



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 08:03 PM UTC

PDB ID : 3MKU / pdb_00003mku
Title : Structure of a Cation-bound Multidrug and Toxin Compound Extrusion (MATE) transporter
Authors : He, X.; Szewczyk, P.; Karyakin, A.; Evin, M.; Hong, W.-X.; Zhang, Q.; Chang, G.
Deposited on : 2010-04-15
Resolution : 4.20 Å(reported)

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

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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

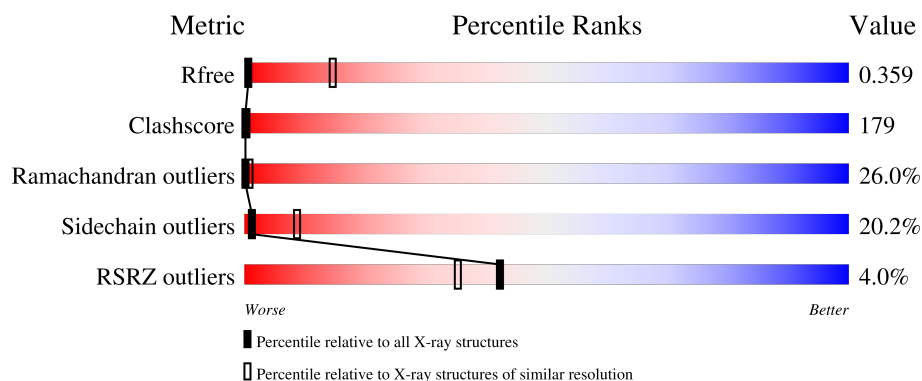
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.20 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	1004 (4.52-3.88)
Clashscore	190562	1019 (4.50-3.90)
Ramachandran outliers	187476	1020 (4.56-3.84)
Sidechain outliers	187428	1006 (4.56-3.84)
RSRZ outliers	180081	1001 (4.52-3.88)

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	460	4% 46% 43% 7%
1	B	460	4% 49% 41% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7013 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 Multi antimicrobial extrusion protein (Na(+)/drug antiporter) MATE-like MDR efflux pump.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	460	Total	C	N	O	S	0	0	0
			3505	2326	569	589	21			
1	B	460	Total	C	N	O	S	0	0	0
			3506	2326	569	590	21			

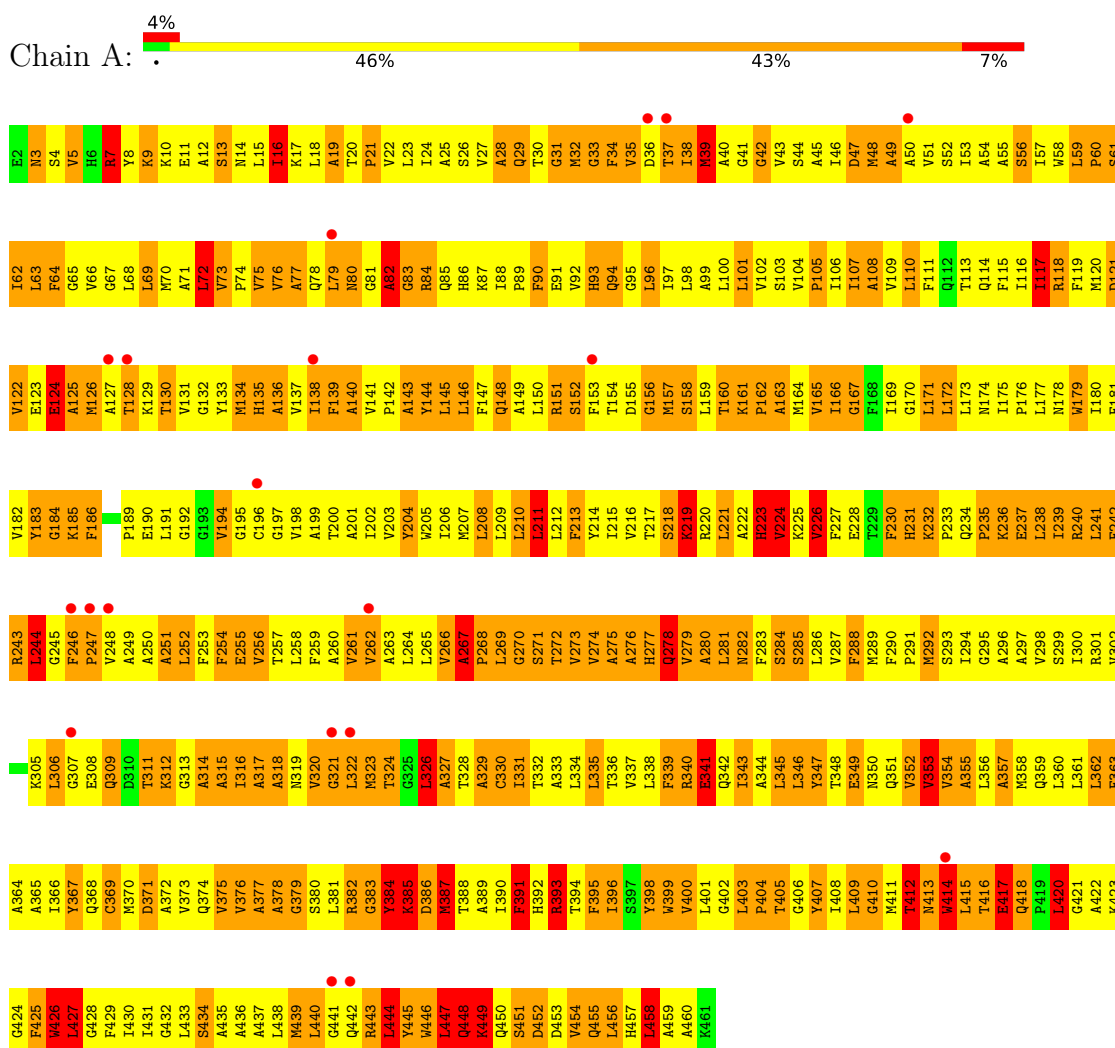
- Molecule 2 is RUBIDIUM ION (CCD ID: RB) (formula: Rb).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Rb	0	0
			1	1		
2	B	1	Total	Rb	0	0
			1	1		

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: Multi antimicrobial extrusion protein (Na(+)/drug antiporter) MATE-like MDR efflux pump



- Molecule 1: Multi antimicrobial extrusion protein (Na(+)/drug antiporter) MATE-like MDR efflux pump



K423	K424	F363	V302	F242	V182	V122	I62
G424	A364	A364	K305	R242	Y183	E123	L63
F425	A365	A365	L306	R244	G184	E124	F64
M426	I366	I366	G307	G245	K185	A125	G65
L427	Y367	Y367	E308	F246	F186	M126	V66
G428	Q368	Q368	Q309	P247	G187	A127	G67
F429	C369	C369	D310	V248	A188	T128	L68
I430	M370	M370	T311	A249	P189	K129	L69
I431	D371	D371	K312	A250	E190	T130	M70
G432	A372	A372	G313	A251	L191	V131	A71
L433	V373	V373	A314	L252	G192	G132	L72
S434	Q374	Q374	A315	F253	G193	Y133	V73
A435	V375	V375	F254	F254	V194	M134	P74
A436	V376	V376	I316	E255	G195	H135	V75
A437	A377	A377	A317	V256	C196	A136	V76
L438	A378	A378	A318	T257	G197	V137	A77
M439	G379	G379	N319	L258	V198	T138	Q78
L440	S380	S380	V320	F259	A199	F139	L79
G441	L381	L381	G321	A260	T200	A140	N80
Q442	R382	R382	L322	V261	A201	V141	T20
R443	G383	G383	M323	V262	I202	P142	G81
L444	Y384	Y384	T324	A263	L203	A143	V22
Y445	K385	K385	G325	A264	V204	Y144	G83
W446	R386	R386	L326	L265	W205	L145	R84
L447	K387	K387	A327	V266	L206	L146	Q85
Q448	T388	T388	T328	A267	I206	H146	H86
K449	A389	A389	A329	P268	M207	F147	S26
Q450	I390	I390	C330	L269	L208	Q148	V27
S451	F391	F391	I331	G270	L209	A149	I88
D452	H392	H392	T332	S271	L210	L150	P89
D453	R393	R393	A333	T272	L211	R151	T30
W454	T394	T394	L334	V273	F213	S152	E91
Q455	F395	F395	L335	V274	G213	F153	V92
L456	I396	I396	T336	A275	Y214	T154	H93
H457	S397	S397	V337	A276	L215	D155	Q94
L458	Y398	Y398	L338	H277	V216	G156	G95
A459	W399	W399	F339	Q278	T217	M157	L96
A460	V400	V400	R340	V279	S218	S158	I97
K461	L401	L401	E341	A280	K219	L159	T37
	G402	G402	Q342	L281	R220	T160	L38
	L403	L403	T343	N282	L221	K161	A99
	P404	P404	A344	F283	A222	P162	M39
	T405	T405	L345	S284	R223	A163	G41
	G406	G406	L346	S285	V224	M164	L101
	Y407	Y407	Y347	L286	V226	V165	G42
	I408	I408	T348	V287	V226	I106	V43
	L409	L409	E349	F288	E228	G167	I46
	G410	G410	N350	M289	T229	F168	D47
	M411	M411	Q351	F290	G230	I169	A48
	T412	T412	V352	H231	H231	L171	V109
	N413	N413	V353	M291	K232	L172	L110
	W414	W414	V354	S293	F233	L173	Q112
	L415	L415	A355	I294	Q234	M174	T113
	T416	T416	L356	Q295	P235	I175	Q114
	E417	E417	A357	A296	K236	P176	F115
	Q418	Q418	M358	A297	E237	L177	I116
	P419	P419	Q359	V298	L238	M178	I117
	L420	L420	L360	S299	I239	W179	R118
	G421	G421	L361	I300	R240	F191	L59
	A422	A422	L362	R301	R240	T180	P60
					L241	F181	S61

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	159.80Å 241.85Å 46.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 4.20 20.00 – 4.20	Depositor EDS
% Data completeness (in resolution range)	99.0 (20.00-4.20) 97.8 (20.00-4.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.87 (at 4.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.309 , 0.342 0.324 , 0.359	Depositor DCC
R_{free} test set	791 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	105.5	Xtriage
Anisotropy	1.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.08 , 29.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	7013	wwPDB-VP
Average B, all atoms (Å ²)	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% 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

Bond lengths and bond angles in the following residue types are not validated in this section: RB

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.84	3/3585 (0.1%)	1.49	89/4879 (1.8%)
1	B	0.83	4/3586 (0.1%)	1.46	75/4879 (1.5%)
All	All	0.83	7/7171 (0.1%)	1.47	164/9758 (1.7%)

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	B	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	73	VAL	CA-CB	7.47	1.57	1.54
1	A	157	MET	SD-CE	7.06	1.97	1.79
1	B	294	ILE	CA-CB	6.63	1.61	1.54
1	A	32	MET	SD-CE	5.62	1.93	1.79
1	B	138	ILE	CA-CB	5.41	1.61	1.54
1	A	38	ILE	CA-CB	5.30	1.60	1.54
1	B	157	MET	SD-CE	5.22	1.92	1.79

All (164) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	413	ASN	N-CA-C	-14.85	95.10	111.14
1	B	413	ASN	N-CA-C	-14.25	95.75	111.14
1	A	236	LYS	N-CA-C	-12.78	97.81	113.41
1	B	236	LYS	N-CA-C	-12.50	98.16	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	VAL	N-CA-C	-12.17	95.03	113.16
1	B	443	ARG	N-CA-C	-11.80	98.31	113.17
1	A	443	ARG	N-CA-C	-11.67	98.47	113.17
1	B	75	VAL	N-CA-C	-11.56	96.40	113.39
1	A	409	LEU	N-CA-C	-11.08	97.94	112.68
1	B	49	ALA	N-CA-C	-10.98	99.40	113.12
1	A	387	MET	N-CA-C	-10.96	99.34	111.28
1	B	73	VAL	N-CA-C	-10.93	99.00	112.67
1	B	409	LEU	N-CA-C	-10.66	98.50	112.68
1	A	241	LEU	N-CA-C	-10.53	99.53	112.38
1	B	387	MET	N-CA-C	-10.39	99.95	111.28
1	B	237	GLU	N-CA-C	-10.28	100.14	112.89
1	B	241	LEU	N-CA-C	-10.26	99.87	112.38
1	A	353	VAL	CB-CA-C	-10.17	94.61	111.29
1	A	49	ALA	N-CA-C	-9.97	99.41	112.68
1	B	343	ILE	N-CA-C	-9.90	100.91	110.42
1	A	391	PHE	N-CA-C	-9.87	101.00	113.23
1	B	271	SER	N-CA-C	-9.81	101.31	113.38
1	A	73	VAL	N-CA-C	-9.77	100.62	112.35
1	A	384	TYR	CB-CA-C	9.67	126.28	110.81
1	A	237	GLU	N-CA-C	-9.65	101.50	113.18
1	B	254	PHE	N-CA-C	-9.54	100.88	111.28
1	A	254	PHE	N-CA-C	-9.52	100.91	111.28
1	A	447	LEU	N-CA-C	-9.50	90.56	110.80
1	B	240	ARG	N-CA-C	-9.48	101.61	113.55
1	A	240	ARG	N-CA-C	-9.30	101.83	113.55
1	A	335	LEU	N-CA-C	-9.30	102.44	113.88
1	A	357	ALA	N-CA-C	-9.28	99.70	111.02
1	A	271	SER	N-CA-C	-9.25	102.01	113.38
1	B	391	PHE	N-CA-C	-9.18	101.85	113.23
1	B	136	ALA	N-CA-C	-9.14	100.05	111.75
1	B	335	LEU	N-CA-C	-9.12	102.73	114.04
1	B	72	LEU	N-CA-C	-8.94	100.97	112.23
1	A	72	LEU	N-CA-C	-8.74	102.05	112.89
1	A	410	GLY	N-CA-C	-8.73	92.50	113.18
1	B	446	TRP	N-CA-C	-8.70	95.08	108.31
1	B	134	MET	N-CA-C	-8.66	102.62	113.01
1	A	412	THR	N-CA-C	-8.58	101.42	112.23
1	B	357	ALA	N-CA-C	-8.46	100.69	111.02
1	A	136	ALA	N-CA-C	-8.26	101.17	111.75
1	A	343	ILE	N-CA-C	-8.25	102.50	110.42
1	B	410	GLY	N-CA-C	-8.24	93.65	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	458	LEU	N-CA-C	-8.19	102.51	114.39
1	B	238	LEU	N-CA-C	-8.15	101.96	112.23
1	B	353	VAL	CB-CA-C	-8.14	97.94	111.29
1	A	239	ILE	N-CA-C	-8.12	102.03	113.07
1	A	139	PHE	N-CA-C	-8.11	103.98	114.04
1	A	238	LEU	N-CA-C	-8.06	102.89	112.89
1	B	69	LEU	N-CA-C	-8.06	102.49	111.28
1	B	139	PHE	N-CA-C	-8.05	104.06	114.04
1	A	448	GLN	N-CA-C	-8.05	93.66	110.80
1	A	270	GLY	N-CA-C	7.96	121.17	110.43
1	B	418	GLN	N-CA-C	7.89	115.32	108.22
1	A	449	LYS	N-CA-CB	-7.86	97.19	110.80
1	A	73	VAL	CA-C-N	7.85	129.66	119.84
1	A	73	VAL	C-N-CA	7.85	129.66	119.84
1	A	48	MET	N-CA-C	-7.84	103.61	113.02
1	B	48	MET	N-CA-C	-7.79	103.67	113.02
1	B	272	THR	N-CA-C	-7.75	101.95	111.33
1	B	407	TYR	N-CA-C	-7.72	102.81	111.14
1	B	326	LEU	N-CA-C	-7.69	102.98	111.36
1	A	458	LEU	N-CA-C	-7.63	101.83	113.89
1	A	134	MET	N-CA-C	-7.63	103.86	113.01
1	B	239	ILE	N-CA-C	-7.50	102.87	113.07
1	A	309	GLN	N-CA-C	-7.42	103.96	113.16
1	A	452	ASP	N-CA-C	-7.41	104.12	113.02
1	B	43	VAL	N-CA-C	-7.34	105.37	111.91
1	B	140	ALA	N-CA-C	-7.31	103.82	112.89
1	A	385	LYS	N-CA-CB	-7.26	98.22	110.49
1	B	309	GLN	N-CA-C	-7.26	104.16	113.16
1	B	452	ASP	N-CA-C	-7.24	104.54	113.15
1	A	459	ALA	N-CA-C	-7.19	102.53	113.89
1	A	326	LEU	N-CA-C	-7.17	103.54	111.36
1	A	385	LYS	N-CA-C	7.17	126.08	110.80
1	A	418	GLN	N-CA-C	7.15	114.66	108.22
1	B	412	THR	N-CA-C	-7.11	103.27	112.23
1	A	69	LEU	N-CA-C	-7.09	103.49	111.07
1	A	16	ILE	N-CA-C	7.04	117.80	110.62
1	B	353	VAL	N-CA-C	7.01	123.92	109.34
1	A	324	THR	N-CA-C	6.97	118.67	111.14
1	A	272	THR	N-CA-C	-6.95	102.92	111.33
1	A	268	PRO	N-CA-C	-6.87	107.53	114.68
1	A	140	ALA	N-CA-C	-6.78	104.48	112.89
1	A	439	MET	N-CA-C	6.78	119.53	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	353	VAL	N-CA-C	6.76	123.41	109.34
1	B	16	ILE	N-CA-C	6.69	116.84	110.42
1	B	414	TRP	N-CA-C	-6.68	104.85	112.87
1	B	446	TRP	CB-CA-C	-6.67	108.87	116.54
1	A	367	TYR	N-CA-C	-6.61	103.76	110.97
1	B	324	THR	N-CA-C	6.58	118.24	111.14
1	B	73	VAL	CA-C-N	6.55	128.03	119.84
1	B	73	VAL	C-N-CA	6.55	128.03	119.84
1	B	436	ALA	N-CA-C	-6.54	104.08	111.07
1	A	393	ARG	N-CA-C	-6.53	103.28	111.11
1	A	288	PHE	N-CA-C	-6.51	104.11	111.07
1	A	246	PHE	N-CA-C	-6.50	103.64	112.35
1	B	367	TYR	N-CA-C	-6.50	103.89	110.97
1	A	107	ILE	CB-CA-C	-6.49	103.54	112.04
1	A	407	TYR	N-CA-C	-6.49	104.14	111.14
1	A	59	LEU	N-CA-C	-6.48	105.22	113.77
1	A	384	TYR	N-CA-C	6.43	118.82	111.11
1	B	91	GLU	N-CA-C	-6.39	104.23	111.07
1	B	459	ALA	N-CA-C	-6.34	103.87	113.89
1	B	270	GLY	N-CA-C	6.33	118.98	110.43
1	B	456	LEU	N-CA-C	-6.33	105.04	112.89
1	B	438	LEU	N-CA-C	-6.32	103.92	111.69
1	A	414	TRP	N-CA-C	-6.29	105.32	112.87
1	B	235	PRO	N-CA-C	-6.28	106.50	114.35
1	B	131	VAL	N-CA-C	-6.22	102.58	111.17
1	B	82	ALA	N-CA-C	-6.21	97.56	110.80
1	B	454	VAL	N-CA-C	-6.21	104.62	113.07
1	B	426	TRP	N-CA-C	-6.14	103.74	111.11
1	A	347	TYR	N-CA-C	-6.11	99.20	108.67
1	B	448	GLN	N-CA-C	-5.98	97.98	108.08
1	A	306	LEU	N-CA-C	-5.92	104.90	111.36
1	A	386	ASP	N-CA-C	-5.91	105.56	112.89
1	B	107	ILE	CB-CA-C	-5.91	103.42	112.05
1	A	442	GLN	N-CA-C	-5.90	105.94	113.02
1	B	439	MET	N-CA-C	5.89	118.45	111.33
1	B	448	GLN	CA-C-N	5.88	130.63	121.76
1	B	448	GLN	C-N-CA	5.88	130.63	121.76
1	A	43	VAL	N-CA-C	-5.84	106.71	111.91
1	B	401	LEU	N-CA-C	-5.84	104.61	110.97
1	A	224	VAL	N-CA-C	5.83	121.46	109.34
1	A	382	ARG	N-CA-C	-5.80	105.09	111.82
1	A	143	ALA	N-CA-C	-5.78	103.97	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	454	VAL	N-CA-C	-5.74	105.26	113.07
1	B	384	TYR	N-CA-C	5.72	118.28	111.71
1	A	426	TRP	N-CA-C	-5.64	104.34	111.11
1	A	451	SER	N-CA-C	-5.63	98.82	110.80
1	A	235	PRO	N-CA-C	-5.53	107.43	114.35
1	B	224	VAL	N-CA-C	5.53	120.85	109.34
1	B	157	MET	N-CA-C	-5.51	102.50	111.04
1	A	82	ALA	N-CA-C	-5.50	99.09	110.80
1	B	268	PRO	N-CA-C	-5.45	107.54	114.35
1	B	329	ALA	N-CA-C	-5.41	105.03	111.03
1	B	384	TYR	CA-CB-CG	5.40	123.62	113.90
1	A	117	ILE	N-CA-C	-5.37	98.18	109.34
1	A	135	HIS	N-CA-C	-5.35	106.43	113.12
1	A	456	LEU	N-CA-C	-5.33	106.04	112.54
1	A	329	ALA	N-CA-C	-5.31	105.19	110.97
1	A	383	GLY	N-CA-C	-5.28	108.54	114.40
1	A	438	LEU	N-CA-C	-5.27	105.21	111.69
1	B	393	ARG	N-CA-C	-5.25	105.45	111.07
1	A	420	LEU	N-CA-C	5.20	116.38	107.28
1	B	382	ARG	N-CA-C	-5.15	105.84	111.82
1	B	80	ASN	N-CA-C	-5.12	104.29	110.44
1	A	403	LEU	CA-C-N	-5.11	113.92	119.24
1	A	403	LEU	C-N-CA	-5.11	113.92	119.24
1	A	118	ARG	N-CA-CB	-5.11	101.86	110.49
1	A	242	PHE	N-CA-C	-5.10	103.76	111.56
1	B	143	ALA	N-CA-C	-5.09	104.81	111.02
1	A	80	ASN	N-CA-C	-5.08	104.34	110.44
1	A	427	LEU	N-CA-C	5.08	116.50	111.07
1	B	259	PHE	N-CA-C	-5.05	104.86	111.02
1	A	255	GLU	N-CA-C	-5.05	105.78	111.28
1	A	267	ALA	CA-C-N	-5.03	115.70	120.83
1	A	267	ALA	C-N-CA	-5.03	115.70	120.83
1	A	434	SER	N-CA-C	-5.02	105.91	112.23
1	B	246	PHE	N-CA-C	-5.01	105.63	112.35

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	133	TYR	Sidechain
1	B	144	TYR	Sidechain

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	3505	0	3676	1286	0
1	B	3506	0	3676	1292	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
All	All	7013	0	7352	2571	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 179.

