



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 27, 2023 – 06:23 AM EDT

PDB ID : 3LRC
Title : Structure of E. coli AdiC (P1)
Authors : Gao, X.; Lu, F.; Zhou, L.; Shi, Y.
Deposited on : 2010-02-11
Resolution : 4.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

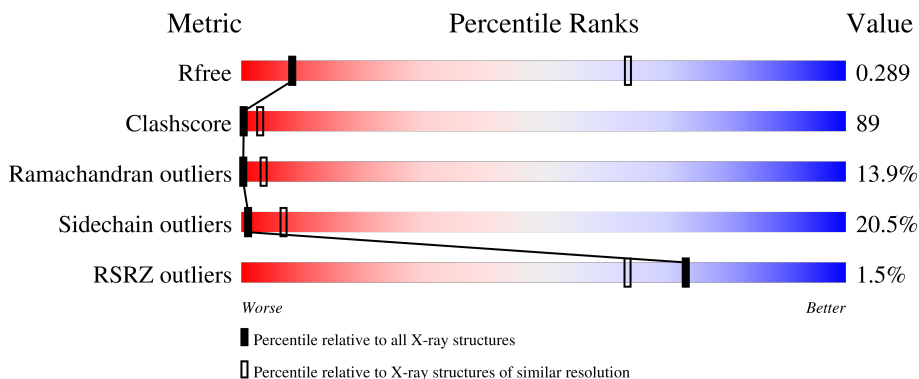
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

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	445	 2% 18% 54% 18% • 8%
1	B	445	 2% 19% 51% 20% • 8%
1	C	445	 % 18% 51% 20% • 8%
1	D	445	 % 18% 53% 19% • 8%

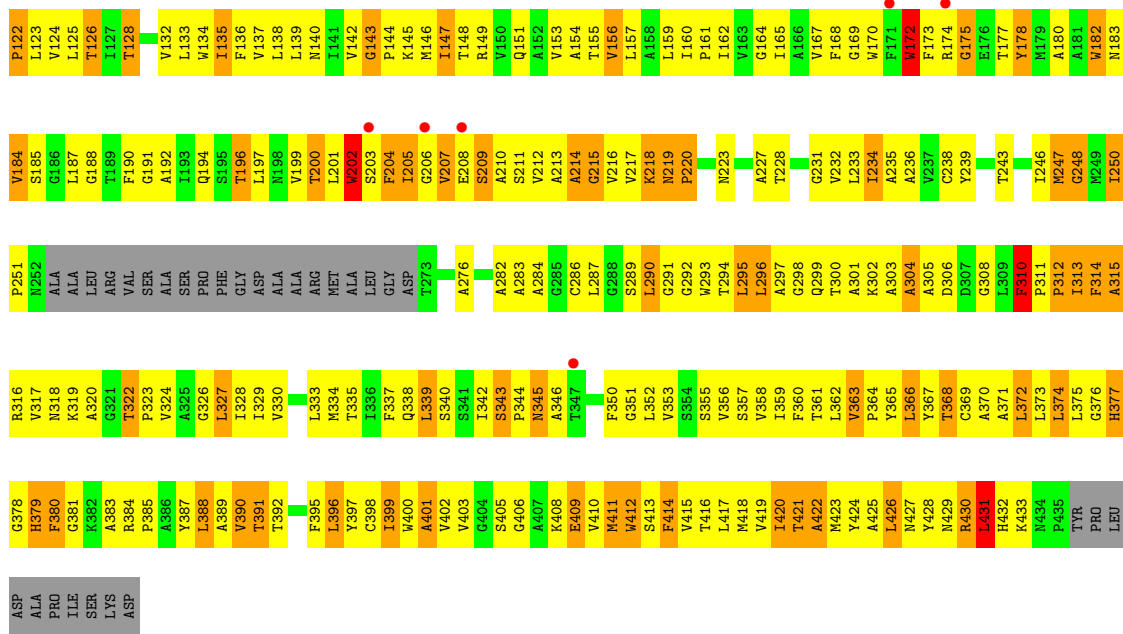
2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12144 atoms, of which 0 are hydrogens and 0 are deuteriums.

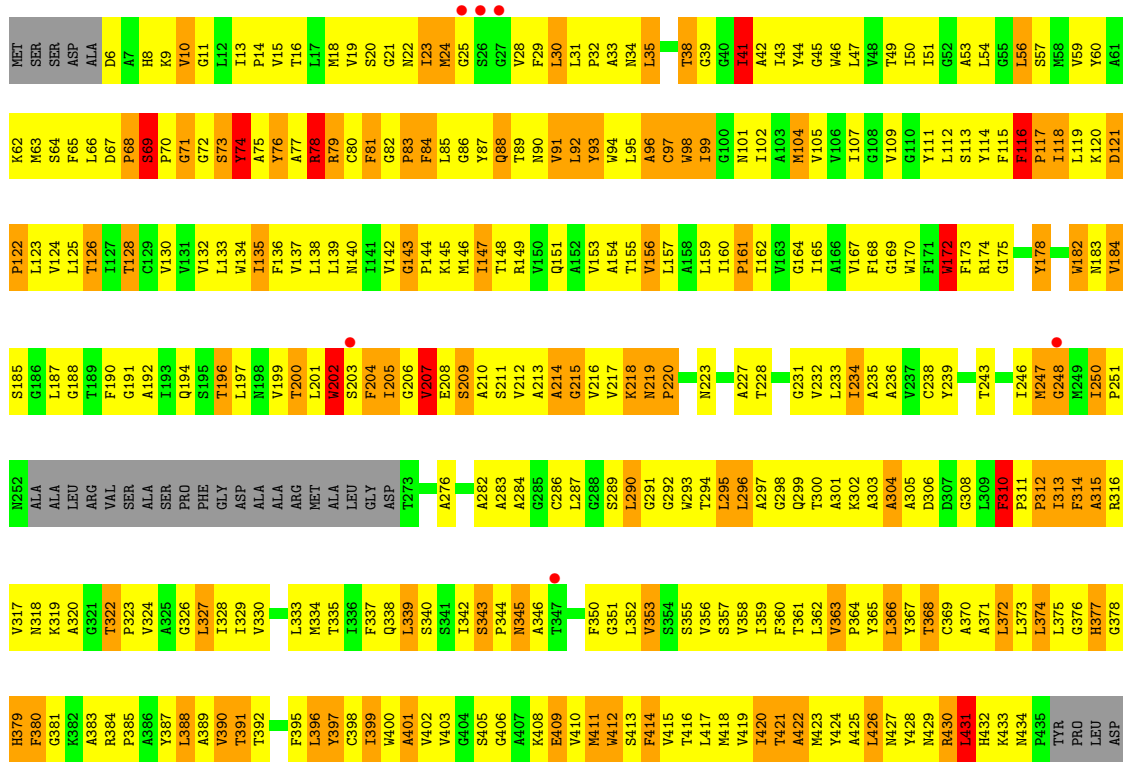
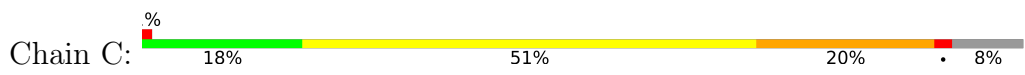
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Arginine/agmatine antiporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	410	Total	C	N	O	S	0	0	0
			3036	2020	481	514	21			
1	B	410	Total	C	N	O	S	0	0	0
			3036	2020	481	514	21			
1	C	410	Total	C	N	O	S	0	0	0
			3036	2020	481	514	21			
1	D	410	Total	C	N	O	S	0	0	0
			3036	2020	481	514	21			

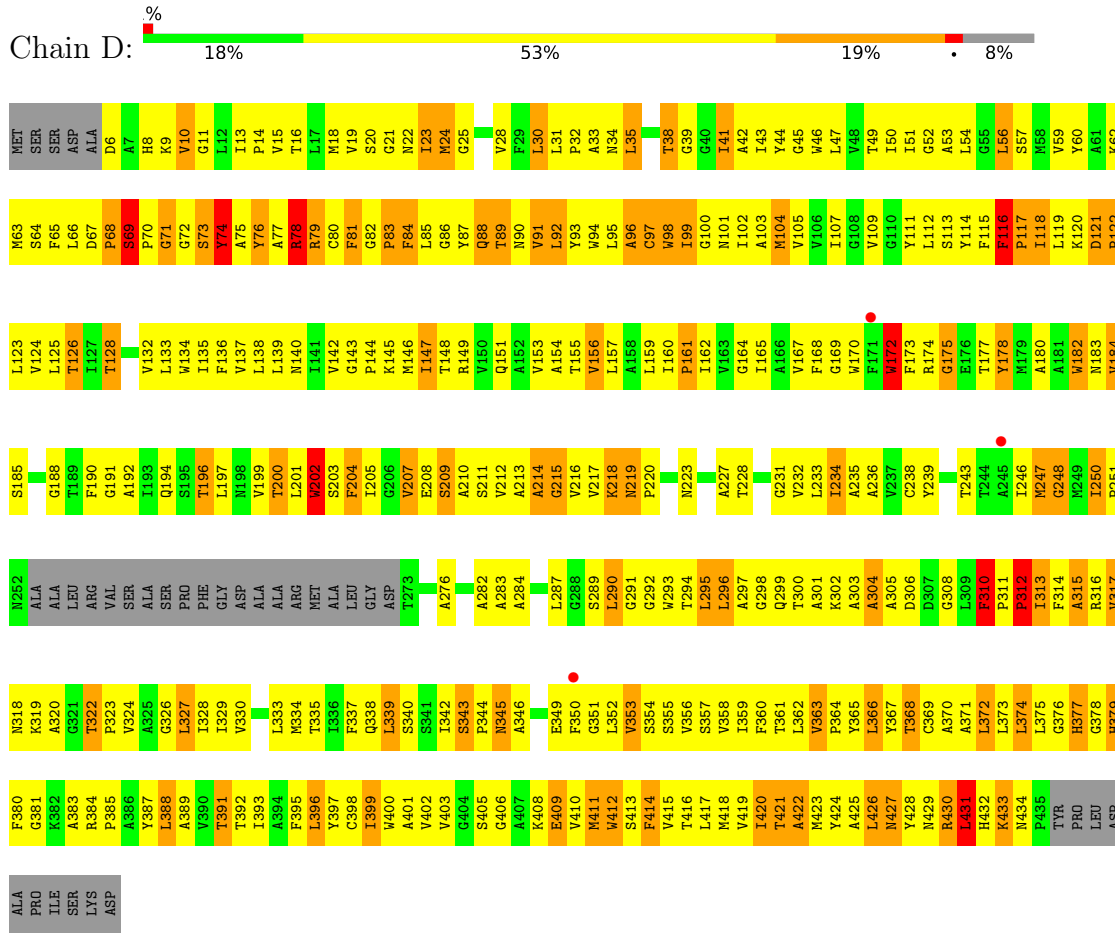


Molecule 1: Arginine/agmatine antiporter



Molecule 1: Arginine/agmatine antiporter





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	81.88Å 111.67Å 113.76Å 80.03° 74.34° 68.83°	Depositor
Resolution (Å)	30.00 – 4.00 32.20 – 4.00	Depositor EDS
% Data completeness (in resolution range)	95.7 (30.00-4.00) 96.9 (32.20-4.00)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 3.99Å)	Xtrriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.319 , 0.331 0.283 , 0.289	Depositor DCC
R_{free} test set	1472 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	184.3	Xtrriage
Anisotropy	0.363	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 219.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	12144	wwPDB-VP
Average B, all atoms (Å ²)	301.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.00% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.47	0/3115	0.68	0/4264
1	B	0.47	0/3115	0.68	0/4264
1	C	0.46	0/3115	0.68	0/4264
1	D	0.47	0/3115	0.69	0/4264
All	All	0.47	0/12460	0.68	0/17056

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	8

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	431	LEU	Peptide
1	A	79	ARG	Peptide
1	B	431	LEU	Peptide
1	B	79	ARG	Peptide
1	C	431	LEU	Peptide
1	C	79	ARG	Peptide
1	D	431	LEU	Peptide
1	D	79	ARG	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3036	0	3141	582	0
1	B	3036	0	3141	589	0
1	C	3036	0	3141	584	0
1	D	3036	0	3141	574	0
All	All	12144	0	12564	2194	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 89.

