



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 05:52 am BST

PDB ID : 2DRD
Title : Crystal structure of a multidrug transporter reveal a functionally rotating mechanism
Authors : Murakami, S.; Nakashima, R.; Yamashita, E.; Matsumoto, T.
Deposited on : 2006-06-08
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

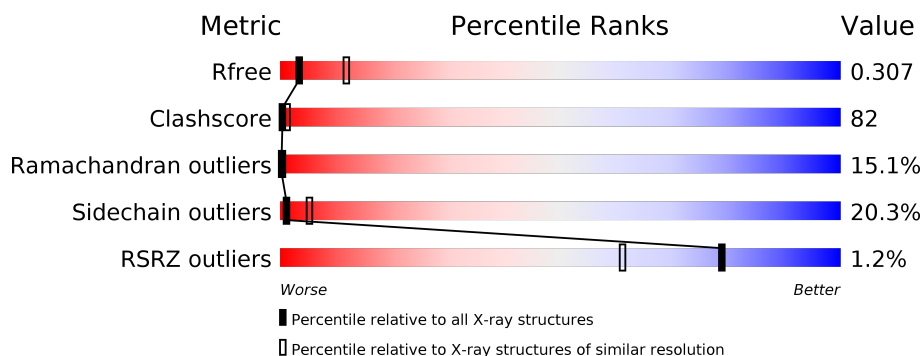
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1053	<div> <div>19%</div> <div>49%</div> <div>24%</div> <div>5%</div> </div>
1	B	1053	<div> <div>17%</div> <div>53%</div> <div>23%</div> </div>
1	C	1053	<div> <div>2%</div> <div>19%</div> <div>50%</div> <div>23%</div> <div>6%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23355 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.

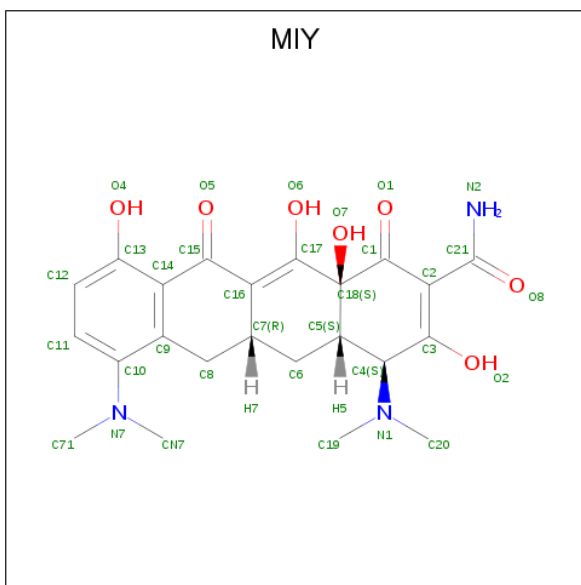
- Molecule 1 is a protein called ACRB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1022	Total	C	N	O	S	0	0	0
			7774	5003	1283	1444	44			
1	B	1022	Total	C	N	O	S	0	0	0
			7774	5003	1283	1444	44			
1	C	1022	Total	C	N	O	S	0	0	0
			7774	5003	1283	1444	44			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1050	HIS	-	EXPRESSION TAG	UNP P31224
A	1051	HIS	-	EXPRESSION TAG	UNP P31224
A	1052	HIS	-	EXPRESSION TAG	UNP P31224
A	1053	HIS	-	EXPRESSION TAG	UNP P31224
B	1050	HIS	-	EXPRESSION TAG	UNP P31224
B	1051	HIS	-	EXPRESSION TAG	UNP P31224
B	1052	HIS	-	EXPRESSION TAG	UNP P31224
B	1053	HIS	-	EXPRESSION TAG	UNP P31224
C	1050	HIS	-	EXPRESSION TAG	UNP P31224
C	1051	HIS	-	EXPRESSION TAG	UNP P31224
C	1052	HIS	-	EXPRESSION TAG	UNP P31224
C	1053	HIS	-	EXPRESSION TAG	UNP P31224

- Molecule 2 is (4S,4AS,5AR,12AS)-4,7-BIS(DIMETHYLAMINO)-3,10,12,12A-TETRAHYDROXY-1,11-DIOXO-1,4,4A,5,5A,6,11,12A-OCTAHYDROTETRACENE-2-CARBOXAMIDE (three-letter code: MIY) (formula: C₂₃H₂₇N₃O₇).

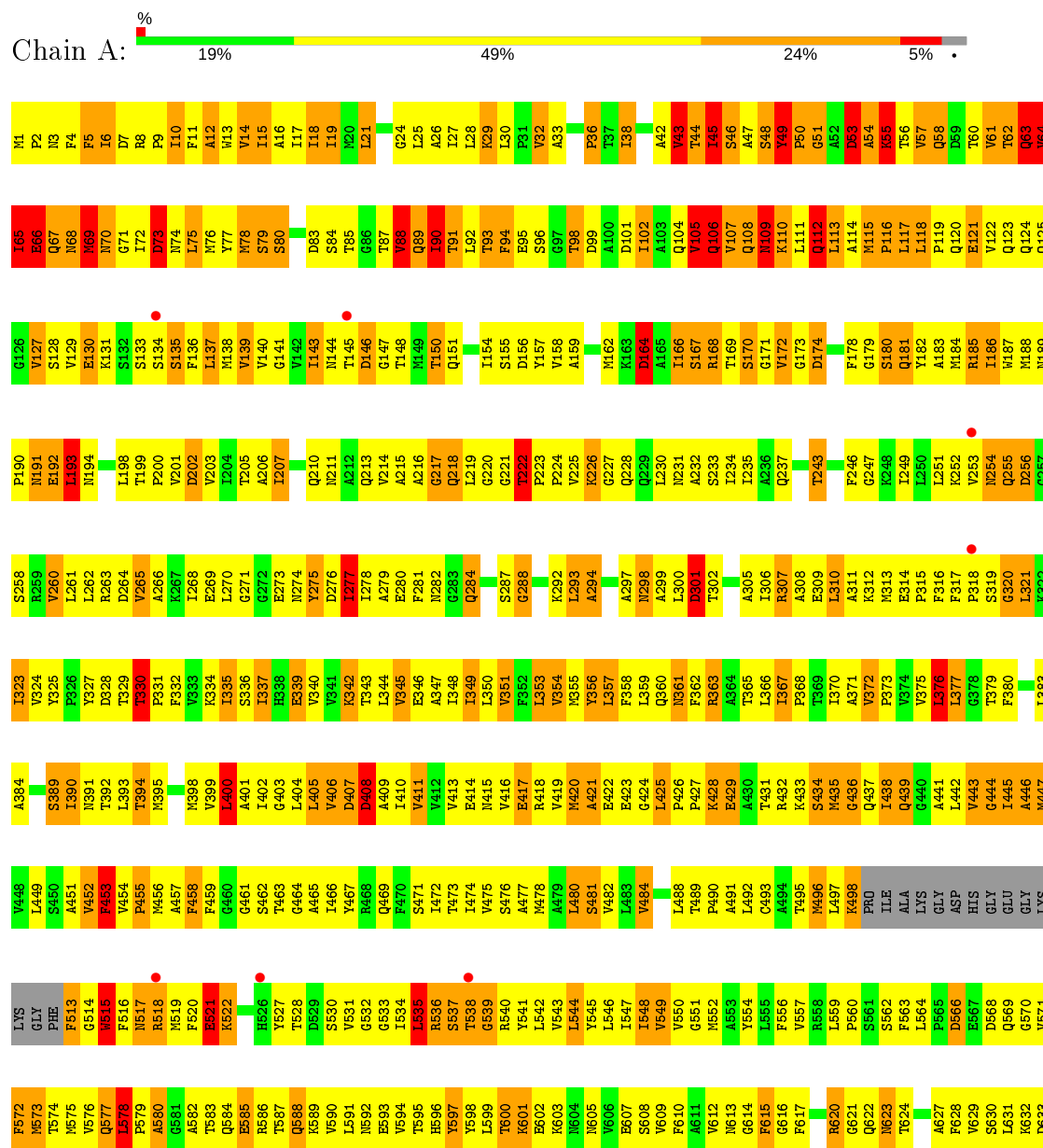


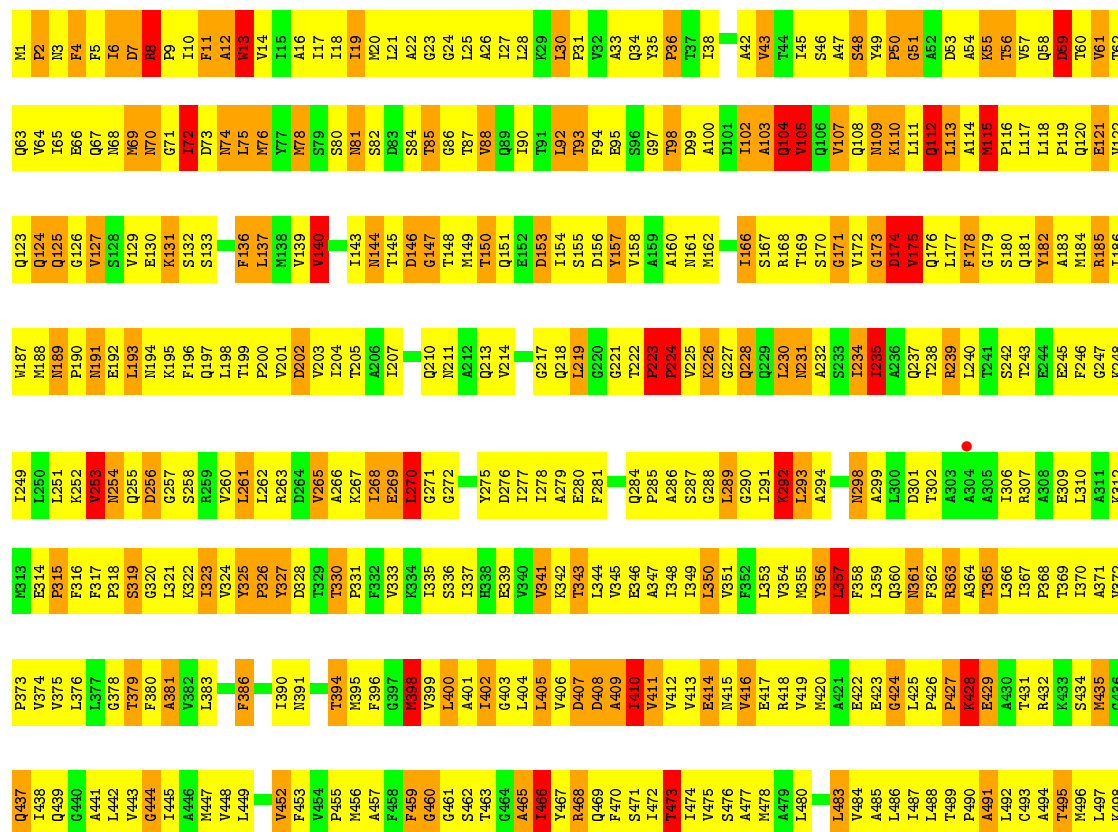
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			33	23	3	7		

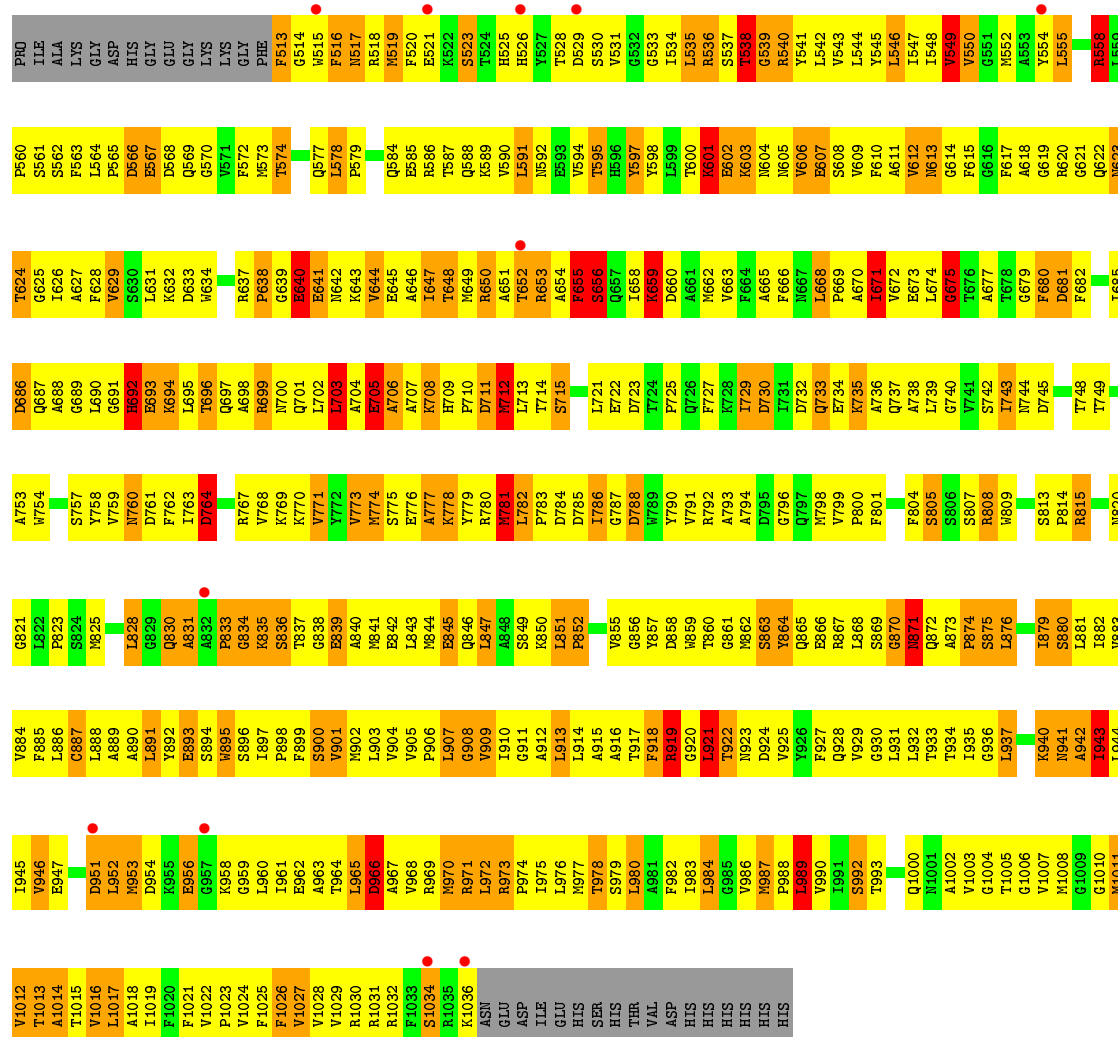
3 Residue-property plots

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

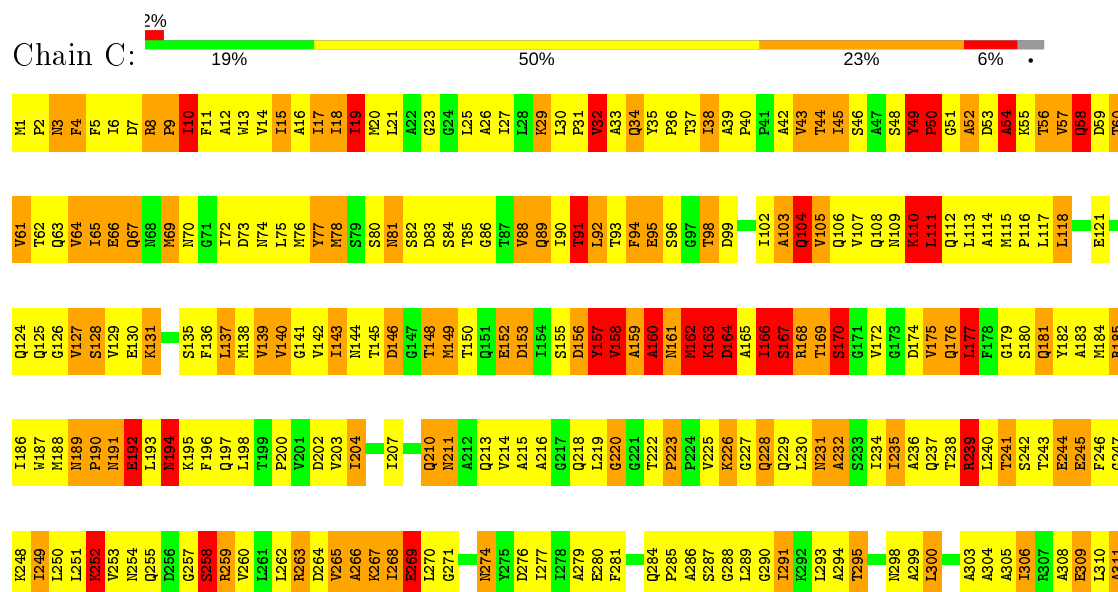
• Molecule 1: ACRB







- Molecule 1: ACRB





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	225.80Å 134.47Å 162.12Å 90.00° 98.17° 90.00°	Depositor
Resolution (Å)	10.00 – 3.10 10.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.5 (10.00-3.10) 97.4 (10.00-3.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 3.10Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.255 , 0.310 0.248 , 0.307	Depositor DCC
R_{free} test set	4181 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	78.1	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 97.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	23355	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.56	90/7920 (1.1%)	1.40	68/10756 (0.6%)
1	B	1.30	22/7920 (0.3%)	1.26	50/10756 (0.5%)
1	C	1.54	90/7920 (1.1%)	1.44	86/10756 (0.8%)
All	All	1.47	202/23760 (0.9%)	1.37	204/32268 (0.6%)

