



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 09:36 PM UTC

PDB ID : 4DJI / pdb_00004dji
Title : Structure of glutamate-GABA antiporter GadC
Authors : Ma, D.; Lu, P.L.; Yan, C.Y.; Fan, C.; Yin, P.; Wang, J.W.; Shi, Y.G.
Deposited on : 2012-02-02
Resolution : 3.19 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

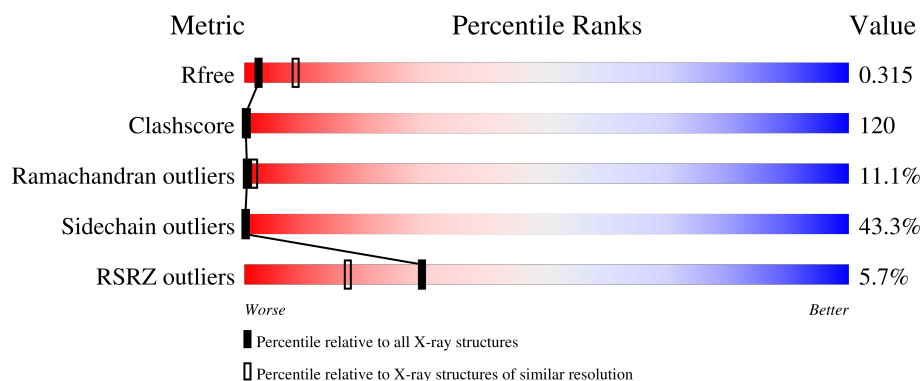
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 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}	180053	2001 (3.20-3.16)
Clashscore	190562	2119 (3.20-3.16)
Ramachandran outliers	187476	2070 (3.20-3.16)
Sidechain outliers	187428	2069 (3.20-3.16)
RSRZ outliers	180081	2001 (3.20-3.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	511	
1	B	511	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7342 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.

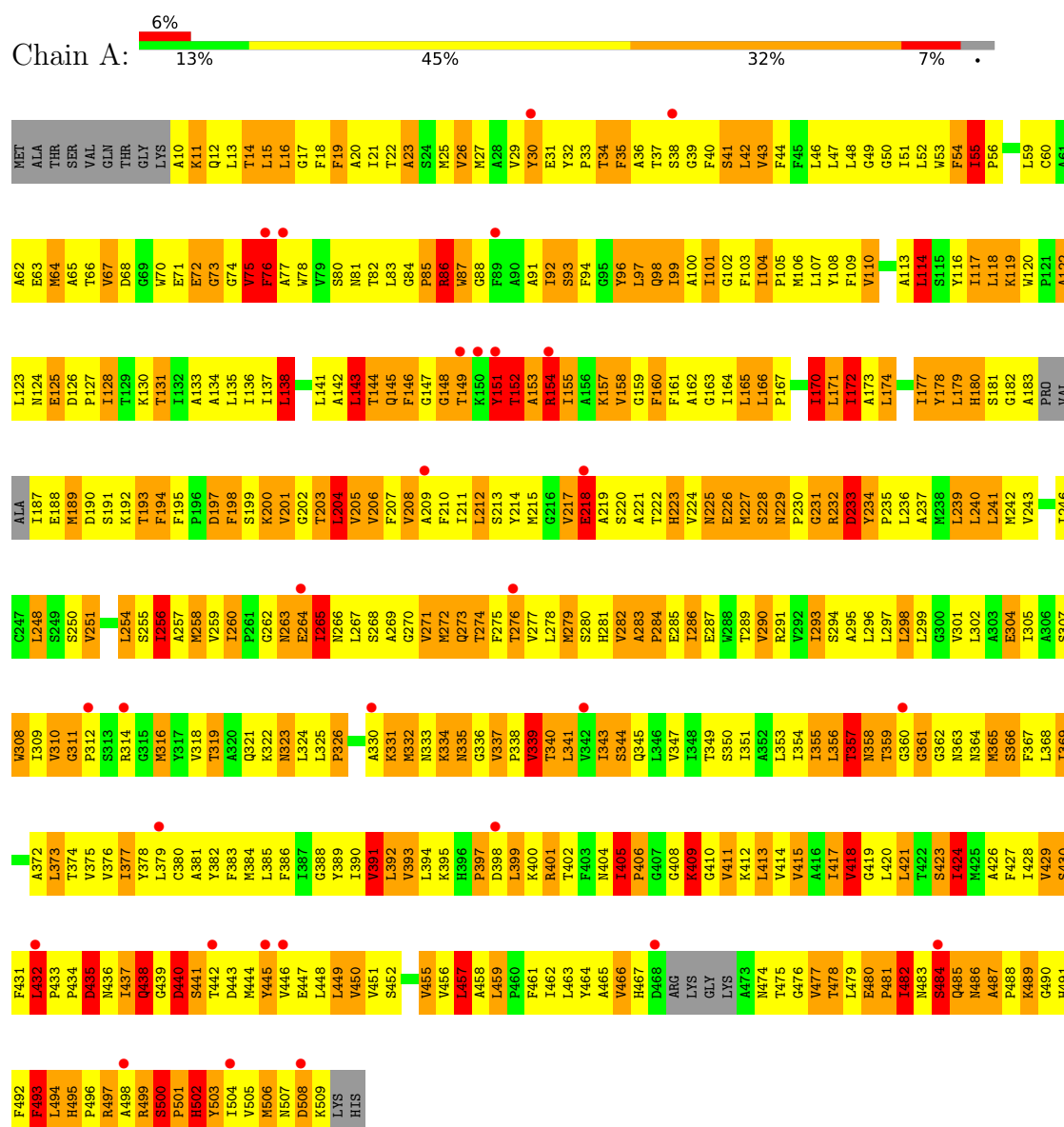
- Molecule 1 is a protein called Probable glutamate/gamma-aminobutyrate antiporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	493	Total	C	N	O	S	0	0	0
			3732	2493	581	636	22			
1	B	480	Total	C	N	O	S	0	0	0
			3610	2417	556	616	21			

3 Residue-property plots

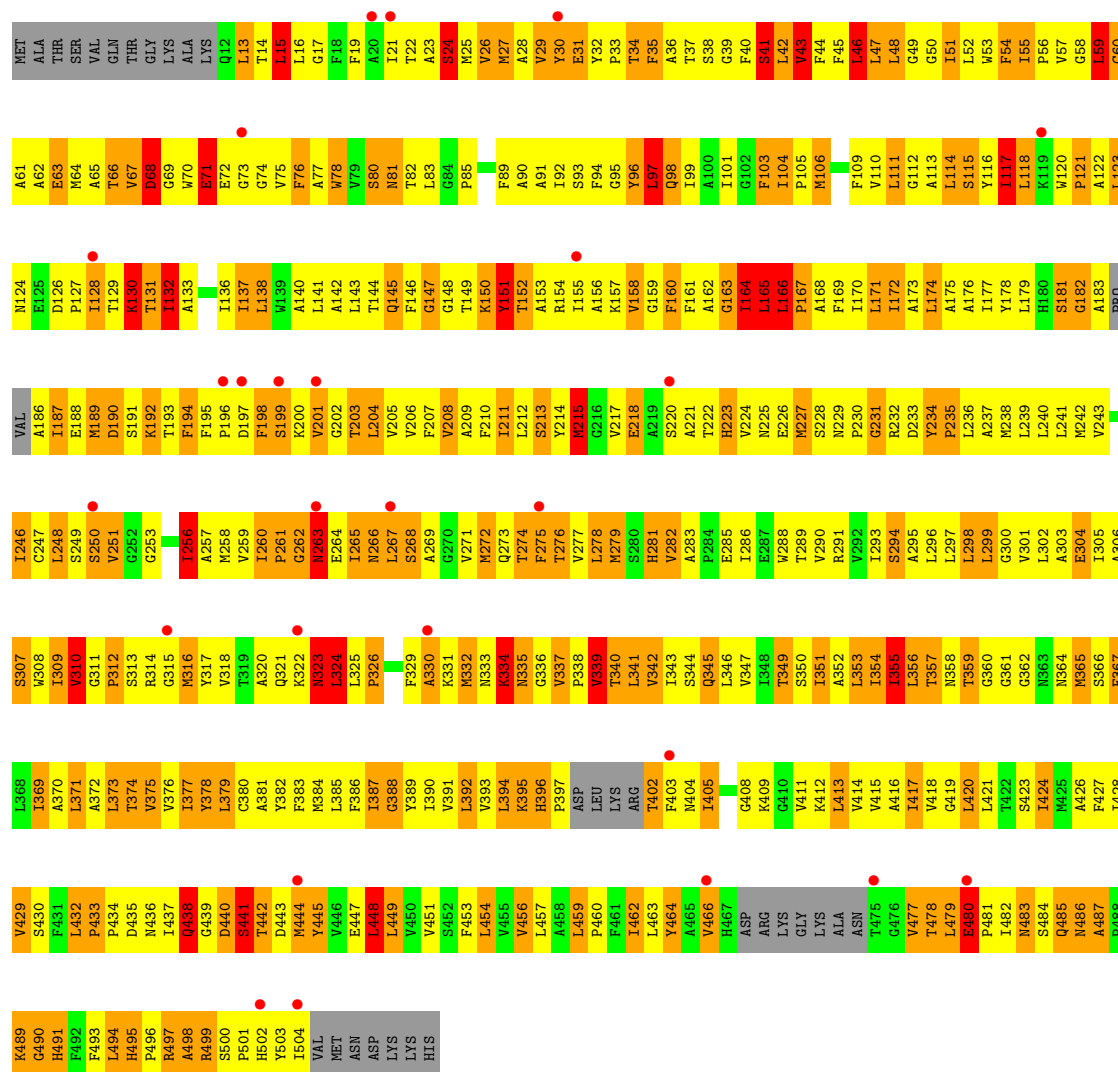
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Probable glutamate/gamma-aminobutyrate antiporter



- Molecule 1: Probable glutamate/gamma-aminobutyrate antiporter





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.62Å 105.42Å 188.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.52 – 3.19 35.52 – 3.19	Depositor EDS
% Data completeness (in resolution range)	84.2 (35.52-3.19) 84.6 (35.52-3.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 3.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.310 , 0.328 0.302 , 0.315	Depositor DCC
R_{free} test set	1138 reflections (4.25%)	wwPDB-VP
Wilson B-factor (Å ²)	107.4	Xtriage
Anisotropy	0.971	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 76.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7342	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.02	0/3826	1.17	40/5222 (0.8%)
1	B	0.90	0/3700	1.14	39/5054 (0.8%)
All	All	0.96	0/7526	1.16	79/10276 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	TYR	N-CA-C	10.27	132.52	109.81
1	A	482	ILE	CB-CA-C	-9.57	96.09	110.82
1	A	234	TYR	CB-CA-C	-8.68	93.07	110.17
1	A	193	THR	N-CA-C	-8.60	102.91	112.72
1	B	42	LEU	CB-CA-C	-8.52	97.84	110.96
1	A	495	HIS	N-CA-C	8.38	120.20	109.65
1	B	263	ASN	N-CA-C	-8.29	103.17	113.20
1	A	499	ARG	N-CA-C	-8.29	98.81	110.50
1	B	153	ALA	N-CA-C	-8.27	102.45	112.54
1	A	256	ILE	CB-CA-C	-8.14	101.14	112.14
1	B	132	ILE	CB-CA-C	-7.99	101.74	111.97
1	A	198	PHE	N-CA-C	-7.99	103.53	113.20
1	B	137	ILE	N-CA-C	7.76	118.35	110.82
1	A	201	VAL	N-CA-C	7.73	117.84	110.42
1	B	94	PHE	N-CA-C	7.68	119.34	110.97
1	B	41	SER	CB-CA-C	7.65	125.65	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	137	ILE	CB-CA-C	-7.65	102.02	112.04
1	B	443	ASP	N-CA-C	-7.49	104.64	114.31
1	B	262	GLY	N-CA-C	-7.38	104.65	114.25
1	A	443	ASP	N-CA-C	-7.18	104.67	113.50
1	A	418	VAL	CB-CA-C	-7.02	102.99	111.97
1	B	43	VAL	N-CA-C	-6.99	103.66	110.72
1	B	24	SER	N-CA-C	-6.89	104.99	113.19
1	A	493	PHE	N-CA-C	-6.82	104.83	113.02
1	A	405	ILE	N-CA-C	-6.75	101.54	108.96
1	A	170	ILE	O-C-N	-6.67	113.24	122.31
1	B	432	LEU	CA-C-N	6.60	127.18	120.38
1	B	432	LEU	C-N-CA	6.60	127.18	120.38
1	B	256	ILE	CB-CA-C	-6.59	103.44	111.88
1	A	76	PHE	N-CA-C	-6.49	103.71	111.69
1	A	114	LEU	N-CA-C	-6.46	103.36	111.11
1	A	500	SER	N-CA-C	-6.41	102.62	110.31
1	A	263	ASN	N-CA-C	6.38	118.23	111.28
1	A	138	LEU	CB-CA-C	-6.04	101.65	110.96
1	A	204	LEU	N-CA-C	5.99	117.89	111.36
1	A	151	TYR	N-CA-C	5.97	118.94	111.24
1	B	165	LEU	N-CA-C	5.96	117.86	111.36
1	A	339	VAL	CB-CA-C	-5.88	104.48	110.88
1	B	339	VAL	CB-CA-C	-5.87	104.48	110.88
1	B	160	PHE	N-CA-C	-5.81	104.85	111.07
1	B	388	GLY	N-CA-C	-5.79	107.16	114.16
1	B	215	MET	CG-SD-CE	5.78	113.62	100.90
1	A	87	TRP	N-CA-C	5.73	117.61	111.36
1	A	122	ALA	N-CA-C	-5.71	105.64	113.30
1	A	265	ILE	CB-CA-C	-5.64	102.39	111.59
1	A	435	ASP	N-CA-CB	-5.61	108.50	114.10
1	A	75	VAL	CB-CA-C	-5.58	102.13	111.29
1	A	267	LEU	N-CA-C	5.55	117.33	111.28
1	A	138	LEU	N-CA-C	5.51	116.98	110.97
1	A	23	ALA	N-CA-C	-5.50	106.41	113.01
1	B	117	ILE	CB-CA-C	-5.49	104.73	112.14
1	B	355	ILE	N-CA-C	5.48	115.69	110.53
1	B	497	ARG	N-CA-C	-5.46	105.33	111.28
1	B	132	ILE	N-CA-C	5.44	115.64	110.42
1	A	488	PRO	N-CA-C	-5.40	103.65	111.22
1	A	262	GLY	N-CA-C	5.38	119.18	112.73
1	B	42	LEU	N-CA-C	5.36	116.81	110.97
1	A	35	PHE	N-CA-C	-5.30	105.96	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	441	SER	N-CA-C	5.30	117.25	108.13
1	B	35	PHE	CB-CA-C	-5.30	102.53	110.90
1	B	309	ILE	CB-CA-C	-5.26	104.00	112.16
1	B	448	LEU	N-CA-C	5.22	116.83	111.03
1	A	256	ILE	N-CA-C	-5.21	105.30	110.62
1	B	480	GLU	CA-C-N	5.21	125.11	119.85
1	B	480	GLU	C-N-CA	5.21	125.11	119.85
1	B	498	ALA	N-CA-C	5.20	117.03	111.36
1	A	391	VAL	N-CA-C	-5.19	105.44	110.42
1	B	359	THR	N-CA-C	5.17	117.01	108.49
1	B	152	THR	CA-C-N	5.16	129.34	120.72
1	B	152	THR	C-N-CA	5.16	129.34	120.72
1	A	201	VAL	CB-CA-C	-5.16	105.37	111.97
1	B	165	LEU	CB-CA-C	-5.13	102.12	110.85
1	A	432	LEU	CA-C-N	5.08	125.61	120.38
1	A	432	LEU	C-N-CA	5.08	125.61	120.38
1	B	163	GLY	N-CA-C	5.07	125.20	113.18
1	A	37	THR	N-CA-C	-5.05	105.77	111.28
1	A	412	LYS	N-CA-C	-5.04	105.67	111.07
1	B	15	LEU	N-CA-C	-5.01	105.82	111.28
1	B	375	VAL	N-CA-C	5.01	116.33	110.62

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	170	ILE	Mainchain
1	A	75	VAL	Peptide

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	3732	0	3867	915	0
1	B	3610	0	3738	881	0
All	All	7342	0	7605	1787	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 120.