All (2194) 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:D:188:GLY:O	1:D:192:ALA:HB2	1.29	1.30
1:B:188:GLY:O	1:B:192:ALA:HB2	1.29	1.29
1:A:188:GLY:O	1:A:192:ALA:HB2	1.29	1.27
1:C:188:GLY:O	1:C:192:ALA:HB2	1.30	1.26
1:B:38:THR:HB	1:B:39:GLY:HA3	1.29	1.14
1:D:38:THR:HB	1:D:39:GLY:HA3	1.29	1.14
1:B:66:LEU:O	1:B:68:PRO:HD3	1.50	1.11
1:C:85:LEU:HD21	1:D:85:LEU:HD21	1.14	1.11
1:C:92:LEU:HD11	1:C:363:VAL:HG21	1.11	1.11
1:C:315:ALA:HB1	1:C:316:ARG:HA	1.10	1.10
1:D:315:ALA:HB1	1:D:316:ARG:HA	1.09	1.09
1:A:85:LEU:HD21	1:B:85:LEU:HD21	1.13	1.09
1:A:38:THR:HB	1:A:39:GLY:HA3	1.28	1.09
1:A:66:LEU:O	1:A:68:PRO:HD3	1.53	1.09
1:C:66:LEU:O	1:C:68:PRO:HD3	1.49	1.08
1:D:66:LEU:O	1:D:68:PRO:HD3	1.53	1.08
1:A:92:LEU:HD11	1:A:363:VAL:HG21	1.11	1.08
1:D:92:LEU:HD11	1:D:363:VAL:HG21	1.10	1.07
1:B:92:LEU:HD11	1:B:363:VAL:HG21	1.09	1.07
1:A:315:ALA:HB1	1:A:316:ARG:HA	1.11	1.05
1:C:16:THR:HG22	1:C:227:ALA:HA	1.37	1.05
1:D:60:TYR:CE2	1:D:368:THR:HG21	1.91	1.05
1:B:311:PRO:HD3	1:B:426:LEU:HD21	1.05	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:ALA:HB1	1:B:316:ARG:HA	1.10	1.04
1:C:38:THR:HB	1:C:39:GLY:HA3	1.29	1.04
1:C:60:TYR:CE2	1:C:368:THR:HG21	1.92	1.04
1:D:60:TYR:HE2	1:D:368:THR:HG21	1.23	1.04
1:A:60:TYR:CE2	1:A:368:THR:HG21	1.92	1.04
1:B:16:THR:HG22	1:B:227:ALA:HA	1.40	1.04
1:B:60:TYR:CE2	1:B:368:THR:HG21	1.93	1.03
1:A:16:THR:HG22	1:A:227:ALA:HA	1.40	1.02
1:C:311:PRO:HD3	1:C:426:LEU:HD21	1.04	1.02
1:D:64:SER:O	1:D:68:PRO:HG3	1.59	1.02
1:A:164:GLY:O	1:A:168:PHE:HB2	1.61	1.01
1:B:360:PHE:HE1	1:B:413:SER:HA	1.23	1.01
1:C:360:PHE:HE1	1:C:413:SER:HA	1.24	1.01
1:C:60:TYR:HE2	1:C:368:THR:HG21	1.25	1.01
1:B:313:ILE:O	1:B:315:ALA:HB3	1.59	1.00
1:D:16:THR:HG22	1:D:227:ALA:HA	1.41	1.00
1:D:313:ILE:O	1:D:315:ALA:HB3	1.62	1.00
1:A:421:THR:HG22	1:A:422:ALA:N	1.76	0.99
1:C:313:ILE:O	1:C:315:ALA:HB3	1.61	0.99
1:D:311:PRO:HD3	1:D:426:LEU:CD2	1.91	0.99
1:B:302:LYS:HG2	1:B:323:PRO:HB3	1.45	0.99
1:B:365:TYR:HB3	1:B:398:CYS:SG	2.02	0.99
1:A:60:TYR:HE2	1:A:368:THR:HG21	1.22	0.99
1:A:414:PHE:HB2	1:B:414:PHE:HD1	1.26	0.99
1:D:311:PRO:CD	1:D:426:LEU:HD21	1.92	0.99
1:B:64:SER:O	1:B:68:PRO:HG3	1.63	0.99
1:D:164:GLY:O	1:D:168:PHE:HB2	1.60	0.98
1:A:64:SER:O	1:A:68:PRO:HG3	1.64	0.98
1:A:313:ILE:O	1:A:315:ALA:HB3	1.62	0.98
1:A:311:PRO:HD3	1:A:426:LEU:CD2	1.93	0.98
1:C:164:GLY:O	1:C:168:PHE:HB2	1.62	0.98
1:D:92:LEU:CD1	1:D:363:VAL:HG21	1.94	0.97
1:A:311:PRO:HD3	1:A:426:LEU:HD21	0.98	0.97
1:B:92:LEU:CD1	1:B:363:VAL:HG21	1.95	0.97
1:C:81:PHE:HB3	1:C:82:GLY:HA2	1.47	0.96
1:A:302:LYS:HG2	1:A:323:PRO:HB3	1.47	0.96
1:B:164:GLY:O	1:B:168:PHE:HB2	1.63	0.96
1:C:64:SER:O	1:C:68:PRO:HG3	1.64	0.96
1:D:302:LYS:HG2	1:D:323:PRO:HB3	1.47	0.96
1:A:365:TYR:HB3	1:A:398:CYS:SG	2.06	0.96
1:A:84:PHE:CE1	1:B:85:LEU:HD11	2.01	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:ILE:HG22	1:C:246:ILE:HD13	1.46	0.96
1:A:311:PRO:CD	1:A:426:LEU:HD21	1.94	0.95
1:D:421:THR:HG22	1:D:422:ALA:N	1.78	0.95
1:C:302:LYS:HG2	1:C:323:PRO:HB3	1.45	0.95
1:B:60:TYR:HE2	1:B:368:THR:HG21	1.27	0.95
1:D:92:LEU:HD21	1:D:363:VAL:HG23	1.48	0.95
1:B:41:ILE:HG22	1:B:246:ILE:HD13	1.48	0.95
1:B:92:LEU:HD21	1:B:363:VAL:HG23	1.49	0.95
1:B:81:PHE:HB3	1:B:82:GLY:HA2	1.47	0.95
1:B:209:SER:HA	1:B:296:LEU:HD11	1.49	0.95
1:C:365:TYR:HB3	1:C:398:CYS:SG	2.05	0.95
1:D:360:PHE:HE1	1:D:413:SER:HA	1.31	0.95
1:A:85:LEU:HD11	1:B:84:PHE:CE1	2.02	0.94
1:A:118:ILE:HD12	1:A:119:LEU:O	1.68	0.94
1:B:421:THR:HG22	1:B:422:ALA:N	1.81	0.94
1:A:360:PHE:HE1	1:A:413:SER:HA	1.33	0.93
1:B:116:PHE:HB3	1:B:117:PRO:HD2	1.49	0.93
1:B:315:ALA:CB	1:B:316:ARG:HA	1.98	0.93
1:A:209:SER:HA	1:A:296:LEU:HD11	1.51	0.92
1:B:118:ILE:HD12	1:B:119:LEU:O	1.69	0.92
1:A:92:LEU:CD1	1:A:363:VAL:HG21	1.97	0.92
1:D:116:PHE:HB3	1:D:117:PRO:HD2	1.50	0.92
1:D:209:SER:HA	1:D:296:LEU:HD11	1.48	0.92
1:C:92:LEU:CD1	1:C:363:VAL:HG21	1.97	0.92
1:C:421:THR:HG22	1:C:422:ALA:N	1.84	0.92
1:C:250:ILE:H	1:C:251:PRO:HD2	1.33	0.92
1:D:119:LEU:HD13	1:D:124:VAL:HG11	1.52	0.92
1:C:116:PHE:HB3	1:C:117:PRO:HD2	1.49	0.92
1:C:315:ALA:HB1	1:C:316:ARG:CA	2.00	0.92
1:B:111:TYR:HB3	1:B:283:ALA:HB2	1.52	0.91
1:D:342:ILE:HB	1:D:343:SER:HB2	1.53	0.91
1:A:116:PHE:HB3	1:A:117:PRO:HD2	1.49	0.91
1:D:365:TYR:HB3	1:D:398:CYS:SG	2.10	0.91
1:A:342:ILE:HB	1:A:343:SER:HB2	1.51	0.91
1:C:119:LEU:HD13	1:C:124:VAL:HG11	1.51	0.91
1:D:84:PHE:CE1	1:D:85:LEU:HD23	2.06	0.91
1:C:92:LEU:HD21	1:C:363:VAL:HG23	1.49	0.91
1:C:414:PHE:HD1	1:D:414:PHE:HB2	1.35	0.91
1:C:111:TYR:HB3	1:C:283:ALA:HB2	1.50	0.91
1:B:315:ALA:HB1	1:B:316:ARG:CA	2.00	0.91
1:D:315:ALA:HB1	1:D:316:ARG:CA	2.00	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:ILE:H	1:B:251:PRO:HD2	1.34	0.90
1:B:342:ILE:HB	1:B:343:SER:HB2	1.53	0.90
1:B:119:LEU:HD13	1:B:124:VAL:HG11	1.51	0.90
1:D:118:ILE:HD12	1:D:119:LEU:O	1.71	0.90
1:A:250:ILE:H	1:A:251:PRO:HD2	1.35	0.90
1:A:85:LEU:HD21	1:B:85:LEU:CD2	2.00	0.90
1:A:315:ALA:HB1	1:A:316:ARG:CA	2.00	0.90
1:A:188:GLY:O	1:A:192:ALA:CB	2.19	0.90
1:D:32:PRO:HG3	1:D:243:THR:HG22	1.54	0.90
1:D:311:PRO:HD3	1:D:426:LEU:HD21	0.96	0.90
1:D:250:ILE:H	1:D:251:PRO:HD2	1.35	0.89
1:D:119:LEU:HD22	1:D:124:VAL:HG21	1.54	0.89
1:A:111:TYR:HB3	1:A:283:ALA:HB2	1.54	0.89
1:A:85:LEU:CD2	1:B:85:LEU:HD21	2.01	0.89
1:C:118:ILE:HD12	1:C:119:LEU:O	1.71	0.89
1:C:63:MET:HG3	1:C:76:TYR:CE2	2.07	0.89
1:A:81:PHE:HB3	1:A:82:GLY:HA2	1.53	0.89
1:A:119:LEU:HD13	1:A:124:VAL:HG11	1.53	0.89
1:D:111:TYR:HB3	1:D:283:ALA:HB2	1.55	0.89
1:C:84:PHE:CE1	1:D:85:LEU:HD11	2.07	0.89
1:A:85:LEU:HD11	1:B:84:PHE:CD1	2.08	0.89
1:C:85:LEU:HD11	1:D:84:PHE:CE1	2.07	0.88
1:A:41:ILE:HG22	1:A:246:ILE:HD13	1.56	0.88
1:A:119:LEU:HD22	1:A:124:VAL:HG21	1.55	0.88
1:C:311:PRO:HD3	1:C:426:LEU:CD2	1.98	0.88
1:A:84:PHE:CE1	1:A:85:LEU:HD23	2.08	0.88
1:B:119:LEU:HD22	1:B:124:VAL:HG21	1.56	0.88
1:C:24:MET:HB3	1:C:25:GLY:HA2	1.56	0.88
1:D:92:LEU:HD21	1:D:363:VAL:CG2	2.04	0.88
1:A:414:PHE:HB2	1:B:414:PHE:CD1	2.08	0.87
1:C:250:ILE:H	1:C:251:PRO:CD	1.87	0.87
1:D:90:ASN:OD1	1:D:300:THR:O	1.91	0.87
1:D:188:GLY:O	1:D:192:ALA:CB	2.20	0.87
1:C:119:LEU:HD22	1:C:124:VAL:HG21	1.56	0.87
1:C:209:SER:HA	1:C:296:LEU:HD11	1.52	0.87
1:C:342:ILE:HB	1:C:343:SER:HB2	1.53	0.87
1:D:24:MET:HB3	1:D:25:GLY:HA2	1.56	0.87
1:B:188:GLY:O	1:B:192:ALA:CB	2.20	0.87
1:B:32:PRO:HG3	1:B:243:THR:HG22	1.57	0.87
1:C:85:LEU:CD2	1:D:85:LEU:HD21	2.04	0.87
1:A:24:MET:HB3	1:A:25:GLY:HA2	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:PHE:HB3	1:D:82:GLY:HA2	1.56	0.86
1:B:250:ILE:H	1:B:251:PRO:CD	1.87	0.86
1:C:92:LEU:HD21	1:C:363:VAL:CG2	2.05	0.86
1:B:84:PHE:CE1	1:B:85:LEU:HD23	2.10	0.86
1:A:250:ILE:H	1:A:251:PRO:CD	1.88	0.86
1:B:311:PRO:HD3	1:B:426:LEU:CD2	1.99	0.86
1:A:373:LEU:HD13	1:B:428:TYR:OH	1.76	0.85
1:A:41:ILE:HG13	1:A:43:ILE:CG1	2.06	0.85
1:C:188:GLY:O	1:C:192:ALA:CB	2.20	0.85
1:D:202:TRP:CE3	1:D:358:VAL:HG11	2.12	0.85
1:D:250:ILE:H	1:D:251:PRO:CD	1.89	0.85
1:B:41:ILE:CG2	1:B:246:ILE:HD13	2.06	0.85
1:B:92:LEU:HD21	1:B:363:VAL:CG2	2.06	0.85
1:C:32:PRO:HG3	1:C:243:THR:HG22	1.58	0.85
1:D:315:ALA:CB	1:D:316:ARG:HA	1.98	0.85
1:A:92:LEU:HD21	1:A:363:VAL:HG23	1.57	0.85
1:A:90:ASN:OD1	1:A:300:THR:O	1.94	0.85
1:A:342:ILE:N	1:A:343:SER:HB2	1.92	0.85
1:D:41:ILE:HG22	1:D:246:ILE:HD13	1.57	0.85
1:C:41:ILE:CG2	1:C:246:ILE:HD13	2.06	0.84
1:A:315:ALA:CB	1:A:316:ARG:HA	1.99	0.84
1:A:78:ARG:HA	1:A:82:GLY:HA3	1.58	0.84
1:B:24:MET:HB3	1:B:25:GLY:HA2	1.57	0.84
1:B:202:TRP:CE3	1:B:358:VAL:HG11	2.11	0.84
1:A:202:TRP:CE3	1:A:358:VAL:HG11	2.13	0.84
1:D:425:ALA:C	1:D:427:ASN:H	1.78	0.84
1:B:365:TYR:HB3	1:B:398:CYS:HG	1.37	0.84
1:C:84:PHE:CE1	1:C:85:LEU:HD23	2.11	0.84
1:C:133:LEU:HD23	1:C:290:LEU:HD11	1.60	0.84
1:D:78:ARG:HA	1:D:82:GLY:HA3	1.57	0.83
1:B:412:TRP:HA	1:B:412:TRP:CE3	2.12	0.83
1:B:425:ALA:C	1:B:427:ASN:H	1.80	0.83
1:D:412:TRP:CE3	1:D:412:TRP:HA	2.12	0.83
1:A:414:PHE:HD1	1:B:414:PHE:HB2	1.43	0.83
1:D:342:ILE:N	1:D:343:SER:HB2	1.94	0.83
1:B:360:PHE:CE1	1:B:413:SER:HA	2.13	0.83
1:C:412:TRP:HA	1:C:412:TRP:CE3	2.12	0.83
1:C:202:TRP:CE3	1:C:358:VAL:HG11	2.13	0.82
1:C:93:TYR:CE2	1:C:97:CYS:SG	2.72	0.82
1:D:412:TRP:HA	1:D:412:TRP:HE3	1.45	0.82
1:A:38:THR:HB	1:A:39:GLY:CA	2.09	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ALA:HB3	1:A:228:THR:HG22	1.61	0.82
1:C:38:THR:HB	1:C:39:GLY:CA	2.09	0.82
1:A:32:PRO:HG3	1:A:243:THR:HG22	1.61	0.82
1:A:425:ALA:C	1:A:427:ASN:H	1.81	0.82
1:B:78:ARG:HA	1:B:82:GLY:HA3	1.61	0.82
1:B:342:ILE:N	1:B:343:SER:HB2	1.94	0.82
1:C:425:ALA:C	1:C:427:ASN:H	1.81	0.82
1:B:38:THR:HB	1:B:39:GLY:CA	2.08	0.81
1:C:311:PRO:CD	1:C:426:LEU:HD21	2.00	0.81
1:D:133:LEU:HD23	1:D:290:LEU:HD11	1.61	0.81
1:B:406:GLY:HA3	1:B:409:GLU:OE2	1.81	0.81
1:C:73:SER:H	1:C:76:TYR:HE1	1.23	0.81
1:D:421:THR:HG22	1:D:422:ALA:H	1.42	0.81
1:C:342:ILE:N	1:C:343:SER:HB2	1.95	0.81
1:A:412:TRP:CE3	1:A:412:TRP:HA	2.11	0.81
1:A:412:TRP:HA	1:A:412:TRP:HE3	1.44	0.81
1:C:85:LEU:HD21	1:D:85:LEU:CD2	2.05	0.81
1:A:38:THR:CB	1:A:39:GLY:HA3	2.10	0.81
1:A:60:TYR:HE2	1:A:368:THR:CG2	1.94	0.81
1:A:342:ILE:CA	1:A:343:SER:HB2	2.11	0.81
1:D:78:ARG:CA	1:D:82:GLY:HA3	2.10	0.81
1:A:133:LEU:HD23	1:A:290:LEU:HD11	1.61	0.81
1:D:210:ALA:HB3	1:D:228:THR:HG22	1.61	0.81
1:A:41:ILE:HG13	1:A:43:ILE:HG13	1.63	0.81
1:B:73:SER:H	1:B:76:TYR:HE1	1.26	0.81
1:D:38:THR:HB	1:D:39:GLY:CA	2.10	0.81
1:D:41:ILE:HG13	1:D:43:ILE:CG1	2.11	0.81
1:C:38:THR:CB	1:C:39:GLY:HA3	2.11	0.81
1:D:60:TYR:HE2	1:D:368:THR:CG2	1.94	0.81
1:A:411:MET:HG3	1:A:412:TRP:N	1.96	0.80
1:B:342:ILE:CA	1:B:343:SER:HB2	2.11	0.80
1:A:421:THR:HG22	1:A:422:ALA:H	1.42	0.80
1:C:412:TRP:HA	1:C:412:TRP:HE3	1.45	0.80
1:C:201:LEU:HG	1:C:401:ALA:HB2	1.63	0.80
1:D:84:PHE:HE1	1:D:85:LEU:HD23	1.44	0.80
1:A:92:LEU:HD21	1:A:363:VAL:CG2	2.11	0.80
1:C:173:PHE:HA	1:C:174:ARG:HB2	1.64	0.80
1:D:342:ILE:CA	1:D:343:SER:HB2	2.11	0.80
1:A:84:PHE:HE1	1:A:85:LEU:HD23	1.46	0.80
1:A:24:MET:O	1:A:28:VAL:HG23	1.82	0.80
1:A:342:ILE:HB	1:A:343:SER:CB	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:PHE:CD1	1:B:85:LEU:HD11	2.16	0.80
1:B:173:PHE:HA	1:B:174:ARG:HB2	1.64	0.80
1:C:78:ARG:HA	1:C:82:GLY:HA3	1.61	0.80
1:A:78:ARG:CA	1:A:82:GLY:HA3	2.11	0.80
1:A:173:PHE:HA	1:A:174:ARG:HB2	1.64	0.80
1:C:35:LEU:HD23	1:C:196:THR:HG22	1.64	0.79
1:C:84:PHE:CD1	1:D:85:LEU:HD11	2.16	0.79
1:C:374:LEU:O	1:C:375:LEU:HD23	1.81	0.79
1:A:95:LEU:HA	1:A:98:TRP:CZ3	2.18	0.79
1:A:140:ASN:HB3	1:A:327:LEU:HD22	1.62	0.79
1:B:133:LEU:HD23	1:B:290:LEU:HD11	1.61	0.79
1:C:56:LEU:HD11	1:C:365:TYR:HD1	1.47	0.79
1:B:210:ALA:HB3	1:B:228:THR:HG22	1.64	0.79
1:C:210:ALA:HB3	1:C:228:THR:HG22	1.64	0.79
1:B:412:TRP:HA	1:B:412:TRP:HE3	1.45	0.79
1:A:19:VAL:HG21	1:A:210:ALA:HB2	1.63	0.79
1:B:19:VAL:HG21	1:B:210:ALA:HB2	1.65	0.79
1:D:355:SER:O	1:D:358:VAL:HB	1.83	0.79
1:A:342:ILE:CB	1:A:343:SER:HB2	2.12	0.79
1:C:78:ARG:CA	1:C:82:GLY:HA3	2.13	0.79
1:C:315:ALA:CB	1:C:316:ARG:HA	1.98	0.79
1:C:342:ILE:CA	1:C:343:SER:HB2	2.12	0.79
1:B:35:LEU:HD23	1:B:196:THR:HG22	1.64	0.79
1:C:406:GLY:HA3	1:C:409:GLU:OE2	1.82	0.79
1:D:73:SER:H	1:D:76:TYR:HE1	1.30	0.79
1:B:342:ILE:CB	1:B:343:SER:HB2	2.13	0.79
1:B:38:THR:CB	1:B:39:GLY:HA3	2.11	0.78
1:B:79:ARG:HB3	1:B:375:LEU:HD21	1.64	0.78
1:C:376:GLY:C	1:C:379:HIS:H	1.87	0.78
1:D:41:ILE:HG13	1:D:43:ILE:HG13	1.65	0.78
1:D:95:LEU:HA	1:D:98:TRP:CZ3	2.18	0.78
1:B:421:THR:HG22	1:B:422:ALA:H	1.47	0.78
1:C:360:PHE:CE1	1:C:413:SER:HA	2.15	0.78
1:C:414:PHE:HB2	1:D:414:PHE:HD1	1.48	0.78
1:C:19:VAL:HG21	1:C:210:ALA:HB2	1.65	0.78
1:A:24:MET:HB3	1:A:25:GLY:CA	2.14	0.78
1:B:409:GLU:O	1:B:412:TRP:HB2	1.83	0.78
1:C:116:PHE:HB3	1:C:117:PRO:CD	2.13	0.78
1:D:24:MET:HB3	1:D:25:GLY:CA	2.14	0.78
1:D:342:ILE:CB	1:D:343:SER:HB2	2.13	0.78
1:A:116:PHE:HB3	1:A:117:PRO:CD	2.14	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:LEU:HD11	1:B:365:TYR:HD1	1.49	0.78
1:A:411:MET:O	1:A:415:VAL:HG23	1.84	0.78
1:C:74:TYR:CZ	1:C:304:ALA:HB2	2.18	0.78
1:B:74:TYR:CZ	1:B:304:ALA:HB2	2.18	0.78
1:B:78:ARG:CA	1:B:82:GLY:HA3	2.13	0.78
1:C:90:ASN:OD1	1:C:300:THR:O	2.02	0.78
1:C:342:ILE:CB	1:C:343:SER:HB2	2.13	0.78
1:D:60:TYR:CE2	1:D:368:THR:CG2	2.67	0.78
1:A:35:LEU:HD23	1:A:196:THR:HG22	1.66	0.78
1:A:93:TYR:CE2	1:A:97:CYS:SG	2.77	0.77
1:C:79:ARG:HB3	1:C:375:LEU:HD21	1.67	0.77
1:D:173:PHE:HA	1:D:174:ARG:HB2	1.64	0.77
1:D:201:LEU:HG	1:D:401:ALA:HB2	1.66	0.77
1:A:414:PHE:CD1	1:B:414:PHE:HB2	2.19	0.77
1:B:24:MET:HB3	1:B:25:GLY:CA	2.15	0.77
1:D:140:ASN:HB3	1:D:327:LEU:HD22	1.64	0.77
1:B:411:MET:O	1:B:415:VAL:HG23	1.84	0.77
1:C:24:MET:HB3	1:C:25:GLY:CA	2.13	0.77
1:D:24:MET:O	1:D:28:VAL:HG23	1.84	0.77
1:B:355:SER:O	1:B:358:VAL:HB	1.85	0.77
1:D:19:VAL:HG21	1:D:210:ALA:HB2	1.63	0.77
1:C:342:ILE:HB	1:C:343:SER:CB	2.15	0.77
1:D:342:ILE:HB	1:D:343:SER:CB	2.15	0.77
1:A:63:MET:HG3	1:A:76:TYR:CE2	2.20	0.77
1:A:355:SER:O	1:A:358:VAL:HB	1.84	0.77
1:B:116:PHE:HB3	1:B:117:PRO:CD	2.14	0.77
1:B:201:LEU:HG	1:B:401:ALA:HB2	1.65	0.77
1:C:310:PHE:HB3	1:C:311:PRO:C	2.06	0.77
1:D:406:GLY:HA3	1:D:409:GLU:OE2	1.85	0.77
1:A:15:VAL:HG21	1:A:217:VAL:HG13	1.65	0.76
1:B:310:PHE:HB3	1:B:311:PRO:C	2.04	0.76
1:B:140:ASN:HB3	1:B:327:LEU:HD22	1.66	0.76
1:C:355:SER:O	1:C:358:VAL:HB	1.85	0.76
1:A:79:ARG:HB3	1:A:375:LEU:HD21	1.68	0.76
1:A:362:LEU:HG	1:A:402:VAL:CG2	2.16	0.76
1:A:374:LEU:O	1:A:375:LEU:HD23	1.85	0.76
1:A:406:GLY:HA3	1:A:409:GLU:OE2	1.85	0.76
1:B:24:MET:O	1:B:28:VAL:HG23	1.85	0.76
1:B:90:ASN:OD1	1:B:300:THR:O	2.02	0.76
1:D:93:TYR:CE2	1:D:97:CYS:SG	2.78	0.76
1:B:115:PHE:HE1	1:B:276:ALA:HA	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:ILE:HG13	1:C:43:ILE:HG13	1.67	0.76
1:D:411:MET:HG3	1:D:412:TRP:N	1.98	0.76
1:D:116:PHE:HB3	1:D:117:PRO:CD	2.15	0.76
1:D:374:LEU:O	1:D:375:LEU:HD23	1.86	0.76
1:B:63:MET:HG3	1:B:76:TYR:CE2	2.20	0.76
1:D:35:LEU:HD23	1:D:196:THR:HG22	1.67	0.76
1:B:311:PRO:CD	1:B:426:LEU:HD21	2.01	0.76
1:B:342:ILE:HB	1:B:343:SER:CB	2.15	0.76
1:C:80:CYS:HA	1:C:374:LEU:HD23	1.68	0.76
1:A:115:PHE:HE1	1:A:276:ALA:HA	1.51	0.75
1:A:346:ALA:HB3	1:A:351:GLY:HA2	1.68	0.75
1:C:84:PHE:HE1	1:C:85:LEU:HD23	1.51	0.75
1:D:15:VAL:HG21	1:D:217:VAL:HG13	1.68	0.75
1:B:411:MET:HG3	1:B:412:TRP:N	2.02	0.75
1:A:366:LEU:CD1	1:B:421:THR:HG21	2.15	0.75
1:A:411:MET:HA	1:B:410:VAL:HG12	1.67	0.75
1:B:376:GLY:C	1:B:379:HIS:H	1.88	0.75
1:A:73:SER:H	1:A:76:TYR:HE1	1.35	0.75
1:C:411:MET:O	1:C:415:VAL:HG23	1.86	0.75
1:C:414:PHE:CD1	1:D:414:PHE:HB2	2.22	0.75
1:C:24:MET:O	1:C:28:VAL:HG23	1.86	0.75
1:B:102:ILE:HG23	1:B:338:GLN:HG2	1.69	0.75
1:C:115:PHE:HE1	1:C:276:ALA:HA	1.51	0.75
1:B:80:CYS:HA	1:B:374:LEU:HD23	1.68	0.75
1:B:374:LEU:O	1:B:375:LEU:HD23	1.86	0.75
1:A:72:GLY:O	1:A:74:TYR:N	2.20	0.75
1:A:421:THR:O	1:A:423:MET:N	2.20	0.75
1:B:346:ALA:HB3	1:B:351:GLY:HA2	1.68	0.75
1:A:201:LEU:HG	1:A:401:ALA:HB2	1.66	0.74
1:B:41:ILE:HG13	1:B:43:ILE:HG13	1.68	0.74
1:C:411:MET:HG3	1:C:412:TRP:N	2.00	0.74
1:C:433:LYS:CB	1:D:78:ARG:HH11	1.99	0.74
1:B:368:THR:HG22	1:B:369:CYS:N	2.00	0.74
1:D:74:TYR:CZ	1:D:304:ALA:HB2	2.23	0.74
1:D:115:PHE:HE1	1:D:276:ALA:HA	1.49	0.74
1:A:62:LYS:HA	1:A:65:PHE:HB2	1.69	0.74
1:A:109:VAL:HG11	1:A:128:THR:HG21	1.70	0.74
1:C:409:GLU:O	1:C:412:TRP:HB2	1.85	0.74
1:A:10:VAL:HG12	1:A:11:GLY:H	1.53	0.74
1:B:63:MET:SD	1:B:372:LEU:HD12	2.27	0.74
1:B:84:PHE:HE1	1:B:85:LEU:HD23	1.50	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:VAL:HG12	1:C:11:GLY:H	1.51	0.74
1:C:346:ALA:HB3	1:C:351:GLY:HA2	1.68	0.74
1:C:15:VAL:HG21	1:C:217:VAL:HG13	1.70	0.74
1:B:56:LEU:HD11	1:B:365:TYR:CD1	2.23	0.74
1:D:79:ARG:HB3	1:D:375:LEU:HD21	1.69	0.74
1:C:41:ILE:HG13	1:C:43:ILE:CG1	2.18	0.74
1:D:81:PHE:HD2	1:D:81:PHE:C	1.91	0.74
1:A:81:PHE:HD2	1:A:81:PHE:C	1.90	0.74
1:D:139:LEU:O	1:D:147:ILE:HD13	1.88	0.73
1:D:346:ALA:HB3	1:D:351:GLY:HA2	1.68	0.73
1:A:366:LEU:HD11	1:B:421:THR:HG21	1.70	0.73
1:C:102:ILE:HG23	1:C:338:GLN:HG2	1.68	0.73
1:A:41:ILE:CG2	1:A:246:ILE:HD13	2.18	0.73
1:B:10:VAL:HG12	1:B:11:GLY:H	1.53	0.73
1:A:310:PHE:HB3	1:A:311:PRO:C	2.08	0.73
1:C:140:ASN:HB3	1:C:327:LEU:HD22	1.68	0.73
1:D:41:ILE:CG2	1:D:246:ILE:HD13	2.18	0.73
1:C:56:LEU:HD11	1:C:365:TYR:CD1	2.22	0.73
1:C:95:LEU:HA	1:C:98:TRP:CZ3	2.23	0.73
1:A:60:TYR:CE2	1:A:368:THR:CG2	2.67	0.73
1:A:80:CYS:HA	1:A:374:LEU:HD23	1.71	0.73
1:B:72:GLY:O	1:B:74:TYR:N	2.21	0.73
1:B:95:LEU:HA	1:B:98:TRP:CZ3	2.23	0.73
1:C:60:TYR:CE2	1:C:368:THR:CG2	2.71	0.73
1:A:74:TYR:CZ	1:A:304:ALA:HB2	2.23	0.73
1:C:85:LEU:HD11	1:D:84:PHE:CD1	2.23	0.73
1:D:202:TRP:HE3	1:D:358:VAL:HG11	1.54	0.73
1:A:292:GLY:O	1:A:296:LEU:HD23	1.89	0.73
1:B:400:TRP:O	1:B:403:VAL:HG12	1.89	0.73
1:B:15:VAL:HG21	1:B:217:VAL:HG13	1.71	0.72
1:D:38:THR:CB	1:D:39:GLY:HA3	2.11	0.72
1:D:292:GLY:O	1:D:296:LEU:HD23	1.88	0.72
1:D:310:PHE:HB3	1:D:311:PRO:C	2.09	0.72
1:A:395:PHE:CD1	1:B:422:ALA:HB2	2.24	0.72
1:A:78:ARG:HH11	1:B:433:LYS:CB	2.01	0.72
1:A:400:TRP:O	1:A:403:VAL:HG12	1.89	0.72
1:B:362:LEU:HG	1:B:402:VAL:CG2	2.19	0.72
1:C:368:THR:HG22	1:C:369:CYS:N	2.02	0.72
1:D:10:VAL:HG12	1:D:11:GLY:H	1.53	0.72
1:D:63:MET:SD	1:D:372:LEU:HD12	2.29	0.72
1:A:63:MET:SD	1:A:372:LEU:HD12	2.30	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:184:VAL:HG12	1:D:185:SER:H	1.54	0.72
1:A:410:VAL:HG12	1:B:411:MET:HA	1.72	0.72
1:D:362:LEU:HG	1:D:402:VAL:CG2	2.18	0.72
1:B:60:TYR:CE2	1:B:368:THR:CG2	2.72	0.72
1:A:116:PHE:O	1:A:118:ILE:HG22	1.90	0.71
1:D:66:LEU:C	1:D:68:PRO:HD3	2.09	0.71
1:B:62:LYS:HA	1:B:65:PHE:HB2	1.70	0.71
1:B:201:LEU:CG	1:B:401:ALA:HB2	2.20	0.71
1:B:416:THR:HA	1:B:419:VAL:HG12	1.71	0.71
1:D:102:ILE:HG23	1:D:338:GLN:HG2	1.72	0.71
1:A:113:SER:O	1:A:118:ILE:HD13	1.91	0.71
1:A:409:GLU:O	1:A:412:TRP:HB2	1.90	0.71
1:C:62:LYS:HA	1:C:65:PHE:HB2	1.72	0.71
1:C:201:LEU:CG	1:C:401:ALA:HB2	2.19	0.71
1:C:362:LEU:HG	1:C:402:VAL:CG2	2.20	0.71
1:D:62:LYS:HA	1:D:65:PHE:HB2	1.71	0.71
1:B:41:ILE:HG13	1:B:43:ILE:CG1	2.20	0.71
1:C:139:LEU:O	1:C:147:ILE:HD13	1.91	0.71
1:D:63:MET:HG3	1:D:76:TYR:CE2	2.26	0.71
1:D:80:CYS:HA	1:D:374:LEU:HD23	1.71	0.71
1:B:109:VAL:HG11	1:B:128:THR:HG21	1.73	0.71
1:C:156:VAL:HA	1:C:159:LEU:HD12	1.73	0.71
1:A:184:VAL:HG12	1:A:185:SER:H	1.55	0.71
1:D:116:PHE:O	1:D:118:ILE:HG22	1.90	0.71
1:D:411:MET:O	1:D:415:VAL:HG23	1.90	0.71
1:A:368:THR:HG22	1:A:369:CYS:N	2.06	0.71
1:C:140:ASN:ND2	1:C:147:ILE:HG12	2.06	0.71
1:C:292:GLY:O	1:C:296:LEU:HD23	1.91	0.71
1:D:140:ASN:ND2	1:D:147:ILE:HG12	2.05	0.71
1:B:93:TYR:CE2	1:B:97:CYS:SG	2.84	0.70
1:A:361:THR:O	1:A:365:TYR:CD2	2.45	0.70
1:B:184:VAL:HG12	1:B:185:SER:H	1.54	0.70
1:B:202:TRP:HE3	1:B:358:VAL:HG11	1.55	0.70
1:D:120:LYS:H	1:D:120:LYS:HE2	1.57	0.70
1:A:361:THR:O	1:A:365:TYR:HD2	1.75	0.70
1:A:362:LEU:O	1:A:365:TYR:HB2	1.91	0.70
1:C:109:VAL:HG11	1:C:128:THR:HG21	1.71	0.70
1:D:314:PHE:HA	1:D:315:ALA:C	2.12	0.70
1:B:60:TYR:HE2	1:B:368:THR:CG2	2.02	0.70
1:A:93:TYR:HB2	1:A:364:PRO:HG2	1.74	0.70
1:A:376:GLY:C	1:A:379:HIS:H	1.95	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:ILE:HG21	1:C:204:PHE:CD1	2.27	0.70
1:C:184:VAL:HG12	1:C:185:SER:H	1.56	0.70
1:C:406:GLY:HA3	1:C:409:GLU:CD	2.12	0.70
1:D:368:THR:HG22	1:D:369:CYS:N	2.06	0.70
1:D:421:THR:CG2	1:D:422:ALA:N	2.53	0.70
1:C:399:ILE:CG1	1:D:418:MET:HE2	2.22	0.70
1:C:421:THR:HG22	1:C:422:ALA:H	1.55	0.70
1:C:120:LYS:HE2	1:C:120:LYS:H	1.56	0.70
1:D:56:LEU:HD11	1:D:365:TYR:HD1	1.57	0.70
1:A:56:LEU:HD11	1:A:365:TYR:HD1	1.56	0.69
1:A:428:TYR:O	1:A:429:ASN:OD1	2.10	0.69
1:C:314:PHE:HA	1:C:315:ALA:C	2.12	0.69
1:D:46:TRP:CZ3	1:D:239:TYR:HB3	2.28	0.69
1:D:302:LYS:H	1:D:302:LYS:HD3	1.57	0.69
1:A:139:LEU:O	1:A:147:ILE:HD13	1.90	0.69
1:B:139:LEU:O	1:B:147:ILE:HD13	1.92	0.69
1:C:410:VAL:HG12	1:D:411:MET:HA	1.74	0.69
1:D:156:VAL:HA	1:D:159:LEU:HD12	1.74	0.69
1:C:72:GLY:O	1:C:74:TYR:N	2.24	0.69
1:A:56:LEU:HD11	1:A:365:TYR:CD1	2.27	0.69
1:A:314:PHE:HA	1:A:315:ALA:C	2.13	0.69
1:D:109:VAL:HG11	1:D:128:THR:HG21	1.73	0.69
1:D:409:GLU:O	1:D:412:TRP:HB2	1.92	0.69
1:B:72:GLY:N	1:B:211:SER:O	2.26	0.69
1:D:360:PHE:CE1	1:D:413:SER:HA	2.22	0.69
1:D:400:TRP:O	1:D:403:VAL:HG12	1.92	0.69
1:A:57:SER:CB	1:A:232:VAL:HG21	2.22	0.69
1:A:301:ALA:HB1	1:A:310:PHE:HE1	1.58	0.69
1:A:416:THR:HA	1:A:419:VAL:HG12	1.73	0.69
1:D:56:LEU:HD11	1:D:365:TYR:CD1	2.28	0.69
1:D:94:TRP:HA	1:D:97:CYS:HB2	1.75	0.69
1:D:421:THR:O	1:D:423:MET:N	2.26	0.69
1:D:428:TYR:O	1:D:429:ASN:OD1	2.11	0.69
1:A:302:LYS:H	1:A:302:LYS:HD3	1.57	0.69
1:A:395:PHE:CE1	1:B:422:ALA:HB2	2.28	0.69
1:C:53:ALA:HB2	1:C:397:TYR:CE2	2.28	0.69
1:A:359:ILE:HD11	1:A:409:GLU:HB3	1.73	0.69
1:B:41:ILE:HG22	1:B:246:ILE:CD1	2.23	0.69
1:C:63:MET:HG3	1:C:76:TYR:CD2	2.28	0.69
1:A:46:TRP:CZ3	1:A:239:TYR:HB3	2.28	0.68
1:C:93:TYR:HB2	1:C:364:PRO:HG2	1.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:TRP:HE3	1:A:358:VAL:HG11	1.56	0.68
1:D:376:GLY:C	1:D:379:HIS:H	1.95	0.68
1:A:81:PHE:C	1:A:81:PHE:CD2	2.65	0.68
1:B:156:VAL:HA	1:B:159:LEU:HD12	1.73	0.68
1:B:361:THR:O	1:B:365:TYR:HD2	1.77	0.68
1:C:102:ILE:HD13	1:C:337:PHE:HD2	1.59	0.68
1:C:178:TYR:HD2	1:C:247:MET:HA	1.59	0.68
1:D:81:PHE:C	1:D:81:PHE:CD2	2.65	0.68
1:D:300:THR:O	1:D:300:THR:HG22	1.93	0.68
1:A:156:VAL:HA	1:A:159:LEU:HD12	1.75	0.68
1:C:202:TRP:HE3	1:C:358:VAL:HG11	1.56	0.68
1:C:302:LYS:HD3	1:C:302:LYS:H	1.58	0.68
1:D:93:TYR:HB2	1:D:364:PRO:HG2	1.74	0.68
1:A:120:LYS:HE2	1:A:120:LYS:H	1.58	0.68
1:B:359:ILE:HD11	1:B:409:GLU:HB3	1.76	0.68
1:D:72:GLY:O	1:D:74:TYR:N	2.26	0.68
1:D:102:ILE:HD13	1:D:337:PHE:HD2	1.59	0.68
1:B:298:GLY:O	1:B:302:LYS:HD3	1.93	0.68
1:D:359:ILE:HD11	1:D:409:GLU:HB3	1.75	0.68
1:B:314:PHE:HA	1:B:315:ALA:C	2.12	0.68
1:C:433:LYS:CB	1:D:78:ARG:NH1	2.55	0.68
1:B:160:ILE:HB	1:B:161:PRO:HD3	1.74	0.68
1:A:23:ILE:HG21	1:A:204:PHE:CD1	2.29	0.68
1:A:102:ILE:HG23	1:A:338:GLN:HG2	1.76	0.68
1:B:46:TRP:CZ3	1:B:239:TYR:HB3	2.29	0.68
1:C:81:PHE:HD2	1:C:81:PHE:C	1.97	0.68
1:C:395:PHE:CE1	1:D:422:ALA:HB2	2.28	0.68
1:C:428:TYR:O	1:C:429:ASN:OD1	2.12	0.68
1:B:301:ALA:HB1	1:B:310:PHE:HE1	1.59	0.68
1:C:66:LEU:C	1:C:68:PRO:HD3	2.13	0.68
1:C:201:LEU:CD2	1:C:401:ALA:HB2	2.23	0.68
1:B:120:LYS:H	1:B:120:LYS:HE2	1.58	0.67
1:B:178:TYR:HD2	1:B:247:MET:HA	1.59	0.67
1:B:184:VAL:HG11	1:C:184:VAL:HG11	1.77	0.67
1:D:57:SER:CB	1:D:232:VAL:HG21	2.24	0.67
1:A:72:GLY:N	1:A:211:SER:O	2.27	0.67
1:B:23:ILE:HG21	1:B:204:PHE:CD1	2.29	0.67
1:C:116:PHE:O	1:C:118:ILE:HG22	1.95	0.67
1:A:54:LEU:HD11	1:A:233:LEU:HD23	1.76	0.67
1:A:92:LEU:HD21	1:A:364:PRO:HD3	1.77	0.67
1:B:201:LEU:CD2	1:B:401:ALA:HB2	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:301:ALA:HB1	1:D:310:PHE:HE1	1.57	0.67
1:B:81:PHE:HD2	1:B:81:PHE:C	1.98	0.67
1:B:361:THR:O	1:B:365:TYR:CD2	2.48	0.67
1:C:60:TYR:HE2	1:C:368:THR:CG2	2.02	0.67
1:A:109:VAL:HG11	1:A:128:THR:CG2	2.25	0.67
1:A:379:HIS:HB3	1:A:381:GLY:O	1.95	0.67
1:C:111:TYR:HE2	1:C:282:ALA:HB1	1.60	0.67
1:C:411:MET:HA	1:D:410:VAL:HG12	1.77	0.67
1:A:140:ASN:ND2	1:A:147:ILE:HG12	2.09	0.67
1:B:53:ALA:HB2	1:B:397:TYR:CE2	2.29	0.67
1:C:160:ILE:HB	1:C:161:PRO:HD3	1.75	0.67
1:C:416:THR:HA	1:C:419:VAL:HG12	1.77	0.67
1:D:178:TYR:HD2	1:D:247:MET:HA	1.60	0.67
1:A:111:TYR:HE2	1:A:282:ALA:HB1	1.59	0.67
1:D:111:TYR:HE2	1:D:282:ALA:HB1	1.59	0.67
1:A:66:LEU:C	1:A:68:PRO:HD3	2.16	0.66
1:A:94:TRP:HA	1:A:97:CYS:HB2	1.77	0.66
1:B:93:TYR:HB2	1:B:364:PRO:HG2	1.76	0.66
1:A:178:TYR:HD2	1:A:247:MET:HA	1.61	0.66
1:A:292:GLY:O	1:A:295:LEU:HB3	1.95	0.66
1:A:300:THR:O	1:A:300:THR:HG22	1.94	0.66
1:B:87:TYR:OH	1:B:308:GLY:HA3	1.94	0.66
1:C:72:GLY:N	1:C:212:VAL:HA	2.11	0.66
1:B:292:GLY:O	1:B:296:LEU:HD23	1.95	0.66
1:C:72:GLY:N	1:C:211:SER:O	2.28	0.66
1:C:72:GLY:H	1:C:212:VAL:HA	1.60	0.66
1:C:359:ILE:HD11	1:C:409:GLU:HB3	1.76	0.66
1:C:414:PHE:HB2	1:D:414:PHE:CD1	2.28	0.66