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	1
1	C	0	4
All	All	0	7

All (202) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	819	TYR	CG-CD1	13.88	1.57	1.39
1	A	45	ILE	CA-CB	-12.79	1.25	1.54
1	A	818	ARG	CG-CD	12.35	1.82	1.51
1	C	167	SER	N-CA	11.14	1.68	1.46
1	A	819	TYR	CE2-CZ	10.84	1.52	1.38
1	A	65	ILE	C-O	10.64	1.43	1.23
1	C	758	TYR	CE2-CZ	10.37	1.52	1.38
1	A	73	ASP	CB-CG	10.05	1.72	1.51
1	A	819	TYR	CE1-CZ	9.80	1.51	1.38
1	C	158	VAL	CB-CG1	9.76	1.73	1.52
1	C	159	ALA	CA-CB	-9.74	1.31	1.52
1	A	275	TYR	CD2-CE2	-9.71	1.24	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	90	ILE	CA-CB	-9.53	1.32	1.54
1	A	46	SER	CA-CB	-9.51	1.38	1.52
1	A	855	VAL	CB-CG2	-9.06	1.33	1.52
1	A	79	SER	C-O	9.05	1.40	1.23
1	A	63	GLN	N-CA	-8.97	1.28	1.46
1	C	767	ARG	CZ-NH2	-8.90	1.21	1.33
1	C	45	ILE	CA-CB	8.82	1.75	1.54
1	C	166	ILE	CA-CB	8.65	1.74	1.54
1	B	459	PHE	CB-CG	8.49	1.65	1.51
1	C	167	SER	CB-OG	8.46	1.53	1.42
1	C	770	LYS	CD-CE	8.42	1.72	1.51
1	A	49	TYR	CE1-CZ	-8.35	1.27	1.38
1	A	67	GLN	CA-CB	8.34	1.72	1.53
1	C	165	ALA	CA-CB	-8.32	1.34	1.52
1	A	801	PHE	CB-CG	8.29	1.65	1.51
1	A	44	THR	C-O	8.27	1.39	1.23
1	C	291	ILE	CA-CB	-8.24	1.35	1.54
1	A	107	VAL	CB-CG1	8.14	1.70	1.52
1	A	725	PRO	C-O	8.13	1.39	1.23
1	C	174	ASP	CA-C	8.11	1.74	1.52
1	B	887	CYS	CB-SG	-7.97	1.68	1.82
1	A	688	ALA	CA-CB	7.95	1.69	1.52
1	A	127	VAL	CB-CG1	7.82	1.69	1.52
1	C	157	TYR	C-O	7.82	1.38	1.23
1	A	66	GLU	CD-OE1	7.80	1.34	1.25
1	A	820	ASN	C-O	7.78	1.38	1.23
1	A	88	VAL	CB-CG1	-7.74	1.36	1.52
1	A	819	TYR	CD1-CE1	7.63	1.50	1.39
1	A	88	VAL	CB-CG2	-7.63	1.36	1.52
1	C	772	TYR	CE2-CZ	-7.57	1.28	1.38
1	B	105	VAL	CA-CB	7.44	1.70	1.54
1	C	91	THR	CA-CB	7.41	1.72	1.53
1	C	105	VAL	CB-CG1	7.39	1.68	1.52
1	A	67	GLN	CB-CG	7.36	1.72	1.52
1	C	167	SER	C-O	7.31	1.37	1.23
1	C	169	THR	CA-CB	7.31	1.72	1.53
1	A	66	GLU	CB-CG	7.31	1.66	1.52
1	C	235	ILE	CA-CB	7.30	1.71	1.54
1	A	105	VAL	C-O	7.29	1.37	1.23
1	C	762	PHE	CE2-CZ	-7.28	1.23	1.37
1	A	275	TYR	CD1-CE1	-7.27	1.28	1.39
1	C	66	GLU	CD-OE2	-7.26	1.17	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	822	LEU	C-O	7.25	1.37	1.23
1	A	823	PRO	C-O	7.17	1.37	1.23
1	A	49	TYR	CD1-CE1	-7.17	1.28	1.39
1	A	43	VAL	CB-CG1	-7.16	1.37	1.52
1	A	70	ASN	CG-ND2	7.09	1.50	1.32
1	A	55	LYS	CD-CE	7.07	1.69	1.51
1	A	893	GLU	CG-CD	7.05	1.62	1.51
1	C	160	ALA	CA-CB	-6.98	1.37	1.52
1	A	808	ARG	CG-CD	6.97	1.69	1.51
1	C	110	LYS	CD-CE	6.96	1.68	1.51
1	C	274	ASN	CB-CG	6.93	1.67	1.51
1	C	161	ASN	N-CA	6.92	1.60	1.46
1	C	772	TYR	CD2-CE2	-6.88	1.29	1.39
1	C	163	LYS	C-O	6.75	1.36	1.23
1	C	165	ALA	C-O	6.72	1.36	1.23
1	C	54	ALA	CA-CB	-6.70	1.38	1.52
1	A	64	VAL	CA-CB	6.68	1.68	1.54
1	C	103	ALA	CA-CB	-6.61	1.38	1.52
1	C	42	ALA	CA-CB	-6.60	1.38	1.52
1	A	819	TYR	CZ-OH	6.55	1.49	1.37
1	C	46	SER	CA-CB	6.54	1.62	1.52
1	C	324	VAL	CB-CG2	-6.49	1.39	1.52
1	C	164	ASP	CG-OD2	6.48	1.40	1.25
1	B	112	GLN	CG-CD	6.47	1.66	1.51
1	B	773	VAL	CB-CG2	-6.47	1.39	1.52
1	C	289	LEU	N-CA	-6.41	1.33	1.46
1	A	691	GLY	C-O	6.40	1.33	1.23
1	B	459	PHE	CG-CD2	6.39	1.48	1.38
1	C	181	GLN	CD-OE1	6.37	1.38	1.24
1	A	58	GLN	CD-OE1	6.36	1.38	1.24
1	C	671	ILE	CA-CB	6.31	1.69	1.54
1	A	43	VAL	CA-CB	-6.31	1.41	1.54
1	A	818	ARG	C-O	6.30	1.35	1.23
1	C	57	VAL	CA-CB	6.28	1.68	1.54
1	B	43	VAL	CB-CG2	-6.27	1.39	1.52
1	C	176	GLN	CG-CD	6.25	1.65	1.51
1	C	136	PHE	CD2-CE2	-6.24	1.26	1.39
1	A	57	VAL	CB-CG2	6.24	1.66	1.52
1	C	49	TYR	CD1-CE1	-6.24	1.29	1.39
1	A	917	THR	CA-CB	6.23	1.69	1.53
1	C	58	GLN	CB-CG	6.20	1.69	1.52
1	A	29	LYS	CB-CG	6.20	1.69	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	807	SER	CB-OG	6.18	1.50	1.42
1	A	70	ASN	N-CA	-6.15	1.34	1.46
1	C	266	ALA	CA-CB	-6.13	1.39	1.52
1	C	46	SER	CB-OG	6.13	1.50	1.42
1	A	819	TYR	C-O	6.12	1.34	1.23
1	A	597	TYR	CB-CG	6.10	1.60	1.51
1	C	139	VAL	CA-CB	-6.10	1.42	1.54
1	C	628	PHE	CB-CG	-6.09	1.41	1.51
1	C	887	CYS	CB-SG	-6.07	1.72	1.82
1	C	152	GLU	CD-OE1	6.02	1.32	1.25
1	C	112	GLN	CG-CD	6.02	1.64	1.51
1	C	110	LYS	CE-NZ	6.01	1.64	1.49
1	C	767	ARG	C-O	5.96	1.34	1.23
1	A	105	VAL	CA-CB	-5.96	1.42	1.54
1	C	316	PHE	CD2-CE2	5.96	1.51	1.39
1	A	585	GLU	CD-OE2	5.96	1.32	1.25
1	C	182	TYR	CE1-CZ	5.96	1.46	1.38
1	A	275	TYR	CE1-CZ	-5.94	1.30	1.38
1	A	68	ASN	C-O	5.90	1.34	1.23
1	B	325	TYR	CE2-CZ	5.87	1.46	1.38
1	B	64	VAL	CA-CB	-5.87	1.42	1.54
1	C	269	GLU	CD-OE1	5.87	1.32	1.25
1	A	61	VAL	CA-C	5.87	1.68	1.52
1	A	521	GLU	CG-CD	5.83	1.60	1.51
1	A	824	SER	CB-OG	5.82	1.49	1.42
1	A	85	THR	N-CA	-5.79	1.34	1.46
1	A	77	TYR	CD2-CE2	5.79	1.48	1.39
1	A	721	LEU	CG-CD2	-5.79	1.30	1.51
1	C	839	GLU	CG-CD	5.78	1.60	1.51
1	B	597	TYR	CE2-CZ	5.78	1.46	1.38
1	C	819	TYR	CD2-CE2	5.77	1.48	1.39
1	A	688	ALA	N-CA	5.76	1.57	1.46
1	A	106	GLN	CD-OE1	5.74	1.36	1.24
1	C	168	ARG	CZ-NH1	5.73	1.40	1.33
1	B	640	GLU	CG-CD	5.73	1.60	1.51
1	A	815	ARG	CG-CD	5.72	1.66	1.51
1	A	615	PHE	CE2-CZ	5.71	1.48	1.37
1	A	94	PHE	CE1-CZ	5.70	1.48	1.37
1	A	108	GLN	CB-CG	5.69	1.68	1.52
1	C	88	VAL	CB-CG2	-5.68	1.41	1.52
1	A	48	SER	CA-CB	-5.64	1.44	1.52
1	A	813	SER	CA-CB	5.62	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	893	GLU	CG-CD	5.61	1.60	1.51
1	C	182	TYR	CD1-CE1	5.61	1.47	1.39
1	A	66	GLU	CA-C	5.61	1.67	1.52
1	A	61	VAL	CB-CG2	-5.61	1.41	1.52
1	A	93	THR	N-CA	5.59	1.57	1.46
1	B	124	GLN	CB-CG	5.57	1.67	1.52
1	C	182	TYR	CD2-CE2	5.57	1.47	1.39
1	C	162	MET	N-CA	-5.53	1.35	1.46
1	C	764	ASP	CB-CG	-5.52	1.40	1.51
1	A	686	ASP	CB-CG	5.50	1.63	1.51
1	C	127	VAL	CA-CB	5.50	1.66	1.54
1	C	131	LYS	C-O	5.47	1.33	1.23
1	C	267	LYS	CD-CE	5.46	1.65	1.51
1	C	43	VAL	CB-CG2	-5.46	1.41	1.52
1	C	688	ALA	CA-CB	-5.46	1.41	1.52
1	C	94	PHE	CD1-CE1	-5.46	1.28	1.39
1	B	46	SER	CA-CB	-5.41	1.44	1.52
1	C	96	SER	CA-C	-5.40	1.39	1.52
1	A	102	ILE	CA-CB	-5.39	1.42	1.54
1	A	768	VAL	CA-CB	-5.38	1.43	1.54
1	C	192	GLU	CB-CG	-5.38	1.42	1.52
1	A	71	GLY	C-O	-5.38	1.15	1.23
1	B	410	ILE	CA-CB	5.38	1.67	1.54
1	A	32	VAL	CB-CG2	-5.36	1.41	1.52
1	C	281	PHE	CE1-CZ	-5.35	1.27	1.37
1	C	53	ASP	CB-CG	5.34	1.62	1.51
1	B	1002	ALA	CA-CB	-5.32	1.41	1.52
1	B	124	GLN	CG-CD	5.32	1.63	1.51
1	C	801	PHE	CD1-CE1	-5.31	1.28	1.39
1	C	317	PHE	CE1-CZ	5.30	1.47	1.37
1	A	899	PHE	CE1-CZ	5.30	1.47	1.37
1	B	429	GLU	CB-CG	5.29	1.62	1.52
1	C	232	ALA	CA-CB	-5.29	1.41	1.52
1	C	244	GLU	CD-OE2	5.26	1.31	1.25
1	A	275	TYR	CG-CD2	-5.26	1.32	1.39
1	C	770	LYS	CB-CG	5.26	1.66	1.52
1	A	57	VAL	CA-CB	-5.25	1.43	1.54
1	C	291	ILE	CG1-CD1	5.25	1.86	1.50
1	C	140	VAL	CA-CB	-5.23	1.43	1.54
1	C	791	VAL	CB-CG2	-5.22	1.41	1.52
1	C	175	VAL	N-CA	-5.22	1.35	1.46
1	C	294	ALA	CA-CB	-5.21	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	90	ILE	C-O	5.20	1.33	1.23
1	C	128	SER	CA-CB	5.19	1.60	1.52
1	A	222	THR	CB-CG2	5.18	1.69	1.52
1	A	73	ASP	CG-OD1	5.17	1.37	1.25
1	A	108	GLN	CA-C	-5.17	1.39	1.52
1	A	597	TYR	CG-CD2	5.14	1.45	1.39
1	A	698	ALA	CA-CB	-5.12	1.41	1.52
1	C	194	ASN	CB-CG	5.12	1.62	1.51
1	A	112	GLN	CG-CD	5.12	1.62	1.51
1	A	645	GLU	CG-CD	5.12	1.59	1.51
1	B	178	PHE	CE1-CZ	5.10	1.47	1.37
1	A	69	MET	CB-CG	5.08	1.67	1.51
1	C	56	THR	CB-CG2	-5.08	1.35	1.52
1	C	612	VAL	CB-CG1	5.08	1.63	1.52
1	C	38	ILE	CA-CB	5.07	1.66	1.54
1	A	816	LEU	C-O	5.05	1.32	1.23
1	B	429	GLU	CG-CD	5.05	1.59	1.51
1	B	675	GLY	N-CA	5.04	1.53	1.46
1	A	68	ASN	CG-OD1	5.04	1.35	1.24
1	C	762	PHE	CD2-CE2	-5.03	1.29	1.39
1	C	98	THR	C-O	5.01	1.32	1.23
1	B	839	GLU	CG-CD	5.00	1.59	1.51

All (204) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	164	ASP	CB-CG-OD1	-15.00	104.80	118.30
1	C	126	GLY	N-CA-C	-11.22	85.04	113.10
1	C	686	ASP	CB-CG-OD2	10.96	128.16	118.30
1	A	717	ARG	NE-CZ-NH2	-10.44	115.08	120.30
1	C	686	ASP	CB-CG-OD1	-9.84	109.44	118.30
1	C	174	ASP	CB-CG-OD2	9.72	127.05	118.30
1	A	586	ARG	NE-CZ-NH1	9.72	125.16	120.30
1	A	185	ARG	NE-CZ-NH1	-9.64	115.48	120.30
1	A	729	ILE	CG1-CB-CG2	-9.57	90.34	111.40
1	B	350	LEU	CB-CG-CD1	-9.43	94.98	111.00
1	C	185	ARG	NE-CZ-NH2	-8.83	115.88	120.30
1	A	695	LEU	CB-CG-CD1	-8.78	96.07	111.00
1	C	767	ARG	NE-CZ-NH1	-8.58	116.01	120.30
1	C	69	MET	CG-SD-CE	-8.56	86.50	100.20
1	A	118	LEU	CB-CG-CD1	8.50	125.44	111.00
1	C	767	ARG	CD-NE-CZ	-8.44	111.78	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	239	ARG	NE-CZ-NH1	-8.42	116.09	120.30
1	B	30	LEU	CA-CB-CG	8.34	134.48	115.30
1	C	681	ASP	CB-CG-OD2	8.29	125.76	118.30
1	C	758	TYR	CB-CG-CD1	-8.26	116.05	121.00
1	A	55	LYS	CD-CE-NZ	8.26	130.69	111.70
1	A	867	ARG	NE-CZ-NH1	8.25	124.42	120.30
1	A	818	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	A	774	MET	CG-SD-CE	8.17	113.28	100.20
1	C	765	ARG	NE-CZ-NH2	8.16	124.38	120.30
1	A	960	LEU	CA-CB-CG	8.10	133.93	115.30
1	C	163	LYS	CD-CE-NZ	-8.03	93.22	111.70
1	B	989	LEU	CA-CB-CG	8.01	133.72	115.30
1	C	761	ASP	CB-CG-OD1	8.00	125.50	118.30
1	B	230	LEU	CA-CB-CG	7.92	133.51	115.30
1	C	761	ASP	CB-CG-OD2	-7.89	111.20	118.30
1	B	705	GLU	N-CA-C	-7.68	90.26	111.00
1	B	289	LEU	CA-CB-CG	7.63	132.86	115.30
1	B	868	LEU	CA-CB-CG	7.62	132.83	115.30
1	B	699	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	C	815	ARG	NE-CZ-NH2	-7.56	116.52	120.30
1	A	168	ARG	NE-CZ-NH1	7.55	124.08	120.30
1	A	130	GLU	OE1-CD-OE2	-7.38	114.45	123.30
1	B	468	ARG	NE-CZ-NH1	-7.36	116.62	120.30
1	B	166	ILE	CG1-CB-CG2	-7.33	95.27	111.40
1	C	425	LEU	CA-CB-CG	7.31	132.12	115.30
1	C	768	VAL	CG1-CB-CG2	-7.29	99.23	110.90
1	C	772	TYR	OH-CZ-CE2	-7.19	100.68	120.10
1	C	65	ILE	CG1-CB-CG2	-7.19	95.59	111.40
1	A	674	LEU	CA-CB-CG	7.15	131.74	115.30
1	C	161	ASN	C-N-CA	-7.12	103.89	121.70
1	C	164	ASP	CB-CG-OD2	7.12	124.70	118.30
1	B	383	LEU	CB-CG-CD2	7.11	123.08	111.00
1	A	49	TYR	CB-CG-CD2	7.06	125.24	121.00
1	B	4	PHE	N-CA-C	-6.97	92.18	111.00
1	A	88	VAL	CB-CA-C	-6.94	98.22	111.40
1	A	383	LEU	CB-CG-CD2	6.93	122.78	111.00
1	A	168	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	A	193	LEU	CA-CB-CG	6.83	131.01	115.30
1	C	960	LEU	CA-CB-CG	6.82	131.00	115.30
1	A	764	ASP	CB-CG-OD2	6.79	124.41	118.30
1	A	586	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	B	558	ARG	NE-CZ-NH1	6.76	123.68	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	772	TYR	CD1-CE1-CZ	-6.72	113.75	119.80
1	B	681	ASP	CB-CG-OD2	-6.71	112.26	118.30
1	A	363	ARG	NE-CZ-NH1	-6.62	116.99	120.30
1	A	785	ASP	CB-CG-OD1	6.60	124.24	118.30
1	A	185	ARG	NE-CZ-NH2	6.58	123.59	120.30
1	C	699	ARG	NE-CZ-NH1	-6.57	117.02	120.30
1	B	913	LEU	CB-CG-CD2	-6.57	99.84	111.00
1	B	263	ARG	NE-CZ-NH2	6.54	123.57	120.30
1	C	135	SER	N-CA-CB	-6.46	100.80	110.50
1	C	313	MET	CG-SD-CE	-6.46	89.86	100.20
1	C	321	LEU	CB-CG-CD2	-6.44	100.06	111.00
1	B	764	ASP	CB-CG-OD2	-6.42	112.52	118.30
1	C	732	ASP	CB-CG-OD2	-6.42	112.52	118.30
1	A	816	LEU	N-CA-C	-6.41	93.68	111.00
1	B	815	ARG	NE-CZ-NH2	-6.41	117.09	120.30
1	A	913	LEU	CA-CB-CG	6.40	130.01	115.30
1	B	117	LEU	CA-CB-CG	6.37	129.95	115.30
1	C	175	VAL	CB-CA-C	-6.35	99.33	111.40
1	C	816	LEU	CB-CG-CD1	6.33	121.76	111.00
1	C	160	ALA	N-CA-C	6.31	128.03	111.00
1	C	772	TYR	CB-CG-CD2	-6.25	117.25	121.00
1	A	383	LEU	CB-CG-CD1	-6.25	100.38	111.00
1	A	66	GLU	CG-CD-OE2	-6.20	105.90	118.30
1	C	555	LEU	CA-CB-CG	6.17	129.48	115.30
1	A	75	LEU	CA-CB-CG	6.13	129.41	115.30
1	B	239	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	A	10	ILE	CG1-CB-CG2	6.13	124.88	111.40
1	B	483	LEU	CB-CG-CD2	6.10	121.37	111.00
1	C	781	MET	CB-CG-SD	-6.10	94.10	112.40
1	B	292	LYS	CD-CE-NZ	-6.09	97.68	111.70
1	A	64	VAL	CB-CA-C	-6.08	99.86	111.40
1	A	812	GLY	N-CA-C	-6.07	97.92	113.10
1	A	164	ASP	CB-CG-OD1	-6.05	112.86	118.30
1	C	156	ASP	CB-CG-OD1	-6.03	112.88	118.30
1	C	73	ASP	CB-CG-OD1	-6.02	112.88	118.30
1	B	175	VAL	CB-CA-C	-5.96	100.07	111.40
1	C	765	ARG	NE-CZ-NH1	-5.92	117.34	120.30
1	C	785	ASP	CB-CG-OD2	5.92	123.63	118.30
1	C	78	MET	CG-SD-CE	5.89	109.62	100.20
1	C	131	LYS	CD-CE-NZ	-5.88	98.18	111.70
1	B	973	ARG	NE-CZ-NH2	5.87	123.24	120.30
1	C	88	VAL	CB-CA-C	-5.86	100.26	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	THR	CA-CB-CG2	-5.86	104.20	112.40
1	A	108	GLN	CB-CA-C	-5.84	98.72	110.40
1	C	717	ARG	NE-CZ-NH1	-5.83	117.39	120.30
1	A	51	GLY	N-CA-C	-5.82	98.55	113.10
1	C	418	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	A	48	SER	CB-CA-C	-5.81	99.06	110.10
1	A	301	ASP	CB-CG-OD2	-5.81	113.07	118.30
1	A	785	ASP	CB-CG-OD2	-5.76	113.11	118.30
1	A	980	LEU	CB-CG-CD2	-5.75	101.22	111.00
1	C	168	ARG	NE-CZ-NH1	-5.73	117.44	120.30
1	C	972	LEU	CA-CB-CG	5.70	128.41	115.30
1	C	156	ASP	CB-CG-OD2	5.68	123.42	118.30
1	B	952	LEU	CA-CB-CG	5.66	128.32	115.30
1	C	162	MET	CG-SD-CE	-5.66	91.15	100.20
1	A	828	LEU	CB-CG-CD1	-5.65	101.39	111.00
1	A	881	LEU	CB-CG-CD2	5.64	120.59	111.00
1	A	566	ASP	CB-CG-OD2	-5.61	113.26	118.30
1	C	111	LEU	CA-CB-CG	5.61	128.19	115.30
1	B	146	ASP	CB-CG-OD1	5.59	123.33	118.30
1	C	309	GLU	N-CA-C	-5.59	95.92	111.00
1	B	353	LEU	CA-CB-CG	5.57	128.12	115.30
1	B	825	MET	CG-SD-CE	5.56	109.09	100.20
1	B	771	VAL	CB-CA-C	-5.55	100.85	111.40
1	B	7	ASP	N-CA-C	-5.55	96.02	111.00
1	C	168	ARG	N-CA-C	5.54	125.97	111.00
1	C	159	ALA	C-N-CA	-5.54	107.86	121.70
1	A	307	ARG	NE-CZ-NH1	-5.54	117.53	120.30
1	C	165	ALA	C-N-CA	-5.52	107.89	121.70
1	A	118	LEU	CB-CA-C	5.52	120.69	110.20
1	A	113	LEU	CB-CG-CD1	5.50	120.35	111.00
1	A	578	LEU	CA-CB-CG	5.50	127.95	115.30
1	A	820	ASN	CB-CA-C	-5.50	99.41	110.40
1	A	366	LEU	CB-CG-CD1	5.49	120.33	111.00
1	B	113	LEU	CB-CG-CD1	5.49	120.33	111.00
1	C	751	GLY	N-CA-C	-5.47	99.42	113.10
1	A	45	ILE	CB-CG1-CD1	-5.47	98.60	113.90
1	C	170	SER	N-CA-CB	5.46	118.69	110.50
1	A	222	THR	N-CA-C	-5.45	96.29	111.00
1	C	249	ILE	CG1-CB-CG2	-5.42	99.48	111.40
1	A	817	GLU	OE1-CD-OE2	5.41	129.79	123.30
1	B	971	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	A	113	LEU	CB-CG-CD2	-5.41	101.81	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	264	ASP	CB-CG-OD2	-5.41	113.44	118.30
1	C	263	ARG	NE-CZ-NH1	-5.40	117.60	120.30
1	A	76	MET	CG-SD-CE	5.39	108.82	100.20
1	C	357	LEU	CA-CB-CG	5.36	127.64	115.30
1	B	764	ASP	CB-CG-OD1	5.36	123.12	118.30
1	B	768	VAL	CB-CA-C	-5.35	101.24	111.40
1	C	252	LYS	CD-CE-NZ	-5.35	99.40	111.70
1	B	230	LEU	CB-CG-CD1	5.34	120.08	111.00
1	B	686	ASP	CB-CG-OD2	5.34	123.11	118.30
1	B	980	LEU	CA-CB-CG	5.34	127.59	115.30
1	C	166	ILE	CB-CA-C	5.34	122.27	111.60
1	C	127	VAL	N-CA-C	-5.33	96.61	111.00
1	C	770	LYS	CA-CB-CG	5.32	125.10	113.40
1	A	688	ALA	N-CA-CB	5.31	117.53	110.10
1	B	546	LEU	CB-CG-CD2	5.31	120.02	111.00
1	B	695	LEU	CA-CB-CG	5.30	127.50	115.30
1	B	971	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	C	816	LEU	CA-CB-CG	-5.28	103.17	115.30
1	C	886	LEU	CB-CG-CD1	-5.27	102.04	111.00
1	C	44	THR	O-C-N	-5.26	114.28	122.70
1	A	973	ARG	NE-CZ-NH1	-5.26	117.67	120.30
1	C	135	SER	N-CA-C	-5.25	96.82	111.00
1	C	127	VAL	CG1-CB-CG2	-5.24	102.51	110.90
1	C	544	LEU	CA-CB-CG	5.24	127.35	115.30
1	C	772	TYR	CE1-CZ-OH	5.24	134.24	120.10
1	C	53	ASP	CB-CG-OD2	5.24	123.01	118.30
1	B	174	ASP	CB-CG-OD1	-5.23	113.59	118.30
1	C	755	GLY	N-CA-C	-5.23	100.03	113.10
1	C	177	LEU	CB-CG-CD2	5.21	119.86	111.00
1	B	774	MET	CG-SD-CE	-5.21	91.87	100.20
1	C	168	ARG	CG-CD-NE	-5.20	100.88	111.80
1	C	773	VAL	N-CA-C	-5.20	96.96	111.00
1	B	919	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	965	LEU	CA-CB-CG	5.18	127.22	115.30
1	C	66	GLU	OE1-CD-OE2	-5.17	117.09	123.30
1	C	558	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	B	650	ARG	NE-CZ-NH2	5.16	122.88	120.30
1	C	322	LYS	CD-CE-NZ	-5.14	99.88	111.70
1	C	32	VAL	CB-CA-C	-5.14	101.64	111.40
1	A	53	ASP	N-CA-C	-5.13	97.15	111.00
1	C	576	VAL	CB-CA-C	-5.12	101.68	111.40
1	B	235	ILE	CB-CA-C	-5.11	101.39	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	398	MET	CB-CG-SD	-5.11	97.08	112.40
1	A	70	ASN	N-CA-C	-5.11	97.22	111.00
1	C	56	THR	CA-CB-CG2	-5.09	105.27	112.40
1	A	653	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	C	624	THR	CB-CA-C	-5.08	97.87	111.60
1	A	67	GLN	CB-CG-CD	5.07	124.78	111.60
1	A	686	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	535	LEU	CA-CB-CG	5.07	126.95	115.30
1	C	241	THR	N-CA-C	5.06	124.66	111.00
1	B	137	LEU	CB-CG-CD2	-5.05	102.41	111.00
1	A	721	LEU	CB-CG-CD2	-5.04	102.43	111.00
1	B	75	LEU	CA-CB-CG	-5.04	103.72	115.30
1	B	231	ASN	CB-CA-C	-5.03	100.34	110.40
1	C	8	ARG	NE-CZ-NH2	5.03	122.81	120.30
1	A	994	GLY	N-CA-C	-5.03	100.54	113.10
1	B	76	MET	CG-SD-CE	5.02	108.23	100.20
1	A	118	LEU	CA-CB-CG	-5.02	103.76	115.30
1	A	107	VAL	N-CA-C	-5.02	97.45	111.00
1	A	739	LEU	CB-CG-CD1	-5.01	102.48	111.00
1	C	650	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	860	THR	Peptide
1	A	949	ALA	Peptide
1	B	706	ALA	Peptide
1	C	157	TYR	Sidechain
1	C	160	ALA	Mainchain
1	C	166	ILE	Peptide
1	C	751	GLY	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	7774	0	7931	1270	0
1	B	7774	0	7931	1386	0
1	C	7774	0	7931	1315	0
2	A	33	0	25	2	0
All	All	23355	0	23818	3853	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 82.