All (1787) 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:157:LYS:HG2	1:A:493:PHE:CD2	1.38	1.57
1:A:117:ILE:HG22	1:A:118:LEU:CD1	1.33	1.55
1:B:395:LYS:CE	1:B:396:HIS:HE1	1.18	1.53
1:A:160:PHE:CE1	1:A:165:LEU:HD23	1.46	1.51
1:A:202:GLY:CA	1:A:434:PRO:HG3	1.05	1.49
1:B:55:ILE:CG2	1:B:56:PRO:HD3	1.00	1.46
1:A:202:GLY:HA3	1:A:434:PRO:CG	1.00	1.45
1:B:395:LYS:HE2	1:B:396:HIS:CE1	1.49	1.44
1:B:55:ILE:HG22	1:B:56:PRO:CD	0.97	1.43
1:B:15:LEU:HD23	1:B:16:LEU:N	1.35	1.37
1:B:53:TRP:CH2	1:B:382:TYR:CE1	2.10	1.37
1:B:395:LYS:CE	1:B:396:HIS:CE1	2.06	1.35
1:B:447:GLU:O	1:B:451:VAL:HG23	1.29	1.33
1:B:160:PHE:CE1	1:B:165:LEU:HD21	1.64	1.31
1:B:15:LEU:CD2	1:B:16:LEU:N	1.95	1.30
1:A:457:LEU:HD12	1:A:457:LEU:O	1.34	1.25
1:B:15:LEU:HD23	1:B:15:LEU:C	1.55	1.25
1:A:15:LEU:HD23	1:A:15:LEU:C	1.58	1.24
1:A:154:ARG:NH2	1:A:489:LYS:HE3	1.47	1.24
1:A:117:ILE:CG2	1:A:118:LEU:CD1	2.16	1.22
1:B:432:LEU:HD12	1:B:432:LEU:O	1.36	1.21
1:A:347:VAL:CG1	1:A:351:ILE:HD11	1.70	1.20
1:A:215:MET:CE	1:A:378:TYR:HB3	1.72	1.20
1:A:143:LEU:HD12	1:A:143:LEU:C	1.55	1.19
1:A:386:PHE:O	1:A:390:ILE:HD12	1.42	1.19
1:A:339:VAL:O	1:A:343:ILE:HG23	1.42	1.19
1:A:154:ARG:HH21	1:A:489:LYS:CG	1.53	1.19
1:A:491:HIS:O	1:A:494:LEU:HB2	1.40	1.18
1:B:53:TRP:CZ2	1:B:382:TYR:CD1	2.32	1.18
1:B:286:ILE:HG22	1:B:289:THR:CG2	1.73	1.18
1:A:154:ARG:NH2	1:A:489:LYS:CE	2.07	1.17
1:B:124:ASN:O	1:B:130:LYS:HE2	1.41	1.17
1:A:224:VAL:O	1:A:227:MET:HB2	1.45	1.17
1:A:117:ILE:CG2	1:A:118:LEU:HD12	1.74	1.16
1:A:76:PHE:HB2	1:A:92:ILE:HG13	1.23	1.15
1:A:215:MET:HE2	1:A:378:TYR:HB3	1.25	1.15
1:A:15:LEU:HD22	1:A:16:LEU:HD23	1.22	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ALA:CB	1:A:353:LEU:HD21	1.77	1.15
1:A:160:PHE:CE1	1:A:165:LEU:CD2	2.30	1.15
1:A:172:ILE:CD1	1:A:251:VAL:HG11	1.77	1.15
1:A:347:VAL:O	1:A:351:ILE:HG13	1.44	1.14
1:A:477:VAL:HG11	1:A:506:MET:HB3	1.26	1.14
1:B:41:SER:HB3	1:B:196:PRO:HG3	1.25	1.14
1:A:449:LEU:HD12	1:A:449:LEU:O	1.41	1.14
1:A:485:GLN:NE2	1:A:485:GLN:HA	1.47	1.14
1:A:145:GLN:HA	1:A:145:GLN:NE2	1.61	1.13
1:A:157:LYS:CG	1:A:493:PHE:HD2	1.62	1.13
1:A:397:PRO:HD2	1:A:398:ASP:H	1.11	1.13
1:B:262:GLY:HA2	1:B:265:ILE:HG13	1.31	1.13
1:A:75:VAL:HG12	1:A:78:TRP:CE3	1.83	1.12
1:A:125:GLU:O	1:A:127:PRO:HD3	1.45	1.12
1:A:128:ILE:HD12	1:A:128:ILE:O	1.48	1.12
1:A:259:VAL:HG21	1:A:278:LEU:HD21	1.13	1.12
1:B:489:LYS:CD	1:B:489:LYS:H	1.62	1.12
1:B:170:ILE:HG22	1:B:275:PHE:CZ	1.85	1.12
1:B:99:ILE:CD1	1:B:312:PRO:HG3	1.80	1.11
1:B:485:GLN:NE2	1:B:485:GLN:HA	1.47	1.11
1:B:166:LEU:HB3	1:B:167:PRO:HD3	1.18	1.11
1:A:432:LEU:O	1:A:432:LEU:HD12	1.52	1.10
1:B:204:LEU:HD23	1:B:204:LEU:N	1.60	1.10
1:A:286:ILE:HG22	1:A:289:THR:HB	1.29	1.09
1:B:53:TRP:CZ2	1:B:382:TYR:CE1	2.38	1.09
1:A:157:LYS:CG	1:A:493:PHE:CD2	2.33	1.09
1:A:154:ARG:HH21	1:A:489:LYS:HG3	1.13	1.09
1:B:47:LEU:HD23	1:B:246:ILE:HD11	1.12	1.09
1:B:215:MET:HE3	1:B:378:TYR:HB3	1.29	1.09
1:B:323:ASN:O	1:B:324:LEU:HD13	1.52	1.08
1:A:44:PHE:HB2	1:A:194:PHE:CE2	1.89	1.07
1:A:203:THR:HG22	1:A:204:LEU:HD23	1.30	1.07
1:B:99:ILE:HD13	1:B:312:PRO:HG3	1.18	1.07
1:B:34:THR:O	1:B:37:THR:HG22	1.53	1.07
1:A:364:ASN:ND2	1:A:438:GLN:HG3	1.70	1.07
1:A:495:HIS:HD2	1:A:497:ARG:HB2	1.18	1.07
1:A:149:THR:CG2	1:A:314:ARG:HH22	1.66	1.06
1:A:337:VAL:O	1:A:337:VAL:HG22	1.56	1.06
1:B:229:ASN:O	1:B:233:ASP:HB2	1.51	1.06
1:B:215:MET:CE	1:B:378:TYR:HB3	1.85	1.06
1:B:489:LYS:N	1:B:489:LYS:HD2	1.54	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ARG:HH21	1:A:489:LYS:CD	1.67	1.06
1:A:272:MET:HE1	1:A:297:LEU:HD12	1.36	1.06
1:B:286:ILE:CG2	1:B:289:THR:CG2	2.33	1.05
1:A:330:ALA:O	1:A:331:LYS:HG2	1.55	1.05
1:B:57:VAL:O	1:B:61:ALA:HB2	1.57	1.05
1:B:160:PHE:HE1	1:B:165:LEU:HD21	0.89	1.05
1:B:337:VAL:O	1:B:337:VAL:HG22	1.55	1.04
1:A:75:VAL:HG12	1:A:78:TRP:CZ3	1.91	1.04
1:B:31:GLU:C	1:B:33:PRO:HD2	1.82	1.04
1:B:161:PHE:CD1	1:B:165:LEU:CD1	2.40	1.04
1:A:15:LEU:CD2	1:A:16:LEU:HD23	1.87	1.04
1:B:36:ALA:HB1	1:B:257:ALA:HB2	1.37	1.03
1:A:234:TYR:HB3	1:A:235:PRO:HD3	1.40	1.03
1:A:117:ILE:O	1:A:291:ARG:NH2	1.92	1.03
1:A:421:LEU:HD11	1:B:424:ILE:HD12	1.40	1.03
1:B:286:ILE:HG22	1:B:289:THR:HG22	1.35	1.03
1:B:501:PRO:O	1:B:502:HIS:HD2	1.42	1.02
1:A:98:GLN:HB2	1:A:377:ILE:HG22	1.41	1.02
1:B:27:MET:HE1	1:B:248:LEU:HG	1.42	1.02
1:B:395:LYS:HE3	1:B:396:HIS:CE1	1.91	1.02
1:A:15:LEU:C	1:A:15:LEU:CD2	2.32	1.01
1:A:353:LEU:O	1:A:357:THR:HG23	1.60	1.01
1:A:157:LYS:O	1:A:161:PHE:HD1	1.42	1.01
1:A:272:MET:CE	1:A:297:LEU:HD12	1.91	1.00
1:B:99:ILE:HD13	1:B:312:PRO:CG	1.90	1.00
1:A:55:ILE:HB	1:A:56:PRO:HD3	1.42	1.00
1:A:74:GLY:O	1:A:75:VAL:HG13	1.61	1.00
1:A:202:GLY:HA3	1:A:434:PRO:CD	1.89	1.00
1:A:74:GLY:O	1:A:75:VAL:HG22	1.61	1.00
1:B:36:ALA:HB2	1:B:253:GLY:O	1.59	1.00
1:B:53:TRP:CH2	1:B:382:TYR:HE1	1.73	1.00
1:B:35:PHE:O	1:B:42:LEU:HD21	1.61	1.00
1:A:21:ILE:HB	1:A:492:PHE:CE2	1.95	1.00
1:B:166:LEU:CD1	1:B:166:LEU:C	2.30	1.00
1:B:194:PHE:CE1	1:B:195:PHE:CE2	2.49	1.00
1:B:67:VAL:HG21	1:B:70:TRP:CE3	1.96	1.00
1:B:98:GLN:OE1	1:B:99:ILE:HG13	1.62	1.00
1:B:266:ASN:HD22	1:B:266:ASN:C	1.70	1.00
1:B:308:TRP:NE1	1:B:498:ALA:HB2	1.75	1.00
1:B:47:LEU:HD23	1:B:246:ILE:CD1	1.91	0.99
1:B:160:PHE:HE1	1:B:165:LEU:CD2	1.74	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ASN:HA	1:A:130:LYS:HE2	1.42	0.99
1:B:53:TRP:HH2	1:B:382:TYR:CE1	1.76	0.99
1:A:347:VAL:HG13	1:A:351:ILE:HD11	1.43	0.99
1:B:166:LEU:HB3	1:B:167:PRO:CD	1.92	0.99
1:A:397:PRO:CD	1:A:398:ASP:H	1.74	0.99
1:B:41:SER:O	1:B:44:PHE:HB3	1.62	0.99
1:B:166:LEU:C	1:B:166:LEU:HD12	1.86	0.99
1:B:187:ILE:O	1:B:187:ILE:HG22	1.59	0.99
1:B:321:GLN:HE22	1:B:479:LEU:CD2	1.76	0.99
1:A:21:ILE:HB	1:A:492:PHE:CD2	1.97	0.99
1:B:42:LEU:O	1:B:46:LEU:HB2	1.60	0.99
1:B:141:LEU:CD1	1:B:306:ALA:HB2	1.91	0.99
1:B:310:VAL:HG22	1:B:310:VAL:O	1.62	0.99
1:B:109:PHE:HD2	1:B:301:VAL:HG21	1.28	0.98
1:B:145:GLN:HA	1:B:145:GLN:HE21	1.20	0.98
1:B:161:PHE:CD1	1:B:165:LEU:HD11	1.99	0.98
1:A:26:VAL:CG1	1:A:248:LEU:HD23	1.93	0.98
1:B:359:THR:O	1:B:359:THR:HG22	1.64	0.98
1:A:172:ILE:HD12	1:A:251:VAL:HG11	1.41	0.98
1:A:250:SER:O	1:A:254:LEU:HD12	1.63	0.98
1:B:30:TYR:CE1	1:B:301:VAL:HG22	1.98	0.98
1:A:506:MET:O	1:A:509:LYS:HD3	1.63	0.98
1:A:134:ALA:HB1	1:A:353:LEU:HD21	1.42	0.98
1:A:264:GLU:HA	1:A:264:GLU:OE2	1.61	0.98
1:B:25:MET:HB2	1:B:495:HIS:CE1	1.99	0.98
1:B:489:LYS:H	1:B:489:LYS:HD2	1.08	0.98
1:B:63:GLU:OE1	1:B:405:ILE:HG13	1.64	0.97
1:A:372:ALA:O	1:A:376:VAL:HG22	1.63	0.97
1:A:483:ASN:O	1:A:485:GLN:N	1.95	0.97
1:B:161:PHE:HD1	1:B:165:LEU:HD12	1.28	0.97
1:A:483:ASN:C	1:A:485:GLN:H	1.72	0.97
1:B:196:PRO:HB2	1:B:198:PHE:CE1	1.98	0.97
1:A:215:MET:HE2	1:A:378:TYR:CB	1.93	0.97
1:B:25:MET:CB	1:B:495:HIS:HE1	1.76	0.97
1:B:76:PHE:C	1:B:76:PHE:CD2	2.43	0.96
1:A:116:TYR:CD1	1:A:272:MET:HB2	2.00	0.96
1:A:364:ASN:HD22	1:A:438:GLN:HG3	1.28	0.96
1:B:96:TYR:CD2	1:B:97:LEU:HD23	2.00	0.96
1:B:151:TYR:CD1	1:B:151:TYR:N	2.30	0.96
1:A:25:MET:HE2	1:A:496:PRO:HG2	1.47	0.96
1:A:486:ASN:HB3	1:A:503:TYR:OH	1.64	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:PHE:HD1	1:B:195:PHE:CD2	1.83	0.96
1:B:70:TRP:CH2	1:B:392:LEU:HD11	1.99	0.96
1:B:362:GLY:H	1:B:440:ASP:HB3	1.28	0.96
1:A:485:GLN:HA	1:A:485:GLN:HE21	1.26	0.96
1:A:67:VAL:HG12	1:A:70:TRP:HB2	1.46	0.96
1:A:135:LEU:CD2	1:A:350:SER:OG	2.14	0.95
1:A:154:ARG:HH22	1:A:489:LYS:CE	1.75	0.95
1:B:82:THR:HG21	1:B:388:GLY:O	1.65	0.95
1:A:431:PHE:O	1:A:446:VAL:HG22	1.65	0.95
1:B:194:PHE:CD1	1:B:195:PHE:CD2	2.54	0.95
1:A:118:LEU:CD1	1:A:118:LEU:N	2.30	0.95
1:B:194:PHE:HD1	1:B:195:PHE:HD2	1.03	0.95
1:A:22:THR:CG2	1:A:25:MET:HE3	1.95	0.95
1:A:478:THR:OG1	1:A:505:VAL:CG2	2.15	0.95
1:A:421:LEU:CD1	1:B:424:ILE:HD12	1.96	0.95
1:A:485:GLN:NE2	1:A:485:GLN:CA	2.30	0.95
1:B:194:PHE:HE1	1:B:195:PHE:CE2	1.83	0.95
1:A:134:ALA:HB3	1:A:353:LEU:HD21	1.49	0.94
1:A:143:LEU:C	1:A:143:LEU:CD1	2.30	0.94
1:A:73:GLY:HA3	1:A:77:ALA:CB	1.97	0.94
1:A:73:GLY:HA3	1:A:77:ALA:HB2	1.49	0.94
1:B:283:ALA:HB1	1:B:286:ILE:HD12	1.46	0.94
1:A:143:LEU:HG	1:A:144:THR:N	1.77	0.94
1:A:160:PHE:HE1	1:A:165:LEU:HD23	1.29	0.94
1:B:53:TRP:HZ2	1:B:382:TYR:CD1	1.83	0.94
1:B:99:ILE:CD1	1:B:312:PRO:CG	2.46	0.94
1:B:109:PHE:CD2	1:B:301:VAL:HG21	2.02	0.94
1:B:215:MET:HE3	1:B:378:TYR:CB	1.95	0.94
1:B:372:ALA:HB1	1:B:449:LEU:HD11	1.49	0.94
1:B:485:GLN:NE2	1:B:485:GLN:CA	2.30	0.94
1:B:160:PHE:CE1	1:B:165:LEU:CD2	2.49	0.94
1:B:13:LEU:HD22	1:B:17:GLY:HA3	1.50	0.93
1:B:194:PHE:CD1	1:B:195:PHE:HD2	1.86	0.93
1:B:286:ILE:HG23	1:B:289:THR:HB	1.46	0.93
1:A:154:ARG:NH2	1:A:489:LYS:HG3	1.83	0.93
1:A:272:MET:HE1	1:A:297:LEU:CD1	1.99	0.93
1:A:149:THR:HG23	1:A:314:ARG:HH22	1.31	0.93
1:B:15:LEU:HD21	1:B:16:LEU:HD13	1.49	0.93
1:B:485:GLN:HA	1:B:485:GLN:HE21	1.26	0.93
1:B:321:GLN:NE2	1:B:479:LEU:HD21	1.82	0.93
1:B:362:GLY:HA3	1:B:440:ASP:OD2	1.65	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:LEU:N	1:B:204:LEU:CD2	2.30	0.92
1:A:67:VAL:HG23	1:A:401:ARG:HG3	1.51	0.92
1:A:172:ILE:HD11	1:A:251:VAL:HG11	1.49	0.92
1:B:15:LEU:HD23	1:B:16:LEU:CA	2.00	0.92
1:B:503:TYR:O	1:B:504:ILE:CB	2.17	0.92
1:A:94:PHE:HB2	1:A:381:ALA:HB2	1.50	0.92
1:B:170:ILE:O	1:B:174:LEU:HB2	1.70	0.92
1:B:141:LEU:HD12	1:B:306:ALA:HB2	1.50	0.91
1:B:69:GLY:C	1:B:70:TRP:HD1	1.78	0.91
1:A:194:PHE:HD2	1:A:194:PHE:O	1.51	0.91
1:B:141:LEU:HD12	1:B:306:ALA:CB	2.01	0.91
1:B:170:ILE:HG22	1:B:275:PHE:CE1	2.04	0.91
1:A:154:ARG:HH22	1:A:489:LYS:HE3	1.11	0.91
1:A:212:LEU:HD12	1:A:375:VAL:HG23	1.50	0.91
1:B:25:MET:CB	1:B:495:HIS:CE1	2.53	0.91
1:B:32:TYR:N	1:B:33:PRO:HD2	1.83	0.91
1:A:435:ASP:HA	1:A:442:THR:OG1	1.71	0.91
1:A:76:PHE:O	1:A:76:PHE:HD1	1.54	0.91
1:A:154:ARG:NH2	1:A:489:LYS:CD	2.32	0.91
1:A:120:TRP:NE1	1:A:122:ALA:HB3	1.85	0.90
1:A:19:PHE:HD2	1:A:19:PHE:C	1.78	0.90
1:A:202:GLY:C	1:A:434:PRO:HG3	1.96	0.90
1:A:310:VAL:HG13	1:A:311:GLY:H	1.36	0.90
1:B:447:GLU:O	1:B:451:VAL:CG2	2.16	0.90
1:B:151:TYR:H	1:B:151:TYR:HD1	0.96	0.90
1:B:76:PHE:C	1:B:76:PHE:HD2	1.75	0.90
1:B:96:TYR:HD2	1:B:97:LEU:HD23	1.35	0.90
1:B:145:GLN:HE21	1:B:145:GLN:CA	1.83	0.90
1:B:286:ILE:CG2	1:B:289:THR:HG21	2.00	0.90
1:A:157:LYS:HG2	1:A:493:PHE:CE2	2.06	0.90
1:A:330:ALA:C	1:A:331:LYS:HG2	1.95	0.90
1:B:30:TYR:HE1	1:B:301:VAL:HG22	1.31	0.90
1:B:151:TYR:N	1:B:151:TYR:HD1	1.69	0.90
1:A:19:PHE:C	1:A:19:PHE:CD2	2.48	0.90
1:A:364:ASN:HD22	1:A:438:GLN:CG	1.84	0.90
1:B:25:MET:HB2	1:B:495:HIS:HE1	1.30	0.90
1:B:427:PHE:HZ	1:B:453:PHE:CE2	1.88	0.90
1:A:178:TYR:C	1:A:178:TYR:CD2	2.50	0.90
1:B:117:ILE:HG13	1:B:294:SER:HB2	1.53	0.90
1:B:51:ILE:HG22	1:B:52:LEU:HD23	1.53	0.89
1:A:101:ILE:HG13	1:A:373:LEU:HD13	1.52	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ILE:HG22	1:A:118:LEU:HD11	1.53	0.89
1:B:269:ALA:HB1	1:B:272:MET:CE	2.01	0.89
1:B:15:LEU:HD22	1:B:16:LEU:N	1.86	0.89
1:B:321:GLN:NE2	1:B:479:LEU:CD2	2.35	0.89
1:A:109:PHE:HE1	1:A:271:VAL:HG21	1.37	0.89
1:A:117:ILE:CG2	1:A:118:LEU:HD11	2.03	0.88
1:B:395:LYS:HG3	1:B:396:HIS:ND1	1.88	0.88
1:A:449:LEU:HD12	1:A:449:LEU:C	1.91	0.88
1:B:48:LEU:N	1:B:48:LEU:HD23	1.87	0.88
1:B:383:PHE:O	1:B:387:ILE:HD12	1.72	0.88
1:A:29:VAL:HG23	1:A:30:TYR:N	1.89	0.88
1:A:504:ILE:O	1:A:504:ILE:HG22	1.72	0.88
1:B:22:THR:O	1:B:241:LEU:HD21	1.72	0.88
1:B:194:PHE:CE1	1:B:195:PHE:HE2	1.90	0.88
1:A:98:GLN:CB	1:A:377:ILE:HG22	2.03	0.88
1:A:347:VAL:CG1	1:A:351:ILE:CD1	2.51	0.88
1:B:283:ALA:CB	1:B:286:ILE:HD12	2.04	0.88
1:B:313:SER:O	1:B:316:MET:N	2.07	0.88
1:B:146:PHE:HE1	1:B:342:VAL:HG11	1.38	0.88
1:B:161:PHE:HD1	1:B:165:LEU:CD1	1.80	0.88
1:B:395:LYS:O	1:B:396:HIS:ND1	2.05	0.88
1:B:25:MET:HA	1:B:495:HIS:CE1	2.09	0.88
1:A:74:GLY:C	1:A:75:VAL:HG13	1.99	0.88
1:B:321:GLN:HE22	1:B:479:LEU:HD22	1.38	0.87
1:A:485:GLN:HE21	1:A:485:GLN:CA	1.87	0.87
1:A:172:ILE:CG2	1:A:173:ALA:N	2.37	0.87
1:A:505:VAL:HG23	1:A:505:VAL:O	1.71	0.87
1:B:124:ASN:HD21	1:B:268:SER:CB	1.87	0.87
1:B:234:TYR:HD2	1:B:234:TYR:C	1.81	0.87
1:A:63:GLU:OE1	1:A:405:ILE:HG13	1.74	0.87
1:A:82:THR:HB	1:A:391:VAL:CG1	2.03	0.87
1:B:157:LYS:HG3	1:B:493:PHE:HE2	1.38	0.87
1:B:308:TRP:CD1	1:B:498:ALA:HB1	2.09	0.87
1:A:98:GLN:HG3	1:A:378:TYR:CD2	2.10	0.87
1:A:393:VAL:HG11	1:A:413:LEU:HD21	1.54	0.87
1:B:347:VAL:O	1:B:351:ILE:HB	1.75	0.87
1:A:145:GLN:NE2	1:A:145:GLN:CA	2.30	0.87
1:A:42:LEU:O	1:A:46:LEU:HG	1.74	0.86
1:A:304:GLU:O	1:A:308:TRP:CE3	2.28	0.86
1:B:395:LYS:C	1:B:396:HIS:HD1	1.83	0.86
1:B:55:ILE:CB	1:B:56:PRO:HD3	2.04	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:LEU:O	1:B:168:ALA:HB3	1.75	0.86
1:B:286:ILE:HG22	1:B:286:ILE:O	1.75	0.86
1:A:356:LEU:HD22	1:A:369:ILE:CG2	2.05	0.86
1:B:166:LEU:CB	1:B:167:PRO:HD3	2.05	0.86
1:A:145:GLN:CA	1:A:145:GLN:HE21	1.85	0.86
1:A:332:MET:HG3	1:A:338:PRO:CA	2.04	0.86
1:B:485:GLN:CA	1:B:485:GLN:HE21	1.87	0.86
1:A:143:LEU:CG	1:A:144:THR:N	2.35	0.86
1:A:172:ILE:HG22	1:A:173:ALA:H	1.41	0.86
1:A:172:ILE:HD12	1:A:251:VAL:CG1	2.05	0.86
1:B:77:ALA:O	1:B:81:ASN:HB2	1.74	0.86
1:A:154:ARG:NH2	1:A:489:LYS:CG	2.39	0.86
1:A:283:ALA:HB1	1:A:285:GLU:OE2	1.75	0.86
1:B:25:MET:CA	1:B:495:HIS:HE1	1.87	0.86
1:A:160:PHE:CD1	1:A:160:PHE:C	2.54	0.86
1:B:35:PHE:C	1:B:42:LEU:HD21	2.01	0.86
1:A:163:GLY:O	1:A:167:PRO:HD2	1.75	0.86
1:B:434:PRO:O	1:B:435:ASP:HB2	1.74	0.86
1:A:109:PHE:HD2	1:A:301:VAL:HG21	1.40	0.85
1:B:145:GLN:HA	1:B:145:GLN:NE2	1.84	0.85
1:A:347:VAL:HG12	1:A:351:ILE:HD11	1.57	0.85
1:A:15:LEU:HD23	1:A:15:LEU:O	1.76	0.85
1:A:26:VAL:HG12	1:A:248:LEU:HD23	1.59	0.85
1:A:286:ILE:O	1:A:289:THR:HG22	1.77	0.85
1:B:37:THR:OG1	1:B:438:GLN:NE2	2.08	0.85
1:B:70:TRP:CZ3	1:B:392:LEU:HD11	2.11	0.85
1:B:269:ALA:HB1	1:B:272:MET:HE1	1.58	0.85
1:B:317:TYR:HD2	1:B:479:LEU:HD11	1.41	0.85
1:A:229:ASN:O	1:A:233:ASP:HB2	1.77	0.84
1:B:55:ILE:HG22	1:B:56:PRO:CG	2.05	0.84
1:B:308:TRP:NE1	1:B:498:ALA:CB	2.39	0.84
1:A:501:PRO:O	1:A:502:HIS:CG	2.30	0.84
1:A:13:LEU:HD12	1:A:226:GLU:HB2	1.58	0.84
1:A:204:LEU:O	1:A:206:VAL:N	2.11	0.84
1:A:495:HIS:CD2	1:A:497:ARG:HB2	2.08	0.84
1:B:194:PHE:CD1	1:B:194:PHE:O	2.30	0.84
1:A:160:PHE:CZ	1:A:165:LEU:CD2	2.60	0.84
1:A:353:LEU:O	1:A:357:THR:CG2	2.25	0.84
1:A:67:VAL:HG11	1:A:70:TRP:CE3	2.13	0.84
1:A:135:LEU:HD21	1:A:350:SER:OG	1.76	0.84
1:A:135:LEU:HD23	1:A:350:SER:OG	1.78	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:LEU:HD12	1:A:143:LEU:O	1.78	0.84
1:B:51:ILE:CG2	1:B:52:LEU:HD23	2.07	0.84
1:B:286:ILE:CG2	1:B:289:THR:HB	2.07	0.84
1:A:399:LEU:CD2	1:A:400:LYS:H	1.90	0.84
1:A:418:VAL:HG12	1:A:419:GLY:N	1.91	0.83
1:B:362:GLY:HA3	1:B:440:ASP:CG	2.02	0.83
1:A:15:LEU:HD23	1:A:16:LEU:N	1.92	0.83
1:A:212:LEU:HD12	1:A:375:VAL:CG2	2.08	0.83
1:B:298:LEU:HG	1:B:302:LEU:CD1	2.08	0.83
1:B:276:THR:HG22	1:B:277:VAL:N	1.92	0.83
1:B:353:LEU:C	1:B:353:LEU:HD12	2.02	0.83
1:B:501:PRO:O	1:B:502:HIS:CD2	2.29	0.83
1:A:149:THR:CG2	1:A:314:ARG:NH2	2.41	0.83
1:B:189:MET:O	1:B:190:ASP:O	1.96	0.83
1:A:44:PHE:HB2	1:A:194:PHE:HE2	1.40	0.83
1:A:85:PRO:O	1:A:87:TRP:N	2.11	0.83
1:A:347:VAL:HG12	1:A:351:ILE:CD1	2.08	0.83
1:B:34:THR:O	1:B:37:THR:CG2	2.25	0.83
1:B:234:TYR:C	1:B:234:TYR:CD2	2.53	0.83
1:B:96:TYR:CD2	1:B:97:LEU:CD2	2.62	0.83
1:A:119:LYS:HG2	1:A:291:ARG:HH12	1.42	0.83
1:B:47:LEU:CD2	1:B:246:ILE:HD11	2.04	0.83
1:B:129:THR:O	1:B:130:LYS:C	2.22	0.83
1:B:221:ALA:O	1:B:224:VAL:HG23	1.79	0.83
1:B:42:LEU:O	1:B:46:LEU:N	2.12	0.82
1:B:395:LYS:HE2	1:B:396:HIS:HE1	0.66	0.82
1:A:234:TYR:HB3	1:A:235:PRO:CD	2.10	0.82
1:B:173:ALA:O	1:B:176:ALA:HB3	1.79	0.82
1:A:73:GLY:CA	1:A:77:ALA:HB2	2.09	0.82
1:A:202:GLY:HA3	1:A:434:PRO:CB	2.06	0.82
1:B:170:ILE:HD13	1:B:293:ILE:HD12	1.60	0.82
1:A:221:ALA:O	1:A:224:VAL:HG23	1.80	0.82
1:A:259:VAL:CG2	1:A:278:LEU:HD21	2.05	0.82
1:B:365:MET:HE2	1:B:442:THR:HA	1.60	0.82
1:A:477:VAL:CG1	1:A:506:MET:HB3	2.10	0.82
1:A:161:PHE:CE1	1:A:493:PHE:CE2	2.67	0.82
1:B:308:TRP:CD1	1:B:498:ALA:CB	2.62	0.81
1:A:433:PRO:HG3	1:A:445:TYR:CD2	2.15	0.81
1:B:62:ALA:O	1:B:66:THR:HG23	1.79	0.81
1:B:353:LEU:C	1:B:353:LEU:CD1	2.53	0.81
1:A:66:THR:HB	1:A:402:THR:HB	1.59	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:VAL:HG21	1:A:278:LEU:CD2	2.05	0.81
1:A:279:MET:SD	1:A:289:THR:CG2	2.68	0.81
1:B:97:LEU:HD23	1:B:97:LEU:H	1.45	0.81
1:A:178:TYR:C	1:A:178:TYR:HD2	1.85	0.81
1:B:51:ILE:HG22	1:B:52:LEU:CD2	2.09	0.81
1:B:246:ILE:HG22	1:B:247:CYS:N	1.95	0.81
1:A:17:GLY:O	1:A:21:ILE:HG23	1.81	0.81
1:A:46:LEU:HD23	1:A:210:PHE:HD1	1.45	0.81
1:A:478:THR:OG1	1:A:505:VAL:HG21	1.79	0.81
1:A:504:ILE:HG22	1:A:506:MET:HG2	1.61	0.81
1:B:27:MET:CE	1:B:248:LEU:HG	2.10	0.81
1:B:30:TYR:HE1	1:B:301:VAL:CG2	1.94	0.81
1:A:26:VAL:CG1	1:A:248:LEU:CD2	2.59	0.80
1:A:177:ILE:O	1:A:180:HIS:HB2	1.81	0.80
1:B:45:PHE:O	1:B:47:LEU:N	2.14	0.80
1:B:99:ILE:HD12	1:B:312:PRO:HB3	1.62	0.80
1:A:166:LEU:CD2	1:A:166:LEU:O	2.30	0.80
1:B:141:LEU:HD11	1:B:306:ALA:HB2	1.63	0.80
1:B:393:VAL:O	1:B:393:VAL:HG12	1.80	0.80
1:A:15:LEU:CD2	1:A:16:LEU:CD2	2.59	0.80
1:B:59:LEU:N	1:B:59:LEU:HD23	1.95	0.80
1:B:128:ILE:HG13	1:B:129:THR:N	1.94	0.80
1:A:109:PHE:CE1	1:A:271:VAL:HG21	2.16	0.80
1:A:120:TRP:CD1	1:A:122:ALA:HB3	2.17	0.80
1:A:173:ALA:O	1:A:177:ILE:HG13	1.82	0.80
1:A:109:PHE:CD2	1:A:301:VAL:HG21	2.16	0.80
1:A:74:GLY:O	1:A:75:VAL:CG1	2.30	0.80
1:A:98:GLN:CA	1:A:98:GLN:HE21	1.94	0.80
1:A:432:LEU:O	1:A:432:LEU:CD1	2.30	0.80
1:B:25:MET:HA	1:B:495:HIS:HE1	1.45	0.80
1:B:50:GLY:HA2	1:B:54:PHE:HB3	1.64	0.80
1:B:371:LEU:HD23	1:B:371:LEU:N	1.94	0.80
1:A:25:MET:CE	1:A:496:PRO:HG2	2.12	0.80
1:A:166:LEU:CD2	1:A:166:LEU:C	2.55	0.80
1:B:60:CYS:HB2	1:B:389:TYR:CD1	2.17	0.80
1:B:163:GLY:O	1:B:167:PRO:HG2	1.82	0.80
1:A:457:LEU:HD12	1:A:457:LEU:C	1.92	0.80
1:B:103:PHE:CZ	1:B:308:TRP:HB2	2.16	0.80
1:B:210:PHE:O	1:B:213:SER:HB2	1.80	0.80
1:A:456:VAL:C	1:A:458:ALA:H	1.90	0.79
1:B:103:PHE:O	1:B:106:MET:HB2	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:LEU:O	1:A:166:LEU:HD23	1.83	0.79
1:A:397:PRO:CD	1:A:398:ASP:N	2.42	0.79
1:B:57:VAL:O	1:B:61:ALA:CB	2.30	0.79
1:B:337:VAL:O	1:B:337:VAL:CG2	2.30	0.79
1:B:353:LEU:CD1	1:B:353:LEU:O	2.30	0.79
1:A:74:GLY:O	1:A:75:VAL:CG2	2.30	0.79
1:A:98:GLN:NE2	1:A:99:ILE:N	2.30	0.79
1:A:362:GLY:H	1:A:440:ASP:HB3	1.45	0.79
1:B:49:GLY:HA3	1:B:214:TYR:CE2	2.18	0.79
1:B:266:ASN:C	1:B:266:ASN:ND2	2.36	0.79
1:B:439:GLY:O	1:B:440:ASP:O	2.01	0.79
1:A:386:PHE:O	1:A:390:ILE:CD1	2.30	0.79
1:A:221:ALA:O	1:A:224:VAL:N	2.16	0.79
1:B:187:ILE:O	1:B:187:ILE:CG2	2.31	0.79
1:A:15:LEU:CD2	1:A:16:LEU:N	2.46	0.79
1:A:340:THR:O	1:A:344:SER:HB3	1.82	0.79
1:A:52:LEU:O	1:A:56:PRO:HG2	1.83	0.78
1:A:96:TYR:C	1:A:96:TYR:CD2	2.61	0.78
1:B:161:PHE:CE1	1:B:165:LEU:HD11	2.18	0.78
1:A:50:GLY:HA2	1:A:54:PHE:HB3	1.64	0.78
1:B:67:VAL:CG2	1:B:70:TRP:CE3	2.66	0.78
1:A:172:ILE:HG22	1:A:173:ALA:N	1.97	0.78
1:B:76:PHE:CD2	1:B:76:PHE:O	2.36	0.78
1:A:484:SER:O	1:A:485:GLN:NE2	2.17	0.78
1:B:286:ILE:CG2	1:B:289:THR:CB	2.60	0.78
1:B:434:PRO:O	1:B:435:ASP:CB	2.31	0.78
1:A:364:ASN:ND2	1:A:438:GLN:CG	2.44	0.78
1:B:152:THR:O	1:B:155:ILE:N	2.17	0.78
1:A:194:PHE:HD2	1:A:194:PHE:C	1.91	0.77
1:B:234:TYR:HE2	1:B:238:MET:CG	1.97	0.77
1:A:157:LYS:O	1:A:161:PHE:CD1	2.33	0.77
1:A:406:PRO:O	1:A:406:PRO:HG2	1.85	0.77
1:B:96:TYR:HD2	1:B:97:LEU:CD2	1.96	0.77
1:B:221:ALA:O	1:B:224:VAL:CG2	2.32	0.77
1:B:332:MET:HE2	1:B:336:GLY:HA2	1.66	0.77