1:C:46:TRP:CZ3	1:C:239:TYR:HB3	2.29	0.66
1:A:78:ARG:C	1:A:82:GLY:HA3	2.16	0.66
1:B:379:HIS:C	1:B:381:GLY:H	1.99	0.66
1:B:109:VAL:HG11	1:B:128:THR:CG2	2.26	0.66
1:C:298:GLY:O	1:C:302:LYS:HD3	1.95	0.66
1:D:23:ILE:HG21	1:D:204:PHE:CD1	2.30	0.66
1:D:78:ARG:C	1:D:82:GLY:HA3	2.14	0.66
1:A:41:ILE:HG13	1:A:43:ILE:HG12	1.74	0.66
1:B:111:TYR:HE2	1:B:282:ALA:HB1	1.59	0.66
1:B:302:LYS:HD3	1:B:302:LYS:H	1.60	0.66
1:C:87:TYR:HB3	1:C:424:TYR:OH	1.95	0.66
1:C:113:SER:O	1:C:118:ILE:HD13	1.95	0.66
1:D:84:PHE:HE1	1:D:85:LEU:CD2	2.08	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:ALA:C	1:B:427:ASN:N	2.49	0.66
1:C:87:TYR:OH	1:C:308:GLY:HA3	1.96	0.66
1:C:301:ALA:HB1	1:C:310:PHE:HE1	1.59	0.66
1:C:302:LYS:HG2	1:C:323:PRO:CB	2.23	0.66
1:C:400:TRP:O	1:C:403:VAL:HG12	1.95	0.66
1:D:379:HIS:HB3	1:D:381:GLY:O	1.95	0.66
1:B:66:LEU:C	1:B:68:PRO:HD3	2.15	0.66
1:C:41:ILE:HG22	1:C:246:ILE:CD1	2.25	0.66
1:C:78:ARG:C	1:C:82:GLY:HA3	2.17	0.66
1:C:94:TRP:HA	1:C:97:CYS:HB2	1.77	0.66
1:C:361:THR:O	1:C:365:TYR:CD2	2.49	0.65
1:A:11:GLY:O	1:A:15:VAL:HG23	1.95	0.65
1:C:143:GLY:HA2	1:C:146:MET:H	1.61	0.65
1:D:136:PHE:CD2	1:D:290:LEU:HB3	2.31	0.65
1:C:102:ILE:HD13	1:C:337:PHE:CD2	2.31	0.65
1:C:428:TYR:OH	1:D:373:LEU:HD13	1.95	0.65
1:D:292:GLY:O	1:D:295:LEU:HB3	1.97	0.65
1:D:379:HIS:C	1:D:381:GLY:H	1.99	0.65
1:A:78:ARG:NH1	1:B:433:LYS:CB	2.59	0.65
1:B:406:GLY:HA3	1:B:409:GLU:CD	2.16	0.65
1:B:428:TYR:O	1:B:429:ASN:OD1	2.13	0.65
1:D:72:GLY:N	1:D:211:SER:O	2.29	0.65
1:B:94:TRP:HA	1:B:97:CYS:HB2	1.77	0.65
1:D:102:ILE:HD13	1:D:337:PHE:CD2	2.31	0.65
1:D:126:THR:HB	1:D:342:ILE:HG23	1.79	0.65
1:A:126:THR:HB	1:A:342:ILE:HG23	1.79	0.65
1:A:418:MET:HE2	1:B:399:ILE:HA	1.79	0.65
1:B:140:ASN:ND2	1:B:147:ILE:HG12	2.11	0.65
1:D:77:ALA:C	1:D:79:ARG:H	1.99	0.65
1:D:420:ILE:O	1:D:421:THR:O	2.14	0.65
1:B:362:LEU:O	1:B:365:TYR:HB2	1.96	0.65
1:C:109:VAL:HG11	1:C:128:THR:CG2	2.26	0.65
1:D:109:VAL:HG11	1:D:128:THR:CG2	2.26	0.65
1:D:350:PHE:HA	1:D:355:SER:HB3	1.79	0.65
1:D:298:GLY:O	1:D:302:LYS:HD3	1.96	0.65
1:A:49:THR:HG21	1:A:200:THR:HB	1.79	0.65
1:B:87:TYR:HB3	1:B:424:TYR:OH	1.97	0.65
1:B:173:PHE:HB3	1:B:178:TYR:OH	1.97	0.65
1:C:422:ALA:HB2	1:D:395:PHE:CD1	2.32	0.64
1:B:78:ARG:C	1:B:82:GLY:HA3	2.17	0.64
1:D:201:LEU:CG	1:D:401:ALA:HB2	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:GLY:O	1:A:302:LYS:HD3	1.98	0.64
1:A:414:PHE:CB	1:B:414:PHE:HD1	2.04	0.64
1:A:422:ALA:HB2	1:B:395:PHE:CE1	2.32	0.64
1:C:91:VAL:HB	1:C:420:ILE:HD11	1.79	0.64
1:B:84:PHE:HE1	1:B:85:LEU:CD2	2.09	0.64
1:B:113:SER:O	1:B:118:ILE:HD13	1.97	0.64
1:C:376:GLY:O	1:C:378:GLY:N	2.30	0.64
1:D:87:TYR:OH	1:D:308:GLY:HA3	1.98	0.64
1:A:57:SER:HB3	1:A:232:VAL:HG21	1.80	0.64
1:A:84:PHE:HE1	1:A:85:LEU:CD2	2.09	0.64
1:A:377:HIS:HE1	1:B:430:ARG:C	2.01	0.64
1:A:425:ALA:C	1:A:427:ASN:N	2.50	0.64
1:B:102:ILE:HD13	1:B:337:PHE:HD2	1.62	0.64
1:B:300:THR:O	1:B:300:THR:HG22	1.96	0.64
1:C:379:HIS:C	1:C:381:GLY:H	2.01	0.64
1:A:111:TYR:CE2	1:A:282:ALA:HB1	2.33	0.64
1:A:420:ILE:HG22	1:A:421:THR:N	2.13	0.64
1:B:344:PRO:O	1:B:345:ASN:HB2	1.97	0.64
1:D:113:SER:O	1:D:118:ILE:HD13	1.97	0.64
1:A:53:ALA:HB2	1:A:397:TYR:CE2	2.32	0.64
1:A:201:LEU:CG	1:A:401:ALA:HB2	2.28	0.64
1:C:57:SER:CB	1:C:232:VAL:HG21	2.28	0.64
1:C:84:PHE:HE1	1:C:85:LEU:CD2	2.11	0.64
1:C:201:LEU:C	1:C:203:SER:H	2.01	0.64
1:D:54:LEU:HD11	1:D:233:LEU:HD23	1.77	0.64
1:A:247:MET:HG2	1:A:248:GLY:N	2.13	0.64
1:C:173:PHE:HB3	1:C:178:TYR:OH	1.97	0.64
1:D:111:TYR:CE2	1:D:282:ALA:HB1	2.33	0.64
1:D:173:PHE:HB3	1:D:178:TYR:OH	1.98	0.64
1:A:360:PHE:CE1	1:A:413:SER:HA	2.24	0.64
1:B:102:ILE:HD13	1:B:337:PHE:CD2	2.33	0.64
1:A:344:PRO:O	1:A:345:ASN:HB2	1.98	0.64
1:B:116:PHE:O	1:B:118:ILE:HG22	1.98	0.64
1:B:420:ILE:HG22	1:B:421:THR:N	2.13	0.64
1:C:362:LEU:O	1:C:365:TYR:HB2	1.98	0.64
1:A:366:LEU:CD2	1:B:421:THR:HG21	2.29	0.63
1:C:344:PRO:O	1:C:345:ASN:HB2	1.98	0.63
1:D:416:THR:HA	1:D:419:VAL:HG12	1.79	0.63
1:D:425:ALA:C	1:D:427:ASN:N	2.47	0.63
1:A:207:VAL:HG12	1:A:232:VAL:CG2	2.28	0.63
1:A:362:LEU:HG	1:A:402:VAL:HG21	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:MET:HG2	1:C:248:GLY:N	2.13	0.63
1:A:337:PHE:CZ	1:A:353:VAL:HG11	2.34	0.63
1:B:136:PHE:CD2	1:B:290:LEU:HB3	2.33	0.63
1:C:207:VAL:HG12	1:C:232:VAL:CG2	2.29	0.63
1:C:361:THR:O	1:C:365:TYR:HD2	1.80	0.63
1:D:384:ARG:HB3	1:D:385:PRO:HD3	1.81	0.63
1:A:87:TYR:OH	1:A:308:GLY:HA3	1.99	0.63
1:A:90:ASN:O	1:A:91:VAL:C	2.37	0.63
1:A:403:VAL:HG23	1:B:415:VAL:HG11	1.80	0.63
1:B:91:VAL:O	1:B:95:LEU:HB3	1.99	0.63
1:B:302:LYS:HG2	1:B:323:PRO:CB	2.24	0.63
1:B:425:ALA:HA	1:B:428:TYR:CZ	2.34	0.63
1:C:78:ARG:HH11	1:D:433:LYS:CB	2.12	0.63
1:D:72:GLY:H	1:D:212:VAL:HA	1.64	0.63
1:B:81:PHE:C	1:B:81:PHE:CD2	2.72	0.63
1:D:93:TYR:HE1	1:D:208:GLU:CD	2.01	0.63
1:D:160:ILE:HB	1:D:161:PRO:HD3	1.81	0.63
1:C:136:PHE:CD2	1:C:290:LEU:HB3	2.33	0.63
1:C:323:PRO:HD2	1:C:327:LEU:HD11	1.81	0.63
1:A:420:ILE:O	1:A:421:THR:O	2.16	0.63
1:B:376:GLY:O	1:B:378:GLY:N	2.32	0.63
1:C:73:SER:N	1:C:76:TYR:HE1	1.96	0.63
1:C:78:ARG:NH1	1:D:433:LYS:CB	2.62	0.63
1:C:93:TYR:HE2	1:C:97:CYS:SG	2.20	0.63
1:C:300:THR:O	1:C:300:THR:HG22	1.99	0.63
1:A:136:PHE:CD2	1:A:290:LEU:HB3	2.34	0.63
1:B:111:TYR:CE2	1:B:282:ALA:HB1	2.33	0.63
1:B:247:MET:HG2	1:B:248:GLY:N	2.14	0.63
1:C:399:ILE:HG13	1:D:418:MET:HE2	1.81	0.63
1:A:379:HIS:C	1:A:381:GLY:H	2.01	0.62
1:C:420:ILE:O	1:C:421:THR:O	2.17	0.62
1:D:247:MET:HG2	1:D:248:GLY:N	2.12	0.62
1:B:72:GLY:H	1:B:212:VAL:HA	1.64	0.62
1:B:143:GLY:HA2	1:B:146:MET:H	1.62	0.62
1:C:292:GLY:O	1:C:295:LEU:HB3	1.98	0.62
1:D:41:ILE:HG13	1:D:43:ILE:HG12	1.80	0.62
1:D:201:LEU:C	1:D:203:SER:H	2.02	0.62
1:A:363:VAL:HG23	1:A:364:PRO:HD3	1.81	0.62
1:B:57:SER:CB	1:B:232:VAL:HG21	2.29	0.62
1:C:111:TYR:CE2	1:C:282:ALA:HB1	2.34	0.62
1:D:57:SER:HB3	1:D:232:VAL:HG21	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:LEU:C	1:B:203:SER:H	2.00	0.62
1:B:346:ALA:CB	1:B:351:GLY:HA2	2.29	0.62
1:C:421:THR:HG21	1:D:366:LEU:CD1	2.30	0.62
1:D:53:ALA:HB2	1:D:397:TYR:CE2	2.35	0.62
1:D:344:PRO:O	1:D:345:ASN:HB2	1.97	0.62
1:A:160:ILE:HB	1:A:161:PRO:HD3	1.81	0.62
1:A:346:ALA:CB	1:A:351:GLY:HA2	2.29	0.62
1:D:90:ASN:O	1:D:91:VAL:C	2.38	0.62
1:D:346:ALA:CB	1:D:351:GLY:HA2	2.29	0.62
1:D:425:ALA:HA	1:D:428:TYR:CZ	2.35	0.62
1:A:173:PHE:HB3	1:A:178:TYR:OH	2.00	0.62
1:B:77:ALA:C	1:B:79:ARG:H	2.03	0.62
1:C:376:GLY:O	1:C:379:HIS:N	2.30	0.62
1:D:13:ILE:HB	1:D:14:PRO:HD3	1.81	0.62
1:A:77:ALA:C	1:A:79:ARG:H	2.03	0.62
1:A:350:PHE:HA	1:A:355:SER:HB3	1.82	0.62
1:B:379:HIS:HB3	1:B:381:GLY:O	1.99	0.62
1:B:337:PHE:CZ	1:B:353:VAL:HG11	2.34	0.62
1:C:10:VAL:HG12	1:C:11:GLY:N	2.14	0.62
1:C:54:LEU:HD11	1:C:233:LEU:HD23	1.82	0.62
1:A:102:ILE:HD13	1:A:337:PHE:HD2	1.65	0.62
1:C:346:ALA:CB	1:C:351:GLY:HA2	2.29	0.62
1:A:302:LYS:HG2	1:A:323:PRO:CB	2.26	0.62
1:A:342:ILE:H	1:A:343:SER:HB2	1.63	0.62
1:C:342:ILE:H	1:C:343:SER:HB2	1.65	0.62
1:D:173:PHE:HA	1:D:174:ARG:CB	2.30	0.62
1:A:81:PHE:CD2	1:A:83:PRO:HD2	2.35	0.61
1:A:201:LEU:C	1:A:203:SER:H	2.03	0.61
1:C:178:TYR:CD2	1:C:247:MET:HA	2.35	0.61
1:D:82:GLY:N	1:D:83:PRO:HD2	2.15	0.61
1:D:246:ILE:O	1:D:246:ILE:HG23	2.00	0.61
1:A:197:LEU:O	1:A:201:LEU:HB2	1.99	0.61
1:A:246:ILE:O	1:A:246:ILE:HG23	2.00	0.61
1:B:10:VAL:HG12	1:B:11:GLY:N	2.15	0.61
1:B:246:ILE:HG23	1:B:246:ILE:O	2.00	0.61
1:D:60:TYR:CD2	1:D:368:THR:HG21	2.35	0.61
1:A:81:PHE:HB3	1:A:82:GLY:CA	2.30	0.61
1:A:425:ALA:HA	1:A:428:TYR:CZ	2.35	0.61
1:B:63:MET:SD	1:B:372:LEU:CD1	2.88	0.61
1:C:421:THR:O	1:C:423:MET:N	2.33	0.61
1:C:422:ALA:HB2	1:D:395:PHE:CE1	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:THR:CG2	1:D:227:ALA:HA	2.24	0.61
1:D:337:PHE:CZ	1:D:353:VAL:HG11	2.35	0.61
1:D:49:THR:HG21	1:D:200:THR:HB	1.82	0.61
1:A:395:PHE:CD1	1:B:422:ALA:CB	2.82	0.61
1:B:72:GLY:N	1:B:212:VAL:HA	2.14	0.61
1:B:292:GLY:O	1:B:295:LEU:HB3	2.00	0.61
1:B:384:ARG:HB3	1:B:385:PRO:HD3	1.82	0.61
1:C:81:PHE:C	1:C:81:PHE:CD2	2.72	0.61
1:C:337:PHE:CZ	1:C:353:VAL:HG11	2.36	0.61
1:C:359:ILE:O	1:C:362:LEU:HB2	2.01	0.61
1:B:60:TYR:CD2	1:B:368:THR:HG21	2.36	0.61
1:B:360:PHE:O	1:B:363:VAL:HG23	2.00	0.61
1:B:421:THR:O	1:B:423:MET:N	2.34	0.61
1:C:368:THR:O	1:C:371:ALA:N	2.31	0.61
1:B:81:PHE:HB3	1:B:82:GLY:CA	2.27	0.61
1:B:178:TYR:CD2	1:B:247:MET:HA	2.35	0.61
1:B:207:VAL:CG1	1:B:232:VAL:CG2	2.78	0.61
1:C:49:THR:HG21	1:C:200:THR:HB	1.83	0.61
1:C:104:MET:HE1	1:C:286:CYS:SG	2.40	0.61
1:C:379:HIS:HB3	1:C:381:GLY:O	2.01	0.61
1:C:421:THR:HG21	1:D:366:LEU:HD11	1.83	0.61
1:C:425:ALA:C	1:C:427:ASN:N	2.50	0.61
1:D:143:GLY:HA2	1:D:146:MET:H	1.66	0.61
1:A:87:TYR:HB3	1:A:424:TYR:OH	2.01	0.61
1:A:102:ILE:HD13	1:A:337:PHE:CD2	2.35	0.61
1:B:207:VAL:HG12	1:B:232:VAL:CG2	2.30	0.61
1:D:24:MET:CE	1:D:162:ILE:HD12	2.31	0.61
1:D:362:LEU:O	1:D:365:TYR:HB2	1.99	0.61
1:A:119:LEU:CD2	1:A:124:VAL:HG21	2.30	0.61
1:A:418:MET:HE2	1:B:399:ILE:CG1	2.31	0.61
1:A:421:THR:CG2	1:A:422:ALA:N	2.52	0.61
1:C:60:TYR:CD2	1:C:368:THR:HG21	2.35	0.61
1:C:77:ALA:C	1:C:79:ARG:H	2.03	0.61
1:C:173:PHE:HA	1:C:174:ARG:CB	2.30	0.61
1:A:143:GLY:HA2	1:A:146:MET:H	1.65	0.61
1:B:91:VAL:HB	1:B:420:ILE:HD11	1.82	0.61
1:B:350:PHE:HA	1:B:355:SER:HB3	1.82	0.61
1:C:418:MET:HE2	1:D:399:ILE:HA	1.82	0.61
1:A:399:ILE:HA	1:B:418:MET:HE2	1.82	0.60
1:B:92:LEU:HD21	1:B:364:PRO:HD3	1.83	0.60
1:C:38:THR:CB	1:C:39:GLY:CA	2.75	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:LYS:HE2	1:D:120:LYS:N	2.16	0.60
1:D:302:LYS:CD	1:D:302:LYS:N	2.64	0.60
1:A:178:TYR:CD2	1:A:247:MET:HA	2.37	0.60
1:B:342:ILE:H	1:B:343:SER:HB2	1.65	0.60
1:C:246:ILE:HG23	1:C:246:ILE:O	2.01	0.60
1:A:63:MET:HG3	1:A:76:TYR:CD2	2.35	0.60
1:B:13:ILE:HB	1:B:14:PRO:HD3	1.83	0.60
1:C:81:PHE:HB3	1:C:82:GLY:CA	2.27	0.60
1:C:144:PRO:HD3	1:C:322:THR:CG2	2.31	0.60
1:C:207:VAL:CG1	1:C:232:VAL:CG2	2.79	0.60
1:D:342:ILE:H	1:D:343:SER:HB2	1.64	0.60
1:A:72:GLY:H	1:A:212:VAL:HA	1.66	0.60
1:A:82:GLY:N	1:A:83:PRO:HD2	2.16	0.60
1:B:88:GLN:HA	1:B:91:VAL:HG23	1.83	0.60
1:C:201:LEU:HD23	1:C:401:ALA:HB2	1.82	0.60
1:C:350:PHE:HA	1:C:355:SER:HB3	1.82	0.60
1:D:10:VAL:HG12	1:D:11:GLY:N	2.16	0.60
1:D:178:TYR:CD2	1:D:247:MET:HA	2.36	0.60
1:D:361:THR:O	1:D:365:TYR:CD2	2.53	0.60
1:A:38:THR:CB	1:A:39:GLY:CA	2.75	0.60
1:A:371:ALA:C	1:A:373:LEU:H	2.04	0.60
1:B:57:SER:HB3	1:B:232:VAL:HG21	1.83	0.60
1:B:201:LEU:HD23	1:B:401:ALA:HB2	1.82	0.60
1:A:302:LYS:N	1:A:302:LYS:CD	2.64	0.60
1:A:421:THR:HG21	1:B:366:LEU:HD11	1.83	0.60
1:C:41:ILE:HA	1:C:42:ALA:C	2.21	0.60
1:C:94:TRP:O	1:C:97:CYS:HB2	2.01	0.60
1:C:197:LEU:O	1:C:201:LEU:HB2	2.02	0.60
1:C:302:LYS:CD	1:C:302:LYS:N	2.65	0.60
1:C:425:ALA:HA	1:C:428:TYR:CZ	2.36	0.60
1:D:54:LEU:HD11	1:D:233:LEU:CD2	2.31	0.60
1:C:420:ILE:HG22	1:C:421:THR:N	2.17	0.60
1:D:24:MET:CE	1:D:238:CYS:SG	2.90	0.60
1:A:207:VAL:CG1	1:A:232:VAL:CG2	2.80	0.60
1:B:155:THR:O	1:B:159:LEU:HG	2.02	0.60
1:D:119:LEU:CD2	1:D:124:VAL:HG21	2.30	0.60
1:A:60:TYR:CD2	1:A:368:THR:HG21	2.36	0.60
1:A:366:LEU:HD21	1:B:421:THR:CG2	2.32	0.60
1:D:197:LEU:O	1:D:201:LEU:HB2	2.00	0.60
1:A:13:ILE:HB	1:A:14:PRO:HD3	1.82	0.60
1:A:93:TYR:HE1	1:A:208:GLU:CD	2.06	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:ASN:ND2	1:B:310:PHE:CZ	2.70	0.60
1:D:89:THR:HG23	1:D:364:PRO:HG3	1.84	0.60
1:D:420:ILE:HG22	1:D:421:THR:N	2.15	0.60
1:A:10:VAL:HG12	1:A:11:GLY:N	2.16	0.59
1:A:24:MET:CE	1:A:162:ILE:HD12	2.31	0.59
1:C:11:GLY:O	1:C:15:VAL:HG23	2.01	0.59
1:D:138:LEU:O	1:D:142:VAL:HG23	2.02	0.59
1:A:41:ILE:HA	1:A:42:ALA:C	2.21	0.59
1:A:422:ALA:HB2	1:B:395:PHE:CD1	2.37	0.59
1:B:144:PRO:HD3	1:B:322:THR:CG2	2.32	0.59
1:D:11:GLY:O	1:D:15:VAL:HG23	2.02	0.59
1:D:72:GLY:N	1:D:212:VAL:HA	2.17	0.59
1:B:49:THR:HG21	1:B:200:THR:HB	1.83	0.59
1:B:54:LEU:HD11	1:B:233:LEU:HD23	1.84	0.59
1:D:91:VAL:HB	1:D:420:ILE:HD11	1.83	0.59
1:D:302:LYS:HG2	1:D:323:PRO:CB	2.27	0.59
1:A:406:GLY:HA3	1:A:409:GLU:CD	2.23	0.59
1:C:79:ARG:HB2	1:C:375:LEU:HD11	1.84	0.59
1:C:88:GLN:HA	1:C:91:VAL:HG23	1.85	0.59
1:C:399:ILE:HA	1:D:418:MET:HE2	1.84	0.59
1:C:421:THR:HG21	1:D:366:LEU:CD2	2.33	0.59
1:D:363:VAL:HG23	1:D:364:PRO:HD3	1.83	0.59
1:B:323:PRO:HD2	1:B:327:LEU:HD11	1.83	0.59
1:D:362:LEU:HG	1:D:402:VAL:HG21	1.84	0.59
1:A:72:GLY:N	1:A:212:VAL:HA	2.18	0.59
1:A:144:PRO:HD3	1:A:322:THR:CG2	2.32	0.59
1:B:371:ALA:C	1:B:373:LEU:H	2.06	0.59
1:C:20:SER:HA	1:C:23:ILE:HD12	1.84	0.59
1:D:41:ILE:HA	1:D:42:ALA:C	2.21	0.59
1:D:361:THR:O	1:D:365:TYR:HD2	1.85	0.59
1:B:120:LYS:NZ	1:B:124:VAL:HG12	2.18	0.59
1:C:395:PHE:CD1	1:D:422:ALA:HB2	2.38	0.59
1:C:418:MET:HE2	1:D:399:ILE:CG1	2.33	0.59
1:D:20:SER:HB2	1:D:231:GLY:HA2	1.85	0.59
1:A:16:THR:CG2	1:A:227:ALA:HA	2.25	0.59
1:B:94:TRP:O	1:B:97:CYS:HB2	2.03	0.59
1:C:107:ILE:O	1:C:111:TYR:HD1	1.85	0.59
1:C:126:THR:HB	1:C:342:ILE:HG23	1.84	0.59
1:C:421:THR:CG2	1:C:422:ALA:N	2.57	0.59
1:B:20:SER:HB2	1:B:231:GLY:HA2	1.85	0.59
1:B:82:GLY:N	1:B:83:PRO:HD2	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:THR:HB	1:B:342:ILE:HG23	1.83	0.59
1:B:368:THR:O	1:B:371:ALA:N	2.35	0.59
1:C:13:ILE:HB	1:C:14:PRO:HD3	1.84	0.59
1:C:421:THR:HG21	1:D:366:LEU:HD21	1.84	0.59
1:D:426:LEU:O	1:D:427:ASN:ND2	2.34	0.59
1:A:120:LYS:HE2	1:A:120:LYS:N	2.17	0.58
1:A:421:THR:HG21	1:B:366:LEU:CD1	2.33	0.58
1:B:119:LEU:CD2	1:B:124:VAL:HG21	2.31	0.58
1:B:376:GLY:O	1:B:379:HIS:N	2.32	0.58
1:C:57:SER:HB3	1:C:232:VAL:HG21	1.83	0.58
1:C:371:ALA:C	1:C:373:LEU:H	2.06	0.58
1:B:362:LEU:HG	1:B:402:VAL:HG21	1.84	0.58
1:A:210:ALA:HB3	1:A:228:THR:CG2	2.33	0.58
1:B:79:ARG:HB2	1:B:375:LEU:HD11	1.84	0.58
1:B:120:LYS:HE2	1:B:120:LYS:N	2.17	0.58
1:B:197:LEU:O	1:B:201:LEU:HB2	2.03	0.58
1:B:302:LYS:CD	1:B:302:LYS:N	2.66	0.58
1:B:315:ALA:HB1	1:B:316:ARG:HD3	1.85	0.58
1:C:384:ARG:HB3	1:C:385:PRO:HD3	1.85	0.58
1:D:24:MET:HE2	1:D:162:ILE:HD12	1.86	0.58
1:D:155:THR:O	1:D:159:LEU:HG	2.03	0.58
1:B:11:GLY:O	1:B:15:VAL:HG23	2.04	0.58
1:C:120:LYS:HE2	1:C:120:LYS:N	2.17	0.58
1:A:54:LEU:HD11	1:A:233:LEU:CD2	2.32	0.58
1:A:365:TYR:HB3	1:A:398:CYS:HG	1.66	0.58
1:A:426:LEU:O	1:A:427:ASN:ND2	2.34	0.58
1:B:81:PHE:CD2	1:B:83:PRO:HD2	2.38	0.58
1:B:209:SER:CA	1:B:296:LEU:HD11	2.30	0.58
1:B:250:ILE:N	1:B:251:PRO:CD	2.60	0.58
1:D:371:ALA:C	1:D:373:LEU:H	2.05	0.58
1:A:366:LEU:HD21	1:B:421:THR:HG21	1.85	0.58
1:A:384:ARG:HB3	1:A:385:PRO:HD3	1.85	0.58
1:B:115:PHE:CE1	1:B:276:ALA:HA	2.37	0.58
1:C:310:PHE:HB3	1:C:311:PRO:CA	2.34	0.58
1:D:63:MET:SD	1:D:372:LEU:CD1	2.91	0.58
1:A:8:HIS:HB3	1:A:9:LYS:HE2	1.85	0.58
1:A:79:ARG:HB2	1:A:375:LEU:HD11	1.85	0.58
1:A:366:LEU:HD13	1:A:367:TYR:CD2	2.39	0.58
1:A:403:VAL:HG23	1:B:415:VAL:CG1	2.34	0.58
1:B:426:LEU:O	1:B:427:ASN:ND2	2.37	0.58
1:C:81:PHE:CD2	1:C:83:PRO:HD2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:LYS:NZ	1:C:124:VAL:HG12	2.18	0.58
1:D:81:PHE:CD2	1:D:83:PRO:HD2	2.38	0.58
1:A:213:ALA:O	1:A:215:GLY:N	2.37	0.58
1:C:284:ALA:HA	1:C:287:LEU:HB2	1.86	0.58
1:D:302:LYS:HD3	1:D:302:LYS:N	2.19	0.58
1:D:368:THR:O	1:D:371:ALA:N	2.36	0.58
1:B:184:VAL:HG11	1:C:184:VAL:CG1	2.34	0.57
1:C:8:HIS:HB3	1:C:9:LYS:HE2	1.85	0.57
1:C:16:THR:CG2	1:C:227:ALA:HA	2.22	0.57
1:D:144:PRO:HD3	1:D:322:THR:CG2	2.33	0.57
1:D:207:VAL:HG12	1:D:232:VAL:CG2	2.33	0.57
1:A:138:LEU:O	1:A:142:VAL:HG23	2.04	0.57
1:A:155:THR:O	1:A:159:LEU:HG	2.03	0.57
1:A:428:TYR:OH	1:B:373:LEU:HD13	2.04	0.57
1:B:213:ALA:O	1:B:215:GLY:N	2.36	0.57
1:C:54:LEU:HD11	1:C:233:LEU:CD2	2.34	0.57
1:D:92:LEU:HD23	1:D:92:LEU:C	2.24	0.57
1:D:115:PHE:CE1	1:D:276:ALA:HA	2.36	0.57
1:A:63:MET:SD	1:A:372:LEU:CD1	2.92	0.57
1:A:120:LYS:NZ	1:A:124:VAL:HG12	2.20	0.57
1:A:191:GLY:O	1:A:194:GLN:HB2	2.04	0.57
1:C:155:THR:O	1:C:159:LEU:HG	2.03	0.57
1:C:357:SER:O	1:C:361:THR:HG23	2.04	0.57
1:D:8:HIS:HB3	1:D:9:LYS:HE2	1.85	0.57
1:D:91:VAL:HG21	1:D:420:ILE:HG12	1.86	0.57
1:B:138:LEU:O	1:B:142:VAL:HG23	2.04	0.57
1:D:49:THR:HB	1:D:197:LEU:HD23	1.86	0.57
1:A:77:ALA:HB1	1:A:86:GLY:HA2	1.87	0.57
1:A:133:LEU:HD22	1:A:334:MET:CE	2.33	0.57
1:A:377:HIS:CE1	1:B:431:LEU:N	2.72	0.57
1:B:41:ILE:HA	1:B:42:ALA:C	2.24	0.57
1:C:63:MET:CG	1:C:76:TYR:CE2	2.85	0.57
1:C:91:VAL:O	1:C:95:LEU:HB3	2.04	0.57
1:C:213:ALA:O	1:C:215:GLY:N	2.36	0.57
1:D:430:ARG:O	1:D:431:LEU:CB	2.53	0.57
1:A:107:ILE:O	1:A:111:TYR:HD1	1.87	0.57
1:B:20:SER:HA	1:B:23:ILE:HD12	1.87	0.57
1:B:99:ILE:HA	1:B:102:ILE:HD12	1.87	0.57
1:C:373:LEU:HD13	1:D:428:TYR:OH	2.05	0.57
1:D:79:ARG:HD3	1:D:375:LEU:HD11	1.87	0.57
1:A:359:ILE:O	1:A:362:LEU:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:ILE:O	1:B:111:TYR:HD1	1.87	0.57
1:B:201:LEU:O	1:B:203:SER:N	2.38	0.57
1:C:53:ALA:HB2	1:C:397:TYR:HE2	1.70	0.57
1:C:119:LEU:CD2	1:C:124:VAL:HG21	2.31	0.57
1:A:68:PRO:HA	1:A:69:SER:CB	2.34	0.57
1:A:302:LYS:HD3	1:A:302:LYS:N	2.19	0.57
1:B:310:PHE:HB3	1:B:311:PRO:CA	2.34	0.57
1:B:421:THR:CG2	1:B:422:ALA:N	2.55	0.57
1:C:63:MET:CG	1:C:76:TYR:CD2	2.87	0.57
1:C:360:PHE:O	1:C:363:VAL:HG23	2.04	0.57
1:D:6:ASP:HB3	1:D:9:LYS:HG2	1.87	0.57
1:D:87:TYR:HB3	1:D:424:TYR:OH	2.04	0.57
1:D:120:LYS:NZ	1:D:124:VAL:HG12	2.19	0.57
1:A:79:ARG:HG2	1:B:433:LYS:O	2.05	0.57
1:C:41:ILE:HG21	1:C:246:ILE:HG21	1.85	0.57
1:C:73:SER:N	1:C:76:TYR:CE1	2.72	0.57
1:C:204:PHE:HB3	1:C:397:TYR:OH	2.05	0.57
1:D:81:PHE:HB3	1:D:82:GLY:CA	2.34	0.57
1:B:84:PHE:CD1	1:B:85:LEU:N	2.73	0.57
1:B:218:LYS:HB2	1:B:223:ASN:HD22	1.70	0.57
1:B:284:ALA:HA	1:B:287:LEU:HB2	1.87	0.57
1:A:99:ILE:HA	1:A:102:ILE:HD12	1.87	0.56
1:C:49:THR:HB	1:C:197:LEU:HD23	1.87	0.56
1:C:90:ASN:ND2	1:C:310:PHE:CZ	2.72	0.56
1:B:357:SER:O	1:B:361:THR:HG23	2.05	0.56
1:B:420:ILE:O	1:B:421:THR:O	2.23	0.56
1:C:214:ALA:O	1:C:216:VAL:N	2.38	0.56
1:C:250:ILE:N	1:C:251:PRO:CD	2.60	0.56
1:C:362:LEU:HG	1:C:402:VAL:HG21	1.86	0.56
1:A:81:PHE:CB	1:A:82:GLY:HA2	2.24	0.56
1:A:140:ASN:CB	1:A:327:LEU:HD22	2.34	0.56
1:A:376:GLY:O	1:A:378:GLY:N	2.38	0.56
1:B:8:HIS:HB3	1:B:9:LYS:HE2	1.87	0.56
1:B:81:PHE:CB	1:B:82:GLY:HA2	2.19	0.56
1:B:210:ALA:HB3	1:B:228:THR:CG2	2.35	0.56
1:C:20:SER:HB2	1:C:231:GLY:HA2	1.86	0.56
1:D:68:PRO:HA	1:D:69:SER:CB	2.35	0.56
1:D:140:ASN:CB	1:D:327:LEU:HD22	2.35	0.56
1:D:204:PHE:HB3	1:D:397:TYR:OH	2.04	0.56
1:A:247:MET:HG2	1:A:248:GLY:H	1.71	0.56
1:A:315:ALA:HB1	1:A:316:ARG:HD3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:LEU:HB3	1:B:428:TYR:CE1	2.41	0.56
1:B:173:PHE:HA	1:B:174:ARG:CB	2.30	0.56
1:B:204:PHE:HB3	1:B:397:TYR:OH	2.06	0.56
1:C:315:ALA:HB1	1:C:316:ARG:HD3	1.87	0.56
1:D:247:MET:HG2	1:D:248:GLY:H	1.70	0.56
1:D:315:ALA:HB1	1:D:316:ARG:HD3	1.87	0.56
1:B:167:VAL:O	1:B:170:TRP:HB3	2.06	0.56
1:C:138:LEU:O	1:C:142:VAL:HG23	2.05	0.56
1:A:234:ILE:HG22	1:A:235:ALA:N	2.20	0.56
1:B:53:ALA:HB2	1:B:397:TYR:HE2	1.70	0.56
1:C:99:ILE:HA	1:C:102:ILE:HD12	1.88	0.56
1:D:212:VAL:CG1	1:D:296:LEU:HD13	2.35	0.56
1:D:310:PHE:HB3	1:D:311:PRO:CA	2.36	0.56
1:A:34:ASN:HB3	1:A:199:VAL:HG11	1.88	0.56
1:A:79:ARG:HD3	1:A:375:LEU:HD11	1.88	0.56
1:A:431:LEU:N	1:B:377:HIS:CE1	2.74	0.56
1:C:92:LEU:HD21	1:C:364:PRO:HD3	1.87	0.56
1:C:426:LEU:O	1:C:427:ASN:ND2	2.37	0.56
1:D:250:ILE:N	1:D:251:PRO:CD	2.61	0.56
1:A:310:PHE:HB3	1:A:311:PRO:CA	2.36	0.56
1:A:430:ARG:O	1:A:431:LEU:CB	2.53	0.56
1:B:73:SER:N	1:B:76:TYR:HE1	2.00	0.56
1:B:213:ALA:O	1:B:214:ALA:C	2.44	0.56
1:B:214:ALA:O	1:B:216:VAL:N	2.39	0.56
1:B:379:HIS:CE1	1:B:387:TYR:HD2	2.24	0.56
1:C:82:GLY:N	1:C:83:PRO:HD2	2.21	0.56
1:C:210:ALA:HB3	1:C:228:THR:CG2	2.35	0.56
1:C:302:LYS:HD3	1:C:302:LYS:N	2.20	0.56
1:C:433:LYS:O	1:D:79:ARG:HG2	2.06	0.56
1:D:88:GLN:HG2	1:D:89:THR:N	2.20	0.56
1:A:88:GLN:HG2	1:A:89:THR:N	2.19	0.56
1:A:284:ALA:HA	1:A:287:LEU:HB2	1.88	0.56
1:B:71:GLY:O	1:B:212:VAL:HA	2.06	0.56
1:C:213:ALA:O	1:C:214:ALA:C	2.45	0.56
1:A:379:HIS:CE1	1:A:387:TYR:HD2	2.24	0.56
1:B:172:TRP:CE3	1:B:173:PHE:HD2	2.24	0.56
1:D:20:SER:HA	1:D:23:ILE:HD12	1.86	0.56
1:D:284:ALA:HA	1:D:287:LEU:HB2	1.88	0.56
1:D:379:HIS:CE1	1:D:387:TYR:HD2	2.24	0.56
1:A:41:ILE:HG21	1:A:246:ILE:HG21	1.88	0.55
1:A:68:PRO:HA	1:A:69:SER:HB3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:VAL:HB	1:A:420:ILE:HD11	1.89	0.55
1:B:24:MET:CE	1:B:162:ILE:HD12	2.36	0.55
1:C:379:HIS:CE1	1:C:387:TYR:HD2	2.23	0.55
1:D:38:THR:CB	1:D:39:GLY:CA	2.76	0.55
1:D:63:MET:HG3	1:D:76:TYR:CD2	2.40	0.55
1:D:213:ALA:O	1:D:215:GLY:N	2.38	0.55
1:D:363:VAL:O	1:D:366:LEU:HB3	2.06	0.55
1:A:123:LEU:O	1:A:126:THR:HG23	2.07	0.55
1:A:20:SER:HB2	1:A:231:GLY:HA2	1.88	0.55
1:A:49:THR:HB	1:A:197:LEU:HD23	1.89	0.55
1:C:172:TRP:CE3	1:C:173:PHE:HD2	2.25	0.55
1:B:119:LEU:HD13	1:B:124:VAL:CG1	2.32	0.55
1:B:133:LEU:HD23	1:B:290:LEU:CD1	2.36	0.55
1:B:359:ILE:O	1:B:362:LEU:HB2	2.06	0.55
1:C:167:VAL:O	1:C:170:TRP:HB3	2.06	0.55
1:C:400:TRP:HA	1:C:403:VAL:HG12	1.88	0.55
1:D:121:ASP:H	1:D:122:PRO:CD	2.19	0.55
1:D:207:VAL:CG1	1:D:232:VAL:CG2	2.84	0.55
1:D:213:ALA:O	1:D:214:ALA:C	2.44	0.55
1:D:359:ILE:O	1:D:362:LEU:HB2	2.05	0.55
1:A:20:SER:HA	1:A:23:ILE:HD12	1.87	0.55
1:A:24:MET:CE	1:A:238:CYS:SG	2.94	0.55
1:C:312:PRO:HA	1:C:313:ILE:HB	1.89	0.55
1:D:81:PHE:CB	1:D:82:GLY:HA2	2.25	0.55
1:D:406:GLY:HA3	1:D:409:GLU:CD	2.26	0.55
1:C:63:MET:SD	1:C:372:LEU:HD12	2.46	0.55
1:A:204:PHE:O	1:A:204:PHE:HD1	1.90	0.55
1:B:121:ASP:H	1:B:122:PRO:CD	2.19	0.55
1:C:173:PHE:CA	1:C:174:ARG:HB2	2.37	0.55
1:C:201:LEU:O	1:C:203:SER:N	2.40	0.55
1:D:167:VAL:O	1:D:170:TRP:HB3	2.07	0.55
1:A:201:LEU:CD2	1:A:401:ALA:HB2	2.37	0.55
1:B:24:MET:CE	1:B:238:CYS:SG	2.95	0.55
1:B:73:SER:N	1:B:76:TYR:CE1	2.74	0.55
1:B:302:LYS:HD3	1:B:302:LYS:N	2.21	0.55
1:C:376:GLY:C	1:C:378:GLY:N	2.59	0.55
1:A:84:PHE:CD1	1:A:85:LEU:N	2.75	0.55
1:B:41:ILE:HG21	1:B:246:ILE:HG21	1.88	0.55
1:B:63:MET:HG3	1:B:76:TYR:CD2	2.41	0.55
1:C:68:PRO:HB2	1:C:220:PRO:HB3	1.88	0.55
1:C:115:PHE:CE1	1:C:276:ALA:HA	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:234:ILE:HG22	1:D:235:ALA:N	2.21	0.55
1:D:376:GLY:O	1:D:378:GLY:N	2.40	0.55
1:A:115:PHE:CE1	1:A:276:ALA:HA	2.37	0.55
1:A:294:THR:O	1:A:297:ALA:HB3	2.07	0.55
1:C:123:LEU:O	1:C:126:THR:HG23	2.06	0.55
1:D:214:ALA:O	1:D:216:VAL:N	2.40	0.55
1:A:204:PHE:HB3	1:A:397:TYR:OH	2.06	0.54
1:A:312:PRO:HA	1:A:313:ILE:HB	1.89	0.54
1:D:34:ASN:HB3	1:D:199:VAL:HG11	1.89	0.54
1:D:88:GLN:HA	1:D:91:VAL:HG23	1.89	0.54
1:D:107:ILE:O	1:D:111:TYR:HD1	1.89	0.54
1:A:92:LEU:HD23	1:A:92:LEU:C	2.28	0.54
1:A:167:VAL:O	1:A:170:TRP:HB3	2.07	0.54
1:B:68:PRO:HA	1:B:69:SER:CB	2.37	0.54
1:C:247:MET:HG2	1:C:248:GLY:H	1.71	0.54
1:B:38:THR:CB	1:B:39:GLY:CA	2.74	0.54
1:B:88:GLN:HG2	1:B:89:THR:N	2.23	0.54
1:C:68:PRO:HA	1:C:69:SER:CB	2.38	0.54
1:C:119:LEU:HD13	1:C:124:VAL:CG1	2.32	0.54
1:A:71:GLY:O	1:A:212:VAL:HA	2.08	0.54
1:A:172:TRP:CE3	1:A:173:PHE:HD2	2.25	0.54
1:D:92:LEU:HD21	1:D:364:PRO:HD3	1.88	0.54
1:D:201:LEU:CD2	1:D:401:ALA:HB2	2.37	0.54
1:D:210:ALA:HB3	1:D:228:THR:CG2	2.34	0.54
1:A:10:VAL:HG22	1:A:145:LYS:HA	1.89	0.54
1:A:400:TRP:HA	1:A:403:VAL:HG12	1.89	0.54
1:B:24:MET:HE1	1:B:238:CYS:SG	2.48	0.54
1:B:430:ARG:O	1:B:431:LEU:CB	2.55	0.54
1:C:71:GLY:O	1:C:212:VAL:HA	2.08	0.54
1:D:172:TRP:CE3	1:D:173:PHE:HD2	2.25	0.54
1:A:212:VAL:CG1	1:A:296:LEU:HD13	2.38	0.54
1:A:213:ALA:O	1:A:214:ALA:C	2.45	0.54
1:A:6:ASP:HB3	1:A:9:LYS:HG2	1.90	0.54
1:A:41:ILE:HG22	1:A:246:ILE:CD1	2.35	0.54
1:A:57:SER:HB2	1:A:232:VAL:HG21	1.89	0.54
1:A:373:LEU:CB	1:B:428:TYR:CE1	2.91	0.54
1:B:54:LEU:HD11	1:B:233:LEU:CD2	2.37	0.54
1:B:77:ALA:HB1	1:B:86:GLY:HA2	1.90	0.54
1:B:132:VAL:O	1:B:135:ILE:HB	2.08	0.54
1:C:218:LYS:HB2	1:C:223:ASN:HD22	1.71	0.54
1:C:323:PRO:HB2	1:C:326:GLY:HA3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:415:VAL:HG11	1:D:403:VAL:HG23	1.88	0.54
1:D:77:ALA:HB1	1:D:86:GLY:HA2	1.90	0.54
1:D:314:PHE:O	1:D:314:PHE:HD2	1.91	0.54
1:B:376:GLY:C	1:B:378:GLY:N	2.60	0.54
1:C:68:PRO:HA	1:C:69:SER:HB3	1.90	0.54