All (3853) 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:C:166:ILE:CA	1:C:166:ILE:CB	1.74	1.60
1:C:45:ILE:CA	1:C:45:ILE:CB	1.75	1.60
1:A:90:ILE:CG1	1:A:90:ILE:CD1	1.80	1.58
1:A:814:PRO:CG	1:A:814:PRO:CB	1.74	1.56
1:A:818:ARG:CD	1:A:818:ARG:CG	1.82	1.55
1:C:167:SER:N	1:C:167:SER:CA	1.68	1.53
1:C:291:ILE:CG1	1:C:291:ILE:CD1	1.86	1.52
1:B:247:GLY:HA2	1:B:268:ILE:CD1	1.52	1.38
1:B:247:GLY:CA	1:B:268:ILE:HD13	1.58	1.33
1:B:946:VAL:HG22	1:B:1026:PHE:CZ	1.64	1.30
1:C:162:MET:HB3	1:C:313:MET:CE	1.65	1.26
1:A:61:VAL:O	1:A:65:ILE:HG22	1.28	1.25
1:A:108:GLN:HG3	1:B:112:GLN:OE1	1.12	1.25
1:C:162:MET:CB	1:C:313:MET:HE3	1.66	1.24
1:B:49:TYR:CE1	1:B:122:VAL:HG13	1.72	1.22
1:A:713:LEU:O	1:A:714:THR:HG23	1.39	1.21
1:C:162:MET:CG	1:C:313:MET:HE3	1.69	1.21
1:A:61:VAL:O	1:A:65:ILE:CG2	1.87	1.21
1:C:115:MET:HE2	1:C:118:LEU:CD2	1.71	1.20
1:B:712:MET:HB3	1:B:713:LEU:HD12	1.23	1.19
1:A:971:ARG:O	1:A:974:PRO:HD2	1.38	1.19
1:B:904:VAL:HG13	1:B:907:LEU:CD1	1.74	1.18
1:C:115:MET:CE	1:C:118:LEU:CD2	2.23	1.17
1:C:162:MET:HG2	1:C:313:MET:CE	1.75	1.16
1:B:990:VAL:HG13	1:B:1005:THR:OG1	1.42	1.16
1:C:115:MET:CE	1:C:118:LEU:HD22	1.73	1.16
1:A:742:SER:OG	1:A:745:ASP:HB2	1.43	1.16
1:B:1:MET:HB2	1:B:2:PRO:HD2	1.17	1.16
1:A:54:ALA:HB1	1:A:816:LEU:HG	1.28	1.15
1:A:979:SER:OG	1:A:1015:THR:HG21	1.45	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:ILE:HD13	1:C:306:ILE:HD13	1.24	1.15
1:A:60:THR:CG2	1:A:119:PRO:HG3	1.77	1.14
1:A:108:GLN:CG	1:B:112:GLN:OE1	1.95	1.14
1:A:729:ILE:HG22	1:A:730:ASP:H	1.02	1.14
1:A:359:LEU:CD1	1:A:417:GLU:HG2	1.78	1.13
1:A:276:ASP:HB3	1:C:222:THR:HG23	1.29	1.13
1:B:42:ALA:HB2	1:B:93:THR:HG22	1.29	1.13
1:B:904:VAL:CG1	1:B:907:LEU:HD12	1.79	1.13
1:C:350:LEU:HD13	1:C:984:LEU:HD22	1.16	1.13
1:A:919:ARG:CG	1:A:920:GLY:H	1.62	1.12
1:A:965:LEU:O	1:A:969:ARG:HG3	1.49	1.12
1:B:291:ILE:HG21	1:B:306:ILE:HD11	1.24	1.12
1:A:531:VAL:HA	1:A:534:ILE:HD11	1.13	1.12
1:A:790:TYR:CE1	1:A:800:PRO:HG3	1.84	1.12
1:B:242:SER:HB2	1:B:245:GLU:OE2	1.50	1.12
1:B:144:ASN:HB2	1:B:320:GLY:O	1.48	1.11
1:C:699:ARG:HG2	1:C:699:ARG:HH11	1.11	1.11
1:B:972:LEU:HD13	1:B:976:LEU:HD23	1.28	1.11
1:C:427:PRO:CA	1:C:498:LYS:HE3	1.80	1.11
1:A:359:LEU:HD12	1:A:417:GLU:HG2	1.18	1.11
1:B:523:SER:HA	1:B:526:HIS:HD2	1.00	1.11
1:B:987:MET:HE3	1:B:987:MET:HA	1.13	1.11
1:C:463:THR:HG22	1:C:464:GLY:H	1.15	1.11
1:A:344:LEU:HD23	1:A:402:ILE:HD13	1.22	1.11
1:A:790:TYR:HE1	1:A:800:PRO:HG3	1.02	1.11
1:A:919:ARG:HG3	1:A:920:GLY:H	1.01	1.11
1:C:431:THR:HG21	1:C:494:ALA:HB2	1.30	1.11
1:A:945:ILE:HG12	1:A:971:ARG:HG2	1.23	1.11
1:C:1025:PHE:O	1:C:1029:VAL:HG23	1.50	1.11
1:B:225:VAL:HG22	1:C:781:MET:CE	1.79	1.10
1:B:225:VAL:HG22	1:C:781:MET:HE3	1.34	1.10
1:A:713:LEU:HB3	1:A:832:ALA:HA	1.28	1.09
1:A:560:PRO:HB2	1:A:922:THR:HG22	1.30	1.09
1:C:410:ILE:HG22	1:C:411:VAL:H	1.11	1.09
1:B:1022:VAL:O	1:B:1024:VAL:O	1.71	1.09
1:A:649:MET:HB3	1:A:653:ARG:HH21	1.11	1.09
1:B:542:LEU:HD11	1:B:1028:VAL:HG11	1.36	1.08
1:B:226:LYS:HA	1:B:226:LYS:HE3	1.27	1.08
1:C:162:MET:CB	1:C:313:MET:CE	2.28	1.08
1:A:713:LEU:HD22	1:A:714:THR:H	0.96	1.08
1:A:253:VAL:HG23	1:A:258:SER:O	1.50	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:GLN:HG3	1:B:105:VAL:N	1.67	1.08
1:A:959:GLY:HA3	1:A:962:GLU:HB2	1.34	1.08
1:B:523:SER:HA	1:B:526:HIS:CD2	1.89	1.07
1:B:49:TYR:CD2	1:B:122:VAL:HA	1.89	1.07
1:B:911:GLY:HA3	1:B:1013:THR:HG21	1.32	1.07
1:A:1024:VAL:O	1:A:1026:PHE:N	1.86	1.07
1:A:713:LEU:HD22	1:A:714:THR:N	1.70	1.07
1:C:729:ILE:HD11	1:C:786:ILE:HD13	1.33	1.07
1:C:712:MET:HB2	1:C:835:LYS:HG3	1.37	1.07
1:A:435:MET:HG2	1:A:490:PRO:HB3	1.37	1.06
1:B:894:SER:HB3	1:B:897:ILE:HG12	1.37	1.06
1:C:162:MET:CG	1:C:313:MET:CE	2.31	1.06
1:C:162:MET:HB3	1:C:313:MET:HE1	1.32	1.06
1:C:513:PHE:HA	1:C:516:PHE:HB3	1.31	1.06
1:C:365:THR:O	1:C:368:PRO:HD2	1.54	1.06
1:C:911:GLY:HA3	1:C:1013:THR:HG21	1.32	1.06
1:A:536:ARG:HG2	1:A:537:SER:H	1.17	1.05
1:B:742:SER:HB3	1:B:745:ASP:OD2	1.56	1.05
1:B:960:LEU:HD12	1:B:961:ILE:HG13	1.32	1.05
1:A:214:VAL:HG12	1:A:215:ALA:H	1.06	1.05
1:C:953:MET:HE1	1:C:1030:ARG:HH22	1.19	1.05
1:B:441:ALA:HB2	1:B:947:GLU:HG2	1.34	1.05
1:B:6:ILE:HD12	1:B:490:PRO:HB2	1.38	1.05
1:C:143:ILE:HD11	1:C:286:ALA:HB2	1.39	1.05
1:C:699:ARG:CG	1:C:699:ARG:HH11	1.68	1.05
1:C:350:LEU:CD1	1:C:984:LEU:HD22	1.86	1.05
1:C:901:VAL:O	1:C:904:VAL:HG23	1.57	1.05
1:B:49:TYR:CD1	1:B:122:VAL:HG13	1.92	1.04
1:C:713:LEU:HG	1:C:832:ALA:O	1.56	1.04
1:B:14:VAL:HG11	1:C:890:ALA:HB2	1.37	1.04
1:C:372:VAL:HG13	1:C:373:PRO:HD3	1.40	1.03
1:A:406:VAL:HG12	1:A:407:ASP:H	1.23	1.03
1:B:463:THR:HG21	1:B:869:SER:HB2	1.40	1.03
1:C:463:THR:HG22	1:C:464:GLY:N	1.71	1.03
1:C:922:THR:HG22	1:C:923:ASN:H	1.21	1.03
1:A:443:VAL:HG12	1:A:444:GLY:H	1.23	1.03
1:C:1022:VAL:HA	1:C:1025:PHE:HD2	1.22	1.03
1:A:30:LEU:HD21	1:A:384:ALA:HB2	1.41	1.02
1:C:778:LYS:HD2	1:C:779:TYR:HE2	1.20	1.02
1:B:1018:ALA:O	1:B:1022:VAL:HG22	1.59	1.02
1:B:544:LEU:HA	1:B:547:ILE:HD12	1.40	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:950:LYS:NZ	1:C:1030:ARG:HD3	1.71	1.02
1:B:171:GLY:HA3	1:B:302:THR:HG22	1.41	1.02
1:B:644:VAL:HG23	1:B:645:GLU:H	1.20	1.02
1:C:674:LEU:HD11	1:C:862:MET:HA	1.40	1.02
1:C:841:MET:O	1:C:845:GLU:HG3	1.59	1.02
1:C:576:VAL:HG12	1:C:663:VAL:HG22	1.37	1.02
1:A:905:VAL:O	1:A:909:VAL:HG23	1.59	1.02
1:C:847:LEU:HA	1:C:850:LYS:HD3	1.37	1.02
1:B:406:VAL:O	1:B:408:ASP:O	1.77	1.02
1:A:406:VAL:CG1	1:A:407:ASP:N	2.22	1.01
1:B:399:VAL:O	1:B:402:ILE:HG22	1.58	1.01
1:A:919:ARG:HG3	1:A:920:GLY:N	1.73	1.01
1:B:431:THR:HG21	1:B:493:CYS:CB	1.91	1.01
1:A:713:LEU:CD2	1:A:714:THR:H	1.72	1.01
1:C:427:PRO:HA	1:C:498:LYS:HE3	1.04	1.01
1:C:432:ARG:HG3	1:C:432:ARG:NH1	1.50	1.01
1:B:431:THR:HG21	1:B:493:CYS:HB2	1.42	1.01
1:A:690:LEU:CD1	1:A:854:GLY:HA3	1.89	1.01
1:B:456:MET:HG3	1:B:467:TYR:HB3	1.43	1.01
1:C:190:PRO:HD3	1:C:779:TYR:HD1	1.25	1.01
1:B:226:LYS:CE	1:B:226:LYS:HA	1.90	1.00
1:B:729:ILE:HG13	1:B:730:ASP:H	1.24	1.00
1:A:690:LEU:HD11	1:A:854:GLY:HA3	1.00	1.00
1:C:350:LEU:HD13	1:C:984:LEU:CD2	1.91	1.00
1:A:5:PHE:CD1	1:A:12:ALA:HB2	1.97	1.00
1:A:200:PRO:HG2	1:A:749:THR:HA	1.44	1.00
1:A:911:GLY:HA3	1:A:1013:THR:HG21	1.41	1.00
1:A:372:VAL:HG22	1:A:405:LEU:CD2	1.92	1.00
1:B:171:GLY:HA3	1:B:302:THR:CG2	1.90	1.00
1:B:792:ARG:HA	1:B:798:MET:HE2	1.44	1.00
1:B:986:VAL:O	1:B:990:VAL:HG23	1.60	1.00
1:C:314:GLU:HB2	1:C:315:PRO:HD3	1.42	1.00
1:C:432:ARG:CG	1:C:432:ARG:HH11	1.74	1.00
1:B:843:LEU:HD23	1:B:847:LEU:HD21	1.39	0.99
1:A:968:VAL:CG2	1:A:1023:PRO:HB3	1.92	0.99
1:B:987:MET:CE	1:B:987:MET:HA	1.90	0.99
1:C:220:GLY:HA3	1:C:231:ASN:ND2	1.75	0.99
1:B:175:VAL:HG12	1:B:175:VAL:O	1.63	0.99
1:B:859:TRP:HB3	1:B:863:SER:HB3	1.42	0.99
1:A:400:LEU:HD13	1:A:1003:VAL:HG13	1.42	0.99
1:B:962:GLU:O	1:B:966:ASP:HB2	1.62	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:GLN:HG3	1:A:249:ILE:HG23	1.44	0.99
1:A:451:ALA:O	1:A:452:VAL:HG22	1.62	0.99
1:B:346:GLU:OE1	1:B:988:PRO:HB3	1.63	0.99
1:B:160:ALA:HB1	1:B:767:ARG:CD	1.92	0.99
1:B:892:TYR:CB	1:B:897:ILE:HD11	1.92	0.99
1:A:214:VAL:HG12	1:A:215:ALA:N	1.75	0.98
1:A:690:LEU:HD11	1:A:854:GLY:CA	1.92	0.98
1:C:427:PRO:HA	1:C:498:LYS:CE	1.94	0.98
1:B:692:HIS:O	1:B:693:GLU:HG3	1.63	0.98
1:A:139:VAL:CG1	1:A:327:TYR:HB3	1.94	0.98
1:A:472:ILE:H	1:A:472:ILE:HD12	1.28	0.98
1:C:317:PHE:HB2	1:C:318:PRO:HD2	1.43	0.98
1:C:950:LYS:HZ3	1:C:1030:ARG:HD3	1.20	0.98
1:B:291:ILE:HG21	1:B:306:ILE:CD1	1.93	0.97
1:B:410:ILE:HG23	1:B:414:GLU:OE2	1.62	0.97
1:B:847:LEU:H	1:B:847:LEU:HD23	1.28	0.97
1:C:410:ILE:HG22	1:C:411:VAL:N	1.70	0.97
1:C:536:ARG:HH11	1:C:961:ILE:HD11	1.25	0.97
1:A:815:ARG:HG2	1:A:815:ARG:HH11	1.27	0.97
1:B:549:VAL:HG22	1:B:550:VAL:H	1.24	0.97
1:A:729:ILE:HG22	1:A:730:ASP:N	1.77	0.97
1:C:4:PHE:HB3	1:C:8:ARG:HH22	1.30	0.97
1:B:574:THR:HG23	1:B:665:ALA:HB2	1.46	0.97
1:C:432:ARG:HG3	1:C:432:ARG:HH11	0.82	0.97
1:C:1:MET:HB2	1:C:2:PRO:HD2	1.44	0.96
1:A:45:ILE:HG22	1:A:45:ILE:O	1.62	0.96
1:B:49:TYR:CG	1:B:122:VAL:HA	1.98	0.96
1:B:904:VAL:HG13	1:B:907:LEU:HD12	1.32	0.96
1:C:415:ASN:ND2	1:C:434:SER:HB2	1.79	0.96
1:A:344:LEU:CD2	1:A:402:ILE:HD13	1.94	0.96
1:A:108:GLN:HG3	1:B:112:GLN:CD	1.86	0.96
1:A:298:ASN:C	1:A:298:ASN:HD22	1.62	0.96
1:B:704:ALA:O	1:B:705:GLU:HG3	1.63	0.96
1:B:445:ILE:HG23	1:B:940:LYS:HG3	1.46	0.96
1:C:352:PHE:HA	1:C:369:THR:HG21	1.46	0.96
1:C:166:ILE:HA	1:C:166:ILE:CB	1.94	0.95
1:B:94:PHE:HB2	1:B:98:THR:HG21	1.48	0.95
1:A:400:LEU:CD1	1:A:1003:VAL:HG13	1.95	0.95
1:A:578:LEU:CD2	1:A:587:THR:HG23	1.95	0.95
1:B:831:ALA:CB	1:B:840:ALA:HB2	1.97	0.95
1:A:578:LEU:HD23	1:A:587:THR:HG23	1.48	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:ARG:HB3	1:A:263:ARG:HH21	1.29	0.95
1:A:32:VAL:HG22	1:A:390:ILE:HB	1.49	0.95
1:C:414:GLU:OE1	1:C:977:MET:HE3	1.67	0.95
1:A:968:VAL:HG21	1:A:1023:PRO:HB3	1.49	0.94
1:B:623:ASN:C	1:B:623:ASN:HD22	1.66	0.94
1:C:190:PRO:HG3	1:C:789:TRP:CZ2	2.03	0.94
1:B:613:ASN:HD22	1:B:614:GLY:N	1.65	0.94
1:A:926:TYR:CE1	1:A:999:ALA:HB2	2.02	0.94
1:C:578:LEU:HD22	1:C:661:ALA:CB	1.97	0.94
1:C:778:LYS:HD2	1:C:779:TYR:CE2	2.02	0.94
1:C:950:LYS:H	1:C:953:MET:HE2	1.33	0.94
1:B:804:PHE:HD1	1:B:804:PHE:O	1.50	0.94
1:B:674:LEU:HD13	1:B:860:THR:HG21	1.50	0.94
1:C:163:LYS:O	1:C:166:ILE:N	1.98	0.94
1:B:713:LEU:H	1:B:713:LEU:HD12	1.32	0.94
1:A:447:MET:HB3	1:A:887:CYS:SG	2.08	0.94
1:A:405:LEU:HD22	1:A:406:VAL:N	1.83	0.93
1:B:921:LEU:CD2	1:B:1005:THR:HG22	1.99	0.93
1:C:162:MET:HG2	1:C:313:MET:HE2	1.47	0.93
1:A:328:ASP:OD1	1:A:330:THR:HB	1.69	0.93
1:A:513:PHE:HD1	1:A:517:ASN:ND2	1.65	0.93
1:B:578:LEU:HD12	1:B:586:ARG:NH2	1.84	0.93
1:B:972:LEU:HD13	1:B:976:LEU:CD2	1.99	0.93
1:C:953:MET:HE1	1:C:1030:ARG:NH2	1.83	0.93
1:C:214:VAL:HG12	1:C:215:ALA:N	1.83	0.93
1:C:418:ARG:O	1:C:420:MET:N	2.00	0.93
1:B:517:ASN:O	1:B:521:GLU:HG3	1.68	0.93
1:B:743:ILE:H	1:B:743:ILE:HD12	1.34	0.93
1:B:537:SER:HB2	1:B:540:ARG:HG2	1.48	0.93
1:B:771:VAL:O	1:B:771:VAL:HG12	1.69	0.93
1:A:418:ARG:HG2	1:A:970:MET:HE3	1.51	0.92
1:B:1022:VAL:HG23	1:B:1023:PRO:HD3	1.50	0.92
1:C:115:MET:HE2	1:C:118:LEU:HD22	0.93	0.92
1:A:63:GLN:O	1:A:66:GLU:N	2.02	0.92
1:B:158:VAL:HA	1:B:162:MET:HG2	1.49	0.92
1:B:525:HIS:HA	1:B:528:THR:HG22	1.48	0.92
1:A:649:MET:HB3	1:A:653:ARG:NH2	1.85	0.92
1:B:219:LEU:HD12	1:B:234:ILE:HG12	1.51	0.92
1:C:513:PHE:HA	1:C:516:PHE:CB	1.97	0.92
1:A:632:LYS:O	1:A:637:ARG:HD3	1.68	0.92
1:A:552:MET:HE1	1:A:906:PRO:HA	1.49	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:PRO:CD	1:C:779:TYR:HD1	1.83	0.92
1:A:531:VAL:HA	1:A:534:ILE:CD1	2.00	0.92
1:B:946:VAL:HG22	1:B:1026:PHE:CE1	2.05	0.91
1:C:277:ILE:HD11	1:C:620:ARG:NH2	1.83	0.91
1:B:713:LEU:CD1	1:B:843:LEU:HD13	2.00	0.91
1:A:105:VAL:O	1:A:108:GLN:HB3	1.70	0.91
1:A:340:VAL:HG13	1:A:399:VAL:HG21	1.51	0.91
1:C:1017:LEU:O	1:C:1017:LEU:HD23	1.69	0.91
1:C:291:ILE:CD1	1:C:306:ILE:HD13	2.00	0.91
1:A:713:LEU:CB	1:A:832:ALA:HA	2.00	0.91
1:B:200:PRO:HD2	1:B:749:THR:HG22	1.52	0.91
1:A:251:LEU:HD11	1:A:262:LEU:HA	1.52	0.91
1:B:405:LEU:HD12	1:B:406:VAL:N	1.85	0.91
1:A:584:GLN:H	1:A:622:GLN:HB3	1.36	0.91
1:C:162:MET:HG2	1:C:313:MET:HE3	1.40	0.91
1:C:167:SER:OG	1:C:168:ARG:N	2.04	0.91
1:C:143:ILE:CD1	1:C:286:ALA:HB2	2.00	0.91
1:C:291:ILE:HD13	1:C:306:ILE:CD1	2.01	0.91
1:C:643:LYS:HG2	1:C:645:GLU:H	1.36	0.91
1:C:980:LEU:HG	1:C:980:LEU:O	1.71	0.91
1:A:314:GLU:N	1:A:315:PRO:CD	2.34	0.90
1:A:166:ILE:HD13	1:A:166:ILE:N	1.84	0.90
1:A:590:VAL:O	1:A:594:VAL:HG23	1.71	0.90
1:C:702:LEU:HB2	1:C:851:LEU:HD21	1.52	0.90
