A:684:LEU:HG	1:A:702:PHE:CE1	2.48	0.49
1:B:241:ILE:HA	1:B:244:VAL:CG1	2.42	0.49
1:B:439:ASP:HB3	1:B:440:PRO:CD	2.41	0.49
1:A:659:GLU:CA	1:A:662:ASN:HD22	2.21	0.49
1:B:271:ILE:HG12	1:B:272:GLN:N	2.21	0.49
1:A:586:ALA:O	1:A:589:PHE:O	2.31	0.49
1:B:511:VAL:HB	1:B:528:LYS:HG3	1.93	0.49
1:A:626:ALA:O	1:A:630:ILE:N	2.33	0.49
1:A:629:THR:CG2	1:A:701:ILE:HD12	2.41	0.49
1:B:237:GLU:HA	1:B:240:GLU:HB3	1.94	0.49
1:B:49:ALA:CB	1:B:252:VAL:HG11	2.40	0.49
1:B:462:ALA:O	1:B:465:VAL:CG1	2.61	0.49
1:A:411:VAL:HG12	1:A:412:PHE:N	2.26	0.49
1:B:532:LEU:HD22	1:B:536:ARG:NH1	2.27	0.49
1:B:473:TYR:O	1:B:618:GLU:HA	2.13	0.49
1:A:564:GLU:O	1:A:567:ARG:HB3	2.12	0.49
1:A:268:GLN:HA	1:A:271:ILE:CG2	2.42	0.49
1:A:65:VAL:O	1:A:68:ASN:OD1	2.30	0.49
1:A:58:ASP:HA	1:A:61:LYS:CD	2.43	0.49
1:B:473:TYR:CE1	1:B:528:LYS:HE2	2.48	0.49
1:A:493:VAL:HA	1:A:496:LEU:CD1	2.39	0.49
1:B:583:LEU:O	1:B:587:PHE:N	2.40	0.49
1:A:420:HIS:HD2	1:A:421:LEU:HD23	1.75	0.49
1:B:298:GLY:O	1:B:299:LEU:C	2.51	0.49
1:A:687:LEU:CA	1:A:698:ALA:HB1	2.42	0.49
1:A:115:PHE:CD2	1:A:204:LEU:HD21	2.47	0.49
1:A:234:SER:CB	1:A:237:GLU:HB2	2.42	0.49
1:A:241:ILE:HA	1:A:244:VAL:CG1	2.42	0.49
1:A:511:VAL:HB	1:A:528:LYS:HG3	1.93	0.49
1:A:402:ILE:O	1:A:403:LEU:C	2.52	0.49
1:A:240:GLU:O	1:A:244:VAL:HG13	2.12	0.49
1:A:659:GLU:CD	1:A:659:GLU:N	2.65	0.49
1:A:663:ARG:HB3	1:A:663:ARG:HE	1.51	0.49
1:B:46:VAL:CG2	1:B:258:GLU:HG2	2.43	0.49
1:A:473:TYR:O	1:A:618:GLU:HA	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:593:PHE:HZ	1:A:642:SER:HA	1.78	0.49
1:B:180:VAL:H	1:B:229:ILE:HG21	1.75	0.49
1:B:193:GLU:CG	1:B:223:THR:HB	2.42	0.49
1:B:288:LEU:C	1:B:288:LEU:HD23	2.34	0.48
1:B:377:VAL:HA	1:B:639:ILE:CD1	2.43	0.48
1:B:326:PRO:O	1:B:399:PHE:HD1	1.96	0.48
1:B:411:VAL:HG12	1:B:412:PHE:N	2.27	0.48
1:A:522:TYR:OH	1:A:550:ALA:HB2	2.12	0.48
1:A:377:VAL:O	1:A:381:HIS:CE1	2.66	0.48
1:B:240:GLU:O	1:B:244:VAL:HG13	2.13	0.48
1:B:574:VAL:HG12	1:B:575:LEU:N	2.28	0.48
1:B:452:THR:HG23	1:B:715:VAL:HG13	1.95	0.48
1:B:232:LEU:HD21	1:B:238:ALA:HA	1.94	0.48
1:A:504:GLY:HA2	1:B:431:ILE:HG12	1.95	0.48
1:B:619:PHE:HB2	1:B:623:THR:CB	2.44	0.48
1:B:539:GLU:O	1:B:540:LEU:C	2.51	0.48
1:A:298:GLY:O	1:A:299:LEU:C	2.51	0.48
1:A:325:LEU:HB3	1:A:326:PRO:CD	2.42	0.48
1:A:377:VAL:HA	1:A:639:ILE:CD1	2.42	0.48
1:A:621:ILE:O	1:A:622:PRO:C	2.51	0.48
1:B:586:ALA:O	1:B:589:PHE:O	2.31	0.48
1:A:13:GLY:O	1:A:16:LEU:HB3	2.13	0.48
1:A:548:LEU:HD23	1:A:550:ALA:N	2.25	0.48
1:A:156:GLY:N	1:A:157:PRO:HD3	2.29	0.48
1:A:288:LEU:HD23	1:A:288:LEU:C	2.33	0.48
1:B:92:LEU:N	1:B:92:LEU:HD12	2.28	0.48
1:B:577:GLY:O	1:B:578:LEU:C	2.51	0.48
1:A:100:GLN:HG2	1:A:101:ASP:N	2.28	0.48
1:B:593:PHE:HZ	1:B:642:SER:HA	1.77	0.48
1:B:683:ILE:O	1:B:687:LEU:N	2.36	0.48
1:A:574:VAL:HG12	1:A:575:LEU:N	2.28	0.48
1:B:115:PHE:HB2	1:B:160:LEU:CD2	2.43	0.48
1:B:505:PHE:CD2	1:B:536:ARG:NH2	2.74	0.48
1:A:232:LEU:HD12	1:A:233:SER:H	1.77	0.48
1:A:711:SER:O	1:A:712:SER:C	2.51	0.48
1:A:436:TRP:CZ3	1:A:438:VAL:HA	2.48	0.48
1:A:444:PHE:O	1:A:447:PRO:HD2	2.12	0.48
1:B:402:ILE:O	1:B:403:LEU:C	2.52	0.48
1:A:327:GLY:O	1:A:328:ILE:C	2.51	0.48
1:B:493:VAL:HA	1:B:496:LEU:CD1	2.39	0.48
1:B:445:MET:O	1:B:445:MET:SD	2.72	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:VAL:H	1:A:229:ILE:HG21	1.76	0.48
1:B:623:THR:O	1:B:626:ALA:HB3	2.14	0.48
1:A:544:PHE:O	1:A:548:LEU:O	2.32	0.48
1:A:702:PHE:HD2	1:A:703:VAL:N	2.12	0.48
1:A:705:ILE:HG23	1:A:706:PHE:H	1.79	0.48
1:B:488:GLU:OE1	1:B:488:GLU:HA	2.14	0.48
1:B:348:ARG:HG2	1:B:366:GLY:HA2	1.95	0.48
1:B:81:GLN:HG2	1:B:82:ILE:N	2.28	0.48
1:B:13:GLY:O	1:B:16:LEU:HB3	2.13	0.48
1:B:144:GLU:O	1:B:147:LYS:HB2	2.13	0.48
1:B:377:VAL:O	1:B:381:HIS:CE1	2.67	0.48
1:B:630:ILE:CG2	1:B:631:VAL:N	2.76	0.48
1:B:522:TYR:OH	1:B:550:ALA:HB2	2.14	0.48
1:A:337:ALA:O	1:A:340:ASP:OD1	2.31	0.48
1:A:565:GLU:O	1:A:569:ASN:ND2	2.47	0.48
1:A:473:TYR:CE1	1:A:528:LYS:HE2	2.48	0.48
1:B:359:LEU:HD23	1:B:426:ALA:CA	2.37	0.48
1:A:144:GLU:O	1:A:147:LYS:HB2	2.14	0.48
1:B:682:PRO:O	1:B:685:ALA:HB3	2.14	0.48
1:A:534:ASP:O	1:A:537:ARG:CG	2.62	0.48
1:A:325:LEU:CB	1:A:326:PRO:HD3	2.41	0.48
1:A:402:ILE:HG22	1:A:403:LEU:N	2.27	0.48
1:A:585:VAL:HG11	1:A:594:GLY:HA2	1.95	0.48
1:A:619:PHE:HB2	1:A:623:THR:CB	2.44	0.48
1:A:630:ILE:CG2	1:A:631:VAL:N	2.77	0.48
1:B:441:ARG:HA	1:B:666:ASN:ND2	2.29	0.48
1:A:496:LEU:O	1:A:500:LEU:HG	2.14	0.48
1:A:81:GLN:HG2	1:A:82:ILE:N	2.28	0.48
1:B:100:GLN:HG2	1:B:101:ASP:N	2.29	0.48
1:B:58:ASP:HA	1:B:61:LYS:CD	2.44	0.48
1:A:348:ARG:HG2	1:A:366:GLY:HA2	1.95	0.48
1:A:53:ASN:OD1	1:A:53:ASN:N	2.43	0.48
1:A:119:LYS:CB	1:A:154:ASP:H	2.22	0.48
1:A:375:MET:O	1:A:376:ASP:C	2.51	0.48
1:A:403:LEU:O	1:A:407:VAL:HG23	2.13	0.48
1:A:381:HIS:ND1	1:A:632:GLY:O	2.46	0.48
1:B:564:GLU:O	1:B:567:ARG:HB3	2.14	0.48
1:B:576:VAL:O	1:B:577:GLY:C	2.52	0.48
1:B:710:TYR:O	1:B:714:TYR:HD1	1.97	0.48
1:B:127:VAL:HG23	1:B:212:VAL:O	2.14	0.48