1:C:144:PRO:HB2	1:C:216:VAL:HG11	1.90	0.54
1:D:8:HIS:HB3	1:D:9:LYS:NZ	2.23	0.54
1:B:247:MET:HG2	1:B:248:GLY:H	1.72	0.54
1:C:23:ILE:HG21	1:C:204:PHE:HD1	1.72	0.54
1:C:81:PHE:CB	1:C:82:GLY:HA2	2.19	0.54
1:B:68:PRO:HB2	1:B:220:PRO:HB3	1.89	0.54
1:C:15:VAL:O	1:C:19:VAL:HG23	2.07	0.54
1:C:67:ASP:OD1	1:C:69:SER:HA	2.08	0.54
1:A:314:PHE:HD2	1:A:314:PHE:O	1.91	0.53
1:B:201:LEU:C	1:B:203:SER:N	2.62	0.53
1:C:69:SER:OG	1:C:70:PRO:HA	2.08	0.53
1:D:15:VAL:O	1:D:19:VAL:HG23	2.06	0.53
1:D:68:PRO:HA	1:D:69:SER:HB3	1.88	0.53
1:B:68:PRO:HA	1:B:69:SER:HB3	1.90	0.53
1:B:323:PRO:HB2	1:B:326:GLY:HA3	1.90	0.53
1:C:84:PHE:CE1	1:C:85:LEU:CD2	2.88	0.53
1:D:77:ALA:C	1:D:79:ARG:N	2.61	0.53
1:D:81:PHE:CE2	1:D:83:PRO:HG2	2.43	0.53
1:A:81:PHE:CE2	1:A:83:PRO:HG2	2.43	0.53
1:A:132:VAL:O	1:A:135:ILE:HB	2.08	0.53
1:A:218:LYS:HB2	1:A:223:ASN:HD22	1.73	0.53
1:C:24:MET:CE	1:C:162:ILE:HD12	2.38	0.53
1:C:132:VAL:O	1:C:135:ILE:HB	2.09	0.53
1:D:133:LEU:HD22	1:D:334:MET:SD	2.48	0.53
1:D:218:LYS:HB2	1:D:223:ASN:HD22	1.72	0.53
1:D:312:PRO:HA	1:D:313:ILE:HB	1.89	0.53
1:D:366:LEU:HD13	1:D:367:TYR:CD2	2.43	0.53
1:A:367:TYR:O	1:A:370:ALA:HB3	2.08	0.53
1:B:312:PRO:HA	1:B:313:ILE:HB	1.89	0.53
1:B:400:TRP:HA	1:B:403:VAL:HG12	1.89	0.53
1:C:24:MET:CE	1:C:238:CYS:SG	2.96	0.53
1:C:54:LEU:HD12	1:C:232:VAL:HG12	1.91	0.53
1:C:133:LEU:HD23	1:C:290:LEU:CD1	2.35	0.53
1:A:15:VAL:O	1:A:19:VAL:HG23	2.08	0.53
1:A:73:SER:N	1:A:76:TYR:HE1	2.06	0.53
1:B:8:HIS:O	1:B:9:LYS:HD3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:TYR:CE1	1:C:304:ALA:HB2	2.43	0.53
1:C:76:TYR:OH	1:C:211:SER:OG	2.15	0.53
1:D:73:SER:N	1:D:76:TYR:CE1	2.76	0.53
1:D:191:GLY:O	1:D:194:GLN:HB2	2.09	0.53
1:D:79:ARG:HB2	1:D:375:LEU:HD11	1.90	0.53
1:D:133:LEU:HD22	1:D:334:MET:CE	2.38	0.53
1:C:6:ASP:HB3	1:C:9:LYS:HG2	1.89	0.53
1:A:121:ASP:H	1:A:122:PRO:CD	2.20	0.53
1:C:121:ASP:H	1:C:122:PRO:CD	2.22	0.53
1:A:323:PRO:HD2	1:A:327:LEU:HD11	1.91	0.53
1:B:144:PRO:HB2	1:B:216:VAL:HG11	1.90	0.53
1:D:201:LEU:O	1:D:203:SER:N	2.41	0.53
1:D:301:ALA:C	1:D:303:ALA:H	2.12	0.53
1:D:400:TRP:HA	1:D:403:VAL:HG12	1.91	0.53
1:D:425:ALA:O	1:D:427:ASN:N	2.42	0.53
1:A:363:VAL:O	1:A:366:LEU:HB3	2.09	0.53
1:B:205:ILE:HD13	1:B:361:THR:OG1	2.09	0.53
1:B:234:ILE:HG22	1:B:235:ALA:N	2.24	0.53
1:D:204:PHE:O	1:D:204:PHE:HD1	1.92	0.53
1:A:173:PHE:CA	1:A:174:ARG:HB2	2.38	0.52
1:B:96:ALA:HA	1:B:357:SER:HB2	1.91	0.52
1:B:426:LEU:O	1:B:426:LEU:HG	2.10	0.52
1:C:41:ILE:HG13	1:C:43:ILE:HG12	1.91	0.52
1:C:77:ALA:HB1	1:C:86:GLY:HA2	1.90	0.52
1:C:367:TYR:O	1:C:370:ALA:HB3	2.09	0.52
1:D:93:TYR:CE1	1:D:208:GLU:CD	2.83	0.52
1:D:139:LEU:HB3	1:D:146:MET:HE1	1.90	0.52
1:A:88:GLN:HA	1:A:91:VAL:HG23	1.90	0.52
1:A:91:VAL:HG21	1:A:420:ILE:HG12	1.91	0.52
1:B:6:ASP:HB3	1:B:9:LYS:HG2	1.90	0.52
1:B:412:TRP:CZ3	1:B:415:VAL:HG21	2.45	0.52
1:D:123:LEU:O	1:D:126:THR:HG23	2.09	0.52
1:A:214:ALA:O	1:A:216:VAL:N	2.42	0.52
1:A:414:PHE:HD1	1:B:414:PHE:CB	2.16	0.52
1:C:96:ALA:HA	1:C:357:SER:HB2	1.90	0.52
1:D:149:ARG:O	1:D:153:VAL:HG23	2.10	0.52
1:D:323:PRO:HB2	1:D:326:GLY:HA3	1.92	0.52
1:A:90:ASN:ND2	1:A:310:PHE:CZ	2.77	0.52
1:B:10:VAL:HG22	1:B:145:LYS:HA	1.92	0.52
1:B:49:THR:HB	1:B:197:LEU:HD23	1.91	0.52
1:C:8:HIS:O	1:C:9:LYS:HD3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:ASP:OD1	1:C:67:ASP:C	2.48	0.52
1:C:84:PHE:CD1	1:C:85:LEU:N	2.77	0.52
1:C:414:PHE:C	1:C:414:PHE:CD2	2.83	0.52
1:D:84:PHE:CD1	1:D:85:LEU:N	2.78	0.52
1:A:433:LYS:CB	1:B:78:ARG:HH11	2.21	0.52
1:C:216:VAL:O	1:C:216:VAL:HG12	2.10	0.52
1:D:41:ILE:HG21	1:D:246:ILE:HG21	1.90	0.52
1:B:15:VAL:O	1:B:19:VAL:HG23	2.09	0.52
1:B:16:THR:CG2	1:B:227:ALA:HA	2.25	0.52
1:B:104:MET:HE1	1:B:286:CYS:SG	2.50	0.52
1:B:389:ALA:O	1:B:392:THR:N	2.43	0.52
1:C:91:VAL:HG21	1:C:420:ILE:HG12	1.91	0.52
1:C:92:LEU:HD23	1:C:92:LEU:C	2.30	0.52
1:C:209:SER:CA	1:C:296:LEU:HD11	2.33	0.52
1:C:377:HIS:HE1	1:D:430:ARG:N	2.08	0.52
1:D:31:LEU:HB2	1:D:32:PRO:HD3	1.91	0.52
1:B:149:ARG:O	1:B:153:VAL:HG23	2.10	0.52
1:B:212:VAL:CG1	1:B:296:LEU:HD13	2.40	0.52
1:C:399:ILE:HA	1:D:418:MET:CE	2.39	0.52
1:C:426:LEU:O	1:C:426:LEU:HG	2.10	0.52
1:A:433:LYS:CB	1:B:78:ARG:NH1	2.73	0.52
1:C:204:PHE:HD1	1:C:204:PHE:O	1.92	0.52
1:D:314:PHE:HA	1:D:315:ALA:O	2.10	0.52
1:A:82:GLY:N	1:A:83:PRO:CD	2.73	0.52
1:A:201:LEU:O	1:A:203:SER:N	2.43	0.52
1:A:216:VAL:HG12	1:A:216:VAL:O	2.09	0.52
1:A:418:MET:HE2	1:B:399:ILE:HG12	1.92	0.52
1:C:10:VAL:HG22	1:C:145:LYS:HA	1.92	0.52
1:C:32:PRO:HA	1:C:35:LEU:HD12	1.91	0.52
1:C:299:GLN:OE1	1:C:299:GLN:HA	2.09	0.52
1:C:389:ALA:O	1:C:392:THR:N	2.43	0.52
1:D:99:ILE:HA	1:D:102:ILE:HD12	1.91	0.52
1:A:24:MET:HE2	1:A:162:ILE:HD12	1.92	0.52
1:A:319:LYS:O	1:A:320:ALA:HB3	2.10	0.52
1:A:425:ALA:O	1:A:427:ASN:N	2.43	0.52
1:C:31:LEU:HB2	1:C:32:PRO:HD3	1.92	0.52
1:A:24:MET:HE1	1:A:238:CYS:SG	2.50	0.51
1:A:323:PRO:HB2	1:A:326:GLY:HA3	1.92	0.51
1:A:418:MET:CE	1:B:399:ILE:HA	2.40	0.51
1:B:204:PHE:O	1:B:204:PHE:HD1	1.92	0.51
1:C:201:LEU:C	1:C:203:SER:N	2.62	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:415:VAL:CG1	1:D:403:VAL:HG23	2.40	0.51
1:D:120:LYS:HZ3	1:D:124:VAL:HG12	1.73	0.51
1:A:85:LEU:CD1	1:B:84:PHE:CE1	2.88	0.51
1:A:412:TRP:CZ3	1:A:415:VAL:HG21	2.45	0.51
1:B:173:PHE:CA	1:B:174:ARG:HB2	2.37	0.51
1:B:184:VAL:O	1:B:185:SER:HB2	2.10	0.51
1:C:184:VAL:O	1:C:185:SER:HB2	2.10	0.51
1:C:430:ARG:O	1:C:431:LEU:CB	2.57	0.51
1:A:377:HIS:HE1	1:B:430:ARG:N	2.08	0.51
1:B:77:ALA:C	1:B:79:ARG:N	2.63	0.51
1:B:123:LEU:O	1:B:126:THR:HG23	2.10	0.51
1:C:88:GLN:HG2	1:C:89:THR:N	2.25	0.51
1:C:149:ARG:O	1:C:153:VAL:HG23	2.10	0.51
1:C:151:GLN:HE22	1:C:289:SER:HA	1.75	0.51
1:D:41:ILE:HG22	1:D:246:ILE:CD1	2.36	0.51
1:D:82:GLY:N	1:D:83:PRO:CD	2.74	0.51
1:D:216:VAL:O	1:D:216:VAL:HG12	2.11	0.51
1:B:67:ASP:C	1:B:67:ASP:OD1	2.49	0.51
1:C:139:LEU:HB3	1:C:146:MET:HE1	1.92	0.51
1:D:144:PRO:HG2	1:D:216:VAL:HG11	1.93	0.51
1:A:119:LEU:HD22	1:A:124:VAL:CG2	2.36	0.51
1:B:216:VAL:O	1:B:216:VAL:HG12	2.10	0.51
1:C:18:MET:HA	1:C:151:GLN:HG2	1.93	0.51
1:C:56:LEU:CD1	1:C:365:TYR:CD1	2.93	0.51
1:C:77:ALA:C	1:C:79:ARG:N	2.64	0.51
1:D:10:VAL:HG22	1:D:145:LYS:HA	1.92	0.51
1:D:372:LEU:HG	1:D:372:LEU:O	2.10	0.51
1:A:31:LEU:HB2	1:A:32:PRO:HD3	1.93	0.51
1:B:32:PRO:HA	1:B:35:LEU:HD12	1.93	0.51
1:C:41:ILE:O	1:C:41:ILE:HG12	2.09	0.51
1:D:367:TYR:O	1:D:370:ALA:HB3	2.11	0.51
1:B:41:ILE:HG13	1:B:43:ILE:HG12	1.93	0.51
1:C:32:PRO:HA	1:C:35:LEU:CD1	2.41	0.51
1:C:111:TYR:CB	1:C:283:ALA:HB2	2.33	0.51
1:D:90:ASN:ND2	1:D:310:PHE:CZ	2.78	0.51
1:D:93:TYR:HE1	1:D:208:GLU:OE2	1.92	0.51
1:A:372:LEU:HG	1:A:372:LEU:O	2.11	0.51
1:B:23:ILE:HG21	1:B:204:PHE:HD1	1.76	0.51
1:B:69:SER:OG	1:B:70:PRO:HA	2.11	0.51
1:B:74:TYR:CE1	1:B:304:ALA:HB2	2.45	0.51
1:B:299:GLN:OE1	1:B:299:GLN:HA	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:LYS:O	1:B:320:ALA:HB3	2.11	0.51
1:D:8:HIS:HB3	1:D:9:LYS:CE	2.41	0.51
1:D:310:PHE:CE1	1:D:314:PHE:HE2	2.29	0.51
1:A:377:HIS:CE1	1:B:430:ARG:N	2.79	0.51
1:B:69:SER:OG	1:B:71:GLY:N	2.43	0.51
1:D:57:SER:HB2	1:D:232:VAL:HG21	1.92	0.51
1:D:132:VAL:O	1:D:135:ILE:HB	2.11	0.51
1:A:80:CYS:O	1:B:81:PHE:CE1	2.64	0.51
1:B:44:TYR:O	1:B:47:LEU:N	2.44	0.51
1:B:92:LEU:C	1:B:92:LEU:HD23	2.31	0.51
1:C:205:ILE:HD13	1:C:361:THR:OG1	2.11	0.51
1:C:421:THR:CG2	1:D:366:LEU:HD21	2.41	0.51
1:C:44:TYR:O	1:C:47:LEU:N	2.44	0.50
1:D:67:ASP:OD1	1:D:69:SER:HA	2.11	0.50
1:D:118:ILE:HA	1:D:119:LEU:C	2.32	0.50
1:A:44:TYR:O	1:A:47:LEU:N	2.44	0.50
1:A:54:LEU:HD12	1:A:232:VAL:HG12	1.92	0.50
1:A:377:HIS:CE1	1:B:430:ARG:C	2.84	0.50
1:B:119:LEU:CD1	1:B:124:VAL:HG11	2.35	0.50
1:C:218:LYS:O	1:C:220:PRO:HD3	2.12	0.50
1:C:319:LYS:O	1:C:320:ALA:HB3	2.12	0.50
1:D:68:PRO:HB2	1:D:220:PRO:HB3	1.93	0.50
1:A:8:HIS:O	1:A:9:LYS:HD3	2.11	0.50
1:A:73:SER:N	1:A:76:TYR:CE1	2.79	0.50
1:A:80:CYS:O	1:B:81:PHE:HE1	1.94	0.50
1:A:133:LEU:HD23	1:A:290:LEU:CD1	2.38	0.50
1:A:154:ALA:O	1:A:157:LEU:HB2	2.11	0.50
1:A:424:TYR:CD1	1:A:430:ARG:NH2	2.79	0.50
1:B:18:MET:HA	1:B:151:GLN:HG2	1.92	0.50
1:B:32:PRO:HA	1:B:35:LEU:CD1	2.42	0.50
1:B:218:LYS:O	1:B:220:PRO:HD3	2.11	0.50
1:A:139:LEU:HB3	1:A:146:MET:HE1	1.92	0.50
1:A:430:ARG:C	1:B:377:HIS:HE1	2.15	0.50
1:B:89:THR:HG23	1:B:364:PRO:HG3	1.93	0.50
1:B:91:VAL:HG21	1:B:420:ILE:HG12	1.92	0.50
1:D:302:LYS:HG3	1:D:314:PHE:HB2	1.94	0.50
1:D:323:PRO:HD2	1:D:327:LEU:HD11	1.93	0.50
1:D:326:GLY:O	1:D:330:VAL:HG23	2.11	0.50
1:A:8:HIS:HB3	1:A:9:LYS:NZ	2.26	0.50
1:A:68:PRO:HB2	1:A:220:PRO:HB3	1.93	0.50
1:A:301:ALA:C	1:A:303:ALA:H	2.13	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:THR:CA	1:A:419:VAL:HG12	2.42	0.50
1:B:67:ASP:OD1	1:B:69:SER:HA	2.11	0.50
1:C:412:TRP:CZ3	1:C:415:VAL:HG21	2.46	0.50
1:D:18:MET:HA	1:D:151:GLN:HG2	1.94	0.50
1:D:56:LEU:HD12	1:D:397:TYR:CE1	2.46	0.50
1:D:92:LEU:O	1:D:360:PHE:HB3	2.12	0.50
1:D:133:LEU:HD23	1:D:290:LEU:CD1	2.34	0.50
1:A:119:LEU:HD13	1:A:124:VAL:CG1	2.33	0.50
1:A:144:PRO:HG2	1:A:216:VAL:HG11	1.93	0.50
1:A:149:ARG:O	1:A:153:VAL:HG23	2.12	0.50
1:A:330:VAL:O	1:A:334:MET:HB2	2.11	0.50
1:B:330:VAL:O	1:B:334:MET:HB2	2.12	0.50
1:C:104:MET:CE	1:C:286:CYS:SG	3.00	0.50
1:C:414:PHE:O	1:C:418:MET:HG3	2.12	0.50
1:D:205:ILE:HD13	1:D:361:THR:OG1	2.12	0.50
1:D:319:LYS:O	1:D:320:ALA:HB3	2.12	0.50
1:A:313:ILE:HG22	1:A:314:PHE:N	2.27	0.50
1:B:31:LEU:HB2	1:B:32:PRO:HD3	1.92	0.50
1:B:72:GLY:C	1:B:74:TYR:H	2.15	0.50
1:B:118:ILE:HA	1:B:119:LEU:C	2.32	0.50
1:B:326:GLY:O	1:B:330:VAL:HG23	2.12	0.50
1:C:314:PHE:HD2	1:C:314:PHE:O	1.95	0.50
1:D:24:MET:HE1	1:D:238:CYS:SG	2.52	0.50
1:D:32:PRO:HA	1:D:35:LEU:HD12	1.93	0.50
1:A:93:TYR:HE1	1:A:208:GLU:OE2	1.95	0.50
1:A:201:LEU:C	1:A:203:SER:N	2.65	0.50
1:A:421:THR:HG21	1:B:366:LEU:HD21	1.93	0.50
1:C:79:ARG:HD3	1:C:375:LEU:HD11	1.93	0.50
1:C:366:LEU:HD11	1:D:421:THR:HG21	1.94	0.50
1:D:32:PRO:HA	1:D:35:LEU:CD1	2.41	0.50
1:D:74:TYR:OH	1:D:304:ALA:HA	2.12	0.50
1:A:50:ILE:HD13	1:A:236:ALA:HB1	1.94	0.50
1:A:84:PHE:CE1	1:A:85:LEU:CD2	2.88	0.50
1:A:89:THR:HG23	1:A:364:PRO:HG3	1.94	0.50
1:A:118:ILE:HA	1:A:119:LEU:C	2.31	0.50
1:A:133:LEU:HD22	1:A:334:MET:SD	2.52	0.50
1:A:420:ILE:HG22	1:A:421:THR:H	1.75	0.50
1:B:90:ASN:O	1:B:91:VAL:C	2.49	0.50
1:C:410:VAL:CG1	1:D:411:MET:HA	2.42	0.50
1:D:24:MET:HE3	1:D:238:CYS:SG	2.51	0.50
1:D:184:VAL:O	1:D:185:SER:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:294:THR:O	1:D:297:ALA:HB3	2.11	0.50
1:B:416:THR:CA	1:B:419:VAL:HG12	2.40	0.49
1:D:71:GLY:O	1:D:212:VAL:HA	2.11	0.49
1:D:313:ILE:HG22	1:D:314:PHE:N	2.26	0.49
1:A:32:PRO:HA	1:A:35:LEU:CD1	2.42	0.49
1:A:53:ALA:HB2	1:A:397:TYR:HE2	1.76	0.49
1:C:119:LEU:CD1	1:C:124:VAL:HG11	2.35	0.49
1:C:310:PHE:CE1	1:C:314:PHE:HE2	2.30	0.49
1:C:418:MET:HE2	1:D:399:ILE:HG12	1.93	0.49
1:B:104:MET:HB3	1:B:290:LEU:HD23	1.94	0.49
1:C:118:ILE:HA	1:C:119:LEU:C	2.32	0.49
1:C:133:LEU:HD22	1:C:334:MET:CE	2.43	0.49
1:C:330:VAL:O	1:C:334:MET:HB2	2.12	0.49
1:C:396:LEU:O	1:C:397:TYR:C	2.50	0.49
1:D:218:LYS:O	1:D:220:PRO:HD3	2.11	0.49
1:D:330:VAL:O	1:D:334:MET:HB2	2.11	0.49
1:D:379:HIS:C	1:D:381:GLY:N	2.65	0.49
1:D:412:TRP:CZ3	1:D:415:VAL:HG21	2.47	0.49
1:A:23:ILE:HG21	1:A:204:PHE:HD1	1.74	0.49
1:A:74:TYR:OH	1:A:304:ALA:HA	2.11	0.49
1:A:111:TYR:CB	1:A:283:ALA:HB2	2.36	0.49
1:A:374:LEU:O	1:A:377:HIS:CD2	2.65	0.49
1:C:23:ILE:HG23	1:C:204:PHE:O	2.13	0.49
1:C:69:SER:OG	1:C:71:GLY:N	2.42	0.49
1:D:140:ASN:HD21	1:D:147:ILE:HG12	1.77	0.49
1:D:357:SER:O	1:D:361:THR:HG23	2.12	0.49
1:A:8:HIS:HB3	1:A:9:LYS:CE	2.43	0.49
1:A:77:ALA:C	1:A:79:ARG:N	2.64	0.49
1:A:165:ILE:O	1:A:169:GLY:HA3	2.11	0.49
1:A:218:LYS:O	1:A:220:PRO:HD3	2.12	0.49
1:A:421:THR:HG21	1:B:366:LEU:CD2	2.43	0.49
1:B:151:GLN:HE22	1:B:289:SER:HA	1.77	0.49
1:B:363:VAL:O	1:B:366:LEU:HB3	2.12	0.49
1:B:366:LEU:HD13	1:B:367:TYR:CD2	2.47	0.49
1:B:385:PRO:HA	1:B:388:LEU:HB2	1.95	0.49
1:C:71:GLY:C	1:C:212:VAL:HA	2.33	0.49
1:C:326:GLY:O	1:C:330:VAL:HG23	2.13	0.49
1:C:430:ARG:N	1:D:377:HIS:HE1	2.10	0.49
1:D:8:HIS:O	1:D:9:LYS:HD3	2.11	0.49
1:D:93:TYR:HE2	1:D:97:CYS:SG	2.35	0.49
1:D:173:PHE:CA	1:D:174:ARG:HB2	2.36	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:209:SER:CA	1:D:296:LEU:HD11	2.30	0.49
1:A:35:LEU:CD2	1:A:196:THR:HG22	2.41	0.49
1:A:379:HIS:CE1	1:A:387:TYR:CD2	3.01	0.49
1:B:23:ILE:HG23	1:B:204:PHE:O	2.13	0.49
1:B:191:GLY:O	1:B:194:GLN:HB2	2.13	0.49
1:B:298:GLY:HA2	1:B:302:LYS:NZ	2.27	0.49
1:B:302:LYS:HG3	1:B:314:PHE:HB2	1.94	0.49
1:B:314:PHE:O	1:B:314:PHE:HD2	1.95	0.49
1:C:24:MET:HE2	1:C:162:ILE:HD12	1.94	0.49
1:C:154:ALA:O	1:C:157:LEU:HB2	2.13	0.49
1:D:54:LEU:HD12	1:D:232:VAL:HG12	1.94	0.49
1:D:165:ILE:O	1:D:169:GLY:HA3	2.13	0.49
1:D:376:GLY:C	1:D:378:GLY:N	2.66	0.49
1:A:360:PHE:O	1:A:363:VAL:HG23	2.13	0.49
1:B:49:THR:OG1	1:B:201:LEU:CD1	2.61	0.49
1:B:119:LEU:HD22	1:B:124:VAL:CG2	2.37	0.49
1:B:339:LEU:HA	1:B:342:ILE:HG13	1.95	0.49
1:B:374:LEU:O	1:B:377:HIS:CD2	2.66	0.49
1:C:76:TYR:HH	1:C:211:SER:HG	1.41	0.49
1:C:78:ARG:C	1:C:79:ARG:HG3	2.33	0.49
1:D:119:LEU:HD22	1:D:124:VAL:CG2	2.35	0.49
1:D:201:LEU:C	1:D:203:SER:N	2.64	0.49
1:D:379:HIS:CE1	1:D:387:TYR:CD2	3.01	0.49
1:A:32:PRO:HA	1:A:35:LEU:HD12	1.94	0.49
1:A:79:ARG:HD3	1:A:375:LEU:CD1	2.42	0.49
1:A:93:TYR:HE2	1:A:97:CYS:SG	2.31	0.49
1:A:363:VAL:CB	1:A:364:PRO:HD3	2.43	0.49
1:B:41:ILE:O	1:B:41:ILE:HG12	2.11	0.49
1:B:56:LEU:CD1	1:B:365:TYR:CD1	2.94	0.49
1:B:63:MET:HB2	1:B:372:LEU:HD13	1.94	0.49
1:C:50:ILE:HD13	1:C:236:ALA:HB1	1.95	0.49
1:C:234:ILE:HG22	1:C:235:ALA:N	2.25	0.49
1:C:422:ALA:CB	1:D:395:PHE:CD1	2.95	0.49
1:C:428:TYR:CE1	1:D:373:LEU:HB3	2.47	0.49
1:D:298:GLY:HA2	1:D:302:LYS:NZ	2.28	0.49
1:A:92:LEU:O	1:A:360:PHE:HB3	2.12	0.49
1:A:376:GLY:HA3	1:A:379:HIS:CD2	2.48	0.49
1:C:104:MET:HB3	1:C:290:LEU:HD23	1.95	0.49
1:D:114:TYR:C	1:D:115:PHE:HD2	2.16	0.49
1:A:24:MET:HE3	1:A:162:ILE:HD12	1.94	0.49
1:A:49:THR:OG1	1:A:201:LEU:CD1	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:LYS:HG3	1:A:314:PHE:HB2	1.94	0.49
1:B:50:ILE:HD13	1:B:236:ALA:HB1	1.93	0.49
1:B:379:HIS:C	1:B:381:GLY:N	2.65	0.49
1:C:376:GLY:O	1:C:377:HIS:C	2.51	0.49
1:C:379:HIS:C	1:C:381:GLY:N	2.66	0.49
1:A:67:ASP:C	1:A:67:ASP:OD1	2.52	0.48
1:A:67:ASP:OD1	1:A:69:SER:HA	2.13	0.48
1:A:314:PHE:HA	1:A:315:ALA:O	2.13	0.48
1:C:79:ARG:HD3	1:C:375:LEU:CD1	2.43	0.48
1:C:379:HIS:CE1	1:C:387:TYR:CD2	3.01	0.48
1:D:79:ARG:HD3	1:D:375:LEU:CD1	2.43	0.48
1:A:14:PRO:HB2	1:A:148:THR:OG1	2.13	0.48
1:A:114:TYR:C	1:A:115:PHE:HD2	2.16	0.48
1:A:151:GLN:HE22	1:A:289:SER:HA	1.77	0.48
1:B:363:VAL:CB	1:B:364:PRO:HD3	2.43	0.48
1:C:8:HIS:HB3	1:C:9:LYS:NZ	2.28	0.48
1:D:21:GLY:HA2	1:D:24:MET:HB2	1.94	0.48
1:D:24:MET:CB	1:D:25:GLY:CA	2.88	0.48
1:A:209:SER:CA	1:A:296:LEU:HD11	2.34	0.48
1:C:8:HIS:HB3	1:C:9:LYS:CE	2.43	0.48
1:C:188:GLY:C	1:C:192:ALA:HB2	2.23	0.48
1:B:363:VAL:HG23	1:B:364:PRO:HD3	1.94	0.48
1:C:90:ASN:O	1:C:91:VAL:C	2.50	0.48
1:C:294:THR:O	1:C:297:ALA:HB3	2.13	0.48
1:D:74:TYR:CE1	1:D:304:ALA:HB2	2.47	0.48
1:D:154:ALA:O	1:D:157:LEU:HB2	2.13	0.48
1:A:310:PHE:CE1	1:A:314:PHE:HE2	2.30	0.48
1:B:74:TYR:OH	1:B:304:ALA:HA	2.13	0.48
1:B:206:GLY:O	1:B:208:GLU:N	2.47	0.48
1:B:372:LEU:O	1:B:373:LEU:HG	2.13	0.48
1:B:379:HIS:CE1	1:B:387:TYR:CD2	3.01	0.48
1:B:396:LEU:O	1:B:397:TYR:C	2.51	0.48
1:B:414:PHE:C	1:B:414:PHE:CD2	2.87	0.48
1:C:49:THR:OG1	1:C:201:LEU:CD1	2.61	0.48
1:C:311:PRO:HG2	1:C:426:LEU:HD11	1.95	0.48
1:A:56:LEU:HD12	1:A:397:TYR:CE1	2.48	0.48
1:A:250:ILE:N	1:A:251:PRO:CD	2.61	0.48
1:B:8:HIS:HB3	1:B:9:LYS:NZ	2.28	0.48
1:B:165:ILE:O	1:B:169:GLY:HA3	2.13	0.48
1:C:74:TYR:OH	1:C:304:ALA:HA	2.14	0.48
1:D:114:TYR:CE1	1:D:118:ILE:HG12	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:PHE:HA	1:B:81:PHE:CZ	2.49	0.48
1:A:205:ILE:HD13	1:A:361:THR:OG1	2.13	0.48
1:A:376:GLY:C	1:A:378:GLY:N	2.65	0.48
1:B:30:LEU:O	1:B:33:ALA:HB3	2.14	0.48
1:B:56:LEU:CD1	1:B:365:TYR:HD1	2.24	0.48
1:B:136:PHE:HB3	1:B:291:GLY:HA2	1.96	0.48
1:B:144:PRO:HD3	1:B:322:THR:HG23	1.96	0.48
1:B:314:PHE:HA	1:B:315:ALA:O	2.13	0.48
1:C:366:LEU:CD1	1:D:421:THR:HG21	2.43	0.48
1:C:430:ARG:C	1:D:377:HIS:HE1	2.16	0.48
1:D:374:LEU:O	1:D:377:HIS:CD2	2.66	0.48
1:A:18:MET:HA	1:A:151:GLN:HG2	1.95	0.48
1:B:24:MET:HE3	1:B:162:ILE:HD12	1.96	0.48
1:B:84:PHE:CE1	1:B:85:LEU:CD2	2.87	0.48
1:B:114:TYR:CE1	1:B:118:ILE:HG12	2.49	0.48
1:B:294:THR:O	1:B:297:ALA:HB3	2.13	0.48
1:C:93:TYR:C	1:C:93:TYR:CD2	2.87	0.48
1:C:191:GLY:O	1:C:194:GLN:HB2	2.13	0.48
1:C:342:ILE:CB	1:C:343:SER:CB	2.86	0.48
1:D:74:TYR:CZ	1:D:304:ALA:CB	2.96	0.48
1:D:93:TYR:CE1	1:D:208:GLU:OE1	2.66	0.48
1:A:74:TYR:CE1	1:A:304:ALA:HB2	2.48	0.48
1:A:218:LYS:HB3	1:A:219:ASN:H	1.52	0.48
1:A:342:ILE:HB	1:A:343:SER:OG	2.13	0.48
1:A:357:SER:O	1:A:361:THR:HG23	2.14	0.48
1:B:46:TRP:CH2	1:B:200:THR:HG22	2.49	0.48
1:B:54:LEU:HD12	1:B:232:VAL:HG12	1.95	0.48
1:B:82:GLY:N	1:B:83:PRO:CD	2.77	0.48
1:B:140:ASN:CB	1:B:327:LEU:HD22	2.38	0.48
1:B:154:ALA:O	1:B:157:LEU:HB2	2.14	0.48
1:C:46:TRP:CH2	1:C:200:THR:HG22	2.49	0.48
1:C:301:ALA:C	1:C:303:ALA:H	2.16	0.48
1:C:302:LYS:HG3	1:C:314:PHE:HB2	1.95	0.48
1:D:69:SER:OG	1:D:70:PRO:HA	2.14	0.48
1:B:71:GLY:C	1:B:212:VAL:HA	2.34	0.48
1:B:218:LYS:HB3	1:B:219:ASN:H	1.52	0.48
1:C:363:VAL:O	1:C:366:LEU:HB3	2.13	0.48
1:D:44:TYR:O	1:D:47:LEU:N	2.47	0.48
1:D:77:ALA:O	1:D:79:ARG:N	2.46	0.48
1:D:424:TYR:CD1	1:D:430:ARG:NH2	2.82	0.48
1:B:19:VAL:CG2	1:B:210:ALA:HB2	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:LEU:HB3	1:B:146:MET:HE1	1.94	0.47
1:B:313:ILE:HG22	1:B:314:PHE:N	2.29	0.47
1:B:376:GLY:O	1:B:377:HIS:C	2.52	0.47
1:C:114:TYR:CE1	1:C:118:ILE:HG12	2.49	0.47
1:C:322:THR:HA	1:C:323:PRO:HD3	1.76	0.47
1:D:56:LEU:HD12	1:D:397:TYR:CD1	2.49	0.47
1:A:74:TYR:CZ	1:A:304:ALA:CB	2.97	0.47
1:B:81:PHE:CE2	1:B:83:PRO:HG2	2.48	0.47
1:C:339:LEU:HA	1:C:342:ILE:HG13	1.96	0.47
1:C:374:LEU:O	1:C:377:HIS:CD2	2.68	0.47
1:A:30:LEU:O	1:A:33:ALA:HB3	2.14	0.47
1:A:95:LEU:HD23	1:A:95:LEU:O	2.14	0.47
1:A:133:LEU:CD1	1:A:338:GLN:HG3	2.44	0.47
1:B:114:TYR:C	1:B:115:PHE:HD2	2.18	0.47
1:C:56:LEU:CD1	1:C:365:TYR:HD1	2.23	0.47
1:C:314:PHE:HA	1:C:315:ALA:O	2.12	0.47
1:C:366:LEU:HD13	1:C:367:TYR:CD2	2.50	0.47
1:A:23:ILE:HG23	1:A:204:PHE:O	2.13	0.47
1:B:311:PRO:HG2	1:B:426:LEU:HD11	1.96	0.47
1:C:92:LEU:O	1:C:360:PHE:HB3	2.14	0.47
1:C:420:ILE:O	1:C:421:THR:C	2.53	0.47
1:D:376:GLY:HA3	1:D:379:HIS:CD2	2.50	0.47
1:A:69:SER:OG	1:A:70:PRO:HA	2.15	0.47
1:A:299:GLN:OE1	1:A:299:GLN:HA	2.14	0.47
1:B:88:GLN:O	1:B:91:VAL:N	2.47	0.47
1:B:301:ALA:C	1:B:303:ALA:H	2.18	0.47
1:B:376:GLY:HA3	1:B:379:HIS:CD2	2.49	0.47
1:C:313:ILE:HG22	1:C:314:PHE:N	2.29	0.47
1:D:14:PRO:HB2	1:D:148:THR:OG1	2.14	0.47
1:D:301:ALA:C	1:D:303:ALA:N	2.68	0.47
1:B:302:LYS:HE3	1:B:326:GLY:CA	2.45	0.47
1:B:420:ILE:HG22	1:B:421:THR:H	1.79	0.47
1:C:144:PRO:HD3	1:C:322:THR:HG23	1.96	0.47
1:C:298:GLY:HA2	1:C:302:LYS:NZ	2.30	0.47
1:D:83:PRO:O	1:D:84:PHE:C	2.52	0.47
1:A:41:ILE:O	1:A:41:ILE:HG12	2.14	0.47
1:A:104:MET:HE1	1:A:286:CYS:SG	2.54	0.47
1:A:326:GLY:O	1:A:330:VAL:HG23	2.15	0.47
1:A:426:LEU:O	1:A:426:LEU:HG	2.15	0.47
1:B:22:ASN:HB3	1:B:293:TRP:HE1	1.79	0.47
1:B:121:ASP:HB2	1:B:122:PRO:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:ALA:O	1:B:238:CYS:HB2	2.15	0.47
1:B:388:LEU:HD23	1:B:388:LEU:HA	1.63	0.47
1:B:421:THR:O	1:B:424:TYR:N	2.37	0.47
1:C:14:PRO:HB2	1:C:148:THR:OG1	2.14	0.47
1:C:31:LEU:HD11	1:C:239:TYR:CE2	2.50	0.47
1:C:34:ASN:HB3	1:C:199:VAL:HG11	1.97	0.47
1:C:165:ILE:O	1:C:169:GLY:HA3	2.14	0.47
1:C:212:VAL:CG1	1:C:296:LEU:HD13	2.45	0.47
1:C:363:VAL:HG23	1:C:364:PRO:HD3	1.97	0.47
1:D:133:LEU:CD1	1:D:338:GLN:HG3	2.44	0.47
1:D:339:LEU:HA	1:D:342:ILE:HG13	1.96	0.47
1:D:360:PHE:O	1:D:363:VAL:HG23	2.15	0.47
1:A:376:GLY:O	1:A:379:HIS:N	2.42	0.47
1:A:379:HIS:C	1:A:381:GLY:N	2.67	0.47
1:B:8:HIS:HB3	1:B:9:LYS:CE	2.44	0.47
1:B:128:THR:O	1:B:132:VAL:HG23	2.15	0.47
1:B:367:TYR:O	1:B:370:ALA:HB3	2.14	0.47
1:C:136:PHE:HB3	1:C:291:GLY:HA2	1.95	0.47
1:C:363:VAL:CB	1:C:364:PRO:HD3	2.45	0.47
1:C:418:MET:CE	1:D:399:ILE:HA	2.44	0.47
1:D:119:LEU:HD13	1:D:124:VAL:CG1	2.33	0.47
1:A:306:ASP:C	1:A:308:GLY:N	2.68	0.47
1:B:14:PRO:HB2	1:B:148:THR:OG1	2.15	0.47
1:B:79:ARG:HD3	1:B:375:LEU:HD11	1.96	0.47
1:C:201:LEU:HD23	1:C:401:ALA:CB	2.44	0.47
1:D:104:MET:HB3	1:D:290:LEU:HD23	1.97	0.47
1:A:93:TYR:CE1	1:A:208:GLU:CD	2.87	0.47
1:A:107:ILE:HG23	1:A:111:TYR:CE1	2.50	0.47
1:A:136:PHE:HB3	1:A:291:GLY:HA2	1.97	0.47
1:A:173:PHE:HA	1:A:174:ARG:CB	2.31	0.47
1:A:400:TRP:HA	1:A:403:VAL:CG1	2.45	0.47
1:C:377:HIS:CE1	1:D:431:LEU:N	2.83	0.47
1:D:19:VAL:CG2	1:D:210:ALA:HB2	2.40	0.47
1:D:67:ASP:OD1	1:D:67:ASP:C	2.52	0.47
1:D:339:LEU:HA	1:D:342:ILE:CG1	2.45	0.47
1:A:22:ASN:HB3	1:A:293:TRP:HE1	1.80	0.46
1:A:161:PRO:O	1:A:165:ILE:HG13	2.15	0.46
1:B:79:ARG:HD3	1:B:375:LEU:CD1	2.45	0.46
1:B:416:THR:O	1:B:419:VAL:HG12	2.15	0.46
1:B:420:ILE:CG2	1:B:421:THR:N	2.78	0.46
1:C:41:ILE:HG21	1:C:246:ILE:CG2	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:GLY:C	1:C:74:TYR:H	2.19	0.46
1:C:114:TYR:C	1:C:115:PHE:HD2	2.18	0.46
1:C:425:ALA:O	1:C:427:ASN:N	2.48	0.46
1:A:21:GLY:HA2	1:A:24:MET:HB2	1.96	0.46
1:A:56:LEU:HD12	1:A:397:TYR:CD1	2.50	0.46
1:A:368:THR:O	1:A:371:ALA:N	2.39	0.46
1:B:305:ALA:HA	1:B:312:PRO:HG2	1.98	0.46
1:C:57:SER:HB2	1:C:232:VAL:HG21	1.96	0.46
1:C:431:LEU:N	1:D:377:HIS:CE1	2.83	0.46
1:D:115:PHE:CD2	1:D:115:PHE:N	2.83	0.46
1:D:217:VAL:O	1:D:218:LYS:O	2.33	0.46
1:D:376:GLY:O	1:D:379:HIS:N	2.43	0.46
1:A:104:MET:HB3	1:A:290:LEU:HD23	1.96	0.46
1:A:184:VAL:O	1:A:185:SER:HB2	2.15	0.46
1:A:363:VAL:CG2	1:A:364:PRO:HD3	2.44	0.46
1:B:88:GLN:O	1:B:91:VAL:HG23	2.14	0.46
1:B:133:LEU:HD22	1:B:334:MET:SD	2.55	0.46
1:B:400:TRP:HA	1:B:403:VAL:CG1	2.46	0.46
1:C:128:THR:O	1:C:132:VAL:HG23	2.15	0.46
1:D:426:LEU:O	1:D:426:LEU:HG	2.16	0.46
1:A:78:ARG:C	1:A:79:ARG:HG3	2.35	0.46
1:B:76:TYR:HH	1:B:211:SER:HG	1.48	0.46
1:C:67:ASP:OD1	1:C:67:ASP:O	2.33	0.46
1:C:82:GLY:N	1:C:83:PRO:CD	2.78	0.46
1:C:144:PRO:HG2	1:C:216:VAL:HG11	1.97	0.46
1:C:206:GLY:O	1:C:208:GLU:N	2.48	0.46
1:D:50:ILE:HD13	1:D:236:ALA:HB1	1.97	0.46
1:D:352:LEU:HD21	1:D:408:LYS:HB2	1.98	0.46
1:A:342:ILE:CB	1:A:343:SER:CB	2.84	0.46
1:B:133:LEU:CD1	1:B:338:GLN:HG3	2.46	0.46
1:B:144:PRO:HG2	1:B:216:VAL:HG11	1.97	0.46
1:B:147:ILE:HD12	1:B:147:ILE:HA	1.70	0.46
1:B:425:ALA:O	1:B:427:ASN:N	2.48	0.46
1:C:99:ILE:HG21	1:C:357:SER:HB3	1.98	0.46
1:D:84:PHE:N	1:D:430:ARG:NH1	2.64	0.46
1:D:151:GLN:HE22	1:D:289:SER:HA	1.80	0.46
1:D:219:ASN:N	1:D:219:ASN:HD22	2.14	0.46
1:D:420:ILE:O	1:D:421:THR:C	2.54	0.46
1:A:62:LYS:HA	1:A:65:PHE:CB	2.42	0.46
1:A:144:PRO:HB2	1:A:216:VAL:HG11	1.98	0.46
1:B:310:PHE:CE1	1:B:314:PHE:HE2	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:ASP:HB2	1:C:122:PRO:HD3	1.97	0.46
1:C:133:LEU:HD22	1:C:334:MET:SD	2.54	0.46
1:C:211:SER:O	1:C:211:SER:OG	2.33	0.46
1:C:219:ASN:HD22	1:C:219:ASN:N	2.12	0.46
1:D:56:LEU:CD1	1:D:365:TYR:CD1	2.99	0.46
1:D:98:TRP:O	1:D:101:ASN:HB2	2.16	0.46
1:A:10:VAL:CG1	1:A:148:THR:HG21	2.46	0.46
1:A:72:GLY:C	1:A:74:TYR:H	2.19	0.46
1:A:201:LEU:HD12	1:A:201:LEU:HA	1.83	0.46
1:A:396:LEU:O	1:A:397:TYR:C	2.54	0.46
1:B:99:ILE:HG21	1:B:357:SER:HB3	1.97	0.46
1:B:111:TYR:CB	1:B:283:ALA:HB2	2.34	0.46
1:B:217:VAL:O	1:B:218:LYS:O	2.34	0.46
1:C:379:HIS:HE1	1:C:387:TYR:CD2	2.34	0.46
1:C:400:TRP:HA	1:C:403:VAL:CG1	2.45	0.46
1:A:376:GLY:O	1:A:377:HIS:C	2.53	0.46
1:C:119:LEU:HD22	1:C:124:VAL:CG2	2.37	0.46
1:C:217:VAL:O	1:C:218:LYS:O	2.34	0.46
1:D:103:ALA:HB2	1:D:354:SER:OG	2.16	0.46
1:D:376:GLY:O	1:D:377:HIS:C	2.53	0.46
1:A:217:VAL:O	1:A:218:LYS:O	2.33	0.46
1:B:74:TYR:CZ	1:B:304:ALA:CB	2.94	0.46
1:B:92:LEU:CD2	1:B:363:VAL:CG2	2.89	0.46
1:B:93:TYR:HE1	1:B:208:GLU:CD	2.19	0.46
1:B:372:LEU:C	1:B:373:LEU:HG	2.36	0.46
1:C:376:GLY:HA3	1:C:379:HIS:CD2	2.51	0.46