1:A:194:PHE:O	1:A:194:PHE:CD2	2.35	0.77
1:A:202:GLY:N	1:A:434:PRO:HG3	1.98	0.77
1:B:70:TRP:CH2	1:B:392:LEU:CD1	2.67	0.77
1:A:98:GLN:CB	1:A:377:ILE:CG2	2.63	0.77
1:A:118:LEU:N	1:A:118:LEU:HD13	1.96	0.77
1:B:70:TRP:O	1:B:72:GLU:N	2.18	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:ILE:CG2	1:B:247:CYS:N	2.47	0.77
1:A:275:PHE:HB3	1:A:290:VAL:HG22	1.67	0.77
1:B:98:GLN:HE22	1:B:497:ARG:HB3	1.50	0.77
1:A:337:VAL:O	1:A:337:VAL:CG2	2.30	0.77
1:B:166:LEU:HD12	1:B:167:PRO:N	1.99	0.77
1:B:259:VAL:HG21	1:B:278:LEU:HD11	1.66	0.77
1:A:215:MET:CE	1:A:378:TYR:CB	2.55	0.77
1:A:19:PHE:CD2	1:A:23:ALA:HB2	2.19	0.77
1:A:44:PHE:CB	1:A:194:PHE:HE2	1.97	0.77
1:A:44:PHE:CB	1:A:194:PHE:CE2	2.68	0.77
1:A:98:GLN:HB2	1:A:377:ILE:CG2	2.14	0.77
1:A:106:MET:HB3	1:A:305:ILE:HD11	1.64	0.77
1:A:215:MET:HE1	1:A:378:TYR:HB3	1.67	0.76
1:A:501:PRO:O	1:A:502:HIS:CB	2.30	0.76
1:B:202:GLY:O	1:B:205:VAL:HG12	1.85	0.76
1:B:395:LYS:HG3	1:B:396:HIS:HD1	1.48	0.76
1:A:161:PHE:HE1	1:A:493:PHE:HE2	1.31	0.76
1:B:286:ILE:HG21	1:B:289:THR:HG21	1.64	0.76
1:B:427:PHE:CZ	1:B:453:PHE:CE2	2.72	0.76
1:A:109:PHE:HE1	1:A:271:VAL:CG2	1.99	0.76
1:A:393:VAL:HG11	1:A:413:LEU:CD2	2.15	0.76
1:B:197:ASP:O	1:B:199:SER:N	2.16	0.76
1:A:125:GLU:O	1:A:127:PRO:CD	2.30	0.76
1:A:203:THR:HG22	1:A:204:LEU:CD2	2.13	0.76
1:A:22:THR:HG23	1:A:25:MET:HE3	1.67	0.76
1:A:55:ILE:HB	1:A:56:PRO:CD	2.15	0.76
1:A:119:LYS:HG2	1:A:291:ARG:NH1	2.00	0.76
1:A:375:VAL:O	1:A:379:LEU:HD23	1.86	0.75
1:B:36:ALA:O	1:B:39:GLY:N	2.16	0.75
1:B:494:LEU:O	1:B:499:ARG:HD3	1.87	0.75
1:A:437:ILE:HD11	1:A:442:THR:CG2	2.15	0.75
1:B:15:LEU:HD22	1:B:16:LEU:H	1.50	0.75
1:B:203:THR:C	1:B:204:LEU:HD23	2.10	0.75
1:A:118:LEU:HD12	1:A:118:LEU:N	2.00	0.75
1:A:336:GLY:O	1:A:337:VAL:CG1	2.34	0.75
1:A:117:ILE:HG22	1:A:118:LEU:HD12	0.77	0.75
1:B:59:LEU:HD23	1:B:59:LEU:H	1.48	0.75
1:B:129:THR:O	1:B:131:THR:N	2.19	0.75
1:B:353:LEU:HD12	1:B:353:LEU:O	1.84	0.75
1:A:279:MET:C	1:A:281:HIS:H	1.95	0.75
1:A:334:LYS:O	1:A:335:ASN:CB	2.34	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:VAL:O	1:B:393:VAL:CG1	2.35	0.75
1:B:482:ILE:C	1:B:483:ASN:OD1	2.30	0.75
1:A:166:LEU:HB3	1:A:167:PRO:HD3	1.69	0.75
1:A:449:LEU:O	1:A:449:LEU:CD1	2.30	0.75
1:B:70:TRP:O	1:B:71:GLU:C	2.29	0.75
1:A:456:VAL:C	1:A:458:ALA:N	2.42	0.75
1:B:200:LYS:O	1:B:201:VAL:C	2.30	0.75
1:A:19:PHE:CE2	1:A:23:ALA:HB2	2.22	0.75
1:A:116:TYR:OH	1:A:273:GLN:HG3	1.87	0.75
1:A:339:VAL:HG23	1:A:343:ILE:CG2	2.17	0.75
1:B:334:LYS:O	1:B:335:ASN:CB	2.34	0.75
1:A:21:ILE:HD12	1:A:223:HIS:ND1	2.00	0.74
1:A:117:ILE:O	1:A:291:ARG:CZ	2.35	0.74
1:B:78:TRP:CD1	1:B:78:TRP:H	2.03	0.74
1:B:126:ASP:O	1:B:130:LYS:HB2	1.87	0.74
1:B:145:GLN:OE1	1:B:152:THR:CG2	2.34	0.74
1:A:29:VAL:CG2	1:A:30:TYR:N	2.51	0.74
1:A:96:TYR:C	1:A:96:TYR:HD2	1.94	0.74
1:B:46:LEU:HD12	1:B:46:LEU:O	1.88	0.74
1:B:113:ALA:HA	1:B:272:MET:SD	2.28	0.74
1:B:233:ASP:O	1:B:236:LEU:HB2	1.87	0.74
1:B:172:ILE:HG12	1:B:251:VAL:HG11	1.67	0.74
1:A:149:THR:HG21	1:A:314:ARG:NH1	2.02	0.74
1:B:70:TRP:C	1:B:72:GLU:N	2.42	0.74
1:B:204:LEU:HD23	1:B:204:LEU:H	1.50	0.74
1:B:267:LEU:HB2	1:B:364:ASN:OD1	1.86	0.74
1:B:310:VAL:O	1:B:310:VAL:CG2	2.36	0.74
1:A:70:TRP:HZ2	1:A:81:ASN:CB	2.01	0.74
1:A:332:MET:HG3	1:A:338:PRO:HA	1.67	0.74
1:B:29:VAL:HA	1:B:32:TYR:CD1	2.23	0.74
1:A:98:GLN:HE21	1:A:98:GLN:N	1.84	0.74
1:A:53:TRP:O	1:A:56:PRO:HD2	1.87	0.74
1:B:355:ILE:HG12	1:B:356:LEU:N	2.03	0.74
1:B:71:GLU:HB3	1:B:225:ASN:HD21	1.53	0.74
1:B:269:ALA:CB	1:B:272:MET:CE	2.66	0.74
1:A:143:LEU:HG	1:A:144:THR:H	1.50	0.73
1:A:437:ILE:C	1:A:438:GLN:HG2	2.11	0.73
1:B:69:GLY:C	1:B:70:TRP:CD1	2.66	0.73
1:B:124:ASN:HD21	1:B:268:SER:HB3	1.50	0.73
1:A:178:TYR:CD1	1:A:278:LEU:HD22	2.23	0.73
1:A:397:PRO:HD2	1:A:398:ASP:N	1.95	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:LEU:C	1:B:166:LEU:HD13	2.11	0.73
1:B:234:TYR:O	1:B:236:LEU:N	2.21	0.73
1:A:98:GLN:CA	1:A:377:ILE:HG21	2.18	0.73
1:A:351:ILE:O	1:A:355:ILE:HG13	1.87	0.73
1:A:70:TRP:CZ2	1:A:81:ASN:CB	2.71	0.73
1:A:282:VAL:O	1:A:283:ALA:HB2	1.86	0.73
1:A:332:MET:HG2	1:A:338:PRO:N	2.02	0.73
1:A:435:ASP:C	1:A:435:ASP:OD2	2.30	0.73
1:B:24:SER:CB	1:B:493:PHE:O	2.36	0.73
1:B:215:MET:CE	1:B:378:TYR:CB	2.60	0.73
1:B:137:ILE:O	1:B:140:ALA:HB3	1.88	0.73
1:B:67:VAL:HG23	1:B:70:TRP:HB2	1.70	0.73
1:B:298:LEU:O	1:B:302:LEU:HD12	1.89	0.73
1:B:315:GLY:CA	1:B:500:SER:HB2	2.18	0.73
1:B:374:THR:CG2	1:B:375:VAL:N	2.51	0.73
1:B:432:LEU:O	1:B:432:LEU:CD1	2.29	0.73
1:A:445:TYR:C	1:A:445:TYR:HD1	1.96	0.73
1:A:205:VAL:O	1:A:208:VAL:HG22	1.88	0.73
1:B:80:SER:OG	1:B:85:PRO:HA	1.88	0.73
1:B:34:THR:C	1:B:37:THR:HG22	2.14	0.73
1:A:23:ALA:HA	1:A:241:LEU:HD21	1.71	0.72
1:B:66:THR:OG1	1:B:403:PHE:N	2.22	0.72
1:B:161:PHE:CD1	1:B:165:LEU:HD12	2.12	0.72
1:A:41:SER:O	1:A:44:PHE:HB3	1.88	0.72
1:A:46:LEU:HD23	1:A:210:PHE:CD1	2.24	0.72
1:A:246:ILE:O	1:A:250:SER:OG	2.06	0.72
1:A:336:GLY:H	1:A:506:MET:HE2	1.54	0.72
1:A:442:THR:HB	1:A:445:TYR:CB	2.19	0.72
1:B:53:TRP:HH2	1:B:382:TYR:CZ	2.06	0.72
1:B:166:LEU:C	1:B:168:ALA:H	1.95	0.72
1:A:506:MET:O	1:A:509:LYS:CD	2.36	0.72
1:A:22:THR:HG1	1:A:220:SER:HG	1.30	0.72
1:B:98:GLN:NE2	1:B:497:ARG:HB3	2.04	0.72
1:B:32:TYR:N	1:B:33:PRO:CD	2.53	0.72
1:B:332:MET:HE2	1:B:336:GLY:CA	2.19	0.72
1:B:311:GLY:H	1:B:312:PRO:CD	2.01	0.72
1:B:323:ASN:O	1:B:324:LEU:CD1	2.35	0.72
1:B:170:ILE:CD1	1:B:293:ILE:HD12	2.19	0.72
1:B:172:ILE:CG1	1:B:251:VAL:HG11	2.19	0.72
1:B:265:ILE:O	1:B:438:GLN:HG2	1.90	0.72
1:A:118:LEU:O	1:A:119:LYS:C	2.29	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:SER:C	1:B:193:THR:H	1.98	0.71
1:B:194:PHE:CD1	1:B:194:PHE:C	2.67	0.71
1:A:149:THR:HG21	1:A:314:ARG:HH12	1.53	0.71
1:A:194:PHE:C	1:A:194:PHE:CD2	2.64	0.71
1:B:145:GLN:OE1	1:B:152:THR:HG22	1.89	0.71
1:B:226:GLU:O	1:B:227:MET:O	2.07	0.71
1:A:215:MET:HE2	1:A:378:TYR:CG	2.25	0.71
1:B:55:ILE:CG2	1:B:56:PRO:CD	1.89	0.71
1:B:365:MET:HG3	1:B:437:ILE:HD12	1.72	0.71
1:B:477:VAL:HG13	1:B:478:THR:N	2.04	0.71
1:A:298:LEU:O	1:A:302:LEU:HG	1.91	0.71
1:A:149:THR:HG21	1:A:314:ARG:NH2	2.04	0.71
1:A:439:GLY:O	1:A:440:ASP:C	2.30	0.71
1:A:442:THR:HB	1:A:445:TYR:HB2	1.71	0.71
1:A:82:THR:HB	1:A:391:VAL:HG12	1.70	0.71
1:B:45:PHE:C	1:B:47:LEU:H	1.98	0.71
1:B:126:ASP:OD1	1:B:127:PRO:HD2	1.90	0.71
1:A:67:VAL:HG11	1:A:70:TRP:CD2	2.26	0.71
1:A:101:ILE:HD13	1:A:101:ILE:N	2.06	0.71
1:A:149:THR:O	1:A:149:THR:OG1	2.09	0.71
1:B:110:VAL:HG23	1:B:301:VAL:HG11	1.72	0.71
1:B:129:THR:O	1:B:132:ILE:N	2.24	0.71
1:B:170:ILE:CG2	1:B:275:PHE:CZ	2.71	0.71
1:A:224:VAL:O	1:A:227:MET:CB	2.34	0.71
1:B:35:PHE:O	1:B:42:LEU:CD2	2.39	0.71
1:B:215:MET:HE3	1:B:378:TYR:CD2	2.26	0.71
1:B:362:GLY:N	1:B:440:ASP:HB3	2.05	0.71
1:A:99:ILE:HG23	1:A:99:ILE:O	1.89	0.70
1:B:82:THR:CG2	1:B:391:VAL:CG1	2.69	0.70
1:A:67:VAL:HG12	1:A:70:TRP:CB	2.21	0.70
1:A:78:TRP:H	1:A:78:TRP:CD1	2.07	0.70
1:A:431:PHE:O	1:A:446:VAL:CG2	2.39	0.70
1:B:24:SER:HB2	1:B:493:PHE:O	1.90	0.70
1:A:22:THR:HG22	1:A:22:THR:O	1.90	0.70
1:A:153:ALA:HB1	1:A:489:LYS:O	1.91	0.70
1:A:399:LEU:HD22	1:A:400:LYS:H	1.55	0.70
1:A:506:MET:O	1:A:507:ASN:HB2	1.91	0.70
1:A:66:THR:HG21	1:A:224:VAL:HG11	1.73	0.70
1:A:98:GLN:NE2	1:A:98:GLN:C	2.50	0.70
1:B:70:TRP:CZ3	1:B:392:LEU:CD1	2.74	0.70
1:B:377:ILE:CD1	1:B:456:VAL:HG11	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:GLU:HG3	1:A:286:ILE:HG12	1.73	0.70
1:A:347:VAL:O	1:A:351:ILE:CG1	2.33	0.70
1:A:106:MET:CB	1:A:305:ILE:HD11	2.22	0.70
1:A:151:TYR:O	1:A:152:THR:C	2.33	0.70
1:A:171:LEU:C	1:A:171:LEU:HD22	2.17	0.70
1:A:166:LEU:HB3	1:A:167:PRO:CD	2.22	0.69
1:A:222:THR:C	1:A:224:VAL:H	2.00	0.69
1:A:476:GLY:O	1:A:477:VAL:CG1	2.40	0.69
1:B:15:LEU:CD2	1:B:16:LEU:HD13	2.22	0.69
1:B:146:PHE:HE1	1:B:342:VAL:CG1	2.03	0.69
1:A:71:GLU:HB2	1:A:72:GLU:OE1	1.92	0.69
1:A:104:ILE:HB	1:A:105:PRO:HD3	1.75	0.69
1:A:272:MET:CE	1:A:297:LEU:CD1	2.66	0.69
1:A:336:GLY:O	1:A:337:VAL:HG13	1.93	0.69
1:B:124:ASN:ND2	1:B:268:SER:OG	2.25	0.69
1:B:194:PHE:CD1	1:B:195:PHE:CE2	2.79	0.69
1:A:143:LEU:CD1	1:A:144:THR:N	2.55	0.69
1:A:124:ASN:ND2	1:A:269:ALA:HB2	2.07	0.69
1:A:445:TYR:C	1:A:445:TYR:CD1	2.70	0.69
1:B:97:LEU:HD23	1:B:97:LEU:N	2.06	0.69
1:B:427:PHE:HZ	1:B:453:PHE:HE2	1.35	0.69
1:A:174:LEU:HD22	1:A:278:LEU:HB3	1.73	0.69
1:A:465:ALA:O	1:A:466:VAL:C	2.35	0.69
1:B:67:VAL:O	1:B:68:ASP:C	2.34	0.69
1:A:160:PHE:CZ	1:A:165:LEU:HD23	2.13	0.69
1:A:283:ALA:O	1:A:285:GLU:HG2	1.93	0.69
1:A:279:MET:HG2	1:A:287:GLU:HA	1.75	0.68
1:B:24:SER:HB3	1:B:493:PHE:HA	1.75	0.68
1:B:414:VAL:O	1:B:418:VAL:HG23	1.93	0.68
1:B:234:TYR:CE2	1:B:238:MET:CG	2.76	0.68
1:A:50:GLY:HA2	1:A:54:PHE:CB	2.24	0.68
1:A:200:LYS:HG3	1:A:201:VAL:N	2.07	0.68
1:B:82:THR:HG22	1:B:391:VAL:HG11	1.74	0.68
1:B:117:ILE:HD11	1:B:295:ALA:N	2.07	0.68
1:A:19:PHE:CE2	1:A:23:ALA:CB	2.76	0.68
1:A:85:PRO:O	1:A:86:ARG:C	2.36	0.68
1:B:258:MET:HE2	1:B:259:VAL:HG23	1.74	0.68
1:B:329:PHE:O	1:B:330:ALA:HB2	1.93	0.68
1:A:98:GLN:HA	1:A:377:ILE:HG21	1.76	0.68
1:A:117:ILE:C	1:A:118:LEU:HD12	2.18	0.68
1:A:279:MET:SD	1:A:289:THR:HG21	2.34	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:THR:OG1	1:A:505:VAL:HG22	1.92	0.68
1:A:173:ALA:O	1:A:177:ILE:CG1	2.42	0.68
1:A:271:VAL:HB	1:A:272:MET:HE3	1.75	0.68
1:B:174:LEU:HD22	1:B:278:LEU:HB3	1.76	0.68
1:A:70:TRP:HZ2	1:A:81:ASN:HB3	1.59	0.68
1:A:76:PHE:HD1	1:A:76:PHE:C	2.01	0.68
1:A:321:GLN:HE22	1:A:476:GLY:HA3	1.59	0.68
1:B:174:LEU:CD2	1:B:278:LEU:HB3	2.23	0.68
1:A:13:LEU:HB2	1:A:227:MET:HA	1.76	0.67
1:A:166:LEU:C	1:A:166:LEU:HD22	2.19	0.67
1:A:74:GLY:O	1:A:75:VAL:CB	2.43	0.67
1:A:171:LEU:C	1:A:171:LEU:CD2	2.66	0.67
1:B:222:THR:C	1:B:224:VAL:N	2.48	0.67
1:A:101:ILE:HG13	1:A:373:LEU:CD1	2.25	0.67
1:A:197:ASP:O	1:A:203:THR:OG1	2.06	0.67
1:B:29:VAL:HB	1:B:32:TYR:CD1	2.30	0.67
1:B:479:LEU:O	1:B:481:PRO:HD3	1.95	0.67
1:A:222:THR:C	1:A:224:VAL:N	2.50	0.67
1:B:194:PHE:CE1	1:B:195:PHE:CD2	2.82	0.67
1:B:377:ILE:HG12	1:B:456:VAL:HG11	1.76	0.67
1:A:55:ILE:CB	1:A:56:PRO:HD3	2.21	0.67
1:B:364:ASN:HB2	1:B:440:ASP:OD1	1.95	0.67
1:A:202:GLY:CA	1:A:434:PRO:CG	1.96	0.67
1:A:282:VAL:O	1:A:283:ALA:CB	2.43	0.67
1:A:503:TYR:CD2	1:A:503:TYR:N	2.62	0.67
1:B:146:PHE:O	1:B:148:GLY:N	2.28	0.67
1:A:336:GLY:C	1:A:337:VAL:HG12	2.20	0.67
1:A:339:VAL:HG23	1:A:343:ILE:HG21	1.76	0.67
1:A:483:ASN:C	1:A:485:GLN:N	2.39	0.67
1:B:269:ALA:CB	1:B:272:MET:HE1	2.25	0.67
1:B:311:GLY:O	1:B:500:SER:HB3	1.94	0.67
1:A:75:VAL:CG1	1:A:78:TRP:CZ3	2.73	0.66
1:A:434:PRO:O	1:A:435:ASP:CB	2.43	0.66
1:A:501:PRO:O	1:A:502:HIS:HB3	1.95	0.66
1:B:126:ASP:CG	1:B:127:PRO:HD2	2.20	0.66
1:B:339:VAL:HG23	1:B:343:ILE:HD12	1.76	0.66
1:A:100:ALA:O	1:A:349:THR:HG23	1.94	0.66
1:A:232:ARG:O	1:A:233:ASP:C	2.36	0.66
1:B:15:LEU:HD22	1:B:16:LEU:HD22	1.76	0.66
1:B:71:GLU:HB3	1:B:225:ASN:ND2	2.10	0.66
1:A:143:LEU:HD12	1:A:144:THR:N	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:ILE:N	1:B:105:PRO:HD2	2.11	0.66
1:B:161:PHE:CE1	1:B:165:LEU:CD1	2.78	0.66
1:B:351:ILE:O	1:B:355:ILE:CG2	2.43	0.66
1:A:26:VAL:HG11	1:A:248:LEU:CD2	2.25	0.66
1:B:78:TRP:CD1	1:B:78:TRP:N	2.60	0.66
1:B:215:MET:HE3	1:B:378:TYR:CG	2.30	0.66
1:B:351:ILE:HG22	1:B:352:ALA:N	2.11	0.66
1:B:99:ILE:HD12	1:B:312:PRO:CB	2.24	0.66
1:B:311:GLY:N	1:B:312:PRO:CD	2.55	0.66
1:B:365:MET:CG	1:B:437:ILE:HD12	2.26	0.66
1:B:489:LYS:O	1:B:490:GLY:C	2.37	0.66
1:A:134:ALA:HB1	1:A:353:LEU:CD2	2.21	0.66
1:A:161:PHE:CE1	1:A:493:PHE:HE2	2.10	0.66
1:B:29:VAL:HB	1:B:32:TYR:CE1	2.30	0.66
1:B:47:LEU:CD2	1:B:246:ILE:CD1	2.69	0.66
1:B:380:CYS:O	1:B:383:PHE:HB2	1.96	0.66
1:B:307:SER:HB2	1:B:494:LEU:HD11	1.77	0.66
1:A:203:THR:CG2	1:A:204:LEU:HD23	2.18	0.66
1:B:298:LEU:CD1	1:B:302:LEU:HD11	2.25	0.66
1:A:30:TYR:O	1:A:33:PRO:HD2	1.96	0.66
1:B:65:ALA:O	1:B:71:GLU:HA	1.95	0.66
1:A:151:TYR:HB2	1:A:155:ILE:HD11	1.78	0.65
1:A:353:LEU:HD12	1:A:357:THR:HG21	1.76	0.65
1:B:127:PRO:O	1:B:131:THR:CG2	2.44	0.65
1:A:70:TRP:CZ2	1:A:81:ASN:HB2	2.31	0.65
1:A:76:PHE:C	1:A:76:PHE:CD1	2.70	0.65
1:A:347:VAL:HG13	1:A:351:ILE:CD1	2.24	0.65
1:A:462:ILE:O	1:A:466:VAL:HG23	1.96	0.65
1:B:29:VAL:C	1:B:31:GLU:H	2.04	0.65
1:B:103:PHE:HZ	1:B:308:TRP:HB2	1.60	0.65
1:B:351:ILE:CG2	1:B:352:ALA:N	2.60	0.65
1:B:420:LEU:HD12	1:B:420:LEU:O	1.95	0.65
1:A:72:GLU:OE1	1:A:72:GLU:N	2.30	0.65
1:A:160:PHE:C	1:A:160:PHE:HD1	2.02	0.65
1:A:242:MET:O	1:A:246:ILE:HG13	1.96	0.65
1:B:359:THR:O	1:B:359:THR:CG2	2.38	0.65
1:A:330:ALA:C	1:A:331:LYS:CG	2.69	0.65
1:A:373:LEU:O	1:A:376:VAL:HG23	1.96	0.65
1:B:22:THR:O	1:B:241:LEU:CD2	2.44	0.65
1:A:22:THR:HG22	1:A:25:MET:HE3	1.76	0.65
1:A:364:ASN:ND2	1:A:438:GLN:HB2	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:LEU:O	1:B:168:ALA:N	2.30	0.65
1:A:125:GLU:N	1:A:125:GLU:OE1	2.30	0.65
1:B:166:LEU:C	1:B:168:ALA:N	2.51	0.65
1:B:181:SER:O	1:B:182:GLY:C	2.40	0.65
1:B:367:PHE:O	1:B:370:ALA:N	2.27	0.65
1:A:149:THR:HG21	1:A:314:ARG:CZ	2.27	0.65
1:B:395:LYS:HG3	1:B:396:HIS:CE1	2.31	0.65
1:B:396:HIS:N	1:B:397:PRO:HD3	2.12	0.65
1:A:205:VAL:O	1:A:205:VAL:HG22	1.94	0.64
1:B:70:TRP:HH2	1:B:392:LEU:CD1	2.10	0.64
1:B:124:ASN:ND2	1:B:268:SER:CB	2.59	0.64
1:A:120:TRP:HE1	1:A:122:ALA:HB3	1.61	0.64
1:A:157:LYS:HD3	1:A:493:PHE:CE2	2.33	0.64
1:B:286:ILE:O	1:B:289:THR:HG22	1.98	0.64
1:A:32:TYR:N	1:A:33:PRO:CD	2.60	0.64
1:A:283:ALA:O	1:A:285:GLU:N	2.30	0.64
1:B:234:TYR:CE2	1:B:238:MET:SD	2.90	0.64
1:A:202:GLY:CA	1:A:434:PRO:CD	2.60	0.64
1:A:435:ASP:OD2	1:A:436:ASN:N	2.30	0.64
1:A:501:PRO:C	1:A:502:HIS:CG	2.72	0.64
1:A:212:LEU:CD1	1:A:375:VAL:HG23	2.26	0.64
1:B:234:TYR:C	1:B:236:LEU:N	2.53	0.64
1:B:259:VAL:HG21	1:B:278:LEU:CD1	2.27	0.64
1:A:152:THR:O	1:A:153:ALA:C	2.39	0.64
1:B:82:THR:CG2	1:B:391:VAL:HG11	2.27	0.64
1:B:95:GLY:O	1:B:98:GLN:HB3	1.97	0.64
1:B:229:ASN:O	1:B:233:ASP:CB	2.38	0.64
1:B:276:THR:CG2	1:B:277:VAL:N	2.60	0.64
1:B:374:THR:HG22	1:B:375:VAL:H	1.63	0.64
1:B:336:GLY:O	1:B:337:VAL:CG1	2.46	0.64
1:A:332:MET:CG	1:A:338:PRO:N	2.60	0.64
1:A:399:LEU:HD23	1:A:400:LYS:H	1.62	0.64
1:B:101:ILE:HG12	1:B:373:LEU:HD13	1.79	0.64
1:B:128:ILE:CG1	1:B:129:THR:N	2.61	0.64
1:A:456:VAL:O	1:A:458:ALA:N	2.30	0.64
1:B:25:MET:CA	1:B:495:HIS:CE1	2.69	0.64
1:B:390:ILE:HG22	1:B:394:LEU:HG	1.80	0.64
1:A:124:ASN:ND2	1:A:269:ALA:CB	2.61	0.63
1:A:266:ASN:O	1:A:270:GLY:HA3	1.98	0.63
1:A:279:MET:O	1:A:281:HIS:N	2.31	0.63
1:B:51:ILE:CG2	1:B:52:LEU:CD2	2.72	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:LYS:HG3	1:B:395:LYS:O	1.98	0.63
1:A:225:ASN:O	1:A:227:MET:N	2.32	0.63
1:B:362:GLY:CA	1:B:440:ASP:CG	2.70	0.63
1:A:98:GLN:CA	1:A:98:GLN:NE2	2.56	0.63
1:A:200:LYS:HZ2	1:A:200:LYS:HB2	1.64	0.63
1:A:128:ILE:HD12	1:A:128:ILE:C	2.17	0.63
1:A:283:ALA:HB1	1:A:285:GLU:CD	2.23	0.63
1:B:98:GLN:OE1	1:B:99:ILE:CG1	2.42	0.63
1:B:376:VAL:HG11	1:B:453:PHE:CG	2.33	0.63
1:B:222:THR:O	1:B:224:VAL:N	2.30	0.63
1:B:311:GLY:H	1:B:312:PRO:HD2	1.64	0.63
1:A:64:MET:HE3	1:A:78:TRP:CE3	2.33	0.63
1:A:154:ARG:HH21	1:A:489:LYS:CE	1.86	0.63
1:A:452:SER:O	1:A:456:VAL:HG23	1.98	0.63
1:A:476:GLY:C	1:A:477:VAL:HG13	2.23	0.63
1:B:36:ALA:CB	1:B:253:GLY:O	2.42	0.63
1:B:357:THR:CG2	1:B:358:ASN:N	2.62	0.63
1:A:321:GLN:HE22	1:A:477:VAL:H	1.44	0.63
1:B:99:ILE:HD12	1:B:312:PRO:CG	2.28	0.63
1:B:409:LYS:O	1:B:413:LEU:HB2	1.99	0.63
1:A:385:LEU:C	1:A:385:LEU:HD23	2.23	0.63
1:A:434:PRO:O	1:A:435:ASP:CG	2.41	0.63
1:A:230:PRO:O	1:A:231:GLY:C	2.39	0.63
1:A:335:ASN:H	1:A:506:MET:CE	2.11	0.63
1:B:308:TRP:CD1	1:B:498:ALA:HB2	2.33	0.63
1:A:124:ASN:O	1:A:130:LYS:HE3	1.98	0.62
1:B:146:PHE:CE1	1:B:342:VAL:HG11	2.29	0.62
1:B:377:ILE:HD11	1:B:456:VAL:HG11	1.81	0.62
1:A:31:GLU:HB3	1:A:35:PHE:CE2	2.34	0.62
1:A:152:THR:CG2	1:A:307:SER:HA	2.29	0.62
1:B:160:PHE:CD1	1:B:165:LEU:HD21	2.27	0.62
1:B:234:TYR:HB3	1:B:235:PRO:CD	2.29	0.62
1:B:262:GLY:HA2	1:B:265:ILE:CG1	2.19	0.62
1:A:232:ARG:O	1:A:236:LEU:HD23	2.00	0.62
1:B:234:TYR:C	1:B:236:LEU:H	2.06	0.62
1:B:234:TYR:HB3	1:B:235:PRO:HD3	1.81	0.62
1:A:70:TRP:HZ3	1:A:392:LEU:HD13	1.65	0.62
1:A:85:PRO:O	1:A:88:GLY:N	2.32	0.62
1:A:163:GLY:O	1:A:167:PRO:CD	2.47	0.62
1:A:208:VAL:HG23	1:A:209:ALA:H	1.65	0.62
1:B:172:ILE:HG22	1:B:173:ALA:N	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:GLY:C	1:B:440:ASP:O	2.41	0.62
1:A:11:LYS:CG	1:A:226:GLU:HA	2.29	0.62
1:A:279:MET:SD	1:A:289:THR:HG22	2.39	0.62
1:A:505:VAL:CG2	1:A:505:VAL:O	2.43	0.62
1:B:117:ILE:HD11	1:B:295:ALA:CA	2.30	0.62
1:A:336:GLY:H	1:A:506:MET:CE	2.12	0.62
1:A:406:PRO:O	1:A:406:PRO:CG	2.46	0.62
1:A:117:ILE:HD12	1:A:294:SER:HB3	1.82	0.61
1:A:332:MET:CG	1:A:338:PRO:CA	2.78	0.61
1:A:399:LEU:HB3	1:A:401:ARG:HH21	1.65	0.61
1:B:374:THR:HG22	1:B:375:VAL:N	2.15	0.61
1:A:163:GLY:O	1:A:167:PRO:HG2	1.99	0.61
1:A:333:ASN:O	1:A:334:LYS:C	2.42	0.61
1:B:60:CYS:HB2	1:B:389:TYR:CE1	2.35	0.61
1:B:124:ASN:C	1:B:124:ASN:OD1	2.43	0.61
1:B:279:MET:O	1:B:283:ALA:N	2.27	0.61
1:B:483:ASN:OD1	1:B:483:ASN:N	2.30	0.61
1:A:68:ASP:HB2	1:A:400:LYS:HB2	1.83	0.61
1:A:75:VAL:HG23	1:A:75:VAL:O	2.00	0.61
1:A:166:LEU:O	1:A:166:LEU:HD22	1.99	0.61
1:A:197:ASP:OD1	1:A:199:SER:HB2	2.00	0.61
1:A:433:PRO:HB3	1:A:442:THR:HG21	1.82	0.61
1:B:317:TYR:CD2	1:B:479:LEU:HD11	2.30	0.61
1:B:353:LEU:O	1:B:353:LEU:HD13	1.98	0.61
1:A:223:HIS:HE1	1:A:492:PHE:CE2	2.19	0.61
1:A:336:GLY:C	1:A:337:VAL:CG1	2.74	0.61
1:A:359:THR:HG22	1:A:360:GLY:N	2.16	0.61
1:A:433:PRO:HG3	1:A:445:TYR:CG	2.36	0.61
1:B:222:THR:O	1:B:225:ASN:N	2.28	0.61
1:A:356:LEU:HD22	1:A:369:ILE:HG21	1.83	0.61
1:B:15:LEU:CD2	1:B:16:LEU:CA	2.70	0.61
1:B:53:TRP:O	1:B:54:PHE:C	2.44	0.61
1:B:341:LEU:HA	1:B:344:SER:HB3	1.83	0.61
1:A:379:LEU:HD12	1:A:383:PHE:CZ	2.36	0.61
1:B:298:LEU:C	1:B:302:LEU:HD12	2.26	0.61
1:B:133:ALA:O	1:B:137:ILE:HG13	2.01	0.60
1:B:178:TYR:OH	1:B:183:ALA:C	2.44	0.60
1:A:53:TRP:O	1:A:54:PHE:C	2.43	0.60
1:A:101:ILE:HG22	1:A:374:THR:OG1	2.01	0.60
1:B:377:ILE:CG1	1:B:456:VAL:HG11	2.30	0.60
1:A:18:PHE:O	1:A:21:ILE:HG12	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:PHE:O	1:B:23:ALA:HB2	2.01	0.60
1:B:67:VAL:HG23	1:B:70:TRP:CB	2.30	0.60
1:B:336:GLY:C	1:B:337:VAL:HG12	2.26	0.60
1:A:392:LEU:O	1:A:393:VAL:C	2.44	0.60
1:A:476:GLY:O	1:A:477:VAL:HG13	2.02	0.60
1:A:484:SER:C	1:A:485:GLN:HE21	2.10	0.60
1:B:63:GLU:OE1	1:B:389:TYR:OH	2.16	0.60
1:A:309:ILE:HG22	1:A:309:ILE:O	2.01	0.60
1:B:390:ILE:O	1:B:394:LEU:HB2	2.01	0.60
1:A:122:ALA:O	1:A:126:ASP:HB2	2.01	0.60
1:A:279:MET:HA	1:A:282:VAL:HG23	1.82	0.60
1:A:78:TRP:CD1	1:A:78:TRP:N	2.64	0.60
1:B:123:LEU:O	1:B:130:LYS:HG2	2.01	0.60
1:B:265:ILE:O	1:B:438:GLN:CG	2.50	0.60
1:B:50:GLY:HA3	1:B:242:MET:CG	2.32	0.60
1:A:202:GLY:O	1:A:205:VAL:HG12	2.02	0.60
1:A:457:LEU:O	1:A:461:PHE:HD2	1.84	0.60
1:B:60:CYS:HA	1:B:405:ILE:HD11	1.83	0.60
1:B:336:GLY:O	1:B:337:VAL:HG13	2.02	0.60
1:B:392:LEU:HA	1:B:396:HIS:HB2	1.84	0.60
1:A:67:VAL:CG1	1:A:70:TRP:HB2	2.29	0.60
1:A:337:VAL:O	1:A:338:PRO:C	2.43	0.60
1:B:56:PRO:O	1:B:60:CYS:SG	2.54	0.60
1:B:157:LYS:CG	1:B:493:PHE:HE2	2.13	0.60
1:B:234:TYR:HD2	1:B:235:PRO:N	1.99	0.60
1:B:307:SER:HG	1:B:308:TRP:CD1	2.20	0.60
1:B:326:PRO:HB2	1:B:329:PHE:CD2	2.37	0.60
1:A:76:PHE:O	1:A:76:PHE:CD1	2.45	0.59
1:A:272:MET:HE2	1:A:297:LEU:HD12	1.83	0.59
1:A:293:ILE:HA	1:A:296:LEU:HD12	1.84	0.59
1:A:433:PRO:CG	1:A:445:TYR:CD2	2.84	0.59
1:B:42:LEU:O	1:B:46:LEU:CB	2.43	0.59