1:A:125:THR:CG2	1:A:130:ILE:HD11	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:SER:O	1:A:100:GLN:N	2.43	0.48
1:A:357:LYS:N	1:A:357:LYS:HD3	2.28	0.48
1:B:337:ALA:O	1:B:340:ASP:OD1	2.32	0.47
1:A:659:GLU:O	1:A:660:LEU:C	2.52	0.47
1:A:44:ARG:HG3	1:A:91:GLU:CG	2.44	0.47
1:A:559:GLY:N	1:A:562:ILE:HD12	2.29	0.47
1:B:49:ALA:HB2	1:B:254:LEU:HD22	1.96	0.47
1:B:47:LEU:HD23	1:B:88:ILE:O	2.14	0.47
1:B:595:VAL:O	1:B:598:ILE:CG2	2.62	0.47
1:B:110:ARG:HG2	1:B:111:ALA:N	2.29	0.47
1:A:483:TYR:CE2	1:A:540:LEU:HD23	2.49	0.47
1:A:674:MET:O	1:A:677:LEU:HB2	2.14	0.47
1:A:115:PHE:HB2	1:A:160:LEU:CD2	2.44	0.47
1:B:132:GLN:HA	1:B:237:GLU:OE2	2.13	0.47
1:B:44:ARG:HG3	1:B:91:GLU:CG	2.42	0.47
1:B:272:GLN:NE2	1:B:276:ARG:NH2	2.62	0.47
1:B:364:PRO:O	1:B:367:PHE:HB3	2.14	0.47
1:A:713:ILE:CG1	1:A:714:TYR:N	2.77	0.47
1:B:304:GLY:HA2	1:B:417:PHE:CD2	2.49	0.47
1:B:232:LEU:HD12	1:B:233:SER:H	1.79	0.47
1:B:376:ASP:O	1:B:377:VAL:C	2.52	0.47
1:B:167:ASP:O	1:B:183:THR:HB	2.14	0.47
1:B:482:ALA:HA	1:B:527:VAL:O	2.15	0.47
1:A:452:THR:HG23	1:A:715:VAL:HG13	1.96	0.47
1:B:357:LYS:HD3	1:B:357:LYS:N	2.29	0.47
1:A:110:ARG:HG2	1:A:111:ALA:N	2.29	0.47
1:A:605:VAL:O	1:A:606:ALA:C	2.52	0.47
1:B:58:ASP:O	1:B:61:LYS:HB2	2.14	0.47
1:B:511:VAL:HB	1:B:528:LYS:HD2	1.96	0.47
1:A:49:ALA:HB2	1:A:254:LEU:HD22	1.95	0.47
1:A:142:ARG:O	1:A:146:GLU:HG3	2.13	0.47
1:B:295:PRO:O	1:B:299:LEU:HB2	2.15	0.47
1:A:539:GLU:O	1:A:540:LEU:C	2.53	0.47
1:B:596:ALA:CB	1:B:716:VAL:HG13	2.44	0.47
1:B:165:LEU:HA	1:B:185:THR:H	1.78	0.47
1:B:45:ILE:CG1	1:B:90:VAL:HB	2.35	0.47
1:A:482:ALA:O	1:A:555:SER:HA	2.14	0.47
1:A:272:GLN:NE2	1:A:276:ARG:NH2	2.62	0.47
1:A:353:LEU:O	1:A:356:GLY:N	2.41	0.47
1:B:577:GLY:O	1:B:581:ILE:HG12	2.14	0.47
1:A:308:THR:CA	1:A:311:LEU:HB2	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:PRO:HA	1:A:450:TYR:HD1	1.79	0.47
1:B:378:ASN:O	1:B:379:ILE:C	2.53	0.47
1:A:116:ARG:HH22	1:A:155:LEU:HB2	1.80	0.47
1:A:326:PRO:O	1:A:399:PHE:HD1	1.97	0.47
1:A:671:ARG:H	1:A:671:ARG:HG2	1.29	0.47
1:A:630:ILE:CD1	1:A:704:GLY:HA3	2.30	0.47
1:A:55:THR:HB	1:A:58:ASP:CB	2.43	0.47
1:A:473:TYR:HD1	1:A:473:TYR:O	1.97	0.47
1:A:353:LEU:CD2	1:A:362:ALA:HB2	2.44	0.47
1:A:176:GLY:C	1:A:177:ARG:HG3	2.35	0.47
1:A:471:PHE:HB3	1:A:613:SER:OG	2.14	0.47
1:B:417:PHE:O	1:B:421:LEU:HG	2.14	0.47
1:B:300:VAL:O	1:B:303:LEU:HB2	2.15	0.47
1:B:330:GLY:O	1:B:331:LEU:C	2.53	0.47
1:B:486:ARG:HG2	1:B:522:TYR:HD2	1.79	0.47
1:B:659:GLU:O	1:B:660:LEU:C	2.52	0.47
1:B:665:ILE:HG23	1:B:666:ASN:H	1.80	0.47
1:A:511:VAL:HB	1:A:528:LYS:HD2	1.97	0.47
1:B:353:LEU:CD2	1:B:362:ALA:HB2	2.45	0.47
1:A:81:GLN:CG	1:A:82:ILE:N	2.78	0.47
1:B:81:GLN:CG	1:B:82:ILE:N	2.78	0.47
1:A:710:TYR:O	1:A:714:TYR:HD1	1.98	0.47
1:A:29:GLU:O	1:A:33:VAL:HG12	2.15	0.47
1:A:481:THR:O	1:A:529:LEU:N	2.35	0.47
1:B:383:LEU:O	1:B:386:ALA:HB3	2.15	0.47
1:B:687:LEU:O	1:B:695:ARG:HG2	2.14	0.47
1:A:285:ILE:O	1:A:286:PHE:C	2.53	0.47
1:A:683:ILE:O	1:A:687:LEU:N	2.37	0.47
1:A:441:ARG:HA	1:A:666:ASN:ND2	2.29	0.47
1:A:441:ARG:HG3	1:A:666:ASN:ND2	2.30	0.47
1:B:473:TYR:CD1	1:B:618:GLU:CB	2.98	0.47
1:A:514:GLN:HG2	1:A:525:PHE:HE2	1.80	0.47
1:A:173:ASP:N	1:A:177:ARG:O	2.47	0.47
1:B:605:VAL:O	1:B:606:ALA:C	2.52	0.47
1:B:403:LEU:O	1:B:407:VAL:HG23	2.14	0.47
1:B:487:ALA:O	1:B:522:TYR:CE2	2.68	0.47
1:B:544:PHE:O	1:B:548:LEU:O	2.32	0.47
1:A:622:PRO:O	1:A:625:ALA:N	2.47	0.47
1:B:81:GLN:CG	1:B:82:ILE:H	2.28	0.47
1:B:406:GLY:O	1:B:407:VAL:C	2.53	0.47
1:A:539:GLU:HA	1:A:542:ARG:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:682:PRO:O	1:A:685:ALA:HB3	2.15	0.47
1:B:55:THR:HB	1:B:58:ASP:CB	2.43	0.47
1:B:660:LEU:O	1:B:661:VAL:C	2.52	0.47
1:A:526:LEU:C	1:A:526:LEU:HD23	2.35	0.47
1:A:473:TYR:CD1	1:A:618:GLU:CB	2.98	0.47
1:B:82:ILE:HG13	1:B:88:ILE:HG13	1.97	0.47
1:A:197:ARG:HA	1:A:200:ILE:HG23	1.96	0.47
1:B:53:ASN:HA	1:B:54:PRO:HD3	1.75	0.47
1:A:116:ARG:HB2	1:A:157:PRO:O	2.15	0.46
1:A:300:VAL:O	1:A:303:LEU:HB2	2.15	0.46
1:A:378:ASN:O	1:A:379:ILE:C	2.54	0.46
1:A:623:THR:O	1:A:626:ALA:HB3	2.15	0.46
1:B:176:GLY:C	1:B:177:ARG:HG3	2.36	0.46
1:A:713:ILE:HG12	1:A:714:TYR:CD1	2.50	0.46
1:A:304:GLY:HA2	1:A:417:PHE:CD2	2.50	0.46
1:B:103:ALA:O	1:B:107:ILE:HG22	2.15	0.46
1:B:327:GLY:O	1:B:328:ILE:C	2.53	0.46
1:B:539:GLU:HA	1:B:542:ARG:HD2	1.98	0.46
1:B:116:ARG:HB2	1:B:157:PRO:O	2.15	0.46
1:B:598:ILE:HG23	1:B:599:LEU:H	1.80	0.46
1:B:713:ILE:CG1	1:B:714:TYR:N	2.78	0.46
1:B:436:TRP:CZ3	1:B:438:VAL:HA	2.50	0.46
1:B:116:ARG:HH22	1:B:155:LEU:HB2	1.79	0.46
1:A:376:ASP:O	1:A:377:VAL:C	2.53	0.46
1:A:377:VAL:HG13	1:A:636:ASN:CB	2.31	0.46
1:A:702:PHE:CD2	1:A:703:VAL:N	2.83	0.46
1:A:488:GLU:HA	1:A:488:GLU:OE1	2.15	0.46
1:A:503:LYS:O	1:A:505:PHE:CD2	2.69	0.46
1:B:65:VAL:O	1:B:68:ASN:OD1	2.33	0.46
1:B:96:SER:O	1:B:99:ASP:CB	2.62	0.46
1:B:18:ALA:O	1:B:22:VAL:HG12	2.16	0.46
1:B:676:SER:O	1:B:677:LEU:C	2.53	0.46
1:B:116:ARG:HH12	1:B:118:VAL:HG13	1.80	0.46
1:A:167:ASP:O	1:A:183:THR:HB	2.14	0.46
1:A:81:GLN:CG	1:A:82:ILE:H	2.28	0.46