1:C:399:ILE:HG12	1:D:418:MET:HE2	1.96	0.46
1:D:92:LEU:CD2	1:D:363:VAL:CG2	2.88	0.46
1:A:113:SER:HA	1:A:120:LYS:HG3	1.98	0.46
1:A:135:ILE:HG22	1:A:136:PHE:N	2.30	0.46
1:A:301:ALA:C	1:A:303:ALA:N	2.70	0.46
1:A:314:PHE:O	1:A:314:PHE:CD2	2.69	0.46
1:A:379:HIS:HE1	1:A:387:TYR:CD2	2.34	0.46
1:B:10:VAL:O	1:B:218:LYS:HG3	2.15	0.46
1:B:31:LEU:HD11	1:B:239:TYR:CE2	2.51	0.46
1:B:205:ILE:O	1:B:205:ILE:HG22	2.16	0.46
1:B:420:ILE:O	1:B:421:THR:C	2.54	0.46
1:C:140:ASN:CB	1:C:327:LEU:HD22	2.40	0.46
1:D:31:LEU:HD13	1:D:46:TRP:HH2	1.81	0.46
1:D:416:THR:O	1:D:419:VAL:HG12	2.16	0.46
1:A:94:TRP:O	1:A:97:CYS:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:MET:HB2	1:B:410:VAL:CG1	2.46	0.45
1:B:93:TYR:HE2	1:B:97:CYS:SG	2.35	0.45
1:C:84:PHE:N	1:C:430:ARG:NH1	2.65	0.45
1:C:107:ILE:O	1:C:111:TYR:CD1	2.68	0.45
1:C:301:ALA:HB1	1:C:310:PHE:CE1	2.47	0.45
1:D:22:ASN:HB3	1:D:293:TRP:HE1	1.81	0.45
1:D:359:ILE:HD11	1:D:409:GLU:CB	2.45	0.45
1:A:385:PRO:HA	1:A:388:LEU:HB2	1.98	0.45
1:A:413:SER:O	1:A:416:THR:HB	2.16	0.45
1:B:115:PHE:CD2	1:B:115:PHE:N	2.84	0.45
1:C:63:MET:SD	1:C:372:LEU:CD1	3.04	0.45
1:C:89:THR:HG23	1:C:364:PRO:HG3	1.97	0.45
1:C:411:MET:HE1	1:D:403:VAL:O	2.16	0.45
1:C:413:SER:O	1:C:416:THR:HB	2.16	0.45
1:D:69:SER:OG	1:D:71:GLY:N	2.45	0.45
1:D:136:PHE:HD2	1:D:290:LEU:HD12	1.82	0.45
1:D:306:ASP:C	1:D:308:GLY:N	2.69	0.45
1:D:379:HIS:HE1	1:D:387:TYR:CD2	2.34	0.45
1:A:41:ILE:HG21	1:A:246:ILE:CG2	2.47	0.45
1:C:115:PHE:N	1:C:115:PHE:CD2	2.84	0.45
1:C:140:ASN:HD21	1:C:147:ILE:HG12	1.79	0.45
1:C:385:PRO:HA	1:C:388:LEU:HB2	1.98	0.45
1:D:201:LEU:HD12	1:D:201:LEU:HA	1.83	0.45
1:A:19:VAL:CG2	1:A:210:ALA:HB2	2.40	0.45
1:A:69:SER:OG	1:A:71:GLY:N	2.45	0.45
1:A:201:LEU:HD23	1:A:401:ALA:HB2	1.99	0.45
1:A:345:ASN:O	1:A:346:ALA:HB3	2.16	0.45
1:A:422:ALA:CB	1:B:395:PHE:CD1	2.99	0.45
1:B:120:LYS:HZ3	1:B:124:VAL:HG12	1.81	0.45
1:C:22:ASN:HB3	1:C:293:TRP:HE1	1.82	0.45
1:C:30:LEU:O	1:C:33:ALA:HB3	2.16	0.45
1:C:81:PHE:HE1	1:D:80:CYS:O	2.00	0.45
1:D:10:VAL:CG1	1:D:148:THR:HG21	2.47	0.45
1:D:41:ILE:O	1:D:41:ILE:HG12	2.16	0.45
1:D:63:MET:HB2	1:D:372:LEU:HD13	1.99	0.45
1:B:339:LEU:HA	1:B:342:ILE:CG1	2.46	0.45
1:C:28:VAL:HA	1:C:31:LEU:HG	1.99	0.45
1:C:98:TRP:O	1:C:101:ASN:HB2	2.17	0.45
1:C:302:LYS:HE3	1:C:326:GLY:CA	2.46	0.45
1:D:363:VAL:CB	1:D:364:PRO:HD3	2.46	0.45
1:A:418:MET:HE2	1:B:399:ILE:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:TRP:O	1:B:101:ASN:HB2	2.16	0.45
1:B:219:ASN:HD22	1:B:219:ASN:N	2.13	0.45
1:C:19:VAL:CG2	1:C:210:ALA:HB2	2.41	0.45
1:C:88:GLN:HG3	1:C:420:ILE:HG21	1.98	0.45
1:D:396:LEU:O	1:D:397:TYR:C	2.54	0.45
1:A:119:LEU:CD1	1:A:124:VAL:HG11	2.36	0.45
1:A:339:LEU:HA	1:A:342:ILE:HG13	1.98	0.45
1:A:373:LEU:HD11	1:A:391:THR:HB	1.97	0.45
1:B:35:LEU:CD2	1:B:196:THR:HG22	2.40	0.45
1:B:72:GLY:C	1:B:74:TYR:N	2.69	0.45
1:B:351:GLY:C	1:B:353:VAL:H	2.19	0.45
1:C:104:MET:HB3	1:C:104:MET:HE2	1.68	0.45
1:C:235:ALA:O	1:C:238:CYS:HB2	2.17	0.45
1:C:342:ILE:HB	1:C:343:SER:OG	2.16	0.45
1:C:411:MET:HA	1:D:410:VAL:CG1	2.46	0.45
1:D:135:ILE:O	1:D:139:LEU:HG	2.16	0.45
1:A:46:TRP:CH2	1:A:200:THR:HG22	2.52	0.45
1:A:83:PRO:O	1:A:84:PHE:C	2.55	0.45
1:B:113:SER:HA	1:B:120:LYS:HG3	1.98	0.45
1:B:342:ILE:HB	1:B:343:SER:OG	2.16	0.45
1:B:371:ALA:C	1:B:373:LEU:N	2.70	0.45
1:C:21:GLY:HA2	1:C:24:MET:HB2	1.98	0.45
1:C:49:THR:OG1	1:C:201:LEU:HD12	2.17	0.45
1:D:107:ILE:HG23	1:D:111:TYR:CE1	2.52	0.45
1:D:172:TRP:HE3	1:D:173:PHE:N	2.15	0.45
1:D:345:ASN:O	1:D:346:ALA:HB3	2.16	0.45
1:A:303:ALA:C	1:A:305:ALA:H	2.20	0.45
1:A:388:LEU:HD23	1:A:388:LEU:HA	1.70	0.45
1:B:41:ILE:HG21	1:B:246:ILE:CG2	2.46	0.45
1:B:92:LEU:O	1:B:360:PHE:HB3	2.17	0.45
1:B:352:LEU:HD21	1:B:408:LYS:HB2	1.99	0.45
1:C:10:VAL:O	1:C:218:LYS:HG3	2.17	0.45
1:C:113:SER:HA	1:C:120:LYS:HG3	1.98	0.45
1:C:345:ASN:O	1:C:346:ALA:HB3	2.17	0.45
1:D:23:ILE:HG21	1:D:204:PHE:HD1	1.79	0.45
1:D:32:PRO:CG	1:D:243:THR:HG22	2.37	0.45
1:D:121:ASP:N	1:D:122:PRO:CD	2.80	0.45
1:D:121:ASP:HB2	1:D:122:PRO:HD3	1.99	0.45
1:D:136:PHE:HB3	1:D:291:GLY:HA2	1.97	0.45
1:D:303:ALA:C	1:D:305:ALA:H	2.20	0.45
1:D:385:PRO:HA	1:D:388:LEU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:LYS:HE3	1:A:326:GLY:CA	2.47	0.45
1:A:352:LEU:HD21	1:A:408:LYS:HB2	1.99	0.45
1:A:373:LEU:HB2	1:B:428:TYR:CE1	2.52	0.45
1:A:376:GLY:HA3	1:A:379:HIS:HD2	1.82	0.45
1:B:78:ARG:C	1:B:79:ARG:HG3	2.37	0.45
1:C:31:LEU:HD13	1:C:46:TRP:HH2	1.82	0.45
1:C:351:GLY:C	1:C:353:VAL:H	2.20	0.45
1:C:426:LEU:C	1:C:427:ASN:HD22	2.21	0.45
1:D:49:THR:OG1	1:D:201:LEU:CD1	2.64	0.45
1:D:135:ILE:HG22	1:D:136:PHE:N	2.32	0.45
1:D:201:LEU:HD23	1:D:401:ALA:HB2	1.99	0.45
1:D:314:PHE:O	1:D:314:PHE:CD2	2.68	0.45
1:D:413:SER:O	1:D:416:THR:HB	2.17	0.45
1:A:298:GLY:HA2	1:A:302:LYS:NZ	2.31	0.44
1:A:371:ALA:C	1:A:373:LEU:N	2.70	0.44
1:A:412:TRP:CE3	1:A:415:VAL:HG21	2.52	0.44
1:A:420:ILE:CG2	1:A:421:THR:N	2.77	0.44
1:B:317:VAL:HA	1:B:322:THR:O	2.17	0.44
1:C:83:PRO:HB2	1:C:84:PHE:H	1.58	0.44
1:C:119:LEU:HB3	1:C:120:LYS:H	1.59	0.44
1:C:136:PHE:HD2	1:C:290:LEU:HD12	1.82	0.44
1:D:311:PRO:HG2	1:D:426:LEU:HD11	2.00	0.44
1:D:342:ILE:CB	1:D:343:SER:CB	2.86	0.44
1:A:98:TRP:O	1:A:101:ASN:HB2	2.17	0.44
1:B:59:VAL:HG22	1:B:391:THR:HG22	1.98	0.44
1:B:379:HIS:HE1	1:B:387:TYR:CD2	2.35	0.44
1:C:19:VAL:HG11	1:C:228:THR:HA	2.00	0.44
1:C:81:PHE:CE2	1:C:83:PRO:HG2	2.52	0.44
1:C:377:HIS:CE1	1:D:430:ARG:N	2.86	0.44
1:D:28:VAL:O	1:D:30:LEU:N	2.45	0.44
1:D:46:TRP:CH2	1:D:200:THR:HG22	2.52	0.44
1:D:113:SER:HA	1:D:120:LYS:HG3	1.99	0.44
1:D:342:ILE:HB	1:D:343:SER:OG	2.17	0.44
1:D:420:ILE:CG2	1:D:421:THR:N	2.80	0.44
1:A:31:LEU:HD13	1:A:46:TRP:HH2	1.81	0.44
1:A:71:GLY:C	1:A:212:VAL:HA	2.37	0.44
1:A:82:GLY:O	1:A:83:PRO:O	2.35	0.44
1:A:135:ILE:O	1:A:139:LEU:HG	2.17	0.44
1:A:136:PHE:HD2	1:A:290:LEU:HD12	1.81	0.44
1:A:219:ASN:N	1:A:219:ASN:HD22	2.14	0.44
1:B:82:GLY:O	1:B:83:PRO:O	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:LEU:HD22	1:B:290:LEU:HA	1.63	0.44
1:B:337:PHE:HZ	1:B:353:VAL:HG11	1.80	0.44
1:C:205:ILE:HG22	1:C:205:ILE:O	2.17	0.44
1:D:136:PHE:CE1	1:D:287:LEU:O	2.71	0.44
1:D:314:PHE:CA	1:D:315:ALA:O	2.65	0.44
1:A:49:THR:HB	1:A:197:LEU:CD2	2.46	0.44
1:A:114:TYR:CE1	1:A:118:ILE:HG12	2.52	0.44
1:A:115:PHE:CD2	1:A:115:PHE:N	2.84	0.44
1:A:305:ALA:HA	1:A:312:PRO:HG2	2.00	0.44
1:A:389:ALA:O	1:A:392:THR:N	2.50	0.44
1:B:21:GLY:HA2	1:B:24:MET:HB2	1.99	0.44
1:B:49:THR:OG1	1:B:201:LEU:HD12	2.17	0.44
1:B:356:VAL:HA	1:B:359:ILE:HD12	1.99	0.44
1:B:412:TRP:CE3	1:B:415:VAL:HG21	2.52	0.44
1:C:74:TYR:CZ	1:C:304:ALA:CB	2.93	0.44
1:C:201:LEU:HD23	1:C:401:ALA:CA	2.48	0.44
1:D:49:THR:HB	1:D:197:LEU:CD2	2.46	0.44
1:D:95:LEU:HD23	1:D:95:LEU:O	2.18	0.44
1:D:363:VAL:CG2	1:D:364:PRO:HD3	2.47	0.44
1:D:389:ALA:O	1:D:392:THR:N	2.50	0.44
1:D:400:TRP:HA	1:D:403:VAL:CG1	2.47	0.44
1:A:28:VAL:O	1:A:30:LEU:N	2.45	0.44
1:A:81:PHE:CB	1:A:82:GLY:CA	2.92	0.44
1:A:93:TYR:CE1	1:A:208:GLU:OE1	2.71	0.44
1:A:420:ILE:O	1:A:421:THR:C	2.56	0.44
1:B:133:LEU:HD22	1:B:334:MET:CE	2.48	0.44
1:B:315:ALA:CB	1:B:316:ARG:CA	2.77	0.44
1:C:59:VAL:HG22	1:C:391:THR:HG22	1.98	0.44
1:C:59:VAL:HG22	1:C:391:THR:CG2	2.48	0.44
1:C:371:ALA:C	1:C:373:LEU:N	2.70	0.44
1:D:128:THR:O	1:D:132:VAL:HG23	2.18	0.44
1:D:161:PRO:O	1:D:165:ILE:HG13	2.17	0.44
1:D:351:GLY:C	1:D:353:VAL:H	2.21	0.44
1:A:121:ASP:HB2	1:A:122:PRO:HD3	1.99	0.44
1:B:34:ASN:HB3	1:B:199:VAL:HG11	1.98	0.44
1:B:346:ALA:HB3	1:B:351:GLY:CA	2.43	0.44
1:C:24:MET:HE1	1:C:238:CYS:SG	2.57	0.44
1:C:120:LYS:HZ3	1:C:124:VAL:HG12	1.83	0.44
1:C:352:LEU:HD21	1:C:408:LYS:HB2	1.99	0.44
1:D:373:LEU:HD11	1:D:391:THR:HB	1.98	0.44
1:A:60:TYR:OH	1:A:368:THR:OG1	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:PHE:HZ	1:A:353:VAL:HG11	1.81	0.44
1:A:351:GLY:C	1:A:353:VAL:H	2.21	0.44
1:B:136:PHE:HD2	1:B:290:LEU:HD12	1.82	0.44
1:B:344:PRO:O	1:B:345:ASN:CB	2.65	0.44
1:C:49:THR:HB	1:C:197:LEU:CD2	2.48	0.44
1:D:78:ARG:C	1:D:79:ARG:HG3	2.38	0.44
1:D:91:VAL:O	1:D:95:LEU:HB3	2.17	0.44
1:D:92:LEU:HD11	1:D:363:VAL:CG2	2.07	0.44
1:D:133:LEU:CD2	1:D:290:LEU:HD11	2.42	0.44
1:A:144:PRO:HD3	1:A:322:THR:HG23	1.99	0.44
1:A:359:ILE:HD11	1:A:409:GLU:CB	2.44	0.44
1:A:414:PHE:HB2	1:B:414:PHE:HB2	2.00	0.44
1:B:201:LEU:HD12	1:B:201:LEU:HA	1.81	0.44
1:D:81:PHE:CB	1:D:82:GLY:CA	2.95	0.44
1:D:104:MET:HB3	1:D:104:MET:HE2	1.67	0.44
1:A:88:GLN:O	1:A:91:VAL:HG23	2.17	0.44
1:A:116:PHE:CB	1:A:117:PRO:CD	2.93	0.44
1:A:373:LEU:HD11	1:A:391:THR:CB	2.48	0.44
1:B:31:LEU:HD13	1:B:46:TRP:HH2	1.82	0.44
1:B:345:ASN:O	1:B:346:ALA:HB3	2.17	0.44
1:C:81:PHE:CE1	1:D:80:CYS:O	2.71	0.44
1:C:339:LEU:HA	1:C:342:ILE:CG1	2.48	0.44
1:C:367:TYR:O	1:C:368:THR:C	2.56	0.44
1:C:396:LEU:HD23	1:C:396:LEU:HA	1.72	0.44
1:D:19:VAL:HG11	1:D:228:THR:HA	2.00	0.44
1:D:53:ALA:HB2	1:D:397:TYR:HE2	1.80	0.44
1:D:210:ALA:C	1:D:212:VAL:H	2.20	0.44
1:D:299:GLN:OE1	1:D:299:GLN:HA	2.17	0.44
1:A:172:TRP:HE3	1:A:173:PHE:N	2.16	0.43
1:B:107:ILE:O	1:B:111:TYR:CD1	2.71	0.43
1:B:121:ASP:N	1:B:122:PRO:CD	2.80	0.43
1:B:318:ASN:HB2	1:B:324:VAL:CG2	2.48	0.43
1:C:403:VAL:HG23	1:D:415:VAL:HG11	2.00	0.43
1:A:311:PRO:HG2	1:A:426:LEU:HD11	1.99	0.43
1:A:311:PRO:HA	1:A:312:PRO:HD3	1.85	0.43
1:A:339:LEU:HA	1:A:342:ILE:CG1	2.48	0.43
1:A:344:PRO:O	1:A:345:ASN:CB	2.65	0.43
1:B:57:SER:HB2	1:B:232:VAL:HG21	1.98	0.43
1:C:91:VAL:HB	1:C:420:ILE:CD1	2.46	0.43
1:C:133:LEU:CD1	1:C:338:GLN:HG3	2.48	0.43
1:D:8:HIS:ND1	1:D:9:LYS:NZ	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:78:ARG:O	1:D:79:ARG:HG3	2.18	0.43
1:D:88:GLN:O	1:D:91:VAL:HG23	2.19	0.43
1:D:94:TRP:O	1:D:97:CYS:HB2	2.17	0.43
1:D:111:TYR:CB	1:D:283:ALA:HB2	2.37	0.43
1:D:174:ARG:HA	1:D:175:GLY:HA3	1.92	0.43
1:D:212:VAL:HG11	1:D:296:LEU:HD13	1.98	0.43
1:A:84:PHE:N	1:A:430:ARG:NH1	2.66	0.43
1:B:212:VAL:HG11	1:B:296:LEU:HD13	1.99	0.43
1:C:359:ILE:H	1:C:359:ILE:HG13	1.69	0.43
1:A:78:ARG:O	1:A:79:ARG:HG3	2.18	0.43
1:A:306:ASP:O	1:A:308:GLY:N	2.52	0.43
1:B:10:VAL:CG1	1:B:148:THR:HG21	2.48	0.43
1:B:83:PRO:HB2	1:B:84:PHE:H	1.56	0.43
1:B:104:MET:CE	1:B:286:CYS:SG	3.06	0.43
1:B:116:PHE:CB	1:B:117:PRO:CD	2.92	0.43
1:B:172:TRP:HE3	1:B:173:PHE:N	2.16	0.43
1:B:201:LEU:HD23	1:B:401:ALA:CB	2.46	0.43
1:B:310:PHE:HB3	1:B:311:PRO:O	2.18	0.43
1:B:376:GLY:HA3	1:B:379:HIS:HD2	1.84	0.43
1:B:413:SER:O	1:B:416:THR:HB	2.18	0.43
1:C:395:PHE:CD1	1:D:422:ALA:CB	3.02	0.43
1:C:430:ARG:N	1:D:377:HIS:CE1	2.85	0.43
1:D:133:LEU:HD11	1:D:338:GLN:HG3	2.00	0.43
1:D:426:LEU:C	1:D:427:ASN:HD22	2.19	0.43
1:A:63:MET:HB2	1:A:372:LEU:HD13	2.00	0.43
1:A:415:VAL:HG11	1:B:403:VAL:HG23	2.00	0.43
1:C:116:PHE:CB	1:C:117:PRO:CD	2.92	0.43
1:C:416:THR:CA	1:C:419:VAL:HG12	2.47	0.43
1:D:99:ILE:HG22	1:D:100:GLY:N	2.33	0.43
1:B:19:VAL:HG11	1:B:228:THR:HA	2.00	0.43
1:C:107:ILE:HG23	1:C:111:TYR:CE1	2.53	0.43
1:C:372:LEU:HG	1:C:372:LEU:O	2.19	0.43
1:C:389:ALA:O	1:C:390:VAL:C	2.56	0.43
1:A:88:GLN:O	1:A:91:VAL:N	2.52	0.43
1:B:28:VAL:O	1:B:30:LEU:N	2.47	0.43
1:C:96:ALA:O	1:C:293:TRP:HZ3	2.00	0.43
1:C:359:ILE:HB	1:C:413:SER:OG	2.19	0.43
1:C:416:THR:O	1:C:419:VAL:HG12	2.19	0.43
1:C:420:ILE:HG22	1:C:421:THR:H	1.82	0.43
1:C:423:MET:HG2	1:C:423:MET:O	2.19	0.43
1:D:116:PHE:CB	1:D:117:PRO:CD	2.93	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:337:PHE:HZ	1:D:353:VAL:HG11	1.82	0.43
1:A:52:GLY:HA2	1:A:393:ILE:CG2	2.49	0.43
1:A:128:THR:O	1:A:132:VAL:HG23	2.19	0.43
1:B:24:MET:HE2	1:B:162:ILE:HD12	2.00	0.43
1:B:56:LEU:HD12	1:B:397:TYR:CE1	2.54	0.43
1:C:10:VAL:CG1	1:C:148:THR:HG21	2.49	0.43
1:C:24:MET:HE3	1:C:238:CYS:SG	2.59	0.43
1:C:56:LEU:HD12	1:C:397:TYR:CE1	2.53	0.43
1:C:172:TRP:HE3	1:C:173:PHE:N	2.17	0.43
1:C:187:LEU:N	1:C:187:LEU:HD23	2.33	0.43
1:C:218:LYS:HB3	1:C:219:ASN:H	1.52	0.43
1:C:414:PHE:HE2	1:C:418:MET:SD	2.42	0.43
1:D:30:LEU:O	1:D:33:ALA:HB3	2.18	0.43
1:A:60:TYR:HH	1:A:368:THR:HG1	1.65	0.43
1:B:156:VAL:HG23	1:B:159:LEU:HD12	2.01	0.43
1:C:82:GLY:O	1:C:83:PRO:O	2.36	0.43
1:C:93:TYR:HE1	1:C:208:GLU:CD	2.22	0.43
1:D:10:VAL:HG11	1:D:148:THR:HG21	2.01	0.43
1:D:41:ILE:HG21	1:D:246:ILE:CG2	2.48	0.43
1:A:56:LEU:CD1	1:A:365:TYR:CD1	2.99	0.43
1:A:72:GLY:C	1:A:74:TYR:N	2.69	0.43
1:A:215:GLY:O	1:A:216:VAL:HG22	2.19	0.43
1:B:81:PHE:CB	1:B:82:GLY:CA	2.90	0.43
1:B:84:PHE:N	1:B:430:ARG:NH1	2.66	0.43
1:C:290:LEU:O	1:C:294:THR:HG23	2.18	0.43
1:C:344:PRO:O	1:C:345:ASN:CB	2.65	0.43
1:D:52:GLY:HA2	1:D:393:ILE:CG2	2.49	0.43
1:D:88:GLN:O	1:D:91:VAL:N	2.52	0.43
1:D:95:LEU:O	1:D:96:ALA:HB2	2.19	0.43
1:D:388:LEU:HD23	1:D:388:LEU:HA	1.70	0.43
1:A:359:ILE:HB	1:A:413:SER:OG	2.19	0.42
1:B:107:ILE:HG23	1:B:111:TYR:CE1	2.54	0.42
1:B:302:LYS:HE3	1:B:326:GLY:HA3	2.01	0.42
1:B:359:ILE:HD11	1:B:409:GLU:CB	2.46	0.42
1:C:311:PRO:HA	1:C:312:PRO:HD3	1.85	0.42
1:C:356:VAL:HA	1:C:359:ILE:HD12	2.01	0.42
1:D:60:TYR:HE2	1:D:368:THR:CB	2.32	0.42
1:A:24:MET:HE3	1:A:238:CYS:SG	2.59	0.42
1:A:188:GLY:C	1:A:192:ALA:HB2	2.24	0.42
1:B:414:PHE:O	1:B:418:MET:HG3	2.19	0.42
1:C:67:ASP:O	1:C:69:SER:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:PRO:HD3	1:D:322:THR:HG23	1.98	0.42
1:A:10:VAL:HG11	1:A:148:THR:HG21	2.01	0.42
1:A:103:ALA:HB2	1:A:354:SER:OG	2.19	0.42
1:B:290:LEU:O	1:B:294:THR:HG23	2.20	0.42
1:C:421:THR:O	1:C:424:TYR:N	2.43	0.42
1:D:144:PRO:HB2	1:D:216:VAL:HG11	2.01	0.42
1:D:412:TRP:CE3	1:D:415:VAL:HG21	2.55	0.42
1:A:421:THR:O	1:A:424:TYR:N	2.44	0.42
1:A:431:LEU:N	1:B:377:HIS:HE1	2.17	0.42
1:B:88:GLN:HG3	1:B:420:ILE:HG21	2.01	0.42
1:C:83:PRO:O	1:C:84:PHE:C	2.57	0.42
1:C:139:LEU:HB3	1:C:147:ILE:HD13	2.00	0.42
1:C:318:ASN:HB2	1:C:324:VAL:CG2	2.49	0.42
1:C:363:VAL:HB	1:C:364:PRO:HD3	2.01	0.42
1:C:420:ILE:CG2	1:C:421:THR:N	2.81	0.42
1:D:59:VAL:HG11	1:D:369:CYS:SG	2.59	0.42
1:D:62:LYS:HA	1:D:65:PHE:CB	2.43	0.42
1:D:318:ASN:HB2	1:D:324:VAL:CG2	2.49	0.42
1:A:114:TYR:O	1:A:115:PHE:HB2	2.19	0.42
1:A:366:LEU:HD11	1:B:421:THR:CG2	2.46	0.42
1:A:372:LEU:C	1:A:373:LEU:HG	2.40	0.42
1:A:421:THR:CG2	1:B:366:LEU:HD21	2.49	0.42
1:A:430:ARG:N	1:B:377:HIS:HE1	2.17	0.42
1:B:67:ASP:OD1	1:B:67:ASP:O	2.38	0.42
1:B:139:LEU:HB3	1:B:147:ILE:HD13	2.01	0.42
1:C:306:ASP:C	1:C:308:GLY:N	2.72	0.42
1:D:147:ILE:HD12	1:D:147:ILE:HA	1.71	0.42
1:D:215:GLY:O	1:D:216:VAL:HG22	2.19	0.42
1:A:8:HIS:ND1	1:A:9:LYS:NZ	2.65	0.42
1:A:50:ILE:CD1	1:A:236:ALA:HB1	2.50	0.42
1:A:318:ASN:HB2	1:A:324:VAL:CG2	2.50	0.42
1:B:50:ILE:CD1	1:B:236:ALA:HB1	2.49	0.42
1:B:59:VAL:HG22	1:B:391:THR:CG2	2.50	0.42
1:B:135:ILE:O	1:B:139:LEU:HG	2.19	0.42
1:B:314:PHE:O	1:B:314:PHE:CD2	2.73	0.42
1:B:359:ILE:H	1:B:359:ILE:HG13	1.69	0.42
1:D:47:LEU:HD13	1:D:47:LEU:C	2.40	0.42
1:D:218:LYS:HB3	1:D:219:ASN:H	1.51	0.42
1:D:306:ASP:C	1:D:308:GLY:H	2.22	0.42
1:D:356:VAL:HA	1:D:359:ILE:HD12	2.02	0.42
1:D:376:GLY:HA3	1:D:379:HIS:HD2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:GLN:HG3	1:A:420:ILE:HG21	2.01	0.42
1:A:136:PHE:CE1	1:A:287:LEU:O	2.72	0.42
1:A:290:LEU:O	1:A:294:THR:HG23	2.19	0.42
1:A:414:PHE:C	1:A:414:PHE:CD2	2.93	0.42
1:B:161:PRO:O	1:B:165:ILE:HG13	2.19	0.42
1:C:135:ILE:HG22	1:C:136:PHE:N	2.34	0.42
1:C:135:ILE:O	1:C:139:LEU:HG	2.19	0.42
1:C:156:VAL:HG23	1:C:159:LEU:HD12	2.01	0.42
1:C:210:ALA:C	1:C:212:VAL:H	2.21	0.42
1:D:119:LEU:CD1	1:D:124:VAL:HG11	2.36	0.42
1:A:19:VAL:HG11	1:A:228:THR:HA	2.01	0.42
1:A:59:VAL:HG11	1:A:369:CYS:SG	2.59	0.42
1:A:77:ALA:O	1:A:79:ARG:N	2.53	0.42
1:A:236:ALA:O	1:A:239:TYR:HB2	2.20	0.42
1:A:306:ASP:C	1:A:308:GLY:H	2.22	0.42
1:B:28:VAL:HA	1:B:31:LEU:HG	2.01	0.42
1:B:46:TRP:CH2	1:B:239:TYR:HB3	2.55	0.42
1:C:50:ILE:CD1	1:C:236:ALA:HB1	2.49	0.42
1:D:172:TRP:HB3	1:D:173:PHE:H	1.65	0.42
1:D:199:VAL:O	1:D:199:VAL:HG12	2.18	0.42
1:D:305:ALA:HA	1:D:312:PRO:HG2	2.01	0.42
1:D:344:PRO:O	1:D:345:ASN:CB	2.64	0.42
1:A:10:VAL:O	1:A:218:LYS:HG3	2.19	0.42
1:A:133:LEU:HD11	1:A:338:GLN:HG3	2.01	0.42
1:A:290:LEU:HA	1:A:290:LEU:HD22	1.64	0.42
1:A:314:PHE:CA	1:A:315:ALA:O	2.68	0.42
1:B:69:SER:N	1:B:70:PRO:HA	2.34	0.42
1:B:104:MET:HB3	1:B:104:MET:HE2	1.66	0.42
1:B:134:TRP:HA	1:B:137:VAL:HB	2.01	0.42
1:B:365:TYR:CB	1:B:398:CYS:SG	2.92	0.42
1:B:389:ALA:O	1:B:390:VAL:C	2.58	0.42
1:C:69:SER:N	1:C:70:PRO:HA	2.35	0.42
1:C:92:LEU:CD2	1:C:363:VAL:CG2	2.88	0.42
1:C:101:ASN:O	1:C:104:MET:HB2	2.20	0.42
1:D:92:LEU:HD21	1:D:363:VAL:HG21	1.94	0.42
1:D:235:ALA:O	1:D:238:CYS:HB2	2.20	0.42
1:D:414:PHE:C	1:D:414:PHE:CD2	2.92	0.42
1:A:147:ILE:HA	1:A:147:ILE:HD12	1.70	0.42
1:B:67:ASP:O	1:B:69:SER:HA	2.20	0.42
1:B:136:PHE:CE1	1:B:287:LEU:O	2.73	0.42
1:C:95:LEU:HD12	1:C:98:TRP:HH2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:ALA:HA	1:C:312:PRO:HG2	2.01	0.42
1:C:359:ILE:HD11	1:C:409:GLU:CB	2.47	0.42
1:C:412:TRP:CE3	1:C:412:TRP:CA	2.96	0.42
1:C:428:TYR:CE1	1:D:373:LEU:CB	3.03	0.42
1:D:60:TYR:OH	1:D:368:THR:OG1	2.35	0.42
1:D:69:SER:N	1:D:70:PRO:HA	2.35	0.42
1:D:156:VAL:HG23	1:D:159:LEU:HD12	2.01	0.42
1:A:368:THR:O	1:A:371:ALA:HB3	2.20	0.41
1:C:136:PHE:CE1	1:C:287:LEU:O	2.73	0.41
1:C:377:HIS:HE1	1:D:430:ARG:C	2.23	0.41
1:D:420:ILE:HG22	1:D:421:THR:H	1.80	0.41
1:A:63:MET:CG	1:A:76:TYR:CD2	3.03	0.41
1:A:96:ALA:HA	1:A:357:SER:HB2	2.02	0.41
1:B:13:ILE:CB	1:B:14:PRO:HD3	2.50	0.41
1:C:88:GLN:O	1:C:91:VAL:HG23	2.21	0.41
1:D:99:ILE:HG21	1:D:357:SER:HB3	2.02	0.41
1:D:107:ILE:O	1:D:111:TYR:CD1	2.72	0.41
1:A:99:ILE:HG21	1:A:357:SER:HB3	2.02	0.41
1:A:107:ILE:O	1:A:111:TYR:CD1	2.71	0.41
1:A:134:TRP:HA	1:A:137:VAL:HB	2.02	0.41
1:B:101:ASN:O	1:B:104:MET:HB2	2.20	0.41
1:B:306:ASP:C	1:B:308:GLY:N	2.73	0.41
1:C:301:ALA:C	1:C:303:ALA:N	2.73	0.41
1:D:24:MET:HE3	1:D:162:ILE:HD12	2.00	0.41
1:D:114:TYR:O	1:D:115:PHE:HB2	2.20	0.41
1:D:317:VAL:HA	1:D:322:THR:O	2.20	0.41
1:D:371:ALA:C	1:D:373:LEU:N	2.72	0.41
1:A:92:LEU:CG	1:A:363:VAL:HG21	2.50	0.41
1:A:121:ASP:N	1:A:122:PRO:CD	2.81	0.41
1:A:212:VAL:HG11	1:A:296:LEU:HD13	2.03	0.41
1:A:352:LEU:HD23	1:A:352:LEU:HA	1.93	0.41
1:B:49:THR:HB	1:B:197:LEU:CD2	2.50	0.41
1:B:51:ILE:HG22	1:B:52:GLY:N	2.35	0.41
1:B:93:TYR:CD2	1:B:93:TYR:C	2.93	0.41
1:C:35:LEU:CD2	1:C:196:THR:HG22	2.42	0.41
1:C:317:VAL:HA	1:C:322:THR:O	2.20	0.41
1:D:290:LEU:O	1:D:294:THR:HG23	2.20	0.41
1:A:49:THR:OG1	1:A:201:LEU:HD12	2.21	0.41
1:A:69:SER:N	1:A:70:PRO:HA	2.35	0.41
1:A:359:ILE:HD13	1:A:410:VAL:HA	2.02	0.41
1:B:135:ILE:HG22	1:B:136:PHE:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:LEU:HD12	1:C:232:VAL:CG1	2.50	0.41
1:C:95:LEU:HD23	1:C:95:LEU:O	2.20	0.41
1:D:311:PRO:HA	1:D:312:PRO:HD3	1.85	0.41
1:D:373:LEU:HD11	1:D:391:THR:CB	2.50	0.41
1:A:174:ARG:HA	1:A:175:GLY:HA3	1.93	0.41
1:A:395:PHE:O	1:A:399:ILE:HB	2.21	0.41
1:B:8:HIS:ND1	1:B:9:LYS:NZ	2.66	0.41
1:B:44:TYR:O	1:B:45:GLY:C	2.58	0.41
1:B:374:LEU:HD12	1:B:374:LEU:HA	1.86	0.41
1:C:28:VAL:O	1:C:30:LEU:N	2.46	0.41
1:C:314:PHE:CA	1:C:315:ALA:O	2.68	0.41
1:C:376:GLY:CA	1:C:379:HIS:H	2.33	0.41
1:D:71:GLY:C	1:D:212:VAL:HA	2.39	0.41
1:D:82:GLY:O	1:D:83:PRO:O	2.39	0.41
1:D:301:ALA:HB1	1:D:310:PHE:CE1	2.46	0.41
1:D:302:LYS:HE3	1:D:326:GLY:CA	2.50	0.41
1:A:366:LEU:HD13	1:A:367:TYR:HD2	1.81	0.41
1:A:410:VAL:C	1:A:412:TRP:N	2.74	0.41
1:C:47:LEU:C	1:C:47:LEU:HD13	2.41	0.41
1:C:310:PHE:HB3	1:C:311:PRO:O	2.20	0.41
1:C:346:ALA:HB3	1:C:351:GLY:CA	2.44	0.41
1:D:35:LEU:CD2	1:D:196:THR:HG22	2.43	0.41
1:D:72:GLY:C	1:D:74:TYR:H	2.23	0.41
1:A:81:PHE:HE1	1:B:80:CYS:O	2.03	0.41
1:A:173:PHE:CE1	1:A:247:MET:SD	3.14	0.41
1:A:299:GLN:C	1:A:301:ALA:H	2.24	0.41
1:A:300:THR:O	1:A:300:THR:CG2	2.64	0.41
1:B:94:TRP:CA	1:B:97:CYS:HB2	2.47	0.41
1:B:359:ILE:HB	1:B:413:SER:OG	2.21	0.41
1:B:363:VAL:HB	1:B:364:PRO:HD3	2.02	0.41
1:C:44:TYR:O	1:C:45:GLY:C	2.58	0.41
1:C:212:VAL:HG11	1:C:296:LEU:HD13	2.02	0.41
1:C:418:MET:HE2	1:D:399:ILE:HG13	2.02	0.41
1:D:69:SER:HB2	1:D:75:ALA:HB2	2.02	0.41
1:D:306:ASP:O	1:D:308:GLY:N	2.54	0.41
1:A:10:VAL:CG2	1:A:145:LYS:HA	2.51	0.41
1:A:426:LEU:C	1:A:427:ASN:HD22	2.19	0.41
1:B:83:PRO:O	1:B:84:PHE:C	2.59	0.41
1:B:133:LEU:HD11	1:B:338:GLN:HG3	2.02	0.41
1:B:187:LEU:N	1:B:187:LEU:HD23	2.35	0.41
1:B:210:ALA:C	1:B:212:VAL:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:SER:O	1:B:292:GLY:N	2.54	0.41
1:B:301:ALA:HB1	1:B:310:PHE:CE1	2.47	0.41
1:B:314:PHE:CA	1:B:315:ALA:O	2.69	0.41
1:B:426:LEU:C	1:B:427:ASN:HD22	2.21	0.41
1:C:69:SER:HB2	1:C:75:ALA:HB2	2.03	0.41
1:C:72:GLY:C	1:C:74:TYR:N	2.71	0.41
1:C:134:TRP:HA	1:C:137:VAL:HB	2.03	0.41
1:C:209:SER:HA	1:C:296:LEU:CD1	2.38	0.41
1:D:88:GLN:HG3	1:D:420:ILE:HG21	2.02	0.41
1:D:299:GLN:C	1:D:301:ALA:H	2.24	0.41
1:D:349:GLU:O	1:D:350:PHE:HB2	2.21	0.41
1:D:368:THR:O	1:D:371:ALA:HB3	2.20	0.41
1:D:372:LEU:C	1:D:373:LEU:HG	2.41	0.41
1:A:47:LEU:C	1:A:47:LEU:HD13	2.40	0.41
1:A:399:ILE:O	1:A:403:VAL:HB	2.21	0.41
1:B:77:ALA:O	1:B:79:ARG:N	2.54	0.41
1:B:92:LEU:CG	1:B:363:VAL:HG21	2.48	0.41
1:B:174:ARG:HA	1:B:175:GLY:HA3	1.93	0.41
1:B:217:VAL:HG12	1:B:218:LYS:N	2.36	0.41
1:B:301:ALA:C	1:B:303:ALA:N	2.74	0.41
1:C:147:ILE:HD12	1:C:147:ILE:HA	1.71	0.41
1:C:215:GLY:O	1:C:216:VAL:HG22	2.21	0.41
1:C:414:PHE:C	1:C:414:PHE:HD2	2.24	0.41
1:D:6:ASP:HB3	1:D:9:LYS:CG	2.49	0.41
1:D:28:VAL:HA	1:D:31:LEU:HG	2.03	0.41
1:D:31:LEU:HD11	1:D:239:TYR:CE2	2.56	0.41
1:D:95:LEU:HA	1:D:98:TRP:HZ3	1.80	0.41
1:D:416:THR:CA	1:D:419:VAL:HG12	2.47	0.41
1:A:433:LYS:O	1:B:79:ARG:HG2	2.21	0.40
1:B:93:TYR:HE1	1:B:208:GLU:OE2	2.04	0.40
1:B:342:ILE:CB	1:B:343:SER:CB	2.86	0.40
1:C:77:ALA:O	1:C:79:ARG:N	2.54	0.40
1:C:92:LEU:HD21	1:C:363:VAL:HG21	1.95	0.40
1:C:366:LEU:HD21	1:D:421:THR:HG21	2.02	0.40
1:D:134:TRP:HA	1:D:137:VAL:HB	2.03	0.40
1:A:28:VAL:HA	1:A:31:LEU:HG	2.03	0.40
1:A:101:ASN:O	1:A:104:MET:HB2	2.21	0.40
1:B:311:PRO:HA	1:B:312:PRO:HD3	1.85	0.40
1:B:322:THR:HA	1:B:323:PRO:HD3	1.76	0.40
1:C:72:GLY:CA	1:C:211:SER:O	2.70	0.40
1:C:114:TYR:O	1:C:115:PHE:HB2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:TRP:CH2	1:C:350:PHE:CE1	3.09	0.40
1:C:376:GLY:HA3	1:C:379:HIS:HD2	1.85	0.40
1:D:84:PHE:CE1	1:D:85:LEU:CD2	2.86	0.40
1:D:117:PRO:O	1:D:118:ILE:CG2	2.68	0.40
1:D:177:THR:O	1:D:180:ALA:HB3	2.21	0.40
1:A:54:LEU:HD12	1:A:232:VAL:CG1	2.51	0.40
1:A:79:ARG:NE	1:B:433:LYS:O	2.55	0.40
1:A:240:VAL:O	1:A:244:THR:HG23	2.22	0.40
1:A:317:VAL:HA	1:A:322:THR:O	2.22	0.40
1:A:349:GLU:O	1:A:350:PHE:HB2	2.22	0.40
1:A:416:THR:O	1:A:419:VAL:HG12	2.21	0.40
1:B:114:TYR:O	1:B:115:PHE:HB2	2.20	0.40
1:C:95:LEU:HD12	1:C:98:TRP:CH2	2.57	0.40
1:C:218:LYS:HB2	1:C:223:ASN:ND2	2.35	0.40
1:C:306:ASP:C	1:C:308:GLY:H	2.25	0.40
1:C:366:LEU:CD2	1:D:421:THR:HG21	2.51	0.40
1:D:54:LEU:HD12	1:D:232:VAL:CG1	2.52	0.40
1:A:67:ASP:OD1	1:A:67:ASP:O	2.39	0.40
1:A:69:SER:HB2	1:A:75:ALA:HB2	2.02	0.40
1:B:207:VAL:HG12	1:B:232:VAL:HG23	2.02	0.40
1:B:378:GLY:O	1:B:379:HIS:O	2.40	0.40
1:C:10:VAL:CG1	1:C:11:GLY:H	2.28	0.40
1:C:29:PHE:O	1:C:30:LEU:HG	2.21	0.40
1:C:302:LYS:HE3	1:C:326:GLY:HA3	2.03	0.40
1:C:412:TRP:CE3	1:C:415:VAL:HG21	2.56	0.40
1:D:44:TYR:O	1:D:45:GLY:C	2.59	0.40
1:D:67:ASP:OD1	1:D:67:ASP:O	2.39	0.40
1:D:72:GLY:C	1:D:74:TYR:N	2.73	0.40
1:A:202:TRP:CH2	1:A:350:PHE:CE1	3.10	0.40
1:A:355:SER:OG	1:A:409:GLU:HG2	2.21	0.40
1:A:395:PHE:CE1	1:B:422:ALA:CB	3.01	0.40
1:B:91:VAL:O	1:B:95:LEU:CB	2.66	0.40
1:B:177:THR:O	1:B:180:ALA:HB3	2.21	0.40
1:B:207:VAL:CG1	1:B:232:VAL:HG21	2.52	0.40
1:B:215:GLY:O	1:B:216:VAL:HG22	2.21	0.40
1:C:60:TYR:CE1	1:C:208:GLU:HA	2.57	0.40
1:C:303:ALA:C	1:C:305:ALA:H	2.24	0.40
1:D:46:TRP:CH2	1:D:239:TYR:HB3	2.56	0.40
1:D:374:LEU:HD12	1:D:374:LEU:HA	1.86	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	406/445 (91%)	275 (68%)	79 (20%)	52 (13%)	0	5
1	B	406/445 (91%)	274 (68%)	76 (19%)	56 (14%)	0	4
1	C	406/445 (91%)	278 (68%)	67 (16%)	61 (15%)	0	3
1	D	406/445 (91%)	274 (68%)	76 (19%)	56 (14%)	0	4
All	All	1624/1780 (91%)	1101 (68%)	298 (18%)	225 (14%)	0	4