1:A:40:PHE:O	1:A:43:VAL:HG23	2.01	0.59
1:B:332:MET:HE3	1:B:338:PRO:CD	2.32	0.59
1:B:337:VAL:O	1:B:338:PRO:C	2.43	0.59
1:A:152:THR:HG21	1:A:307:SER:HA	1.84	0.59
1:A:172:ILE:HG23	1:A:173:ALA:N	2.17	0.59
1:A:225:ASN:C	1:A:227:MET:H	2.10	0.59
1:A:225:ASN:C	1:A:227:MET:N	2.58	0.59
1:B:103:PHE:CE1	1:B:308:TRP:CE3	2.90	0.59
1:B:131:THR:CG2	1:B:357:THR:HG21	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:PHE:O	1:B:194:PHE:CG	2.54	0.59
1:B:332:MET:HE3	1:B:338:PRO:HD3	1.84	0.59
1:B:403:PHE:C	1:B:404:ASN:HD22	2.09	0.59
1:A:68:ASP:HB2	1:A:400:LYS:CB	2.32	0.59
1:A:94:PHE:CB	1:A:381:ALA:HB2	2.27	0.59
1:A:503:TYR:H	1:A:503:TYR:HD2	1.45	0.59
1:B:103:PHE:CE1	1:B:308:TRP:HE3	2.20	0.59
1:A:113:ALA:HA	1:A:272:MET:SD	2.41	0.59
1:B:44:PHE:CD2	1:B:196:PRO:CD	2.86	0.59
1:B:157:LYS:HG3	1:B:493:PHE:CE2	2.30	0.59
1:A:339:VAL:O	1:A:339:VAL:HG23	2.03	0.59
1:B:43:VAL:O	1:B:47:LEU:HB2	2.03	0.59
1:B:230:PRO:O	1:B:231:GLY:C	2.46	0.59
1:B:351:ILE:HG22	1:B:352:ALA:H	1.66	0.59
1:B:376:VAL:CG1	1:B:453:PHE:CD1	2.85	0.59
1:B:21:ILE:HD11	1:B:484:SER:HB2	1.85	0.59
1:B:339:VAL:HG23	1:B:339:VAL:O	2.03	0.59
1:A:373:LEU:HD22	1:A:377:ILE:HD12	1.85	0.59
1:A:423:SER:O	1:A:424:ILE:C	2.46	0.59
1:B:59:LEU:N	1:B:59:LEU:CD2	2.63	0.59
1:B:170:ILE:HD13	1:B:293:ILE:CD1	2.32	0.59
1:B:332:MET:HE2	1:B:336:GLY:C	2.27	0.59
1:B:106:MET:HB3	1:B:305:ILE:HD11	1.85	0.58
1:B:127:PRO:O	1:B:131:THR:HG22	2.03	0.58
1:B:222:THR:C	1:B:224:VAL:H	2.09	0.58
1:A:166:LEU:C	1:A:166:LEU:HD23	2.25	0.58
1:B:15:LEU:HD23	1:B:16:LEU:HA	1.83	0.58
1:B:171:LEU:HG	1:B:172:ILE:N	2.17	0.58
1:B:321:GLN:C	1:B:323:ASN:H	2.10	0.58
1:A:98:GLN:C	1:A:98:GLN:CD	2.69	0.58
1:A:128:ILE:O	1:A:128:ILE:CD1	2.38	0.58
1:A:157:LYS:HD3	1:A:493:PHE:HE2	1.67	0.58
1:B:234:TYR:HE2	1:B:238:MET:HG3	1.69	0.58
1:A:203:THR:HG22	1:A:204:LEU:N	2.19	0.58
1:A:319:THR:HA	1:A:324:LEU:HD12	1.84	0.58
1:A:421:LEU:HD12	1:B:424:ILE:HD12	1.85	0.58
1:B:120:TRP:HD1	1:B:121:PRO:HD2	1.68	0.58
1:B:332:MET:HE3	1:B:338:PRO:N	2.17	0.58
1:A:417:ILE:HD11	1:B:424:ILE:HG22	1.85	0.58
1:B:234:TYR:HE2	1:B:238:MET:SD	2.23	0.58
1:A:73:GLY:HA3	1:A:77:ALA:HB3	1.82	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:GLY:C	1:A:75:VAL:CG1	2.69	0.58
1:A:101:ILE:CG1	1:A:373:LEU:HD13	2.31	0.58
1:B:437:ILE:O	1:B:438:GLN:C	2.45	0.58
1:A:172:ILE:CD1	1:A:251:VAL:CG1	2.65	0.58
1:A:272:MET:HE3	1:A:272:MET:N	2.19	0.58
1:A:482:ILE:HG22	1:A:483:ASN:N	2.19	0.58
1:B:286:ILE:CG2	1:B:286:ILE:O	2.48	0.58
1:B:30:TYR:OH	1:B:164:ILE:HD11	2.04	0.58
1:B:191:SER:O	1:B:193:THR:N	2.37	0.58
1:B:491:HIS:C	1:B:491:HIS:CD2	2.81	0.58
1:A:138:LEU:C	1:A:138:LEU:CD2	2.77	0.58
1:B:170:ILE:CG2	1:B:275:PHE:CE1	2.82	0.58
1:B:44:PHE:CE2	1:B:196:PRO:HD2	2.39	0.58
1:B:234:TYR:O	1:B:237:ALA:N	2.36	0.58
1:B:444:MET:O	1:B:445:TYR:C	2.45	0.58
1:A:198:PHE:O	1:B:395:LYS:HD3	2.03	0.57
1:B:26:VAL:HG23	1:B:27:MET:CE	2.34	0.57
1:A:101:ILE:N	1:A:101:ILE:CD1	2.68	0.57
1:A:204:LEU:C	1:A:206:VAL:N	2.62	0.57
1:B:46:LEU:O	1:B:46:LEU:CD1	2.52	0.57
1:B:246:ILE:HG22	1:B:247:CYS:H	1.69	0.57
1:A:445:TYR:HE1	1:A:449:LEU:HD23	1.68	0.57
1:B:23:ALA:C	1:B:25:MET:H	2.11	0.57
1:B:462:ILE:O	1:B:466:VAL:HB	2.04	0.57
1:B:495:HIS:O	1:B:498:ALA:N	2.37	0.57
1:A:98:GLN:HG3	1:A:378:TYR:HD2	1.67	0.57
1:A:146:PHE:C	1:A:148:GLY:H	2.12	0.57
1:B:82:THR:CG2	1:B:391:VAL:HB	2.33	0.57
1:A:80:SER:HA	1:A:84:GLY:O	2.04	0.57
1:A:465:ALA:O	1:A:467:HIS:N	2.37	0.57
1:B:70:TRP:C	1:B:72:GLU:H	2.13	0.57
1:B:215:MET:HE1	1:B:378:TYR:HB3	1.81	0.57
1:A:19:PHE:HE2	1:A:23:ALA:CB	2.17	0.57
1:A:242:MET:CE	1:A:246:ILE:HD11	2.34	0.57
1:B:47:LEU:O	1:B:51:ILE:HB	2.05	0.57
1:B:152:THR:O	1:B:156:ALA:N	2.36	0.57
1:B:204:LEU:O	1:B:207:PHE:N	2.30	0.57
1:A:146:PHE:O	1:A:148:GLY:N	2.30	0.57
1:A:67:VAL:CG2	1:A:401:ARG:HG3	2.30	0.57
1:A:154:ARG:CZ	1:A:489:LYS:HG3	2.35	0.57
1:A:365:MET:O	1:A:369:ILE:HB	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:LEU:HD11	1:B:424:ILE:CD1	2.25	0.57
1:A:44:PHE:CG	1:A:194:PHE:HE2	2.23	0.57
1:A:67:VAL:HA	1:A:400:LYS:O	2.05	0.57
1:A:200:LYS:CB	1:A:200:LYS:NZ	2.67	0.57
1:B:212:LEU:O	1:B:213:SER:C	2.45	0.57
1:A:256:ILE:HA	1:A:274:THR:OG1	2.04	0.56
1:A:286:ILE:O	1:A:289:THR:CG2	2.51	0.56
1:A:353:LEU:HD12	1:A:357:THR:CG2	2.35	0.56
1:A:399:LEU:HD23	1:A:400:LYS:N	2.19	0.56
1:B:40:PHE:C	1:B:42:LEU:H	2.13	0.56
1:B:126:ASP:OD2	1:B:128:ILE:HG23	2.05	0.56
1:B:390:ILE:HD11	1:B:416:ALA:HB3	1.86	0.56
1:B:392:LEU:C	1:B:394:LEU:H	2.12	0.56
1:A:491:HIS:O	1:A:494:LEU:CB	2.34	0.56
1:B:336:GLY:C	1:B:337:VAL:CG1	2.79	0.56
1:B:60:CYS:CA	1:B:405:ILE:HD11	2.35	0.56
1:B:92:ILE:CG2	1:B:93:SER:N	2.69	0.56
1:B:163:GLY:HA2	1:B:167:PRO:HG2	1.88	0.56
1:B:377:ILE:HG12	1:B:456:VAL:CG1	2.35	0.56
1:A:389:TYR:O	1:A:392:LEU:HB3	2.06	0.56
1:A:435:ASP:O	1:A:441:SER:HA	2.05	0.56
1:B:342:VAL:O	1:B:346:LEU:HG	2.06	0.56
1:A:427:PHE:O	1:A:430:SER:HB2	2.05	0.56
1:B:396:HIS:N	1:B:397:PRO:CD	2.68	0.56
1:A:12:GLN:HG3	1:A:228:SER:HB2	1.86	0.56
1:B:227:MET:HE2	1:B:227:MET:HA	1.88	0.56
1:B:269:ALA:HB1	1:B:272:MET:HE2	1.84	0.56
1:A:373:LEU:HA	1:A:376:VAL:CG2	2.35	0.56
1:A:143:LEU:O	1:A:144:THR:C	2.45	0.56
1:A:178:TYR:CD2	1:A:178:TYR:O	2.59	0.56
1:B:120:TRP:CE3	1:B:123:LEU:HD22	2.40	0.56
1:B:146:PHE:C	1:B:148:GLY:H	2.14	0.56
1:B:186:ALA:C	1:B:188:GLU:H	2.13	0.56
1:B:226:GLU:OE2	1:B:483:ASN:HB3	2.06	0.56
1:A:67:VAL:O	1:A:68:ASP:C	2.46	0.55
1:A:242:MET:HE3	1:A:246:ILE:HD11	1.86	0.55
1:A:477:VAL:HG21	1:A:504:ILE:HG23	1.88	0.55
1:B:41:SER:CB	1:B:196:PRO:HG3	2.18	0.55
1:B:54:PHE:CE2	1:B:238:MET:HE3	2.42	0.55
1:B:103:PHE:CZ	1:B:308:TRP:CB	2.89	0.55
1:A:263:ASN:O	1:A:438:GLN:HB3	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:PHE:O	1:B:47:LEU:HB2	2.06	0.55
1:B:289:THR:CG2	1:B:290:VAL:N	2.70	0.55
1:A:38:SER:O	1:A:39:GLY:C	2.46	0.55
1:A:266:ASN:O	1:A:270:GLY:CA	2.54	0.55
1:B:92:ILE:HG23	1:B:93:SER:N	2.21	0.55
1:A:170:ILE:O	1:A:174:LEU:HB2	2.06	0.55
1:A:364:ASN:ND2	1:A:438:GLN:CB	2.69	0.55
1:A:378:TYR:CD1	1:A:382:TYR:CE2	2.94	0.55
1:B:48:LEU:N	1:B:48:LEU:CD2	2.60	0.55
1:A:11:LYS:HG3	1:A:226:GLU:HB3	1.88	0.55
1:B:65:ALA:O	1:B:71:GLU:CA	2.55	0.55
1:B:277:VAL:O	1:B:281:HIS:HB2	2.06	0.55
1:A:11:LYS:HA	1:A:11:LYS:CE	2.36	0.55
1:A:217:VAL:C	1:A:219:ALA:N	2.62	0.55
1:A:373:LEU:O	1:A:376:VAL:CG2	2.55	0.55
1:A:399:LEU:CD2	1:A:400:LYS:N	2.67	0.55
1:B:47:LEU:HA	1:B:246:ILE:HD11	1.87	0.55
1:B:131:THR:HB	1:B:357:THR:HG21	1.88	0.55
1:B:298:LEU:HG	1:B:302:LEU:HD12	1.88	0.55
1:B:32:TYR:HB3	1:B:256:ILE:HD11	1.88	0.55
1:B:408:GLY:O	1:B:412:LYS:HB2	2.06	0.55
1:A:117:ILE:HD11	1:A:295:ALA:N	2.21	0.55
1:B:279:MET:HE2	1:B:289:THR:HG21	1.89	0.55
1:A:117:ILE:CB	1:A:118:LEU:CD1	2.84	0.55
1:A:179:LEU:O	1:A:179:LEU:HD22	2.07	0.55
1:A:182:GLY:O	1:A:183:ALA:HB2	2.07	0.55
1:A:204:LEU:C	1:A:206:VAL:H	2.14	0.55
1:A:217:VAL:C	1:A:219:ALA:H	2.15	0.55
1:B:82:THR:HG23	1:B:391:VAL:CG1	2.37	0.55
1:B:171:LEU:HA	1:B:275:PHE:CE1	2.42	0.55
1:B:340:THR:O	1:B:344:SER:HB2	2.07	0.55
1:A:286:ILE:HG22	1:A:289:THR:CB	2.20	0.54
1:A:501:PRO:O	1:A:502:HIS:CD2	2.59	0.54
1:B:323:ASN:O	1:B:324:LEU:HD22	2.06	0.54
1:B:352:ALA:HA	1:B:355:ILE:HG23	1.88	0.54
1:A:11:LYS:HA	1:A:11:LYS:HE3	1.89	0.54
1:A:343:ILE:HG13	1:A:344:SER:N	2.18	0.54
1:A:93:SER:O	1:A:97:LEU:HB2	2.07	0.54
1:A:154:ARG:HE	1:A:489:LYS:HG3	1.71	0.54
1:A:331:LYS:O	1:A:338:PRO:HA	2.07	0.54
1:A:394:LEU:HD11	1:A:413:LEU:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:PHE:C	1:B:148:GLY:N	2.65	0.54
1:B:308:TRP:HE1	1:B:498:ALA:CB	2.20	0.54
1:A:117:ILE:HD11	1:A:294:SER:C	2.32	0.54
1:B:89:PHE:O	1:B:92:ILE:HG22	2.07	0.54
1:B:129:THR:C	1:B:131:THR:N	2.65	0.54
1:B:496:PRO:O	1:B:497:ARG:C	2.45	0.54
1:A:116:TYR:OH	1:A:273:GLN:CG	2.56	0.54
1:A:336:GLY:O	1:A:337:VAL:HG12	2.06	0.54
1:A:434:PRO:O	1:A:435:ASP:HB3	2.08	0.54
1:B:36:ALA:HB1	1:B:257:ALA:CB	2.25	0.54
1:B:116:TYR:OH	1:B:273:GLN:HG3	2.08	0.54
1:B:237:ALA:O	1:B:241:LEU:N	2.29	0.54
1:B:298:LEU:HG	1:B:302:LEU:HD11	1.87	0.54
1:B:325:LEU:HB3	1:B:326:PRO:HD2	1.89	0.54
1:A:19:PHE:O	1:A:23:ALA:HB2	2.07	0.54
1:A:223:HIS:CE1	1:A:492:PHE:CE2	2.96	0.54
1:A:339:VAL:HG23	1:A:343:ILE:HG23	1.89	0.54
1:A:480:GLU:O	1:A:481:PRO:C	2.51	0.54
1:B:117:ILE:HD11	1:B:295:ALA:HA	1.89	0.54
1:B:395:LYS:O	1:B:395:LYS:CG	2.54	0.54
1:A:207:PHE:O	1:A:210:PHE:N	2.40	0.54
1:A:232:ARG:O	1:A:234:TYR:N	2.40	0.54
1:A:357:THR:OG1	1:A:358:ASN:N	2.38	0.54
1:A:380:CYS:O	1:A:384:MET:HE3	2.06	0.54
1:A:25:MET:HB2	1:A:495:HIS:CE1	2.42	0.54
1:A:197:ASP:CG	1:A:199:SER:HB2	2.33	0.54
1:A:260:ILE:HD12	1:A:273:GLN:HE21	1.72	0.54
1:A:428:ILE:C	1:A:430:SER:N	2.66	0.54
1:B:162:ALA:O	1:B:296:LEU:HD22	2.08	0.54
1:B:267:LEU:O	1:B:268:SER:C	2.49	0.54
1:B:432:LEU:HD12	1:B:432:LEU:C	2.23	0.54
1:A:15:LEU:HD22	1:A:16:LEU:N	2.22	0.54
1:A:19:PHE:HE2	1:A:23:ALA:HB1	1.71	0.54
1:B:58:GLY:O	1:B:61:ALA:HB3	2.08	0.54
1:B:70:TRP:CD1	1:B:70:TRP:N	2.71	0.54
1:B:299:LEU:O	1:B:300:GLY:C	2.49	0.54
1:A:336:GLY:N	1:A:506:MET:HE2	2.22	0.54
1:A:363:ASN:N	1:A:440:ASP:OD2	2.41	0.54
1:B:82:THR:HG22	1:B:391:VAL:CG1	2.36	0.54
1:B:93:SER:CB	1:B:460:PRO:HB3	2.39	0.54
1:B:197:ASP:C	1:B:199:SER:N	2.65	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:LEU:CD2	1:B:369:ILE:HG21	2.38	0.54
1:B:411:VAL:HA	1:B:414:VAL:HG12	1.89	0.54
1:A:275:PHE:HB3	1:A:290:VAL:CG2	2.34	0.53
1:A:360:GLY:O	1:A:361:GLY:O	2.26	0.53
1:B:189:MET:O	1:B:190:ASP:C	2.49	0.53
1:B:350:SER:O	1:B:354:ILE:HG13	2.08	0.53
1:A:71:GLU:CD	1:A:71:GLU:H	2.16	0.53
1:A:204:LEU:O	1:A:205:VAL:C	2.51	0.53
1:A:217:VAL:O	1:A:219:ALA:N	2.41	0.53
1:A:410:GLY:O	1:A:411:VAL:C	2.52	0.53
1:B:55:ILE:CB	1:B:56:PRO:CD	2.68	0.53
1:A:120:TRP:C	1:A:122:ALA:H	2.16	0.53
1:A:222:THR:O	1:A:224:VAL:N	2.41	0.53
1:A:504:ILE:O	1:A:504:ILE:CG2	2.45	0.53
1:B:333:ASN:O	1:B:334:LYS:C	2.49	0.53
1:A:75:VAL:HG12	1:A:78:TRP:CD2	2.41	0.53
1:A:160:PHE:CZ	1:A:165:LEU:HD21	2.43	0.53
1:A:405:ILE:CG2	1:A:406:PRO:HD2	2.38	0.53
1:B:351:ILE:O	1:B:355:ILE:HG22	2.07	0.53
1:A:117:ILE:HG21	1:A:118:LEU:HD11	1.89	0.53
1:A:272:MET:HE3	1:A:272:MET:H	1.73	0.53
1:B:40:PHE:O	1:B:40:PHE:HD2	1.92	0.53
1:B:96:TYR:O	1:B:97:LEU:C	2.51	0.53
1:B:308:TRP:HE1	1:B:498:ALA:HB2	1.69	0.53
1:A:96:TYR:HB2	1:A:316:MET:HG3	1.89	0.53
1:A:161:PHE:HE1	1:A:493:PHE:CE2	2.07	0.53
1:A:492:PHE:C	1:A:494:LEU:H	2.15	0.53
1:B:484:SER:C	1:B:485:GLN:HE21	2.17	0.53
1:A:86:ARG:HD2	1:A:87:TRP:CZ2	2.43	0.53
1:A:321:GLN:NE2	1:A:476:GLY:HA3	2.24	0.53
1:B:142:ALA:HA	1:B:309:ILE:HG21	1.90	0.53
1:A:123:LEU:O	1:A:130:LYS:HG2	2.08	0.53
1:A:44:PHE:HB2	1:A:194:PHE:CD2	2.42	0.53
1:B:50:GLY:HA3	1:B:242:MET:SD	2.49	0.52
1:B:53:TRP:CZ2	1:B:382:TYR:HD1	2.17	0.52
1:B:60:CYS:N	1:B:405:ILE:HD11	2.24	0.52
1:B:138:LEU:HD22	1:B:138:LEU:C	2.33	0.52
1:B:166:LEU:HD13	1:B:166:LEU:O	2.08	0.52
1:A:124:ASN:HD21	1:A:269:ALA:HB2	1.71	0.52
1:B:82:THR:O	1:B:83:LEU:HD23	2.09	0.52
1:B:433:PRO:HB2	1:B:434:PRO:CD	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:GLU:C	1:A:127:PRO:HD3	2.29	0.52
1:A:476:GLY:C	1:A:477:VAL:CG1	2.82	0.52
1:B:29:VAL:HA	1:B:32:TYR:CE1	2.43	0.52
1:B:32:TYR:O	1:B:35:PHE:HB2	2.09	0.52
1:A:15:LEU:HD22	1:A:16:LEU:CD2	2.13	0.52
1:A:229:ASN:C	1:A:229:ASN:OD1	2.51	0.52
1:A:239:LEU:O	1:A:243:VAL:HG23	2.10	0.52
1:B:103:PHE:O	1:B:106:MET:CB	2.56	0.52
1:B:163:GLY:C	1:B:167:PRO:HG2	2.34	0.52
1:B:131:THR:HG22	1:B:357:THR:HG21	1.92	0.52
1:B:160:PHE:O	1:B:164:ILE:HB	2.09	0.52
1:B:175:ALA:O	1:B:178:TYR:HB3	2.09	0.52
1:A:224:VAL:O	1:A:227:MET:N	2.36	0.52
1:A:332:MET:HG3	1:A:338:PRO:CB	2.40	0.52
1:A:408:GLY:O	1:A:410:GLY:N	2.41	0.52
1:B:208:VAL:CG1	1:B:371:LEU:HB3	2.40	0.52
1:B:226:GLU:O	1:B:227:MET:C	2.53	0.52
1:A:160:PHE:HE1	1:A:165:LEU:CD2	1.97	0.52
1:A:142:ALA:O	1:A:143:LEU:C	2.52	0.52
1:A:323:ASN:O	1:A:324:LEU:C	2.53	0.52
1:A:428:ILE:O	1:A:430:SER:N	2.43	0.52
1:A:476:GLY:O	1:A:477:VAL:HG12	2.09	0.52
1:A:15:LEU:HD21	1:A:16:LEU:CD2	2.37	0.52
1:A:205:VAL:O	1:A:205:VAL:CG2	2.56	0.52
1:A:206:VAL:O	1:A:207:PHE:C	2.53	0.52
1:B:376:VAL:HG11	1:B:453:PHE:CD1	2.45	0.52
1:A:65:ALA:O	1:A:71:GLU:HA	2.10	0.52
1:A:399:LEU:CB	1:A:401:ARG:HH21	2.23	0.52
1:B:82:THR:HG21	1:B:391:VAL:HB	1.90	0.52
1:B:109:PHE:CD2	1:B:301:VAL:CG2	2.87	0.52
1:B:266:ASN:HD21	1:B:268:SER:HB3	1.75	0.52
1:A:310:VAL:CG1	1:A:311:GLY:H	2.18	0.51
1:B:349:THR:O	1:B:353:LEU:N	2.43	0.51
1:A:128:ILE:C	1:A:128:ILE:CD1	2.81	0.51
1:A:250:SER:O	1:A:254:LEU:CD1	2.50	0.51
1:B:294:SER:O	1:B:295:ALA:C	2.49	0.51
1:A:13:LEU:CB	1:A:227:MET:HA	2.41	0.51
1:A:55:ILE:CB	1:A:56:PRO:CD	2.77	0.51
1:A:283:ALA:O	1:A:284:PRO:C	2.53	0.51
1:B:40:PHE:C	1:B:42:LEU:N	2.68	0.51
1:A:504:ILE:CG2	1:A:506:MET:HG2	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:LEU:HD21	1:A:254:LEU:HG	1.93	0.51
1:B:75:VAL:HG23	1:B:76:PHE:N	2.26	0.51
1:B:111:LEU:HD12	1:B:130:LYS:HD3	1.92	0.51
1:B:395:LYS:C	1:B:396:HIS:ND1	2.61	0.51
1:B:484:SER:O	1:B:485:GLN:NE2	2.40	0.51
1:B:312:PRO:O	1:B:313:SER:C	2.54	0.51
1:B:395:LYS:CG	1:B:396:HIS:CE1	2.94	0.51
1:A:10:ALA:O	1:A:11:LYS:HD2	2.11	0.51
1:A:64:MET:CE	1:A:78:TRP:CE3	2.94	0.51
1:A:124:ASN:HD21	1:A:269:ALA:CB	2.22	0.51
1:A:124:ASN:CA	1:A:130:LYS:HE2	2.29	0.51
1:A:226:GLU:OE2	1:A:484:SER:HB3	2.10	0.51
1:B:338:PRO:HB2	1:B:341:LEU:CD1	2.41	0.51
1:B:393:VAL:HG11	1:B:413:LEU:CD2	2.41	0.51
1:A:408:GLY:O	1:A:409:LYS:C	2.54	0.51
1:B:59:LEU:O	1:B:61:ALA:N	2.44	0.51
1:A:98:GLN:CA	1:A:377:ILE:CG2	2.89	0.51
1:A:433:PRO:HG2	1:A:445:TYR:HB3	1.93	0.51
1:B:24:SER:HB3	1:B:493:PHE:O	2.10	0.51
1:A:29:VAL:HA	1:A:32:TYR:CD2	2.46	0.50
1:B:29:VAL:HA	1:B:32:TYR:CG	2.46	0.50
1:B:175:ALA:O	1:B:178:TYR:CB	2.59	0.50
1:A:96:TYR:CD1	1:A:316:MET:HG3	2.46	0.50
1:A:154:ARG:NE	1:A:489:LYS:HG3	2.26	0.50
1:A:310:VAL:HG13	1:A:311:GLY:N	2.16	0.50
1:A:434:PRO:O	1:A:435:ASP:OD2	2.30	0.50
1:A:442:THR:HG21	1:A:445:TYR:HD2	1.75	0.50
1:B:222:THR:O	1:B:223:HIS:C	2.54	0.50
1:B:374:THR:HG23	1:B:375:VAL:N	2.27	0.50
1:B:437:ILE:O	1:B:439:GLY:N	2.44	0.50
1:B:493:PHE:O	1:B:494:LEU:C	2.51	0.50
1:A:221:ALA:C	1:A:223:HIS:N	2.68	0.50
1:B:138:LEU:HD22	1:B:138:LEU:O	2.10	0.50
1:B:159:GLY:HA2	1:B:162:ALA:HB3	1.93	0.50
1:B:307:SER:CB	1:B:494:LEU:HD11	2.39	0.50
1:A:55:ILE:O	1:A:56:PRO:C	2.53	0.50
1:A:131:THR:O	1:A:135:LEU:HD12	2.12	0.50
1:A:338:PRO:HG2	1:A:338:PRO:O	2.12	0.50
1:A:347:VAL:HG12	1:A:351:ILE:HD12	1.91	0.50
1:A:442:THR:HB	1:A:445:TYR:HB3	1.90	0.50
1:B:51:ILE:HG22	1:B:52:LEU:CG	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:ALA:HB2	1:B:371:LEU:HD12	1.93	0.50
1:B:436:ASN:OD1	1:B:436:ASN:O	2.30	0.50
1:B:489:LYS:H	1:B:489:LYS:HD3	1.66	0.50
1:A:19:PHE:HD2	1:A:20:ALA:N	2.10	0.50
1:A:212:LEU:O	1:A:213:SER:C	2.54	0.50
1:B:45:PHE:O	1:B:46:LEU:C	2.54	0.50
1:A:67:VAL:HG12	1:A:70:TRP:CG	2.46	0.50
1:A:101:ILE:HG22	1:A:374:THR:HG1	1.76	0.50
1:A:263:ASN:O	1:A:263:ASN:OD1	2.30	0.50
1:B:76:PHE:O	1:B:80:SER:HB2	2.12	0.50
1:B:124:ASN:O	1:B:124:ASN:OD1	2.30	0.50
1:A:31:GLU:O	1:A:35:PHE:CD2	2.65	0.50
1:A:355:ILE:O	1:A:359:THR:HB	2.11	0.50
1:A:356:LEU:HD22	1:A:369:ILE:HG22	1.91	0.50
1:A:423:SER:O	1:A:426:ALA:N	2.45	0.50
1:B:67:VAL:O	1:B:69:GLY:N	2.45	0.50
1:B:115:SER:O	1:B:116:TYR:C	2.54	0.50
1:B:170:ILE:HG22	1:B:275:PHE:HZ	1.63	0.50
1:A:170:ILE:HG22	1:A:275:PHE:CZ	2.47	0.50
1:A:187:ILE:CB	1:A:258:MET:O	2.60	0.50
1:A:208:VAL:HG23	1:A:209:ALA:N	2.26	0.50
1:B:234:TYR:CD2	1:B:235:PRO:N	2.77	0.50
1:A:55:ILE:HG22	1:A:56:PRO:N	2.26	0.50
1:A:163:GLY:O	1:A:167:PRO:CG	2.59	0.50
1:A:254:LEU:O	1:A:258:MET:HG2	2.12	0.50
1:A:433:PRO:HB2	1:A:442:THR:OG1	2.12	0.50
1:A:486:ASN:O	1:A:487:ALA:O	2.30	0.50
1:B:29:VAL:C	1:B:31:GLU:N	2.69	0.50
1:B:200:LYS:O	1:B:201:VAL:O	2.30	0.50
1:B:279:MET:CE	1:B:286:ILE:HG21	2.41	0.50
1:B:486:ASN:O	1:B:487:ALA:O	2.30	0.50
1:A:29:VAL:CG2	1:A:30:TYR:H	2.25	0.49
1:A:85:PRO:HB2	1:A:464:TYR:OH	2.12	0.49
1:A:85:PRO:C	1:A:87:TRP:N	2.69	0.49
1:A:98:GLN:HG2	1:A:374:THR:HG23	1.92	0.49
1:B:31:GLU:O	1:B:34:THR:HG23	2.11	0.49
1:A:71:GLU:HB3	1:A:225:ASN:HD21	1.76	0.49
1:A:265:ILE:O	1:A:265:ILE:HG22	2.08	0.49
1:A:308:TRP:N	1:A:308:TRP:HE3	2.10	0.49
1:A:312:PRO:HG3	1:A:498:ALA:HA	1.93	0.49
1:B:204:LEU:O	1:B:205:VAL:C	2.56	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:VAL:C	1:B:208:VAL:H	2.19	0.49
1:B:386:PHE:CE1	1:B:419:GLY:HA3	2.47	0.49
1:B:444:MET:O	1:B:445:TYR:O	2.30	0.49
1:A:34:THR:O	1:A:34:THR:OG1	2.30	0.49
1:A:38:SER:OG	1:A:41:SER:HB2	2.13	0.49
1:B:128:ILE:O	1:B:131:THR:HG23	2.12	0.49
1:B:338:PRO:O	1:B:338:PRO:HG2	2.12	0.49
1:A:118:LEU:HD13	1:A:118:LEU:H	1.71	0.49
1:B:31:GLU:C	1:B:33:PRO:CD	2.71	0.49
1:B:437:ILE:HD11	1:B:442:THR:HG22	1.95	0.49
1:A:200:LYS:HG3	1:A:201:VAL:H	1.76	0.49
1:A:357:THR:O	1:A:359:THR:N	2.44	0.49
1:A:379:LEU:CD1	1:A:423:SER:HB3	2.42	0.49
1:B:117:ILE:CG1	1:B:294:SER:HB2	2.35	0.49
1:B:266:ASN:ND2	1:B:268:SER:N	2.61	0.49
1:A:82:THR:HB	1:A:391:VAL:HG11	1.89	0.49
1:A:439:GLY:O	1:A:440:ASP:O	2.30	0.49
1:B:27:MET:HA	1:B:27:MET:HE2	1.94	0.49
1:B:141:LEU:HD12	1:B:306:ALA:CA	2.42	0.49
1:B:362:GLY:H	1:B:440:ASP:CB	2.11	0.49
1:B:428:ILE:O	1:B:430:SER:N	2.45	0.49
1:B:234:TYR:O	1:B:235:PRO:C	2.54	0.49
1:B:426:ALA:O	1:B:430:SER:OG	2.25	0.49
1:A:18:PHE:HB2	1:A:227:MET:HE3	1.95	0.49
1:A:224:VAL:O	1:A:225:ASN:C	2.55	0.49
1:B:50:GLY:O	1:B:55:ILE:HB	2.13	0.49
1:A:38:SER:O	1:A:38:SER:OG	2.30	0.49
1:A:170:ILE:HG21	1:A:293:ILE:HD12	1.95	0.49
1:A:198:PHE:O	1:B:395:LYS:CD	2.61	0.49
1:A:274:THR:CG2	1:A:275:PHE:N	2.75	0.49
1:A:160:PHE:HD1	1:A:161:PHE:N	2.11	0.49
1:A:223:HIS:CE1	1:A:492:PHE:HE2	2.31	0.49
1:A:229:ASN:O	1:A:229:ASN:OD1	2.30	0.49
1:A:256:ILE:HG22	1:A:257:ALA:N	2.20	0.49
1:B:150:LYS:HE3	1:B:150:LYS:HB3	1.47	0.49
1:B:266:ASN:HD22	1:B:267:LEU:N	2.09	0.49
1:B:480:GLU:HA	1:B:481:PRO:HD2	1.67	0.49
1:A:96:TYR:CD2	1:A:96:TYR:O	2.66	0.48
1:A:264:GLU:OE2	1:A:264:GLU:CA	2.45	0.48
1:A:466:VAL:HG12	1:A:467:HIS:HB2	1.94	0.48
1:B:276:THR:HG22	1:B:277:VAL:H	1.74	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:TRP:NE1	1:B:122:ALA:HB3	2.28	0.48
1:B:206:VAL:C	1:B:208:VAL:N	2.71	0.48
1:A:91:ALA:HB2	1:A:384:MET:SD	2.53	0.48
1:A:101:ILE:HG21	1:A:373:LEU:HB3	1.95	0.48
1:B:181:SER:O	1:B:182:GLY:O	2.30	0.48
1:A:157:LYS:CD	1:A:493:PHE:CE2	2.96	0.48
1:A:207:PHE:O	1:A:208:VAL:C	2.55	0.48
1:A:433:PRO:HD3	1:A:446:VAL:CG2	2.44	0.48
1:B:63:GLU:OE2	1:B:404:ASN:HA	2.13	0.48
1:B:66:THR:OG1	1:B:402:THR:HA	2.14	0.48
1:B:203:THR:C	1:B:204:LEU:CD2	2.81	0.48
1:B:234:TYR:CB	1:B:235:PRO:CD	2.90	0.48
1:B:236:LEU:O	1:B:237:ALA:C	2.57	0.48
1:A:449:LEU:C	1:A:449:LEU:CD1	2.66	0.48
1:A:456:VAL:O	1:A:459:LEU:N	2.44	0.48
1:B:31:GLU:HB2	1:B:35:PHE:CE2	2.49	0.48
1:B:44:PHE:CD2	1:B:196:PRO:HD2	2.48	0.48
1:B:90:ALA:O	1:B:91:ALA:C	2.56	0.48
1:B:263:ASN:OD1	1:B:263:ASN:O	2.30	0.48
1:A:63:GLU:OE1	1:A:405:ILE:CG1	2.57	0.48
1:A:157:LYS:CG	1:A:493:PHE:CE2	2.84	0.48
1:A:161:PHE:O	1:A:162:ALA:C	2.57	0.48
1:A:283:ALA:C	1:A:285:GLU:N	2.70	0.48
1:B:51:ILE:HG23	1:B:52:LEU:HD23	1.92	0.48
1:B:266:ASN:ND2	1:B:267:LEU:N	2.61	0.48
1:B:389:TYR:CE2	1:B:393:VAL:HG21	2.49	0.48
1:B:459:LEU:CB	1:B:460:PRO:CD	2.92	0.48
1:B:21:ILE:CD1	1:B:484:SER:HB2	2.42	0.48
1:B:98:GLN:CD	1:B:497:ARG:HH11	2.22	0.48
1:A:32:TYR:N	1:A:33:PRO:HD2	2.27	0.48
1:A:54:PHE:CD1	1:A:214:TYR:CD1	3.02	0.48
1:A:104:ILE:HB	1:A:105:PRO:CD	2.43	0.48
1:A:117:ILE:CD1	1:A:294:SER:HB3	2.44	0.48