All (2571) 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:447:LEU:CD1	1:A:450:GLN:HE21	1.27	1.48
1:A:447:LEU:CD1	1:A:450:GLN:NE2	1.96	1.27
1:A:447:LEU:HD13	1:A:450:GLN:NE2	1.50	1.24
1:A:447:LEU:C	1:A:447:LEU:HD12	1.65	1.19
1:B:162:PRO:O	1:B:165:VAL:HG12	1.38	1.17
1:A:162:PRO:O	1:A:165:VAL:HG12	1.43	1.17
1:A:320:VAL:HG13	1:A:321:GLY:H	1.04	1.17
1:A:151:ARG:HG3	1:A:162:PRO:HG2	1.27	1.16
1:A:358:MET:HA	1:A:361:LEU:HD12	1.22	1.16
1:A:231:HIS:HB3	1:A:235:PRO:HD3	1.27	1.15
1:B:320:VAL:HG13	1:B:321:GLY:H	0.99	1.15
1:B:235:PRO:HA	1:B:238:LEU:HB2	1.26	1.15
1:B:73:VAL:HB	1:B:74:PRO:HD3	1.19	1.14
1:B:398:TYR:HB3	1:B:436:ALA:HB2	1.18	1.14
1:A:447:LEU:HD12	1:A:447:LEU:O	1.45	1.14
1:B:408:ILE:HA	1:B:411:MET:HB2	1.16	1.14
1:A:398:TYR:CB	1:A:436:ALA:HB2	1.77	1.13
1:B:151:ARG:HG3	1:B:162:PRO:HG2	1.23	1.13
1:B:165:VAL:HG13	1:B:166:ILE:H	1.09	1.13
1:A:447:LEU:CD1	1:A:447:LEU:O	1.97	1.12
1:A:398:TYR:HB3	1:A:436:ALA:HB2	1.11	1.11
1:A:266:VAL:HG12	1:A:269:LEU:HD11	1.33	1.11
1:A:45:ALA:HB3	1:A:49:ALA:HB2	1.31	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ILE:HG22	1:A:118:ARG:H	1.15	1.10
1:B:398:TYR:CB	1:B:436:ALA:HB2	1.80	1.10
1:A:73:VAL:HB	1:A:74:PRO:HD3	1.20	1.10
1:A:165:VAL:HG13	1:A:166:ILE:H	1.13	1.09
1:A:447:LEU:HD11	1:A:450:GLN:HE21	0.94	1.08
1:A:235:PRO:HA	1:A:238:LEU:HB2	1.34	1.08
1:A:408:ILE:HA	1:A:411:MET:HB2	1.11	1.08
1:B:445:TYR:HB2	1:B:448:GLN:HA	1.31	1.07
1:B:118:ARG:HE	1:B:119:PHE:HB2	1.14	1.07
1:B:420:LEU:HD12	1:B:423:LYS:H	1.18	1.07
1:B:231:HIS:HB3	1:B:235:PRO:HD3	1.32	1.07
1:B:11:GLU:HA	1:B:301:ARG:HH22	1.13	1.07
1:A:118:ARG:HE	1:A:119:PHE:HB2	1.12	1.06
1:B:4:SER:O	1:B:8:TYR:CD2	2.08	1.06
1:B:266:VAL:HG12	1:B:269:LEU:HD11	1.30	1.06
1:B:147:PHE:HB2	1:B:211:LEU:HD13	1.39	1.05
1:B:45:ALA:HB3	1:B:49:ALA:HB2	1.34	1.05
1:B:340:ARG:HD2	1:B:358:MET:HG2	1.32	1.04
1:B:358:MET:HA	1:B:361:LEU:HD12	1.08	1.04
1:A:420:LEU:HD12	1:A:423:LYS:H	1.22	1.03
1:B:262:VAL:HG11	1:B:403:LEU:HD22	1.41	1.02
1:B:353:VAL:O	1:B:357:ALA:N	1.92	1.01
1:A:145:LEU:HD13	1:A:146:LEU:N	1.74	1.01
1:B:145:LEU:HD13	1:B:146:LEU:N	1.74	1.01
1:A:12:ALA:O	1:A:15:LEU:HG	1.58	1.01
1:B:165:VAL:CG1	1:B:166:ILE:H	1.71	1.01
1:A:165:VAL:CG1	1:A:166:ILE:H	1.73	1.00
1:A:11:GLU:HA	1:A:301:ARG:HH22	1.27	1.00
1:A:262:VAL:HG11	1:A:403:LEU:HD22	1.44	0.99
1:A:231:HIS:HB3	1:A:235:PRO:CD	1.90	0.99
1:B:12:ALA:O	1:B:15:LEU:HG	1.62	0.99
1:A:385:LYS:O	1:A:388:THR:OG1	1.80	0.98
1:B:231:HIS:HB3	1:B:235:PRO:CD	1.94	0.98
1:A:151:ARG:HA	1:A:155:ASP:HA	1.46	0.97
1:B:76:VAL:HA	1:B:78:GLN:HE21	1.28	0.97
1:B:165:VAL:HG13	1:B:166:ILE:N	1.78	0.97
1:B:376:VAL:HG13	1:B:377:ALA:H	1.27	0.97
1:A:287:VAL:HG11	1:A:368:GLN:OE1	1.64	0.97
1:A:312:LYS:O	1:A:316:ILE:HG12	1.65	0.97
1:A:244:LEU:HD23	1:A:385:LYS:O	1.65	0.97
1:A:340:ARG:HD2	1:A:358:MET:HG2	1.43	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:ILE:HG22	1:B:101:LEU:HD11	1.45	0.96
1:A:343:ILE:O	1:A:346:LEU:HB2	1.65	0.96
1:B:272:THR:HG23	1:B:275:ALA:HB3	1.47	0.96
1:A:272:THR:HG23	1:A:275:ALA:HB3	1.44	0.96
1:B:208:LEU:HD23	1:B:209:LEU:N	1.80	0.96
1:B:177:LEU:HD12	1:B:202:ILE:HD13	1.45	0.96
1:A:420:LEU:HB3	1:A:423:LYS:HG2	1.48	0.96
1:B:17:LYS:O	1:B:21:PRO:HG2	1.63	0.95
1:A:17:LYS:O	1:A:21:PRO:HG2	1.64	0.95
1:B:76:VAL:C	1:B:78:GLN:H	1.74	0.95
1:A:62:ILE:HG13	1:A:63:LEU:N	1.78	0.95
1:A:165:VAL:HG13	1:A:166:ILE:N	1.80	0.95
1:A:28:ALA:O	1:A:32:MET:HG2	1.65	0.95
1:A:118:ARG:NE	1:A:119:PHE:HB2	1.80	0.95
1:B:235:PRO:CA	1:B:238:LEU:HB2	1.97	0.95
1:A:262:VAL:HG21	1:A:403:LEU:HD13	1.46	0.95
1:A:177:LEU:HD12	1:A:202:ILE:HD13	1.47	0.95
1:B:343:ILE:O	1:B:346:LEU:HB2	1.66	0.95
1:A:445:TYR:CB	1:A:448:GLN:HA	1.97	0.95
1:A:147:PHE:HB2	1:A:211:LEU:HD13	1.46	0.94
1:A:203:VAL:O	1:A:206:ILE:HG12	1.67	0.94
1:B:358:MET:CA	1:B:361:LEU:HD12	1.98	0.94
1:B:369:CYS:SG	1:B:370:MET:HE2	2.08	0.94
1:B:320:VAL:HG13	1:B:321:GLY:N	1.80	0.94
1:B:177:LEU:HG	1:B:202:ILE:HG21	1.50	0.94
1:A:76:VAL:C	1:A:78:GLN:H	1.74	0.93
1:A:398:TYR:HB3	1:A:436:ALA:CB	1.99	0.93
1:B:203:VAL:O	1:B:206:ILE:HG12	1.67	0.93
1:A:180:ILE:HA	1:A:184:GLY:HA3	1.49	0.93
1:B:407:TYR:HA	1:B:425:PHE:HD2	1.34	0.93
1:B:118:ARG:NE	1:B:119:PHE:HB2	1.82	0.93
1:A:445:TYR:HB2	1:A:448:GLN:HA	1.51	0.93
1:B:16:ILE:HA	1:B:19:ALA:CB	1.99	0.93
1:B:353:VAL:HG12	1:B:357:ALA:N	1.83	0.92
1:A:208:LEU:HD23	1:A:209:LEU:N	1.83	0.92
1:A:222:ALA:O	1:A:224:VAL:HG13	1.68	0.92
1:A:94:GLN:NE2	1:A:231:HIS:HB2	1.85	0.92
1:B:62:ILE:HG13	1:B:63:LEU:N	1.80	0.92
1:B:16:ILE:HA	1:B:19:ALA:HB3	1.52	0.92
1:B:96:LEU:O	1:B:99:ALA:HB3	1.67	0.92
1:A:407:TYR:HA	1:A:425:PHE:HD2	1.35	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:SER:O	1:B:8:TYR:CE2	2.22	0.92
1:B:88:ILE:HG12	1:B:89:PRO:HD3	1.52	0.92
1:A:110:LEU:O	1:A:114:GLN:HG2	1.69	0.92
1:A:74:PRO:HB3	1:A:149:ALA:HB1	1.51	0.91
1:B:222:ALA:O	1:B:224:VAL:HG13	1.71	0.91
1:A:63:LEU:HD23	1:A:64:PHE:H	1.33	0.91
1:A:276:ALA:HB1	1:A:426:TRP:CZ2	2.04	0.91
1:B:315:ALA:O	1:B:319:ASN:HB2	1.71	0.91
1:B:73:VAL:CB	1:B:74:PRO:HD3	2.01	0.91
1:A:231:HIS:C	1:A:235:PRO:HG2	1.96	0.90
1:B:262:VAL:HG21	1:B:403:LEU:HD13	1.52	0.90
1:A:76:VAL:HA	1:A:78:GLN:HE21	1.33	0.90
1:A:320:VAL:HG13	1:A:321:GLY:N	1.85	0.90
1:B:287:VAL:HG11	1:B:368:GLN:OE1	1.71	0.90
1:B:391:PHE:HD2	1:B:392:HIS:N	1.70	0.90
1:A:11:GLU:HB3	1:A:320:VAL:CG2	2.02	0.90
1:A:88:ILE:HG12	1:A:89:PRO:HD3	1.50	0.90
1:A:382:ARG:NH2	1:A:445:TYR:H	1.68	0.90
1:A:73:VAL:CB	1:A:74:PRO:HD3	2.02	0.90
1:A:177:LEU:HG	1:A:202:ILE:HG21	1.54	0.90
1:A:418:GLN:NE2	1:A:421:GLY:HA2	1.87	0.90
1:B:382:ARG:NH2	1:B:445:TYR:H	1.70	0.90
1:B:385:LYS:O	1:B:388:THR:OG1	1.89	0.90
1:B:238:LEU:HA	1:B:241:LEU:HB2	1.52	0.89
1:A:97:ILE:HG22	1:A:101:LEU:HD11	1.53	0.89
1:A:59:LEU:H	1:A:59:LEU:HD12	1.37	0.89
1:A:123:GLU:O	1:A:124:GLU:O	1.88	0.89
1:B:11:GLU:HB3	1:B:320:VAL:CG2	2.02	0.89
1:A:206:ILE:O	1:A:210:LEU:HD22	1.72	0.89
1:A:253:PHE:HA	1:A:256:VAL:HB	1.53	0.89
1:A:353:VAL:O	1:A:357:ALA:N	2.06	0.89
1:B:232:LYS:HB3	1:B:233:PRO:HD3	1.55	0.88
1:B:398:TYR:HB3	1:B:436:ALA:CB	2.03	0.88
1:A:315:ALA:O	1:A:319:ASN:HB2	1.73	0.88
1:A:117:ILE:HG22	1:A:118:ARG:N	1.88	0.88
1:A:16:ILE:HA	1:A:19:ALA:HB3	1.56	0.88
1:B:320:VAL:CG1	1:B:321:GLY:H	1.82	0.88
1:B:327:ALA:O	1:B:331:ILE:HG22	1.72	0.88
1:A:391:PHE:HD2	1:A:392:HIS:N	1.71	0.88
1:A:16:ILE:HA	1:A:19:ALA:CB	2.04	0.88
1:B:276:ALA:HB1	1:B:426:TRP:CZ2	2.09	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:VAL:HG13	1:A:377:ALA:H	1.37	0.88
1:A:71:ALA:C	1:A:74:PRO:HD2	1.99	0.87
1:A:238:LEU:HA	1:A:241:LEU:HB2	1.54	0.87
1:A:113:THR:HA	1:A:116:ILE:HG22	1.56	0.87
1:B:15:LEU:HD12	1:B:16:ILE:N	1.89	0.87
1:A:4:SER:O	1:A:8:TYR:CD2	2.26	0.87
1:A:231:HIS:O	1:A:235:PRO:HG2	1.73	0.87
1:B:46:ILE:C	1:B:48:MET:H	1.81	0.87
1:A:15:LEU:HD12	1:A:16:ILE:N	1.89	0.87
1:A:369:CYS:SG	1:A:370:MET:HE2	2.14	0.87
1:B:110:LEU:O	1:B:114:GLN:HG2	1.75	0.87
1:B:266:VAL:CG1	1:B:269:LEU:HD11	2.05	0.87
1:A:211:LEU:O	1:A:215:ILE:HG22	1.75	0.87
1:B:353:VAL:O	1:B:353:VAL:HG12	1.73	0.86
1:A:93:HIS:CE1	1:A:225:LYS:HB3	2.09	0.86
1:A:173:LEU:O	1:A:177:LEU:HD23	1.75	0.86
1:B:420:LEU:HB3	1:B:423:LYS:HG2	1.54	0.86
1:A:155:ASP:HB2	1:A:159:LEU:H	1.38	0.86
1:A:235:PRO:O	1:A:239:ILE:HG13	1.76	0.86
1:A:408:ILE:HA	1:A:411:MET:CB	2.02	0.86
1:B:28:ALA:O	1:B:32:MET:HG2	1.75	0.86
1:B:71:ALA:C	1:B:74:PRO:HD2	2.00	0.86
1:B:94:GLN:NE2	1:B:231:HIS:HB2	1.89	0.86
1:A:327:ALA:O	1:A:331:ILE:HG22	1.74	0.86
1:A:420:LEU:CD1	1:A:423:LYS:H	1.89	0.86
1:A:96:LEU:O	1:A:99:ALA:HB3	1.76	0.86
1:A:276:ALA:HA	1:A:426:TRP:HE1	1.38	0.86
1:B:63:LEU:HD23	1:B:64:PHE:H	1.40	0.86
1:B:72:LEU:HD12	1:B:244:LEU:HD21	1.58	0.86
1:B:206:ILE:O	1:B:209:LEU:HB3	1.75	0.86
1:B:401:LEU:O	1:B:405:THR:HB	1.76	0.86
1:B:26:SER:HB2	1:B:289:MET:SD	2.14	0.86
1:B:395:PHE:O	1:B:398:TYR:HD1	1.58	0.86
1:A:265:LEU:O	1:A:268:PRO:HD3	1.75	0.86
1:A:353:VAL:HG12	1:A:357:ALA:N	1.91	0.86
1:B:72:LEU:O	1:B:75:VAL:HG22	1.76	0.85
1:B:235:PRO:HA	1:B:238:LEU:CB	2.05	0.85
1:B:107:ILE:HA	1:B:139:PHE:CZ	2.09	0.85
1:A:251:ALA:O	1:A:255:GLU:HB3	1.77	0.85
1:B:173:LEU:O	1:B:177:LEU:HD23	1.75	0.85
1:B:395:PHE:O	1:B:398:TYR:CD1	2.29	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:ILE:HA	1:B:184:GLY:HA3	1.59	0.85
1:B:231:HIS:O	1:B:235:PRO:HG2	1.77	0.85
1:A:235:PRO:CA	1:A:238:LEU:HB2	2.05	0.84
1:A:395:PHE:O	1:A:398:TYR:CD1	2.30	0.84
1:B:154:THR:O	1:B:158:SER:HA	1.77	0.84
1:A:206:ILE:O	1:A:209:LEU:HB3	1.78	0.84
1:A:320:VAL:CG1	1:A:321:GLY:H	1.88	0.84
1:B:211:LEU:O	1:B:215:ILE:HG22	1.77	0.84
1:B:93:HIS:CE1	1:B:225:LYS:HB3	2.12	0.84
1:A:401:LEU:O	1:A:405:THR:HB	1.74	0.84
1:A:46:ILE:C	1:A:48:MET:H	1.85	0.84
1:A:327:ALA:C	1:A:331:ILE:HG22	2.02	0.84
1:B:312:LYS:O	1:B:316:ILE:HG12	1.76	0.84
1:A:232:LYS:HB3	1:A:233:PRO:HD3	1.59	0.84
1:A:408:ILE:CA	1:A:411:MET:HB2	2.03	0.83
1:B:445:TYR:HB2	1:B:448:GLN:CA	2.08	0.83
1:B:151:ARG:HA	1:B:155:ASP:HA	1.60	0.83
1:B:206:ILE:O	1:B:210:LEU:HD22	1.76	0.83
1:B:251:ALA:O	1:B:255:GLU:HB3	1.76	0.83
1:A:59:LEU:HB2	1:A:60:PRO:HD3	1.60	0.83
1:B:235:PRO:O	1:B:239:ILE:HG13	1.76	0.83
1:B:420:LEU:CD1	1:B:423:LYS:H	1.90	0.83
1:B:72:LEU:HA	1:B:75:VAL:HG13	1.60	0.83
1:A:341:GLU:CD	1:A:342:GLN:H	1.87	0.83
1:B:55:ALA:O	1:B:58:TRP:HB2	1.78	0.83
1:B:406:GLY:O	1:B:409:LEU:HB3	1.77	0.83
1:B:418:GLN:NE2	1:B:421:GLY:HA2	1.93	0.83
1:A:124:GLU:O	1:A:125:ALA:C	2.22	0.83
1:A:118:ARG:HE	1:A:119:PHE:CB	1.92	0.83
1:B:74:PRO:HB3	1:B:149:ALA:HB1	1.60	0.83
1:A:74:PRO:CB	1:A:149:ALA:HB1	2.08	0.82
1:B:118:ARG:HE	1:B:119:PHE:CB	1.92	0.82
1:A:72:LEU:HA	1:A:75:VAL:HG13	1.59	0.82
1:B:231:HIS:C	1:B:235:PRO:HG2	2.03	0.82
1:A:142:PRO:HA	1:A:145:LEU:HB3	1.58	0.82
1:A:244:LEU:HB2	1:A:385:LYS:HZ3	1.44	0.82
1:A:266:VAL:CG1	1:A:269:LEU:HD11	2.07	0.82
1:A:72:LEU:O	1:A:75:VAL:HG22	1.78	0.82
1:A:137:VAL:CG1	1:A:201:ALA:HA	2.10	0.82
1:A:445:TYR:O	1:A:446:TRP:HB3	1.80	0.82
1:A:266:VAL:HG12	1:A:269:LEU:CD1	2.10	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:LEU:HD21	1:B:429:PHE:HD2	1.44	0.82
1:A:107:ILE:HA	1:A:139:PHE:CZ	2.15	0.82
1:A:151:ARG:CG	1:A:162:PRO:HG2	2.08	0.82
1:A:236:LYS:HA	1:A:239:ILE:HD12	1.61	0.82
1:A:353:VAL:O	1:A:353:VAL:HG12	1.79	0.82
1:B:71:ALA:CA	1:B:74:PRO:HD2	2.10	0.82
1:B:420:LEU:HD12	1:B:423:LYS:N	1.95	0.81
1:B:266:VAL:HG12	1:B:269:LEU:CD1	2.10	0.81
1:B:276:ALA:HB1	1:B:426:TRP:CE2	2.15	0.81
1:A:420:LEU:HD12	1:A:423:LYS:N	1.95	0.81
1:B:398:TYR:CG	1:B:436:ALA:HB2	2.16	0.81
1:B:427:LEU:HD23	1:B:428:GLY:N	1.95	0.81
1:A:72:LEU:HD12	1:A:244:LEU:HD21	1.61	0.81
1:A:75:VAL:C	1:A:77:ALA:H	1.85	0.81
1:A:77:ALA:CB	1:A:154:THR:HG23	2.11	0.81
1:B:58:TRP:O	1:B:61:SER:HB3	1.79	0.81
1:A:226:VAL:HG12	1:A:227:PHE:N	1.94	0.81
1:B:70:MET:HE2	1:B:99:ALA:HB2	1.63	0.81
1:B:155:ASP:HB2	1:B:159:LEU:H	1.46	0.81
1:A:208:LEU:O	1:A:211:LEU:HB3	1.80	0.81
1:A:137:VAL:HG11	1:A:201:ALA:HA	1.62	0.81
1:A:252:LEU:O	1:A:255:GLU:HG2	1.81	0.80
1:B:137:VAL:CG1	1:B:201:ALA:HA	2.09	0.80
1:B:296:ALA:O	1:B:300:ILE:HG23	1.82	0.80
1:A:57:ILE:HA	1:A:60:PRO:HG2	1.62	0.80
1:A:329:ALA:HB1	1:A:369:CYS:HA	1.63	0.80
1:A:395:PHE:O	1:A:398:TYR:HD1	1.62	0.80
1:B:151:ARG:CG	1:B:162:PRO:HG2	2.08	0.80
1:A:63:LEU:HD12	1:A:106:ILE:HG21	1.61	0.80
1:B:327:ALA:C	1:B:331:ILE:HG22	2.05	0.80
1:A:57:ILE:C	1:A:60:PRO:HD2	2.06	0.80
1:A:74:PRO:CG	1:A:149:ALA:HB1	2.11	0.80
1:B:73:VAL:HB	1:B:74:PRO:CD	2.07	0.80
1:B:226:VAL:HG12	1:B:227:PHE:N	1.97	0.80
1:B:276:ALA:HA	1:B:426:TRP:HE1	1.47	0.80
1:A:447:LEU:CD1	1:A:447:LEU:C	2.36	0.80
1:B:407:TYR:HA	1:B:425:PHE:CD2	2.16	0.80
1:A:267:ALA:N	1:A:268:PRO:CD	2.45	0.80
1:B:59:LEU:HD22	1:B:59:LEU:H	1.47	0.80
1:B:266:VAL:HB	1:B:425:PHE:CZ	2.16	0.80
1:A:87:LYS:HZ1	1:B:308:GLU:HG2	1.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:LEU:HD22	1:A:145:LEU:C	2.06	0.80
1:A:407:TYR:HA	1:A:425:PHE:CD2	2.16	0.80
1:A:447:LEU:HD11	1:A:450:GLN:NE2	1.76	0.80
1:B:74:PRO:CG	1:B:149:ALA:HB1	2.12	0.80
1:A:53:ILE:O	1:A:56:SER:HB3	1.80	0.80
1:A:154:THR:O	1:A:158:SER:HA	1.82	0.80
1:B:211:LEU:HG	1:B:212:LEU:H	1.47	0.80
1:B:11:GLU:HA	1:B:301:ARG:NH2	1.95	0.79
1:A:398:TYR:CG	1:A:436:ALA:HB2	2.16	0.79
1:A:447:LEU:O	1:A:448:GLN:HB2	1.82	0.79
1:B:77:ALA:CB	1:B:154:THR:HG23	2.11	0.79
1:B:80:ASN:C	1:B:82:ALA:H	1.88	0.79
1:A:272:THR:O	1:A:273:VAL:C	2.24	0.79
1:B:329:ALA:HB1	1:B:369:CYS:HA	1.63	0.79
1:A:272:THR:O	1:A:275:ALA:N	2.15	0.79
1:A:379:GLY:O	1:A:383:GLY:HA3	1.83	0.79
1:B:98:LEU:HA	1:B:101:LEU:HD12	1.65	0.79
1:B:200:THR:HA	1:B:203:VAL:HG23	1.64	0.79
1:B:208:LEU:O	1:B:211:LEU:HB3	1.82	0.79
1:B:340:ARG:HD2	1:B:358:MET:CG	2.12	0.79
1:A:332:THR:O	1:A:335:LEU:HG	1.83	0.79
1:A:444:LEU:O	1:A:446:TRP:N	2.12	0.79
1:A:276:ALA:HB1	1:A:426:TRP:CE2	2.16	0.79
1:A:84:ARG:HB3	1:A:87:LYS:HD2	1.65	0.79
1:A:98:LEU:HA	1:A:101:LEU:HD12	1.64	0.79
1:B:236:LYS:HA	1:B:239:ILE:HD12	1.64	0.79
1:B:353:VAL:HG12	1:B:357:ALA:CA	2.13	0.79
1:A:155:ASP:HB2	1:A:159:LEU:N	1.98	0.79
1:B:55:ALA:HB3	1:B:123:GLU:OE2	1.83	0.79
1:A:104:VAL:HA	1:A:107:ILE:HG13	1.63	0.78
1:A:445:TYR:HB2	1:A:448:GLN:CA	2.12	0.78
1:A:150:LEU:O	1:A:155:ASP:N	2.16	0.78
1:B:203:VAL:HG12	1:B:207:MET:SD	2.23	0.78
1:A:382:ARG:HH22	1:A:445:TYR:H	1.32	0.78
1:A:63:LEU:HD23	1:A:64:PHE:N	1.98	0.78
1:A:358:MET:CA	1:A:361:LEU:HD12	2.10	0.78
1:B:420:LEU:HD11	1:B:422:ALA:HB3	1.66	0.78
1:B:341:GLU:O	1:B:344:ALA:HB3	1.84	0.78
1:A:235:PRO:HA	1:A:238:LEU:CB	2.12	0.78
1:B:32:MET:HG3	1:B:33:GLY:N	1.98	0.78
1:B:391:PHE:C	1:B:391:PHE:CD2	2.60	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:GLU:HB3	1:A:320:VAL:HG21	1.64	0.78
1:A:272:THR:CG2	1:A:275:ALA:HB3	2.13	0.78
1:B:253:PHE:HA	1:B:256:VAL:HB	1.63	0.78
1:A:341:GLU:O	1:A:344:ALA:HB3	1.83	0.77
1:B:137:VAL:HG11	1:B:201:ALA:HA	1.64	0.77
1:A:70:MET:HE2	1:A:99:ALA:HB2	1.65	0.77
1:B:379:GLY:O	1:B:383:GLY:HA3	1.85	0.77
1:A:403:LEU:HD21	1:A:429:PHE:HD2	1.49	0.77
1:B:31:GLY:O	1:B:35:VAL:HG23	1.84	0.77
1:B:267:ALA:N	1:B:268:PRO:CD	2.47	0.77
1:B:340:ARG:CB	1:B:361:LEU:HD13	2.14	0.77
1:A:161:LYS:H	1:A:162:PRO:CD	1.98	0.77
1:A:166:ILE:HB	1:A:210:LEU:CD2	2.12	0.77
1:B:104:VAL:HB	1:B:105:PRO:HD3	1.65	0.77
1:A:387:MET:HA	1:A:443:ARG:HH21	1.49	0.77
1:A:146:LEU:O	1:A:149:ALA:HB3	1.83	0.77
1:A:406:GLY:O	1:A:409:LEU:HB3	1.84	0.77
1:B:96:LEU:HD12	1:B:146:LEU:HD12	1.66	0.77
1:A:47:ASP:C	1:A:48:MET:HE2	2.10	0.77
1:B:146:LEU:O	1:B:149:ALA:HB3	1.85	0.77
1:B:44:SER:C	1:B:46:ILE:H	1.93	0.77
1:A:447:LEU:HD13	1:A:447:LEU:O	1.85	0.76
1:B:77:ALA:HB1	1:B:154:THR:HG23	1.65	0.76
1:A:385:LYS:C	1:A:385:LYS:HD3	2.10	0.76
1:B:75:VAL:C	1:B:77:ALA:H	1.91	0.76
1:B:116:ILE:HG23	1:B:117:ILE:O	1.85	0.76
1:A:391:PHE:C	1:A:391:PHE:CD2	2.63	0.76
1:B:161:LYS:H	1:B:162:PRO:CD	1.98	0.76
1:B:272:THR:O	1:B:275:ALA:N	2.17	0.76
1:B:411:MET:HA	1:B:414:TRP:CG	2.21	0.76
1:A:152:SER:O	1:A:160:THR:HA	1.85	0.76
1:A:272:THR:O	1:A:274:VAL:N	2.19	0.76
1:A:316:ILE:O	1:A:320:VAL:HG12	1.86	0.76
1:B:63:LEU:HD12	1:B:106:ILE:HG21	1.67	0.76
1:A:246:PHE:HB3	1:A:247:PRO:HD3	1.68	0.76
1:B:246:PHE:HB3	1:B:247:PRO:HD3	1.66	0.76
1:A:20:THR:OG1	1:A:21:PRO:HD3	1.85	0.76
1:A:151:ARG:HD2	1:A:155:ASP:HA	1.67	0.76
1:A:411:MET:HA	1:A:414:TRP:CG	2.21	0.76
1:B:142:PRO:HA	1:B:145:LEU:HB3	1.66	0.76
1:B:266:VAL:HG13	1:B:407:TYR:CE2	2.21	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ILE:CG1	1:A:89:PRO:HD3	2.15	0.76
1:A:73:VAL:O	1:A:76:VAL:HB	1.85	0.76
1:A:273:VAL:HG13	1:A:274:VAL:H	1.50	0.76
1:B:24:ILE:HG21	1:B:164:MET:HG3	1.68	0.76
1:B:90:PHE:HE2	1:B:228:GLU:HA	1.51	0.76
1:B:275:ALA:CB	1:B:353:VAL:HG11	2.15	0.76
1:A:71:ALA:CA	1:A:74:PRO:HD2	2.17	0.75
1:A:90:PHE:CE2	1:A:228:GLU:HA	2.21	0.75
1:A:155:ASP:CB	1:A:159:LEU:H	1.98	0.75
1:B:182:VAL:HG22	1:B:195:GLY:HA3	1.68	0.75
1:B:74:PRO:CB	1:B:149:ALA:HB1	2.16	0.75
1:B:341:GLU:CD	1:B:342:GLN:H	1.94	0.75
1:A:276:ALA:HA	1:A:426:TRP:NE1	2.00	0.75
1:A:445:TYR:CD2	1:A:448:GLN:HG2	2.22	0.75
1:B:46:ILE:O	1:B:48:MET:N	2.19	0.75
1:A:265:LEU:O	1:A:268:PRO:CD	2.35	0.75
1:A:407:TYR:O	1:A:411:MET:N	2.19	0.75
1:A:45:ALA:CB	1:A:49:ALA:HB2	2.13	0.75
1:A:76:VAL:HG23	1:A:78:GLN:NE2	2.02	0.75
1:A:266:VAL:HG13	1:A:407:TYR:CE2	2.21	0.75
1:A:314:ALA:HB1	1:A:445:TYR:CE1	2.21	0.75
1:A:413:ASN:HB3	1:A:414:TRP:CE3	2.21	0.75
1:B:252:LEU:O	1:B:255:GLU:HG2	1.87	0.75
1:B:358:MET:HA	1:B:361:LEU:CD1	2.04	0.75
1:A:191:LEU:HB3	1:A:194:VAL:HG23	1.67	0.75
1:A:232:LYS:C	1:A:235:PRO:HD2	2.11	0.75
1:B:117:ILE:HG22	1:B:118:ARG:N	2.02	0.75
1:B:123:GLU:O	1:B:124:GLU:O	2.04	0.75
1:A:142:PRO:O	1:A:145:LEU:HB3	1.86	0.75
1:A:326:LEU:O	1:A:330:CYS:CB	2.34	0.75
1:B:272:THR:CG2	1:B:275:ALA:HB3	2.15	0.75
1:A:117:ILE:CG2	1:A:118:ARG:H	1.90	0.74
1:B:41:GLY:C	1:B:49:ALA:HB1	2.13	0.74
1:B:90:PHE:CE2	1:B:228:GLU:HA	2.22	0.74
1:B:185:LYS:HB2	1:B:189:PRO:HB3	1.68	0.74
1:B:216:VAL:HG22	1:B:225:LYS:HD3	1.68	0.74
1:B:273:VAL:HG13	1:B:274:VAL:H	1.52	0.74
1:A:211:LEU:HG	1:A:212:LEU:H	1.50	0.74
1:A:412:THR:C	1:A:415:LEU:H	1.96	0.74
1:B:166:ILE:HB	1:B:210:LEU:CD2	2.18	0.74
1:B:141:VAL:HB	1:B:142:PRO:HD3	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:PRO:O	1:B:145:LEU:HB3	1.88	0.74
1:B:265:LEU:O	1:B:268:PRO:HD3	1.87	0.74
1:B:332:THR:O	1:B:335:LEU:HG	1.86	0.74
1:A:171:LEU:HD23	1:A:172:LEU:N	2.01	0.74
1:A:340:ARG:CA	1:A:361:LEU:HD13	2.18	0.74
1:A:80:ASN:C	1:A:82:ALA:H	1.94	0.74
1:B:210:LEU:HD22	1:B:210:LEU:H	1.51	0.74
1:B:57:ILE:C	1:B:60:PRO:HD2	2.12	0.74
1:A:36:ASP:HB2	1:A:178:ASN:ND2	2.03	0.73
1:B:93:HIS:HD2	1:B:228:GLU:HB3	1.51	0.73
1:B:113:THR:HA	1:B:116:ILE:HG22	1.69	0.73
1:B:123:GLU:HG2	1:B:127:ALA:HB3	1.70	0.73
1:A:267:ALA:H	1:A:268:PRO:CD	2.01	0.73
1:B:20:THR:OG1	1:B:21:PRO:HD3	1.88	0.73
1:A:202:ILE:O	1:A:205:TRP:HB3	1.88	0.73
1:B:53:ILE:O	1:B:56:SER:HB3	1.89	0.73
1:B:211:LEU:HG	1:B:212:LEU:N	2.03	0.73
1:A:93:HIS:HD2	1:A:228:GLU:HB3	1.52	0.73
1:A:409:LEU:HD12	1:A:424:GLY:O	1.88	0.73
1:A:116:ILE:HG23	1:A:117:ILE:O	1.88	0.73
1:B:238:LEU:HD12	1:B:241:LEU:HD13	1.71	0.73
1:B:332:THR:HA	1:B:335:LEU:CD2	2.18	0.73
1:B:449:LYS:O	1:B:449:LYS:HG2	1.89	0.73
1:B:134:MET:O	1:B:137:VAL:HB	1.88	0.73
1:B:267:ALA:H	1:B:268:PRO:CD	2.00	0.73
1:B:423:LYS:HG3	1:B:424:GLY:N	2.04	0.73
1:A:45:ALA:HB3	1:A:49:ALA:CB	2.15	0.73
1:A:113:THR:CA	1:A:116:ILE:HG22	2.18	0.73
1:A:275:ALA:CA	1:A:353:VAL:HG21	2.18	0.73
1:A:427:LEU:HD23	1:A:428:GLY:N	2.04	0.73
1:B:45:ALA:HB3	1:B:49:ALA:CB	2.16	0.73
1:B:117:ILE:HG22	1:B:118:ARG:H	1.54	0.73
1:B:200:THR:HA	1:B:203:VAL:CG2	2.18	0.73
1:B:300:ILE:HG13	1:B:301:ARG:N	2.04	0.73
1:B:416:THR:O	1:B:417:GLU:HB2	1.86	0.73
1:A:123:GLU:HG2	1:A:127:ALA:HB3	1.71	0.72
1:B:208:LEU:HD23	1:B:209:LEU:H	1.55	0.72
1:B:232:LYS:C	1:B:235:PRO:HD2	2.13	0.72
1:A:253:PHE:O	1:A:256:VAL:HG12	1.88	0.72
1:B:275:ALA:HA	1:B:353:VAL:HG11	1.71	0.72
1:A:26:SER:HB2	1:A:289:MET:SD	2.28	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:PHE:HE2	1:A:228:GLU:HA	1.55	0.72
1:A:141:VAL:HB	1:A:142:PRO:HD3	1.70	0.72
1:A:244:LEU:HB2	1:A:385:LYS:NZ	2.04	0.72
1:B:266:VAL:HG22	1:B:407:TYR:CE1	2.24	0.72
1:B:433:LEU:O	1:B:437:ALA:HB2	1.89	0.72
1:B:76:VAL:HG23	1:B:78:GLN:NE2	2.05	0.72
1:B:385:LYS:HD3	1:B:386:ASP:N	2.05	0.72
1:A:27:VAL:O	1:A:31:GLY:HA3	1.89	0.72
1:A:35:VAL:O	1:A:39:MET:HB3	1.89	0.72
1:B:215:ILE:HG23	1:B:216:VAL:H	1.54	0.72
1:A:21:PRO:HA	1:A:164:MET:HE1	1.70	0.72
1:A:250:ALA:O	1:A:254:PHE:HB3	1.88	0.72
1:B:124:GLU:O	1:B:125:ALA:C	2.31	0.72
1:B:213:PHE:O	1:B:217:THR:HG22	1.89	0.72
1:A:73:VAL:HB	1:A:74:PRO:CD	2.10	0.72
1:A:327:ALA:O	1:A:331:ILE:N	2.22	0.72
1:B:77:ALA:HB2	1:B:154:THR:OG1	1.89	0.72
1:B:185:LYS:HD3	1:B:185:LYS:C	2.15	0.72
1:B:272:THR:O	1:B:273:VAL:C	2.32	0.72
1:A:46:ILE:O	1:A:48:MET:N	2.23	0.72
1:A:340:ARG:CB	1:A:361:LEU:HD13	2.19	0.72
1:A:393:ARG:HH11	1:A:393:ARG:HG3	1.55	0.72
1:B:46:ILE:O	1:B:46:ILE:HG22	1.88	0.72
1:B:132:GLY:O	1:B:135:HIS:HB2	1.89	0.72
1:B:171:LEU:HD23	1:B:172:LEU:N	2.04	0.72
1:B:275:ALA:CA	1:B:353:VAL:HG21	2.19	0.72
1:B:326:LEU:O	1:B:330:CYS:CB	2.37	0.72
1:B:316:ILE:O	1:B:320:VAL:HG12	1.90	0.72
1:A:145:LEU:HD22	1:A:145:LEU:O	1.90	0.71
1:A:234:GLN:N	1:A:235:PRO:CD	2.53	0.71
1:A:326:LEU:O	1:A:330:CYS:N	2.19	0.71
1:A:340:ARG:HA	1:A:361:LEU:HD13	1.72	0.71
1:A:353:VAL:HG12	1:A:357:ALA:CA	2.21	0.71
1:A:34:PHE:CD1	1:A:34:PHE:C	2.68	0.71
1:A:252:LEU:HD22	1:A:255:GLU:OE2	1.90	0.71
1:A:266:VAL:HB	1:A:425:PHE:CZ	2.25	0.71
1:A:272:THR:HG23	1:A:275:ALA:CB	2.20	0.71
1:B:46:ILE:C	1:B:48:MET:N	2.47	0.71
1:A:299:SER:O	1:A:302:VAL:HG12	1.88	0.71
1:B:88:ILE:CG1	1:B:89:PRO:HD3	2.19	0.71
1:A:151:ARG:O	1:A:155:ASP:N	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:ASP:C	1:B:48:MET:HE2	2.16	0.71
1:B:63:LEU:HD23	1:B:64:PHE:N	2.03	0.71
1:A:18:LEU:C	1:A:21:PRO:HD2	2.15	0.71
1:A:104:VAL:HB	1:A:105:PRO:HD3	1.72	0.71
1:B:411:MET:O	1:B:414:TRP:HB2	1.90	0.71
1:B:24:ILE:O	1:B:27:VAL:HB	1.91	0.71
1:B:316:ILE:C	1:B:320:VAL:HG12	2.16	0.71
1:A:275:ALA:CB	1:A:353:VAL:HG11	2.20	0.71
1:A:148:GLN:O	1:A:152:SER:HB3	1.90	0.71
1:B:96:LEU:CA	1:B:146:LEU:HG	2.20	0.71
1:B:150:LEU:O	1:B:155:ASP:N	2.24	0.71
1:B:244:LEU:HB2	1:B:385:LYS:HZ3	1.55	0.71
1:B:409:LEU:HD12	1:B:424:GLY:O	1.91	0.71
1:A:59:LEU:H	1:A:59:LEU:CD1	2.04	0.71
1:A:94:GLN:OE1	1:A:238:LEU:HD11	1.91	0.71
1:A:130:THR:HG21	1:A:194:VAL:HG22	1.72	0.71
1:B:69:LEU:HG	1:B:245:GLY:HA3	1.72	0.71
1:A:44:SER:C	1:A:46:ILE:H	1.97	0.71
1:A:77:ALA:HB1	1:A:154:THR:HG23	1.71	0.71
1:A:433:LEU:O	1:A:437:ALA:HB2	1.91	0.71
1:B:145:LEU:C	1:B:145:LEU:HD22	2.16	0.71
1:B:11:GLU:HB3	1:B:320:VAL:HG21	1.71	0.70
1:B:251:ALA:HB1	1:B:395:PHE:CD1	2.26	0.70
1:B:104:VAL:HA	1:B:107:ILE:HG13	1.74	0.70
1:B:155:ASP:HB2	1:B:159:LEU:N	2.04	0.70
1:B:340:ARG:CA	1:B:361:LEU:HD13	2.21	0.70
1:B:420:LEU:CD1	1:B:422:ALA:HB3	2.21	0.70
1:A:173:LEU:O	1:A:176:PRO:HD2	1.91	0.70
1:B:408:ILE:HA	1:B:411:MET:CB	2.10	0.70
1:A:191:LEU:HB3	1:A:194:VAL:CG2	2.22	0.70
1:A:216:VAL:HG22	1:A:225:LYS:HD3	1.71	0.70
1:A:423:LYS:HG3	1:A:424:GLY:N	2.04	0.70
1:B:326:LEU:O	1:B:330:CYS:N	2.24	0.70
1:B:408:ILE:CA	1:B:411:MET:HB2	2.09	0.70
1:A:32:MET:HG3	1:A:33:GLY:N	2.07	0.70
1:A:68:LEU:HD13	1:A:68:LEU:O	1.91	0.70
1:A:150:LEU:O	1:A:154:THR:HB	1.92	0.70
1:B:40:ALA:O	1:B:44:SER:HB2	1.91	0.70
1:B:68:LEU:O	1:B:68:LEU:HD13	1.91	0.70
1:A:416:THR:O	1:A:417:GLU:HB2	1.92	0.70
1:A:76:VAL:C	1:A:78:GLN:N	2.46	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:GLY:O	1:A:135:HIS:HB2	1.91	0.70
1:B:151:ARG:HD2	1:B:155:ASP:HA	1.73	0.70
1:B:155:ASP:CB	1:B:159:LEU:H	2.03	0.70
1:B:235:PRO:C	1:B:238:LEU:HB2	2.16	0.70
1:A:211:LEU:HG	1:A:212:LEU:N	2.06	0.70
1:A:215:ILE:HG23	1:A:216:VAL:N	2.07	0.70
1:A:215:ILE:HG23	1:A:216:VAL:H	1.57	0.70
1:A:244:LEU:HG	1:A:385:LYS:NZ	2.07	0.70
1:B:252:LEU:HD22	1:B:255:GLU:OE2	1.92	0.70
1:A:182:VAL:HG22	1:A:195:GLY:HA3	1.73	0.69
1:A:390:ILE:O	1:A:390:ILE:HG22	1.92	0.69
1:A:444:LEU:C	1:A:446:TRP:H	1.98	0.69
1:B:118:ARG:HH21	1:B:119:PHE:HB2	1.57	0.69
1:B:21:PRO:HA	1:B:164:MET:HE1	1.73	0.69
1:B:152:SER:O	1:B:160:THR:HA	1.92	0.69
1:B:173:LEU:O	1:B:176:PRO:HD2	1.92	0.69
1:B:423:LYS:HG3	1:B:424:GLY:H	1.57	0.69
1:A:266:VAL:HG22	1:A:407:TYR:CE1	2.27	0.69
1:A:421:GLY:O	1:A:425:PHE:HB3	1.92	0.69
1:B:45:ALA:CB	1:B:49:ALA:HB2	2.15	0.69
1:A:75:VAL:O	1:A:77:ALA:N	2.26	0.69
1:A:203:VAL:HG12	1:A:207:MET:SD	2.33	0.69
1:A:236:LYS:HA	1:A:239:ILE:CD1	2.22	0.69
1:A:366:ILE:O	1:A:369:CYS:HB3	1.91	0.69
1:A:410:GLY:CA	1:A:425:PHE:HB2	2.22	0.69
1:A:300:ILE:HG13	1:A:301:ARG:N	2.05	0.69
1:A:74:PRO:HB3	1:A:149:ALA:CB	2.22	0.69
1:A:118:ARG:HH21	1:A:119:PHE:HB2	1.58	0.69
1:A:353:VAL:HG12	1:A:357:ALA:HB2	1.73	0.69
1:B:165:VAL:O	1:B:169:ILE:HB	1.92	0.69
1:B:264:LEU:O	1:B:265:LEU:C	2.34	0.69
1:B:403:LEU:HD21	1:B:429:PHE:CD2	2.27	0.69
1:A:131:VAL:HA	1:A:134:MET:HB2	1.74	0.69
1:A:174:ASN:HD21	1:A:203:VAL:HG22	1.58	0.69
1:A:314:ALA:HB2	1:A:449:LYS:NZ	2.07	0.69
1:A:449:LYS:HG2	1:A:449:LYS:O	1.93	0.69
1:B:18:LEU:C	1:B:21:PRO:HD2	2.18	0.69
1:B:215:ILE:HG23	1:B:216:VAL:N	2.07	0.69
1:B:236:LYS:HA	1:B:239:ILE:CD1	2.23	0.69
1:B:328:THR:HA	1:B:331:ILE:CG2	2.23	0.69
1:A:124:GLU:O	1:A:126:MET:N	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:LYS:HD2	1:A:220:ARG:HG2	1.75	0.69
1:A:353:VAL:CG1	1:A:357:ALA:HB2	2.23	0.69
1:A:411:MET:O	1:A:414:TRP:HB2	1.92	0.69
1:B:55:ALA:HA	1:B:58:TRP:CD1	2.27	0.69
1:B:166:ILE:O	1:B:166:ILE:HD13	1.93	0.69
1:B:191:LEU:HB3	1:B:194:VAL:HG23	1.73	0.69
1:B:250:ALA:O	1:B:254:PHE:HB3	1.93	0.69
1:B:339:PHE:HB3	1:B:343:ILE:CG1	2.23	0.69
1:B:393:ARG:HG3	1:B:393:ARG:HH11	1.56	0.69
1:A:24:ILE:HG21	1:A:164:MET:HG3	1.75	0.69
1:A:92:VAL:HG12	1:A:93:HIS:N	2.08	0.69
1:A:185:LYS:C	1:A:185:LYS:HD3	2.18	0.69
1:A:410:GLY:HA3	1:A:425:PHE:HB2	1.75	0.69
1:B:13:SER:O	1:B:16:ILE:HG22	1.92	0.69
1:B:272:THR:HG23	1:B:275:ALA:CB	2.20	0.69
1:B:353:VAL:HG12	1:B:357:ALA:H	1.54	0.69
1:A:251:ALA:HB1	1:A:395:PHE:CD1	2.27	0.68
1:A:274:VAL:O	1:A:275:ALA:C	2.35	0.68
1:A:281:LEU:HD22	1:A:282:ASN:HD22	1.59	0.68
1:B:240:ARG:HD3	1:B:460:ALA:HA	1.75	0.68
1:A:232:LYS:H	1:A:233:PRO:CD	2.05	0.68
1:A:354:VAL:HA	1:A:357:ALA:HB3	1.74	0.68
1:A:441:GLY:O	1:A:444:LEU:HB2	1.93	0.68
1:B:86:HIS:CG	1:B:87:LYS:N	2.61	0.68
1:B:102:VAL:C	1:B:105:PRO:HD2	2.19	0.68
1:B:144:TYR:CD1	1:B:145:LEU:N	2.62	0.68
1:B:362:LEU:HD23	1:B:363:PHE:N	2.08	0.68
1:A:4:SER:O	1:A:8:TYR:CE2	2.47	0.68
1:A:173:LEU:C	1:A:177:LEU:HD23	2.18	0.68
1:A:275:ALA:HA	1:A:353:VAL:HG11	1.75	0.68
1:A:185:LYS:HB2	1:A:189:PRO:HB3	1.73	0.68
1:A:420:LEU:HB3	1:A:423:LYS:CG	2.20	0.68
1:B:173:LEU:C	1:B:177:LEU:HD23	2.17	0.68
1:B:244:LEU:HB2	1:B:385:LYS:NZ	2.09	0.68
1:B:247:PRO:O	1:B:251:ALA:HB2	1.93	0.68
1:A:130:THR:CG2	1:A:194:VAL:HG22	2.23	0.68
1:A:213:PHE:O	1:A:217:THR:HG22	1.93	0.68
1:A:295:GLY:O	1:A:299:SER:N	2.25	0.68
1:A:312:LYS:HA	1:A:312:LYS:NZ	2.08	0.68
1:B:11:GLU:CD	1:B:320:VAL:HB	2.18	0.68
1:B:93:HIS:CD2	1:B:228:GLU:HB3	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:MET:O	1:B:373:VAL:HG12	1.93	0.68
1:A:362:LEU:HD23	1:A:363:PHE:N	2.09	0.68
1:A:13:SER:O	1:A:16:ILE:HG22	1.94	0.68
1:A:46:ILE:C	1:A:48:MET:N	2.51	0.68
1:A:63:LEU:C	1:A:65:GLY:N	2.50	0.68
1:A:96:LEU:O	1:A:96:LEU:HD23	1.93	0.68
1:A:166:ILE:HD13	1:A:166:ILE:O	1.93	0.68
1:A:457:HIS:HA	1:A:460:ALA:HB3	1.75	0.68
1:A:359:GLN:O	1:A:362:LEU:HB3	1.94	0.68
1:A:447:LEU:HD21	1:A:450:GLN:HG2	1.76	0.68
1:A:423:LYS:HG3	1:A:424:GLY:H	1.58	0.68
1:B:387:MET:HG3	1:B:446:TRP:HZ2	1.59	0.68
1:A:264:LEU:O	1:A:265:LEU:C	2.36	0.68
1:B:244:LEU:HG	1:B:385:LYS:NZ	2.09	0.68
1:B:72:LEU:CD1	1:B:244:LEU:HD21	2.24	0.67
1:B:76:VAL:C	1:B:78:GLN:N	2.47	0.67
1:B:443:ARG:O	1:B:445:TYR:N	2.26	0.67
1:A:93:HIS:CD2	1:A:228:GLU:HB3	2.28	0.67
1:A:387:MET:O	1:A:391:PHE:N	2.28	0.67
1:B:296:ALA:HA	1:B:299:SER:HB3	1.76	0.67
1:B:299:SER:O	1:B:302:VAL:HG12	1.95	0.67
1:A:238:LEU:HD12	1:A:241:LEU:HD13	1.77	0.67
1:A:200:THR:HA	1:A:203:VAL:HG23	1.77	0.67
1:A:316:ILE:C	1:A:320:VAL:HG12	2.20	0.67
1:A:414:TRP:N	1:A:414:TRP:HE3	1.92	0.67
1:B:290:PHE:CB	1:B:291:PRO:HD3	2.24	0.67
1:A:46:ILE:O	1:A:46:ILE:HG22	1.93	0.67
1:A:413:ASN:HB2	1:A:418:GLN:HE21	1.57	0.67
1:B:63:LEU:C	1:B:65:GLY:N	2.50	0.67
1:B:73:VAL:O	1:B:76:VAL:HB	1.95	0.67
1:B:76:VAL:HA	1:B:78:GLN:NE2	2.08	0.67
1:B:275:ALA:N	1:B:353:VAL:HG21	2.10	0.67
1:B:445:TYR:CB	1:B:448:GLN:HA	2.17	0.67
1:A:225:LYS:O	1:A:226:VAL:HG23	1.95	0.67
1:A:238:LEU:HA	1:A:241:LEU:HD13	1.77	0.67
1:A:273:VAL:HG13	1:A:274:VAL:N	2.10	0.67
1:A:328:THR:HA	1:A:331:ILE:CG2	2.23	0.67
1:B:134:MET:HG3	1:B:197:GLY:HA3	1.75	0.67
1:A:231:HIS:HB3	1:A:235:PRO:CG	2.25	0.67