1:A:462:ALA:O	1:A:465:VAL:CG1	2.63	0.46
1:B:671:ARG:H	1:B:671:ARG:HG2	1.28	0.46
1:A:343:VAL:HG13	1:A:344:LEU:N	2.30	0.46
1:A:577:GLY:O	1:A:578:LEU:C	2.52	0.46
1:A:58:ASP:O	1:A:61:LYS:HB2	2.15	0.46
1:B:566:LEU:O	1:B:567:ARG:C	2.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:GLU:C	1:A:503:LYS:N	2.69	0.46
1:B:124:GLY:CA	1:B:150:ILE:HD11	2.43	0.46
1:A:18:ALA:O	1:A:22:VAL:HG12	2.16	0.46
1:B:444:PHE:O	1:B:447:PRO:HD2	2.15	0.46
1:B:638:SER:O	1:B:639:ILE:C	2.54	0.46
1:B:702:PHE:HD2	1:B:703:VAL:N	2.13	0.46
1:A:330:GLY:O	1:A:331:LEU:C	2.52	0.46
1:A:665:ILE:HG23	1:A:666:ASN:H	1.80	0.46
1:B:559:GLY:N	1:B:562:ILE:HD12	2.30	0.46
1:B:65:VAL:O	1:B:66:LEU:C	2.52	0.46
1:B:142:ARG:O	1:B:146:GLU:HG3	2.15	0.46
1:B:287:LEU:HG	1:B:288:LEU:N	2.29	0.46
1:B:483:TYR:CE2	1:B:540:LEU:HD23	2.51	0.46
1:A:35:LEU:HB3	1:A:322:THR:HG22	1.98	0.46
1:A:683:ILE:HD11	1:A:702:PHE:CA	2.46	0.46
1:A:684:LEU:O	1:A:685:ALA:C	2.54	0.46
1:A:596:ALA:CB	1:A:716:VAL:HG13	2.44	0.46
1:A:482:ALA:HA	1:A:527:VAL:O	2.15	0.46
1:B:308:THR:CA	1:B:311:LEU:HB2	2.42	0.46
1:B:447:PRO:HA	1:B:450:TYR:HD1	1.80	0.46
1:B:381:HIS:ND1	1:B:632:GLY:O	2.47	0.46
1:A:375:MET:C	1:A:379:ILE:HG12	2.36	0.46
1:A:677:LEU:O	1:A:678:THR:C	2.54	0.46
1:A:243:LEU:O	1:A:244:VAL:C	2.54	0.46
1:B:526:LEU:C	1:B:526:LEU:HD23	2.36	0.46
1:B:125:THR:CG2	1:B:130:ILE:HD11	2.45	0.46
1:B:651:LEU:O	1:B:652:LEU:HD23	2.16	0.46
1:A:379:ILE:O	1:A:382:LEU:HB2	2.16	0.46
1:B:496:LEU:O	1:B:500:LEU:HG	2.16	0.46
1:B:209:ASP:N	1:B:209:ASP:OD1	2.49	0.46
1:A:304:GLY:HA2	1:A:417:PHE:CE2	2.51	0.46
1:A:352:GLU:O	1:A:355:ALA:HB3	2.15	0.46
1:B:379:ILE:O	1:B:382:LEU:HB2	2.15	0.46
1:B:116:ARG:HD3	1:B:158:PRO:N	2.30	0.46
1:A:295:PRO:O	1:A:299:LEU:N	2.41	0.46
1:A:331:LEU:O	1:A:334:THR:HB	2.16	0.46
1:B:482:ALA:O	1:B:555:SER:HA	2.15	0.46
1:B:578:LEU:O	1:B:579:GLY:C	2.55	0.46
1:B:473:TYR:O	1:B:473:TYR:HD1	1.99	0.45
1:A:445:MET:SD	1:A:445:MET:O	2.74	0.45
1:B:35:LEU:HB3	1:B:322:THR:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:683:ILE:HD11	1:B:702:PHE:CA	2.46	0.45
1:A:486:ARG:HG2	1:A:522:TYR:HD2	1.80	0.45
1:A:119:LYS:CD	1:A:153:GLU:HB2	2.46	0.45
1:A:301:ALA:HB2	1:A:346:PHE:CE2	2.52	0.45
1:A:638:SER:O	1:A:639:ILE:C	2.55	0.45
1:B:501:GLU:C	1:B:503:LYS:N	2.70	0.45
1:A:308:THR:CG2	1:A:309:SER:N	2.79	0.45
1:A:53:ASN:HA	1:A:54:PRO:HD3	1.76	0.45
1:B:548:LEU:HD23	1:B:550:ALA:N	2.25	0.45
1:B:116:ARG:HA	1:B:159:LEU:CG	2.43	0.45
1:B:119:LYS:CD	1:B:153:GLU:HB2	2.44	0.45
1:A:103:ALA:O	1:A:107:ILE:HG22	2.15	0.45
1:B:705:ILE:HG23	1:B:706:PHE:H	1.82	0.45
1:A:116:ARG:HD3	1:A:158:PRO:N	2.30	0.45
1:A:324:THR:CG2	1:A:395:PRO:HA	2.38	0.45
1:A:576:VAL:O	1:A:577:GLY:C	2.55	0.45
1:B:258:GLU:HB3	1:B:562:ILE:CD1	2.43	0.45
1:A:503:LYS:O	1:A:505:PHE:N	2.49	0.45
1:B:352:GLU:O	1:B:355:ALA:HB3	2.17	0.45
1:A:383:LEU:O	1:A:386:ALA:HB3	2.17	0.45
1:B:534:ASP:HA	1:B:537:ARG:CD	2.46	0.45
1:B:538:LEU:O	1:B:539:GLU:C	2.55	0.45
1:B:692:SER:O	1:B:696:ASP:OD1	2.34	0.45
1:A:541:GLU:O	1:A:544:PHE:HB2	2.17	0.45
1:A:692:SER:O	1:A:696:ASP:OD1	2.35	0.45
1:A:342:ASN:O	1:A:346:PHE:CD2	2.70	0.45
1:A:403:LEU:HA	1:A:403:LEU:HD12	1.79	0.45
1:A:439:ASP:HB3	1:A:440:PRO:CD	2.40	0.45
1:A:501:GLU:O	1:A:503:LYS:N	2.49	0.45
1:A:611:MET:C	1:A:611:MET:SD	2.94	0.45
1:B:304:GLY:HA2	1:B:417:PHE:CE2	2.51	0.45
1:B:343:VAL:HG13	1:B:344:LEU:N	2.30	0.45
1:B:702:PHE:CD2	1:B:703:VAL:N	2.85	0.45
1:B:541:GLU:O	1:B:544:PHE:HB2	2.16	0.45
1:A:486:ARG:HB2	1:A:553:LEU:HD21	1.97	0.45
1:A:283:LEU:O	1:A:286:PHE:N	2.50	0.45
1:A:676:SER:O	1:A:677:LEU:C	2.54	0.45
1:B:501:GLU:O	1:B:503:LYS:N	2.50	0.45
1:B:561:ALA:O	1:B:565:GLU:HB2	2.16	0.45
1:A:65:VAL:O	1:A:66:LEU:C	2.54	0.45
1:A:310:ALA:O	1:A:311:LEU:C	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:THR:O	1:B:285:ILE:HB	2.16	0.45
1:B:295:PRO:O	1:B:299:LEU:N	2.41	0.45
1:B:674:MET:O	1:B:677:LEU:HB2	2.16	0.45
1:B:118:VAL:HG13	1:B:155:LEU:HA	1.97	0.45
1:B:119:LYS:CB	1:B:154:ASP:H	2.20	0.45
1:A:282:THR:O	1:A:285:ILE:HB	2.16	0.45
1:A:578:LEU:O	1:A:579:GLY:C	2.55	0.45
1:A:635:ILE:O	1:A:638:SER:N	2.50	0.45
1:A:636:ASN:HA	1:A:639:ILE:CG1	2.47	0.45
1:A:596:ALA:CA	1:A:719:LEU:HD13	2.46	0.45
1:B:503:LYS:O	1:B:505:PHE:CD2	2.70	0.45
1:A:258:GLU:HB3	1:A:562:ILE:CD1	2.41	0.45
1:B:581:ILE:O	1:B:582:LEU:C	2.55	0.45
1:B:585:VAL:HG11	1:B:594:GLY:HA2	1.97	0.45
1:B:101:ASP:C	1:B:101:ASP:OD1	2.55	0.45
1:B:310:ALA:O	1:B:311:LEU:C	2.54	0.45
1:B:515:VAL:O	1:B:524:GLU:HB3	2.17	0.45
1:B:156:GLY:C	1:B:158:PRO:HD3	2.29	0.45
1:A:327:GLY:C	1:A:402:ILE:HD12	2.38	0.45
1:A:583:LEU:O	1:A:587:PHE:N	2.39	0.45
1:A:458:LEU:O	1:A:459:ALA:C	2.55	0.45
1:B:111:ALA:HB3	1:B:251:PRO:HB3	1.98	0.45
1:A:111:ALA:HB3	1:A:251:PRO:HB3	1.98	0.45
1:B:56:LEU:O	1:B:59:LEU:HB2	2.17	0.45
1:B:285:ILE:O	1:B:286:PHE:C	2.54	0.45
1:B:375:MET:C	1:B:379:ILE:HG12	2.37	0.45
1:B:636:ASN:HA	1:B:639:ILE:CG1	2.46	0.45
1:A:691:GLY:O	1:A:692:SER:C	2.55	0.45
1:A:116:ARG:HA	1:A:159:LEU:CG	2.41	0.45
1:A:370:SER:O	1:A:371:THR:C	2.54	0.45