1:A:272:MET:HE1	1:A:297:LEU:HD13	1.92	0.48
1:A:401:ARG:HB2	1:A:404:ASN:OD1	2.13	0.48
1:A:455:VAL:O	1:A:455:VAL:HG13	2.14	0.48
1:B:40:PHE:O	1:B:40:PHE:CD2	2.66	0.48
1:B:141:LEU:CD1	1:B:306:ALA:CB	2.69	0.48
1:B:221:ALA:O	1:B:224:VAL:CB	2.62	0.48
1:B:260:ILE:HD11	1:B:274:THR:HA	1.95	0.48
1:A:155:ILE:H	1:A:155:ILE:HG12	1.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:GLU:C	1:A:227:MET:O	2.51	0.48
1:A:275:PHE:CE2	1:A:293:ILE:HG21	2.49	0.48
1:A:393:VAL:CG1	1:A:413:LEU:HD21	2.36	0.48
1:B:22:THR:HG21	1:B:220:SER:OG	2.14	0.48
1:A:27:MET:HE1	1:A:248:LEU:HG	1.96	0.48
1:A:417:ILE:HG23	1:B:421:LEU:HD23	1.95	0.48
1:A:433:PRO:CG	1:A:445:TYR:CG	2.97	0.48
1:B:69:GLY:O	1:B:70:TRP:HD1	1.94	0.48
1:A:124:ASN:HA	1:A:130:LYS:CE	2.29	0.47
1:A:304:GLU:O	1:A:308:TRP:CZ3	2.67	0.47
1:B:166:LEU:CD1	1:B:166:LEU:O	2.57	0.47
1:B:341:LEU:O	1:B:342:VAL:C	2.56	0.47
1:B:356:LEU:HD22	1:B:369:ILE:HG21	1.96	0.47
1:B:357:THR:HG22	1:B:358:ASN:N	2.29	0.47
1:A:66:THR:O	1:A:401:ARG:HA	2.14	0.47
1:A:162:ALA:O	1:A:166:LEU:HB2	2.14	0.47
1:B:501:PRO:C	1:B:502:HIS:CD2	2.91	0.47
1:A:141:LEU:HA	1:A:144:THR:HG23	1.97	0.47
1:A:279:MET:HE2	1:A:282:VAL:HG21	1.94	0.47
1:A:332:MET:SD	1:A:504:ILE:HG21	2.54	0.47
1:B:59:LEU:HB3	1:B:405:ILE:HD13	1.95	0.47
1:B:386:PHE:H	1:B:386:PHE:HD2	1.63	0.47
1:A:19:PHE:HE1	1:A:240:LEU:HD22	1.80	0.47
1:A:200:LYS:HB2	1:A:200:LYS:NZ	2.27	0.47
1:B:67:VAL:CG2	1:B:70:TRP:CD2	2.97	0.47
1:B:163:GLY:O	1:B:167:PRO:CG	2.59	0.47
1:B:303:ALA:O	1:B:304:GLU:C	2.53	0.47
1:B:495:HIS:O	1:B:499:ARG:HG2	2.14	0.47
1:A:456:VAL:O	1:A:457:LEU:C	2.57	0.47
1:B:222:THR:HG23	1:B:223:HIS:N	2.29	0.47
1:A:62:ALA:O	1:A:63:GLU:C	2.56	0.47
1:A:70:TRP:CZ3	1:A:392:LEU:HD13	2.48	0.47
1:A:83:LEU:O	1:A:87:TRP:HD1	1.96	0.47
1:A:117:ILE:C	1:A:118:LEU:CD1	2.81	0.47
1:A:386:PHE:HB2	1:A:420:LEU:HD13	1.97	0.47
1:B:54:PHE:O	1:B:55:ILE:C	2.57	0.47
1:B:261:PRO:HD2	1:B:264:GLU:CB	2.44	0.47
1:A:21:ILE:CD1	1:A:223:HIS:ND1	2.74	0.47
1:A:22:THR:CG2	1:A:22:THR:O	2.61	0.47
1:A:154:ARG:O	1:A:155:ILE:C	2.57	0.47
1:A:155:ILE:O	1:A:159:GLY:N	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:LEU:CD2	1:A:369:ILE:CG2	2.87	0.47
1:A:408:GLY:C	1:A:410:GLY:N	2.73	0.47
1:A:435:ASP:OD2	1:A:436:ASN:ND2	2.48	0.47
1:B:76:PHE:HD2	1:B:76:PHE:O	1.81	0.47
1:A:46:LEU:CD2	1:A:210:PHE:CD1	2.95	0.47
1:A:146:PHE:C	1:A:148:GLY:N	2.71	0.47
1:B:82:THR:CG2	1:B:391:VAL:CB	2.93	0.47
1:A:437:ILE:HD11	1:A:442:THR:HG21	1.95	0.47
1:B:44:PHE:CE2	1:B:198:PHE:HZ	2.33	0.47
1:B:221:ALA:O	1:B:224:VAL:HB	2.14	0.47
1:B:260:ILE:O	1:B:262:GLY:N	2.47	0.47
1:B:436:ASN:O	1:B:436:ASN:CG	2.57	0.47
1:B:479:LEU:O	1:B:481:PRO:CD	2.62	0.47
1:A:52:LEU:N	1:A:52:LEU:HD23	2.30	0.47
1:B:78:TRP:N	1:B:78:TRP:HD1	2.12	0.47
1:B:351:ILE:O	1:B:355:ILE:HG23	2.14	0.46
1:B:380:CYS:O	1:B:383:PHE:N	2.48	0.46
1:A:83:LEU:O	1:A:87:TRP:CD1	2.69	0.46
1:A:411:VAL:HA	1:A:414:VAL:HG12	1.97	0.46
1:B:22:THR:CG2	1:B:220:SER:OG	2.64	0.46
1:B:99:ILE:CD1	1:B:312:PRO:CB	2.89	0.46
1:B:109:PHE:CE2	1:B:301:VAL:HG21	2.47	0.46
1:A:67:VAL:CG1	1:A:70:TRP:CD2	2.98	0.46
1:B:49:GLY:HA3	1:B:214:TYR:HE2	1.75	0.46
1:B:127:PRO:HG2	1:B:128:ILE:H	1.80	0.46
1:B:417:ILE:O	1:B:421:LEU:HD12	2.15	0.46
1:A:11:LYS:HG3	1:A:226:GLU:HA	1.95	0.46
1:A:143:LEU:O	1:A:146:PHE:HB2	2.14	0.46
1:A:259:VAL:O	1:A:259:VAL:HG12	2.15	0.46
1:A:364:ASN:N	1:A:440:ASP:OD2	2.49	0.46
1:A:397:PRO:CG	1:A:398:ASP:N	2.78	0.46
1:A:448:LEU:O	1:A:452:SER:OG	2.30	0.46
1:A:489:LYS:H	1:A:489:LYS:HG2	1.26	0.46
1:B:127:PRO:O	1:B:131:THR:HG23	2.15	0.46
1:B:131:THR:CB	1:B:357:THR:HG21	2.45	0.46
1:B:373:LEU:HD22	1:B:377:ILE:HD12	1.97	0.46
1:A:64:MET:HE2	1:A:64:MET:HB2	1.70	0.46
1:A:102:GLY:C	1:A:105:PRO:HD2	2.40	0.46
1:A:138:LEU:C	1:A:138:LEU:HD23	2.41	0.46
1:A:178:TYR:HD2	1:A:179:LEU:N	2.13	0.46
1:A:232:ARG:C	1:A:234:TYR:N	2.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:VAL:HG12	1:A:291:ARG:N	2.31	0.46
1:A:332:MET:HG2	1:A:336:GLY:C	2.40	0.46
1:A:15:LEU:HD23	1:A:16:LEU:CA	2.46	0.46
1:A:29:VAL:HA	1:A:32:TYR:CE2	2.50	0.46
1:A:160:PHE:HA	1:A:164:ILE:HD12	1.97	0.46
1:A:202:GLY:CA	1:A:434:PRO:HD3	2.43	0.46
1:B:279:MET:HE3	1:B:286:ILE:HB	1.98	0.46
1:B:372:ALA:CB	1:B:449:LEU:HD11	2.33	0.46
1:A:60:CYS:HB3	1:A:389:TYR:CD1	2.51	0.46
1:A:118:LEU:O	1:A:119:LYS:O	2.33	0.46
1:A:221:ALA:O	1:A:222:THR:C	2.59	0.46
1:A:507:ASN:O	1:A:508:ASP:O	2.34	0.46
1:B:131:THR:CG2	1:B:357:THR:CG2	2.93	0.46
1:B:246:ILE:O	1:B:250:SER:HB3	2.16	0.46
1:B:437:ILE:CD1	1:B:442:THR:HG22	2.46	0.46
1:B:29:VAL:O	1:B:31:GLU:N	2.48	0.46
1:B:110:VAL:HG23	1:B:301:VAL:CG1	2.42	0.46
1:B:211:ILE:HG22	1:B:215:MET:SD	2.55	0.46
1:B:289:THR:HG23	1:B:290:VAL:N	2.30	0.46
1:B:380:CYS:O	1:B:381:ALA:C	2.59	0.46
1:A:157:LYS:HA	1:A:493:PHE:HD2	1.80	0.46
1:A:220:SER:O	1:A:220:SER:OG	2.31	0.46
1:A:279:MET:HA	1:A:279:MET:HE2	1.98	0.46
1:A:340:THR:O	1:A:344:SER:CB	2.60	0.46
1:B:98:GLN:NE2	1:B:497:ARG:HD2	2.31	0.46
1:A:123:LEU:HD23	1:A:123:LEU:HA	1.80	0.46
1:B:28:ALA:O	1:B:31:GLU:HG3	2.16	0.46
1:B:71:GLU:H	1:B:71:GLU:HG3	1.38	0.46
1:B:112:GLY:HA3	1:B:269:ALA:HB3	1.97	0.46
1:B:146:PHE:CE1	1:B:342:VAL:CG1	2.93	0.46
1:B:151:TYR:HB2	1:B:152:THR:H	1.55	0.46
1:B:166:LEU:CB	1:B:167:PRO:CD	2.66	0.46
1:B:376:VAL:HG13	1:B:427:PHE:HE1	1.81	0.46
1:A:198:PHE:O	1:B:395:LYS:HB2	2.15	0.45
1:A:225:ASN:O	1:A:226:GLU:C	2.60	0.45
1:A:350:SER:O	1:A:354:ILE:HG13	2.16	0.45
1:B:47:LEU:HD23	1:B:47:LEU:HA	1.52	0.45
1:B:148:GLY:C	1:B:150:LYS:H	2.24	0.45
1:B:191:SER:C	1:B:193:THR:N	2.64	0.45
1:A:96:TYR:HD1	1:A:316:MET:HG3	1.79	0.45
1:B:137:ILE:O	1:B:140:ALA:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:GLY:O	1:B:440:ASP:C	2.58	0.45
1:B:495:HIS:O	1:B:496:PRO:C	2.57	0.45
1:A:457:LEU:HD11	1:A:461:PHE:CE2	2.51	0.45
1:B:13:LEU:O	1:B:227:MET:HE2	2.17	0.45
1:B:114:LEU:HA	1:B:114:LEU:HD23	1.47	0.45
1:B:444:MET:O	1:B:448:LEU:HB2	2.16	0.45
1:A:401:ARG:CB	1:A:404:ASN:OD1	2.64	0.45
1:B:262:GLY:CA	1:B:265:ILE:HG13	2.22	0.45
1:A:231:GLY:O	1:A:235:PRO:HD2	2.16	0.45
1:B:308:TRP:CE2	1:B:498:ALA:HB2	2.48	0.45
1:A:116:TYR:CE1	1:A:272:MET:HB2	2.49	0.45
1:A:157:LYS:HG3	1:A:490:GLY:HA3	1.98	0.45
1:B:298:LEU:CG	1:B:302:LEU:HD11	2.45	0.45
1:B:329:PHE:O	1:B:330:ALA:CB	2.58	0.45
1:B:484:SER:O	1:B:484:SER:OG	2.30	0.45
1:A:157:LYS:HA	1:A:493:PHE:CD2	2.52	0.45
1:A:495:HIS:CD2	1:A:497:ARG:H	2.34	0.45
1:B:36:ALA:O	1:B:37:THR:C	2.59	0.45
1:B:65:ALA:O	1:B:71:GLU:N	2.50	0.45
1:B:72:GLU:HA	1:B:73:GLY:HA3	1.64	0.45
1:B:208:VAL:O	1:B:375:VAL:HG21	2.17	0.45
1:B:325:LEU:O	1:B:326:PRO:C	2.58	0.45
1:B:433:PRO:CB	1:B:434:PRO:CD	2.95	0.45
1:B:436:ASN:OD1	1:B:436:ASN:C	2.60	0.45
1:A:32:TYR:HB2	1:A:33:PRO:HD3	1.99	0.45
1:B:272:MET:HE2	1:B:272:MET:HB2	1.68	0.45
1:B:299:LEU:HD22	1:B:299:LEU:HA	1.78	0.45
1:B:394:LEU:HD22	1:B:394:LEU:HA	1.80	0.45
1:A:204:LEU:HD23	1:A:204:LEU:N	2.32	0.45
1:A:404:ASN:O	1:A:405:ILE:C	2.56	0.45
1:B:117:ILE:HG22	1:B:118:LEU:N	2.29	0.45
1:B:127:PRO:HB2	1:B:358:ASN:OD1	2.16	0.45
1:B:428:ILE:C	1:B:430:SER:N	2.75	0.45
1:A:54:PHE:O	1:A:55:ILE:C	2.60	0.45
1:A:232:ARG:HG3	1:A:236:LEU:HD23	1.98	0.45
1:B:279:MET:HE3	1:B:286:ILE:CG2	2.47	0.45
1:B:376:VAL:HG13	1:B:427:PHE:CE1	2.52	0.45
1:B:441:SER:O	1:B:441:SER:OG	2.31	0.45
1:A:103:PHE:O	1:A:104:ILE:C	2.59	0.44
1:A:152:THR:O	1:A:154:ARG:N	2.49	0.44
1:B:279:MET:HE3	1:B:286:ILE:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:THR:O	1:B:293:ILE:HG12	2.17	0.44
1:B:379:LEU:HD23	1:B:379:LEU:HA	1.65	0.44
1:B:483:ASN:C	1:B:485:GLN:H	2.23	0.44
1:B:15:LEU:O	1:B:16:LEU:C	2.58	0.44
1:B:42:LEU:C	1:B:46:LEU:HB2	2.35	0.44
1:B:74:GLY:O	1:B:77:ALA:N	2.41	0.44
1:B:278:LEU:O	1:B:282:VAL:N	2.48	0.44
1:B:386:PHE:HE1	1:B:419:GLY:HA3	1.83	0.44
1:A:83:LEU:HD21	1:A:388:GLY:HA2	1.99	0.44
1:A:88:GLY:O	1:A:92:ILE:HB	2.18	0.44
1:B:60:CYS:CB	1:B:389:TYR:CE1	3.00	0.44
1:B:145:GLN:HG3	1:B:310:VAL:CG1	2.47	0.44
1:B:157:LYS:CG	1:B:493:PHE:CE2	2.94	0.44
1:B:177:ILE:HD11	1:B:282:VAL:HG21	1.99	0.44
1:B:309:ILE:O	1:B:309:ILE:HG22	2.18	0.44
1:B:315:GLY:N	1:B:500:SER:HB2	2.31	0.44
1:B:356:LEU:CD2	1:B:369:ILE:CG2	2.95	0.44
1:B:366:SER:O	1:B:367:PHE:C	2.58	0.44
1:A:82:THR:CB	1:A:391:VAL:HG12	2.46	0.44
1:A:171:LEU:HD21	1:A:255:SER:HB3	1.99	0.44
1:B:313:SER:O	1:B:314:ARG:C	2.61	0.44
1:A:19:PHE:CE1	1:A:240:LEU:HD22	2.53	0.44
1:A:338:PRO:O	1:A:338:PRO:CG	2.65	0.44
1:B:307:SER:OG	1:B:308:TRP:HD1	2.01	0.44
1:B:405:ILE:HB	1:B:412:LYS:HG2	1.99	0.44
1:B:428:ILE:O	1:B:429:VAL:C	2.61	0.44
1:A:19:PHE:CE2	1:A:23:ALA:HB1	2.47	0.44
1:A:66:THR:CG2	1:A:224:VAL:HG11	2.45	0.44
1:A:321:GLN:NE2	1:A:477:VAL:H	2.14	0.44
1:A:368:LEU:HD22	1:A:437:ILE:HG21	1.99	0.44
1:A:373:LEU:O	1:A:373:LEU:HD22	2.17	0.44
1:A:399:LEU:CB	1:A:401:ARG:NH2	2.80	0.44
1:A:474:ASN:O	1:A:475:THR:OG1	2.31	0.44
1:A:494:LEU:HA	1:A:494:LEU:HD12	1.72	0.44
1:B:137:ILE:O	1:B:140:ALA:CB	2.62	0.44
1:A:14:THR:O	1:A:17:GLY:N	2.49	0.44
1:A:49:GLY:O	1:A:54:PHE:N	2.51	0.44
1:A:154:ARG:HH22	1:A:489:LYS:NZ	2.13	0.44
1:A:154:ARG:O	1:A:158:VAL:HG23	2.18	0.44
1:A:167:PRO:HG2	1:A:297:LEU:HD23	1.98	0.44
1:A:435:ASP:CA	1:A:442:THR:OG1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:LEU:C	1:B:61:ALA:N	2.74	0.44
1:B:98:GLN:OE1	1:B:99:ILE:N	2.50	0.44
1:B:224:VAL:O	1:B:227:MET:HB2	2.18	0.44
1:B:315:GLY:HA2	1:B:500:SER:HB2	1.98	0.44
1:B:365:MET:CG	1:B:437:ILE:CD1	2.95	0.44
1:A:202:GLY:C	1:A:434:PRO:CG	2.74	0.44
1:A:442:THR:CG2	1:A:445:TYR:HD2	2.31	0.44
1:B:36:ALA:CB	1:B:257:ALA:HB2	2.27	0.44
1:B:158:VAL:O	1:B:162:ALA:CB	2.65	0.44
1:B:196:PRO:HB2	1:B:198:PHE:CD1	2.48	0.44
1:B:298:LEU:HD11	1:B:302:LEU:HD11	2.00	0.44
1:B:381:ALA:O	1:B:382:TYR:C	2.59	0.44
1:B:417:ILE:HD12	1:B:417:ILE:HA	1.88	0.44
1:A:98:GLN:N	1:A:377:ILE:HG21	2.32	0.44
1:A:178:TYR:OH	1:A:183:ALA:HA	2.18	0.44
1:A:332:MET:HG3	1:A:338:PRO:HB3	1.99	0.44
1:B:29:VAL:CB	1:B:32:TYR:CE1	2.98	0.44
1:B:117:ILE:HG22	1:B:118:LEU:CD1	2.48	0.44
1:B:360:GLY:O	1:B:361:GLY:C	2.61	0.44
1:A:50:GLY:CA	1:A:54:PHE:HB3	2.44	0.43
1:A:192:LYS:C	1:A:194:PHE:H	2.23	0.43
1:A:360:GLY:O	1:A:361:GLY:C	2.60	0.43
1:B:30:TYR:HD1	1:B:109:PHE:CD2	2.36	0.43
1:B:51:ILE:HG22	1:B:52:LEU:HG	2.00	0.43
1:B:332:MET:CE	1:B:338:PRO:HD3	2.48	0.43
1:A:283:ALA:HB1	1:A:285:GLU:HG2	2.00	0.43
1:A:478:THR:O	1:A:505:VAL:HG22	2.17	0.43
1:B:177:ILE:HD11	1:B:282:VAL:CG2	2.48	0.43
1:B:212:LEU:O	1:B:212:LEU:HD12	2.17	0.43
1:B:286:ILE:C	1:B:288:TRP:H	2.27	0.43
1:B:338:PRO:O	1:B:338:PRO:CG	2.66	0.43
1:A:104:ILE:HG22	1:A:108:TYR:CZ	2.53	0.43
1:A:145:GLN:HE21	1:A:145:GLN:N	2.14	0.43
1:A:231:GLY:O	1:A:235:PRO:CD	2.66	0.43
1:B:196:PRO:HB2	1:B:198:PHE:HE1	1.67	0.43
1:B:369:ILE:HG13	1:B:445:TYR:CE1	2.53	0.43
1:A:26:VAL:CG1	1:A:26:VAL:O	2.62	0.43
1:A:102:GLY:O	1:A:105:PRO:HD2	2.18	0.43
1:A:151:TYR:O	1:A:154:ARG:N	2.52	0.43
1:A:355:ILE:O	1:A:359:THR:CB	2.67	0.43
1:B:23:ALA:C	1:B:25:MET:N	2.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:SER:O	1:B:316:MET:CA	2.67	0.43
1:B:340:THR:O	1:B:344:SER:CB	2.65	0.43
1:A:170:ILE:HD13	1:A:293:ILE:CD1	2.48	0.43
1:A:218:GLU:H	1:A:218:GLU:HG3	1.40	0.43
1:A:377:ILE:HG22	1:A:378:TYR:N	2.33	0.43
1:A:405:ILE:HG23	1:A:406:PRO:HD2	2.00	0.43
1:A:428:ILE:C	1:A:430:SER:H	2.27	0.43
1:B:74:GLY:O	1:B:75:VAL:C	2.62	0.43
1:B:199:SER:O	1:B:199:SER:OG	2.30	0.43
1:B:186:ALA:C	1:B:188:GLU:N	2.76	0.43
1:B:325:LEU:HD23	1:B:463:LEU:HD23	1.99	0.43
1:B:350:SER:O	1:B:354:ILE:CG1	2.66	0.43
1:A:18:PHE:CB	1:A:227:MET:HE3	2.49	0.43
1:A:104:ILE:O	1:A:105:PRO:C	2.62	0.43
1:A:266:ASN:HB2	1:A:273:GLN:OE1	2.19	0.43
1:A:417:ILE:HD13	1:A:417:ILE:HA	1.67	0.43
1:B:106:MET:HG2	1:B:305:ILE:HG12	2.00	0.43
1:B:454:LEU:HD12	1:B:454:LEU:HA	1.80	0.43
1:B:494:LEU:HA	1:B:494:LEU:HD12	1.77	0.43
1:A:64:MET:HE3	1:A:78:TRP:CB	2.49	0.43
1:A:73:GLY:HA2	1:A:77:ALA:HB2	1.98	0.43
1:A:248:LEU:HD12	1:A:248:LEU:HA	1.81	0.43
1:A:411:VAL:O	1:A:415:VAL:HB	2.18	0.43
1:B:59:LEU:O	1:B:60:CYS:C	2.60	0.43
1:B:70:TRP:HZ3	1:B:392:LEU:CD1	2.25	0.43
1:B:261:PRO:HD2	1:B:264:GLU:HB2	2.01	0.43
1:A:29:VAL:O	1:A:30:TYR:C	2.62	0.43
1:A:31:GLU:HB3	1:A:35:PHE:HE2	1.79	0.43
1:A:34:THR:HG21	1:A:367:PHE:HE2	1.84	0.43
1:A:428:ILE:O	1:A:429:VAL:C	2.60	0.43
1:A:447:GLU:O	1:A:450:VAL:N	2.50	0.43
1:B:51:ILE:HA	1:B:51:ILE:HD13	1.74	0.43
1:B:90:ALA:O	1:B:93:SER:HB2	2.19	0.43
1:B:96:TYR:O	1:B:98:GLN:N	2.52	0.43
1:B:259:VAL:CG2	1:B:278:LEU:HD11	2.42	0.43
1:B:345:GLN:HG2	1:B:346:LEU:N	2.32	0.43
1:A:76:PHE:HB2	1:A:92:ILE:CG1	2.18	0.43
1:A:124:ASN:O	1:A:363:ASN:OD1	2.37	0.43
1:B:50:GLY:HA2	1:B:54:PHE:CB	2.41	0.43
1:B:312:PRO:O	1:B:315:GLY:N	2.51	0.43
1:B:466:VAL:O	1:B:466:VAL:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:SER:OG	1:A:501:PRO:N	2.49	0.42
1:B:122:ALA:O	1:B:123:LEU:C	2.61	0.42
1:B:243:VAL:O	1:B:246:ILE:HG22	2.19	0.42
1:A:44:PHE:O	1:A:47:LEU:HB2	2.18	0.42
1:A:130:LYS:O	1:A:134:ALA:N	2.50	0.42
1:A:206:VAL:CG1	1:A:207:PHE:N	2.82	0.42
1:B:49:GLY:CA	1:B:214:TYR:CE2	2.98	0.42
1:B:145:GLN:HG3	1:B:310:VAL:HG12	2.00	0.42
1:B:349:THR:O	1:B:353:LEU:HB2	2.19	0.42
1:B:392:LEU:C	1:B:394:LEU:N	2.69	0.42
1:B:427:PHE:CZ	1:B:453:PHE:CZ	3.07	0.42
1:A:67:VAL:CG1	1:A:70:TRP:CG	3.03	0.42
1:A:217:VAL:O	1:A:218:GLU:C	2.62	0.42
1:A:256:ILE:HD11	1:A:270:GLY:O	2.20	0.42
1:A:413:LEU:N	1:A:413:LEU:HD23	2.33	0.42
1:A:495:HIS:HD2	1:A:497:ARG:CB	2.08	0.42
1:B:55:ILE:CG2	1:B:56:PRO:N	2.50	0.42
1:B:93:SER:OG	1:B:460:PRO:HB3	2.19	0.42
1:B:170:ILE:CD1	1:B:293:ILE:CD1	2.94	0.42
1:B:172:ILE:CG1	1:B:251:VAL:CG1	2.96	0.42
1:A:29:VAL:O	1:A:32:TYR:HB2	2.19	0.42
1:A:447:GLU:C	1:A:449:LEU:N	2.76	0.42
1:B:101:ILE:HG22	1:B:374:THR:CB	2.50	0.42
1:B:345:GLN:O	1:B:349:THR:CG2	2.67	0.42
1:A:96:TYR:HD2	1:A:96:TYR:O	2.02	0.42
1:A:107:LEU:O	1:A:110:VAL:HB	2.20	0.42
1:A:165:LEU:HA	1:A:165:LEU:HD13	1.86	0.42
1:A:259:VAL:HG12	1:A:277:VAL:HG11	2.00	0.42
1:A:335:ASN:H	1:A:506:MET:HE1	1.83	0.42
1:A:338:PRO:HB2	1:A:341:LEU:CD1	2.49	0.42
1:A:486:ASN:HB3	1:A:503:TYR:HH	1.76	0.42
1:B:390:ILE:O	1:B:394:LEU:CB	2.67	0.42
1:B:495:HIS:ND1	1:B:496:PRO:HD2	2.34	0.42
1:B:208:VAL:HG12	1:B:371:LEU:HB3	2.02	0.42
1:A:33:PRO:O	1:A:36:ALA:HB3	2.19	0.42
1:A:97:LEU:HA	1:A:97:LEU:HD13	1.53	0.42
1:A:373:LEU:CA	1:A:376:VAL:HG22	2.49	0.42
1:A:457:LEU:CD1	1:A:461:PHE:HE2	2.33	0.42
1:B:64:MET:O	1:B:67:VAL:CG2	2.68	0.42
1:B:95:GLY:HA2	1:B:378:TYR:CE1	2.55	0.42
1:B:356:LEU:HD21	1:B:369:ILE:CG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:437:ILE:C	1:B:439:GLY:N	2.78	0.42
1:A:279:MET:C	1:A:281:HIS:N	2.61	0.42
1:A:457:LEU:CD1	1:A:461:PHE:CE2	3.03	0.42
1:B:29:VAL:CB	1:B:32:TYR:CD1	3.02	0.42
1:B:55:ILE:HD12	1:B:55:ILE:HA	1.91	0.42
1:B:233:ASP:O	1:B:236:LEU:CB	2.65	0.42
1:B:339:VAL:CG2	1:B:343:ILE:HD12	2.47	0.42
1:A:325:LEU:O	1:A:326:PRO:C	2.61	0.42
1:A:445:TYR:HD1	1:A:445:TYR:O	2.00	0.42
1:B:112:GLY:HA3	1:B:269:ALA:CB	2.50	0.42
1:B:124:ASN:O	1:B:130:LYS:CE	2.35	0.42
1:B:311:GLY:N	1:B:312:PRO:HD2	2.29	0.42
1:B:393:VAL:HG11	1:B:413:LEU:HD23	2.01	0.42
1:B:447:GLU:OE2	1:B:447:GLU:N	2.45	0.42
1:A:19:PHE:CD2	1:A:19:PHE:O	2.70	0.42
1:A:104:ILE:N	1:A:105:PRO:CD	2.82	0.42
1:A:124:ASN:O	1:A:130:LYS:CE	2.66	0.42
1:A:474:ASN:C	1:A:475:THR:OG1	2.63	0.42
1:A:506:MET:O	1:A:507:ASN:CB	2.63	0.42
1:B:145:GLN:CA	1:B:145:GLN:NE2	2.55	0.42
1:A:170:ILE:HG22	1:A:275:PHE:CE1	2.55	0.41
1:A:171:LEU:O	1:A:172:ILE:C	2.63	0.41
1:A:309:ILE:O	1:A:309:ILE:CG2	2.67	0.41
1:B:60:CYS:HA	1:B:389:TYR:CE1	2.55	0.41
1:B:234:TYR:CE2	1:B:238:MET:HG2	2.53	0.41
1:A:120:TRP:O	1:A:122:ALA:N	2.49	0.41
1:A:188:GLU:O	1:A:189:MET:O	2.37	0.41
1:A:362:GLY:N	1:A:440:ASP:HB3	2.24	0.41
1:A:432:LEU:CD1	1:A:432:LEU:C	2.90	0.41
1:A:492:PHE:C	1:A:494:LEU:N	2.78	0.41
1:B:207:PHE:HA	1:B:210:PHE:CD2	2.55	0.41
1:A:83:LEU:CD2	1:A:388:GLY:HA2	2.51	0.41
1:A:197:ASP:C	1:A:199:SER:N	2.78	0.41
1:B:29:VAL:CA	1:B:32:TYR:CD1	2.97	0.41
1:B:433:PRO:HA	1:B:434:PRO:HD3	1.89	0.41
1:A:405:ILE:HG22	1:A:406:PRO:HD2	2.01	0.41
1:B:32:TYR:CE2	1:B:249:SER:HA	2.56	0.41
1:B:70:TRP:HH2	1:B:392:LEU:HD11	1.64	0.41
1:B:85:PRO:HB2	1:B:464:TYR:HH	1.85	0.41
1:B:103:PHE:CE1	1:B:308:TRP:HB2	2.52	0.41
1:B:320:ALA:HB1	1:B:330:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:TRP:C	1:A:56:PRO:HD2	2.45	0.41
1:A:114:LEU:O	1:A:118:LEU:HD13	2.20	0.41
1:A:161:PHE:CE1	1:A:493:PHE:CZ	3.07	0.41
1:A:276:THR:OG1	1:A:290:VAL:HG11	2.21	0.41
1:B:66:THR:CB	1:B:402:THR:HA	2.50	0.41
1:B:131:THR:HG22	1:B:357:THR:CG2	2.50	0.41
1:B:158:VAL:O	1:B:162:ALA:N	2.35	0.41
1:A:48:LEU:HD12	1:A:207:PHE:HE2	1.86	0.41
1:A:83:LEU:HD12	1:A:384:MET:HB3	2.02	0.41
1:A:114:LEU:HA	1:A:114:LEU:HD23	1.52	0.41
1:B:44:PHE:HE2	1:B:198:PHE:HZ	1.68	0.41
1:B:218:GLU:H	1:B:218:GLU:HG3	1.41	0.41
1:A:96:TYR:CB	1:A:316:MET:HG3	2.50	0.41
1:A:191:SER:OG	1:A:192:LYS:N	2.54	0.41
1:A:229:ASN:O	1:A:229:ASN:CG	2.62	0.41
1:A:232:ARG:CG	1:A:233:ASP:N	2.84	0.41
1:A:260:ILE:HD12	1:A:273:GLN:NE2	2.35	0.41
1:B:110:VAL:O	1:B:114:LEU:HB2	2.20	0.41
1:B:205:VAL:HG13	1:B:206:VAL:N	2.36	0.41
1:B:297:LEU:O	1:B:298:LEU:C	2.64	0.41
1:A:64:MET:HE3	1:A:78:TRP:HB3	2.02	0.41
1:A:263:ASN:OD1	1:A:263:ASN:C	2.64	0.41
1:A:495:HIS:HA	1:A:496:PRO:HD3	1.91	0.41
1:B:67:VAL:HG23	1:B:70:TRP:CG	2.56	0.41
1:B:214:TYR:O	1:B:215:MET:C	2.61	0.41
1:A:52:LEU:C	1:A:56:PRO:HG2	2.44	0.41
1:A:104:ILE:N	1:A:105:PRO:HD2	2.36	0.41
1:A:104:ILE:H	1:A:104:ILE:HG12	1.54	0.41
1:A:133:ALA:O	1:A:137:ILE:HG13	2.21	0.41
1:A:194:PHE:CD2	1:A:195:PHE:CD1	3.08	0.41
1:A:242:MET:HE2	1:A:246:ILE:CD1	2.51	0.41
1:A:322:LYS:C	1:A:324:LEU:H	2.29	0.41
1:A:333:ASN:OD1	1:A:339:VAL:HG11	2.21	0.41
1:A:357:THR:HA	1:A:366:SER:HB3	2.02	0.41
1:A:373:LEU:HA	1:A:373:LEU:HD23	1.90	0.41
1:A:379:LEU:HD12	1:A:383:PHE:CE1	2.54	0.41
1:A:433:PRO:HD3	1:A:446:VAL:HG23	2.02	0.41
1:B:13:LEU:O	1:B:227:MET:CE	2.68	0.41
1:B:13:LEU:CD2	1:B:17:GLY:HA3	2.36	0.41
1:B:24:SER:HB3	1:B:493:PHE:CA	2.48	0.41
1:B:82:THR:HG23	1:B:391:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:LEU:O	1:B:168:ALA:CB	2.58	0.41
1:B:200:LYS:HB2	1:B:203:THR:HG21	2.03	0.41
1:B:371:LEU:O	1:B:374:THR:HG22	2.21	0.41
1:B:376:VAL:HG12	1:B:453:PHE:CD1	2.56	0.41
1:B:435:ASP:HA	1:B:442:THR:OG1	2.20	0.41
1:B:485:GLN:O	1:B:486:ASN:O	2.39	0.41
1:A:230:PRO:O	1:A:231:GLY:O	2.38	0.41
1:B:51:ILE:HG22	1:B:52:LEU:N	2.35	0.41
1:B:106:MET:O	1:B:109:PHE:N	2.54	0.41
1:A:197:ASP:C	1:A:199:SER:H	2.28	0.40
1:A:455:VAL:HG12	1:A:456:VAL:HG22	2.04	0.40
1:B:146:PHE:O	1:B:147:GLY:C	2.62	0.40
1:B:163:GLY:CA	1:B:167:PRO:HG2	2.51	0.40
1:A:53:TRP:O	1:A:56:PRO:CD	2.63	0.40
1:A:124:ASN:ND2	1:A:269:ALA:HB3	2.36	0.40
1:B:27:MET:HE2	1:B:27:MET:CA	2.50	0.40
1:B:58:GLY:HA3	1:B:238:MET:CE	2.51	0.40
1:B:390:ILE:CD1	1:B:416:ALA:HB3	2.50	0.40
1:A:178:TYR:HD1	1:A:278:LEU:HD22	1.83	0.40
1:A:236:LEU:O	1:A:237:ALA:C	2.63	0.40
1:A:250:SER:O	1:A:254:LEU:HB2	2.20	0.40
1:B:46:LEU:HD12	1:B:246:ILE:HG13	2.04	0.40
1:B:103:PHE:CD1	1:B:308:TRP:HE3	2.39	0.40
1:B:293:ILE:O	1:B:296:LEU:HB2	2.21	0.40
1:B:300:GLY:O	1:B:303:ALA:HB3	2.22	0.40
1:A:59:LEU:HB3	1:A:405:ILE:HD13	2.04	0.40
1:A:113:ALA:O	1:A:114:LEU:C	2.64	0.40
1:A:485:GLN:O	1:A:486:ASN:O	2.39	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	487/511 (95%)	374 (77%)	59 (12%)	54 (11%)	0	1
1	B	472/511 (92%)	336 (71%)	84 (18%)	52 (11%)	0	1
All	All	959/1022 (94%)	710 (74%)	143 (15%)	106 (11%)	0	1