1:C:847:LEU:H	1:C:847:LEU:HD22	1.36	0.90
1:A:987:MET:N	1:A:988:PRO:HD2	1.86	0.90
1:A:513:PHE:HD1	1:A:517:ASN:HD21	1.14	0.90
1:A:568:ASP:HB3	1:A:634:TRP:HZ3	1.34	0.90
1:A:223:PRO:HD3	1:B:275:TYR:CD2	2.07	0.90
1:C:423:GLU:HB3	1:C:426:PRO:CG	2.02	0.90
1:A:60:THR:HG21	1:A:119:PRO:HG3	1.52	0.90
1:B:280:GLU:HB2	1:B:284:GLN:O	1.72	0.90
1:B:225:VAL:H	1:C:781:MET:HE2	1.37	0.89
1:A:1018:ALA:O	1:A:1022:VAL:HG13	1.72	0.89
1:C:144:ASN:ND2	1:C:149:MET:H	1.70	0.89
1:C:922:THR:HG22	1:C:923:ASN:N	1.88	0.89
1:B:1:MET:CB	1:B:2:PRO:HD2	1.99	0.89
1:B:517:ASN:HB3	1:B:521:GLU:OE1	1.71	0.89
1:A:372:VAL:HG22	1:A:405:LEU:HD21	1.54	0.89
1:A:989:LEU:HG	1:A:993:THR:HG23	1.55	0.89
1:A:138:MET:HE3	1:A:306:ILE:HD13	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:VAL:HG12	1:A:407:ASP:N	1.83	0.89
1:A:355:MET:HE3	1:A:410:ILE:HG12	1.55	0.89
1:A:515:TRP:HA	1:A:519:MET:SD	2.13	0.89
1:B:68:ASN:O	1:B:70:ASN:ND2	2.05	0.89
1:A:813:SER:HB3	1:A:816:LEU:HD21	1.53	0.89
1:B:674:LEU:HD13	1:B:860:THR:CG2	2.02	0.88
1:C:1:MET:CE	1:C:439:GLN:HE22	1.84	0.88
1:A:454:VAL:O	1:A:456:MET:O	1.90	0.88
1:A:713:LEU:O	1:A:714:THR:CG2	2.21	0.88
1:A:418:ARG:HD3	1:A:970:MET:HG3	1.55	0.88
1:C:417:GLU:HA	1:C:417:GLU:OE2	1.73	0.88
1:A:139:VAL:HG13	1:A:327:TYR:HB3	1.56	0.88
1:A:909:VAL:HG12	1:A:913:LEU:CD2	2.03	0.88
1:A:1018:ALA:HB1	1:A:1022:VAL:CG1	2.03	0.88
1:A:750:LEU:HD11	1:C:216:ALA:HB2	1.53	0.88
1:C:344:LEU:HD22	1:C:402:ILE:HD11	1.53	0.88
1:C:463:THR:O	1:C:465:ALA:N	2.07	0.88
1:B:1:MET:HB2	1:B:2:PRO:CD	2.02	0.88
1:B:892:TYR:HB2	1:B:897:ILE:HD11	1.56	0.88
1:B:104:GLN:CG	1:B:105:VAL:N	2.37	0.88
1:B:115:MET:CE	1:B:115:MET:HA	2.03	0.88
1:C:588:GLN:HG2	1:C:613:ASN:HD22	1.38	0.88
1:C:785:ASP:C	1:C:787:GLY:H	1.72	0.88
1:C:911:GLY:CA	1:C:1013:THR:HG21	2.04	0.88
1:A:536:ARG:HG2	1:A:537:SER:N	1.90	0.87
1:C:60:THR:HG22	1:C:61:VAL:HG23	1.55	0.87
1:B:235:ILE:HD13	1:B:235:ILE:H	1.39	0.87
1:C:115:MET:HE1	1:C:118:LEU:CD2	2.02	0.87
1:B:160:ALA:HB1	1:B:767:ARG:HD3	1.54	0.87
1:C:713:LEU:HD11	1:C:834:GLY:HA3	1.56	0.87
1:A:531:VAL:CA	1:A:534:ILE:HD11	2.03	0.87
1:B:360:GLN:O	1:B:361:ASN:HB2	1.74	0.87
1:B:876:LEU:HD13	1:B:932:LEU:HD11	1.55	0.87
1:C:951:ASP:C	1:C:953:MET:H	1.76	0.87
1:C:699:ARG:HG2	1:C:699:ARG:NH1	1.89	0.87
1:A:780:ARG:HG2	1:A:780:ARG:HH11	1.38	0.86
1:C:58:GLN:CD	1:C:82:SER:OG	2.13	0.86
1:A:571:VAL:HG12	1:A:630:SER:HA	1.56	0.86
1:B:291:ILE:CG2	1:B:306:ILE:HD11	2.05	0.86
1:A:819:TYR:H	1:A:824:SER:HB3	1.38	0.86
1:A:528:THR:HG21	1:A:969:ARG:HE	1.41	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:729:ILE:HG13	1:B:730:ASP:N	1.90	0.86
1:B:549:VAL:HG22	1:B:550:VAL:N	1.89	0.86
1:B:418:ARG:NE	1:B:970:MET:SD	2.48	0.86
1:B:70:ASN:H	1:B:70:ASN:HD22	1.24	0.86
1:B:280:GLU:CB	1:B:284:GLN:O	2.24	0.86
1:B:1005:THR:O	1:B:1005:THR:HG22	1.74	0.86
1:A:228:GLN:HG2	1:B:781:MET:HG2	1.57	0.86
1:B:945:ILE:CD1	1:B:1026:PHE:HE2	1.88	0.86
1:A:9:PRO:HB3	1:A:491:ALA:HB1	1.57	0.85
1:B:404:LEU:HD13	1:B:449:LEU:HD13	1.56	0.85
1:B:714:THR:HG21	1:B:833:PRO:HD2	1.57	0.85
1:C:190:PRO:HG3	1:C:789:TRP:CH2	2.10	0.85
1:A:782:LEU:O	1:A:784:ASP:O	1.93	0.85
1:C:190:PRO:CD	1:C:779:TYR:CD1	2.58	0.85
1:C:463:THR:HA	1:C:466:ILE:HD13	1.55	0.85
1:C:713:LEU:HD11	1:C:835:LYS:H	1.41	0.85
1:C:1022:VAL:HA	1:C:1025:PHE:CD2	2.10	0.85
1:A:190:PRO:HG3	1:A:789:TRP:CE2	2.12	0.85
1:C:222:THR:HB	1:C:223:PRO:HD3	1.57	0.85
1:B:644:VAL:HG23	1:B:645:GLU:N	1.92	0.85
1:C:141:GLY:HA3	1:C:324:VAL:HG22	1.57	0.85
1:B:136:PHE:HE1	1:B:617:PHE:CZ	1.95	0.85
1:A:729:ILE:CG2	1:A:730:ASP:H	1.87	0.85
1:A:90:ILE:O	1:A:90:ILE:HG22	1.72	0.85
1:B:542:LEU:HD11	1:B:1028:VAL:CG1	2.07	0.85
1:B:115:MET:HA	1:B:115:MET:HE3	1.58	0.85
1:B:966:ASP:O	1:B:970:MET:HB2	1.77	0.85
1:A:298:ASN:ND2	1:A:300:LEU:H	1.74	0.84
1:B:356:TYR:C	1:B:358:PHE:H	1.81	0.84
1:B:707:ALA:O	1:B:708:LYS:HB3	1.76	0.84
1:C:872:GLN:HB2	1:C:875:SER:HB3	1.56	0.84
1:A:428:LYS:HG3	1:A:429:GLU:H	1.42	0.84
1:A:971:ARG:C	1:A:974:PRO:HD2	1.97	0.84
1:B:561:SER:HB2	1:B:838:GLY:HA3	1.57	0.84
1:C:393:LEU:HD13	1:C:466:ILE:HG23	1.58	0.84
1:A:355:MET:CE	1:A:977:MET:HE1	2.06	0.84
1:B:545:TYR:OH	1:B:906:PRO:HG3	1.78	0.84
1:C:92:LEU:HD12	1:C:92:LEU:N	1.91	0.84
1:C:592:ASN:O	1:C:593:GLU:HB3	1.76	0.84
1:C:713:LEU:HD11	1:C:835:LYS:N	1.92	0.84
1:A:950:LYS:HA	1:A:953:MET:HB3	1.57	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:540:ARG:HE	1:C:541:TYR:HE1	1.25	0.84
1:B:372:VAL:HG22	1:B:373:PRO:HD3	1.59	0.84
1:B:525:HIS:HA	1:B:528:THR:CG2	2.08	0.84
1:C:950:LYS:NZ	1:C:1030:ARG:CD	2.39	0.84
1:A:214:VAL:CG1	1:A:215:ALA:H	1.90	0.84
1:A:719:ASN:HD22	1:A:719:ASN:C	1.75	0.84
1:C:847:LEU:O	1:C:850:LYS:HG2	1.77	0.84
1:A:493:CYS:O	1:A:497:LEU:HB2	1.78	0.84
1:B:416:VAL:HG21	1:B:431:THR:HA	1.59	0.83
1:A:1024:VAL:HG12	1:A:1028:VAL:HG23	1.58	0.83
1:B:185:ARG:HG3	1:B:185:ARG:HH11	1.41	0.83
1:B:697:GLN:O	1:B:699:ARG:O	1.95	0.83
1:B:763:ILE:HD11	1:C:59:ASP:HB3	1.60	0.83
1:C:578:LEU:HB3	1:C:579:PRO:HD2	1.59	0.83
1:A:472:ILE:N	1:A:472:ILE:HD12	1.92	0.83
1:B:904:VAL:HG13	1:B:907:LEU:HD11	1.58	0.83
1:C:713:LEU:CD1	1:C:834:GLY:HA3	2.09	0.83
1:A:44:THR:CG2	1:A:89:GLN:HG3	2.09	0.83
1:A:951:ASP:O	1:A:955:LYS:HB2	1.78	0.83
1:B:900:SER:HA	1:B:903:LEU:HD12	1.59	0.83
1:A:443:VAL:HG12	1:A:444:GLY:N	1.93	0.83
1:B:804:PHE:CD1	1:B:804:PHE:O	2.31	0.83
1:C:644:VAL:CG1	1:C:667:ASN:HB2	2.08	0.83
1:A:210:GLN:HG3	1:A:249:ILE:CG2	2.07	0.83
1:A:243:THR:HG22	1:A:268:ILE:HG22	1.58	0.83
1:B:528:THR:O	1:B:531:VAL:HG12	1.78	0.83
1:C:951:ASP:O	1:C:953:MET:N	2.12	0.83
1:B:946:VAL:CG2	1:B:1026:PHE:CZ	2.57	0.83
1:B:584:GLN:HB2	1:B:622:GLN:HE21	1.44	0.83
1:C:44:THR:HG22	1:C:91:THR:HB	1.60	0.83
1:B:659:LYS:NZ	1:B:659:LYS:HA	1.93	0.83
1:B:713:LEU:HD13	1:B:843:LEU:HD13	1.59	0.83
1:C:919:ARG:HB3	1:C:921:LEU:HD23	1.61	0.83
1:B:356:TYR:O	1:B:358:PHE:N	2.12	0.83
1:A:513:PHE:CD1	1:A:517:ASN:ND2	2.47	0.82
1:A:836:SER:OG	1:A:839:GLU:HG2	1.78	0.82
1:A:205:THR:O	1:A:205:THR:HG22	1.76	0.82
1:B:184:MET:HG3	1:B:184:MET:O	1.77	0.82
1:B:219:LEU:CD2	1:C:783:PRO:HG3	2.10	0.82
1:B:81:ASN:O	1:B:81:ASN:ND2	2.11	0.82
1:A:90:ILE:CD1	1:A:90:ILE:CB	2.57	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:ALA:O	1:C:30:LEU:HG	1.79	0.82
1:C:713:LEU:HB2	1:C:832:ALA:HB3	1.62	0.82
1:A:255:GLN:H	1:A:255:GLN:CD	1.81	0.82
1:B:261:LEU:HD13	1:B:261:LEU:H	1.43	0.82
1:C:915:ALA:HA	1:C:918:PHE:HB3	1.61	0.82
1:A:451:ALA:O	1:A:452:VAL:CG2	2.27	0.82
1:B:361:ASN:O	1:B:365:THR:HB	1.80	0.82
1:B:790:TYR:HE1	1:B:800:PRO:HB3	1.45	0.82
1:C:214:VAL:HG12	1:C:215:ALA:H	1.43	0.82
1:C:457:ALA:HB1	1:C:468:ARG:HA	1.60	0.82
1:B:408:ASP:O	1:B:410:ILE:N	2.13	0.82
1:A:740:GLY:O	1:A:793:ALA:HB1	1.79	0.82
1:A:154:ILE:O	1:A:158:VAL:HG23	1.80	0.82
1:B:894:SER:CB	1:B:897:ILE:HG12	2.08	0.82
1:C:578:LEU:HD22	1:C:661:ALA:HB2	1.62	0.82
1:C:184:MET:HE3	1:C:184:MET:HA	1.62	0.82
1:A:896:SER:O	1:A:899:PHE:HB2	1.79	0.81
1:B:851:LEU:N	1:B:852:PRO:CD	2.43	0.81
1:B:412:VAL:HG13	1:B:435:MET:HE1	1.63	0.81
1:B:904:VAL:HG12	1:B:907:LEU:HD12	1.62	0.81
1:B:555:LEU:HD22	1:B:555:LEU:H	1.45	0.81
1:B:568:ASP:OD1	1:B:644:VAL:HG22	1.81	0.81
1:A:90:ILE:HG21	1:A:90:ILE:CD1	2.10	0.81
1:B:129:VAL:HG12	1:B:129:VAL:O	1.80	0.81
1:B:157:TYR:HA	1:B:161:ASN:ND2	1.94	0.81
1:C:167:SER:H	1:C:175:VAL:HG21	1.44	0.81
1:A:418:ARG:HH12	1:A:973:ARG:HB3	1.45	0.81
1:A:425:LEU:HD12	1:A:425:LEU:H	1.45	0.81
1:A:649:MET:CB	1:A:653:ARG:HH21	1.93	0.81
1:B:767:ARG:HD3	1:B:769:LYS:HE2	1.62	0.81
1:C:190:PRO:HD2	1:C:779:TYR:CD1	2.15	0.81
1:C:252:LYS:O	1:C:260:VAL:HG12	1.80	0.81
1:C:592:ASN:O	1:C:593:GLU:CB	2.28	0.81
1:A:495:THR:O	1:A:496:MET:HB2	1.79	0.81
1:A:843:LEU:O	1:A:846:GLN:N	2.13	0.81
1:C:131:LYS:O	1:C:295:THR:HG22	1.79	0.81
1:C:244:GLU:HA	1:C:263:ARG:HH22	1.46	0.81
1:C:361:ASN:HB2	1:C:364:ALA:HB3	1.62	0.81
1:A:568:ASP:OD2	1:A:637:ARG:NH1	2.13	0.81
1:B:150:THR:H	1:B:153:ASP:HB3	1.44	0.81
1:C:685:ILE:HG12	1:C:687:GLN:OE1	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:VAL:O	1:A:544:LEU:HB3	1.80	0.81
1:C:790:TYR:CD1	1:C:800:PRO:HB3	2.15	0.81
1:A:419:VAL:O	1:A:424:GLY:HA3	1.81	0.81
1:A:585:GLU:OE2	1:C:227:GLY:HA2	1.81	0.81
1:C:953:MET:CE	1:C:1030:ARG:HH22	1.93	0.81
1:C:54:ALA:HB2	1:C:84:SER:HB2	1.63	0.80
1:A:456:MET:O	1:A:457:ALA:HB3	1.79	0.80
1:B:775:SER:HB3	1:B:780:ARG:HG3	1.61	0.80
1:C:644:VAL:HG11	1:C:667:ASN:HB2	1.63	0.80
1:C:728:LYS:HG3	1:C:729:ILE:N	1.95	0.80
1:B:739:LEU:O	1:B:793:ALA:HB1	1.81	0.80
1:C:531:VAL:O	1:C:533:GLY:N	2.15	0.80
1:C:682:PHE:CE2	1:C:702:LEU:HD11	2.16	0.80
1:C:897:ILE:HG12	1:C:950:LYS:HZ2	1.45	0.80
1:B:178:PHE:HA	1:B:277:ILE:HG21	1.63	0.80
1:B:930:GLY:O	1:B:934:THR:HG23	1.80	0.80
1:C:45:ILE:CA	1:C:45:ILE:CG2	2.57	0.80
1:C:927:PHE:O	1:C:931:LEU:HB2	1.82	0.80
1:A:60:THR:HG23	1:A:119:PRO:HG3	1.62	0.80
1:A:688:ALA:O	1:A:689:GLY:C	2.18	0.80
1:B:223:PRO:HG2	1:B:223:PRO:O	1.82	0.80
1:B:642:ASN:H	1:B:650:ARG:HH12	1.29	0.80
1:B:880:SER:O	1:B:884:VAL:HG23	1.81	0.80
1:C:536:ARG:NH1	1:C:961:ILE:HD11	1.95	0.80
1:B:225:VAL:HG22	1:C:781:MET:HE2	1.62	0.80
1:B:773:VAL:O	1:B:773:VAL:HG13	1.78	0.80
1:C:420:MET:SD	1:C:498:LYS:CE	2.70	0.80
1:A:534:ILE:HB	1:A:540:ARG:NH1	1.96	0.80
1:A:991:ILE:HD13	1:A:1008:MET:HG3	1.61	0.80
1:A:1023:PRO:O	1:A:1027:VAL:HG23	1.82	0.80
1:A:909:VAL:HG12	1:A:913:LEU:HD21	1.61	0.80
1:C:530:SER:O	1:C:534:ILE:HG23	1.81	0.80
1:B:42:ALA:CB	1:B:93:THR:HG22	2.10	0.80
1:C:713:LEU:H	1:C:713:LEU:HD13	1.47	0.80
1:A:10:ILE:HD11	1:B:895:TRP:HB2	1.64	0.79
1:C:721:LEU:CD1	1:C:815:ARG:O	2.30	0.79
1:C:721:LEU:HD12	1:C:815:ARG:O	1.82	0.79
1:C:144:ASN:HD21	1:C:149:MET:H	1.30	0.79
1:C:31:PRO:O	1:C:389:SER:HB2	1.82	0.79
1:C:925:VAL:O	1:C:927:PHE:N	2.15	0.79
1:A:389:SER:O	1:A:394:THR:HG21	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:901:VAL:O	1:A:904:VAL:HG23	1.81	0.79
1:C:901:VAL:HG11	1:C:943:ILE:HD13	1.64	0.79
1:A:713:LEU:HB3	1:A:832:ALA:CA	2.10	0.79
1:B:407:ASP:O	1:B:408:ASP:O	2.01	0.79
1:C:694:LYS:O	1:C:697:GLN:HB2	1.81	0.79
1:B:1022:VAL:HG23	1:B:1023:PRO:CD	2.13	0.79
1:B:560:PRO:HB2	1:B:836:SER:HB3	1.63	0.79
1:B:987:MET:HE3	1:B:987:MET:CA	2.05	0.79
1:C:420:MET:SD	1:C:498:LYS:CD	2.70	0.79
1:C:682:PHE:HE2	1:C:702:LEU:HD11	1.44	0.79
1:C:844:MET:HA	1:C:847:LEU:HD21	1.62	0.79
1:A:919:ARG:CG	1:A:920:GLY:N	2.33	0.79
1:A:355:MET:HA	1:A:977:MET:HE3	1.65	0.79
1:B:973:ARG:CG	1:B:974:PRO:HD3	2.12	0.79
1:A:731:ILE:HD12	1:A:731:ILE:N	1.96	0.79
1:C:1016:VAL:O	1:C:1019:ILE:HG22	1.82	0.79
1:A:961:ILE:O	1:A:965:LEU:HD23	1.83	0.79
1:A:340:VAL:HG13	1:A:399:VAL:CG2	2.13	0.79
1:A:355:MET:HE2	1:A:977:MET:HE1	1.64	0.79
1:B:6:ILE:CD1	1:B:490:PRO:HB2	2.11	0.79
1:B:278:ILE:HD11	1:B:584:GLN:NE2	1.97	0.79
1:B:699:ARG:HG2	1:B:700:ASN:N	1.99	0.78
1:A:324:VAL:HG12	1:A:325:TYR:H	1.46	0.78
1:A:61:VAL:O	1:A:65:ILE:HG23	1.82	0.78
1:A:90:ILE:CG2	1:A:90:ILE:CD1	2.60	0.78
1:C:910:ILE:HG23	1:C:911:GLY:N	1.97	0.78
1:B:644:VAL:O	1:B:648:THR:OG1	2.00	0.78
1:B:973:ARG:HG2	1:B:974:PRO:CD	2.12	0.78
1:C:497:LEU:CD1	1:C:498:LYS:H	1.95	0.78
1:C:519:MET:O	1:C:523:SER:OG	2.01	0.78
1:A:987:MET:N	1:A:988:PRO:CD	2.46	0.78
1:B:419:VAL:O	1:B:426:PRO:HG3	1.83	0.78
1:B:573:MET:CE	1:B:626:ILE:HD12	2.14	0.78
1:C:939:ALA:O	1:C:943:ILE:HG12	1.83	0.78
1:C:962:GLU:O	1:C:965:LEU:HB3	1.83	0.78
1:A:168:ARG:HG3	1:A:168:ARG:O	1.82	0.78
1:C:60:THR:CG2	1:C:61:VAL:HG23	2.14	0.78
1:A:124:GLN:HG2	1:A:758:TYR:CE2	2.19	0.78
1:B:946:VAL:CG2	1:B:1026:PHE:CE1	2.65	0.78
1:C:188:MET:HA	1:C:266:ALA:HB1	1.66	0.78