1:A:264:LEU:O	1:A:267:ALA:N	2.27	0.67
1:B:412:THR:C	1:B:415:LEU:H	2.02	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ALA:O	1:A:58:TRP:HB3	1.94	0.67
1:A:340:ARG:HD2	1:A:358:MET:CG	2.24	0.67
1:B:34:PHE:CD1	1:B:34:PHE:C	2.72	0.67
1:B:161:LYS:H	1:B:162:PRO:HD2	1.60	0.67
1:B:376:VAL:HG13	1:B:377:ALA:N	2.07	0.67
1:A:77:ALA:HB2	1:A:154:THR:OG1	1.94	0.67
1:A:86:HIS:CG	1:A:87:LYS:N	2.63	0.67
1:B:413:ASN:HB2	1:B:418:GLN:NE2	2.10	0.67
1:A:118:ARG:CZ	1:A:119:PHE:HB2	2.24	0.66
1:B:53:ILE:C	1:B:53:ILE:HD12	2.19	0.66
1:B:238:LEU:HA	1:B:241:LEU:HD13	1.76	0.66
1:B:279:VAL:HG21	1:B:357:ALA:HA	1.77	0.66
1:A:102:VAL:C	1:A:105:PRO:HD2	2.19	0.66
1:B:118:ARG:CZ	1:B:119:PHE:HB2	2.26	0.66
1:B:130:THR:HG21	1:B:194:VAL:HG22	1.77	0.66
1:B:247:PRO:CB	1:B:389:ALA:HA	2.25	0.66
1:B:340:ARG:HA	1:B:361:LEU:HD13	1.77	0.66
1:B:148:GLN:O	1:B:152:SER:HB3	1.95	0.66
1:B:234:GLN:O	1:B:238:LEU:N	2.29	0.66
1:B:281:LEU:HD22	1:B:282:ASN:HD22	1.59	0.66
1:A:262:VAL:CG2	1:A:403:LEU:HD13	2.23	0.66
1:A:353:VAL:HG12	1:A:357:ALA:H	1.59	0.66
1:A:413:ASN:HB2	1:A:418:GLN:NE2	2.10	0.66
1:A:417:GLU:OE1	1:A:417:GLU:HA	1.95	0.66
1:B:225:LYS:O	1:B:226:VAL:HG23	1.95	0.66
1:B:327:ALA:O	1:B:331:ILE:N	2.29	0.66
1:A:84:ARG:C	1:A:86:HIS:H	2.02	0.66
1:A:144:TYR:CD1	1:A:145:LEU:N	2.63	0.66
1:A:165:VAL:O	1:A:169:ILE:HB	1.96	0.66
1:A:210:LEU:HD22	1:A:210:LEU:H	1.59	0.66
1:B:234:GLN:N	1:B:235:PRO:CD	2.58	0.66
1:B:253:PHE:O	1:B:256:VAL:HG12	1.96	0.66
1:B:353:VAL:HG12	1:B:357:ALA:HB2	1.76	0.66
1:A:118:ARG:NH2	1:A:119:PHE:HB2	2.10	0.66
1:A:423:LYS:O	1:A:426:TRP:HB2	1.95	0.66
1:B:389:ALA:O	1:B:392:HIS:HB3	1.95	0.66
1:A:113:THR:HA	1:A:116:ILE:CG2	2.24	0.66
1:A:284:SER:O	1:A:286:LEU:N	2.29	0.66
1:A:290:PHE:CB	1:A:291:PRO:HD3	2.25	0.66
1:A:391:PHE:HD2	1:A:391:PHE:C	2.02	0.66
1:B:92:VAL:O	1:B:93:HIS:C	2.38	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:VAL:HG21	1:B:321:GLY:HA3	1.77	0.66
1:A:183:TYR:O	1:A:185:LYS:N	2.28	0.66
1:B:118:ARG:NH2	1:B:119:PHE:HB2	2.11	0.66
1:B:276:ALA:HA	1:B:426:TRP:NE1	2.10	0.66
1:A:63:LEU:O	1:A:65:GLY:N	2.29	0.66
1:A:296:ALA:HA	1:A:299:SER:HB3	1.78	0.66
1:A:379:GLY:HA2	1:A:391:PHE:HE1	1.61	0.66
1:B:69:LEU:C	1:B:69:LEU:HD23	2.20	0.66
1:B:354:VAL:CA	1:B:357:ALA:HB3	2.26	0.66
1:A:87:LYS:NZ	1:B:308:GLU:HG2	2.10	0.66
1:A:96:LEU:CA	1:A:146:LEU:HG	2.26	0.66
1:A:208:LEU:HD23	1:A:209:LEU:H	1.57	0.66
1:B:236:LYS:O	1:B:239:ILE:HB	1.96	0.66
1:B:420:LEU:HB3	1:B:423:LYS:CG	2.25	0.66
1:A:161:LYS:H	1:A:162:PRO:HD2	1.60	0.65
1:B:12:ALA:HA	1:B:15:LEU:HD21	1.76	0.65
1:B:354:VAL:HA	1:B:357:ALA:HB3	1.78	0.65
1:B:382:ARG:O	1:B:387:MET:HB2	1.96	0.65
1:B:385:LYS:HD3	1:B:385:LYS:C	2.21	0.65
1:A:41:GLY:C	1:A:49:ALA:HB1	2.21	0.65
1:A:296:ALA:O	1:A:300:ILE:HG23	1.97	0.65
1:B:63:LEU:O	1:B:65:GLY:N	2.28	0.65
1:A:73:VAL:O	1:A:76:VAL:CB	2.44	0.65
1:A:114:GLN:O	1:A:128:THR:HG23	1.95	0.65
1:A:378:ALA:HB2	1:A:440:LEU:HG	1.78	0.65
1:A:420:LEU:HD11	1:A:422:ALA:HB3	1.78	0.65
1:B:11:GLU:CG	1:B:320:VAL:HB	2.26	0.65
1:B:262:VAL:CG2	1:B:403:LEU:HD13	2.25	0.65
1:A:240:ARG:HD3	1:A:460:ALA:HA	1.76	0.65
1:B:94:GLN:HE21	1:B:231:HIS:HB2	1.61	0.65
1:B:146:LEU:HD22	1:B:149:ALA:HB3	1.78	0.65
1:B:413:ASN:HB2	1:B:418:GLN:HE21	1.61	0.65
1:A:53:ILE:C	1:A:53:ILE:HD12	2.22	0.65
1:A:146:LEU:HD22	1:A:149:ALA:HB3	1.79	0.65
1:B:128:THR:HG22	1:B:129:LYS:N	2.11	0.65
1:B:130:THR:CG2	1:B:194:VAL:HG22	2.27	0.65
1:B:244:LEU:HD23	1:B:385:LYS:O	1.97	0.65
1:B:247:PRO:CG	1:B:389:ALA:HA	2.27	0.65
1:B:407:TYR:O	1:B:411:MET:N	2.23	0.65
1:A:11:GLU:CD	1:A:320:VAL:HB	2.21	0.65
1:B:96:LEU:O	1:B:99:ALA:CB	2.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:HIS:HA	1:B:138:ILE:HG22	1.78	0.65
1:A:275:ALA:N	1:A:353:VAL:HG21	2.11	0.65
1:A:301:ARG:O	1:A:301:ARG:HD3	1.95	0.65
1:A:332:THR:HA	1:A:335:LEU:CD2	2.27	0.65
1:B:428:GLY:O	1:B:431:ILE:HB	1.97	0.65
1:A:279:VAL:HG21	1:A:357:ALA:HA	1.79	0.65
1:B:247:PRO:HB3	1:B:389:ALA:HA	1.79	0.65
1:B:290:PHE:HB3	1:B:291:PRO:HD3	1.79	0.65
1:A:134:MET:HG3	1:A:197:GLY:HA3	1.79	0.65
1:A:290:PHE:HB3	1:A:291:PRO:HD3	1.79	0.65
1:A:326:LEU:O	1:A:330:CYS:HB2	1.96	0.65
1:A:339:PHE:HB3	1:A:343:ILE:CG1	2.27	0.65
1:B:314:ALA:O	1:B:315:ALA:C	2.40	0.65
1:A:94:GLN:HE21	1:A:231:HIS:HB2	1.62	0.64
1:A:258:LEU:O	1:A:261:VAL:HB	1.97	0.64
1:A:69:LEU:HD23	1:A:69:LEU:C	2.23	0.64
1:A:96:LEU:HD12	1:A:146:LEU:HD12	1.79	0.64
1:A:258:LEU:HD22	1:A:399:TRP:CZ2	2.32	0.64
1:B:134:MET:SD	1:B:198:VAL:HA	2.37	0.64
1:B:275:ALA:CA	1:B:353:VAL:HG11	2.27	0.64
1:A:93:HIS:HE1	1:A:225:LYS:HB3	1.61	0.64
1:A:131:VAL:HB	1:A:135:HIS:NE2	2.13	0.64
1:A:235:PRO:C	1:A:238:LEU:HB2	2.23	0.64
1:A:273:VAL:O	1:A:277:HIS:N	2.30	0.64
1:B:125:ALA:O	1:B:126:MET:O	2.16	0.64
1:B:301:ARG:NH2	1:B:316:ILE:HG22	2.11	0.64
1:B:353:VAL:CG1	1:B:357:ALA:HB2	2.28	0.64
1:B:382:ARG:HH22	1:B:445:TYR:H	1.44	0.64
1:A:98:LEU:HA	1:A:101:LEU:CD1	2.27	0.64
1:A:137:VAL:HG11	1:A:201:ALA:CA	2.28	0.64
1:B:36:ASP:HB2	1:B:178:ASN:ND2	2.11	0.64
1:B:96:LEU:O	1:B:96:LEU:HD23	1.98	0.64
1:B:359:GLN:O	1:B:362:LEU:HB3	1.98	0.64
1:A:251:ALA:HB2	1:A:392:HIS:ND1	2.13	0.64
1:A:354:VAL:CA	1:A:357:ALA:HB3	2.27	0.64
1:B:80:ASN:C	1:B:82:ALA:N	2.54	0.64
1:B:263:ALA:O	1:B:266:VAL:C	2.41	0.64
1:B:273:VAL:HG13	1:B:274:VAL:N	2.11	0.64
1:A:5:VAL:HA	1:A:8:TYR:CZ	2.32	0.64
1:A:75:VAL:C	1:A:77:ALA:N	2.53	0.64
1:B:145:LEU:HA	1:B:148:GLN:NE2	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:ALA:CB	1:B:353:VAL:CG1	2.74	0.64
1:B:350:ASN:OD1	1:B:352:VAL:HB	1.98	0.64
1:B:436:ALA:O	1:B:439:MET:N	2.31	0.64
1:A:144:TYR:CD2	1:A:207:MET:HB3	2.33	0.64
1:A:177:LEU:CD1	1:A:202:ILE:HD13	2.25	0.64
1:B:35:VAL:O	1:B:39:MET:HB3	1.98	0.64
1:B:51:VAL:O	1:B:54:ALA:HB3	1.97	0.64
1:B:70:MET:CE	1:B:99:ALA:HB2	2.27	0.64
1:B:145:LEU:HD22	1:B:145:LEU:O	1.97	0.64
1:B:326:LEU:O	1:B:330:CYS:HB2	1.97	0.64
1:A:207:MET:HA	1:A:210:LEU:HD23	1.80	0.64
1:B:63:LEU:O	1:B:66:VAL:HG22	1.98	0.64
1:B:353:VAL:HG12	1:B:357:ALA:CB	2.28	0.64
1:A:275:ALA:CB	1:A:353:VAL:CG1	2.76	0.64
1:A:276:ALA:CA	1:A:426:TRP:HE1	2.09	0.64
1:A:314:ALA:O	1:A:315:ALA:C	2.40	0.64
1:A:394:THR:HG23	1:A:439:MET:HB3	1.80	0.64
1:B:302:VAL:O	1:B:306:LEU:HB2	1.98	0.64
1:B:366:ILE:O	1:B:369:CYS:HB3	1.97	0.64
1:B:390:ILE:HG22	1:B:390:ILE:O	1.97	0.64
1:B:12:ALA:HA	1:B:15:LEU:CD2	2.27	0.63
1:B:236:LYS:HA	1:B:239:ILE:CG1	2.29	0.63
1:A:17:LYS:O	1:A:21:PRO:CG	2.43	0.63
1:A:128:THR:HG22	1:A:129:LYS:N	2.12	0.63
1:A:148:GLN:HA	1:A:152:SER:HB2	1.80	0.63
1:B:378:ALA:HB2	1:B:440:LEU:HG	1.80	0.63
1:B:439:MET:HE2	1:B:439:MET:HA	1.79	0.63
1:B:441:GLY:O	1:B:444:LEU:HB2	1.97	0.63
1:A:125:ALA:O	1:A:126:MET:O	2.16	0.63
1:B:96:LEU:HA	1:B:146:LEU:HG	1.80	0.63
1:B:117:ILE:HG22	1:B:119:PHE:H	1.63	0.63
1:B:181:PHE:CD2	1:B:198:VAL:HG11	2.34	0.63
1:B:191:LEU:HB3	1:B:194:VAL:CG2	2.28	0.63
1:B:272:THR:O	1:B:274:VAL:N	2.31	0.63
1:B:373:VAL:HG13	1:B:437:ALA:HB1	1.80	0.63
1:A:12:ALA:HA	1:A:15:LEU:HD21	1.80	0.63
1:A:72:LEU:CD1	1:A:244:LEU:HD21	2.26	0.63
1:A:135:HIS:HA	1:A:138:ILE:HG22	1.79	0.63
1:A:342:GLN:O	1:A:345:LEU:HB2	1.99	0.63
1:B:231:HIS:HB3	1:B:235:PRO:CG	2.27	0.63
1:A:40:ALA:O	1:A:44:SER:HB2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ALA:O	1:A:48:MET:HB2	1.99	0.63
1:A:92:VAL:O	1:A:93:HIS:C	2.40	0.63
1:A:386:ASP:O	1:A:389:ALA:N	2.31	0.63
1:A:407:TYR:C	1:A:409:LEU:H	2.06	0.63
1:B:264:LEU:O	1:B:267:ALA:N	2.31	0.63
1:B:414:TRP:N	1:B:414:TRP:HE3	1.96	0.63
1:B:420:LEU:HD13	1:B:422:ALA:H	1.62	0.63
1:A:63:LEU:O	1:A:66:VAL:HG22	1.98	0.63
1:A:287:VAL:O	1:A:290:PHE:HB2	1.99	0.63
1:B:363:PHE:CE2	1:B:426:TRP:HB3	2.33	0.63
1:B:445:TYR:O	1:B:448:GLN:N	2.32	0.63
1:A:25:ALA:O	1:A:28:ALA:HB3	1.99	0.63
1:A:52:SER:O	1:A:123:GLU:OE2	2.16	0.63
1:B:238:LEU:CA	1:B:241:LEU:HB2	2.27	0.63
1:B:274:VAL:O	1:B:275:ALA:C	2.41	0.63
1:A:55:ALA:HB3	1:A:123:GLU:OE2	1.99	0.63
1:A:89:PRO:O	1:A:93:HIS:ND1	2.32	0.63
1:A:267:ALA:N	1:A:268:PRO:HD2	2.13	0.63
1:A:373:VAL:HG13	1:A:437:ALA:HB1	1.81	0.63
1:A:408:ILE:HG22	1:A:408:ILE:O	1.99	0.63
1:B:16:ILE:HA	1:B:19:ALA:HB2	1.76	0.63
1:B:45:ALA:O	1:B:48:MET:HB2	1.99	0.63
1:B:53:ILE:C	1:B:56:SER:HB3	2.24	0.63
1:B:178:ASN:CG	1:B:199:ALA:HB2	2.23	0.63
1:A:351:GLN:C	1:A:351:GLN:CD	2.67	0.63
1:B:25:ALA:O	1:B:28:ALA:HB3	1.98	0.63
1:B:113:THR:CA	1:B:116:ILE:HG22	2.29	0.63
1:A:149:ALA:O	1:A:154:THR:HB	1.98	0.62
1:A:299:SER:CB	1:A:380:SER:HA	2.28	0.62
1:B:351:GLN:O	1:B:352:VAL:C	2.41	0.62
1:A:59:LEU:HD12	1:A:59:LEU:N	2.12	0.62
1:A:117:ILE:HG22	1:A:119:PHE:H	1.64	0.62
1:A:147:PHE:HE2	1:A:215:ILE:HB	1.64	0.62
1:A:298:VAL:HG21	1:A:321:GLY:HA3	1.81	0.62
1:B:344:ALA:HB1	1:B:354:VAL:HG22	1.80	0.62
1:A:445:TYR:O	1:A:446:TRP:CB	2.47	0.62
1:B:7:ARG:HB3	1:B:11:GLU:OE1	1.98	0.62
1:B:333:ALA:O	1:B:336:THR:HB	1.99	0.62
1:A:284:SER:O	1:A:287:VAL:N	2.33	0.62
1:A:391:PHE:CD2	1:A:392:HIS:N	2.61	0.62
1:A:428:GLY:O	1:A:431:ILE:HB	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:LEU:HD22	1:B:59:LEU:N	2.13	0.62
1:B:147:PHE:HE2	1:B:215:ILE:HB	1.64	0.62
1:B:353:VAL:C	1:B:357:ALA:HB2	2.25	0.62
1:B:444:LEU:O	1:B:446:TRP:O	2.18	0.62
1:B:219:LYS:HD2	1:B:220:ARG:HG2	1.81	0.62
1:B:339:PHE:HB3	1:B:343:ILE:HG13	1.79	0.62
1:B:423:LYS:O	1:B:426:TRP:HB2	1.99	0.62
1:A:40:ALA:HB1	1:A:182:VAL:HG11	1.81	0.62
1:A:215:ILE:HG23	1:A:216:VAL:HG23	1.81	0.62
1:A:314:ALA:O	1:A:318:ALA:HB3	1.99	0.62
1:B:262:VAL:O	1:B:266:VAL:HG23	2.00	0.62
1:B:265:LEU:O	1:B:268:PRO:CD	2.48	0.62
1:B:408:ILE:O	1:B:408:ILE:HG22	1.98	0.62
1:A:141:VAL:HG22	1:A:204:TYR:HB3	1.81	0.62
1:B:284:SER:O	1:B:287:VAL:N	2.33	0.62
1:B:407:TYR:C	1:B:409:LEU:H	2.06	0.62
1:B:417:GLU:OE1	1:B:417:GLU:HA	1.99	0.62
1:A:15:LEU:O	1:A:19:ALA:N	2.30	0.62
1:A:120:MET:O	1:A:120:MET:HG2	1.99	0.62
1:B:14:ASN:N	1:B:14:ASN:HD22	1.97	0.62
1:B:52:SER:O	1:B:123:GLU:OE2	2.17	0.62
1:B:141:VAL:HG22	1:B:204:TYR:HB3	1.81	0.62
1:B:174:ASN:HD21	1:B:203:VAL:HG22	1.63	0.62
1:B:328:THR:O	1:B:332:THR:HG23	2.00	0.62
1:B:387:MET:HE2	1:B:456:LEU:HD13	1.81	0.62
1:A:200:THR:HA	1:A:203:VAL:CG2	2.30	0.62
1:A:203:VAL:O	1:A:207:MET:HG3	2.00	0.62
1:A:398:TYR:HB2	1:A:432:GLY:O	2.00	0.62
1:B:238:LEU:HG	1:B:241:LEU:HD22	1.81	0.62
1:A:353:VAL:HG12	1:A:357:ALA:CB	2.29	0.62
1:B:40:ALA:HB1	1:B:182:VAL:HG11	1.82	0.62
1:B:60:PRO:O	1:B:63:LEU:HD23	2.00	0.62
1:B:92:VAL:HG12	1:B:93:HIS:N	2.15	0.62
1:B:211:LEU:O	1:B:212:LEU:C	2.43	0.62
1:B:421:GLY:O	1:B:425:PHE:HB3	2.00	0.62
1:A:171:LEU:HD23	1:A:172:LEU:H	1.63	0.61
1:B:32:MET:CG	1:B:33:GLY:N	2.63	0.61
1:B:100:LEU:N	1:B:100:LEU:HD12	2.15	0.61
1:B:126:MET:HE3	1:B:191:LEU:HD21	1.82	0.61
1:B:137:VAL:HG11	1:B:201:ALA:CA	2.28	0.61
1:B:221:LEU:HD12	1:B:221:LEU:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:PRO:CG	1:A:389:ALA:HA	2.30	0.61
1:A:403:LEU:HD21	1:A:429:PHE:CD2	2.32	0.61
1:B:74:PRO:HB3	1:B:149:ALA:CB	2.30	0.61
1:B:250:ALA:O	1:B:251:ALA:O	2.18	0.61
1:B:423:LYS:CG	1:B:424:GLY:H	2.13	0.61
1:A:139:PHE:C	1:A:142:PRO:HD2	2.26	0.61
1:B:73:VAL:HG13	1:B:241:LEU:HG	1.83	0.61
1:B:342:GLN:O	1:B:345:LEU:HB2	2.00	0.61
1:B:98:LEU:HA	1:B:101:LEU:CD1	2.29	0.61
1:B:340:ARG:HB2	1:B:361:LEU:HD13	1.83	0.61
1:A:178:ASN:CG	1:A:199:ALA:HB2	2.25	0.61
1:A:314:ALA:HB2	1:A:449:LYS:HZ1	1.65	0.61
1:B:26:SER:HB2	1:B:289:MET:CG	2.30	0.61
1:B:284:SER:O	1:B:286:LEU:N	2.34	0.61
1:B:295:GLY:O	1:B:299:SER:N	2.27	0.61
1:B:376:VAL:O	1:B:377:ALA:C	2.43	0.61
1:A:57:ILE:HA	1:A:60:PRO:CG	2.29	0.61
1:A:126:MET:O	1:A:130:THR:HG23	2.01	0.61
1:A:144:TYR:CG	1:A:207:MET:HB3	2.35	0.61
1:A:339:PHE:HB3	1:A:343:ILE:HG12	1.81	0.61
1:A:387:MET:HE2	1:A:456:LEU:HD13	1.81	0.61
1:B:74:PRO:HG3	1:B:149:ALA:HB1	1.82	0.61
1:B:84:ARG:C	1:B:86:HIS:H	2.09	0.61
1:B:94:GLN:OE1	1:B:238:LEU:HD11	2.00	0.61
1:B:202:ILE:O	1:B:205:TRP:HB3	2.00	0.61
1:A:423:LYS:CG	1:A:424:GLY:H	2.13	0.61
1:B:126:MET:O	1:B:130:THR:HG23	2.01	0.61
1:A:86:HIS:O	1:A:87:LYS:HB2	2.01	0.61
1:A:376:VAL:O	1:A:377:ALA:C	2.44	0.61
1:A:443:ARG:O	1:A:445:TYR:N	2.33	0.61
1:B:84:ARG:HB3	1:B:87:LYS:HD2	1.81	0.61
1:B:131:VAL:HB	1:B:135:HIS:NE2	2.16	0.61
1:B:251:ALA:HB2	1:B:392:HIS:ND1	2.16	0.61
1:B:276:ALA:CA	1:B:426:TRP:HE1	2.13	0.61
1:B:312:LYS:HA	1:B:312:LYS:NZ	2.15	0.61
1:A:58:TRP:O	1:A:61:SER:HB3	2.00	0.61
1:A:245:GLY:HA2	1:A:248:VAL:HG22	1.83	0.61
1:A:252:LEU:HA	1:A:255:GLU:OE2	2.00	0.61
1:A:352:VAL:O	1:A:352:VAL:HG13	1.99	0.61
1:B:21:PRO:CB	1:B:160:THR:HG23	2.31	0.61
1:B:33:GLY:O	1:B:37:THR:HB	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:PHE:O	1:B:155:ASP:OD1	2.19	0.61
1:A:33:GLY:O	1:A:37:THR:HB	2.01	0.61
1:A:72:LEU:HD12	1:A:244:LEU:HD11	1.81	0.61
1:A:220:ARG:HG3	1:A:221:LEU:HD12	1.83	0.61
1:A:238:LEU:CA	1:A:241:LEU:HB2	2.30	0.61
1:A:328:THR:O	1:A:332:THR:HG23	2.01	0.61
1:A:414:TRP:CE3	1:A:414:TRP:N	2.68	0.61
1:B:387:MET:HG3	1:B:446:TRP:CZ2	2.35	0.61
1:A:96:LEU:HA	1:A:146:LEU:HG	1.83	0.60
1:B:89:PRO:O	1:B:93:HIS:ND1	2.34	0.60
1:B:320:VAL:O	1:B:321:GLY:C	2.44	0.60
1:B:391:PHE:HD2	1:B:391:PHE:C	2.00	0.60
1:A:7:ARG:HB3	1:A:11:GLU:OE1	2.02	0.60
1:A:24:ILE:O	1:A:27:VAL:HB	2.01	0.60
1:A:406:GLY:HA2	1:A:428:GLY:HA3	1.81	0.60
1:B:75:VAL:O	1:B:77:ALA:N	2.34	0.60
1:B:181:PHE:CG	1:B:198:VAL:HG11	2.35	0.60
1:A:69:LEU:HG	1:A:245:GLY:HA3	1.82	0.60
1:B:131:VAL:HA	1:B:134:MET:HB2	1.84	0.60
1:B:314:ALA:HB2	1:B:449:LYS:NZ	2.15	0.60
1:B:353:VAL:O	1:B:353:VAL:CG1	2.46	0.60
1:A:31:GLY:O	1:A:35:VAL:HG23	2.02	0.60
1:A:431:ILE:O	1:A:435:ALA:HB2	2.01	0.60
1:B:100:LEU:C	1:B:102:VAL:H	2.08	0.60
1:B:114:GLN:O	1:B:128:THR:HG23	2.01	0.60
1:B:183:TYR:O	1:B:185:LYS:N	2.35	0.60
1:B:301:ARG:HH12	1:B:320:VAL:HG11	1.66	0.60
1:B:343:ILE:O	1:B:344:ALA:C	2.45	0.60
1:B:248:VAL:O	1:B:251:ALA:HB3	2.02	0.60
1:B:252:LEU:HA	1:B:255:GLU:OE2	2.02	0.60
1:A:151:ARG:O	1:A:152:SER:C	2.45	0.60
1:B:250:ALA:HA	1:B:254:PHE:HB2	1.84	0.60
1:A:166:ILE:O	1:A:170:GLY:HA3	2.01	0.60
1:A:439:MET:HE2	1:A:439:MET:HA	1.84	0.60
1:B:72:LEU:HB3	1:B:244:LEU:HD13	1.83	0.60
1:B:147:PHE:CG	1:B:211:LEU:HA	2.37	0.60
1:B:151:ARG:O	1:B:152:SER:C	2.44	0.60
1:B:166:ILE:O	1:B:170:GLY:N	2.35	0.60
1:B:273:VAL:O	1:B:277:HIS:N	2.33	0.60
1:B:398:TYR:HB2	1:B:432:GLY:O	2.02	0.60
1:A:129:LYS:HA	1:A:132:GLY:HA3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:MET:O	1:A:373:VAL:HG12	2.01	0.60
1:B:5:VAL:HA	1:B:8:TYR:CZ	2.37	0.60
1:A:53:ILE:C	1:A:56:SER:HB3	2.26	0.60
1:A:196:CYS:SG	1:A:197:GLY:N	2.74	0.60
1:A:239:ILE:HA	1:A:242:PHE:HB2	1.83	0.60
1:B:59:LEU:H	1:B:59:LEU:CD2	2.14	0.60
1:B:232:LYS:H	1:B:233:PRO:CD	2.15	0.60
1:B:267:ALA:N	1:B:268:PRO:HD2	2.15	0.60
1:A:221:LEU:HD12	1:A:221:LEU:N	2.17	0.60
1:B:211:LEU:CG	1:B:212:LEU:N	2.64	0.60
1:A:146:LEU:C	1:A:146:LEU:HD13	2.27	0.59
1:A:366:ILE:C	1:A:430:ILE:HD11	2.27	0.59
1:B:177:LEU:CD1	1:B:202:ILE:HD13	2.25	0.59
1:B:202:ILE:O	1:B:206:ILE:HG23	2.02	0.59
1:B:209:LEU:HD12	1:B:210:LEU:HD13	1.82	0.59
1:B:387:MET:HA	1:B:443:ARG:HH21	1.66	0.59
1:A:118:ARG:HH21	1:A:119:PHE:CB	2.15	0.59
1:A:217:THR:O	1:A:218:SER:C	2.44	0.59
1:A:250:ALA:O	1:A:251:ALA:O	2.20	0.59
1:A:420:LEU:CD1	1:A:422:ALA:HB3	2.32	0.59
1:A:420:LEU:CB	1:A:423:LYS:HG2	2.28	0.59
1:B:123:GLU:CG	1:B:127:ALA:HB3	2.32	0.59
1:B:146:LEU:HD13	1:B:146:LEU:C	2.27	0.59
1:B:147:PHE:CE2	1:B:215:ILE:HB	2.37	0.59
1:B:207:MET:HA	1:B:210:LEU:HD23	1.84	0.59
1:B:367:TYR:HA	1:B:430:ILE:HG13	1.84	0.59
1:A:81:GLY:HA3	1:A:307:GLY:O	2.02	0.59
1:A:123:GLU:CG	1:A:127:ALA:HB3	2.32	0.59
1:A:166:ILE:HB	1:A:210:LEU:HD21	1.83	0.59
1:A:275:ALA:CA	1:A:353:VAL:HG11	2.31	0.59
1:A:299:SER:OG	1:A:380:SER:HA	2.02	0.59
1:A:343:ILE:O	1:A:344:ALA:C	2.46	0.59
1:A:354:VAL:O	1:A:358:MET:N	2.28	0.59
1:B:21:PRO:HB3	1:B:160:THR:O	2.03	0.59
1:B:65:GLY:HA2	1:B:253:PHE:CD2	2.37	0.59
1:B:127:ALA:O	1:B:131:VAL:HG22	2.01	0.59
1:A:191:LEU:O	1:A:195:GLY:N	2.34	0.59
1:B:147:PHE:CD2	1:B:211:LEU:HA	2.37	0.59
1:B:171:LEU:HD23	1:B:172:LEU:H	1.67	0.59
1:A:16:ILE:HA	1:A:19:ALA:HB2	1.81	0.59
1:A:68:LEU:HD22	1:A:71:ALA:HB3	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:PHE:CD2	1:A:211:LEU:HA	2.38	0.59
1:A:234:GLN:O	1:A:238:LEU:HD13	2.02	0.59
1:A:333:ALA:O	1:A:336:THR:HB	2.02	0.59
1:A:445:TYR:HD2	1:A:448:GLN:HG2	1.64	0.59
1:B:88:ILE:N	1:B:89:PRO:CD	2.65	0.59
1:B:233:PRO:O	1:B:236:LYS:HB3	2.02	0.59
1:B:379:GLY:HA2	1:B:391:PHE:HE1	1.68	0.59
1:A:202:ILE:O	1:A:206:ILE:HG23	2.03	0.59
1:A:234:GLN:O	1:A:238:LEU:N	2.36	0.59
1:B:23:LEU:C	1:B:23:LEU:HD13	2.28	0.59
1:B:277:HIS:HD2	1:B:278:GLN:OE1	1.86	0.59
1:A:7:ARG:HB3	1:A:7:ARG:HH11	1.68	0.59
1:A:235:PRO:HA	1:A:238:LEU:HD22	1.84	0.59
1:A:354:VAL:O	1:A:358:MET:CB	2.51	0.59
1:B:106:ILE:HG22	1:B:139:PHE:HE1	1.68	0.59
1:B:366:ILE:C	1:B:430:ILE:HD11	2.27	0.59
1:A:11:GLU:OE2	1:A:320:VAL:HB	2.03	0.59
1:B:443:ARG:CZ	1:B:446:TRP:NE1	2.66	0.59
1:B:452:ASP:O	1:B:456:LEU:HG	2.03	0.59
1:A:11:GLU:CG	1:A:320:VAL:HB	2.32	0.59
1:A:142:PRO:CA	1:A:145:LEU:HB3	2.30	0.59
1:A:151:ARG:HG3	1:A:152:SER:N	2.18	0.59
1:A:382:ARG:HH21	1:A:443:ARG:C	2.11	0.59
1:B:151:ARG:HG3	1:B:152:SER:H	1.67	0.59
1:A:23:LEU:HD13	1:A:23:LEU:C	2.27	0.59
1:B:11:GLU:HG2	1:B:316:ILE:CG2	2.33	0.59
1:B:86:HIS:CG	1:B:87:LYS:H	2.21	0.59
1:B:382:ARG:CD	1:B:382:ARG:N	2.65	0.59
1:A:142:PRO:O	1:A:145:LEU:HD12	2.03	0.58
1:A:236:LYS:O	1:A:239:ILE:HB	2.02	0.58
1:A:351:GLN:O	1:A:354:VAL:HG23	2.03	0.58
1:B:17:LYS:O	1:B:21:PRO:CG	2.46	0.58
1:B:63:LEU:CG	1:B:64:PHE:N	2.66	0.58
1:B:151:ARG:O	1:B:155:ASP:N	2.35	0.58
1:B:251:ALA:HB1	1:B:395:PHE:HD1	1.67	0.58
1:B:301:ARG:NH1	1:B:320:VAL:HG11	2.18	0.58
1:B:313:GLY:O	1:B:317:ALA:HB3	2.03	0.58
1:A:74:PRO:HG3	1:A:149:ALA:HB1	1.85	0.58
1:A:116:ILE:O	1:A:117:ILE:C	2.46	0.58
1:A:355:ALA:O	1:A:358:MET:HB3	2.02	0.58
1:A:370:MET:HG3	1:A:434:SER:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:LEU:HD12	1:B:244:LEU:HD11	1.85	0.58
1:B:351:GLN:CD	1:B:351:GLN:C	2.70	0.58
1:A:55:ALA:O	1:A:59:LEU:CD1	2.50	0.58
1:A:141:VAL:HA	1:A:204:TYR:HB2	1.86	0.58
1:A:250:ALA:O	1:A:254:PHE:N	2.36	0.58
1:A:281:LEU:HD22	1:A:282:ASN:ND2	2.17	0.58
1:A:363:PHE:CD1	1:A:364:ALA:N	2.71	0.58
1:A:408:ILE:HG12	1:A:411:MET:SD	2.44	0.58
1:A:426:TRP:HA	1:A:426:TRP:CE3	2.38	0.58
1:A:65:GLY:HA2	1:A:253:PHE:CD2	2.38	0.58
1:A:219:LYS:HD3	1:A:220:ARG:HE	1.68	0.58
1:A:302:VAL:O	1:A:306:LEU:HB2	2.03	0.58
1:B:144:TYR:O	1:B:145:LEU:C	2.46	0.58
1:B:178:ASN:ND2	1:B:199:ALA:CB	2.67	0.58
1:B:244:LEU:HG	1:B:385:LYS:HZ1	1.67	0.58
1:B:340:ARG:HG3	1:B:341:GLU:H	1.66	0.58
1:B:354:VAL:O	1:B:358:MET:CB	2.51	0.58
1:B:353:VAL:O	1:B:357:ALA:CB	2.52	0.58
1:A:301:ARG:HD3	1:A:301:ARG:C	2.29	0.58
1:A:320:VAL:O	1:A:321:GLY:C	2.46	0.58
1:B:151:ARG:HG3	1:B:152:SER:N	2.19	0.58
1:B:281:LEU:HD22	1:B:282:ASN:ND2	2.18	0.58
1:B:314:ALA:O	1:B:318:ALA:HB3	2.03	0.58
1:B:413:ASN:HB2	1:B:418:GLN:HG2	1.85	0.58
1:B:417:GLU:CD	1:B:418:GLN:H	2.12	0.58
1:A:80:ASN:C	1:A:82:ALA:N	2.60	0.58
1:A:326:LEU:HD13	1:A:330:CYS:HB2	1.85	0.58
1:B:15:LEU:CD1	1:B:16:ILE:N	2.66	0.58
1:B:245:GLY:HA2	1:B:248:VAL:HG22	1.86	0.58
1:A:21:PRO:HB3	1:A:160:THR:O	2.03	0.58
1:A:247:PRO:CB	1:A:389:ALA:HA	2.34	0.58
1:A:251:ALA:HB1	1:A:395:PHE:HD1	1.67	0.58
1:A:367:TYR:HA	1:A:430:ILE:HG13	1.86	0.58
1:B:302:VAL:HG23	1:B:317:ALA:HB3	1.86	0.58
1:A:72:LEU:HA	1:A:75:VAL:CG1	2.33	0.58
1:A:236:LYS:HA	1:A:239:ILE:CG1	2.34	0.58
1:B:141:VAL:HA	1:B:204:TYR:HB2	1.86	0.58
1:B:398:TYR:CD1	1:B:399:TRP:N	2.71	0.58
1:B:461:LYS:OXT	1:B:461:LYS:HD2	2.04	0.58
1:A:12:ALA:HA	1:A:15:LEU:CD2	2.33	0.58
1:A:147:PHE:CE2	1:A:215:ILE:HB	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:TYR:HE2	1:A:429:PHE:CD1	2.21	0.58
1:B:410:GLY:HA3	1:B:425:PHE:HB2	1.86	0.58
1:A:178:ASN:O	1:A:179:TRP:C	2.46	0.57
1:A:379:GLY:HA2	1:A:391:PHE:CE1	2.39	0.57
1:A:409:LEU:O	1:A:410:GLY:C	2.43	0.57
1:B:418:GLN:CD	1:B:421:GLY:HA2	2.29	0.57
1:B:455:GLN:HA	1:B:458:LEU:HB2	1.85	0.57
1:A:160:THR:O	1:A:160:THR:HG23	2.04	0.57
1:A:250:ALA:O	1:A:254:PHE:CB	2.52	0.57
1:A:363:PHE:CE2	1:A:426:TRP:HB3	2.40	0.57
1:A:447:LEU:O	1:A:448:GLN:CB	2.51	0.57
1:B:443:ARG:CZ	1:B:446:TRP:HE1	2.16	0.57
1:A:74:PRO:CG	1:A:149:ALA:CB	2.82	0.57
1:A:96:LEU:O	1:A:99:ALA:CB	2.52	0.57
1:A:389:ALA:O	1:A:392:HIS:HB3	2.04	0.57
1:B:73:VAL:CB	1:B:74:PRO:CD	2.77	0.57
1:B:144:TYR:CD2	1:B:207:MET:HB3	2.39	0.57
1:B:413:ASN:HB3	1:B:414:TRP:CE3	2.39	0.57
1:A:57:ILE:O	1:A:60:PRO:HB2	2.04	0.57
1:B:57:ILE:HA	1:B:60:PRO:HG2	1.87	0.57
1:B:318:ALA:HA	1:B:381:LEU:HD11	1.86	0.57
1:B:406:GLY:HA2	1:B:428:GLY:HA3	1.86	0.57
1:A:63:LEU:CD2	1:A:64:PHE:N	2.65	0.57
1:A:145:LEU:HA	1:A:148:GLN:NE2	2.18	0.57
1:A:263:ALA:O	1:A:266:VAL:C	2.46	0.57
1:A:275:ALA:HA	1:A:353:VAL:HG21	1.85	0.57
1:B:86:HIS:O	1:B:87:LYS:HB2	2.04	0.57
1:B:149:ALA:O	1:B:154:THR:HB	2.04	0.57
1:B:172:LEU:O	1:B:176:PRO:HD2	2.04	0.57
1:A:287:VAL:HG11	1:A:368:GLN:CD	2.29	0.57
1:B:324:THR:O	1:B:327:ALA:HB3	2.05	0.57
1:B:376:VAL:O	1:B:380:SER:HB3	2.04	0.57
1:A:19:ALA:O	1:A:22:VAL:HG22	2.03	0.57
1:A:106:ILE:HG22	1:A:139:PHE:HE1	1.70	0.57
1:A:120:MET:O	1:A:121:ASP:C	2.47	0.57
1:B:63:LEU:C	1:B:65:GLY:H	2.12	0.57
1:B:70:MET:HE2	1:B:99:ALA:CB	2.34	0.57
1:B:97:ILE:HG22	1:B:101:LEU:CD1	2.29	0.57
1:B:460:ALA:O	1:B:461:LYS:O	2.23	0.57
1:A:130:THR:C	1:A:132:GLY:N	2.60	0.57
1:A:350:ASN:ND2	1:A:352:VAL:H	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:ALA:HB1	1:B:126:MET:HE1	1.85	0.57
1:B:314:ALA:HB2	1:B:449:LYS:HZ1	1.68	0.57
1:B:352:VAL:HG13	1:B:352:VAL:O	2.04	0.57
1:A:147:PHE:CG	1:A:211:LEU:HA	2.40	0.57
1:A:152:SER:O	1:A:155:ASP:OD1	2.23	0.57
1:A:420:LEU:HD13	1:A:422:ALA:H	1.69	0.57
1:B:107:ILE:O	1:B:110:LEU:HB3	2.05	0.57
1:B:215:ILE:HG23	1:B:216:VAL:HG23	1.85	0.57
1:B:235:PRO:HA	1:B:238:LEU:CG	2.35	0.57
1:B:237:GLU:O	1:B:241:LEU:HD12	2.05	0.57
1:A:63:LEU:C	1:A:65:GLY:H	2.12	0.57
1:A:88:ILE:CG1	1:A:89:PRO:CD	2.82	0.57
1:A:191:LEU:HG	1:A:192:GLY:N	2.19	0.57
1:A:360:LEU:O	1:A:361:LEU:C	2.46	0.57
1:B:239:ILE:HA	1:B:242:PHE:HB2	1.87	0.57
1:A:14:ASN:HD22	1:A:14:ASN:N	2.03	0.56
1:A:63:LEU:CG	1:A:64:PHE:N	2.67	0.56
1:A:72:LEU:HD13	1:A:75:VAL:HG21	1.86	0.56
1:B:299:SER:CB	1:B:380:SER:HA	2.35	0.56
1:A:88:ILE:N	1:A:89:PRO:CD	2.68	0.56
1:A:123:GLU:C	1:A:124:GLU:O	2.47	0.56
1:A:292:MET:HA	1:A:375:VAL:HG11	1.86	0.56
1:A:418:GLN:HE22	1:A:421:GLY:HA2	1.69	0.56
1:B:83:GLY:O	1:B:85:GLN:N	2.37	0.56
1:B:136:ALA:HA	1:B:139:PHE:HD2	1.70	0.56
1:B:332:THR:HA	1:B:335:LEU:HG	1.87	0.56
1:B:426:TRP:HA	1:B:426:TRP:CE3	2.40	0.56
1:A:68:LEU:HD12	1:A:248:VAL:HB	1.87	0.56
1:A:110:LEU:HD13	1:A:114:GLN:HG3	1.86	0.56
1:A:237:GLU:O	1:A:240:ARG:HB3	2.05	0.56
1:A:247:PRO:HB3	1:A:389:ALA:HA	1.88	0.56
1:A:311:THR:C	1:A:312:LYS:HZ3	2.13	0.56
1:A:353:VAL:O	1:A:353:VAL:CG1	2.51	0.56
1:A:398:TYR:CD1	1:A:399:TRP:N	2.73	0.56
1:B:21:PRO:CA	1:B:164:MET:HE1	2.34	0.56
1:B:81:GLY:HA3	1:B:307:GLY:O	2.04	0.56
1:B:118:ARG:HH21	1:B:119:PHE:CB	2.17	0.56
1:B:146:LEU:O	1:B:149:ALA:CB	2.52	0.56
1:B:159:LEU:O	1:B:161:LYS:N	2.38	0.56
1:B:181:PHE:O	1:B:190:GLU:HG2	2.05	0.56
1:B:248:VAL:HG12	1:B:391:PHE:CZ	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:LEU:C	1:B:335:LEU:HD12	2.30	0.56
1:B:391:PHE:CD2	1:B:392:HIS:N	2.60	0.56
1:B:427:LEU:O	1:B:430:ILE:N	2.38	0.56
1:A:237:GLU:O	1:A:241:LEU:HD12	2.05	0.56
1:A:261:VAL:HG12	1:A:262:VAL:N	2.20	0.56
1:A:367:TYR:N	1:A:430:ILE:HD11	2.20	0.56
1:A:390:ILE:O	1:A:390:ILE:CG2	2.53	0.56
1:A:407:TYR:CD2	1:A:411:MET:HG3	2.41	0.56
1:B:15:LEU:O	1:B:19:ALA:N	2.32	0.56
1:B:104:VAL:C	1:B:106:ILE:H	2.13	0.56
1:B:199:ALA:O	1:B:203:VAL:HG23	2.06	0.56
1:B:235:PRO:HA	1:B:238:LEU:HD22	1.86	0.56
1:A:73:VAL:CB	1:A:74:PRO:CD	2.79	0.56
1:A:144:TYR:CD1	1:A:144:TYR:C	2.83	0.56
1:B:74:PRO:CG	1:B:149:ALA:CB	2.84	0.56
1:B:78:GLN:HG3	1:B:79:LEU:HD12	1.86	0.56
1:B:160:THR:HG23	1:B:160:THR:O	2.05	0.56
1:B:382:ARG:HA	1:B:387:MET:HG2	1.86	0.56
1:B:384:TYR:HE1	1:B:446:TRP:HH2	1.52	0.56
1:A:88:ILE:HG13	1:A:89:PRO:N	2.20	0.56
1:A:127:ALA:O	1:A:128:THR:C	2.48	0.56
1:B:79:LEU:O	1:B:84:ARG:O	2.24	0.56
1:B:178:ASN:O	1:B:181:PHE:N	2.39	0.56
1:B:209:LEU:O	1:B:213:PHE:HB2	2.05	0.56
1:B:394:THR:HG23	1:B:439:MET:HB3	1.87	0.56
1:B:400:VAL:O	1:B:404:PRO:HD2	2.06	0.56
1:A:70:MET:HE2	1:A:99:ALA:CB	2.35	0.56
1:A:175:ILE:HG22	1:A:176:PRO:N	2.19	0.56
1:B:63:LEU:CD2	1:B:64:PHE:N	2.69	0.56
1:B:97:ILE:CG2	1:B:101:LEU:HD11	2.29	0.56
1:B:114:GLN:NE2	1:B:135:HIS:CE1	2.74	0.56
1:B:145:LEU:HD13	1:B:146:LEU:CA	2.35	0.56
1:B:150:LEU:O	1:B:154:THR:HB	2.06	0.56
1:B:320:VAL:O	1:B:322:LEU:N	2.39	0.56
1:B:348:THR:C	1:B:349:GLU:HG3	2.30	0.56
1:B:398:TYR:HD2	1:B:432:GLY:C	2.12	0.56
1:A:13:SER:O	1:A:16:ILE:CG2	2.53	0.56
1:A:77:ALA:HB2	1:A:154:THR:HG23	1.87	0.56
1:A:220:ARG:HG3	1:A:221:LEU:CD1	2.35	0.56
1:A:222:ALA:O	1:A:223:HIS:C	2.49	0.56
1:A:423:LYS:CG	1:A:424:GLY:N	2.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:LEU:HD13	1:B:75:VAL:HG21	1.86	0.56
1:B:257:THR:O	1:B:261:VAL:HG23	2.06	0.56
1:B:414:TRP:N	1:B:414:TRP:CE3	2.74	0.56
1:B:457:HIS:HA	1:B:460:ALA:HB3	1.86	0.56
1:A:141:VAL:CG2	1:A:204:TYR:HB3	2.36	0.56
1:A:382:ARG:CD	1:A:382:ARG:N	2.69	0.56
1:B:130:THR:C	1:B:132:GLY:N	2.61	0.56
1:B:219:LYS:HD3	1:B:220:ARG:HE	1.71	0.56
1:B:275:ALA:HA	1:B:353:VAL:HG21	1.87	0.56
1:B:350:ASN:ND2	1:B:352:VAL:H	2.04	0.56
1:B:387:MET:O	1:B:391:PHE:N	2.39	0.56
1:A:165:VAL:HG13	1:A:210:LEU:HG	1.87	0.56
1:A:356:LEU:O	1:A:360:LEU:N	2.27	0.56
1:A:400:VAL:O	1:A:404:PRO:HD2	2.06	0.56
1:B:97:ILE:O	1:B:98:LEU:C	2.48	0.56
1:B:151:ARG:O	1:B:153:PHE:N	2.39	0.56
1:B:166:ILE:O	1:B:170:GLY:HA3	2.06	0.56
1:B:222:ALA:O	1:B:223:HIS:C	2.49	0.56
1:A:240:ARG:C	1:A:242:PHE:N	2.63	0.55
1:A:250:ALA:HA	1:A:254:PHE:HB2	1.88	0.55
1:B:3:ASN:C	1:B:5:VAL:H	2.14	0.55
1:A:30:THR:O	1:A:31:GLY:C	2.49	0.55
1:A:98:LEU:HA	1:A:101:LEU:CG	2.36	0.55
1:A:117:ILE:CG2	1:A:118:ARG:N	2.58	0.55
1:A:166:ILE:O	1:A:170:GLY:N	2.38	0.55
1:B:27:VAL:O	1:B:31:GLY:HA3	2.06	0.55
1:B:138:ILE:HA	1:B:141:VAL:CG2	2.36	0.55
1:B:208:LEU:CD2	1:B:209:LEU:N	2.63	0.55
1:A:151:ARG:HG3	1:A:152:SER:H	1.70	0.55
1:A:213:PHE:O	1:A:215:ILE:N	2.40	0.55
1:A:262:VAL:O	1:A:266:VAL:HG23	2.05	0.55
1:B:287:VAL:O	1:B:290:PHE:HB2	2.05	0.55
1:B:382:ARG:N	1:B:382:ARG:HD3	2.22	0.55
1:A:70:MET:CE	1:A:99:ALA:HB2	2.34	0.55
1:A:100:LEU:N	1:A:100:LEU:HD12	2.22	0.55
1:A:122:VAL:O	1:A:124:GLU:OE1	2.23	0.55
1:A:211:LEU:CG	1:A:212:LEU:N	2.67	0.55
1:A:233:PRO:O	1:A:236:LYS:HB3	2.06	0.55
1:A:238:LEU:HG	1:A:241:LEU:HD22	1.88	0.55
1:A:286:LEU:O	1:A:289:MET:HB3	2.05	0.55
1:A:348:THR:C	1:A:349:GLU:HG3	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:ASN:HB3	1:A:414:TRP:CZ3	2.40	0.55
1:B:137:VAL:HG21	1:B:201:ALA:HB2	1.87	0.55
1:B:144:TYR:O	1:B:147:PHE:N	2.39	0.55
1:B:144:TYR:CG	1:B:207:MET:HB3	2.41	0.55
1:B:145:LEU:HA	1:B:148:GLN:HE21	1.70	0.55
1:A:409:LEU:HD12	1:A:424:GLY:C	2.31	0.55
1:B:129:LYS:HA	1:B:132:GLY:HA3	1.88	0.55
1:B:213:PHE:O	1:B:215:ILE:N	2.39	0.55
1:B:218:SER:O	1:B:220:ARG:N	2.40	0.55
1:B:220:ARG:HG3	1:B:221:LEU:HD12	1.88	0.55
1:B:242:PHE:O	1:B:244:LEU:N	2.35	0.55
1:A:134:MET:SD	1:A:198:VAL:HA	2.46	0.55
1:A:146:LEU:O	1:A:149:ALA:CB	2.52	0.55
1:A:165:VAL:CG1	1:A:166:ILE:N	2.42	0.55
1:A:398:TYR:HD2	1:A:432:GLY:C	2.15	0.55
1:B:127:ALA:O	1:B:128:THR:C	2.50	0.55
1:B:180:ILE:HG23	1:B:181:PHE:HD1	1.71	0.55
1:A:28:ALA:O	1:A:29:GLN:C	2.50	0.55
1:A:81:GLY:HA3	1:A:307:GLY:C	2.30	0.55
1:A:97:ILE:O	1:A:101:LEU:HG	2.07	0.55
1:A:134:MET:O	1:A:137:VAL:HB	2.06	0.55
1:A:324:THR:O	1:A:327:ALA:HB3	2.06	0.55
1:B:72:LEU:HD13	1:B:75:VAL:CG2	2.36	0.55
1:B:166:ILE:HB	1:B:210:LEU:HD21	1.89	0.55
1:B:258:LEU:O	1:B:261:VAL:HB	2.06	0.55