1:A:574:VAL:O	1:A:577:GLY:N	2.50	0.45
1:A:562:ILE:O	1:A:565:GLU:CB	2.65	0.45
1:A:501:GLU:HG3	1:A:507:GLY:HA3	1.99	0.45
1:A:82:ILE:HG13	1:A:88:ILE:HG13	1.99	0.45
1:B:100:GLN:O	1:B:101:ASP:C	2.56	0.45
1:B:370:SER:O	1:B:371:THR:C	2.55	0.44
1:B:485:LEU:HB2	1:B:552:VAL:CA	2.26	0.44
1:B:549:LYS:HE3	1:B:549:LYS:HB2	1.77	0.44
1:A:118:VAL:HG13	1:A:155:LEU:HA	1.99	0.44
1:A:295:PRO:O	1:A:299:LEU:HB2	2.17	0.44
1:A:55:THR:CB	1:A:58:ASP:HB3	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:THR:CB	1:B:58:ASP:HB3	2.46	0.44
1:A:386:ALA:O	1:A:387:ALA:C	2.56	0.44
1:A:105:LYS:O	1:A:109:GLN:N	2.50	0.44
1:A:188:GLY:O	1:A:192:PHE:HB2	2.17	0.44
1:B:635:ILE:O	1:B:638:SER:N	2.50	0.44
1:A:287:LEU:HG	1:A:288:LEU:N	2.31	0.44
1:A:331:LEU:O	1:A:334:THR:N	2.50	0.44
1:B:596:ALA:CA	1:B:719:LEU:HD13	2.46	0.44
1:A:58:ASP:HA	1:A:61:LYS:HD2	2.00	0.44
1:B:493:VAL:HG22	1:B:525:PHE:HE2	1.82	0.44
1:B:562:ILE:O	1:B:565:GLU:CB	2.65	0.44
1:A:462:ALA:CB	1:A:610:GLY:HA3	2.40	0.44
1:B:471:PHE:CD1	1:B:471:PHE:C	2.91	0.44
1:B:142:ARG:O	1:B:145:LEU:N	2.51	0.44
1:B:442:PHE:CE1	1:B:445:MET:HB2	2.39	0.44
1:B:411:VAL:O	1:B:412:PHE:C	2.56	0.44
1:A:35:LEU:O	1:A:322:THR:CA	2.66	0.44
1:A:403:LEU:O	1:A:404:ALA:C	2.54	0.44
1:A:581:ILE:O	1:A:582:LEU:C	2.55	0.44
1:A:237:GLU:O	1:A:241:ILE:HG13	2.16	0.44
1:B:441:ARG:HG3	1:B:666:ASN:ND2	2.31	0.44
1:A:45:ILE:CG1	1:A:90:VAL:HB	2.36	0.44
1:B:101:ASP:CA	1:B:104:LEU:HD12	2.43	0.44
1:B:113:LEU:HG	1:B:208:LEU:CD2	2.47	0.44
1:B:188:GLY:O	1:B:192:PHE:HB2	2.17	0.44
1:A:534:ASP:HA	1:A:537:ARG:CD	2.46	0.44
1:B:119:LYS:HB3	1:B:153:GLU:CG	2.48	0.44
1:B:252:VAL:HG12	1:B:254:LEU:CD2	2.46	0.44
1:B:582:LEU:O	1:B:583:LEU:C	2.55	0.44
1:B:283:LEU:O	1:B:286:PHE:N	2.51	0.44
1:B:331:LEU:O	1:B:334:THR:HB	2.16	0.44
1:B:342:ASN:O	1:B:346:PHE:CD2	2.70	0.44
1:A:293:TYR:OH	1:A:343:VAL:HG23	2.17	0.44
1:B:713:ILE:HG12	1:B:714:TYR:CD1	2.52	0.44
1:A:193:GLU:HB2	1:A:223:THR:HA	1.99	0.44
1:B:323:LEU:CD1	1:B:328:ILE:N	2.69	0.44
1:A:504:GLY:CA	1:B:431:ILE:HG23	2.47	0.44
1:A:538:LEU:O	1:A:539:GLU:C	2.55	0.44
1:A:620:SER:O	1:A:623:THR:CB	2.65	0.44
1:A:16:LEU:HD23	1:A:17:LEU:HD23	2.00	0.44
1:B:79:LEU:HD23	1:B:79:LEU:HA	1.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:ARG:HH12	1:A:156:GLY:H	1.63	0.44
1:A:595:VAL:O	1:A:598:ILE:CG2	2.65	0.44
1:A:599:LEU:O	1:A:600:ALA:C	2.55	0.44
1:A:113:LEU:HG	1:A:208:LEU:CD2	2.47	0.44
1:B:662:ASN:C	1:B:665:ILE:HG22	2.38	0.44
1:B:565:GLU:O	1:B:569:ASN:ND2	2.50	0.44
1:A:67:GLU:OE2	1:A:71:ASN:ND2	2.51	0.44
1:B:462:ALA:CB	1:B:610:GLY:HA3	2.41	0.44
1:B:574:VAL:O	1:B:577:GLY:N	2.51	0.44
1:B:649:GLN:HG3	1:B:650:LYS:H	1.80	0.44
1:A:444:PHE:C	1:A:447:PRO:HD2	2.38	0.44
1:B:105:LYS:O	1:B:109:GLN:N	2.51	0.44
1:A:119:LYS:HB3	1:A:153:GLU:CG	2.48	0.44
1:A:113:LEU:HD21	1:A:206:ILE:HG23	1.99	0.44
1:B:135:ARG:HD2	1:B:237:GLU:OE2	2.18	0.44
1:B:243:LEU:O	1:B:244:VAL:C	2.55	0.44
1:A:101:ASP:OD1	1:A:101:ASP:C	2.55	0.44
1:B:308:THR:CG2	1:B:309:SER:N	2.80	0.44
1:B:308:THR:HG23	1:B:309:SER:N	2.32	0.44
1:B:193:GLU:HG3	1:B:223:THR:N	2.33	0.44
1:B:193:GLU:HB2	1:B:223:THR:HA	1.98	0.44
1:A:41:GLY:HA2	1:A:262:ILE:O	2.17	0.44
1:B:324:THR:CG2	1:B:395:PRO:HA	2.39	0.44
1:A:337:ALA:O	1:A:338:ALA:C	2.55	0.44
1:A:598:ILE:O	1:A:601:VAL:N	2.51	0.44
1:B:501:GLU:HG3	1:B:507:GLY:HA3	2.00	0.44
1:A:43:LEU:CB	1:A:92:LEU:HD22	2.48	0.44
1:B:647:GLU:O	1:B:651:LEU:HB2	2.18	0.44
1:B:474:SER:O	1:B:474:SER:OG	2.34	0.44
1:B:331:LEU:O	1:B:334:THR:N	2.51	0.43
1:B:403:LEU:O	1:B:404:ALA:C	2.55	0.43
1:B:553:LEU:H	1:B:553:LEU:HG	1.44	0.43
1:B:486:ARG:HB2	1:B:553:LEU:HD21	1.98	0.43
1:A:347:GLU:CG	1:A:671:ARG:CD	2.92	0.43
1:A:595:VAL:HG12	1:A:599:LEU:CD1	2.48	0.43
1:B:237:GLU:O	1:B:241:ILE:HG13	2.17	0.43
1:A:46:VAL:HG12	1:A:257:ALA:HB3	2.00	0.43
1:A:561:ALA:O	1:A:565:GLU:HB2	2.17	0.43
1:B:458:LEU:O	1:B:459:ALA:C	2.57	0.43
1:B:127:VAL:CA	1:B:130:ILE:HD12	2.42	0.43
1:A:709:THR:HG22	1:A:710:TYR:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:PHE:O	1:A:421:LEU:HG	2.17	0.43
1:A:106:LEU:HA	1:A:109:GLN:HB2	2.00	0.43
1:A:75:VAL:HG21	1:A:95:LEU:HD11	1.99	0.43
1:B:337:ALA:O	1:B:338:ALA:C	2.55	0.43
1:B:620:SER:O	1:B:623:THR:CB	2.65	0.43
1:A:515:VAL:O	1:A:524:GLU:HB3	2.18	0.43
1:B:116:ARG:HH22	1:B:155:LEU:HA	1.83	0.43
1:A:471:PHE:CD1	1:A:471:PHE:C	2.91	0.43
1:B:709:THR:HG22	1:B:710:TYR:N	2.33	0.43
1:A:12:LEU:O	1:A:15:PHE:HB3	2.18	0.43
1:B:316:LEU:O	1:B:320:GLY:N	2.34	0.43
1:A:312:ILE:O	1:A:315:LEU:N	2.52	0.43
1:A:344:LEU:HA	1:A:344:LEU:HD23	1.76	0.43
1:A:598:ILE:HG23	1:A:599:LEU:H	1.83	0.43
1:A:165:LEU:C	1:A:165:LEU:HD12	2.39	0.43
1:B:663:ARG:O	1:B:664:SER:C	2.57	0.43
1:B:611:MET:C	1:B:611:MET:SD	2.97	0.43
1:A:308:THR:HG23	1:A:309:SER:N	2.32	0.43
1:B:669:LEU:O	1:B:670:SER:C	2.56	0.43
1:B:386:ALA:O	1:B:387:ALA:C	2.56	0.43
1:B:41:GLY:HA2	1:B:262:ILE:O	2.18	0.43
1:B:325:LEU:CB	1:B:326:PRO:HD3	2.42	0.43
1:B:684:LEU:O	1:B:685:ALA:C	2.55	0.43
1:A:406:GLY:O	1:A:407:VAL:C	2.55	0.43