All (225) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	VAL
1	A	30	LEU
1	A	41	ILE
1	A	69	SER
1	A	73	SER
1	A	83	PRO
1	A	96	ALA
1	A	117	PRO
1	A	121	ASP
1	A	172	TRP
1	A	182	TRP
1	A	183	ASN
1	A	184	VAL
1	A	214	ALA
1	A	218	LYS
1	A	345	ASN
1	A	377	HIS
1	A	421	THR
1	A	422	ALA
1	A	426	LEU
1	A	431	LEU
1	B	10	VAL

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Mol	Chain	Res	Type
1	B	30	LEU
1	B	41	ILE
1	B	69	SER
1	B	73	SER
1	B	83	PRO
1	B	96	ALA
1	B	117	PRO
1	B	121	ASP
1	B	172	TRP
1	B	182	TRP
1	B	183	ASN
1	B	184	VAL
1	B	214	ALA
1	B	218	LYS
1	B	345	ASN
1	B	377	HIS
1	B	421	THR
1	B	431	LEU
1	C	10	VAL
1	C	30	LEU
1	C	41	ILE
1	C	69	SER
1	C	73	SER
1	C	83	PRO
1	C	96	ALA
1	C	117	PRO
1	C	121	ASP
1	C	172	TRP
1	C	182	TRP
1	C	183	ASN
1	C	184	VAL
1	C	214	ALA
1	C	218	LYS
1	C	345	ASN
1	C	377	HIS
1	C	421	THR
1	C	431	LEU
1	D	10	VAL
1	D	30	LEU
1	D	41	ILE
1	D	69	SER
1	D	73	SER