1:A:83:GLY:O	1:A:85:GLN:N	2.40	0.55
1:A:84:ARG:HG2	1:B:309:GLN:HG2	1.89	0.55
1:B:13:SER:O	1:B:16:ILE:CG2	2.55	0.55
1:B:240:ARG:C	1:B:242:PHE:N	2.64	0.55
1:B:410:GLY:CA	1:B:425:PHE:HB2	2.37	0.55
1:A:159:LEU:O	1:A:161:LYS:N	2.40	0.55
1:A:197:GLY:O	1:A:200:THR:HB	2.06	0.55
1:A:207:MET:HA	1:A:210:LEU:CD2	2.37	0.55
1:B:120:MET:O	1:B:120:MET:HG2	2.06	0.55
1:B:122:VAL:O	1:B:124:GLU:OE1	2.25	0.55
1:B:162:PRO:HA	1:B:165:VAL:HB	1.87	0.55
1:B:299:SER:OG	1:B:380:SER:HA	2.07	0.55
1:B:443:ARG:O	1:B:444:LEU:C	2.50	0.55
1:A:114:GLN:NE2	1:A:135:HIS:CE1	2.75	0.55
1:A:344:ALA:O	1:A:345:LEU:C	2.49	0.55
1:A:382:ARG:NH2	1:A:445:TYR:N	2.47	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:GLY:O	1:B:47:ASP:HA	2.07	0.55
1:B:81:GLY:HA3	1:B:307:GLY:C	2.33	0.55
1:B:283:PHE:O	1:B:284:SER:C	2.49	0.55
1:A:45:ALA:HB1	1:A:126:MET:HE1	1.88	0.54
1:A:78:GLN:HG3	1:A:79:LEU:HD12	1.88	0.54
1:A:178:ASN:ND2	1:A:199:ALA:CB	2.71	0.54
1:A:275:ALA:HB1	1:A:353:VAL:HG11	1.89	0.54
1:A:302:VAL:HG23	1:A:317:ALA:HB3	1.88	0.54
1:B:203:VAL:O	1:B:207:MET:HG3	2.07	0.54
1:A:276:ALA:CA	1:A:426:TRP:NE1	2.70	0.54
1:A:394:THR:HG21	1:A:440:LEU:HD13	1.89	0.54
1:B:73:VAL:O	1:B:76:VAL:CB	2.54	0.54
1:B:367:TYR:HE2	1:B:429:PHE:CD1	2.24	0.54
1:A:137:VAL:HG21	1:A:201:ALA:HB2	1.90	0.54
1:A:199:ALA:O	1:A:203:VAL:HG23	2.08	0.54
1:A:244:LEU:HG	1:A:385:LYS:CE	2.38	0.54
1:B:93:HIS:HE1	1:B:225:LYS:HB3	1.65	0.54
1:B:120:MET:O	1:B:121:ASP:C	2.51	0.54
1:B:217:THR:O	1:B:218:SER:C	2.48	0.54
1:B:275:ALA:HB1	1:B:353:VAL:HG11	1.88	0.54
1:A:86:HIS:CG	1:A:87:LYS:H	2.25	0.54
1:A:137:VAL:HG13	1:A:201:ALA:HA	1.89	0.54
1:A:209:LEU:O	1:A:213:PHE:HB2	2.08	0.54
1:A:328:THR:O	1:A:332:THR:OG1	2.21	0.54
1:B:68:LEU:HD12	1:B:248:VAL:HB	1.89	0.54
1:B:176:PRO:O	1:B:180:ILE:HG22	2.07	0.54
1:B:367:TYR:N	1:B:430:ILE:HD11	2.23	0.54
1:A:21:PRO:CA	1:A:164:MET:HE1	2.37	0.54
1:A:72:LEU:HB3	1:A:244:LEU:HD13	1.88	0.54
1:A:155:ASP:O	1:A:157:MET:N	2.40	0.54
1:A:350:ASN:OD1	1:A:352:VAL:HB	2.08	0.54
1:A:418:GLN:CD	1:A:421:GLY:HA2	2.32	0.54
1:A:44:SER:C	1:A:46:ILE:N	2.66	0.54
1:A:398:TYR:CB	1:A:436:ALA:CB	2.68	0.54
1:A:455:GLN:C	1:A:455:GLN:NE2	2.66	0.54
1:B:78:GLN:HG3	1:B:79:LEU:CD1	2.38	0.54
1:B:113:THR:HA	1:B:116:ILE:CG2	2.38	0.54
1:B:191:LEU:HG	1:B:192:GLY:N	2.22	0.54
1:A:104:VAL:HA	1:A:107:ILE:CG1	2.37	0.54
1:A:151:ARG:O	1:A:153:PHE:N	2.41	0.54
1:A:345:LEU:O	1:A:347:TYR:O	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:VAL:CG1	1:B:407:TYR:CE2	2.89	0.54
1:A:56:SER:O	1:A:60:PRO:HD2	2.07	0.54
1:A:142:PRO:C	1:A:145:LEU:HB3	2.32	0.54
1:A:181:PHE:CD2	1:A:198:VAL:HG11	2.43	0.54
1:A:422:ALA:O	1:A:423:LYS:C	2.51	0.54
1:A:455:GLN:C	1:A:455:GLN:HE21	2.16	0.54
1:B:44:SER:C	1:B:46:ILE:N	2.61	0.54
1:B:206:ILE:O	1:B:209:LEU:CB	2.52	0.54
1:B:226:VAL:CG1	1:B:227:PHE:N	2.68	0.54
1:B:237:GLU:O	1:B:241:LEU:N	2.41	0.54
1:B:250:ALA:O	1:B:254:PHE:N	2.40	0.54
1:A:231:HIS:C	1:A:235:PRO:CG	2.77	0.54
1:A:235:PRO:HA	1:A:238:LEU:CG	2.37	0.54
1:A:339:PHE:C	1:A:341:GLU:OE1	2.51	0.54
1:A:345:LEU:O	1:A:347:TYR:N	2.41	0.54
1:B:273:VAL:O	1:B:277:HIS:CB	2.56	0.54
1:B:420:LEU:O	1:B:423:LYS:HG2	2.08	0.54
1:A:72:LEU:HD13	1:A:75:VAL:CG2	2.37	0.54
1:A:140:ALA:HB1	1:A:204:TYR:CE2	2.43	0.54
1:A:178:ASN:O	1:A:181:PHE:N	2.40	0.54
1:A:266:VAL:HG13	1:A:269:LEU:HD21	1.90	0.54
1:A:406:GLY:CA	1:A:428:GLY:HA3	2.38	0.54
1:A:410:GLY:HA2	1:A:421:GLY:O	2.08	0.54
1:A:426:TRP:HA	1:A:426:TRP:HE3	1.73	0.54
1:A:455:GLN:HA	1:A:458:LEU:HB2	1.90	0.54
1:B:11:GLU:OE2	1:B:320:VAL:HB	2.08	0.54
1:B:28:ALA:O	1:B:29:GLN:C	2.50	0.54
1:B:60:PRO:HA	1:B:63:LEU:HB3	1.90	0.54
1:B:137:VAL:HG13	1:B:201:ALA:HA	1.88	0.54
1:B:220:ARG:HG3	1:B:221:LEU:CD1	2.38	0.54
1:B:328:THR:O	1:B:332:THR:OG1	2.22	0.54
1:B:418:GLN:HE22	1:B:421:GLY:HA2	1.71	0.54
1:B:436:ALA:HA	1:B:439:MET:CG	2.38	0.54
1:A:73:VAL:HG13	1:A:241:LEU:HG	1.90	0.53
1:A:142:PRO:O	1:A:145:LEU:CD1	2.56	0.53
1:A:191:LEU:HG	1:A:192:GLY:H	1.73	0.53
1:B:8:TYR:O	1:B:12:ALA:CB	2.56	0.53
1:B:100:LEU:CD1	1:B:100:LEU:H	2.20	0.53
1:B:197:GLY:O	1:B:200:THR:HB	2.08	0.53
1:B:301:ARG:O	1:B:301:ARG:HD3	2.08	0.53
1:B:423:LYS:CG	1:B:424:GLY:N	2.69	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:GLU:OE1	1:A:124:GLU:C	2.50	0.53
1:A:218:SER:O	1:A:220:ARG:N	2.41	0.53
1:A:339:PHE:O	1:A:340:ARG:C	2.52	0.53
1:A:454:VAL:O	1:A:458:LEU:HD13	2.08	0.53
1:B:116:ILE:O	1:B:117:ILE:C	2.49	0.53
1:B:178:ASN:O	1:B:179:TRP:C	2.50	0.53
1:B:180:ILE:HG23	1:B:181:PHE:CD1	2.43	0.53
1:B:369:CYS:O	1:B:372:ALA:HB3	2.08	0.53
1:B:392:HIS:O	1:B:395:PHE:HB2	2.08	0.53
1:A:4:SER:HA	1:A:7:ARG:HB2	1.91	0.53
1:A:35:VAL:HG12	1:A:36:ASP:N	2.23	0.53
1:A:277:HIS:HD2	1:A:278:GLN:OE1	1.91	0.53
1:B:18:LEU:O	1:B:22:VAL:HG13	2.08	0.53
1:B:47:ASP:C	1:B:49:ALA:H	2.14	0.53
1:B:146:LEU:O	1:B:147:PHE:C	2.50	0.53
1:B:191:LEU:O	1:B:195:GLY:N	2.42	0.53
1:B:236:LYS:HG3	1:B:239:ILE:HD12	1.90	0.53
1:B:340:ARG:HB2	1:B:361:LEU:CD1	2.38	0.53
1:B:454:VAL:O	1:B:458:LEU:HD13	2.07	0.53
1:A:107:ILE:O	1:A:110:LEU:HB3	2.07	0.53
1:A:144:TYR:O	1:A:145:LEU:C	2.50	0.53
1:A:318:ALA:HA	1:A:381:LEU:HD11	1.90	0.53
1:A:407:TYR:C	1:A:409:LEU:N	2.66	0.53
1:B:22:VAL:HG23	1:B:293:SER:HB3	1.89	0.53
1:B:148:GLN:HA	1:B:152:SER:HB2	1.89	0.53
1:A:72:LEU:CA	1:A:75:VAL:HG13	2.34	0.53
1:A:136:ALA:HA	1:A:139:PHE:HD2	1.74	0.53
1:A:181:PHE:CG	1:A:198:VAL:HG11	2.43	0.53
1:A:272:THR:O	1:A:274:VAL:C	2.50	0.53
1:A:340:ARG:HG3	1:A:341:GLU:H	1.72	0.53
1:A:432:GLY:O	1:A:435:ALA:HB3	2.08	0.53
1:B:234:GLN:O	1:B:238:LEU:HD13	2.08	0.53
1:B:314:ALA:C	1:B:318:ALA:HB3	2.33	0.53
1:B:353:VAL:C	1:B:357:ALA:CB	2.82	0.53
1:B:382:ARG:NH2	1:B:445:TYR:N	2.49	0.53
1:B:72:LEU:CA	1:B:75:VAL:HG13	2.36	0.53
1:B:409:LEU:HD12	1:B:424:GLY:C	2.32	0.53
1:A:68:LEU:O	1:A:71:ALA:HB3	2.09	0.53
1:A:84:ARG:C	1:A:86:HIS:N	2.64	0.53
1:A:123:GLU:O	1:A:123:GLU:HG2	2.07	0.53
1:A:279:VAL:HG12	1:A:280:ALA:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:HIS:O	1:B:97:ILE:HG13	2.08	0.53
1:B:238:LEU:O	1:B:242:PHE:HD1	1.91	0.53
1:A:146:LEU:O	1:A:147:PHE:C	2.51	0.53
1:A:244:LEU:HG	1:A:385:LYS:HE2	1.91	0.53
1:A:335:LEU:C	1:A:335:LEU:HD12	2.34	0.53
1:A:367:TYR:HE2	1:A:429:PHE:CE1	2.27	0.53
1:A:382:ARG:HA	1:A:387:MET:HG2	1.91	0.53
1:A:411:MET:HA	1:A:414:TRP:CD2	2.43	0.53
1:B:94:GLN:OE1	1:B:238:LEU:HD21	2.09	0.53
1:B:139:PHE:C	1:B:142:PRO:HD2	2.33	0.53
1:B:144:TYR:CD1	1:B:144:TYR:C	2.85	0.53
1:B:238:LEU:O	1:B:242:PHE:N	2.41	0.53
1:B:344:ALA:O	1:B:345:LEU:C	2.50	0.53
1:A:7:ARG:HH11	1:A:7:ARG:CB	2.21	0.53
1:A:276:ALA:O	1:A:277:HIS:C	2.51	0.53
1:A:433:LEU:O	1:A:437:ALA:CB	2.55	0.53
1:B:35:VAL:HG12	1:B:36:ASP:N	2.23	0.53
1:B:182:VAL:HG22	1:B:195:GLY:CA	2.37	0.53
1:B:200:THR:CA	1:B:203:VAL:HG23	2.38	0.53
1:A:239:ILE:CA	1:A:242:PHE:HB2	2.39	0.53
1:A:266:VAL:CG1	1:A:407:TYR:CE2	2.90	0.53
1:A:284:SER:O	1:A:285:SER:C	2.52	0.53
1:A:345:LEU:O	1:A:346:LEU:C	2.51	0.53
1:A:447:LEU:HD12	1:A:448:GLN:N	2.23	0.53
1:B:96:LEU:HD23	1:B:96:LEU:C	2.34	0.53
1:A:165:VAL:C	1:A:167:GLY:H	2.17	0.52
1:A:267:ALA:H	1:A:268:PRO:HD3	1.72	0.52
1:A:387:MET:CE	1:A:456:LEU:HD13	2.39	0.52
1:A:436:ALA:O	1:A:439:MET:N	2.43	0.52
1:B:12:ALA:O	1:B:13:SER:C	2.52	0.52
1:B:218:SER:C	1:B:220:ARG:H	2.16	0.52
1:B:326:LEU:HD13	1:B:330:CYS:HB2	1.92	0.52
1:B:411:MET:HA	1:B:414:TRP:CD2	2.45	0.52
1:B:413:ASN:HB2	1:B:418:GLN:CG	2.39	0.52
1:B:433:LEU:O	1:B:437:ALA:CB	2.56	0.52
1:A:18:LEU:O	1:A:21:PRO:HD2	2.09	0.52
1:A:447:LEU:HD21	1:A:450:GLN:CG	2.39	0.52
1:B:72:LEU:HA	1:B:75:VAL:CG1	2.36	0.52
1:B:353:VAL:CB	1:B:357:ALA:HB2	2.39	0.52
1:A:101:LEU:O	1:A:105:PRO:HG2	2.09	0.52
1:A:274:VAL:O	1:A:278:GLN:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:LEU:O	1:A:404:PRO:C	2.48	0.52
1:B:45:ALA:HB1	1:B:126:MET:CE	2.39	0.52
1:B:113:THR:O	1:B:116:ILE:HG22	2.09	0.52
1:B:398:TYR:CB	1:B:436:ALA:CB	2.72	0.52
1:A:234:GLN:O	1:A:237:GLU:HB3	2.09	0.52
1:A:320:VAL:O	1:A:322:LEU:N	2.42	0.52
1:A:382:ARG:O	1:A:387:MET:HB2	2.09	0.52
1:B:101:LEU:O	1:B:105:PRO:HG2	2.09	0.52
1:B:155:ASP:O	1:B:157:MET:N	2.42	0.52
1:B:161:LYS:C	1:B:163:ALA:H	2.17	0.52
1:B:409:LEU:O	1:B:410:GLY:C	2.49	0.52
1:B:430:ILE:CG2	1:B:431:ILE:N	2.72	0.52
1:A:60:PRO:O	1:A:61:SER:C	2.52	0.52
1:A:68:LEU:HD22	1:A:71:ALA:CB	2.40	0.52
1:A:127:ALA:O	1:A:131:VAL:HG22	2.09	0.52
1:B:141:VAL:CG2	1:B:204:TYR:HB3	2.39	0.52
1:B:154:THR:O	1:B:158:SER:CA	2.54	0.52
1:B:165:VAL:HG13	1:B:210:LEU:HG	1.91	0.52
1:B:165:VAL:C	1:B:167:GLY:H	2.17	0.52
1:B:298:VAL:HA	1:B:301:ARG:HB3	1.91	0.52
1:B:390:ILE:O	1:B:390:ILE:CG2	2.57	0.52
1:A:26:SER:HB2	1:A:289:MET:CG	2.39	0.52
1:A:32:MET:CG	1:A:33:GLY:N	2.72	0.52
1:A:236:LYS:HG3	1:A:239:ILE:HD12	1.92	0.52
1:A:376:VAL:HG13	1:A:377:ALA:N	2.17	0.52
1:A:394:THR:HG23	1:A:439:MET:CB	2.39	0.52
1:A:430:ILE:CG2	1:A:431:ILE:N	2.72	0.52
1:B:152:SER:O	1:B:155:ASP:OD1	2.28	0.52
1:A:21:PRO:CB	1:A:160:THR:HG23	2.40	0.52
1:A:145:LEU:HD13	1:A:146:LEU:CA	2.39	0.52
1:A:238:LEU:O	1:A:242:PHE:N	2.43	0.52
1:B:11:GLU:HG2	1:B:316:ILE:HG22	1.90	0.52
1:B:185:LYS:C	1:B:185:LYS:CD	2.82	0.52
1:B:248:VAL:HG23	1:B:249:ALA:H	1.75	0.52
1:B:267:ALA:H	1:B:268:PRO:HD3	1.72	0.52
1:B:332:THR:HA	1:B:335:LEU:CG	2.39	0.52
1:B:351:GLN:O	1:B:354:VAL:HG23	2.08	0.52
1:B:379:GLY:HA2	1:B:391:PHE:CE1	2.45	0.52
1:A:86:HIS:O	1:A:87:LYS:CB	2.57	0.52
1:A:104:VAL:C	1:A:106:ILE:H	2.18	0.52
1:A:212:LEU:O	1:A:215:ILE:HG22	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:LEU:HB3	1:A:423:LYS:CD	2.40	0.52
1:B:142:PRO:O	1:B:145:LEU:HD12	2.09	0.52
1:B:165:VAL:C	1:B:167:GLY:N	2.67	0.52
1:B:345:LEU:O	1:B:346:LEU:C	2.53	0.52
1:B:445:TYR:O	1:B:446:TRP:C	2.53	0.52
1:A:96:LEU:HD23	1:A:96:LEU:C	2.34	0.52
1:A:113:THR:O	1:A:116:ILE:HG22	2.10	0.52
1:A:145:LEU:HA	1:A:148:GLN:HE21	1.75	0.52
1:A:159:LEU:HD21	1:A:220:ARG:HH11	1.75	0.52
1:A:226:VAL:HG12	1:A:227:PHE:H	1.71	0.52
1:A:394:THR:HG21	1:A:440:LEU:HD22	1.91	0.52
1:A:451:SER:HA	1:A:453:ASP:OD1	2.09	0.52
1:B:11:GLU:HB3	1:B:320:VAL:CB	2.40	0.52
1:B:42:GLY:CA	1:B:49:ALA:HB3	2.40	0.52
1:B:100:LEU:C	1:B:102:VAL:N	2.66	0.52
1:B:161:LYS:N	1:B:162:PRO:CD	2.68	0.52
1:B:298:VAL:HG21	1:B:321:GLY:CA	2.40	0.52
1:B:332:THR:C	1:B:335:LEU:HG	2.34	0.52
1:B:339:PHE:HB3	1:B:343:ILE:HG12	1.91	0.52
1:B:382:ARG:HH21	1:B:443:ARG:C	2.17	0.52
1:B:387:MET:CE	1:B:456:LEU:HD13	2.40	0.52
1:B:413:ASN:C	1:B:415:LEU:H	2.18	0.52
1:A:62:ILE:CG1	1:A:63:LEU:N	2.63	0.52
1:A:69:LEU:HB2	1:A:249:ALA:HB2	1.92	0.52
1:A:72:LEU:HD22	1:A:75:VAL:HG11	1.92	0.52
1:A:182:VAL:HG22	1:A:195:GLY:CA	2.40	0.52
1:A:340:ARG:HB2	1:A:361:LEU:HD13	1.91	0.52
1:A:367:TYR:HA	1:A:430:ILE:CG1	2.40	0.52
1:B:75:VAL:C	1:B:77:ALA:N	2.58	0.52
1:B:104:VAL:C	1:B:106:ILE:N	2.65	0.52
1:B:191:LEU:HG	1:B:192:GLY:H	1.75	0.52
1:B:431:ILE:O	1:B:435:ALA:HB2	2.09	0.52
1:A:78:GLN:C	1:A:80:ASN:H	2.18	0.51
1:A:166:ILE:HB	1:A:210:LEU:CG	2.40	0.51
1:A:166:ILE:HB	1:A:210:LEU:HG	1.90	0.51
1:A:181:PHE:O	1:A:190:GLU:HG2	2.09	0.51
1:A:436:ALA:HA	1:A:439:MET:CG	2.40	0.51
1:B:237:GLU:O	1:B:240:ARG:HB3	2.10	0.51
1:B:367:TYR:HE2	1:B:429:PHE:CE1	2.28	0.51
1:B:385:LYS:N	1:B:387:MET:SD	2.83	0.51
1:B:445:TYR:O	1:B:448:GLN:O	2.27	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:VAL:O	1:A:54:ALA:HB3	2.10	0.51
1:A:181:PHE:C	1:A:183:TYR:N	2.66	0.51
1:A:206:ILE:CG1	1:A:207:MET:N	2.72	0.51
1:A:3:ASN:C	1:A:5:VAL:H	2.18	0.51
1:A:15:LEU:CD1	1:A:16:ILE:N	2.66	0.51
1:A:53:ILE:HD12	1:A:54:ALA:N	2.25	0.51
1:A:211:LEU:O	1:A:212:LEU:C	2.52	0.51
1:A:218:SER:C	1:A:220:ARG:H	2.19	0.51
1:A:316:ILE:O	1:A:317:ALA:C	2.53	0.51
1:B:234:GLN:O	1:B:237:GLU:HB3	2.09	0.51
1:B:250:ALA:O	1:B:254:PHE:CB	2.59	0.51
1:B:258:LEU:HD22	1:B:399:TRP:CZ2	2.45	0.51
1:B:314:ALA:O	1:B:318:ALA:N	2.42	0.51
1:A:316:ILE:O	1:A:318:ALA:N	2.44	0.51
1:A:392:HIS:O	1:A:395:PHE:HB2	2.09	0.51
1:B:145:LEU:HD13	1:B:145:LEU:C	2.35	0.51
1:B:290:PHE:CB	1:B:291:PRO:CD	2.88	0.51
1:B:420:LEU:CB	1:B:423:LYS:HG2	2.34	0.51
1:A:131:VAL:CA	1:A:134:MET:HB2	2.41	0.51
1:A:155:ASP:CG	1:A:159:LEU:H	2.17	0.51
1:A:382:ARG:C	1:A:384:TYR:N	2.67	0.51
1:A:408:ILE:O	1:A:412:THR:N	2.44	0.51
1:B:212:LEU:O	1:B:215:ILE:HG22	2.10	0.51
1:B:386:ASP:O	1:B:389:ALA:N	2.43	0.51
1:A:104:VAL:C	1:A:106:ILE:N	2.68	0.51
1:A:242:PHE:O	1:A:244:LEU:N	2.42	0.51
1:A:273:VAL:CG1	1:A:274:VAL:H	2.23	0.51
1:A:353:VAL:CB	1:A:357:ALA:HB2	2.40	0.51
1:B:32:MET:CG	1:B:33:GLY:H	2.23	0.51
1:B:77:ALA:HB2	1:B:154:THR:CG2	2.41	0.51
1:B:96:LEU:CB	1:B:146:LEU:HG	2.40	0.51
1:B:173:LEU:O	1:B:174:ASN:C	2.53	0.51
1:B:268:PRO:C	1:B:270:GLY:H	2.19	0.51
1:B:360:LEU:O	1:B:361:LEU:C	2.53	0.51
1:A:84:ARG:CG	1:B:309:GLN:HG2	2.41	0.51
1:A:135:HIS:C	1:A:137:VAL:N	2.67	0.51
1:A:209:LEU:HD12	1:A:210:LEU:HD13	1.92	0.51
1:A:226:VAL:CG1	1:A:227:PHE:N	2.66	0.51
1:A:301:ARG:NH2	1:A:316:ILE:HG22	2.26	0.51
1:A:332:THR:HA	1:A:335:LEU:HD21	1.91	0.51
1:A:385:LYS:HB3	1:A:387:MET:HE1	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:THR:O	1:B:31:GLY:C	2.53	0.51
1:B:332:THR:HA	1:B:335:LEU:HD21	1.90	0.51
1:B:393:ARG:HH11	1:B:393:ARG:CG	2.23	0.51
1:A:74:PRO:O	1:A:154:THR:OG1	2.29	0.51
1:A:146:LEU:O	1:A:146:LEU:HD22	2.10	0.51
1:A:166:ILE:O	1:A:170:GLY:CA	2.58	0.51
1:A:274:VAL:HG12	1:A:275:ALA:N	2.26	0.51
1:A:353:VAL:HB	1:A:357:ALA:HB2	1.93	0.51
1:A:371:ASP:O	1:A:375:VAL:HG23	2.10	0.51
1:A:433:LEU:N	1:A:433:LEU:HD12	2.26	0.51
1:B:353:VAL:HB	1:B:357:ALA:HB2	1.93	0.51
1:B:413:ASN:C	1:B:415:LEU:N	2.68	0.51
1:B:98:LEU:HA	1:B:101:LEU:CG	2.41	0.51
1:B:313:GLY:O	1:B:317:ALA:N	2.44	0.51
1:B:363:PHE:CD1	1:B:364:ALA:N	2.79	0.51
1:B:409:LEU:C	1:B:409:LEU:HD13	2.36	0.51
1:B:436:ALA:O	1:B:439:MET:HB2	2.10	0.51
1:A:100:LEU:C	1:A:102:VAL:H	2.18	0.51
1:A:142:PRO:O	1:A:145:LEU:CB	2.55	0.51
1:A:145:LEU:O	1:A:148:GLN:HB3	2.11	0.51
1:A:173:LEU:O	1:A:174:ASN:C	2.52	0.51
1:A:260:ALA:O	1:A:261:VAL:C	2.54	0.51
1:A:290:PHE:CB	1:A:291:PRO:CD	2.89	0.51
1:B:146:LEU:O	1:B:149:ALA:N	2.44	0.51
1:B:455:GLN:HE21	1:B:455:GLN:C	2.18	0.51
1:A:73:VAL:O	1:A:76:VAL:CG1	2.59	0.50
1:A:76:VAL:HG23	1:A:78:GLN:HE21	1.76	0.50
1:A:154:THR:O	1:A:158:SER:CA	2.56	0.50
1:A:176:PRO:O	1:A:180:ILE:HG22	2.09	0.50
1:A:238:LEU:O	1:A:242:PHE:HD1	1.93	0.50
1:A:244:LEU:CD2	1:A:385:LYS:O	2.49	0.50
1:A:301:ARG:C	1:A:301:ARG:CD	2.84	0.50
1:B:14:ASN:HD22	1:B:14:ASN:H	1.57	0.50
1:B:62:ILE:CG1	1:B:63:LEU:N	2.63	0.50
1:B:142:PRO:CA	1:B:145:LEU:HB3	2.39	0.50
1:A:73:VAL:O	1:A:76:VAL:HG12	2.11	0.50
1:A:255:GLU:HG2	1:A:256:VAL:N	2.27	0.50
1:A:410:GLY:HA3	1:A:425:PHE:CB	2.41	0.50
1:B:76:VAL:C	1:B:78:GLN:HG2	2.36	0.50
1:B:88:ILE:CG1	1:B:89:PRO:CD	2.88	0.50
1:B:386:ASP:O	1:B:389:ALA:HB3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:PRO:HA	1:A:165:VAL:HB	1.92	0.50
1:A:339:PHE:HB3	1:A:343:ILE:HG13	1.94	0.50
1:A:341:GLU:CD	1:A:342:GLN:N	2.65	0.50
1:A:385:LYS:HD3	1:A:386:ASP:N	2.26	0.50
1:B:19:ALA:O	1:B:20:THR:C	2.55	0.50
1:B:69:LEU:HG	1:B:245:GLY:CA	2.40	0.50
1:B:76:VAL:CA	1:B:78:GLN:HE21	2.11	0.50
1:B:282:ASN:O	1:B:285:SER:HB3	2.11	0.50
1:B:312:LYS:HA	1:B:312:LYS:HZ2	1.74	0.50
1:B:398:TYR:HE2	1:B:433:LEU:HG	1.77	0.50
1:A:387:MET:O	1:A:391:PHE:HB3	2.12	0.50
1:A:395:PHE:O	1:A:398:TYR:CE1	2.64	0.50
1:B:102:VAL:O	1:B:105:PRO:HD2	2.11	0.50
1:B:261:VAL:HG12	1:B:262:VAL:N	2.27	0.50
1:B:299:SER:HA	1:B:380:SER:OG	2.12	0.50
1:B:343:ILE:O	1:B:346:LEU:N	2.45	0.50
1:B:367:TYR:HA	1:B:430:ILE:CG1	2.41	0.50
1:B:394:THR:HG23	1:B:439:MET:CB	2.42	0.50
1:A:445:TYR:HB3	1:A:448:GLN:HA	1.88	0.50
1:A:447:LEU:HD12	1:A:448:GLN:C	2.36	0.50
1:B:18:LEU:HD13	1:B:300:ILE:HD11	1.92	0.50
1:B:100:LEU:HD12	1:B:100:LEU:H	1.74	0.50
1:B:345:LEU:O	1:B:347:TYR:O	2.30	0.50
1:A:69:LEU:C	1:A:71:ALA:H	2.20	0.50
1:A:76:VAL:HA	1:A:78:GLN:NE2	2.14	0.50
1:A:89:PRO:O	1:A:93:HIS:CE1	2.64	0.50
1:A:232:LYS:N	1:A:235:PRO:HD2	2.26	0.50
1:A:233:PRO:N	1:A:235:PRO:HD2	2.27	0.50
1:A:353:VAL:C	1:A:357:ALA:HB2	2.36	0.50
1:A:445:TYR:CB	1:A:448:GLN:CA	2.76	0.50
1:B:97:ILE:O	1:B:101:LEU:HG	2.12	0.50
1:B:185:LYS:HD3	1:B:186:PHE:N	2.26	0.50
1:B:239:ILE:CA	1:B:242:PHE:HB2	2.41	0.50
1:B:420:LEU:HB3	1:B:423:LYS:CD	2.41	0.50
1:A:45:ALA:HB1	1:A:126:MET:CE	2.42	0.50
1:A:58:TRP:HE3	1:A:59:LEU:HD12	1.76	0.50
1:A:126:MET:HE3	1:A:191:LEU:HD21	1.93	0.50
1:A:151:ARG:CA	1:A:155:ASP:HA	2.31	0.50
1:A:208:LEU:CD2	1:A:209:LEU:N	2.66	0.50
1:B:84:ARG:C	1:B:86:HIS:N	2.70	0.50
1:B:110:LEU:HD13	1:B:114:GLN:HG3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:LEU:HB2	1:B:404:PRO:HD3	1.94	0.50
1:B:406:GLY:O	1:B:409:LEU:CB	2.53	0.50
1:A:120:MET:O	1:A:121:ASP:O	2.30	0.50
1:A:195:GLY:C	1:A:197:GLY:N	2.68	0.50
1:A:287:VAL:O	1:A:291:PRO:CD	2.60	0.50
1:A:382:ARG:HE	1:A:443:ARG:HB3	1.77	0.50
1:A:393:ARG:HH11	1:A:393:ARG:CG	2.23	0.50
1:A:413:ASN:HD22	1:A:421:GLY:H	1.59	0.50
1:B:20:THR:O	1:B:21:PRO:O	2.29	0.50
1:B:33:GLY:O	1:B:37:THR:CB	2.60	0.50
1:B:63:LEU:O	1:B:64:PHE:C	2.55	0.50
1:B:63:LEU:HG	1:B:64:PHE:N	2.27	0.50
1:B:100:LEU:N	1:B:100:LEU:CD1	2.75	0.50
1:B:137:VAL:HG11	1:B:201:ALA:N	2.27	0.50
1:B:178:ASN:ND2	1:B:199:ALA:HB2	2.27	0.50
1:B:406:GLY:CA	1:B:428:GLY:HA3	2.42	0.50
1:B:407:TYR:C	1:B:409:LEU:N	2.68	0.50
1:A:87:LYS:HZ1	1:B:308:GLU:C	2.19	0.50
1:A:183:TYR:O	1:A:184:GLY:C	2.55	0.50
1:B:22:VAL:O	1:B:25:ALA:HB3	2.12	0.50
1:B:95:GLY:O	1:B:96:LEU:C	2.55	0.50
1:B:173:LEU:O	1:B:176:PRO:CD	2.58	0.50
1:B:178:ASN:HD21	1:B:199:ALA:CB	2.25	0.50
1:B:207:MET:HA	1:B:210:LEU:CD2	2.42	0.50
1:B:215:ILE:CG2	1:B:216:VAL:H	2.23	0.50
1:B:341:GLU:CD	1:B:342:GLN:N	2.68	0.50
1:B:398:TYR:HD2	1:B:432:GLY:O	1.94	0.50
1:B:403:LEU:O	1:B:404:PRO:C	2.54	0.50
1:A:97:ILE:O	1:A:98:LEU:C	2.55	0.49
1:A:332:THR:C	1:A:335:LEU:HG	2.37	0.49
1:A:386:ASP:O	1:A:389:ALA:HB3	2.12	0.49
1:B:72:LEU:HB3	1:B:244:LEU:CD1	2.41	0.49
1:B:140:ALA:HB1	1:B:204:TYR:CE2	2.47	0.49
1:B:226:VAL:HG12	1:B:227:PHE:H	1.76	0.49
1:B:354:VAL:O	1:B:358:MET:N	2.40	0.49
1:A:60:PRO:O	1:A:63:LEU:HD23	2.13	0.49
1:A:244:LEU:HD23	1:A:388:THR:OG1	2.11	0.49
1:A:313:GLY:O	1:A:317:ALA:N	2.45	0.49
1:A:409:LEU:C	1:A:412:THR:H	2.20	0.49
1:A:447:LEU:HD11	1:A:450:GLN:HG2	1.93	0.49
1:B:145:LEU:CD1	1:B:146:LEU:N	2.64	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:SER:C	1:B:220:ARG:N	2.70	0.49
1:B:276:ALA:CA	1:B:426:TRP:NE1	2.75	0.49
1:A:5:VAL:HA	1:A:8:TYR:OH	2.12	0.49
1:A:72:LEU:HD12	1:A:244:LEU:CD2	2.37	0.49
1:A:413:ASN:C	1:A:415:LEU:N	2.69	0.49
1:B:248:VAL:HG23	1:B:249:ALA:N	2.28	0.49
1:B:279:VAL:HG12	1:B:280:ALA:N	2.26	0.49
1:B:314:ALA:O	1:B:316:ILE:N	2.45	0.49
1:B:316:ILE:O	1:B:317:ALA:C	2.54	0.49
1:B:455:GLN:C	1:B:455:GLN:NE2	2.70	0.49
1:A:314:ALA:O	1:A:318:ALA:N	2.44	0.49
1:A:354:VAL:O	1:A:358:MET:HB2	2.12	0.49
1:B:7:ARG:HB3	1:B:7:ARG:HH11	1.77	0.49
1:B:72:LEU:HD12	1:B:244:LEU:CD2	2.36	0.49
1:B:77:ALA:HB2	1:B:154:THR:HG23	1.90	0.49
1:B:126:MET:CE	1:B:191:LEU:HD21	2.42	0.49
1:B:133:TYR:C	1:B:135:HIS:H	2.20	0.49
1:B:175:ILE:HG22	1:B:176:PRO:N	2.27	0.49
1:A:78:GLN:HG3	1:A:79:LEU:CD1	2.41	0.49
1:A:118:ARG:CD	1:A:118:ARG:C	2.86	0.49
1:A:206:ILE:HG13	1:A:207:MET:N	2.27	0.49
1:A:218:SER:C	1:A:220:ARG:N	2.70	0.49
1:B:162:PRO:O	1:B:165:VAL:CG1	2.33	0.49
1:A:77:ALA:HB2	1:A:154:THR:CG2	2.43	0.49
1:A:244:LEU:CG	1:A:385:LYS:NZ	2.76	0.49
1:A:274:VAL:HG13	1:A:278:GLN:CD	2.37	0.49
1:A:279:VAL:HG13	1:A:361:LEU:HD23	1.94	0.49
1:A:314:ALA:C	1:A:318:ALA:HB3	2.36	0.49
1:A:413:ASN:C	1:A:415:LEU:H	2.20	0.49
1:B:144:TYR:O	1:B:147:PHE:HB3	2.13	0.49
1:B:166:ILE:O	1:B:170:GLY:CA	2.61	0.49
1:B:250:ALA:O	1:B:251:ALA:C	2.54	0.49
1:B:279:VAL:HG13	1:B:361:LEU:HD23	1.94	0.49
1:B:358:MET:SD	1:B:358:MET:C	2.96	0.49
1:B:422:ALA:O	1:B:423:LYS:C	2.55	0.49
1:A:19:ALA:O	1:A:20:THR:C	2.53	0.49
1:A:102:VAL:CA	1:A:105:PRO:HD2	2.43	0.49
1:A:161:LYS:O	1:A:163:ALA:N	2.45	0.49
1:B:155:ASP:CB	1:B:159:LEU:N	2.71	0.49
1:B:176:PRO:HG2	1:B:177:LEU:HD22	1.95	0.49
1:B:274:VAL:O	1:B:278:GLN:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:LEU:C	1:B:412:THR:H	2.20	0.49
1:A:145:LEU:HD13	1:A:146:LEU:H	1.70	0.49
1:A:339:PHE:O	1:A:340:ARG:O	2.30	0.49
1:B:59:LEU:O	1:B:60:PRO:C	2.55	0.49
1:B:155:ASP:CG	1:B:159:LEU:H	2.21	0.49
1:A:87:LYS:NZ	1:B:308:GLU:C	2.70	0.49
1:A:106:ILE:HG22	1:A:139:PHE:CE1	2.48	0.49
1:A:338:LEU:O	1:A:340:ARG:HG2	2.12	0.49
1:A:362:LEU:HD23	1:A:362:LEU:C	2.37	0.49
1:B:244:LEU:HG	1:B:385:LYS:CE	2.42	0.49
1:B:271:SER:O	1:B:273:VAL:HG12	2.13	0.49
1:B:407:TYR:CD2	1:B:411:MET:HG3	2.47	0.49
1:A:18:LEU:O	1:A:22:VAL:HG13	2.13	0.49
1:A:92:VAL:O	1:A:95:GLY:N	2.45	0.49
1:A:257:THR:O	1:A:260:ALA:HB3	2.12	0.49
1:A:279:VAL:O	1:A:280:ALA:C	2.55	0.49
1:B:41:GLY:C	1:B:49:ALA:CB	2.85	0.49
1:B:123:GLU:O	1:B:123:GLU:HG2	2.13	0.49
1:B:236:LYS:HA	1:B:239:ILE:HG13	1.94	0.49
1:B:292:MET:HA	1:B:375:VAL:HG11	1.95	0.49
1:A:63:LEU:O	1:A:64:PHE:C	2.55	0.48
1:A:76:VAL:CA	1:A:78:GLN:HE21	2.17	0.48
1:A:118:ARG:HD2	1:A:118:ARG:O	2.12	0.48
1:A:165:VAL:C	1:A:167:GLY:N	2.69	0.48
1:A:185:LYS:C	1:A:185:LYS:CD	2.86	0.48
1:A:420:LEU:HD12	1:A:423:LYS:HG2	1.95	0.48
1:A:427:LEU:O	1:A:430:ILE:N	2.46	0.48
1:B:76:VAL:HA	1:B:78:GLN:HG2	1.95	0.48
1:B:142:PRO:C	1:B:145:LEU:HB3	2.38	0.48
1:B:248:VAL:HG12	1:B:391:PHE:HZ	1.77	0.48
1:B:290:PHE:O	1:B:293:SER:HB2	2.13	0.48
1:A:133:TYR:C	1:A:135:HIS:H	2.21	0.48
1:A:161:LYS:N	1:A:162:PRO:CD	2.67	0.48
1:A:345:LEU:HD23	1:A:345:LEU:HA	1.57	0.48
1:B:68:LEU:O	1:B:71:ALA:HB3	2.13	0.48
1:B:106:ILE:HG22	1:B:139:PHE:CE1	2.46	0.48
1:B:205:TRP:CE3	1:B:206:ILE:HG22	2.48	0.48
1:B:317:ALA:CA	1:B:320:VAL:HG12	2.42	0.48
1:B:446:TRP:CH2	1:B:456:LEU:HD11	2.48	0.48
1:A:162:PRO:O	1:A:165:VAL:CG1	2.37	0.48
1:A:257:THR:O	1:A:261:VAL:HG23	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:SER:HB2	1:A:380:SER:HA	1.94	0.48
1:A:376:VAL:O	1:A:380:SER:HB3	2.13	0.48
1:A:381:LEU:O	1:A:384:TYR:CD2	2.66	0.48
1:B:20:THR:O	1:B:21:PRO:C	2.56	0.48
1:B:183:TYR:O	1:B:184:GLY:C	2.57	0.48
1:B:266:VAL:HG22	1:B:407:TYR:CZ	2.47	0.48
1:B:322:LEU:O	1:B:323:MET:C	2.56	0.48
1:A:137:VAL:HG11	1:A:201:ALA:N	2.28	0.48
1:A:250:ALA:O	1:A:251:ALA:C	2.56	0.48
1:A:331:ILE:HG13	1:A:335:LEU:HD23	1.95	0.48
1:A:357:ALA:O	1:A:358:MET:C	2.56	0.48
1:A:387:MET:HB3	1:A:443:ARG:HE	1.78	0.48
1:A:394:THR:HG21	1:A:440:LEU:CD1	2.43	0.48
1:B:78:GLN:C	1:B:80:ASN:H	2.20	0.48
1:B:89:PRO:O	1:B:93:HIS:CE1	2.67	0.48
1:B:159:LEU:O	1:B:160:THR:C	2.56	0.48
1:B:316:ILE:O	1:B:318:ALA:N	2.46	0.48
1:A:161:LYS:C	1:A:163:ALA:H	2.20	0.48
1:A:258:LEU:HA	1:A:261:VAL:CG2	2.43	0.48
1:A:272:THR:C	1:A:274:VAL:N	2.71	0.48
1:A:370:MET:HA	1:A:373:VAL:HG12	1.96	0.48
1:A:386:ASP:C	1:A:386:ASP:OD1	2.56	0.48
1:B:161:LYS:O	1:B:163:ALA:N	2.46	0.48
1:B:195:GLY:C	1:B:197:GLY:N	2.70	0.48
1:B:215:ILE:CG2	1:B:216:VAL:N	2.76	0.48
1:A:65:GLY:C	1:A:67:GLY:N	2.67	0.48
1:A:163:ALA:HB3	1:A:164:MET:SD	2.54	0.48
1:A:271:SER:O	1:A:273:VAL:HG12	2.13	0.48
1:A:410:GLY:CA	1:A:425:PHE:CB	2.92	0.48
1:A:417:GLU:CD	1:A:418:GLN:H	2.21	0.48
1:B:60:PRO:O	1:B:61:SER:C	2.55	0.48
1:B:65:GLY:C	1:B:67:GLY:N	2.69	0.48
1:B:100:LEU:O	1:B:102:VAL:N	2.47	0.48
1:B:208:LEU:HD23	1:B:209:LEU:CA	2.44	0.48
1:B:260:ALA:O	1:B:261:VAL:C	2.56	0.48
1:B:426:TRP:HA	1:B:426:TRP:HE3	1.77	0.48
1:A:22:VAL:HG23	1:A:293:SER:HB3	1.95	0.48
1:A:195:GLY:O	1:A:196:CYS:C	2.57	0.48
1:A:244:LEU:CB	1:A:385:LYS:HZ3	2.22	0.48
1:A:287:VAL:O	1:A:291:PRO:HD2	2.13	0.48
1:A:385:LYS:N	1:A:387:MET:SD	2.83	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:TYR:C	1:B:135:HIS:N	2.71	0.48
1:B:181:PHE:C	1:B:183:TYR:N	2.70	0.48
1:B:244:LEU:HG	1:B:385:LYS:HE2	1.96	0.48
1:B:284:SER:O	1:B:285:SER:C	2.57	0.48
1:B:382:ARG:C	1:B:384:TYR:H	2.22	0.48
1:A:20:THR:O	1:A:21:PRO:C	2.51	0.48
1:A:192:GLY:O	1:A:195:GLY:N	2.47	0.48
1:A:312:LYS:HA	1:A:312:LYS:HZ3	1.75	0.48
1:A:314:ALA:O	1:A:316:ILE:N	2.46	0.48
1:A:326:LEU:O	1:A:330:CYS:HB3	2.11	0.48
1:A:360:LEU:CD2	1:A:423:LYS:CB	2.92	0.48
1:A:386:ASP:O	1:A:387:MET:C	2.54	0.48
1:A:391:PHE:O	1:A:394:THR:HB	2.13	0.48
1:B:92:VAL:O	1:B:95:GLY:N	2.46	0.48
1:B:130:THR:O	1:B:131:VAL:C	2.56	0.48
1:B:134:MET:SD	1:B:198:VAL:N	2.87	0.48
1:B:283:PHE:CE1	1:B:287:VAL:HG21	2.49	0.48
1:A:144:TYR:O	1:A:147:PHE:HB3	2.14	0.48
1:A:273:VAL:O	1:A:277:HIS:CB	2.62	0.48
1:B:18:LEU:O	1:B:21:PRO:HD2	2.14	0.48
1:B:69:LEU:HD23	1:B:69:LEU:O	2.14	0.48
1:B:116:ILE:CG2	1:B:117:ILE:N	2.76	0.48
1:B:118:ARG:C	1:B:118:ARG:CD	2.87	0.48
1:B:410:GLY:O	1:B:413:ASN:HB3	2.14	0.48
1:A:28:ALA:C	1:A:32:MET:HG2	2.37	0.48
1:A:288:PHE:O	1:A:289:MET:C	2.57	0.48
1:B:81:GLY:O	1:B:82:ALA:CB	2.62	0.48
1:B:354:VAL:O	1:B:358:MET:HB2	2.13	0.48
1:B:408:ILE:O	1:B:408:ILE:CG2	2.61	0.48
1:A:145:LEU:CD1	1:A:146:LEU:N	2.64	0.47
1:A:215:ILE:CG2	1:A:216:VAL:N	2.75	0.47
1:A:223:HIS:ND1	1:A:223:HIS:N	2.62	0.47
1:A:408:ILE:O	1:A:408:ILE:CG2	2.62	0.47
1:B:71:ALA:HA	1:B:74:PRO:HD2	1.94	0.47
1:B:275:ALA:HB2	1:B:353:VAL:CG1	2.43	0.47
1:A:48:MET:HE2	1:A:48:MET:N	2.28	0.47
1:A:141:VAL:HG22	1:A:204:TYR:CB	2.43	0.47
1:A:178:ASN:OD1	1:A:199:ALA:HB2	2.14	0.47
1:A:224:VAL:HB	1:A:225:LYS:H	1.43	0.47
1:A:271:SER:C	1:A:273:VAL:HG12	2.39	0.47
1:A:374:GLN:HB2	1:A:437:ALA:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:GLN:O	1:B:97:ILE:HB	2.13	0.47
1:B:196:CYS:SG	1:B:197:GLY:N	2.87	0.47
1:B:427:LEU:C	1:B:429:PHE:N	2.70	0.47
1:A:172:LEU:O	1:A:176:PRO:HD2	2.14	0.47
1:A:180:ILE:HG23	1:A:181:PHE:HD1	1.78	0.47
1:A:255:GLU:CG	1:A:256:VAL:N	2.76	0.47
1:A:328:THR:HA	1:A:331:ILE:HG23	1.96	0.47
1:B:4:SER:C	1:B:8:TYR:CE2	2.92	0.47
1:B:61:SER:O	1:B:253:PHE:CE1	2.67	0.47
1:B:77:ALA:CB	1:B:154:THR:CG2	2.90	0.47
1:B:266:VAL:HG22	1:B:407:TYR:CD1	2.49	0.47
1:B:346:LEU:HB3	1:B:347:TYR:H	1.50	0.47
1:B:394:THR:HG21	1:B:440:LEU:HD22	1.96	0.47
1:B:451:SER:HA	1:B:453:ASP:OD1	2.14	0.47
1:A:403:LEU:HB2	1:A:404:PRO:HD3	1.96	0.47
1:B:146:LEU:HD22	1:B:149:ALA:CB	2.45	0.47
1:B:273:VAL:CG1	1:B:274:VAL:H	2.24	0.47
1:B:287:VAL:O	1:B:291:PRO:CD	2.63	0.47
1:B:301:ARG:NH2	1:B:316:ILE:CG2	2.76	0.47
1:A:58:TRP:O	1:A:59:LEU:C	2.55	0.47
1:A:203:VAL:C	1:A:205:TRP:N	2.71	0.47
1:A:244:LEU:HG	1:A:385:LYS:HZ1	1.76	0.47
1:A:344:ALA:HB1	1:A:354:VAL:HG22	1.97	0.47
1:B:10:LYS:HA	1:B:13:SER:OG	2.14	0.47
1:B:332:THR:CA	1:B:335:LEU:HG	2.43	0.47
1:B:394:THR:HG21	1:B:440:LEU:HD13	1.96	0.47
1:A:234:GLN:C	1:A:238:LEU:HD13	2.40	0.47
1:B:314:ALA:HB1	1:B:445:TYR:CZ	2.49	0.47
1:B:405:THR:HG22	1:B:406:GLY:N	2.30	0.47
1:A:72:LEU:HB3	1:A:244:LEU:CD1	2.45	0.47
1:A:74:PRO:HB3	1:A:149:ALA:CA	2.45	0.47
1:A:178:ASN:HD21	1:A:199:ALA:CB	2.28	0.47
1:A:215:ILE:CG2	1:A:216:VAL:H	2.24	0.47
1:A:259:PHE:O	1:A:260:ALA:C	2.58	0.47
1:A:266:VAL:HG22	1:A:407:TYR:CZ	2.49	0.47
1:A:283:PHE:O	1:A:284:SER:C	2.58	0.47
1:A:358:MET:C	1:A:358:MET:SD	2.98	0.47
1:A:382:ARG:HB3	1:A:387:MET:HB2	1.96	0.47
1:B:18:LEU:HA	1:B:160:THR:CG2	2.45	0.47
1:B:21:PRO:HA	1:B:164:MET:CE	2.43	0.47
1:B:42:GLY:N	1:B:49:ALA:CB	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:MET:N	1:B:48:MET:HE2	2.30	0.47
1:B:53:ILE:HA	1:B:56:SER:HB3	1.97	0.47
1:B:68:LEU:HD22	1:B:71:ALA:HB3	1.96	0.47
1:B:69:LEU:O	1:B:73:VAL:HG23	2.14	0.47
1:B:86:HIS:O	1:B:87:LYS:CB	2.62	0.47
1:B:142:PRO:O	1:B:143:ALA:C	2.56	0.47
1:B:206:ILE:CG1	1:B:207:MET:N	2.77	0.47
1:B:208:LEU:C	1:B:211:LEU:HB3	2.40	0.47
1:B:210:LEU:HD13	1:B:210:LEU:N	2.30	0.47
1:B:281:LEU:HD23	1:B:281:LEU:C	2.40	0.47
1:B:299:SER:CA	1:B:380:SER:OG	2.63	0.47
1:B:331:ILE:HG13	1:B:335:LEU:HD23	1.97	0.47
1:B:403:LEU:O	1:B:407:TYR:N	2.30	0.47
1:B:435:ALA:O	1:B:439:MET:HG2	2.15	0.47
1:A:149:ALA:O	1:A:154:THR:CB	2.62	0.47
1:A:150:LEU:O	1:A:154:THR:CB	2.60	0.47
1:A:311:THR:OG1	1:A:312:LYS:N	2.47	0.47