1:A:474:SER:O	1:A:474:SER:OG	2.35	0.43
1:A:626:ALA:O	1:A:627:LEU:C	2.57	0.43
1:A:640:VAL:HG12	1:A:668:THR:HG23	1.99	0.43
1:B:182:LEU:O	1:B:226:GLN:CA	2.49	0.43
1:A:559:GLY:HA3	1:A:562:ILE:CG1	2.48	0.43
1:A:473:TYR:CE1	1:A:528:LYS:CE	3.01	0.43
1:A:193:GLU:HG3	1:A:223:THR:N	2.32	0.43
1:B:18:ALA:O	1:B:21:PHE:HB2	2.18	0.43
1:B:327:GLY:C	1:B:402:ILE:HD12	2.38	0.43
1:B:346:PHE:HA	1:B:349:ILE:CD1	2.34	0.43
1:B:410:SER:O	1:B:411:VAL:C	2.56	0.43
1:B:691:GLY:O	1:B:692:SER:C	2.57	0.43
1:A:116:ARG:HH12	1:A:118:VAL:HG13	1.82	0.43
1:B:360:ARG:O	1:B:364:PRO:HD2	2.19	0.43
1:B:423:GLU:O	1:B:424:ARG:C	2.56	0.43
1:A:423:GLU:O	1:A:424:ARG:C	2.56	0.43
1:B:598:ILE:O	1:B:601:VAL:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:LEU:O	1:B:15:PHE:HB3	2.19	0.43
1:B:16:LEU:HD23	1:B:17:LEU:HD23	1.99	0.43
1:B:312:ILE:O	1:B:315:LEU:N	2.51	0.43
1:B:621:ILE:N	1:B:622:PRO:CD	2.82	0.43
1:A:349:ILE:O	1:A:350:LYS:C	2.56	0.43
1:A:623:THR:O	1:A:624:ILE:C	2.57	0.43
1:A:663:ARG:O	1:A:664:SER:C	2.57	0.43
1:A:360:ARG:O	1:A:364:PRO:HD2	2.18	0.43
1:A:593:PHE:HE2	1:A:642:SER:HB3	1.83	0.43
1:A:669:LEU:O	1:A:670:SER:C	2.56	0.43
1:B:106:LEU:HA	1:B:109:GLN:HB2	2.01	0.43
1:B:293:TYR:O	1:B:297:LEU:HB2	2.18	0.43
1:A:151:LYS:CG	1:A:153:GLU:OE2	2.65	0.43
1:A:329:ALA:O	1:A:330:GLY:C	2.57	0.43
1:B:473:TYR:CE1	1:B:528:LYS:CE	3.01	0.43
1:A:43:LEU:O	1:A:92:LEU:HD13	2.19	0.43
1:A:353:LEU:HD21	1:A:362:ALA:CB	2.47	0.43
1:A:430:GLU:O	1:A:430:GLU:CG	2.67	0.43
1:A:48:GLU:O	1:A:255:LYS:HB3	2.19	0.43
1:A:121:GLY:O	1:A:150:ILE:HG23	2.19	0.43
1:A:73:LEU:HG	1:A:75:VAL:HG23	2.01	0.43
1:A:79:LEU:HA	1:A:79:LEU:HD23	1.83	0.43
1:A:76:ALA:O	1:A:78:PRO:HD3	2.19	0.43
1:B:301:ALA:HB2	1:B:346:PHE:CE2	2.53	0.43
1:B:372:LEU:HB3	1:B:588:ARG:HH22	1.83	0.43
1:A:574:VAL:HG12	1:A:575:LEU:HD23	2.01	0.43
1:A:582:LEU:O	1:A:583:LEU:C	2.57	0.43
1:A:177:ARG:HA	1:A:178:PRO:HD3	1.73	0.43
1:B:574:VAL:HG12	1:B:575:LEU:HD23	2.00	0.43
1:A:125:THR:HG22	1:A:130:ILE:HD11	2.01	0.43
1:A:647:GLU:O	1:A:651:LEU:HB2	2.17	0.43
1:B:343:VAL:O	1:B:344:LEU:C	2.57	0.43
1:B:680:LEU:HA	1:B:680:LEU:HD12	1.75	0.43
1:A:485:LEU:O	1:A:524:GLU:HG3	2.18	0.43
1:A:135:ARG:HD2	1:A:237:GLU:OE2	2.17	0.43
1:B:473:TYR:HB3	1:B:618:GLU:HA	2.00	0.43
1:B:353:LEU:HD21	1:B:362:ALA:CB	2.47	0.43
1:A:651:LEU:O	1:A:652:LEU:HD23	2.19	0.43
1:B:35:LEU:O	1:B:322:THR:CA	2.66	0.43
1:B:323:LEU:HD11	1:B:328:ILE:CG1	2.49	0.43
1:B:344:LEU:O	1:B:345:SER:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:582:LEU:HD21	1:A:598:ILE:CG2	2.49	0.43
1:B:115:PHE:HD2	1:B:204:LEU:HD21	1.83	0.43
1:B:44:ARG:NH1	1:B:260:ARG:HH22	2.11	0.43
1:A:257:ALA:O	1:A:559:GLY:HA2	2.19	0.43
1:A:44:ARG:NH1	1:A:260:ARG:HH22	2.10	0.43
1:A:493:VAL:HG22	1:A:525:PHE:HE2	1.83	0.43
1:B:366:GLY:O	1:B:367:PHE:C	2.57	0.43
1:A:209:ASP:N	1:A:209:ASP:OD1	2.50	0.43
1:A:104:LEU:H	1:A:104:LEU:HG	1.65	0.43
1:A:193:GLU:HG3	1:A:223:THR:CA	2.49	0.43
1:B:111:ALA:HB3	1:B:251:PRO:CB	2.49	0.43
1:B:106:LEU:O	1:B:109:GLN:HB3	2.19	0.43
1:B:73:LEU:HG	1:B:75:VAL:HG23	2.01	0.43
1:B:323:LEU:HD12	1:B:327:GLY:HA3	2.00	0.42
1:B:623:THR:O	1:B:624:ILE:C	2.57	0.42
1:B:677:LEU:O	1:B:678:THR:C	2.57	0.42
1:A:293:TYR:O	1:A:297:LEU:HB2	2.19	0.42
1:A:627:LEU:HA	1:A:627:LEU:HD12	1.63	0.42
1:B:441:ARG:N	1:B:441:ARG:CD	2.82	0.42
1:A:471:PHE:CD1	1:A:472:ASN:N	2.82	0.42
1:B:113:LEU:HD21	1:B:206:ILE:HG23	2.00	0.42
1:A:56:LEU:O	1:A:59:LEU:HB2	2.18	0.42
1:B:118:VAL:CG1	1:B:152:PRO:CB	2.87	0.42
1:A:284:ALA:O	1:A:287:LEU:HB3	2.20	0.42
1:A:37:LEU:C	1:A:39:LEU:N	2.72	0.42
1:A:411:VAL:O	1:A:412:PHE:C	2.57	0.42
1:A:687:LEU:HD11	1:A:699:LEU:HB2	2.01	0.42
1:B:165:LEU:C	1:B:165:LEU:HD12	2.39	0.42
1:B:430:GLU:CG	1:B:430:GLU:O	2.66	0.42
1:B:47:LEU:C	1:B:48:GLU:HG3	2.39	0.42
1:A:142:ARG:O	1:A:145:LEU:N	2.52	0.42
1:A:230:GLU:O	1:A:231:GLY:C	2.58	0.42
1:B:29:GLU:O	1:B:33:VAL:HG12	2.18	0.42
1:B:626:ALA:HA	1:B:629:THR:HB	2.02	0.42
1:A:117:ILE:C	1:A:157:PRO:HG2	2.35	0.42
1:A:333:LEU:O	1:A:334:THR:C	2.57	0.42
1:A:333:LEU:HD13	1:A:403:LEU:HD11	2.02	0.42
1:A:621:ILE:N	1:A:622:PRO:CD	2.81	0.42
1:A:441:ARG:CD	1:A:441:ARG:N	2.83	0.42
1:B:514:GLN:HG2	1:B:525:PHE:HE2	1.79	0.42
1:B:258:GLU:HG3	1:B:259:ILE:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:564:GLU:O	1:B:565:GLU:C	2.57	0.42
1:A:473:TYR:HB3	1:A:618:GLU:HA	2.01	0.42
1:B:68:ASN:HB2	1:B:211:ARG:HH11	1.75	0.42
1:B:644:ARG:O	1:B:648:ASN:HB2	2.20	0.42
1:A:487:ALA:O	1:A:522:TYR:CE2	2.73	0.42
1:B:156:GLY:H	1:B:157:PRO:HD2	1.82	0.42
1:A:405:ILE:CG2	1:A:406:GLY:N	2.82	0.42
1:A:412:PHE:O	1:A:413:SER:C	2.58	0.42
1:A:626:ALA:HA	1:A:629:THR:HB	2.01	0.42
1:B:503:LYS:O	1:B:505:PHE:N	2.52	0.42
1:A:493:VAL:HG13	1:A:512:ILE:HD13	2.02	0.42
1:A:359:LEU:O	1:A:363:ILE:HD12	2.20	0.42
1:B:48:GLU:O	1:B:255:LYS:HB3	2.19	0.42
1:B:286:PHE:O	1:B:289:ILE:CG2	2.66	0.42
1:B:339:VAL:O	1:B:341:GLY:N	2.53	0.42
1:B:694:LEU:O	1:B:695:ARG:C	2.58	0.42
1:A:343:VAL:O	1:A:344:LEU:C	2.57	0.42
1:A:410:SER:O	1:A:411:VAL:C	2.57	0.42