1:C:164:ASP:O	1:C:167:SER:OG	2.02	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:887:CYS:O	1:C:890:ALA:HB3	1.84	0.78
1:A:105:VAL:O	1:A:109:ASN:N	2.13	0.78
1:A:376:LEU:O	1:A:377:LEU:C	2.17	0.78
1:A:583:THR:HG22	1:A:585:GLU:H	1.47	0.78
1:B:714:THR:HG23	1:B:830:GLN:NE2	1.99	0.78
1:C:983:ILE:HG23	1:C:1008:MET:HG3	1.65	0.78
1:A:911:GLY:HA3	1:A:1013:THR:CG2	2.14	0.77
1:B:49:TYR:CE1	1:B:122:VAL:CG1	2.62	0.77
1:C:442:LEU:O	1:C:445:ILE:HG13	1.83	0.77
1:A:277:ILE:O	1:A:277:ILE:HG23	1.82	0.77
1:A:815:ARG:HG2	1:A:815:ARG:NH1	1.99	0.77
1:A:298:ASN:C	1:A:298:ASN:ND2	2.38	0.77
1:A:355:MET:CE	1:A:410:ILE:HG12	2.13	0.77
1:B:213:GLN:HE21	1:B:239:ARG:HD2	1.48	0.77
1:B:601:LYS:O	1:B:603:LYS:N	2.17	0.77
1:B:760:ASN:HD22	1:B:761:ASP:H	1.31	0.77
1:B:843:LEU:CD2	1:B:847:LEU:HD21	2.12	0.77
1:C:888:LEU:HB3	1:C:898:PRO:HB3	1.64	0.77
1:A:30:LEU:CD2	1:A:384:ALA:HB2	2.14	0.77
1:A:596:HIS:O	1:A:598:TYR:N	2.17	0.77
1:A:638:PRO:HG2	1:A:639:GLY:H	1.49	0.77
1:B:705:GLU:O	1:B:707:ALA:N	2.17	0.77
1:B:712:MET:CB	1:B:713:LEU:HD12	2.10	0.77
1:C:418:ARG:C	1:C:420:MET:H	1.84	0.77
1:C:729:ILE:HD11	1:C:786:ILE:CD1	2.14	0.77
1:A:124:GLN:HG2	1:A:758:TYR:HE2	1.49	0.77
1:A:801:PHE:HD2	1:A:805:SER:OG	1.67	0.77
1:A:979:SER:HG	1:A:1015:THR:HG21	1.44	0.77
1:B:974:PRO:O	1:B:978:THR:HB	1.84	0.77
1:C:459:PHE:HD2	1:C:459:PHE:H	1.30	0.77
1:A:263:ARG:HB3	1:A:263:ARG:NH2	1.98	0.77
1:A:60:THR:HG22	1:A:61:VAL:HG23	1.64	0.77
1:A:69:MET:C	1:A:70:ASN:HD22	1.87	0.77
1:A:983:ILE:HD12	1:A:983:ILE:C	2.05	0.77
1:B:346:GLU:OE1	1:B:988:PRO:CB	2.32	0.77
1:B:987:MET:O	1:B:990:VAL:HB	1.83	0.77
1:A:634:TRP:CE3	1:A:995:ALA:HB1	2.20	0.77
1:B:213:GLN:HG3	1:C:56:THR:HG23	1.67	0.77
1:B:261:LEU:HD13	1:B:261:LEU:N	1.98	0.77
1:C:213:GLN:NE2	1:C:238:THR:HA	2.00	0.77
1:C:44:THR:HG22	1:C:91:THR:CB	2.15	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:393:LEU:CD1	1:C:466:ILE:HG23	2.15	0.77
1:C:560:PRO:O	1:C:922:THR:HG23	1.84	0.77
1:B:833:PRO:HG2	1:B:834:GLY:H	1.50	0.77
1:C:346:GLU:OE1	1:C:988:PRO:HG3	1.84	0.77
1:A:1009:GLY:O	1:A:1011:MET:N	2.17	0.76
1:A:888:LEU:HD11	1:A:943:ILE:HG12	1.67	0.76
1:B:919:ARG:HG3	1:B:1005:THR:CG2	2.14	0.76
1:B:520:PHE:HA	1:B:523:SER:OG	1.85	0.76
1:B:572:PHE:HB2	1:B:666:PHE:O	1.85	0.76
1:B:713:LEU:H	1:B:713:LEU:CD1	1.99	0.76
1:B:416:VAL:CG2	1:B:431:THR:HA	2.15	0.76
1:C:728:LYS:HG3	1:C:729:ILE:H	1.50	0.76
1:B:709:HIS:N	1:B:710:PRO:HD3	1.99	0.76
1:B:431:THR:CG2	1:B:493:CYS:CB	2.64	0.76
1:B:701:GLN:HA	1:B:704:ALA:HB3	1.66	0.76
1:B:894:SER:HB3	1:B:897:ILE:CG1	2.15	0.76
1:B:944:LEU:O	1:B:971:ARG:HD2	1.84	0.76
1:C:692:HIS:HE1	1:C:721:LEU:HD21	1.50	0.76
1:C:911:GLY:HA3	1:C:1013:THR:CG2	2.13	0.76
1:A:400:LEU:HD13	1:A:1003:VAL:CG1	2.14	0.76
1:A:274:ASN:ND2	1:A:276:ASP:H	1.83	0.76
1:A:926:TYR:CE1	1:A:999:ALA:CB	2.69	0.76
1:B:626:ILE:HD11	1:B:628:PHE:CZ	2.20	0.76
1:B:714:THR:HG23	1:B:830:GLN:HE22	1.50	0.76
1:C:684:LEU:HG	1:C:684:LEU:O	1.85	0.76
1:A:552:MET:HE1	1:A:906:PRO:CA	2.15	0.76
1:B:945:ILE:HD11	1:B:1026:PHE:CE2	2.20	0.76
1:B:407:ASP:C	1:B:408:ASP:O	2.21	0.76
1:B:835:LYS:HD2	1:B:839:GLU:OE1	1.86	0.76
1:C:673:GLU:O	1:C:674:LEU:HB3	1.86	0.76
1:A:400:LEU:HG	1:A:929:VAL:HG12	1.67	0.76
1:B:941:ASN:ND2	1:B:1015:THR:HA	2.00	0.76
1:C:463:THR:CG2	1:C:464:GLY:N	2.42	0.76
1:C:497:LEU:HD13	1:C:498:LYS:H	1.50	0.76
1:B:708:LYS:HG2	1:B:708:LYS:O	1.85	0.76
1:C:1024:VAL:O	1:C:1028:VAL:HG23	1.86	0.76
1:C:584:GLN:HB2	1:C:622:GLN:HE21	1.51	0.76
1:C:7:ASP:O	1:C:9:PRO:HD3	1.87	0.76
1:A:314:GLU:N	1:A:315:PRO:HD3	2.01	0.75
1:A:466:ILE:O	1:A:469:GLN:HB2	1.86	0.75
1:A:801:PHE:CD2	1:A:805:SER:OG	2.39	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:775:SER:HB3	1:B:780:ARG:CD	2.16	0.75
1:C:542:LEU:HD23	1:C:542:LEU:O	1.85	0.75
1:A:986:VAL:C	1:A:988:PRO:HD2	2.05	0.75
1:B:172:VAL:HG12	1:B:172:VAL:O	1.84	0.75
1:C:847:LEU:N	1:C:847:LEU:HD22	2.01	0.75
1:A:543:VAL:O	1:A:544:LEU:CB	2.35	0.75
1:B:3:ASN:H	1:B:6:ILE:HG12	1.50	0.75
1:C:457:ALA:CB	1:C:468:ARG:HA	2.15	0.75
1:A:227:GLY:HA2	1:B:585:GLU:OE1	1.86	0.75
1:A:443:VAL:O	1:A:445:ILE:N	2.19	0.75
1:B:1031:ARG:N	1:B:1034:SER:OG	2.20	0.75
1:B:973:ARG:CG	1:B:974:PRO:CD	2.64	0.75
1:A:106:GLN:O	1:A:110:LYS:HB2	1.86	0.75
1:A:54:ALA:O	1:A:58:GLN:N	2.20	0.75
1:B:852:PRO:HA	1:B:855:VAL:HB	1.69	0.75
1:C:415:ASN:HD21	1:C:434:SER:HB2	1.51	0.75
1:A:117:LEU:HD11	1:C:124:GLN:O	1.85	0.75
1:A:90:ILE:HD13	1:A:90:ILE:HG21	1.67	0.75
1:B:137:LEU:HD11	1:B:299:ALA:HB1	1.68	0.75
1:B:485:ALA:HA	1:B:489:THR:HB	1.67	0.75
1:B:659:LYS:HD3	1:B:660:ASP:N	2.01	0.75
1:B:190:PRO:HG2	1:B:779:TYR:CG	2.21	0.75
1:B:350:LEU:HB3	1:B:984:LEU:HD12	1.67	0.75
1:C:114:ALA:O	1:C:115:MET:C	2.22	0.75
1:C:410:ILE:CG2	1:C:411:VAL:H	1.91	0.75
1:C:979:SER:O	1:C:983:ILE:HG13	1.86	0.75
1:B:411:VAL:O	1:B:438:ILE:HG12	1.86	0.75
1:B:674:LEU:CD1	1:B:860:THR:HG21	2.17	0.75
1:B:792:ARG:CA	1:B:798:MET:HE2	2.16	0.75
1:C:758:TYR:CD2	1:C:770:LYS:HE2	2.22	0.75
1:A:1024:VAL:HG12	1:A:1028:VAL:CG2	2.17	0.74
1:A:425:LEU:HD12	1:A:425:LEU:N	2.02	0.74
1:A:713:LEU:HG	1:A:833:PRO:HD3	1.68	0.74
1:A:935:ILE:O	1:A:935:ILE:HG22	1.86	0.74
1:B:602:GLU:OE2	1:B:650:ARG:HD2	1.86	0.74
1:B:531:VAL:HG13	1:B:965:LEU:HD21	1.69	0.74
1:C:727:PHE:CZ	1:C:783:PRO:HB3	2.22	0.74
1:A:43:VAL:O	1:A:43:VAL:HG12	1.85	0.74
1:A:65:ILE:O	1:A:68:ASN:HB2	1.87	0.74
1:A:795:ASP:OD1	1:A:797:GLN:HG2	1.87	0.74
1:B:262:LEU:HD22	1:B:266:ALA:HB3	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:GLN:HA	1:B:442:LEU:HD12	1.69	0.74
1:B:740:GLY:O	1:B:794:ALA:N	2.20	0.74
1:B:988:PRO:O	1:B:989:LEU:HB3	1.85	0.74
1:C:44:THR:O	1:C:45:ILE:C	2.21	0.74
1:A:539:GLY:HA2	1:A:542:LEU:HB2	1.69	0.74
1:A:559:LEU:HD12	1:A:560:PRO:HD2	1.67	0.74
1:A:719:ASN:HB2	1:A:828:LEU:HD23	1.69	0.74
1:B:11:PHE:O	1:B:14:VAL:HB	1.87	0.74
1:B:431:THR:CG2	1:B:493:CYS:HB2	2.16	0.74
1:A:949:ALA:HB1	1:A:1026:PHE:CE2	2.23	0.74
1:B:850:LYS:C	1:B:852:PRO:HD3	2.07	0.74
1:C:345:VAL:O	1:C:348:ILE:HG12	1.86	0.74
1:C:431:THR:O	1:C:435:MET:HG2	1.86	0.74
1:C:58:GLN:OE1	1:C:82:SER:OG	2.04	0.74
1:C:713:LEU:CG	1:C:832:ALA:O	2.34	0.74
1:A:719:ASN:ND2	1:A:719:ASN:C	2.36	0.74
1:B:699:ARG:O	1:B:700:ASN:HB2	1.85	0.74
1:B:704:ALA:O	1:B:705:GLU:CG	2.35	0.74
1:C:115:MET:HE1	1:C:118:LEU:HD23	1.68	0.74
1:C:758:TYR:H	1:C:758:TYR:HD1	1.33	0.74
1:C:910:ILE:CG2	1:C:911:GLY:N	2.50	0.74
1:B:986:VAL:O	1:B:990:VAL:CG2	2.36	0.74
1:C:247:GLY:HA3	1:C:263:ARG:NE	2.01	0.74
1:C:43:VAL:HA	1:C:130:GLU:O	1.88	0.74
1:C:785:ASP:O	1:C:787:GLY:N	2.20	0.74
1:B:24:GLY:HA2	1:B:27:ILE:HG23	1.70	0.74
1:C:420:MET:SD	1:C:498:LYS:HD3	2.28	0.74
1:C:785:ASP:C	1:C:787:GLY:N	2.37	0.74
1:A:115:MET:O	1:A:117:LEU:N	2.21	0.74
1:B:1021:PHE:HB3	1:B:1025:PHE:HE1	1.52	0.74
1:B:109:ASN:HD22	1:B:112:GLN:NE2	1.86	0.74
1:C:176:GLN:NE2	1:C:620:ARG:HH11	1.85	0.74
1:C:159:ALA:HB3	1:C:181:GLN:HG3	1.70	0.74
1:C:190:PRO:O	1:C:191:ASN:C	2.26	0.74
1:C:444:GLY:O	1:C:448:VAL:HG23	1.88	0.74
1:C:946:VAL:HG12	1:C:946:VAL:O	1.87	0.74
1:A:113:LEU:HD21	1:C:128:SER:HA	1.68	0.73
1:A:518:ARG:CZ	1:A:518:ARG:HB3	2.16	0.73
1:A:596:HIS:C	1:A:598:TYR:H	1.91	0.73
1:A:186:ILE:HB	1:A:773:VAL:HG23	1.69	0.73
1:B:847:LEU:HD23	1:B:847:LEU:N	2.01	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:657:GLN:O	1:C:659:LYS:N	2.21	0.73
1:B:644:VAL:CG2	1:B:645:GLU:H	2.00	0.73
1:C:16:ALA:O	1:C:20:MET:HG3	1.87	0.73
1:C:143:ILE:HG23	1:C:284:GLN:NE2	2.03	0.73
1:A:189:ASN:HD21	1:A:192:GLU:HB2	1.54	0.73
1:B:26:ALA:O	1:B:30:LEU:HB2	1.87	0.73
1:B:435:MET:HE2	1:B:435:MET:HA	1.68	0.73
1:B:905:VAL:HG23	1:B:935:ILE:HG12	1.68	0.73
1:C:743:ILE:HD12	1:C:743:ILE:H	1.53	0.73
1:A:225:VAL:HG12	1:A:226:LYS:O	1.88	0.73
1:A:56:THR:O	1:A:56:THR:HG22	1.88	0.73
1:C:159:ALA:O	1:C:161:ASN:N	2.21	0.73
1:C:337:ILE:HD13	1:C:338:HIS:N	2.04	0.73
1:C:380:PHE:CE1	1:C:398:MET:SD	2.82	0.73
1:C:60:THR:HG23	1:C:60:THR:O	1.88	0.73
1:A:61:VAL:HG13	1:A:118:LEU:HD13	1.67	0.73
1:A:594:VAL:HA	1:A:655:PHE:CE2	2.23	0.73
1:A:104:GLN:NE2	1:B:109:ASN:HB3	2.04	0.73
1:C:907:LEU:O	1:C:910:ILE:HG22	1.88	0.73
1:A:731:ILE:CD1	1:A:731:ILE:N	2.52	0.73
1:B:104:GLN:CG	1:B:105:VAL:H	2.02	0.73
1:B:188:MET:HE3	1:B:203:VAL:HG11	1.68	0.73
1:B:431:THR:HG21	1:B:493:CYS:HB3	1.69	0.73
1:B:48:SER:OG	1:B:48:SER:O	2.06	0.73
1:C:190:PRO:O	1:C:192:GLU:N	2.22	0.73
1:C:45:ILE:C	1:C:45:ILE:CB	2.55	0.73
1:A:28:LEU:N	1:A:28:LEU:CD1	2.51	0.73
1:A:1:MET:N	1:A:2:PRO:HD2	2.04	0.73
1:A:605:ASN:OD1	1:A:637:ARG:HG2	1.89	0.73
1:B:327:TYR:CD2	1:B:628:PHE:HB3	2.23	0.73
1:B:773:VAL:CG1	1:B:773:VAL:O	2.36	0.73
1:C:314:GLU:HB2	1:C:315:PRO:CD	2.17	0.73
1:C:402:ILE:O	1:C:406:VAL:HG23	1.88	0.73
1:C:713:LEU:HD11	1:C:834:GLY:CA	2.18	0.73
1:C:686:ASP:CG	1:C:690:LEU:HB2	2.09	0.73
1:B:945:ILE:CD1	1:B:1026:PHE:CE2	2.71	0.73
1:B:590:VAL:O	1:B:594:VAL:HG23	1.88	0.73
1:B:778:LYS:HZ2	1:B:778:LYS:H	1.34	0.73
1:C:753:ALA:HB1	1:C:775:SER:HB2	1.69	0.73
1:A:1013:THR:O	1:A:1017:LEU:HB3	1.89	0.73
1:A:191:ASN:O	1:A:193:LEU:N	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:ASN:HB3	1:A:434:SER:OG	1.89	0.73
1:B:979:SER:O	1:B:1011:MET:HE3	1.88	0.73
1:B:345:VAL:HA	1:B:348:ILE:HD12	1.70	0.73
1:C:1035:ARG:HA	1:C:1035:ARG:HE	1.54	0.73
1:C:247:GLY:HA2	1:C:268:ILE:HD13	1.71	0.73
1:A:5:PHE:CE1	1:A:12:ALA:HB2	2.24	0.72
1:A:58:GLN:NE2	1:A:816:LEU:CD1	2.52	0.72
1:B:493:CYS:O	1:B:494:ALA:HB3	1.89	0.72
1:C:190:PRO:HD3	1:C:779:TYR:CD1	2.16	0.72
1:C:1:MET:CB	1:C:2:PRO:HD2	2.19	0.72
1:C:219:LEU:HD12	1:C:232:ALA:HB3	1.69	0.72
1:B:70:ASN:N	1:B:70:ASN:HD22	1.86	0.72
1:C:185:ARG:HB2	1:C:269:GLU:O	1.88	0.72
1:C:3:ASN:HD21	1:C:432:ARG:HD3	1.53	0.72
1:C:4:PHE:CB	1:C:8:ARG:HH22	2.02	0.72
1:C:713:LEU:O	1:C:831:ALA:HA	1.88	0.72
1:C:562:SER:O	1:C:924:ASP:HA	1.89	0.72
1:A:729:ILE:O	1:A:730:ASP:HB2	1.89	0.72
1:A:790:TYR:HE1	1:A:800:PRO:CG	1.92	0.72
1:A:885:PHE:HD2	1:A:886:LEU:HD12	1.53	0.72
1:B:355:MET:CE	1:B:369:THR:HG23	2.19	0.72
1:B:356:TYR:O	1:B:359:LEU:N	2.22	0.72
1:C:210:GLN:O	1:C:240:LEU:HD21	1.89	0.72
1:C:626:ILE:HD13	1:C:627:ALA:H	1.54	0.72
1:B:412:VAL:HG13	1:B:435:MET:CE	2.19	0.72
1:B:962:GLU:O	1:B:966:ASP:CB	2.37	0.72
1:B:538:THR:O	1:B:540:ARG:N	2.21	0.72
1:C:873:ALA:O	1:C:876:LEU:N	2.20	0.72
1:C:560:PRO:O	1:C:922:THR:CG2	2.38	0.72
1:A:298:ASN:HB3	1:A:301:ASP:OD1	1.88	0.72
1:A:324:VAL:HG12	1:A:325:TYR:N	2.04	0.72
1:B:210:GLN:HG3	1:B:249:ILE:HG23	1.72	0.72
1:B:613:ASN:ND2	1:B:614:GLY:N	2.37	0.72
1:C:568:ASP:OD2	1:C:644:VAL:HG23	1.89	0.72
1:A:1018:ALA:HB1	1:A:1022:VAL:HG11	1.69	0.72
1:A:1029:VAL:HG12	1:A:1030:ARG:H	1.55	0.72
1:B:20:MET:O	1:B:23:GLY:O	2.08	0.72
1:B:262:LEU:HB3	1:B:268:ILE:HD11	1.70	0.72
1:A:223:PRO:HD3	1:B:275:TYR:HB2	1.72	0.72
1:B:468:ARG:O	1:B:469:GLN:C	2.25	0.72
1:B:659:LYS:HA	1:B:659:LYS:HZ3	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:545:TYR:OH	1:C:1021:PHE:CB	2.38	0.72
1:C:781:MET:O	1:C:782:LEU:HD23	1.90	0.72
1:C:959:GLY:H	1:C:962:GLU:HB2	1.55	0.72
1:B:57:VAL:HG23	1:B:58:GLN:H	1.55	0.71
1:B:714:THR:HG21	1:B:833:PRO:CD	2.18	0.71
1:B:972:LEU:CD1	1:B:976:LEU:CD2	2.68	0.71
1:A:182:TYR:HB3	1:A:270:LEU:HD12	1.70	0.71
1:A:64:VAL:O	1:A:65:ILE:C	2.28	0.71
1:B:990:VAL:CG1	1:B:1005:THR:OG1	2.30	0.71
1:C:545:TYR:OH	1:C:1021:PHE:CG	2.42	0.71
1:C:899:PHE:HD1	1:C:899:PHE:N	1.87	0.71
1:A:95:GLU:O	1:A:98:THR:HG23	1.91	0.71
1:B:360:GLN:O	1:B:361:ASN:CB	2.38	0.71
1:B:418:ARG:HE	1:B:970:MET:CE	2.04	0.71
1:C:310:LEU:O	1:C:313:MET:N	2.22	0.71
1:C:450:SER:O	1:C:451:ALA:CB	2.38	0.71
1:A:269:GLU:HG3	1:A:270:LEU:O	1.90	0.71
1:B:30:LEU:HD23	1:B:390:ILE:HG13	1.73	0.71
1:B:418:ARG:HE	1:B:970:MET:HE3	1.55	0.71