1:A:436:ALA:O	1:A:439:MET:HB2	2.14	0.47
1:B:71:ALA:N	1:B:74:PRO:HD2	2.30	0.47
1:B:135:HIS:C	1:B:137:VAL:N	2.66	0.47
1:B:143:ALA:O	1:B:146:LEU:HB3	2.15	0.47
1:B:235:PRO:HA	1:B:238:LEU:CD2	2.45	0.47
1:B:294:ILE:O	1:B:295:GLY:C	2.57	0.47
1:B:376:VAL:CG1	1:B:377:ALA:H	2.10	0.47
1:A:10:LYS:NZ	1:A:305:LYS:NZ	2.62	0.47
1:A:191:LEU:H	1:A:194:VAL:HB	1.79	0.47
1:A:206:ILE:O	1:A:209:LEU:CB	2.55	0.47
1:A:244:LEU:CD2	1:A:388:THR:OG1	2.63	0.47
1:A:275:ALA:HB2	1:A:353:VAL:CG2	2.45	0.47
1:A:399:TRP:NE1	1:A:403:LEU:HD12	2.30	0.47
1:B:42:GLY:N	1:B:49:ALA:HB3	2.30	0.47
1:B:120:MET:O	1:B:121:ASP:O	2.32	0.47
1:A:42:GLY:O	1:A:47:ASP:HA	2.14	0.47
1:A:61:SER:O	1:A:253:PHE:CE1	2.68	0.47
1:A:208:LEU:C	1:A:211:LEU:HB3	2.40	0.47
1:A:210:LEU:HD13	1:A:210:LEU:N	2.30	0.47
1:A:235:PRO:HA	1:A:238:LEU:CD2	2.45	0.47
1:A:351:GLN:O	1:A:352:VAL:C	2.58	0.47
1:A:443:ARG:O	1:A:444:LEU:C	2.57	0.47
1:B:412:THR:HG23	1:B:416:THR:HB	1.96	0.47
1:A:47:ASP:C	1:A:49:ALA:H	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:PHE:O	1:A:155:ASP:OD1	2.32	0.46
1:B:102:VAL:CA	1:B:105:PRO:HD2	2.45	0.46
1:B:104:VAL:O	1:B:106:ILE:N	2.48	0.46
1:B:178:ASN:HD21	1:B:199:ALA:HB1	1.80	0.46
1:B:300:ILE:CG1	1:B:301:ARG:N	2.77	0.46
1:B:387:MET:O	1:B:391:PHE:HB3	2.15	0.46
1:B:427:LEU:HD23	1:B:427:LEU:C	2.40	0.46
1:B:433:LEU:HD12	1:B:433:LEU:N	2.30	0.46
1:A:5:VAL:O	1:A:9:LYS:HB2	2.15	0.46
1:A:173:LEU:O	1:A:177:LEU:CD2	2.57	0.46
1:B:38:ILE:O	1:B:39:MET:C	2.58	0.46
1:B:98:LEU:O	1:B:99:ALA:C	2.57	0.46
1:B:219:LYS:HD3	1:B:220:ARG:NE	2.30	0.46
1:B:276:ALA:O	1:B:277:HIS:C	2.57	0.46
1:B:339:PHE:O	1:B:343:ILE:HB	2.15	0.46
1:B:348:THR:O	1:B:349:GLU:HG3	2.15	0.46
1:B:355:ALA:O	1:B:358:MET:HB3	2.15	0.46
1:A:11:GLU:HA	1:A:301:ARG:NH2	2.11	0.46
1:A:233:PRO:HA	1:A:236:LYS:HB2	1.96	0.46
1:A:340:ARG:HB2	1:A:361:LEU:CD1	2.44	0.46
1:B:16:ILE:CA	1:B:19:ALA:HB3	2.35	0.46
1:B:23:LEU:O	1:B:24:ILE:C	2.57	0.46
1:B:69:LEU:C	1:B:71:ALA:H	2.23	0.46
1:B:191:LEU:CG	1:B:192:GLY:H	2.29	0.46
1:B:232:LYS:CB	1:B:233:PRO:HD3	2.30	0.46
1:A:59:LEU:HB2	1:A:60:PRO:CD	2.40	0.46
1:A:100:LEU:CD1	1:A:100:LEU:H	2.28	0.46
1:A:206:ILE:O	1:A:210:LEU:CD2	2.55	0.46
1:A:230:PHE:CG	1:A:231:HIS:N	2.81	0.46
1:A:367:TYR:O	1:A:368:GLN:C	2.57	0.46
1:A:381:LEU:O	1:A:384:TYR:CG	2.68	0.46
1:A:386:ASP:C	1:A:389:ALA:H	2.23	0.46
1:B:118:ARG:HD2	1:B:118:ARG:O	2.15	0.46
1:B:161:LYS:C	1:B:163:ALA:N	2.73	0.46
1:B:178:ASN:OD1	1:B:199:ALA:HB2	2.14	0.46
1:A:69:LEU:HG	1:A:245:GLY:C	2.40	0.46
1:A:76:VAL:C	1:A:78:GLN:HG2	2.41	0.46
1:A:145:LEU:HD13	1:A:145:LEU:C	2.37	0.46
1:A:178:ASN:ND2	1:A:199:ALA:HB2	2.29	0.46
1:A:232:LYS:N	1:A:233:PRO:CD	2.70	0.46
1:A:298:VAL:HA	1:A:301:ARG:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:ILE:HB	1:B:210:LEU:HG	1.96	0.46
1:B:311:THR:OG1	1:B:312:LYS:N	2.47	0.46
1:A:139:PHE:O	1:A:142:PRO:HD2	2.16	0.46
1:A:237:GLU:O	1:A:241:LEU:N	2.48	0.46
1:A:312:LYS:HA	1:A:312:LYS:HZ2	1.78	0.46
1:A:410:GLY:O	1:A:413:ASN:HB3	2.16	0.46
1:B:14:ASN:H	1:B:14:ASN:ND2	2.14	0.46
1:B:19:ALA:O	1:B:22:VAL:HG22	2.15	0.46
1:B:97:ILE:C	1:B:99:ALA:N	2.72	0.46
1:B:131:VAL:O	1:B:134:MET:HB2	2.16	0.46
1:B:274:VAL:HG13	1:B:278:GLN:NE2	2.31	0.46
1:B:318:ALA:HA	1:B:381:LEU:CD1	2.45	0.46
1:B:328:THR:CA	1:B:331:ILE:CG2	2.94	0.46
1:B:382:ARG:C	1:B:384:TYR:N	2.67	0.46
1:B:443:ARG:NH2	1:B:446:TRP:HE1	2.13	0.46
1:A:232:LYS:CB	1:A:233:PRO:HD3	2.32	0.46
1:A:238:LEU:HA	1:A:241:LEU:CB	2.37	0.46
1:A:290:PHE:HB3	1:A:291:PRO:CD	2.46	0.46
1:A:317:ALA:CA	1:A:320:VAL:HG12	2.46	0.46
1:A:322:LEU:O	1:A:323:MET:C	2.58	0.46
1:A:445:TYR:HD2	1:A:448:GLN:CG	2.29	0.46
1:B:388:THR:O	1:B:391:PHE:CD2	2.69	0.46
1:A:38:ILE:O	1:A:39:MET:C	2.57	0.46
1:A:63:LEU:HG	1:A:64:PHE:N	2.28	0.46
1:A:131:VAL:HB	1:A:135:HIS:HE2	1.80	0.46
1:A:161:LYS:C	1:A:163:ALA:N	2.72	0.46
1:A:238:LEU:HA	1:A:241:LEU:CD1	2.45	0.46
1:A:300:ILE:CG1	1:A:301:ARG:N	2.75	0.46
1:A:431:ILE:O	1:A:435:ALA:CB	2.63	0.46
1:B:88:ILE:HG13	1:B:89:PRO:N	2.30	0.46
1:B:110:LEU:O	1:B:111:PHE:C	2.59	0.46
1:B:116:ILE:HG23	1:B:117:ILE:N	2.31	0.46
1:B:166:ILE:HB	1:B:210:LEU:CG	2.46	0.46
1:B:238:LEU:CA	1:B:241:LEU:HD13	2.46	0.46
1:A:299:SER:N	1:A:380:SER:OG	2.49	0.46
1:A:335:LEU:HD12	1:A:336:THR:N	2.31	0.46
1:B:32:MET:HG3	1:B:33:GLY:H	1.74	0.46
1:B:65:GLY:CA	1:B:253:PHE:CG	2.99	0.46
1:B:178:ASN:ND2	1:B:199:ALA:HB1	2.31	0.46
1:B:213:PHE:O	1:B:217:THR:CG2	2.63	0.46
1:B:232:LYS:N	1:B:235:PRO:HD2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:461:LYS:HD2	1:B:461:LYS:C	2.41	0.46
1:A:21:PRO:HA	1:A:164:MET:CE	2.44	0.46
1:A:81:GLY:O	1:A:82:ALA:CB	2.63	0.46
1:A:86:HIS:NE2	1:B:83:GLY:HA2	2.31	0.46
1:A:135:HIS:O	1:A:138:ILE:HG22	2.16	0.46
1:A:205:TRP:CE3	1:A:206:ILE:HG22	2.50	0.46
1:A:299:SER:CA	1:A:380:SER:OG	2.64	0.46
1:B:7:ARG:HH11	1:B:7:ARG:CB	2.29	0.46
1:B:76:VAL:CA	1:B:78:GLN:HG2	2.46	0.46
1:B:191:LEU:H	1:B:194:VAL:HB	1.81	0.46
1:B:329:ALA:O	1:B:333:ALA:CB	2.64	0.46
1:A:15:LEU:HD12	1:A:15:LEU:C	2.39	0.45
1:A:69:LEU:HG	1:A:245:GLY:CA	2.46	0.45
1:A:94:GLN:OE1	1:A:238:LEU:HD21	2.16	0.45
1:A:180:ILE:HG23	1:A:181:PHE:CD1	2.51	0.45
1:A:339:PHE:O	1:A:343:ILE:HB	2.16	0.45
1:A:369:CYS:O	1:A:372:ALA:HB3	2.16	0.45
1:A:386:ASP:OD1	1:A:387:MET:N	2.50	0.45
1:B:3:ASN:O	1:B:5:VAL:HG23	2.15	0.45
1:B:145:LEU:O	1:B:148:GLN:HB3	2.15	0.45
1:B:238:LEU:HA	1:B:241:LEU:CB	2.35	0.45
1:B:247:PRO:HG2	1:B:389:ALA:HA	1.98	0.45
1:B:381:LEU:O	1:B:384:TYR:CD2	2.69	0.45
1:A:18:LEU:HD13	1:A:300:ILE:HD11	1.98	0.45
1:A:94:GLN:O	1:A:95:GLY:C	2.57	0.45
1:A:328:THR:O	1:A:332:THR:CG2	2.64	0.45
1:A:358:MET:O	1:A:361:LEU:HB2	2.17	0.45
1:A:407:TYR:O	1:A:410:GLY:N	2.49	0.45
1:B:172:LEU:C	1:B:172:LEU:HD13	2.41	0.45
1:B:262:VAL:HG12	1:B:263:ALA:N	2.29	0.45
1:B:272:THR:O	1:B:274:VAL:C	2.59	0.45
1:B:399:TRP:NE1	1:B:403:LEU:HD12	2.30	0.45
1:A:73:VAL:N	1:A:74:PRO:CD	2.79	0.45
1:A:76:VAL:O	1:A:78:GLN:N	2.46	0.45
1:A:124:GLU:HB2	1:A:125:ALA:H	1.59	0.45
1:A:244:LEU:CB	1:A:385:LYS:NZ	2.76	0.45
1:A:409:LEU:O	1:A:410:GLY:O	2.34	0.45
1:A:427:LEU:C	1:A:429:PHE:N	2.72	0.45
1:B:31:GLY:O	1:B:35:VAL:CG2	2.59	0.45
1:B:77:ALA:HB2	1:B:154:THR:CB	2.46	0.45
1:B:81:GLY:O	1:B:308:GLU:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:ILE:O	1:B:91:GLU:HB3	2.17	0.45
1:A:58:TRP:O	1:A:61:SER:N	2.49	0.45
1:A:125:ALA:O	1:A:126:MET:C	2.60	0.45
1:A:148:GLN:HA	1:A:152:SER:CB	2.45	0.45
1:A:180:ILE:HD11	1:A:186:PHE:HB2	1.98	0.45
1:A:319:ASN:O	1:A:323:MET:HB2	2.16	0.45
1:A:382:ARG:C	1:A:384:TYR:H	2.24	0.45
1:B:277:HIS:O	1:B:278:GLN:C	2.59	0.45
1:B:429:PHE:CE1	1:B:433:LEU:HD11	2.52	0.45
1:A:79:LEU:O	1:A:84:ARG:O	2.34	0.45
1:A:93:HIS:N	1:A:93:HIS:ND1	2.65	0.45
1:A:413:ASN:HB3	1:A:414:TRP:HE3	1.74	0.45
1:A:445:TYR:CG	1:A:448:GLN:HA	2.49	0.45
1:B:185:LYS:HG2	1:B:189:PRO:HD3	1.97	0.45
1:B:195:GLY:O	1:B:196:CYS:C	2.60	0.45
1:B:301:ARG:HD3	1:B:301:ARG:C	2.41	0.45
1:B:335:LEU:HD12	1:B:336:THR:N	2.31	0.45
1:B:439:MET:HE2	1:B:439:MET:CA	2.46	0.45
1:A:122:VAL:C	1:A:124:GLU:N	2.72	0.45
1:A:266:VAL:HG22	1:A:407:TYR:CD1	2.51	0.45
1:A:282:ASN:O	1:A:283:PHE:C	2.60	0.45
1:A:286:LEU:N	1:A:286:LEU:CD1	2.80	0.45
1:B:53:ILE:HD12	1:B:54:ALA:N	2.31	0.45
1:B:204:TYR:HA	1:B:207:MET:SD	2.57	0.45
1:B:231:HIS:C	1:B:235:PRO:CG	2.84	0.45
1:B:275:ALA:H	1:B:353:VAL:HG21	1.82	0.45
1:A:8:TYR:O	1:A:12:ALA:CB	2.65	0.45
1:A:275:ALA:HB2	1:A:353:VAL:CG1	2.45	0.45
1:A:281:LEU:CD2	1:A:282:ASN:HD22	2.27	0.45
1:A:394:THR:HG21	1:A:440:LEU:CD2	2.46	0.45
1:B:18:LEU:HB2	1:B:297:ALA:HB1	1.99	0.45
1:B:172:LEU:HD13	1:B:173:LEU:N	2.32	0.45
1:B:239:ILE:C	1:B:242:PHE:HB2	2.42	0.45
1:A:20:THR:O	1:A:21:PRO:O	2.34	0.45
1:A:98:LEU:O	1:A:99:ALA:C	2.59	0.45
1:A:346:LEU:HB3	1:A:347:TYR:H	1.57	0.45
1:B:93:HIS:CD2	1:B:228:GLU:OE2	2.70	0.45
1:B:165:VAL:CG1	1:B:166:ILE:N	2.41	0.45
1:B:206:ILE:HG13	1:B:207:MET:N	2.30	0.45
1:B:234:GLN:C	1:B:237:GLU:H	2.24	0.45
1:B:244:LEU:CG	1:B:385:LYS:NZ	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:LEU:CD2	1:B:282:ASN:HD22	2.28	0.45
1:B:328:THR:HA	1:B:331:ILE:HG23	1.96	0.45
1:B:370:MET:HG3	1:B:434:SER:HB2	1.97	0.45
1:A:88:ILE:HG13	1:A:89:PRO:CD	2.46	0.45
1:A:128:THR:HG22	1:A:129:LYS:HG2	1.99	0.45
1:A:150:LEU:C	1:A:154:THR:HB	2.41	0.45
1:B:69:LEU:C	1:B:69:LEU:CD2	2.89	0.45
1:B:142:PRO:O	1:B:145:LEU:CD1	2.65	0.45
1:B:279:VAL:O	1:B:280:ALA:C	2.59	0.45
1:B:290:PHE:HB3	1:B:291:PRO:CD	2.46	0.45
1:B:326:LEU:O	1:B:330:CYS:HB3	2.16	0.45
1:B:447:LEU:H	1:B:447:LEU:HG	1.56	0.45
1:A:39:MET:CG	1:A:40:ALA:N	2.78	0.45
1:A:299:SER:HA	1:A:380:SER:OG	2.16	0.45
1:B:148:GLN:HE21	1:B:148:GLN:HB3	1.56	0.45
1:B:262:VAL:HG21	1:B:403:LEU:CD1	2.35	0.45
1:B:271:SER:C	1:B:273:VAL:HG12	2.42	0.45
1:A:33:GLY:O	1:A:37:THR:CB	2.65	0.44
1:A:266:VAL:HG12	1:A:269:LEU:CG	2.46	0.44
1:A:313:GLY:O	1:A:317:ALA:HB3	2.17	0.44
1:B:15:LEU:HD12	1:B:16:ILE:CA	2.47	0.44
1:B:210:LEU:O	1:B:211:LEU:O	2.35	0.44
1:B:292:MET:C	1:B:292:MET:HE2	2.42	0.44
1:A:95:GLY:O	1:A:96:LEU:C	2.59	0.44
1:A:103:SER:HB2	1:A:139:PHE:HD1	1.82	0.44
1:A:281:LEU:HD23	1:A:281:LEU:C	2.42	0.44
1:B:108:ALA:O	1:B:109:VAL:C	2.61	0.44
1:B:124:GLU:HB2	1:B:125:ALA:H	1.62	0.44
1:A:142:PRO:O	1:A:143:ALA:C	2.60	0.44
1:A:239:ILE:C	1:A:242:PHE:HB2	2.42	0.44
1:A:294:ILE:O	1:A:297:ALA:HB3	2.17	0.44
1:A:429:PHE:CE1	1:A:433:LEU:HD11	2.52	0.44
1:B:141:VAL:CB	1:B:142:PRO:HD3	2.44	0.44
1:B:275:ALA:O	1:B:279:VAL:HB	2.17	0.44
1:B:299:SER:N	1:B:380:SER:OG	2.51	0.44
1:A:72:LEU:HD13	1:A:75:VAL:HG11	2.00	0.44
1:A:277:HIS:O	1:A:278:GLN:C	2.59	0.44
1:A:444:LEU:HD22	1:A:445:TYR:CD2	2.52	0.44
1:B:7:ARG:O	1:B:11:GLU:HG3	2.18	0.44
1:B:11:GLU:CG	1:B:316:ILE:HG23	2.47	0.44
1:B:80:ASN:ND2	1:B:157:MET:HG2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:THR:O	1:B:332:THR:CG2	2.64	0.44
1:A:10:LYS:HA	1:A:13:SER:OG	2.17	0.44
1:A:145:LEU:C	1:A:145:LEU:CD2	2.78	0.44
1:A:151:ARG:HA	1:A:155:ASP:CA	2.31	0.44
1:A:185:LYS:HG2	1:A:189:PRO:HD3	1.99	0.44
1:A:242:PHE:O	1:A:246:PHE:N	2.31	0.44
1:A:427:LEU:O	1:A:428:GLY:C	2.59	0.44
1:B:93:HIS:N	1:B:93:HIS:ND1	2.62	0.44
1:B:181:PHE:O	1:B:183:TYR:N	2.51	0.44
1:A:11:GLU:HB3	1:A:320:VAL:HG23	1.93	0.44
1:A:80:ASN:OD1	1:A:80:ASN:O	2.35	0.44
1:A:329:ALA:O	1:A:333:ALA:CB	2.66	0.44
1:A:420:LEU:O	1:A:423:LYS:HG2	2.18	0.44
1:A:159:LEU:O	1:A:160:THR:C	2.59	0.44
1:A:219:LYS:HD3	1:A:220:ARG:NE	2.32	0.44
1:A:328:THR:CA	1:A:331:ILE:CG2	2.92	0.44
1:B:103:SER:HB2	1:B:139:PHE:HD1	1.81	0.44
1:B:179:TRP:O	1:B:184:GLY:N	2.51	0.44
1:B:452:ASP:HA	1:B:455:GLN:HB2	2.00	0.44
1:A:14:ASN:HD22	1:A:14:ASN:H	1.65	0.44
1:A:15:LEU:HD12	1:A:16:ILE:CA	2.48	0.44
1:A:100:LEU:HD12	1:A:100:LEU:H	1.81	0.44
1:A:146:LEU:HD22	1:A:149:ALA:CB	2.46	0.44
1:A:207:MET:O	1:A:208:LEU:C	2.58	0.44
1:A:452:ASP:O	1:A:456:LEU:HG	2.18	0.44
1:B:11:GLU:HB3	1:B:320:VAL:HG23	1.93	0.44
1:B:69:LEU:HB2	1:B:249:ALA:HB2	1.98	0.44
1:B:86:HIS:CD2	1:B:87:LYS:HG3	2.53	0.44
1:B:135:HIS:O	1:B:136:ALA:C	2.61	0.44
1:B:320:VAL:CG1	1:B:321:GLY:N	2.53	0.44
1:A:20:THR:OG1	1:A:21:PRO:CD	2.61	0.44
1:A:97:ILE:HG22	1:A:101:LEU:CD1	2.37	0.44
1:A:148:GLN:C	1:A:152:SER:HB3	2.43	0.44
1:A:234:GLN:O	1:A:238:LEU:CD1	2.65	0.44
1:A:268:PRO:C	1:A:270:GLY:H	2.26	0.44
1:A:273:VAL:CG1	1:A:274:VAL:N	2.78	0.44
1:A:367:TYR:O	1:A:371:ASP:HB3	2.18	0.44
1:B:20:THR:OG1	1:B:21:PRO:CD	2.63	0.44
1:B:72:LEU:HG	1:B:388:THR:HG21	1.99	0.44
1:B:238:LEU:HA	1:B:241:LEU:CD1	2.45	0.44
1:B:298:VAL:HG11	1:B:317:ALA:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:GLU:HB3	1:B:309:GLN:H	1.63	0.44
1:B:360:LEU:HD21	1:B:423:LYS:HB3	2.00	0.44
1:B:443:ARG:NH1	1:B:446:TRP:CD1	2.85	0.44
1:A:86:HIS:C	1:A:88:ILE:H	2.26	0.43
1:A:116:ILE:CG2	1:A:117:ILE:N	2.80	0.43
1:A:144:TYR:O	1:A:147:PHE:N	2.51	0.43
1:A:178:ASN:HD21	1:A:199:ALA:HB1	1.83	0.43
1:B:110:LEU:HD13	1:B:110:LEU:C	2.43	0.43
1:B:151:ARG:CG	1:B:152:SER:N	2.78	0.43
1:B:223:HIS:ND1	1:B:223:HIS:N	2.65	0.43
1:B:367:TYR:O	1:B:368:GLN:C	2.61	0.43
1:B:374:GLN:HB2	1:B:437:ALA:HB2	2.00	0.43
1:A:3:ASN:O	1:A:4:SER:OG	2.23	0.43
1:A:133:TYR:C	1:A:135:HIS:N	2.74	0.43
1:A:135:HIS:CA	1:A:138:ILE:HG22	2.45	0.43
1:A:155:ASP:CB	1:A:159:LEU:N	2.69	0.43
1:A:280:ALA:O	1:A:281:LEU:C	2.61	0.43
1:A:318:ALA:HA	1:A:381:LEU:CD1	2.48	0.43
1:A:322:LEU:O	1:A:324:THR:N	2.51	0.43
1:A:332:THR:HA	1:A:335:LEU:HG	1.98	0.43
1:A:410:GLY:N	1:A:425:PHE:HB2	2.32	0.43
1:B:4:SER:HA	1:B:7:ARG:HB2	2.00	0.43
1:B:94:GLN:O	1:B:95:GLY:C	2.62	0.43
1:B:404:PRO:O	1:B:408:ILE:HB	2.18	0.43
1:A:72:LEU:HD11	1:A:383:GLY:O	2.18	0.43
1:A:77:ALA:HB2	1:A:154:THR:CB	2.48	0.43
1:A:100:LEU:C	1:A:102:VAL:N	2.76	0.43
1:A:151:ARG:HD2	1:A:155:ASP:CA	2.44	0.43
1:A:185:LYS:HD3	1:A:186:PHE:N	2.32	0.43
1:A:208:LEU:HD23	1:A:209:LEU:CA	2.47	0.43
1:A:234:GLN:HB3	1:A:235:PRO:HD3	2.00	0.43
1:B:44:SER:O	1:B:46:ILE:N	2.51	0.43
1:B:69:LEU:HG	1:B:245:GLY:C	2.43	0.43
1:B:72:LEU:HD22	1:B:75:VAL:HG11	2.00	0.43
1:B:135:HIS:CA	1:B:138:ILE:HG22	2.47	0.43
1:A:146:LEU:O	1:A:149:ALA:N	2.52	0.43
1:A:247:PRO:O	1:A:251:ALA:HB2	2.18	0.43
1:A:276:ALA:O	1:A:277:HIS:O	2.36	0.43
1:A:327:ALA:O	1:A:330:CYS:HB3	2.18	0.43
1:A:412:THR:O	1:A:416:THR:N	2.51	0.43
1:B:53:ILE:CA	1:B:56:SER:HB3	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:MET:SD	1:B:197:GLY:C	3.01	0.43
1:A:130:THR:HB	1:A:194:VAL:HA	2.00	0.43
1:A:173:LEU:O	1:A:176:PRO:CD	2.64	0.43
1:A:262:VAL:O	1:A:263:ALA:C	2.61	0.43
1:A:353:VAL:O	1:A:357:ALA:CB	2.66	0.43
1:A:388:THR:O	1:A:391:PHE:CD2	2.71	0.43
1:B:127:ALA:C	1:B:130:THR:HG1	2.25	0.43
1:B:128:THR:HG22	1:B:129:LYS:HG2	2.00	0.43
1:B:236:LYS:C	1:B:239:ILE:H	2.26	0.43
1:B:238:LEU:O	1:B:242:PHE:CD1	2.71	0.43
1:B:288:PHE:O	1:B:289:MET:C	2.60	0.43
1:B:316:ILE:HB	1:B:317:ALA:H	1.53	0.43
1:B:412:THR:O	1:B:416:THR:N	2.52	0.43
1:B:420:LEU:HD12	1:B:423:LYS:HG2	2.01	0.43
1:A:18:LEU:HB2	1:A:297:ALA:HB1	1.99	0.43
1:A:191:LEU:CG	1:A:192:GLY:H	2.30	0.43
1:A:191:LEU:CG	1:A:192:GLY:N	2.81	0.43
1:A:343:ILE:O	1:A:346:LEU:N	2.52	0.43
1:A:363:PHE:CD2	1:A:426:TRP:HB3	2.53	0.43
1:B:53:ILE:C	1:B:53:ILE:CD1	2.87	0.43
1:B:109:VAL:O	1:B:113:THR:HG22	2.17	0.43
1:B:111:PHE:C	1:B:111:PHE:CD2	2.96	0.43
1:B:141:VAL:HG22	1:B:204:TYR:CB	2.47	0.43
1:B:212:LEU:O	1:B:213:PHE:O	2.36	0.43
1:B:247:PRO:HB3	1:B:388:THR:O	2.18	0.43
1:B:273:VAL:CG1	1:B:274:VAL:N	2.79	0.43
1:B:378:ALA:O	1:B:380:SER:N	2.51	0.43
1:B:427:LEU:O	1:B:428:GLY:C	2.61	0.43
1:B:451:SER:C	1:B:453:ASP:H	2.27	0.43
1:A:130:THR:O	1:A:131:VAL:C	2.61	0.43
1:A:131:VAL:O	1:A:135:HIS:CG	2.72	0.43
1:B:32:MET:O	1:B:33:GLY:C	2.60	0.43
1:B:56:SER:O	1:B:60:PRO:HD2	2.18	0.43
1:B:131:VAL:HB	1:B:135:HIS:HE2	1.84	0.43
1:B:173:LEU:O	1:B:177:LEU:CD2	2.56	0.43
1:B:230:PHE:CG	1:B:231:HIS:N	2.83	0.43
1:B:262:VAL:O	1:B:263:ALA:C	2.59	0.43
1:B:345:LEU:HD23	1:B:345:LEU:HA	1.54	0.43
1:B:420:LEU:HB3	1:B:423:LYS:HE2	2.01	0.43
1:A:4:SER:C	1:A:8:TYR:CE2	2.96	0.43
1:A:8:TYR:CD1	1:A:9:LYS:N	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:VAL:O	1:A:31:GLY:CA	2.64	0.43
1:A:69:LEU:C	1:A:69:LEU:CD2	2.92	0.43
1:A:72:LEU:HD13	1:A:75:VAL:CG1	2.49	0.43
1:A:179:TRP:O	1:A:184:GLY:N	2.50	0.43
1:A:234:GLN:C	1:A:237:GLU:H	2.27	0.43
1:A:275:ALA:HB1	1:A:353:VAL:CG1	2.47	0.43
1:A:298:VAL:HG21	1:A:321:GLY:CA	2.46	0.43
1:B:11:GLU:HG2	1:B:316:ILE:HG23	1.99	0.43
1:B:60:PRO:O	1:B:63:LEU:HB3	2.18	0.43
1:B:60:PRO:O	1:B:63:LEU:CD2	2.66	0.43
1:B:65:GLY:HA2	1:B:253:PHE:CG	2.54	0.43
1:B:72:LEU:O	1:B:73:VAL:C	2.62	0.43
1:B:147:PHE:CD1	1:B:211:LEU:HA	2.54	0.43
1:B:244:LEU:C	1:B:247:PRO:HD2	2.43	0.43
1:B:294:ILE:O	1:B:297:ALA:HB3	2.19	0.43
1:A:86:HIS:CE1	1:A:87:LYS:H	2.35	0.43
1:A:166:ILE:C	1:A:170:GLY:H	2.26	0.43
1:A:212:LEU:O	1:A:213:PHE:O	2.37	0.43
1:A:287:VAL:HB	1:A:368:GLN:HG2	2.00	0.43
1:A:356:LEU:O	1:A:357:ALA:C	2.61	0.43
1:B:60:PRO:HA	1:B:63:LEU:HD22	2.01	0.43
1:B:129:LYS:O	1:B:132:GLY:HA3	2.19	0.43
1:B:311:THR:C	1:B:312:LYS:HZ3	2.26	0.43
1:B:366:ILE:HG22	1:B:430:ILE:HD11	2.01	0.43
1:B:386:ASP:O	1:B:387:MET:C	2.59	0.43
1:A:93:HIS:O	1:A:97:ILE:HG13	2.19	0.43
1:A:109:VAL:O	1:A:113:THR:HG22	2.19	0.43
1:A:113:THR:O	1:A:116:ILE:N	2.48	0.43
1:A:218:SER:HB3	1:A:221:LEU:O	2.19	0.43
1:A:252:LEU:HA	1:A:255:GLU:CD	2.44	0.43
1:A:352:VAL:C	1:A:353:VAL:HG23	2.44	0.43
1:A:364:ALA:O	1:A:365:ALA:C	2.62	0.43
1:A:382:ARG:CA	1:A:387:MET:HB2	2.49	0.43
1:B:104:VAL:HA	1:B:107:ILE:CG1	2.47	0.43
1:B:126:MET:O	1:B:127:ALA:C	2.62	0.43
1:B:266:VAL:HG21	1:B:407:TYR:CG	2.54	0.43
1:A:181:PHE:O	1:A:183:TYR:N	2.52	0.42
1:A:235:PRO:HA	1:A:238:LEU:HD13	2.01	0.42
1:A:271:SER:O	1:A:272:THR:C	2.62	0.42
1:B:24:ILE:HB	1:B:164:MET:SD	2.59	0.42
1:B:118:ARG:C	1:B:118:ARG:HD2	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:PHE:C	1:B:215:ILE:N	2.77	0.42
1:B:317:ALA:HA	1:B:320:VAL:CG1	2.49	0.42
1:B:413:ASN:HD22	1:B:421:GLY:H	1.67	0.42
1:B:416:THR:HB	1:B:417:GLU:H	1.54	0.42
1:B:444:LEU:O	1:B:445:TYR:C	2.62	0.42
1:A:58:TRP:CE3	1:A:59:LEU:N	2.87	0.42
1:A:66:VAL:O	1:A:69:LEU:HB3	2.19	0.42
1:A:113:THR:C	1:A:116:ILE:H	2.26	0.42
1:A:134:MET:SD	1:A:198:VAL:N	2.92	0.42
1:A:180:ILE:CA	1:A:184:GLY:HA3	2.35	0.42
1:A:396:ILE:O	1:A:399:TRP:HB3	2.19	0.42
1:B:95:GLY:O	1:B:97:ILE:N	2.52	0.42
1:B:213:PHE:O	1:B:214:TYR:C	2.61	0.42
1:B:237:GLU:O	1:B:241:LEU:CD1	2.66	0.42
1:B:432:GLY:O	1:B:435:ALA:HB3	2.20	0.42
1:B:447:LEU:HD12	1:B:447:LEU:O	2.19	0.42
1:A:104:VAL:O	1:A:106:ILE:N	2.52	0.42
1:A:116:ILE:HG23	1:A:117:ILE:N	2.35	0.42
1:A:118:ARG:C	1:A:118:ARG:HD2	2.44	0.42
1:A:236:LYS:HA	1:A:239:ILE:HG13	2.02	0.42
1:A:298:VAL:HG11	1:A:317:ALA:O	2.20	0.42
1:A:360:LEU:HD21	1:A:423:LYS:HB3	1.99	0.42
1:A:393:ARG:CG	1:A:393:ARG:NH1	2.82	0.42
1:B:134:MET:SD	1:B:198:VAL:CA	3.05	0.42
1:B:191:LEU:CG	1:B:192:GLY:N	2.82	0.42
1:B:203:VAL:C	1:B:205:TRP:N	2.77	0.42
1:A:11:GLU:O	1:A:12:ALA:C	2.63	0.42
1:A:138:ILE:HA	1:A:141:VAL:CG2	2.49	0.42
1:A:176:PRO:HG2	1:A:177:LEU:HD22	2.00	0.42
1:A:200:THR:CA	1:A:203:VAL:HG23	2.48	0.42
1:A:353:VAL:C	1:A:357:ALA:CB	2.93	0.42
1:A:413:ASN:HD22	1:A:421:GLY:N	2.17	0.42
1:B:11:GLU:HB3	1:B:320:VAL:HB	2.00	0.42
1:B:244:LEU:HD23	1:B:388:THR:OG1	2.20	0.42
1:B:266:VAL:HG13	1:B:269:LEU:HD21	2.02	0.42
1:B:356:LEU:O	1:B:357:ALA:C	2.62	0.42
1:B:358:MET:O	1:B:361:LEU:HB2	2.19	0.42
1:B:393:ARG:CG	1:B:393:ARG:NH1	2.82	0.42
1:A:92:VAL:C	1:A:94:GLN:N	2.77	0.42
1:A:181:PHE:C	1:A:183:TYR:H	2.28	0.42
1:A:290:PHE:O	1:A:293:SER:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:LEU:HD12	1:B:15:LEU:C	2.43	0.42
1:B:73:VAL:O	1:B:76:VAL:HG12	2.20	0.42
1:B:73:VAL:N	1:B:74:PRO:CD	2.82	0.42
1:B:96:LEU:HB2	1:B:146:LEU:HG	2.01	0.42
1:B:163:ALA:HB3	1:B:164:MET:SD	2.60	0.42
1:B:206:ILE:O	1:B:210:LEU:CD2	2.58	0.42
1:B:334:LEU:C	1:B:337:VAL:HG12	2.45	0.42
1:B:387:MET:HE2	1:B:446:TRP:CH2	2.55	0.42
1:B:403:LEU:HD23	1:B:403:LEU:HA	1.78	0.42
1:A:135:HIS:O	1:A:136:ALA:C	2.62	0.42
1:A:180:ILE:CD1	1:A:186:PHE:HB2	2.50	0.42
1:A:274:VAL:HA	1:A:277:HIS:HB3	2.01	0.42
1:A:332:THR:HA	1:A:335:LEU:CG	2.49	0.42
1:B:142:PRO:O	1:B:145:LEU:CB	2.61	0.42
1:B:339:PHE:O	1:B:343:ILE:HG12	2.20	0.42
1:B:395:PHE:O	1:B:398:TYR:CE1	2.71	0.42
1:A:12:ALA:O	1:A:13:SER:C	2.60	0.42
1:A:108:ALA:O	1:A:109:VAL:C	2.62	0.42
1:A:131:VAL:HG23	1:A:135:HIS:CE1	2.54	0.42
1:A:266:VAL:CG1	1:A:269:LEU:HD21	2.49	0.42
1:A:436:ALA:HA	1:A:439:MET:HG2	2.00	0.42
1:B:159:LEU:HD21	1:B:220:ARG:HH11	1.83	0.42
1:B:234:GLN:C	1:B:238:LEU:HD13	2.45	0.42
1:B:287:VAL:O	1:B:291:PRO:HD2	2.18	0.42
1:B:318:ALA:CB	1:B:381:LEU:HD13	2.50	0.42
1:B:399:TRP:HE1	1:B:403:LEU:HD12	1.85	0.42
1:A:88:ILE:O	1:A:91:GLU:HB3	2.20	0.42
1:A:216:VAL:CG2	1:A:225:LYS:HD3	2.47	0.42
1:A:392:HIS:O	1:A:395:PHE:CB	2.67	0.42
1:B:34:PHE:O	1:B:35:VAL:O	2.37	0.42
1:B:72:LEU:HD11	1:B:383:GLY:O	2.19	0.42
1:B:134:MET:C	1:B:137:VAL:HB	2.45	0.42
1:B:162:PRO:C	1:B:165:VAL:HG12	2.31	0.42
1:B:452:ASP:O	1:B:455:GLN:HB3	2.19	0.42
1:A:49:ALA:O	1:A:53:ILE:HG13	2.20	0.42
1:A:198:VAL:O	1:A:199:ALA:C	2.62	0.42
1:A:238:LEU:CA	1:A:241:LEU:HD13	2.48	0.42
1:A:247:PRO:HG2	1:A:389:ALA:HA	1.99	0.42
1:A:348:THR:O	1:A:349:GLU:HG3	2.20	0.42
1:B:71:ALA:O	1:B:74:PRO:HB2	2.19	0.42
1:B:138:ILE:HA	1:B:141:VAL:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:LEU:CB	1:B:385:LYS:NZ	2.81	0.42
1:B:339:PHE:O	1:B:340:ARG:C	2.61	0.42
1:B:342:GLN:O	1:B:343:ILE:C	2.63	0.42
1:A:98:LEU:HA	1:A:101:LEU:HG	2.01	0.42
1:A:181:PHE:O	1:A:182:VAL:C	2.63	0.42
1:A:314:ALA:C	1:A:316:ILE:N	2.76	0.42
1:A:382:ARG:N	1:A:382:ARG:HD3	2.34	0.42
1:A:409:LEU:C	1:A:409:LEU:HD13	2.45	0.42
1:B:86:HIS:CE1	1:B:87:LYS:H	2.38	0.42
1:B:96:LEU:CD1	1:B:146:LEU:HD12	2.46	0.42
1:B:339:PHE:O	1:B:340:ARG:O	2.38	0.42
1:B:381:LEU:O	1:B:384:TYR:CG	2.73	0.42
1:B:392:HIS:O	1:B:395:PHE:CB	2.68	0.42
1:B:400:VAL:CG1	1:B:401:LEU:N	2.81	0.42
1:B:413:ASN:HB3	1:B:414:TRP:CZ3	2.55	0.42
1:B:415:LEU:HB3	1:B:416:THR:H	1.54	0.42
1:A:97:ILE:CG2	1:A:101:LEU:HD11	2.39	0.41
1:A:308:GLU:HB3	1:A:309:GLN:H	1.67	0.41
1:A:357:ALA:O	1:A:360:LEU:N	2.53	0.41
1:A:386:ASP:C	1:A:388:THR:N	2.71	0.41
1:B:427:LEU:HD23	1:B:428:GLY:CA	2.50	0.41
1:A:39:MET:SD	1:A:40:ALA:HB2	2.60	0.41
1:A:100:LEU:N	1:A:100:LEU:CD1	2.82	0.41
1:A:263:ALA:O	1:A:264:LEU:C	2.63	0.41
1:A:275:ALA:O	1:A:279:VAL:HB	2.20	0.41
1:A:388:THR:HA	1:A:391:PHE:CG	2.55	0.41
1:B:72:LEU:HD13	1:B:75:VAL:CG1	2.50	0.41
1:B:97:ILE:O	1:B:99:ALA:N	2.53	0.41
1:B:125:ALA:O	1:B:126:MET:C	2.63	0.41
1:B:147:PHE:CE2	1:B:211:LEU:HA	2.55	0.41
1:B:187:GLY:O	1:B:188:ALA:HB2	2.19	0.41
1:B:274:VAL:HG13	1:B:278:GLN:CD	2.44	0.41
1:B:287:VAL:O	1:B:291:PRO:HD3	2.20	0.41
1:A:155:ASP:O	1:A:156:GLY:C	2.62	0.41
1:A:219:LYS:CD	1:A:220:ARG:NE	2.83	0.41
1:A:454:VAL:O	1:A:458:LEU:HB2	2.20	0.41
1:B:18:LEU:HA	1:B:160:THR:HG21	2.02	0.41
1:B:86:HIS:C	1:B:88:ILE:H	2.28	0.41
1:B:181:PHE:C	1:B:183:TYR:H	2.28	0.41
1:B:276:ALA:O	1:B:277:HIS:O	2.38	0.41
1:B:408:ILE:HG12	1:B:411:MET:SD	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:GLU:CD	1:B:418:GLN:N	2.77	0.41
1:A:248:VAL:HG12	1:A:391:PHE:CZ	2.55	0.41
1:A:363:PHE:HD1	1:A:364:ALA:N	2.16	0.41
1:B:8:TYR:O	1:B:12:ALA:HB2	2.21	0.41
1:B:74:PRO:HB3	1:B:149:ALA:CA	2.50	0.41
1:B:185:LYS:O	1:B:186:PHE:CD2	2.73	0.41
1:B:219:LYS:CD	1:B:220:ARG:NE	2.84	0.41
1:B:408:ILE:O	1:B:412:THR:N	2.53	0.41
1:A:7:ARG:O	1:A:11:GLU:HG3	2.21	0.41
1:A:102:VAL:O	1:A:105:PRO:HD2	2.21	0.41
1:A:178:ASN:ND2	1:A:199:ALA:HB1	2.35	0.41
1:A:275:ALA:H	1:A:353:VAL:HG21	1.83	0.41
1:A:409:LEU:HA	1:A:412:THR:HB	2.01	0.41
1:B:80:ASN:OD1	1:B:80:ASN:O	2.39	0.41
1:B:117:ILE:CG2	1:B:118:ARG:H	2.18	0.41
1:B:122:VAL:C	1:B:124:GLU:N	2.73	0.41
1:B:266:VAL:CG2	1:B:407:TYR:CD1	3.03	0.41
1:B:275:ALA:HB2	1:B:353:VAL:CG2	2.49	0.41
1:B:276:ALA:HB1	1:B:426:TRP:NE1	2.34	0.41
1:B:363:PHE:CD2	1:B:426:TRP:HB3	2.55	0.41
1:A:235:PRO:CA	1:A:238:LEU:HD22	2.50	0.41
1:A:248:VAL:HG23	1:A:249:ALA:N	2.35	0.41
1:A:253:PHE:O	1:A:254:PHE:C	2.62	0.41
1:A:317:ALA:HA	1:A:320:VAL:CG1	2.50	0.41
1:B:42:GLY:HA2	1:B:49:ALA:HB3	2.01	0.41
1:B:237:GLU:C	1:B:240:ARG:H	2.29	0.41
1:B:380:SER:O	1:B:383:GLY:N	2.53	0.41
1:A:15:LEU:CG	1:A:16:ILE:N	2.84	0.41
1:A:131:VAL:O	1:A:134:MET:HB2	2.20	0.41
1:B:146:LEU:HD13	1:B:147:PHE:N	2.35	0.41
1:B:296:ALA:O	1:B:300:ILE:HG12	2.20	0.41
1:B:339:PHE:C	1:B:341:GLU:OE1	2.64	0.41
1:A:34:PHE:CD1	1:A:35:VAL:N	2.88	0.41
1:A:81:GLY:O	1:A:308:GLU:HG3	2.20	0.41
1:A:262:VAL:HG12	1:A:263:ALA:N	2.36	0.41
1:A:287:VAL:O	1:A:291:PRO:HD3	2.21	0.41
1:A:360:LEU:CD2	1:A:423:LYS:HB2	2.51	0.41
1:B:21:PRO:HB2	1:B:160:THR:HG23	2.03	0.41
1:B:92:VAL:C	1:B:94:GLN:N	2.74	0.41
1:B:137:VAL:O	1:B:141:VAL:HG23	2.21	0.41
1:B:273:VAL:O	1:B:277:HIS:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:LEU:O	1:B:289:MET:HB3	2.21	0.41
1:B:287:VAL:HG11	1:B:368:GLN:CD	2.40	0.41
1:A:11:GLU:HG2	1:A:316:ILE:CG2	2.50	0.41
1:A:23:LEU:C	1:A:23:LEU:CD1	2.94	0.41
1:A:58:TRP:CE3	1:A:59:LEU:HA	2.56	0.41
1:A:63:LEU:O	1:A:66:VAL:N	2.53	0.41
1:A:73:VAL:HG11	1:A:241:LEU:HD23	2.02	0.41
1:A:195:GLY:O	1:A:198:VAL:N	2.54	0.41
1:A:203:VAL:C	1:A:205:TRP:H	2.29	0.41
1:A:238:LEU:O	1:A:242:PHE:CD1	2.73	0.41
1:A:247:PRO:HB3	1:A:388:THR:O	2.21	0.41
1:A:251:ALA:O	1:A:255:GLU:CB	2.58	0.41
1:A:314:ALA:O	1:A:318:ALA:CB	2.66	0.41
1:A:382:ARG:HB3	1:A:387:MET:CB	2.51	0.41
1:A:398:TYR:CD2	1:A:432:GLY:C	2.98	0.41
1:B:8:TYR:O	1:B:12:ALA:HB3	2.21	0.41
1:B:47:ASP:C	1:B:49:ALA:N	2.75	0.41
1:B:72:LEU:CD1	1:B:75:VAL:HG21	2.51	0.41
1:B:107:ILE:CA	1:B:139:PHE:CZ	2.94	0.41
1:B:131:VAL:CA	1:B:134:MET:HB2	2.50	0.41
1:B:143:ALA:O	1:B:144:TYR:C	2.64	0.41
1:B:180:ILE:HD11	1:B:186:PHE:HB2	2.01	0.41
1:B:225:LYS:O	1:B:226:VAL:CG2	2.68	0.41
1:B:252:LEU:HA	1:B:255:GLU:CD	2.46	0.41
1:B:271:SER:O	1:B:272:THR:C	2.64	0.41
1:B:311:THR:HG23	1:B:312:LYS:N	2.36	0.41
1:B:314:ALA:C	1:B:316:ILE:N	2.79	0.41
1:B:320:VAL:C	1:B:322:LEU:N	2.79	0.41
1:B:339:PHE:O	1:B:343:ILE:CG1	2.69	0.41
1:B:356:LEU:O	1:B:360:LEU:N	2.34	0.41
1:B:384:TYR:CE1	1:B:446:TRP:HH2	2.36	0.41
1:B:388:THR:HA	1:B:391:PHE:CG	2.56	0.41
1:A:13:SER:O	1:A:14:ASN:C	2.62	0.41
1:A:88:ILE:CG1	1:A:89:PRO:N	2.84	0.41
1:A:97:ILE:C	1:A:99:ALA:N	2.75	0.41
1:A:111:PHE:C	1:A:111:PHE:CD2	2.96	0.41
1:A:126:MET:O	1:A:127:ALA:C	2.62	0.41
1:A:130:THR:O	1:A:134:MET:HG2	2.21	0.41
1:B:65:GLY:C	1:B:67:GLY:H	2.28	0.41
1:A:195:GLY:O	1:A:197:GLY:N	2.54	0.40
1:A:451:SER:C	1:A:453:ASP:H	2.27	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:GLY:HA3	1:B:253:PHE:CG	2.56	0.40
1:B:198:VAL:O	1:B:199:ALA:C	2.63	0.40
1:B:240:ARG:C	1:B:242:PHE:H	2.29	0.40
1:B:284:SER:C	1:B:286:LEU:N	2.79	0.40
1:B:341:GLU:OE1	1:B:341:GLU:N	2.53	0.40
1:B:447:LEU:O	1:B:450:GLN:NE2	2.53	0.40
1:A:3:ASN:O	1:A:5:VAL:HG23	2.21	0.40
1:A:60:PRO:HA	1:A:63:LEU:HB3	2.02	0.40
1:A:172:LEU:HD13	1:A:173:LEU:N	2.36	0.40
1:A:258:LEU:O	1:A:259:PHE:C	2.64	0.40
1:A:385:LYS:CB	1:A:387:MET:HE1	2.50	0.40
1:B:166:ILE:C	1:B:170:GLY:H	2.28	0.40
1:B:350:ASN:CG	1:B:352:VAL:H	2.29	0.40
1:B:362:LEU:HD23	1:B:362:LEU:C	2.46	0.40
1:B:364:ALA:O	1:B:365:ALA:C	2.64	0.40
1:B:447:LEU:HD13	1:B:450:GLN:HG2	2.04	0.40
1:A:57:ILE:O	1:A:57:ILE:HG22	2.22	0.40
1:A:96:LEU:CB	1:A:146:LEU:HG	2.51	0.40
1:A:232:LYS:H	1:A:233:PRO:HD3	1.85	0.40
1:A:360:LEU:HD13	1:A:426:TRP:CD1	2.56	0.40
1:B:66:VAL:O	1:B:69:LEU:HB3	2.21	0.40
1:B:70:MET:SD	1:B:99:ALA:N	2.94	0.40
1:B:233:PRO:N	1:B:235:PRO:HD2	2.37	0.40
1:B:412:THR:O	1:B:415:LEU:C	2.65	0.40
1:B:461:LYS:C	1:B:461:LYS:CD	2.94	0.40
1:A:71:ALA:HA	1:A:74:PRO:HD2	1.98	0.40
1:A:113:THR:C	1:A:116:ILE:HG22	2.46	0.40
1:A:129:LYS:O	1:A:132:GLY:HA3	2.22	0.40
1:A:326:LEU:O	1:A:327:ALA:C	2.65	0.40
1:A:412:THR:HA	1:A:415:LEU:HB2	2.03	0.40
1:B:26:SER:C	1:B:28:ALA:N	2.78	0.40
1:B:34:PHE:O	1:B:35:VAL:C	2.64	0.40
1:B:72:LEU:HD13	1:B:75:VAL:HG11	2.03	0.40
1:B:257:THR:O	1:B:260:ALA:HB3	2.21	0.40
1:B:357:ALA:O	1:B:358:MET:C	2.64	0.40
1:A:110:LEU:HD13	1:A:110:LEU:C	2.47	0.40
1:A:398:TYR:HD2	1:A:432:GLY:O	2.04	0.40
1:B:10:LYS:NZ	1:B:305:LYS:NZ	2.70	0.40
1:B:24:ILE:HD13	1:B:24:ILE:HA	1.99	0.40
1:B:76:VAL:HG23	1:B:78:GLN:HE21	1.83	0.40
1:B:186:PHE:HD2	1:B:186:PHE:HA	1.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:LEU:CD1	1:B:210:LEU:HD13	2.49	0.40
1:B:218:SER:HB3	1:B:221:LEU:O	2.21	0.40
1:B:259:PHE:O	1:B:260:ALA:C	2.65	0.40
1:B:353:VAL:O	1:B:357:ALA:CA	2.68	0.40
1:B:411:MET:C	1:B:414:TRP:HB2	2.46	0.40
1:B:461:LYS:HB3	1:B:461:LYS:HE3	1.88	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	458/460 (100%)	218 (48%)	118 (26%)	122 (27%)	0	0
1	B	458/460 (100%)	221 (48%)	121 (26%)	116 (25%)	0	1
All	All	916/920 (100%)	439 (48%)	239 (26%)	238 (26%)	0	1