1:B:58:ASP:HA	1:B:61:LYS:HD2	2.01	0.42
1:B:67:GLU:OE2	1:B:71:ASN:ND2	2.53	0.42
1:B:359:LEU:O	1:B:363:ILE:HD12	2.20	0.42
1:B:391:TYR:CD1	1:B:391:TYR:N	2.88	0.42
1:B:576:VAL:O	1:B:579:GLY:N	2.53	0.42
1:A:649:GLN:HG3	1:A:650:LYS:H	1.80	0.42
1:A:351:GLU:OE1	1:A:644:ARG:NH1	2.53	0.42
1:B:284:ALA:O	1:B:287:LEU:HB3	2.20	0.42
1:B:325:LEU:HB3	1:B:326:PRO:CD	2.42	0.42
1:B:333:LEU:O	1:B:334:THR:C	2.58	0.42
1:B:405:ILE:CG2	1:B:406:GLY:N	2.82	0.42
1:B:687:LEU:HD11	1:B:699:LEU:HB2	2.01	0.42
1:B:697:PHE:O	1:B:698:ALA:C	2.57	0.42
1:B:485:LEU:HB3	1:B:552:VAL:HB	2.02	0.42
1:B:155:LEU:H	1:B:155:LEU:HD12	1.85	0.42
1:A:323:LEU:HD12	1:A:327:GLY:HA3	2.01	0.42
1:A:570:ALA:O	1:A:571:VAL:C	2.58	0.42
1:A:719:LEU:O	1:A:720:VAL:C	2.58	0.42
1:A:241:ILE:O	1:A:242:ALA:C	2.58	0.42
1:B:452:THR:HG23	1:B:715:VAL:HG22	2.02	0.42
1:B:193:GLU:HG3	1:B:223:THR:CA	2.49	0.42
1:B:293:TYR:OH	1:B:343:VAL:HG23	2.20	0.42
1:B:372:LEU:HG	1:B:372:LEU:H	1.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:PHE:O	1:B:413:SER:C	2.58	0.42
1:A:259:ILE:O	1:A:260:ARG:HG3	2.19	0.42
1:A:305:LEU:O	1:A:309:SER:N	2.34	0.42
1:B:117:ILE:C	1:B:157:PRO:HG2	2.36	0.42
1:A:474:SER:OG	1:A:477:PHE:CD1	2.64	0.42
1:B:260:ARG:CG	1:B:556:GLU:HB3	2.49	0.42
1:B:480:GLY:O	1:B:557:THR:HA	2.20	0.42
1:B:125:THR:HG22	1:B:130:ILE:HD11	2.02	0.42
1:A:30:GLU:N	1:A:31:PRO:CD	2.83	0.42
1:B:444:PHE:C	1:B:447:PRO:HD2	2.40	0.42
1:B:374:ILE:O	1:B:377:VAL:HB	2.20	0.42
1:B:588:ARG:HD2	1:B:588:ARG:HA	1.75	0.42
1:A:537:ARG:HG3	1:A:538:LEU:H	1.84	0.42
1:B:116:ARG:NH1	1:B:118:VAL:HG13	2.35	0.42
1:A:165:LEU:CD2	1:A:182:LEU:HB3	2.50	0.42
1:B:570:ALA:O	1:B:571:VAL:C	2.57	0.42
1:B:308:THR:O	1:B:309:SER:C	2.58	0.42
1:B:24:LYS:HA	1:B:25:PRO:HD3	1.84	0.42
1:A:484:THR:O	1:A:554:ALA:O	2.37	0.42
1:A:543:LEU:O	1:A:547:GLU:HB2	2.20	0.42
1:B:349:ILE:O	1:B:350:LYS:C	2.57	0.41
1:A:323:LEU:CD1	1:A:328:ILE:N	2.69	0.41
1:A:372:LEU:H	1:A:372:LEU:HG	1.57	0.41
1:A:687:LEU:HD22	1:A:699:LEU:HA	2.01	0.41
1:A:687:LEU:CD1	1:A:699:LEU:HB2	2.50	0.41
1:B:719:LEU:O	1:B:720:VAL:C	2.57	0.41
1:A:258:GLU:HG3	1:A:259:ILE:N	2.34	0.41
1:B:600:ALA:O	1:B:604:ASP:OD2	2.37	0.41
1:B:14:VAL:O	1:B:17:LEU:HB2	2.20	0.41
1:B:76:ALA:O	1:B:78:PRO:HD3	2.20	0.41
1:B:290:PHE:CE1	1:B:299:LEU:N	2.88	0.41
1:B:333:LEU:HD13	1:B:403:LEU:HD11	2.02	0.41
1:B:403:LEU:HD12	1:B:403:LEU:HA	1.78	0.41
1:B:695:ARG:HD3	1:B:695:ARG:O	2.20	0.41
1:A:485:LEU:HB3	1:A:552:VAL:HB	2.00	0.41
1:A:372:LEU:HB3	1:A:588:ARG:HH22	1.85	0.41
1:A:160:LEU:N	1:A:160:LEU:HD23	2.34	0.41
1:B:46:VAL:HG12	1:B:257:ALA:HB3	2.02	0.41
1:B:581:ILE:O	1:B:585:VAL:HG23	2.19	0.41
1:A:308:THR:O	1:A:309:SER:C	2.58	0.41
1:B:16:LEU:CD2	1:B:17:LEU:HD23	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ALA:O	1:A:21:PHE:HB2	2.20	0.41
1:A:269:ASP:O	1:A:270:ALA:C	2.59	0.41
1:B:373:THR:O	1:B:374:ILE:C	2.58	0.41
1:A:344:LEU:O	1:A:345:SER:C	2.58	0.41
1:A:409:ALA:O	1:A:410:SER:C	2.58	0.41
1:B:663:ARG:HB3	1:B:663:ARG:HE	1.52	0.41
1:B:664:SER:CA	1:B:667:GLN:HE21	2.16	0.41
1:A:662:ASN:C	1:A:665:ILE:HG22	2.40	0.41
1:A:200:ILE:HG22	1:A:218:ILE:HG22	2.02	0.41
1:B:447:PRO:O	1:B:448:ALA:C	2.58	0.41
1:B:537:ARG:HG3	1:B:538:LEU:H	1.85	0.41
1:A:485:LEU:HB2	1:A:552:VAL:CA	2.26	0.41
1:A:391:TYR:N	1:A:391:TYR:CD1	2.88	0.41
1:A:581:ILE:O	1:A:585:VAL:HG23	2.20	0.41
1:A:588:ARG:HD2	1:A:588:ARG:HA	1.73	0.41
1:B:43:LEU:CB	1:B:92:LEU:HD22	2.50	0.41
1:A:366:GLY:O	1:A:367:PHE:C	2.59	0.41
1:A:47:LEU:C	1:A:48:GLU:HG3	2.39	0.41
1:B:595:VAL:HG12	1:B:599:LEU:CD1	2.51	0.41
1:A:16:LEU:CD2	1:A:17:LEU:HD23	2.51	0.41
1:B:30:GLU:N	1:B:31:PRO:CD	2.84	0.41
1:B:221:ALA:O	1:B:222:ILE:HD13	2.20	0.41
1:B:248:GLY:O	1:B:251:PRO:HD3	2.21	0.41
1:A:111:ALA:HB3	1:A:251:PRO:CB	2.50	0.41
1:B:118:VAL:CG1	1:B:154:ASP:O	2.68	0.41
1:A:290:PHE:CE1	1:A:299:LEU:N	2.89	0.41
1:A:299:LEU:O	1:A:303:LEU:HG	2.20	0.41
1:A:624:ILE:O	1:A:625:ALA:C	2.58	0.41
1:A:631:VAL:C	1:A:633:TYR:N	2.74	0.41
1:A:58:ASP:HA	1:A:61:LYS:HG3	2.03	0.41
1:A:564:GLU:O	1:A:565:GLU:C	2.59	0.41
1:A:126:THR:OG1	1:A:129:GLN:CG	2.68	0.41
1:A:100:GLN:O	1:A:101:ASP:C	2.57	0.41
1:B:377:VAL:HG13	1:B:636:ASN:CB	2.33	0.41
1:B:431:ILE:H	1:B:431:ILE:HG13	1.59	0.41
1:A:155:LEU:HD12	1:A:155:LEU:H	1.85	0.41
1:A:655:LEU:HA	1:A:656:PRO:HD3	1.84	0.41
1:B:493:VAL:HG13	1:B:512:ILE:HD13	2.02	0.41
1:B:276:ARG:HD2	1:B:689:LEU:HD11	2.01	0.41
1:B:456:LEU:HD23	1:B:456:LEU:HA	1.83	0.41
1:B:266:LEU:HD22	1:B:553:LEU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:VAL:O	1:A:341:GLY:N	2.54	0.41
1:A:115:PHE:HD2	1:A:204:LEU:HD21	1.84	0.41
1:A:497:ARG:HH21	1:A:508:LYS:HA	1.84	0.41
1:B:271:ILE:O	1:B:274:GLY:N	2.52	0.41
1:B:71:ASN:HB3	1:B:211:ARG:NH2	2.34	0.41
1:A:271:ILE:O	1:A:274:GLY:N	2.54	0.41
1:B:19:LEU:HA	1:B:22:VAL:CG1	2.50	0.41
1:A:106:LEU:O	1:A:109:GLN:HB3	2.20	0.41
1:B:102:ARG:O	1:B:106:LEU:HG	2.21	0.41
1:B:351:GLU:OE1	1:B:644:ARG:NH1	2.53	0.41
1:B:329:ALA:O	1:B:330:GLY:C	2.56	0.41
1:B:640:VAL:HG12	1:B:668:THR:HG23	2.02	0.41