1:C:449:LEU:HB2	1:C:478:MET:HE3	1.72	0.71
1:A:1024:VAL:HG12	1:A:1025:PHE:H	1.54	0.71
1:A:522:LYS:H	1:A:522:LYS:HE2	1.56	0.71
1:B:158:VAL:HA	1:B:162:MET:CG	2.19	0.71
1:B:235:ILE:CD1	1:B:235:ILE:N	2.53	0.71
1:B:517:ASN:C	1:B:521:GLU:HG3	2.11	0.71
1:B:952:LEU:HB3	1:B:963:ALA:HB1	1.71	0.71
1:B:987:MET:HE2	1:B:987:MET:O	1.90	0.71
1:C:568:ASP:OD1	1:C:634:TRP:NE1	2.24	0.71
1:A:344:LEU:CD2	1:A:402:ILE:CD1	2.68	0.71
1:A:44:THR:HG22	1:A:89:GLN:HG3	1.72	0.71
1:A:780:ARG:HG2	1:A:780:ARG:NH1	2.06	0.71
1:A:552:MET:SD	1:A:909:VAL:HG11	2.30	0.71
1:B:100:ALA:O	1:B:103:ALA:HB3	1.91	0.71
1:B:365:THR:O	1:B:368:PRO:HD2	1.91	0.71
1:B:45:ILE:HD13	1:B:65:ILE:CG2	2.20	0.71
1:C:214:VAL:CG1	1:C:215:ALA:N	2.53	0.71
1:C:997:SER:O	1:C:998:GLY:C	2.27	0.71
1:A:60:THR:CG2	1:A:119:PRO:CG	2.64	0.71
1:B:538:THR:N	1:B:540:ARG:HH21	1.88	0.71
1:B:851:LEU:N	1:B:852:PRO:HD3	2.04	0.71
1:C:786:ILE:O	1:C:786:ILE:HG22	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:GLN:O	1:A:108:GLN:HB2	1.90	0.71
1:A:476:SER:O	1:A:480:LEU:HB2	1.91	0.71
1:B:775:SER:HB3	1:B:780:ARG:CG	2.19	0.71
1:C:868:LEU:O	1:C:869:SER:HB3	1.89	0.71
1:A:62:THR:O	1:A:63:GLN:O	2.07	0.71
1:B:139:VAL:O	1:B:139:VAL:HG12	1.90	0.71
1:B:804:PHE:O	1:B:805:SER:HB3	1.91	0.71
1:C:229:GLN:O	1:C:230:LEU:HB3	1.91	0.71
1:B:921:LEU:HD23	1:B:1005:THR:O	1.91	0.70
1:B:1012:VAL:CG2	1:B:1013:THR:H	2.03	0.70
1:B:226:LYS:CA	1:B:226:LYS:CE	2.69	0.70
1:B:687:GLN:NE2	1:B:856:GLY:HA3	2.06	0.70
1:C:423:GLU:HB3	1:C:426:PRO:HG2	1.72	0.70
1:A:359:LEU:HD12	1:A:417:GLU:CG	2.10	0.70
1:B:831:ALA:HB2	1:B:840:ALA:HB2	1.72	0.70
1:B:45:ILE:HD12	1:B:90:ILE:HB	1.71	0.70
1:C:344:LEU:CD2	1:C:402:ILE:HD11	2.20	0.70
1:A:991:ILE:CD1	1:A:1008:MET:HG3	2.21	0.70
1:A:274:ASN:HD21	1:A:276:ASP:H	1.36	0.70
1:A:30:LEU:HD21	1:A:384:ALA:CB	2.20	0.70
1:B:892:TYR:HB3	1:B:897:ILE:HD11	1.72	0.70
1:C:450:SER:O	1:C:451:ALA:HB2	1.91	0.70
1:C:972:LEU:H	1:C:974:PRO:HD2	1.55	0.70
1:A:185:ARG:O	1:A:186:ILE:CG1	2.38	0.70
1:A:246:PHE:O	1:A:249:ILE:CD1	2.39	0.70
1:B:987:MET:CE	1:B:987:MET:CA	2.66	0.70
1:C:899:PHE:CD1	1:C:899:PHE:N	2.60	0.70
1:A:105:VAL:O	1:A:108:GLN:CB	2.39	0.70
1:A:441:ALA:O	1:A:445:ILE:HG23	1.90	0.70
1:A:578:LEU:HD21	1:A:587:THR:HG23	1.72	0.70
1:A:901:VAL:HG11	1:A:943:ILE:HG13	1.74	0.70
1:B:245:GLU:HA	1:B:248:LYS:HG2	1.74	0.70
1:B:534:ILE:HG23	1:B:541:TYR:CZ	2.26	0.70
1:B:549:VAL:CG2	1:B:550:VAL:N	2.53	0.70
1:C:395:MET:O	1:C:398:MET:N	2.25	0.70
1:C:426:PRO:HB2	1:C:429:GLU:HB2	1.73	0.70
1:A:832:ALA:HB3	1:A:835:LYS:HB2	1.73	0.70
1:A:90:ILE:O	1:A:90:ILE:CG2	2.38	0.70
1:A:961:ILE:O	1:A:965:LEU:CD2	2.38	0.70
1:B:157:TYR:HA	1:B:161:ASN:HD22	1.54	0.70
1:B:151:GLN:HE22	1:B:279:ALA:H	1.37	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:GLU:O	1:B:346:GLU:HG2	1.91	0.70
1:B:743:ILE:H	1:B:743:ILE:CD1	2.01	0.70
1:B:940:LYS:O	1:B:941:ASN:C	2.30	0.70
1:C:184:MET:HB3	1:C:771:VAL:HG13	1.73	0.70
1:C:417:GLU:HB3	1:C:973:ARG:HH12	1.55	0.70
1:A:246:PHE:O	1:A:249:ILE:HD12	1.92	0.70
1:A:190:PRO:HG3	1:A:789:TRP:CD2	2.26	0.70
1:B:136:PHE:HE1	1:B:617:PHE:HZ	1.36	0.70
1:C:945:ILE:O	1:C:946:VAL:HG23	1.91	0.70
1:A:488:LEU:O	1:A:492:LEU:HB2	1.90	0.70
1:B:7:ASP:O	1:B:8:ARG:HB2	1.89	0.70
1:A:143:ILE:HG21	1:A:281:PHE:CD2	2.26	0.70
1:A:90:ILE:HD13	1:A:90:ILE:CG2	2.22	0.70
1:B:525:HIS:CA	1:B:528:THR:HG22	2.21	0.70
1:A:78:MET:CG	1:A:78:MET:O	2.39	0.69
1:A:790:TYR:CE1	1:A:800:PRO:CG	2.71	0.69
1:A:968:VAL:HG21	1:A:1023:PRO:CB	2.21	0.69
1:B:413:VAL:HG13	1:B:414:GLU:N	2.06	0.69
1:C:459:PHE:O	1:C:460:GLY:O	2.09	0.69
1:C:758:TYR:HB3	1:C:772:TYR:CE2	2.26	0.69
1:C:953:MET:SD	1:C:963:ALA:HB2	2.32	0.69
1:B:699:ARG:O	1:B:701:GLN:N	2.26	0.69
1:C:220:GLY:HA3	1:C:231:ASN:HD22	1.57	0.69
1:C:463:THR:CG2	1:C:464:GLY:H	1.87	0.69
1:A:733:GLN:OE1	1:A:743:ILE:HG12	1.92	0.69
1:B:130:GLU:OE1	1:C:110:LYS:HE2	1.92	0.69
1:C:317:PHE:HB2	1:C:318:PRO:CD	2.20	0.69
1:A:463:THR:HA	1:A:466:ILE:HD12	1.73	0.69
1:A:46:SER:O	1:A:127:VAL:HG13	1.92	0.69
1:B:150:THR:H	1:B:153:ASP:CB	2.04	0.69
1:B:356:TYR:C	1:B:358:PHE:N	2.43	0.69
1:B:649:MET:O	1:B:653:ARG:HB2	1.93	0.69
1:C:990:VAL:HG13	1:C:1005:THR:HG22	1.75	0.69
1:C:474:ILE:O	1:C:476:SER:O	2.10	0.69
1:A:375:VAL:O	1:A:379:THR:HG23	1.91	0.69
1:B:932:LEU:HA	1:B:935:ILE:HD12	1.75	0.69
1:C:191:ASN:HA	1:C:194:ASN:OD1	1.92	0.69
1:C:1:MET:HB2	1:C:2:PRO:CD	2.22	0.69
1:C:251:LEU:HB2	1:C:260:VAL:HG13	1.72	0.69
1:A:406:VAL:HG13	1:A:407:ASP:N	2.04	0.69
1:A:596:HIS:O	1:A:599:LEU:O	2.11	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:973:ARG:HG2	1:B:974:PRO:HD3	1.72	0.69
1:C:925:VAL:C	1:C:927:PHE:H	1.94	0.69
1:A:166:ILE:N	1:A:166:ILE:CD1	2.56	0.69
1:B:156:ASP:OD2	1:B:182:TYR:HB2	1.91	0.69
1:B:55:LYS:O	1:B:57:VAL:N	2.25	0.69
1:B:187:TRP:CZ3	1:B:774:MET:HE3	2.27	0.69
1:A:750:LEU:HD11	1:C:216:ALA:CB	2.21	0.69
1:C:44:THR:CG2	1:C:91:THR:HB	2.22	0.69
1:A:687:GLN:NE2	1:A:856:GLY:HA3	2.08	0.69
1:C:317:PHE:CB	1:C:318:PRO:HD2	2.22	0.69
1:A:49:TYR:HE2	1:A:121:GLU:HG2	1.57	0.69
1:A:528:THR:CG2	1:A:969:ARG:HE	2.05	0.69
1:A:607:GLU:OE2	1:A:607:GLU:O	2.11	0.69
1:B:169:THR:HB	1:B:172:VAL:HG21	1.74	0.69
1:B:1012:VAL:HG23	1:B:1013:THR:N	2.08	0.69
1:B:219:LEU:HD12	1:B:234:ILE:CG1	2.21	0.69
1:B:235:ILE:N	1:B:235:ILE:HD13	2.08	0.69
1:C:159:ALA:CB	1:C:181:GLN:HG3	2.23	0.69
1:C:164:ASP:N	1:C:164:ASP:OD1	2.21	0.69
1:A:367:ILE:HG12	1:A:413:VAL:HG21	1.75	0.69
1:A:548:ILE:HG23	1:A:910:ILE:HG12	1.75	0.69
1:B:523:SER:CA	1:B:526:HIS:HD2	1.93	0.69
1:B:6:ILE:HA	1:B:491:ALA:HA	1.74	0.69
1:B:881:LEU:HD21	1:B:905:VAL:HG21	1.75	0.69
1:A:661:ALA:O	1:A:663:VAL:HG23	1.93	0.68
1:B:30:LEU:HD23	1:B:390:ILE:CG1	2.23	0.68
1:C:410:ILE:CG2	1:C:411:VAL:N	2.44	0.68
1:A:48:SER:HB2	1:A:125:GLN:HG3	1.75	0.68
1:B:653:ARG:O	1:B:656:SER:OG	2.07	0.68
1:B:563:PHE:O	1:B:925:VAL:HG12	1.92	0.68
1:B:324:VAL:O	1:B:326:PRO:HD2	1.93	0.68
1:C:431:THR:HG21	1:C:494:ALA:CB	2.16	0.68
1:B:942:ALA:HA	1:B:1022:VAL:HG11	1.74	0.68
1:B:252:LYS:HG2	1:B:253:VAL:H	1.57	0.68
1:C:17:ILE:N	1:C:17:ILE:CD1	2.56	0.68
1:C:792:ARG:HB2	1:C:798:MET:HE2	1.73	0.68
1:B:109:ASN:ND2	1:B:112:GLN:NE2	2.41	0.68
1:B:157:TYR:CA	1:B:161:ASN:HD22	2.07	0.68
1:B:973:ARG:HG3	1:B:974:PRO:HD3	1.75	0.68
1:A:890:ALA:HB2	1:C:10:ILE:O	1.94	0.68
1:C:418:ARG:HD2	1:C:970:MET:CE	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:ASN:ND2	1:A:790:TYR:CD2	2.61	0.68
1:A:261:LEU:HD12	1:A:263:ARG:HH22	1.59	0.68
1:A:600:THR:O	1:A:600:THR:HG22	1.91	0.68
1:B:136:PHE:HD2	1:B:290:GLY:O	1.75	0.68
1:B:555:LEU:HB2	1:B:913:LEU:HD23	1.75	0.68
1:C:922:THR:CG2	1:C:923:ASN:H	2.04	0.68
1:A:15:ILE:O	1:A:19:ILE:HG13	1.93	0.68
1:A:583:THR:HG22	1:A:585:GLU:N	2.09	0.68
1:B:1012:VAL:CG2	1:B:1013:THR:N	2.57	0.68
1:C:420:MET:SD	1:C:498:LYS:NZ	2.66	0.68
1:C:975:ILE:HG22	1:C:976:LEU:N	2.07	0.68
1:B:558:ARG:HH11	1:B:558:ARG:HG2	1.59	0.68
1:C:176:GLN:HE21	1:C:620:ARG:HH11	1.42	0.68
1:C:358:PHE:HB3	1:C:977:MET:CE	2.24	0.68
1:C:933:THR:O	1:C:937:LEU:HB2	1.94	0.68
1:A:184:MET:HB3	1:A:771:VAL:HG13	1.76	0.68
1:B:1005:THR:CG2	1:B:1005:THR:O	2.42	0.68
1:B:945:ILE:HG13	1:B:1026:PHE:CE2	2.27	0.68
1:C:214:VAL:CG1	1:C:215:ALA:H	2.06	0.68
1:C:241:THR:OG1	1:C:241:THR:O	2.10	0.68
1:C:572:PHE:HE2	1:C:631:LEU:HD21	1.58	0.68
1:A:58:GLN:OE1	1:A:818:ARG:NH2	2.25	0.68
1:B:139:VAL:O	1:B:140:VAL:C	2.31	0.68
1:B:7:ASP:C	1:B:8:ARG:HD2	2.14	0.68
1:C:1024:VAL:HG12	1:C:1028:VAL:HG21	1.74	0.68
1:A:601:LYS:O	1:A:601:LYS:HG3	1.94	0.67
1:B:945:ILE:HD11	1:B:1026:PHE:HE2	1.56	0.67
1:B:24:GLY:HA2	1:B:27:ILE:CG2	2.24	0.67
1:B:463:THR:HA	1:B:466:ILE:HG13	1.75	0.67
1:B:276:ASP:O	1:B:614:GLY:HA3	1.94	0.67
1:B:399:VAL:HG11	1:B:989:LEU:HG	1.75	0.67
1:B:651:ALA:O	1:B:655:PHE:CE2	2.47	0.67
1:B:940:LYS:NZ	1:B:978:THR:HG23	2.09	0.67
1:C:244:GLU:HA	1:C:263:ARG:NH2	2.09	0.67
1:B:10:ILE:HG13	1:C:893:GLU:O	1.94	0.67
1:A:138:MET:HE3	1:A:306:ILE:CD1	2.24	0.67
1:B:65:ILE:HD11	1:B:118:LEU:HD21	1.77	0.67
1:B:26:ALA:O	1:B:30:LEU:HD22	1.94	0.67
1:B:452:VAL:O	1:B:453:PHE:HB2	1.94	0.67
1:A:139:VAL:O	1:A:139:VAL:HG22	1.95	0.67
1:C:102:ILE:HG22	1:C:106:GLN:HG3	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:934:THR:O	1:C:936:GLY:N	2.28	0.67
1:A:548:ILE:CG2	1:A:910:ILE:HG12	2.25	0.67
1:A:945:ILE:CG1	1:A:971:ARG:HG2	2.14	0.67
1:B:116:PRO:HA	1:B:123:GLN:HE22	1.59	0.67
1:B:252:LYS:HB3	1:B:260:VAL:CG1	2.24	0.67
1:B:140:VAL:HG13	1:B:291:ILE:HD12	1.77	0.67
1:B:897:ILE:HG13	1:B:898:PRO:HD3	1.77	0.67
1:C:514:GLY:O	1:C:518:ARG:HG3	1.95	0.67
1:C:790:TYR:CE1	1:C:800:PRO:HB3	2.29	0.67
1:A:883:VAL:O	1:A:887:CYS:HB2	1.94	0.67
1:A:945:ILE:HG12	1:A:971:ARG:CG	2.14	0.67
1:A:952:LEU:HD12	1:A:953:MET:N	2.10	0.67
1:B:115:MET:HE1	1:B:127:VAL:HG21	1.77	0.67
1:A:498:LYS:O	1:A:498:LYS:NZ	2.25	0.67
1:A:418:ARG:NH1	1:A:973:ARG:HB3	2.08	0.67
1:B:952:LEU:HD12	1:B:956:GLU:OE2	1.94	0.67
1:C:358:PHE:HB3	1:C:977:MET:HE1	1.74	0.67
1:C:39:ALA:HB2	1:C:673:GLU:HB3	1.77	0.67
1:C:576:VAL:CG1	1:C:663:VAL:HG22	2.21	0.67
1:B:355:MET:O	1:B:365:THR:OG1	2.13	0.67
1:B:537:SER:CA	1:B:540:ARG:HE	2.07	0.67
1:C:905:VAL:HB	1:C:906:PRO:HD3	1.76	0.67
1:B:181:GLN:OE1	1:B:767:ARG:NE	2.24	0.67
1:B:314:GLU:HA	1:B:317:PHE:CD2	2.30	0.67
1:B:420:MET:CE	1:B:425:LEU:HD23	2.25	0.67
1:B:51:GLY:O	1:B:53:ASP:OD2	2.13	0.67
1:B:225:VAL:CG2	1:C:781:MET:HE3	2.21	0.67
1:C:879:ILE:O	1:C:883:VAL:HG23	1.95	0.67
1:C:924:ASP:C	1:C:925:VAL:O	2.33	0.67
1:C:418:ARG:CD	1:C:970:MET:HE2	2.25	0.67
1:A:540:ARG:HG3	1:A:541:TYR:H	1.59	0.66
1:C:189:ASN:CG	1:C:779:TYR:HE1	1.99	0.66
1:C:554:TYR:HD1	1:C:558:ARG:HH21	1.35	0.66
1:B:293:LEU:HD22	1:B:294:ALA:O	1.95	0.66
1:C:950:LYS:HZ1	1:C:1030:ARG:CD	2.07	0.66
1:B:213:GLN:CG	1:C:56:THR:HG23	2.25	0.66
1:C:686:ASP:OD1	1:C:690:LEU:HB2	1.95	0.66
1:A:355:MET:HE3	1:A:977:MET:HE1	1.77	0.66
1:B:600:THR:OG1	1:B:601:LYS:NZ	2.26	0.66
1:B:641:GLU:HA	1:B:650:ARG:NH1	2.10	0.66
1:B:940:LYS:HZ2	1:B:978:THR:HG23	1.58	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:721:LEU:HD23	1:C:721:LEU:O	1.95	0.66
1:C:843:LEU:HA	1:C:846:GLN:NE2	2.10	0.66
1:A:255:GLN:CD	1:A:255:GLN:N	2.49	0.66
1:B:42:ALA:HB2	1:B:93:THR:CG2	2.16	0.66
1:C:5:PHE:HE2	1:C:11:PHE:HD2	1.43	0.66
1:A:188:MET:HA	1:A:266:ALA:HB2	1.76	0.66
1:B:371:ALA:O	1:B:375:VAL:HG23	1.95	0.66
1:A:119:PRO:HG2	1:A:122:VAL:HG23	1.77	0.66
1:A:742:SER:HG	1:A:745:ASP:HB2	1.57	0.66
1:B:13:TRP:HA	1:B:13:TRP:CE3	2.30	0.66
1:B:562:SER:O	1:B:924:ASP:HA	1.95	0.66
1:A:28:LEU:N	1:A:28:LEU:HD12	2.10	0.66
1:A:348:ILE:HA	1:A:351:VAL:HG23	1.76	0.66
1:A:418:ARG:HH11	1:A:973:ARG:HE	1.44	0.66
1:A:38:ILE:O	1:A:462:SER:HA	1.95	0.66
1:A:820:ASN:O	1:A:822:LEU:CD2	2.43	0.66
1:B:178:PHE:CA	1:B:277:ILE:HG21	2.25	0.66
1:B:416:VAL:HG11	1:B:431:THR:HG22	1.76	0.66
1:B:518:ARG:HA	1:B:521:GLU:HB2	1.78	0.66
1:B:574:THR:HG23	1:B:665:ALA:CB	2.25	0.66
1:B:807:SER:C	1:B:808:ARG:HG3	2.15	0.66
1:C:4:PHE:HB3	1:C:8:ARG:NH2	2.08	0.66
1:C:82:SER:HB3	1:C:88:VAL:HA	1.76	0.66
1:A:13:TRP:O	1:A:17:ILE:HG13	1.96	0.66
1:A:155:SER:HA	1:A:287:SER:OG	1.96	0.66
1:B:219:LEU:HD23	1:C:783:PRO:HG3	1.77	0.66
1:B:692:HIS:HD1	1:B:692:HIS:C	1.97	0.66
1:A:367:ILE:HD12	1:A:368:PRO:N	2.11	0.66
1:A:428:LYS:HE3	1:A:429:GLU:OE2	1.96	0.66
1:A:521:GLU:HB3	1:A:522:LYS:HZ3	1.61	0.66
1:B:68:ASN:HD22	1:B:114:ALA:HB2	1.61	0.66
1:C:449:LEU:HB2	1:C:478:MET:CE	2.26	0.66
1:C:82:SER:CB	1:C:88:VAL:HA	2.26	0.66
1:A:568:ASP:O	1:A:634:TRP:HH2	1.79	0.66
1:B:2:PRO:HD3	1:B:486:LEU:HD12	1.78	0.66
1:C:527:TYR:CE2	1:C:972:LEU:HD23	2.31	0.66
1:C:742:SER:O	1:C:746:ILE:HG13	1.96	0.66