All (238) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	ALA
1	A	35	VAL
1	A	56	SER
1	A	76	VAL
1	A	121	ASP
1	A	124	GLU
1	A	125	ALA
1	A	126	MET
1	A	128	THR
1	A	152	SER
1	A	165	VAL
1	A	184	GLY

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Mol	Chain	Res	Type
1	A	211	LEU
1	A	213	PHE
1	A	226	VAL
1	A	251	ALA
1	A	261	VAL
1	A	273	VAL
1	A	277	HIS
1	A	279	VAL
1	A	280	ALA
1	A	282	ASN
1	A	285	SER
1	A	311	THR
1	A	314	ALA
1	A	316	ILE
1	A	340	ARG
1	A	346	LEU
1	A	352	VAL
1	A	353	VAL
1	A	376	VAL
1	A	378	ALA
1	A	416	THR
1	A	444	LEU
1	A	445	TYR
1	B	19	ALA
1	B	35	VAL
1	B	110	LEU
1	B	121	ASP
1	B	124	GLU
1	B	126	MET
1	B	128	THR
1	B	152	SER
1	B	165	VAL
1	B	184	GLY
1	B	211	LEU
1	B	213	PHE
1	B	226	VAL
1	B	251	ALA
1	B	261	VAL
1	B	273	VAL
1	B	277	HIS
1	B	279	VAL
1	B	280	ALA