1:A:116:ARG:HH22	1:A:155:LEU:HA	1.84	0.41
1:A:572:MET:O	1:A:576:VAL:HG23	2.20	0.41
1:A:595:VAL:HG12	1:A:599:LEU:HD11	2.02	0.41
1:B:491:VAL:HG12	1:B:496:LEU:HD21	2.02	0.41
1:B:89:VAL:HG22	1:B:90:VAL:N	2.36	0.41
1:A:480:GLY:O	1:A:557:THR:HA	2.20	0.41
1:A:92:LEU:N	1:A:92:LEU:CD1	2.84	0.41
1:B:121:GLY:O	1:B:150:ILE:HG23	2.19	0.41
1:B:326:PRO:HG2	1:B:395:PRO:C	2.41	0.41
1:B:624:ILE:O	1:B:625:ALA:C	2.57	0.41
1:B:674:MET:O	1:B:675:THR:C	2.60	0.41
1:B:409:ALA:O	1:B:410:SER:C	2.59	0.41
1:A:285:ILE:O	1:A:288:LEU:N	2.53	0.41
1:A:289:ILE:O	1:A:290:PHE:C	2.59	0.41
1:A:373:THR:O	1:A:374:ILE:C	2.58	0.41
1:A:695:ARG:O	1:A:695:ARG:HD3	2.21	0.41
1:A:704:GLY:O	1:A:708:GLY:N	2.28	0.41
1:A:283:LEU:O	1:A:284:ALA:C	2.58	0.41
1:A:334:THR:O	1:A:338:ALA:N	2.45	0.41
1:A:401:VAL:O	1:A:402:ILE:C	2.59	0.41
1:A:600:ALA:O	1:A:604:ASP:OD2	2.39	0.41
1:A:115:PHE:CE2	1:A:206:ILE:HG12	2.55	0.41
1:B:167:ASP:O	1:B:183:THR:CB	2.69	0.41
1:B:656:PRO:O	1:B:660:LEU:HB2	2.21	0.41
1:B:505:PHE:CD2	1:B:505:PHE:N	2.85	0.41
1:B:512:ILE:HD12	1:B:512:ILE:N	2.36	0.41
1:B:488:GLU:HB3	1:B:491:VAL:CG2	2.50	0.41
1:B:559:GLY:HA3	1:B:562:ILE:CG1	2.49	0.41
1:A:276:ARG:HD2	1:A:689:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:454:ALA:HA	1:B:457:LEU:HD12	2.03	0.41
1:B:599:LEU:O	1:B:600:ALA:C	2.57	0.41
1:A:453:ALA:O	1:A:456:LEU:HB2	2.21	0.41
1:A:129:GLN:H	1:A:129:GLN:HG2	1.68	0.41
1:A:23:TRP:O	1:A:24:LYS:C	2.59	0.41
1:A:248:GLY:O	1:A:251:PRO:HD3	2.20	0.41
1:B:75:VAL:HG21	1:B:95:LEU:HD11	2.01	0.41
1:B:687:LEU:CD1	1:B:699:LEU:HB2	2.51	0.41
1:B:485:LEU:O	1:B:524:GLU:HG3	2.21	0.41
1:B:151:LYS:CG	1:B:153:GLU:OE2	2.67	0.41
1:A:694:LEU:O	1:A:695:ARG:C	2.59	0.41
1:A:185:THR:HG23	1:A:186:PRO:HD2	2.03	0.41
1:B:160:LEU:HD23	1:B:160:LEU:N	2.36	0.41
1:A:559:GLY:HA3	1:A:562:ILE:CD1	2.51	0.41
1:A:67:GLU:O	1:A:70:ILE:CG2	2.65	0.41
1:B:453:ALA:O	1:B:456:LEU:HB2	2.20	0.41
1:B:572:MET:O	1:B:576:VAL:HG23	2.21	0.41
1:A:454:ALA:HA	1:A:457:LEU:HD12	2.03	0.41
1:A:14:VAL:O	1:A:17:LEU:HB2	2.21	0.41
1:B:422:LEU:HD12	1:B:422:LEU:HA	1.91	0.41
1:B:134:LEU:O	1:B:138:PRO:HA	2.21	0.41
1:B:289:ILE:HG12	1:B:290:PHE:N	2.36	0.40
1:A:574:VAL:O	1:A:575:LEU:C	2.60	0.40
1:A:622:PRO:O	1:A:625:ALA:CB	2.66	0.40
1:A:164:ASP:O	1:A:185:THR:N	2.54	0.40
1:B:657:TYR:O	1:B:661:VAL:N	2.46	0.40
1:B:268:GLN:HA	1:B:271:ILE:HG23	2.03	0.40
1:B:590:ASP:HB2	1:B:646:ARG:HH21	1.83	0.40
1:A:134:LEU:O	1:A:138:PRO:HA	2.21	0.40
1:A:116:ARG:NH1	1:A:118:VAL:HG13	2.36	0.40
1:A:576:VAL:O	1:A:579:GLY:N	2.54	0.40
1:A:585:VAL:CG1	1:A:594:GLY:HA2	2.51	0.40
1:B:164:ASP:O	1:B:185:THR:N	2.54	0.40
1:B:58:ASP:HA	1:B:61:LYS:HG3	2.04	0.40
1:B:257:ALA:CB	1:B:562:ILE:HD11	2.51	0.40
1:B:459:ALA:HB2	1:B:603:HIS:CD2	2.57	0.40
1:A:452:THR:HG23	1:A:715:VAL:HG22	2.04	0.40
1:B:126:THR:OG1	1:B:129:GLN:CG	2.69	0.40
1:A:717:SER:O	1:A:718:ALA:C	2.58	0.40
1:B:400:ALA:O	1:B:401:VAL:C	2.60	0.40
1:B:687:LEU:HD22	1:B:699:LEU:HA	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ASP:O	1:A:183:THR:CB	2.70	0.40
1:B:662:ASN:O	1:B:665:ILE:CG2	2.70	0.40
1:A:491:VAL:HG12	1:A:496:LEU:HD21	2.02	0.40
1:A:505:PHE:CD2	1:A:505:PHE:N	2.85	0.40
1:A:101:ASP:CA	1:A:104:LEU:HD12	2.43	0.40
1:A:644:ARG:O	1:A:648:ASN:HB2	2.21	0.40
1:B:484:THR:O	1:B:554:ALA:O	2.39	0.40
1:B:263:GLY:HA2	1:B:264:PRO:HD3	1.76	0.40
1:B:285:ILE:O	1:B:288:LEU:N	2.54	0.40
1:B:296:HIS:O	1:B:297:LEU:C	2.60	0.40
1:B:668:THR:O	1:B:671:ARG:CG	2.70	0.40
1:B:678:THR:HB	1:B:679:THR:H	1.54	0.40
1:B:533:SER:O	1:B:534:ASP:C	2.59	0.40
1:B:117:ILE:CD1	1:B:159:LEU:HD21	2.51	0.40
1:A:323:LEU:HD11	1:A:328:ILE:CG1	2.50	0.40
1:B:259:ILE:O	1:B:260:ARG:HG3	2.21	0.40
1:B:423:GLU:OE1	1:B:427:ASP:OD1	2.39	0.40
1:B:585:VAL:CG1	1:B:594:GLY:HA2	2.52	0.40
1:A:100:GLN:HG3	1:A:101:ASP:N	2.37	0.40
1:B:23:TRP:O	1:B:24:LYS:C	2.59	0.40
1:B:717:SER:O	1:B:718:ALA:C	2.59	0.40
1:B:269:ASP:O	1:B:270:ALA:C	2.59	0.40
1:B:293:TYR:CE2	1:B:350:LYS:HE3	2.57	0.40
1:B:347:GLU:CG	1:B:671:ARG:CD	2.91	0.40
1:B:37:LEU:C	1:B:39:LEU:N	2.74	0.40
1:B:626:ALA:O	1:B:627:LEU:C	2.59	0.40
1:A:580:LEU:O	1:A:583:LEU:HB3	2.22	0.40
1:A:582:LEU:HD21	1:A:598:ILE:HG21	2.03	0.40
1:A:687:LEU:CD2	1:A:699:LEU:HD12	2.39	0.40
1:B:165:LEU:CD2	1:B:182:LEU:HB3	2.50	0.40
1:A:89:VAL:HG22	1:A:90:VAL:N	2.35	0.40
1:A:423:GLU:OE1	1:A:427:ASP:OD1	2.40	0.40
1:A:648:ASN:O	1:A:651:LEU:CB	2.70	0.40
1:A:19:LEU:HA	1:A:22:VAL:CG1	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	715/741 (96%)	463 (65%)	193 (27%)	59 (8%)	1	8
1	B	715/741 (96%)	456 (64%)	198 (28%)	61 (8%)	1	7
All	All	1430/1482 (96%)	919 (64%)	391 (27%)	120 (8%)	1	7

All (120) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	PRO
1	A	76	ALA
1	A	331	LEU
1	A	410	SER
1	A	574	VAL
1	A	661	VAL
1	A	678	THR
1	A	692	SER
1	A	713	ILE
1	B	28	PRO
1	B	76	ALA
1	B	331	LEU
1	B	410	SER
1	B	574	VAL
1	B	661	VAL
1	B	678	THR
1	B	692	SER
1	B	713	ILE
1	A	102	ARG
1	A	231	GLY
1	A	280	ILE
1	A	296	HIS
1	A	300	VAL
1	A	376	ASP
1	A	386	ALA