All (106) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	VAL
1	A	86	ARG
1	A	152	THR
1	A	231	GLY
1	A	280	SER
1	A	283	ALA
1	A	335	ASN
1	A	466	VAL
1	A	484	SER
1	A	486	ASN
1	A	501	PRO
1	A	502	HIS
1	B	46	LEU
1	B	59	LEU
1	B	71	GLU
1	B	96	TYR
1	B	151	TYR
1	B	182	GLY
1	B	190	ASP
1	B	227	MET
1	B	330	ALA
1	B	335	ASN
1	B	440	ASP
1	B	442	THR
1	B	486	ASN
1	A	54	PHE
1	A	85	PRO
1	A	153	ALA
1	A	205	VAL
1	A	226	GLU
1	A	311	GLY
1	A	356	LEU
1	A	361	GLY
1	A	393	VAL
1	A	409	LYS

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Mol	Chain	Res	Type
1	A	429	VAL
1	A	457	LEU
1	A	477	VAL
1	B	30	TYR
1	B	68	ASP
1	B	130	LYS
1	B	147	GLY
1	B	201	VAL
1	B	223	HIS
1	B	231	GLY
1	B	324	LEU
1	B	367	PHE
1	B	429	VAL
1	B	433	PRO
1	B	438	GLN
1	B	445	TYR
1	A	55	ILE
1	A	143	LEU
1	A	154	ARG
1	A	218	GLU
1	A	223	HIS
1	A	284	PRO
1	A	334	LYS
1	A	357	THR
1	A	358	ASN
1	A	359	THR
1	A	508	ASP
1	B	54	PHE
1	B	115	SER
1	B	192	LYS
1	B	198	PHE
1	B	235	PRO
1	B	312	PRO
1	B	322	LYS
1	A	110	VAL
1	A	147	GLY
1	A	189	MET
1	A	225	ASN
1	A	233	ASP
1	A	326	PRO
1	A	423	SER
1	A	424	ILE