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Mol	Chain	Res	Type
1	B	282	ASN
1	B	285	SER
1	B	311	THR
1	B	314	ALA
1	B	316	ILE
1	B	340	ARG
1	B	352	VAL
1	B	354	VAL
1	B	376	VAL
1	B	378	ALA
1	B	399	TRP
1	B	416	THR
1	B	444	LEU
1	A	7	ARG
1	A	9	LYS
1	A	33	GLY
1	A	47	ASP
1	A	50	ALA
1	A	110	LEU
1	A	160	THR
1	A	167	GLY
1	A	179	TRP
1	A	183	TYR
1	A	214	TYR
1	A	219	LYS
1	A	230	PHE
1	A	244	LEU
1	A	262	VAL
1	A	276	ALA
1	A	278	GLN
1	A	281	LEU
1	A	317	ALA
1	A	318	ALA
1	A	321	GLY
1	A	322	LEU
1	A	323	MET
1	A	399	TRP
1	A	402	GLY
1	A	417	GLU
1	A	446	TRP
1	A	448	GLN
1	B	7	ARG

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Mol	Chain	Res	Type
1	B	21	PRO
1	B	33	GLY
1	B	47	ASP
1	B	50	ALA
1	B	56	SER
1	B	64	PHE
1	B	76	VAL
1	B	156	GLY
1	B	160	THR
1	B	167	GLY
1	B	183	TYR
1	B	214	TYR
1	B	219	LYS
1	B	230	PHE
1	B	244	LEU
1	B	262	VAL
1	B	269	LEU
1	B	278	GLN
1	B	317	ALA
1	B	318	ALA
1	B	321	GLY
1	B	323	MET
1	B	346	LEU
1	B	353	VAL
1	B	369	CYS
1	B	379	GLY
1	B	402	GLY
1	B	417	GLU
1	A	21	PRO
1	A	39	MET
1	A	64	PHE
1	A	82	ALA
1	A	84	ARG
1	A	158	SER
1	A	163	ALA
1	A	223	HIS
1	A	275	ALA
1	A	284	SER
1	A	327	ALA
1	A	334	LEU
1	A	339	PHE
1	B	9	LYS