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Mol	Chain	Res	Type
1	A	402	ILE
1	A	404	ALA
1	A	408	VAL
1	A	411	VAL
1	A	660	LEU
1	A	673	VAL
1	A	696	ASP
1	B	102	ARG
1	B	231	GLY
1	B	296	HIS
1	B	300	VAL
1	B	376	ASP
1	B	386	ALA
1	B	402	ILE
1	B	404	ALA
1	B	408	VAL
1	B	411	VAL
1	B	632	GLY
1	B	660	LEU
1	B	673	VAL
1	B	696	ASP
1	A	101	ASP
1	A	270	ALA
1	A	278	ALA
1	A	332	VAL
1	A	340	ASP
1	A	368	ARG
1	A	375	MET
1	A	377	VAL
1	A	502	GLU
1	A	565	GLU
1	A	632	GLY
1	A	700	ALA
1	B	101	ASP
1	B	270	ALA
1	B	278	ALA
1	B	280	ILE
1	B	332	VAL
1	B	340	ASP
1	B	368	ARG
1	B	375	MET
1	B	377	VAL

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Mol	Chain	Res	Type
1	B	502	GLU
1	B	565	GLU
1	B	700	ALA
1	A	10	PHE
1	A	93	PRO
1	A	156	GLY
1	A	450	TYR
1	A	567	ARG
1	A	581	ILE
1	A	640	VAL
1	B	10	PHE
1	B	93	PRO
1	B	156	GLY
1	B	287	LEU
1	B	450	TYR
1	B	567	ARG
1	B	571	VAL
1	A	276	ARG
1	A	287	LEU
1	A	571	VAL
1	A	573	ALA
1	A	677	LEU
1	A	709	THR
1	B	276	ARG
1	B	573	ALA
1	B	578	LEU
1	B	581	ILE
1	B	605	VAL
1	B	640	VAL
1	B	677	LEU
1	B	709	THR
1	A	244	VAL
1	A	538	LEU
1	A	605	VAL
1	A	717	SER
1	B	344	LEU
1	B	538	LEU
1	A	298	GLY
1	B	244	VAL
1	A	294	GLY
1	A	295	PRO
1	B	65	VAL

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Mol	Chain	Res	Type
1	B	298	GLY
1	A	65	VAL
1	A	560	PRO
1	B	295	PRO
1	B	560	PRO
1	B	635	ILE
1	A	635	ILE
1	B	117	ILE
1	B	576	VAL
1	A	117	ILE
1	B	693	VAL

5.3.2 Protein sidechains ⓘ

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	581/597 (97%)	496 (85%)	85 (15%)	4	18
1	B	581/597 (97%)	497 (86%)	84 (14%)	4	18
All	All	1162/1194 (97%)	993 (86%)	169 (14%)	4	18

All (169) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LEU
1	A	22	VAL
1	A	26	TRP
1	A	34	ARG
1	A	45	ILE
1	A	47	LEU
1	A	63	ARG
1	A	68	ASN
1	A	70	ILE
1	A	80	ILE
1	A	88	ILE
1	A	99	ASP

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Mol	Chain	Res	Type
1	A	100	GLN
1	A	107	ILE
1	A	116	ARG
1	A	123	THR
1	A	126	THR
1	A	129	GLN
1	A	143	GLU
1	A	148	ASP
1	A	151	LYS
1	A	155	LEU
1	A	164	ASP
1	A	165	LEU
1	A	167	ASP
1	A	196	THR
1	A	209	ASP
1	A	220	GLN
1	A	229	ILE
1	A	247	SER
1	A	265	THR
1	A	271	ILE
1	A	289	ILE
1	A	296	HIS
1	A	297	LEU
1	A	299	LEU
1	A	324	THR
1	A	359	LEU
1	A	361	GLN
1	A	388	LEU
1	A	402	ILE
1	A	403	LEU
1	A	414	ASN
1	A	437	LEU
1	A	441	ARG
1	A	442	PHE
1	A	443	ASN
1	A	471	PHE
1	A	473	TYR
1	A	477	PHE
1	A	512	ILE
1	A	514	GLN
1	A	526	LEU
1	A	528	LYS

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Mol	Chain	Res	Type
1	A	532	LEU
1	A	543	LEU
1	A	590	ASP
1	A	598	ILE
1	A	607	ILE
1	A	620	SER
1	A	628	LEU
1	A	629	THR
1	A	630	ILE
1	A	634	SER
1	A	636	ASN
1	A	637	ASP
1	A	641	VAL
1	A	642	SER
1	A	651	LEU
1	A	654	HIS
1	A	662	ASN
1	A	663	ARG
1	A	670	SER
1	A	671	ARG
1	A	676	SER
1	A	679	THR
1	A	680	LEU
1	A	683	ILE
1	A	684	LEU
1	A	693	VAL
1	A	695	ARG
1	A	705	ILE
1	A	711	SER
1	A	713	ILE
1	A	723	TRP
1	B	16	LEU
1	B	22	VAL
1	B	26	TRP
1	B	34	ARG
1	B	45	ILE
1	B	47	LEU
1	B	63	ARG
1	B	68	ASN
1	B	70	ILE
1	B	80	ILE
1	B	88	ILE

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Mol	Chain	Res	Type
1	B	99	ASP
1	B	100	GLN
1	B	107	ILE
1	B	116	ARG
1	B	123	THR
1	B	126	THR
1	B	129	GLN
1	B	143	GLU
1	B	148	ASP
1	B	151	LYS
1	B	155	LEU
1	B	164	ASP
1	B	165	LEU
1	B	196	THR
1	B	209	ASP
1	B	220	GLN
1	B	229	ILE
1	B	247	SER
1	B	265	THR
1	B	271	ILE
1	B	289	ILE
1	B	296	HIS
1	B	297	LEU
1	B	299	LEU
1	B	324	THR
1	B	359	LEU
1	B	361	GLN
1	B	388	LEU
1	B	402	ILE
1	B	403	LEU
1	B	414	ASN
1	B	437	LEU
1	B	441	ARG
1	B	442	PHE
1	B	443	ASN
1	B	471	PHE
1	B	473	TYR
1	B	477	PHE
1	B	512	ILE
1	B	514	GLN
1	B	526	LEU
1	B	528	LYS

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Mol	Chain	Res	Type
1	B	532	LEU
1	B	543	LEU
1	B	590	ASP
1	B	598	ILE
1	B	607	ILE
1	B	620	SER
1	B	628	LEU
1	B	629	THR
1	B	630	ILE
1	B	634	SER
1	B	636	ASN
1	B	637	ASP
1	B	641	VAL
1	B	642	SER
1	B	651	LEU
1	B	654	HIS
1	B	662	ASN
1	B	663	ARG
1	B	670	SER
1	B	671	ARG
1	B	676	SER
1	B	679	THR
1	B	680	LEU
1	B	683	ILE
1	B	684	LEU
1	B	693	VAL
1	B	695	ARG
1	B	705	ILE
1	B	711	SER
1	B	713	ILE
1	B	723	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	GLN
1	A	272	GLN
1	A	296	HIS
1	A	414	ASN
1	A	420	HIS
1	A	569	ASN
1	A	662	ASN

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Mol	Chain	Res	Type
1	A	667	GLN
1	B	68	ASN
1	B	129	GLN
1	B	272	GLN
1	B	296	HIS
1	B	414	ASN
1	B	420	HIS
1	B	569	ASN
1	B	662	ASN
1	B	667	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	719/741 (97%)	-0.43	7 (0%) 84 80	31, 111, 181, 242	0
1	B	719/741 (97%)	-0.40	8 (1%) 82 78	33, 111, 184, 240	0
All	All	1438/1482 (97%)	-0.41	15 (1%) 84 80	31, 111, 183, 242	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	213	TYR	3.7
1	A	122	ALA	3.5
1	A	511	VAL	3.3
1	A	34	ARG	3.2
1	A	123	THR	3.0
1	B	483	TYR	2.8
1	B	714	TYR	2.6
1	A	213	TYR	2.5
1	B	415	LEU	2.5
1	A	483	TYR	2.4
1	A	549	LYS	2.2
1	B	192	PHE	2.1
1	B	180	VAL	2.0
1	B	256	VAL	2.0
1	B	182	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.