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Mol	Chain	Res	Type
1	A	440	ASP
1	A	487	ALA
1	B	41	SER
1	B	60	CYS
1	B	97	LEU
1	B	166	LEU
1	B	167	PRO
1	B	268	SER
1	B	487	ALA
1	A	481	PRO
1	B	164	ILE
1	B	298	LEU
1	B	323	ASN
1	B	334	LYS
1	B	396	HIS
1	A	406	PRO
1	A	438	GLN
1	B	121	PRO
1	B	490	GLY
1	A	73	GLY
1	A	172	ILE
1	B	251	VAL
1	B	261	PRO
1	A	148	GLY
1	B	310	VAL
1	B	459	LEU
1	A	397	PRO
1	B	326	PRO
1	A	208	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	394/414 (95%)	226 (57%)	168 (43%)	0	0
1	B	380/414 (92%)	213 (56%)	167 (44%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	774/828 (94%)	439 (57%)	335 (43%)	0 0

All (335) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	14	THR
1	A	15	LEU
1	A	16	LEU
1	A	19	PHE
1	A	26	VAL
1	A	30	TYR
1	A	34	THR
1	A	41	SER
1	A	42	LEU
1	A	43	VAL
1	A	51	ILE
1	A	55	ILE
1	A	64	MET
1	A	67	VAL
1	A	72	GLU
1	A	75	VAL
1	A	76	PHE
1	A	86	ARG
1	A	92	ILE
1	A	93	SER
1	A	96	TYR
1	A	97	LEU
1	A	98	GLN
1	A	99	ILE
1	A	101	ILE
1	A	104	ILE
1	A	114	LEU
1	A	117	ILE
1	A	118	LEU
1	A	119	LYS
1	A	125	GLU
1	A	128	ILE
1	A	131	THR
1	A	136	ILE
1	A	138	LEU
1	A	143	LEU