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Mol	Chain	Res	Type
1	D	83	PRO
1	D	96	ALA
1	D	117	PRO
1	D	121	ASP
1	D	172	TRP
1	D	182	TRP
1	D	183	ASN
1	D	184	VAL
1	D	214	ALA
1	D	218	LYS
1	D	345	ASN
1	D	377	HIS
1	D	421	THR
1	D	422	ALA
1	D	426	LEU
1	D	431	LEU
1	D	432	HIS
1	A	24	MET
1	A	68	PRO
1	A	116	PHE
1	A	118	ILE
1	A	122	PRO
1	A	190	PHE
1	A	202	TRP
1	A	215	GLY
1	A	250	ILE
1	A	310	PHE
1	A	372	LEU
1	A	379	HIS
1	A	432	HIS
1	B	24	MET
1	B	116	PHE
1	B	118	ILE
1	B	122	PRO
1	B	190	PHE
1	B	202	TRP
1	B	215	GLY
1	B	250	ILE
1	B	310	PHE
1	B	379	HIS
1	B	422	ALA
1	B	426	LEU

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Mol	Chain	Res	Type
1	C	24	MET
1	C	116	PHE
1	C	118	ILE
1	C	122	PRO
1	C	190	PHE
1	C	202	TRP
1	C	215	GLY
1	C	250	ILE
1	C	310	PHE
1	C	379	HIS
1	C	401	ALA
1	C	422	ALA
1	C	426	LEU
1	D	24	MET
1	D	116	PHE
1	D	118	ILE
1	D	122	PRO
1	D	190	PHE
1	D	202	TRP
1	D	215	GLY
1	D	250	ILE
1	D	310	PHE
1	D	372	LEU
1	D	379	HIS
1	A	248	GLY
1	A	312	PRO
1	A	313	ILE
1	A	315	ALA
1	A	343	SER
1	B	68	PRO
1	B	143	GLY
1	B	248	GLY
1	B	312	PRO
1	B	313	ILE
1	B	315	ALA
1	B	340	SER
1	B	368	THR
1	B	372	LEU
1	B	390	VAL
1	B	432	HIS
1	C	68	PRO
1	C	78	ARG