1:C:848:ALA:HA	1:C:851:LEU:HD11	1.77	0.66
1:A:323:ILE:HG12	1:A:325:TYR:HE1	1.60	0.65
1:B:1021:PHE:HB3	1:B:1025:PHE:CE1	2.30	0.65
1:C:344:LEU:HD23	1:C:399:VAL:HG22	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:963:ALA:O	1:A:965:LEU:N	2.30	0.65
1:B:247:GLY:HA2	1:B:268:ILE:HD13	0.72	0.65
1:C:17:ILE:N	1:C:17:ILE:HD12	2.10	0.65
1:C:260:VAL:O	1:C:260:VAL:HG13	1.94	0.65
1:C:459:PHE:CD2	1:C:459:PHE:N	2.59	0.65
1:A:568:ASP:HB3	1:A:634:TRP:CZ3	2.25	0.65
1:A:64:VAL:O	1:A:65:ILE:O	2.14	0.65
1:A:815:ARG:HH11	1:A:815:ARG:CG	2.06	0.65
1:A:781:MET:HE2	1:C:225:VAL:H	1.61	0.65
1:C:244:GLU:O	1:C:263:ARG:NH2	2.29	0.65
1:C:188:MET:HA	1:C:266:ALA:CB	2.25	0.65
1:A:185:ARG:O	1:A:186:ILE:HG13	1.97	0.65
1:A:521:GLU:HB3	1:A:522:LYS:NZ	2.12	0.65
1:B:48:SER:HA	1:B:87:THR:HA	1.77	0.65
1:C:102:ILE:HG22	1:C:106:GLN:CG	2.26	0.65
1:C:338:HIS:O	1:C:338:HIS:ND1	2.30	0.65
1:C:476:SER:C	1:C:478:MET:H	1.99	0.65
1:C:65:ILE:HD13	1:C:111:LEU:HD23	1.77	0.65
1:A:463:THR:O	1:A:465:ALA:N	2.28	0.65
1:B:562:SER:HA	1:B:837:THR:OG1	1.97	0.65
1:B:200:PRO:CD	1:B:749:THR:HG22	2.26	0.65
1:B:160:ALA:HB1	1:B:767:ARG:HD2	1.78	0.65
1:B:792:ARG:HB2	1:B:798:MET:HE1	1.79	0.65
1:B:919:ARG:HG3	1:B:1005:THR:HG21	1.76	0.65
1:B:970:MET:HE2	1:B:970:MET:HA	1.77	0.65
1:C:378:GLY:O	1:C:382:VAL:HG23	1.97	0.65
1:C:35:TYR:CD1	1:C:671:ILE:HG12	2.31	0.65
1:C:928:GLN:OE1	1:C:928:GLN:N	2.28	0.65
1:A:545:TYR:HB2	1:A:1021:PHE:CE1	2.31	0.65
1:B:262:LEU:HD22	1:B:266:ALA:CB	2.26	0.65
1:C:423:GLU:O	1:C:426:PRO:HD3	1.96	0.65
1:A:78:MET:HG2	1:A:78:MET:O	1.96	0.65
1:A:418:ARG:CD	1:A:970:MET:HG3	2.27	0.65
1:A:350:LEU:HD11	1:A:984:LEU:HB2	1.79	0.65
1:B:6:ILE:HD12	1:B:490:PRO:CB	2.22	0.65
1:B:972:LEU:CD1	1:B:976:LEU:HD23	2.16	0.65
1:C:404:LEU:CD2	1:C:937:LEU:HD13	2.27	0.65
1:C:519:MET:HG3	1:C:520:PHE:N	2.10	0.65
1:C:536:ARG:NH1	1:C:961:ILE:CD1	2.60	0.65
1:C:626:ILE:HD13	1:C:627:ALA:N	2.10	0.65
1:A:754:TRP:CZ2	1:A:786:ILE:HG12	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:LEU:HD12	1:B:178:PHE:N	2.12	0.65
1:B:431:THR:CG2	1:B:493:CYS:HB3	2.25	0.65
1:B:587:THR:O	1:B:591:LEU:HB2	1.97	0.65
1:B:713:LEU:N	1:B:713:LEU:HD12	2.09	0.65
1:A:113:LEU:HD13	1:C:108:GLN:HE22	1.62	0.65
1:A:200:PRO:CD	1:A:749:THR:HG23	2.27	0.65
1:A:58:GLN:HE21	1:A:816:LEU:HD12	1.60	0.65
1:B:537:SER:O	1:B:540:ARG:HB2	1.97	0.65
1:C:251:LEU:HB2	1:C:260:VAL:O	1.97	0.65
1:C:4:PHE:O	1:C:8:ARG:HG2	1.97	0.65
1:C:527:TYR:OH	1:C:968:VAL:HG12	1.96	0.65
1:A:51:GLY:O	1:C:215:ALA:HB1	1.97	0.64
1:C:713:LEU:HD23	1:C:831:ALA:C	2.16	0.64
1:C:674:LEU:HD21	1:C:862:MET:N	2.11	0.64
1:C:897:ILE:HG12	1:C:950:LYS:NZ	2.12	0.64
1:A:188:MET:HA	1:A:266:ALA:CB	2.27	0.64
1:B:372:VAL:HG22	1:B:373:PRO:CD	2.26	0.64
1:B:831:ALA:HB3	1:B:840:ALA:HB2	1.78	0.64
1:B:953:MET:O	1:B:953:MET:HG2	1.96	0.64
1:C:1025:PHE:C	1:C:1029:VAL:HG23	2.16	0.64
1:B:189:ASN:HD22	1:B:190:PRO:HD2	1.61	0.64
1:C:790:TYR:C	1:C:791:VAL:HG23	2.17	0.64
1:C:950:LYS:HZ3	1:C:1030:ARG:CD	1.99	0.64
1:A:983:ILE:O	1:A:983:ILE:HD12	1.96	0.64
1:B:453:PHE:HA	1:B:456:MET:SD	2.37	0.64
1:B:489:THR:O	1:B:492:LEU:HB2	1.97	0.64
1:B:537:SER:HB2	1:B:540:ARG:CG	2.23	0.64
1:B:555:LEU:HG	1:B:914:LEU:HD23	1.79	0.64
1:B:632:LYS:O	1:B:637:ARG:HD2	1.98	0.64
1:B:640:GLU:O	1:B:643:LYS:HB2	1.98	0.64
1:B:418:ARG:HG3	1:B:970:MET:CE	2.28	0.64
1:C:72:ILE:HG22	1:C:94:PHE:HE2	1.62	0.64
1:A:313:MET:C	1:A:315:PRO:HD2	2.18	0.64
1:A:736:ALA:O	1:A:741:VAL:CG1	2.45	0.64
1:A:108:GLN:CG	1:B:112:GLN:CD	2.57	0.64
1:B:699:ARG:HG2	1:B:700:ASN:H	1.59	0.64
1:C:934:THR:O	1:C:935:ILE:C	2.35	0.64
1:A:193:LEU:HB2	1:A:265:VAL:HG13	1.79	0.64
1:A:418:ARG:HG2	1:A:970:MET:CE	2.25	0.64
1:A:616:GLY:HA3	1:A:624:THR:OG1	1.98	0.64
1:A:69:MET:C	1:A:70:ASN:ND2	2.51	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1010:GLY:HA2	1:C:1013:THR:CG2	2.28	0.64
1:C:166:ILE:HA	1:C:166:ILE:CD1	2.28	0.64
1:C:435:MET:HA	1:C:438:ILE:HG22	1.80	0.64
1:A:686:ASP:OD1	1:A:686:ASP:O	2.15	0.64
1:B:591:LEU:O	1:B:595:THR:HG22	1.98	0.64
1:B:74:ASN:O	1:B:94:PHE:HB3	1.97	0.64
1:C:115:MET:HE2	1:C:115:MET:HA	1.78	0.64
1:C:673:GLU:O	1:C:674:LEU:CB	2.44	0.64
1:B:223:PRO:CG	1:B:223:PRO:O	2.45	0.64
1:B:545:TYR:O	1:B:547:ILE:N	2.31	0.64
1:B:707:ALA:O	1:B:708:LYS:CB	2.45	0.64
1:A:846:GLN:O	1:A:849:SER:HB3	1.98	0.64
1:C:184:MET:CE	1:C:184:MET:HA	2.28	0.64
1:C:291:ILE:CB	1:C:291:ILE:CD1	2.73	0.64
1:C:513:PHE:CA	1:C:516:PHE:HB3	2.18	0.64
1:B:911:GLY:CA	1:B:1013:THR:HG21	2.18	0.64
1:B:1014:ALA:O	1:B:1018:ALA:HB2	1.98	0.64
1:B:409:ALA:HB2	1:B:485:ALA:HB2	1.79	0.64
1:A:115:MET:O	1:A:116:PRO:C	2.35	0.63
1:A:359:LEU:CD1	1:A:417:GLU:CG	2.68	0.63
1:A:950:LYS:O	1:A:951:ASP:HB3	1.98	0.63
1:B:144:ASN:OD1	1:B:149:MET:HG3	1.98	0.63
1:B:230:LEU:HD21	1:C:809:TRP:CH2	2.34	0.63
1:B:171:GLY:HA3	1:B:302:THR:HG21	1.78	0.63
1:B:910:ILE:O	1:B:914:LEU:HG	1.97	0.63
1:C:453:PHE:O	1:C:456:MET:HG2	1.97	0.63
1:C:564:LEU:CD2	1:C:671:ILE:HD12	2.28	0.63
1:C:552:MET:CE	1:C:909:VAL:HG21	2.28	0.63
1:A:298:ASN:ND2	1:A:300:LEU:N	2.46	0.63
1:B:921:LEU:CD2	1:B:1005:THR:CG2	2.75	0.63
1:B:1025:PHE:H	1:B:1028:VAL:CG2	2.11	0.63
1:B:602:GLU:OE1	1:B:650:ARG:NH2	2.31	0.63
1:C:202:ASP:OD2	1:C:792:ARG:NH2	2.27	0.63
1:A:298:ASN:HD22	1:A:299:ALA:N	1.97	0.63
1:A:344:LEU:HD23	1:A:402:ILE:CD1	2.13	0.63
1:A:686:ASP:O	1:A:688:ALA:N	2.30	0.63
1:B:448:VAL:O	1:B:452:VAL:HG22	1.99	0.63
1:B:693:GLU:O	1:B:696:THR:OG1	2.16	0.63
1:B:85:THR:HG23	1:B:87:THR:HB	1.79	0.63
1:A:727:PHE:O	1:C:234:ILE:HA	1.99	0.63
1:C:238:THR:HG22	1:C:239:ARG:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:775:SER:O	1:C:776:GLU:C	2.35	0.63
1:A:659:LYS:O	1:A:661:ALA:N	2.32	0.63
1:A:69:MET:HA	1:A:69:MET:HE2	1.81	0.63
1:B:622:GLN:O	1:B:622:GLN:CG	2.44	0.63
1:B:785:ASP:O	1:B:787:GLY:N	2.31	0.63
1:B:790:TYR:CE1	1:B:800:PRO:HB3	2.30	0.63
1:B:901:VAL:HG21	1:B:943:ILE:HD13	1.81	0.63
1:C:164:ASP:O	1:C:168:ARG:HG2	1.98	0.63
1:C:695:LEU:HD22	1:C:825:MET:CE	2.28	0.63
1:A:426:PRO:HG2	1:A:429:GLU:OE2	1.99	0.63
1:A:911:GLY:H	1:A:914:LEU:HD13	1.63	0.63
1:A:983:ILE:HG13	1:A:984:LEU:N	2.13	0.63
1:B:904:VAL:CG1	1:B:907:LEU:CD1	2.52	0.63
1:B:80:SER:OG	1:B:90:ILE:HG12	1.99	0.63
1:C:102:ILE:O	1:C:103:ALA:C	2.34	0.63
1:C:45:ILE:CA	1:C:45:ILE:CG1	2.73	0.63
1:B:116:PRO:HA	1:B:123:GLN:NE2	2.13	0.63
1:B:137:LEU:CD1	1:B:299:ALA:HB1	2.28	0.63
1:B:905:VAL:CG2	1:B:935:ILE:HG12	2.29	0.63
1:C:637:ARG:HB3	1:C:642:ASN:HB3	1.81	0.63
1:A:316:PHE:O	1:A:321:LEU:HD11	1.99	0.63
1:A:372:VAL:O	1:A:375:VAL:N	2.32	0.63
1:A:760:ASN:O	1:A:771:VAL:HB	1.99	0.63
1:B:355:MET:HE3	1:B:369:THR:HG23	1.78	0.63
1:B:845:GLU:HG3	1:B:857:TYR:OH	1.97	0.63
1:B:876:LEU:CD1	1:B:932:LEU:HD11	2.28	0.63
1:C:701:GLN:O	1:C:704:ALA:HB3	1.99	0.63
1:C:713:LEU:HD21	1:C:835:LYS:H	1.62	0.63
1:C:910:ILE:CG2	1:C:911:GLY:H	2.10	0.63
1:A:11:PHE:CD1	1:B:890:ALA:HB1	2.34	0.63
1:A:193:LEU:HB2	1:A:265:VAL:CG1	2.29	0.63
1:A:58:GLN:NE2	1:A:816:LEU:HD12	2.14	0.63
1:A:47:ALA:HB3	1:A:88:VAL:CG2	2.28	0.63
1:B:49:TYR:CE2	1:B:122:VAL:HA	2.34	0.63
1:C:538:THR:O	1:C:540:ARG:HG2	1.99	0.63
1:A:520:PHE:H	1:A:522:LYS:HE3	1.63	0.63
1:A:736:ALA:O	1:A:741:VAL:HG12	1.99	0.63
1:B:125:GLN:CG	1:B:125:GLN:O	2.47	0.63
1:B:186:ILE:HG23	1:B:266:ALA:HB1	1.81	0.63
1:B:587:THR:HG22	1:B:613:ASN:OD1	1.99	0.63
1:B:712:MET:HB3	1:B:713:LEU:CD1	2.16	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:352:PHE:CA	1:C:369:THR:HG21	2.26	0.63
1:C:919:ARG:HB3	1:C:921:LEU:CD2	2.29	0.63
1:A:324:VAL:C	1:A:325:TYR:HD1	2.02	0.62
1:B:335:ILE:C	1:B:337:ILE:H	2.03	0.62
1:B:785:ASP:O	1:B:786:ILE:C	2.36	0.62
1:C:801:PHE:O	1:C:805:SER:OG	2.16	0.62
1:A:311:ALA:O	1:A:312:LYS:HB2	1.99	0.62
1:A:936:GLY:O	1:A:940:LYS:HB2	1.99	0.62
1:B:537:SER:C	1:B:540:ARG:HE	2.01	0.62
1:C:1007:VAL:HG12	1:C:1008:MET:N	2.14	0.62
1:A:781:MET:HB3	1:C:228:GLN:OE1	1.99	0.62
1:B:115:MET:CE	1:B:118:LEU:HD22	2.30	0.62
1:B:403:GLY:O	1:B:404:LEU:HD23	1.98	0.62
1:B:418:ARG:HH21	1:B:970:MET:CG	2.12	0.62
1:B:860:THR:HG22	1:B:861:GLY:N	2.14	0.62
1:C:418:ARG:HG3	1:C:419:VAL:HG13	1.82	0.62
1:C:92:LEU:HD22	1:C:107:VAL:CG2	2.29	0.62
1:C:945:ILE:HD12	1:C:945:ILE:C	2.18	0.62
1:A:282:ASN:HD21	1:A:609:VAL:H	1.47	0.62
1:A:95:GLU:O	1:A:98:THR:CG2	2.47	0.62
1:B:437:GLN:HA	1:B:437:GLN:HE21	1.64	0.62
1:A:170:SER:OG	1:A:170:SER:O	2.16	0.62
1:A:655:PHE:C	1:A:656:SER:O	2.31	0.62
1:B:298:ASN:HB2	1:B:301:ASP:OD1	2.00	0.62
1:B:573:MET:HE3	1:B:626:ILE:HD12	1.81	0.62
1:A:10:ILE:HD11	1:B:895:TRP:CB	2.30	0.62
1:B:973:ARG:HG2	1:B:974:PRO:HD2	1.80	0.62
1:C:427:PRO:O	1:C:431:THR:HG22	2.00	0.62
1:C:476:SER:O	1:C:478:MET:N	2.32	0.62
1:B:953:MET:HA	1:B:958:LYS:HA	1.81	0.62
1:C:144:ASN:ND2	1:C:149:MET:HG3	2.13	0.62
1:C:492:LEU:O	1:C:496:MET:HG2	2.00	0.62
1:C:686:ASP:HB3	1:C:823:PRO:HG2	1.82	0.62
1:C:685:ILE:HD12	1:C:686:ASP:N	2.15	0.62
1:A:635:ALA:C	1:A:637:ARG:H	2.01	0.62
1:B:1024:VAL:O	1:B:1025:PHE:HB2	1.98	0.62
1:B:804:PHE:O	1:B:805:SER:CB	2.48	0.62
1:B:902:MET:O	1:B:905:VAL:HG12	1.98	0.62
1:C:80:SER:O	1:C:89:GLN:O	2.17	0.62
1:A:653:ARG:O	1:A:656:SER:N	2.31	0.62
1:A:781:MET:HE1	1:C:228:GLN:HG2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1026:PHE:HB3	1:B:1030:ARG:CZ	2.30	0.62
1:B:190:PRO:HG2	1:B:779:TYR:CD1	2.35	0.62
1:B:681:ASP:O	1:B:859:TRP:HE3	1.82	0.62
1:C:685:ILE:HD11	1:C:687:GLN:HA	1.81	0.62
1:C:965:LEU:HG	1:C:966:ASP:H	1.64	0.62
1:C:166:ILE:HA	1:C:166:ILE:HD13	1.82	0.62
1:A:472:ILE:H	1:A:472:ILE:CD1	2.08	0.62
1:A:588:GLN:O	1:A:591:LEU:N	2.32	0.62
1:B:612:VAL:HG23	1:B:626:ILE:O	2.00	0.62
1:B:631:LEU:HD13	1:B:637:ARG:NH2	2.15	0.62
1:C:527:TYR:CD2	1:C:972:LEU:HD23	2.35	0.62
1:C:686:ASP:OD2	1:C:690:LEU:HB2	1.99	0.62
1:C:699:ARG:CG	1:C:699:ARG:NH1	2.43	0.62
1:A:1020:PHE:O	1:A:1024:VAL:HG23	2.00	0.61
1:A:199:THR:HB	1:A:200:PRO:CD	2.30	0.61
1:A:818:ARG:HA	1:A:824:SER:N	2.15	0.61
1:A:902:MET:O	1:A:905:VAL:HG23	2.00	0.61
1:C:58:GLN:HG3	1:C:62:THR:OG1	1.99	0.61
1:A:298:ASN:HD22	1:A:300:LEU:H	1.47	0.61
1:A:527:TYR:CD2	1:A:972:LEU:HG	2.35	0.61
1:A:588:GLN:HG2	1:A:613:ASN:ND2	2.14	0.61
1:A:61:VAL:HG21	1:A:122:VAL:HG21	1.81	0.61
1:A:578:LEU:O	1:A:623:ASN:ND2	2.34	0.61
1:A:924:ASP:O	1:A:927:PHE:HB3	2.00	0.61
1:B:328:ASP:OD2	1:B:330:THR:N	2.33	0.61
1:B:623:ASN:HD22	1:B:624:THR:N	1.97	0.61
1:C:344:LEU:HD21	1:C:399:VAL:HG23	1.81	0.61
1:A:64:VAL:O	1:A:68:ASN:OD1	2.18	0.61
1:B:56:THR:O	1:B:60:THR:HB	2.00	0.61
1:B:732:ASP:HB2	1:B:735:LYS:HG3	1.82	0.61
1:B:743:ILE:N	1:B:743:ILE:HD12	2.12	0.61
1:B:57:VAL:HG11	1:B:86:GLY:HA2	1.82	0.61
1:B:908:GLY:C	1:B:910:ILE:H	2.02	0.61
1:C:190:PRO:HG3	1:C:789:TRP:CE2	2.35	0.61
1:C:189:ASN:HD21	1:C:191:ASN:HD22	1.48	0.61
1:C:551:GLY:O	1:C:555:LEU:HD23	2.00	0.61
1:C:846:GLN:O	1:C:849:SER:OG	2.18	0.61
1:A:359:LEU:HD11	1:A:417:GLU:HG2	1.79	0.61
1:A:543:VAL:HG22	1:A:544:LEU:H	1.64	0.61
1:A:1016:VAL:HG12	1:A:1016:VAL:O	2.00	0.61
1:A:461:GLY:O	1:A:463:THR:O	2.19	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:GLY:O	1:A:554:TYR:HB3	2.00	0.61
1:A:60:THR:HG22	1:A:61:VAL:CG2	2.30	0.61
1:B:109:ASN:ND2	1:B:112:GLN:HE22	1.98	0.61
1:B:543:VAL:O	1:B:547:ILE:CD1	2.48	0.61
1:B:791:VAL:CG2	1:B:801:PHE:HE2	2.13	0.61
1:B:922:THR:OG1	1:B:923:ASN:N	2.33	0.61
1:A:223:PRO:HD3	1:B:275:TYR:CG	2.34	0.61
1:A:894:SER:OG	1:A:897:ILE:HB	1.99	0.61
1:B:623:ASN:C	1:B:623:ASN:ND2	2.42	0.61
1:C:682:PHE:HE2	1:C:702:LEU:CD1	2.13	0.61
1:C:695:LEU:HD22	1:C:825:MET:HE2	1.83	0.61
1:C:848:ALA:HA	1:C:851:LEU:CD1	2.30	0.61
1:A:1021:PHE:O	1:A:1024:VAL:HB	2.00	0.61
1:A:169:THR:O	1:A:172:VAL:HG22	2.00	0.61