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Mol	Chain	Res	Type
1	A	144	THR
1	A	145	GLN
1	A	146	PHE
1	A	149	THR
1	A	151	TYR
1	A	152	THR
1	A	154	ARG
1	A	155	ILE
1	A	157	LYS
1	A	158	VAL
1	A	160	PHE
1	A	165	LEU
1	A	166	LEU
1	A	170	ILE
1	A	171	LEU
1	A	172	ILE
1	A	174	LEU
1	A	177	ILE
1	A	178	TYR
1	A	179	LEU
1	A	180	HIS
1	A	181	SER
1	A	190	ASP
1	A	193	THR
1	A	194	PHE
1	A	197	ASP
1	A	200	LYS
1	A	203	THR
1	A	204	LEU
1	A	206	VAL
1	A	211	ILE
1	A	212	LEU
1	A	217	VAL
1	A	218	GLU
1	A	227	MET
1	A	228	SER
1	A	229	ASN
1	A	232	ARG
1	A	233	ASP
1	A	239	LEU
1	A	240	LEU
1	A	241	LEU

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Mol	Chain	Res	Type
1	A	248	LEU
1	A	251	VAL
1	A	254	LEU
1	A	256	ILE
1	A	258	MET
1	A	260	ILE
1	A	264	GLU
1	A	265	ILE
1	A	268	SER
1	A	271	VAL
1	A	272	MET
1	A	273	GLN
1	A	274	THR
1	A	276	THR
1	A	279	MET
1	A	282	VAL
1	A	286	ILE
1	A	290	VAL
1	A	293	ILE
1	A	298	LEU
1	A	299	LEU
1	A	304	GLU
1	A	308	TRP
1	A	310	VAL
1	A	316	MET
1	A	318	VAL
1	A	319	THR
1	A	323	ASN
1	A	331	LYS
1	A	332	MET
1	A	337	VAL
1	A	339	VAL
1	A	340	THR
1	A	341	LEU
1	A	343	ILE
1	A	344	SER
1	A	345	GLN
1	A	355	ILE
1	A	357	THR
1	A	365	MET
1	A	366	SER
1	A	369	ILE

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Mol	Chain	Res	Type
1	A	373	LEU
1	A	377	ILE
1	A	391	VAL
1	A	392	LEU
1	A	395	LYS
1	A	399	LEU
1	A	401	ARG
1	A	405	ILE
1	A	409	LYS
1	A	411	VAL
1	A	413	LEU
1	A	415	VAL
1	A	417	ILE
1	A	418	VAL
1	A	421	LEU
1	A	424	ILE
1	A	430	SER
1	A	432	LEU
1	A	435	ASP
1	A	437	ILE
1	A	438	GLN
1	A	440	ASP
1	A	441	SER
1	A	444	MET
1	A	445	TYR
1	A	449	LEU
1	A	450	VAL
1	A	451	VAL
1	A	455	VAL
1	A	457	LEU
1	A	459	LEU
1	A	463	LEU
1	A	478	THR
1	A	479	LEU
1	A	480	GLU
1	A	482	ILE
1	A	484	SER
1	A	485	GLN
1	A	489	LYS
1	A	493	PHE
1	A	494	LEU
1	A	497	ARG

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Mol	Chain	Res	Type
1	A	499	ARG
1	A	500	SER
1	A	502	HIS
1	A	503	TYR
1	A	506	MET
1	B	13	LEU
1	B	14	THR
1	B	15	LEU
1	B	24	SER
1	B	26	VAL
1	B	27	MET
1	B	29	VAL
1	B	31	GLU
1	B	34	THR
1	B	38	SER
1	B	41	SER
1	B	43	VAL
1	B	46	LEU
1	B	47	LEU
1	B	48	LEU
1	B	51	ILE
1	B	55	ILE
1	B	59	LEU
1	B	63	GLU
1	B	66	THR
1	B	67	VAL
1	B	68	ASP
1	B	71	GLU
1	B	76	PHE
1	B	78	TRP
1	B	80	SER
1	B	81	ASN
1	B	97	LEU
1	B	98	GLN
1	B	103	PHE
1	B	104	ILE
1	B	106	MET
1	B	111	LEU
1	B	114	LEU
1	B	117	ILE
1	B	118	LEU
1	B	123	LEU

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Mol	Chain	Res	Type
1	B	128	ILE
1	B	130	LYS
1	B	131	THR
1	B	132	ILE
1	B	136	ILE
1	B	138	LEU
1	B	143	LEU
1	B	144	THR
1	B	145	GLN
1	B	149	THR
1	B	150	LYS
1	B	151	TYR
1	B	154	ARG
1	B	158	VAL
1	B	164	ILE
1	B	165	LEU
1	B	166	LEU
1	B	169	PHE
1	B	171	LEU
1	B	172	ILE
1	B	174	LEU
1	B	179	LEU
1	B	181	SER
1	B	187	ILE
1	B	189	MET
1	B	192	LYS
1	B	194	PHE
1	B	199	SER
1	B	203	THR
1	B	204	LEU
1	B	208	VAL
1	B	211	ILE
1	B	213	SER
1	B	215	MET
1	B	217	VAL
1	B	218	GLU
1	B	228	SER
1	B	232	ARG
1	B	234	TYR
1	B	239	LEU
1	B	240	LEU
1	B	246	ILE

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Mol	Chain	Res	Type
1	B	248	LEU
1	B	250	SER
1	B	256	ILE
1	B	260	ILE
1	B	263	ASN
1	B	265	ILE
1	B	266	ASN
1	B	267	LEU
1	B	271	VAL
1	B	272	MET
1	B	274	THR
1	B	275	PHE
1	B	276	THR
1	B	278	LEU
1	B	279	MET
1	B	281	HIS
1	B	282	VAL
1	B	285	GLU
1	B	291	ARG
1	B	294	SER
1	B	299	LEU
1	B	304	GLU
1	B	307	SER
1	B	310	VAL
1	B	316	MET
1	B	318	VAL
1	B	323	ASN
1	B	324	LEU
1	B	331	LYS
1	B	332	MET
1	B	334	LYS
1	B	337	VAL
1	B	339	VAL
1	B	340	THR
1	B	341	LEU
1	B	342	VAL
1	B	345	GLN
1	B	349	THR
1	B	351	ILE
1	B	353	LEU
1	B	354	ILE
1	B	355	ILE

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Mol	Chain	Res	Type
1	B	356	LEU
1	B	357	THR
1	B	365	MET
1	B	369	ILE
1	B	371	LEU
1	B	373	LEU
1	B	374	THR
1	B	377	ILE
1	B	378	TYR
1	B	379	LEU
1	B	384	MET
1	B	385	LEU
1	B	387	ILE
1	B	392	LEU
1	B	394	LEU
1	B	395	LYS
1	B	402	THR
1	B	405	ILE
1	B	413	LEU
1	B	415	VAL
1	B	417	ILE
1	B	420	LEU
1	B	423	SER
1	B	424	ILE
1	B	438	GLN
1	B	441	SER
1	B	444	MET
1	B	448	LEU
1	B	449	LEU
1	B	454	LEU
1	B	456	VAL
1	B	457	LEU
1	B	462	ILE
1	B	464	TYR
1	B	466	VAL
1	B	477	VAL
1	B	478	THR
1	B	479	LEU
1	B	480	GLU
1	B	483	ASN
1	B	485	GLN
1	B	489	LYS

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Mol	Chain	Res	Type
1	B	491	HIS
1	B	494	LEU
1	B	495	HIS
1	B	499	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	GLN
1	A	145	GLN
1	A	223	HIS
1	A	225	ASN
1	A	321	GLN
1	A	364	ASN
1	A	436	ASN
1	A	485	GLN
1	A	486	ASN
1	A	495	HIS
1	B	124	ASN
1	B	145	GLN
1	B	225	ASN
1	B	229	ASN
1	B	266	ASN
1	B	321	GLN
1	B	323	ASN
1	B	333	ASN
1	B	345	GLN
1	B	404	ASN
1	B	438	GLN
1	B	485	GLN
1	B	486	ASN
1	B	491	HIS
1	B	495	HIS
1	B	502	HIS

5.3.3 RNA ⓘ

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 oligosaccharides 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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	493/511 (96%)	0.32	29 (5%)	28 16	47, 95, 150, 198	0
1	B	480/511 (93%)	0.40	26 (5%)	31 18	51, 115, 177, 251	0
All	All	973/1022 (95%)	0.36	55 (5%)	29 17	47, 105, 168, 251	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	504	ILE	5.3
1	B	480	GLU	5.2
1	A	89	PHE	5.1
1	B	502	HIS	5.0
1	B	30	TYR	4.6
1	A	342	VAL	4.0
1	A	446	VAL	3.9
1	B	21	ILE	3.9
1	B	315	GLY	3.8
1	A	398	ASP	3.5
1	B	20	ALA	3.3
1	B	444	MET	3.3
1	A	154	ARG	3.2
1	A	432	LEU	3.1
1	A	77	ALA	3.1
1	A	76	PHE	3.0
1	B	275	PHE	3.0
1	A	445	TYR	2.9
1	B	466	VAL	2.9
1	A	218	GLU	2.9
1	B	128	ILE	2.9
1	B	267	LEU	2.8
1	B	197	ASP	2.8
1	B	475	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	150	LYS	2.6
1	A	276	THR	2.6
1	A	484	SER	2.6
1	B	196	PRO	2.6
1	A	314	ARG	2.5
1	B	155	ILE	2.5
1	B	330	ALA	2.4
1	B	403	PHE	2.4
1	A	149	THR	2.4
1	A	498	ALA	2.4
1	A	38	SER	2.4
1	A	508	ASP	2.4
1	A	468	ASP	2.4
1	B	119	LYS	2.4
1	B	199	SER	2.4
1	B	250	SER	2.4
1	A	209	ALA	2.3
1	B	220	SER	2.3
1	B	73	GLY	2.3
1	A	330	ALA	2.2
1	A	360	GLY	2.2
1	A	312	PRO	2.2
1	A	504	ILE	2.2
1	A	151	TYR	2.1
1	B	322	LYS	2.1
1	A	442	THR	2.1
1	A	379	LEU	2.0
1	B	263	ASN	2.0
1	A	30	TYR	2.0
1	A	264	GLU	2.0
1	B	201	VAL	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 oligosaccharides 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.