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Mol	Chain	Res	Type
1	C	248	GLY
1	C	312	PRO
1	C	313	ILE
1	C	315	ALA
1	C	340	SER
1	C	368	THR
1	C	372	LEU
1	C	432	HIS
1	D	68	PRO
1	D	78	ARG
1	D	248	GLY
1	D	312	PRO
1	D	313	ILE
1	D	315	ALA
1	D	340	SER
1	D	343	SER
1	A	38	THR
1	A	74	TYR
1	A	78	ARG
1	A	322	THR
1	A	340	SER
1	A	368	THR
1	A	380	PHE
1	B	38	THR
1	B	78	ARG
1	B	322	THR
1	B	343	SER
1	B	401	ALA
1	C	38	THR
1	C	143	GLY
1	C	322	THR
1	C	343	SER
1	C	390	VAL
1	C	396	LEU
1	D	38	THR
1	D	74	TYR
1	D	322	THR
1	D	368	THR
1	D	434	ASN
1	A	383	ALA
1	B	304	ALA
1	B	380	PHE

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Mol	Chain	Res	Type
1	B	383	ALA
1	B	396	LEU
1	C	74	TYR
1	C	304	ALA
1	C	380	PHE
1	C	383	ALA
1	D	383	ALA
1	D	433	LYS
1	B	74	TYR
1	B	220	PRO
1	C	397	TYR
1	D	89	THR
1	D	304	ALA
1	D	396	LEU
1	A	175	GLY
1	B	71	GLY
1	B	175	GLY
1	C	71	GLY
1	C	175	GLY
1	D	175	GLY
1	A	71	GLY
1	A	434	ASN
1	C	220	PRO
1	D	71	GLY
1	B	205	ILE
1	C	207	VAL
1	C	161	PRO
1	C	205	ILE
1	C	434	ASN
1	A	353	VAL
1	A	390	VAL
1	C	353	VAL
1	D	161	PRO
1	D	317	VAL
1	D	353	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	314/343 (92%)	251 (80%)	63 (20%)	1	8
1	B	314/343 (92%)	250 (80%)	64 (20%)	1	7
1	C	314/343 (92%)	247 (79%)	67 (21%)	1	6
1	D	314/343 (92%)	250 (80%)	64 (20%)	1	7
All	All	1256/1372 (92%)	998 (80%)	258 (20%)	1	7

All (258) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ILE
1	A	35	LEU
1	A	51	ILE
1	A	56	LEU
1	A	69	SER
1	A	74	TYR
1	A	76	TYR
1	A	81	PHE
1	A	84	PHE
1	A	88	GLN
1	A	91	VAL
1	A	92	LEU
1	A	97	CYS
1	A	98	TRP
1	A	99	ILE
1	A	104	MET
1	A	105	VAL
1	A	112	LEU
1	A	116	PHE
1	A	125	LEU
1	A	126	THR
1	A	128	THR
1	A	147	ILE
1	A	156	VAL
1	A	172	TRP
1	A	178	TYR
1	A	182	TRP
1	A	196	THR
1	A	200	THR
1	A	202	TRP
1	A	204	PHE

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Mol	Chain	Res	Type
1	A	207	VAL
1	A	209	SER
1	A	219	ASN
1	A	234	ILE
1	A	247	MET
1	A	290	LEU
1	A	295	LEU
1	A	296	LEU
1	A	310	PHE
1	A	312	PRO
1	A	314	PHE
1	A	327	LEU
1	A	328	ILE
1	A	329	ILE
1	A	333	LEU
1	A	335	THR
1	A	339	LEU
1	A	363	VAL
1	A	366	LEU
1	A	374	LEU
1	A	380	PHE
1	A	388	LEU
1	A	391	THR
1	A	399	ILE
1	A	405	SER
1	A	409	GLU
1	A	411	MET
1	A	412	TRP
1	A	414	PHE
1	A	417	LEU
1	A	420	ILE
1	A	430	ARG
1	B	23	ILE
1	B	35	LEU
1	B	51	ILE
1	B	56	LEU
1	B	69	SER
1	B	74	TYR
1	B	76	TYR
1	B	78	ARG
1	B	81	PHE
1	B	84	PHE

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Mol	Chain	Res	Type
1	B	88	GLN
1	B	91	VAL
1	B	92	LEU
1	B	97	CYS
1	B	98	TRP
1	B	99	ILE
1	B	104	MET
1	B	105	VAL
1	B	112	LEU
1	B	116	PHE
1	B	125	LEU
1	B	126	THR
1	B	128	THR
1	B	135	ILE
1	B	147	ILE
1	B	156	VAL
1	B	172	TRP
1	B	178	TYR
1	B	182	TRP
1	B	196	THR
1	B	200	THR
1	B	202	TRP
1	B	204	PHE
1	B	207	VAL
1	B	209	SER
1	B	219	ASN
1	B	234	ILE
1	B	247	MET
1	B	290	LEU
1	B	295	LEU
1	B	296	LEU
1	B	310	PHE
1	B	314	PHE
1	B	327	LEU
1	B	328	ILE
1	B	329	ILE
1	B	333	LEU
1	B	335	THR
1	B	339	LEU
1	B	363	VAL
1	B	366	LEU
1	B	374	LEU

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Mol	Chain	Res	Type
1	B	380	PHE
1	B	388	LEU
1	B	391	THR
1	B	399	ILE
1	B	405	SER
1	B	409	GLU
1	B	411	MET
1	B	412	TRP
1	B	414	PHE
1	B	417	LEU
1	B	420	ILE
1	B	430	ARG
1	C	23	ILE
1	C	35	LEU
1	C	41	ILE
1	C	51	ILE
1	C	56	LEU
1	C	69	SER
1	C	74	TYR
1	C	76	TYR
1	C	78	ARG
1	C	81	PHE
1	C	84	PHE
1	C	88	GLN
1	C	91	VAL
1	C	92	LEU
1	C	93	TYR
1	C	97	CYS
1	C	98	TRP
1	C	99	ILE
1	C	104	MET
1	C	105	VAL
1	C	112	LEU
1	C	116	PHE
1	C	125	LEU
1	C	126	THR
1	C	128	THR
1	C	130	VAL
1	C	135	ILE
1	C	147	ILE
1	C	156	VAL
1	C	172	TRP

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Mol	Chain	Res	Type
1	C	178	TYR
1	C	182	TRP
1	C	196	THR
1	C	200	THR
1	C	202	TRP
1	C	204	PHE
1	C	207	VAL
1	C	209	SER
1	C	219	ASN
1	C	234	ILE
1	C	247	MET
1	C	290	LEU
1	C	295	LEU
1	C	296	LEU
1	C	310	PHE
1	C	314	PHE
1	C	327	LEU
1	C	328	ILE
1	C	329	ILE
1	C	333	LEU
1	C	335	THR
1	C	339	LEU
1	C	363	VAL
1	C	366	LEU
1	C	374	LEU
1	C	380	PHE
1	C	388	LEU
1	C	391	THR
1	C	399	ILE
1	C	405	SER
1	C	409	GLU
1	C	411	MET
1	C	412	TRP
1	C	414	PHE
1	C	417	LEU
1	C	420	ILE
1	C	430	ARG
1	D	23	ILE
1	D	35	LEU
1	D	51	ILE
1	D	56	LEU
1	D	69	SER

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Mol	Chain	Res	Type
1	D	74	TYR
1	D	76	TYR
1	D	78	ARG
1	D	81	PHE
1	D	84	PHE
1	D	88	GLN
1	D	91	VAL
1	D	92	LEU
1	D	97	CYS
1	D	98	TRP
1	D	99	ILE
1	D	104	MET
1	D	105	VAL
1	D	112	LEU
1	D	116	PHE
1	D	125	LEU
1	D	126	THR
1	D	128	THR
1	D	147	ILE
1	D	156	VAL
1	D	172	TRP
1	D	178	TYR
1	D	182	TRP
1	D	196	THR
1	D	200	THR
1	D	202	TRP
1	D	204	PHE
1	D	207	VAL
1	D	209	SER
1	D	219	ASN
1	D	234	ILE
1	D	247	MET
1	D	290	LEU
1	D	295	LEU
1	D	296	LEU
1	D	310	PHE
1	D	312	PRO
1	D	327	LEU
1	D	328	ILE
1	D	329	ILE
1	D	333	LEU
1	D	335	THR

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Mol	Chain	Res	Type
1	D	339	LEU
1	D	363	VAL
1	D	366	LEU
1	D	374	LEU
1	D	380	PHE
1	D	388	LEU
1	D	391	THR
1	D	399	ILE
1	D	405	SER
1	D	409	GLU
1	D	411	MET
1	D	412	TRP
1	D	414	PHE
1	D	417	LEU
1	D	420	ILE
1	D	427	ASN
1	D	430	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	151	GLN
1	A	219	ASN
1	A	223	ASN
1	A	377	HIS
1	A	379	HIS
1	B	22	ASN
1	B	151	GLN
1	B	219	ASN
1	B	223	ASN
1	B	345	ASN
1	B	377	HIS
1	B	379	HIS
1	C	22	ASN
1	C	151	GLN
1	C	219	ASN
1	C	223	ASN
1	C	377	HIS
1	C	379	HIS
1	D	22	ASN
1	D	151	GLN

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Mol	Chain	Res	Type
1	D	219	ASN
1	D	223	ASN
1	D	377	HIS
1	D	379	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	410/445 (92%)	-0.23	7 (1%) 70 60	144, 300, 447, 565	0
1	B	410/445 (92%)	-0.23	9 (2%) 62 52	133, 299, 453, 567	0
1	C	410/445 (92%)	-0.31	6 (1%) 73 64	136, 297, 453, 569	0
1	D	410/445 (92%)	-0.32	3 (0%) 87 82	141, 299, 442, 563	0
All	All	1640/1780 (92%)	-0.27	25 (1%) 73 64	133, 299, 452, 569	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	347	THR	6.0
1	C	26	SER	5.2
1	B	26	SER	5.0
1	D	350	PHE	4.8
1	A	352	LEU	3.6
1	C	27	GLY	3.5
1	A	184	VAL	3.4
1	A	183	ASN	3.3
1	C	347	THR	3.0
1	B	27	GLY	3.0
1	B	203	SER	3.0
1	A	174	ARG	2.7
1	C	248	GLY	2.6
1	B	171	PHE	2.6
1	D	171	PHE	2.5
1	B	174	ARG	2.5
1	B	208	GLU	2.5
1	C	25	GLY	2.4
1	A	171	PHE	2.4
1	C	203	SER	2.2
1	B	206	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	342	ILE	2.1
1	A	203	SER	2.1
1	B	25	GLY	2.1
1	D	245	ALA	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 monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.