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Mol	Chain	Res	Type
1	B	39	MET
1	B	82	ALA
1	B	84	ARG
1	B	108	ALA
1	B	118	ARG
1	B	158	SER
1	B	179	TRP
1	B	186	PHE
1	B	243	ARG
1	B	275	ALA
1	B	276	ALA
1	B	281	LEU
1	B	284	SER
1	B	322	LEU
1	B	334	LEU
1	B	339	PHE
1	B	341	GLU
1	B	349	GLU
1	B	385	LYS
1	B	445	TYR
1	A	13	SER
1	A	29	GLN
1	A	31	GLY
1	A	37	THR
1	A	79	LEU
1	A	108	ALA
1	A	117	ILE
1	A	130	THR
1	A	151	ARG
1	A	156	GLY
1	A	186	PHE
1	A	218	SER
1	A	231	HIS
1	A	232	LYS
1	A	269	LEU
1	A	320	VAL
1	A	330	CYS
1	A	341	GLU
1	A	349	GLU
1	A	354	VAL
1	A	369	CYS
1	A	379	GLY

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Mol	Chain	Res	Type
1	A	447	LEU
1	B	13	SER
1	B	37	THR
1	B	45	ALA
1	B	79	LEU
1	B	101	LEU
1	B	125	ALA
1	B	130	THR
1	B	163	ALA
1	B	223	HIS
1	B	231	HIS
1	B	232	LYS
1	B	320	VAL
1	A	28	ALA
1	A	42	GLY
1	A	77	ALA
1	A	122	VAL
1	A	161	LYS
1	A	162	PRO
1	A	172	LEU
1	A	185	LYS
1	A	243	ARG
1	A	315	ALA
1	A	355	ALA
1	B	29	GLN
1	B	42	GLY
1	B	96	LEU
1	B	117	ILE
1	B	122	VAL
1	B	161	LYS
1	B	315	ALA
1	B	327	ALA
1	B	330	CYS
1	B	377	ALA
1	A	96	LEU
1	A	101	LEU
1	A	375	VAL
1	A	377	ALA
1	A	385	LYS
1	B	28	ALA
1	B	31	GLY
1	B	83	GLY

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Mol	Chain	Res	Type
1	B	138	ILE
1	B	151	ARG
1	B	162	PRO
1	A	83	GLY
1	A	138	ILE
1	B	5	VAL
1	B	267	ALA
1	B	295	GLY
1	B	92	VAL
1	A	5	VAL
1	A	224	VAL
1	A	266	VAL
1	A	267	ALA
1	B	97	ILE
1	A	274	VAL
1	B	224	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	364/364 (100%)	292 (80%)	72 (20%)	1	9
1	B	364/364 (100%)	289 (79%)	75 (21%)	1	7
All	All	728/728 (100%)	581 (80%)	147 (20%)	1	9

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	7	ARG
1	A	16	ILE
1	A	34	PHE
1	A	39	MET
1	A	60	PRO
1	A	61	SER

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Mol	Chain	Res	Type
1	A	62	ILE
1	A	63	LEU
1	A	72	LEU
1	A	90	PHE
1	A	93	HIS
1	A	94	GLN
1	A	105	PRO
1	A	115	PHE
1	A	124	GLU
1	A	144	TYR
1	A	145	LEU
1	A	146	LEU
1	A	148	GLN
1	A	166	ILE
1	A	171	LEU
1	A	194	VAL
1	A	204	TYR
1	A	208	LEU
1	A	210	LEU
1	A	211	LEU
1	A	219	LYS
1	A	221	LEU
1	A	223	HIS
1	A	226	VAL
1	A	243	ARG
1	A	244	LEU
1	A	247	PRO
1	A	252	LEU
1	A	256	VAL
1	A	278	GLN
1	A	292	MET
1	A	312	LYS
1	A	326	LEU
1	A	331	ILE
1	A	337	VAL
1	A	341	GLU
1	A	345	LEU
1	A	362	LEU
1	A	363	PHE
1	A	371	ASP
1	A	384	TYR
1	A	385	LYS

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Mol	Chain	Res	Type
1	A	387	MET
1	A	391	PHE
1	A	393	ARG
1	A	395	PHE
1	A	396	ILE
1	A	398	TYR
1	A	400	VAL
1	A	404	PRO
1	A	405	THR
1	A	412	THR
1	A	414	TRP
1	A	415	LEU
1	A	417	GLU
1	A	420	LEU
1	A	425	PHE
1	A	426	TRP
1	A	427	LEU
1	A	440	LEU
1	A	444	LEU
1	A	447	LEU
1	A	449	LYS
1	A	455	GLN
1	A	458	LEU
1	B	3	ASN
1	B	5	VAL
1	B	7	ARG
1	B	14	ASN
1	B	16	ILE
1	B	29	GLN
1	B	34	PHE
1	B	39	MET
1	B	57	ILE
1	B	60	PRO
1	B	61	SER
1	B	62	ILE
1	B	63	LEU
1	B	72	LEU
1	B	90	PHE
1	B	93	HIS
1	B	94	GLN
1	B	105	PRO
1	B	115	PHE

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Mol	Chain	Res	Type
1	B	119	PHE
1	B	124	GLU
1	B	144	TYR
1	B	145	LEU
1	B	148	GLN
1	B	166	ILE
1	B	171	LEU
1	B	186	PHE
1	B	194	VAL
1	B	204	TYR
1	B	208	LEU
1	B	210	LEU
1	B	211	LEU
1	B	219	LYS
1	B	221	LEU
1	B	223	HIS
1	B	226	VAL
1	B	243	ARG
1	B	244	LEU
1	B	252	LEU
1	B	256	VAL
1	B	266	VAL
1	B	278	GLN
1	B	292	MET
1	B	312	LYS
1	B	326	LEU
1	B	331	ILE
1	B	337	VAL
1	B	341	GLU
1	B	345	LEU
1	B	362	LEU
1	B	363	PHE
1	B	371	ASP
1	B	385	LYS
1	B	387	MET
1	B	391	PHE
1	B	393	ARG
1	B	395	PHE
1	B	396	ILE
1	B	398	TYR
1	B	400	VAL
1	B	404	PRO

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Mol	Chain	Res	Type
1	B	405	THR
1	B	412	THR
1	B	414	TRP
1	B	415	LEU
1	B	420	LEU
1	B	425	PHE
1	B	426	TRP
1	B	427	LEU
1	B	444	LEU
1	B	445	TYR
1	B	449	LYS
1	B	455	GLN
1	B	458	LEU
1	B	461	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	78	GLN
1	A	85	GLN
1	A	148	GLN
1	A	174	ASN
1	A	277	HIS
1	A	282	ASN
1	A	350	ASN
1	A	359	GLN
1	A	442	GLN
1	A	448	GLN
1	A	450	GLN
1	A	455	GLN
1	B	3	ASN
1	B	14	ASN
1	B	78	GLN
1	B	85	GLN
1	B	114	GLN
1	B	148	GLN
1	B	174	ASN
1	B	277	HIS
1	B	282	ASN
1	B	309	GLN
1	B	350	ASN

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Mol	Chain	Res	Type
1	B	359	GLN
1	B	442	GLN
1	B	455	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	460/460 (100%)	0.28	19 (4%) 41 35	34, 111, 174, 267	0
1	B	460/460 (100%)	0.28	18 (3%) 43 36	28, 117, 180, 253	0
All	All	920/920 (100%)	0.28	37 (4%) 42 35	28, 114, 180, 267	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	324	THR	5.6
1	B	244	LEU	4.7
1	B	325	GLY	4.6
1	A	196	CYS	4.5
1	B	379	GLY	4.3
1	A	79	LEU	4.2
1	B	196	CYS	3.9
1	B	386	ASP	3.9
1	A	247	PRO	3.8
1	A	442	GLN	3.7
1	B	153	PHE	3.7
1	B	41	GLY	3.6
1	A	128	THR	3.3
1	A	37	THR	3.3
1	A	441	GLY	3.0
1	B	442	GLN	2.9
1	A	127	ALA	2.8
1	A	248	VAL	2.8
1	B	113	THR	2.8
1	A	36	ASP	2.8
1	B	414	TRP	2.7
1	A	50	ALA	2.7
1	B	42	GLY	2.6
1	A	153	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	367	TYR	2.6
1	B	38	ILE	2.6
1	A	246	PHE	2.5
1	A	414	TRP	2.5
1	B	50	ALA	2.5
1	A	321	GLY	2.4
1	A	322	LEU	2.4
1	A	307	GLY	2.2
1	B	68	LEU	2.2
1	A	138	ILE	2.1
1	A	262	VAL	2.1
1	B	363	PHE	2.1
1	B	449	LYS	2.1

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	RB	A	5001	1/1	0.82	0.17	182,182,182,182	0
2	RB	B	5002	1/1	0.82	0.25	186,186,186,186	0

6.5 Other polymers [i](#)

There are no such residues in this entry.