1:B:1027:VAL:O	1:B:1030:ARG:O	2.19	0.61
1:B:9:PRO:O	1:B:12:ALA:HB3	1.99	0.61
1:B:423:GLU:OE1	1:B:427:PRO:CD	2.49	0.61
1:B:573:MET:HE1	1:B:626:ILE:HD12	1.81	0.61
1:B:3:ASN:N	1:B:6:ILE:HG12	2.15	0.61
1:B:921:LEU:HD13	1:B:921:LEU:H	1.64	0.61
1:C:549:VAL:C	1:C:551:GLY:N	2.53	0.61
1:C:641:GLU:H	1:C:641:GLU:CD	2.04	0.61
1:C:688:ALA:C	1:C:690:LEU:H	2.03	0.61
1:A:73:ASP:CG	1:A:106:GLN:NE2	2.54	0.61
1:A:746:ILE:HD13	1:A:804:PHE:CE1	2.36	0.61
1:A:200:PRO:CG	1:A:749:THR:HG23	2.31	0.61
1:B:160:ALA:CB	1:B:767:ARG:HD3	2.27	0.61
1:C:445:ILE:HD13	1:C:940:LYS:HE3	1.83	0.61
1:C:584:GLN:HB2	1:C:622:GLN:NE2	2.13	0.61
1:C:819:TYR:O	1:C:820:ASN:HB2	1.99	0.61
1:A:953:MET:HE1	1:A:960:LEU:O	2.01	0.61
1:B:476:SER:O	1:B:477:ALA:C	2.39	0.61
1:B:588:GLN:HA	1:B:588:GLN:OE1	2.01	0.61
1:B:68:ASN:ND2	1:B:114:ALA:HB2	2.15	0.61
1:A:818:ARG:NE	1:A:818:ARG:CG	2.62	0.61
1:A:885:PHE:CD2	1:A:886:LEU:HD12	2.36	0.61
1:A:901:VAL:O	1:A:904:VAL:CG2	2.49	0.61
1:B:136:PHE:CE1	1:B:617:PHE:HZ	2.17	0.61
1:B:777:ALA:O	1:B:780:ARG:HB2	2.01	0.61
1:C:115:MET:N	1:C:116:PRO:HD2	2.16	0.61
1:A:56:THR:HG23	1:C:213:GLN:HG3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:415:ASN:HD21	1:C:434:SER:CB	2.14	0.61
1:C:38:ILE:HG21	1:C:466:ILE:HD11	1.83	0.61
1:C:540:ARG:HG3	1:C:541:TYR:CD1	2.35	0.61
1:C:588:GLN:HG2	1:C:613:ASN:ND2	2.13	0.61
1:C:843:LEU:O	1:C:846:GLN:HB2	2.01	0.61
1:A:436:GLY:HA2	1:A:439:GLN:HB2	1.83	0.60
1:A:528:THR:O	1:A:532:GLY:N	2.33	0.60
1:B:1026:PHE:HB3	1:B:1030:ARG:NH2	2.15	0.60
1:A:108:GLN:CD	1:B:112:GLN:CD	2.59	0.60
1:B:172:VAL:O	1:B:173:GLY:O	2.18	0.60
1:B:622:GLN:HG3	1:B:622:GLN:O	2.00	0.60
1:B:709:HIS:N	1:B:710:PRO:CD	2.63	0.60
1:A:210:GLN:CG	1:A:249:ILE:HG23	2.27	0.60
1:A:594:VAL:HA	1:A:655:PHE:CZ	2.35	0.60
1:A:73:ASP:CB	1:A:106:GLN:HE22	2.14	0.60
1:A:780:ARG:HH21	1:C:223:PRO:HD2	1.67	0.60
1:B:193:LEU:HD22	1:B:198:LEU:O	2.01	0.60
1:B:413:VAL:CG1	1:B:414:GLU:N	2.63	0.60
1:B:680:PHE:O	1:B:680:PHE:CD1	2.54	0.60
1:A:10:ILE:CD1	1:B:895:TRP:HB2	2.31	0.60
1:A:542:LEU:HD23	1:A:1028:VAL:HG11	1.84	0.60
1:A:634:TRP:O	1:A:637:ARG:O	2.18	0.60
1:A:644:VAL:O	1:A:648:THR:HG23	2.01	0.60
1:A:949:ALA:HB1	1:A:1026:PHE:CZ	2.36	0.60
1:A:952:LEU:HD11	1:A:963:ALA:HB1	1.82	0.60
1:B:149:MET:SD	1:B:154:ILE:HG22	2.42	0.60
1:B:408:ASP:C	1:B:410:ILE:H	2.04	0.60
1:B:418:ARG:HG3	1:B:970:MET:HE3	1.83	0.60
1:B:58:GLN:HA	1:B:62:THR:CB	2.30	0.60
1:C:350:LEU:CD1	1:C:984:LEU:CD2	2.66	0.60
1:C:951:ASP:C	1:C:953:MET:N	2.44	0.60
1:A:1021:PHE:HB3	1:A:1025:PHE:CZ	2.36	0.60
1:B:184:MET:HB3	1:B:771:VAL:HG22	1.82	0.60
1:B:605:ASN:OD1	1:B:642:ASN:HB3	2.02	0.60
1:B:784:ASP:O	1:B:785:ASP:C	2.38	0.60
1:B:115:MET:HA	1:B:118:LEU:HD13	1.83	0.60
1:B:184:MET:CG	1:B:184:MET:O	2.50	0.60
1:B:370:ILE:O	1:B:370:ILE:HG22	2.01	0.60
1:B:569:GLN:OE1	1:B:569:GLN:HA	2.00	0.60
1:B:602:GLU:C	1:B:604:ASN:H	2.04	0.60
1:C:375:VAL:HB	1:C:405:LEU:HD13	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:MET:HG2	1:A:490:PRO:CB	2.25	0.60
1:B:187:TRP:O	1:B:266:ALA:HA	2.02	0.60
1:C:1024:VAL:HG12	1:C:1028:VAL:CG2	2.31	0.60
1:C:404:LEU:O	1:C:405:LEU:HD23	2.02	0.60
1:B:534:ILE:HA	1:B:541:TYR:CE1	2.37	0.60
1:C:1016:VAL:O	1:C:1018:ALA:N	2.31	0.60
1:C:118:LEU:N	1:C:118:LEU:HD13	2.16	0.60
1:A:520:PHE:N	1:A:522:LYS:HE3	2.17	0.60
1:A:571:VAL:HG12	1:A:630:SER:CA	2.30	0.60
1:B:160:ALA:CB	1:B:767:ARG:CD	2.75	0.60
1:B:62:THR:OG1	1:B:88:VAL:HG11	2.01	0.60
1:C:229:GLN:O	1:C:230:LEU:CB	2.48	0.60
1:C:284:GLN:HG3	1:C:285:PRO:HD2	1.83	0.60
1:A:340:VAL:CG1	1:A:399:VAL:CG2	2.80	0.60
1:A:428:LYS:HG3	1:A:429:GLU:N	2.15	0.60
1:B:1029:VAL:HG23	1:B:1032:ARG:HD2	1.83	0.60
1:B:120:GLN:HG2	1:B:124:GLN:HG2	1.84	0.60
1:B:13:TRP:HE3	1:B:13:TRP:HA	1.67	0.60
1:C:115:MET:HA	1:C:115:MET:CE	2.32	0.60
1:A:62:THR:HG22	1:A:62:THR:O	2.02	0.60
1:B:314:GLU:H	1:B:315:PRO:CD	2.14	0.60
1:C:527:TYR:O	1:C:531:VAL:HG13	2.02	0.60
1:C:686:ASP:C	1:C:686:ASP:OD1	2.37	0.60
1:A:314:GLU:H	1:A:315:PRO:HD3	1.67	0.59
1:A:407:ASP:O	1:A:408:ASP:C	2.41	0.59
1:A:584:GLN:N	1:A:622:GLN:HB3	2.12	0.59
1:A:726:GLN:N	1:A:810:GLU:O	2.35	0.59
1:A:813:SER:HB3	1:A:816:LEU:CD2	2.28	0.59
1:B:983:ILE:HD13	1:B:1012:VAL:HG12	1.84	0.59
1:B:343:THR:O	1:B:347:ALA:N	2.35	0.59
1:B:58:GLN:HA	1:B:62:THR:HB	1.83	0.59
1:B:655:PHE:C	1:B:658:ILE:HG12	2.22	0.59
1:B:776:GLU:HG2	1:B:777:ALA:N	2.17	0.59
1:B:792:ARG:HB2	1:B:798:MET:CE	2.31	0.59
1:B:916:ALA:HB2	1:B:1005:THR:O	2.02	0.59
1:C:54:ALA:HB2	1:C:84:SER:CB	2.32	0.59
1:A:1024:VAL:HG12	1:A:1025:PHE:N	2.16	0.59
1:A:277:ILE:O	1:A:277:ILE:CG2	2.49	0.59
1:A:437:GLN:HG2	1:A:948:PHE:CE2	2.36	0.59
1:A:993:THR:HG22	1:A:994:GLY:H	1.67	0.59
1:B:199:THR:HB	1:B:749:THR:CG2	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:482:VAL:O	1:C:486:LEU:HG	2.03	0.59
1:A:379:THR:CG2	1:A:477:ALA:HA	2.33	0.59
1:A:73:ASP:CG	1:A:106:GLN:HE22	2.06	0.59
1:A:99:ASP:O	1:A:102:ILE:HG22	2.02	0.59
1:B:407:ASP:OD1	1:B:407:ASP:N	2.33	0.59
1:B:569:GLN:HG3	1:B:668:LEU:CD1	2.32	0.59
1:C:685:ILE:HD11	1:C:687:GLN:CD	2.22	0.59
1:C:324:VAL:HG23	1:C:326:PRO:HD3	1.85	0.59
1:C:457:ALA:HB1	1:C:468:ARG:CA	2.32	0.59
1:C:84:SER:C	1:C:86:GLY:H	2.06	0.59
1:C:897:ILE:CD1	1:C:950:LYS:HD2	2.33	0.59
1:A:687:GLN:HG2	1:C:316:PHE:CG	2.36	0.59
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.84	0.59
1:B:405:LEU:HD12	1:B:406:VAL:H	1.66	0.59
1:B:943:ILE:O	1:B:947:GLU:HB3	2.02	0.59
1:C:423:GLU:OE1	1:C:426:PRO:HG2	2.03	0.59
1:C:633:ASP:CG	1:C:633:ASP:O	2.40	0.59
1:B:168:ARG:HD3	1:C:69:MET:O	2.00	0.59
1:B:221:GLY:HA3	1:C:780:ARG:NH1	2.18	0.59
1:A:191:ASN:C	1:A:193:LEU:H	2.05	0.59
1:A:418:ARG:HH21	1:A:970:MET:HA	1.66	0.59
1:A:634:TRP:HE3	1:A:995:ALA:HB1	1.65	0.59
1:A:988:PRO:O	1:A:990:VAL:O	2.20	0.59
1:B:35:TYR:HB3	1:B:38:ILE:HG13	1.84	0.59
1:B:835:LYS:HB2	1:B:839:GLU:OE2	2.03	0.59
1:B:914:LEU:O	1:B:917:THR:HB	2.02	0.59
1:C:792:ARG:HB2	1:C:798:MET:CE	2.32	0.59
1:A:843:LEU:HA	1:A:846:GLN:NE2	2.17	0.59
1:B:185:ARG:HG3	1:B:185:ARG:NH1	2.16	0.59
1:B:415:ASN:ND2	1:B:438:ILE:HD13	2.17	0.59
1:B:601:LYS:C	1:B:603:LYS:H	2.05	0.59
1:B:690:LEU:HB2	1:B:694:LYS:CB	2.33	0.59
1:C:102:ILE:O	1:C:105:VAL:N	2.36	0.59
1:C:726:GLN:NE2	1:C:812:GLY:HA3	2.17	0.59
1:A:1025:PHE:O	1:A:1029:VAL:HG23	2.03	0.59
1:A:888:LEU:HD21	1:A:901:VAL:HB	1.84	0.59
1:B:269:GLU:O	1:B:270:LEU:HB2	2.03	0.59
1:B:520:PHE:O	1:B:523:SER:N	2.30	0.59
1:B:598:TYR:HB3	1:B:606:VAL:HG11	1.84	0.59
1:C:110:LYS:HA	1:C:113:LEU:HD12	1.84	0.59
1:C:564:LEU:HD21	1:C:671:ILE:HD12	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:VAL:HG21	1:A:745:ASP:OD2	2.02	0.59
1:A:733:GLN:O	1:A:736:ALA:HB3	2.03	0.59
1:C:144:ASN:ND2	1:C:149:MET:N	2.48	0.59
1:A:324:VAL:C	1:A:325:TYR:CD1	2.77	0.59
1:A:686:ASP:OD1	1:A:690:LEU:HB2	2.03	0.59
1:B:642:ASN:N	1:B:650:ARG:HH12	2.01	0.59
1:B:679:GLY:HA2	1:B:830:GLN:HB3	1.85	0.59
1:B:686:ASP:HB3	1:B:823:PRO:O	2.03	0.59
1:C:158:VAL:HG11	1:C:177:LEU:HD21	1.85	0.59
1:C:425:LEU:N	1:C:426:PRO:HD3	2.18	0.59
1:C:644:VAL:HG11	1:C:667:ASN:CB	2.33	0.59
1:A:166:ILE:HD13	1:A:166:ILE:H	1.63	0.58
1:A:58:GLN:NE2	1:A:816:LEU:HD13	2.17	0.58
1:A:773:VAL:O	1:A:773:VAL:CG1	2.50	0.58
1:A:813:SER:CB	1:A:816:LEU:HD21	2.30	0.58
1:C:65:ILE:HG23	1:C:111:LEU:HD23	1.85	0.58
1:C:786:ILE:O	1:C:786:ILE:CG2	2.50	0.58
1:A:251:LEU:CD1	1:A:262:LEU:HA	2.31	0.58
1:A:263:ARG:NH2	1:A:263:ARG:CB	2.66	0.58
1:A:44:THR:CG2	1:A:89:GLN:CG	2.80	0.58
1:B:328:ASP:OD2	1:B:330:THR:HB	2.04	0.58
1:B:362:PHE:HA	1:B:365:THR:HG22	1.84	0.58
1:B:207:ILE:HG21	1:B:759:VAL:HG11	1.85	0.58
1:B:552:MET:SD	1:B:909:VAL:HG23	2.44	0.58
1:B:918:PHE:CD1	1:B:919:ARG:HD3	2.39	0.58
1:C:452:VAL:O	1:C:932:LEU:HD13	2.02	0.58
1:C:708:LYS:C	1:C:710:PRO:HD3	2.24	0.58
1:A:740:GLY:O	1:A:793:ALA:CB	2.50	0.58
1:B:438:ILE:HD12	1:B:971:ARG:NH1	2.18	0.58
1:B:439:GLN:HE21	1:B:486:LEU:HD11	1.68	0.58
1:B:682:PHE:HD1	1:B:859:TRP:CH2	2.21	0.58
1:A:1:MET:N	1:A:2:PRO:CD	2.65	0.58
1:A:752:ALA:O	1:A:774:MET:HG3	2.02	0.58
1:A:740:GLY:C	1:A:793:ALA:HB1	2.23	0.58
1:B:921:LEU:HD23	1:B:1005:THR:HG22	1.85	0.58
1:B:946:VAL:HG13	1:B:1026:PHE:CD1	2.39	0.58
1:B:198:LEU:HD13	1:B:251:LEU:HD23	1.86	0.58
1:B:144:ASN:CB	1:B:320:GLY:O	2.37	0.58
1:B:366:LEU:O	1:B:369:THR:N	2.36	0.58
1:B:674:LEU:HD23	1:B:675:GLY:N	2.18	0.58
1:B:792:ARG:CB	1:B:798:MET:CE	2.82	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:352:PHE:HD1	1:C:369:THR:HG1	1.51	0.58
1:C:1:MET:HE3	1:C:439:GLN:HE22	1.65	0.58
1:C:914:LEU:O	1:C:915:ALA:HB3	2.03	0.58
1:A:156:ASP:O	1:A:159:ALA:HB3	2.03	0.58
1:A:988:PRO:O	1:A:989:LEU:C	2.42	0.58
1:A:991:ILE:HG22	1:A:991:ILE:O	2.04	0.58
1:B:3:ASN:H	1:B:6:ILE:CG1	2.16	0.58
1:B:973:ARG:N	1:B:974:PRO:HD2	2.17	0.58
1:C:908:GLY:HA2	1:C:1014:ALA:HB2	1.85	0.58
1:C:131:LYS:HB2	1:C:295:THR:CG2	2.33	0.58
1:C:332:PHE:O	1:C:336:SER:HB3	2.03	0.58
1:C:650:ARG:O	1:C:653:ARG:HG2	2.04	0.58
1:C:705:GLU:O	1:C:707:ALA:N	2.36	0.58
1:A:164:ASP:HA	1:A:167:SER:HB2	1.84	0.58
1:A:568:ASP:O	1:A:634:TRP:CH2	2.57	0.58
1:B:414:GLU:O	1:B:973:ARG:HD3	2.04	0.58
1:C:894:SER:CB	1:C:897:ILE:HG13	2.34	0.58
1:C:559:LEU:HD13	1:C:917:THR:HG23	1.86	0.58
1:C:972:LEU:N	1:C:974:PRO:HD2	2.19	0.58
1:A:114:ALA:O	1:A:117:LEU:N	2.34	0.58
1:A:139:VAL:HG12	1:A:327:TYR:HB3	1.84	0.58
1:A:819:TYR:N	1:A:824:SER:HB3	2.13	0.58
1:B:104:GLN:HE21	1:B:108:GLN:HE21	1.50	0.58
1:B:729:ILE:CG1	1:B:730:ASP:H	2.08	0.58
1:B:873:ALA:O	1:B:875:SER:N	2.37	0.58
1:C:1010:GLY:HA2	1:C:1013:THR:HG21	1.86	0.58
1:C:143:ILE:HG23	1:C:284:GLN:HE22	1.68	0.58
1:C:358:PHE:CD1	1:C:977:MET:HE2	2.38	0.58
1:C:764:ASP:O	1:C:765:ARG:C	2.42	0.58
1:A:112:GLN:HG3	1:A:112:GLN:O	2.02	0.58
1:A:350:LEU:HD11	1:A:984:LEU:CB	2.32	0.58
1:B:65:ILE:O	1:B:69:MET:HG2	2.03	0.58
1:C:490:PRO:C	1:C:491:ALA:O	2.37	0.58
1:C:759:VAL:O	1:C:760:ASN:HB3	2.04	0.58
1:A:171:GLY:O	1:A:172:VAL:C	2.42	0.58
1:A:191:ASN:C	1:A:193:LEU:N	2.57	0.58
1:A:400:LEU:HG	1:A:929:VAL:CG1	2.32	0.58
1:A:937:LEU:HD12	1:A:1011:MET:SD	2.43	0.58
1:B:18:ILE:HG22	1:B:19:ILE:N	2.19	0.58
1:B:281:PHE:CE1	1:B:608:SER:HB2	2.39	0.58
1:B:680:PHE:O	1:B:680:PHE:HD1	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:ASN:HD21	1:C:149:MET:N	1.99	0.58
1:C:33:ALA:HB2	1:C:298:ASN:ND2	2.18	0.58
1:C:50:PRO:CD	1:C:125:GLN:HG3	2.34	0.58
1:C:74:ASN:HB3	1:C:95:GLU:HB2	1.86	0.58
1:A:348:ILE:HD11	1:A:372:VAL:CG1	2.34	0.58
1:A:413:VAL:HG23	1:A:493:CYS:HB2	1.86	0.58
1:B:1017:LEU:N	1:B:1017:LEU:HD12	2.18	0.58
1:B:124:GLN:O	1:B:125:GLN:HB2	2.04	0.58
1:C:418:ARG:HD2	1:C:970:MET:HE3	1.85	0.58
1:C:590:VAL:O	1:C:594:VAL:HG23	2.03	0.58
1:C:894:SER:OG	1:C:897:ILE:N	2.25	0.58
1:C:953:MET:SD	1:C:963:ALA:CB	2.92	0.58
1:A:350:LEU:CD1	1:A:984:LEU:HB2	2.34	0.57
1:A:464:GLY:HA2	1:A:467:TYR:HB2	1.86	0.57
1:B:401:ALA:HA	1:B:404:LEU:HB2	1.85	0.57
1:B:639:GLY:HA2	1:B:643:LYS:NZ	2.19	0.57
1:B:929:VAL:O	1:B:933:THR:OG1	2.17	0.57
1:C:576:VAL:HG12	1:C:663:VAL:CG2	2.24	0.57
1:A:2:PRO:O	1:A:6:ILE:HG23	2.04	0.57
1:A:719:ASN:HB2	1:A:828:LEU:CD2	2.33	0.57
1:B:183:ALA:H	1:B:272:GLY:HA2	1.68	0.57
1:B:441:ALA:O	1:B:445:ILE:HG13	2.03	0.57
1:B:670:ALA:H	1:B:862:MET:HE1	1.68	0.57
1:B:699:ARG:CG	1:B:700:ASN:N	2.67	0.57
1:B:1010:GLY:HA2	1:B:1013:THR:CG2	2.35	0.57
1:B:456:MET:HG3	1:B:467:TYR:CB	2.26	0.57
1:C:15:ILE:O	1:C:16:ALA:C	2.41	0.57
1:C:188:MET:HE3	1:C:200:PRO:HB3	1.85	0.57
1:C:415:ASN:ND2	1:C:434:SER:CB	2.62	0.57
1:A:29:LYS:HG2	1:A:29:LYS:O	2.04	0.57
1:A:946:VAL:O	1:A:946:VAL:HG12	2.03	0.57
1:B:1021:PHE:O	1:B:1025:PHE:CD1	2.57	0.57
1:B:445:ILE:CG2	1:B:940:LYS:HG3	2.28	0.57
1:B:975:ILE:O	1:B:979:SER:HB2	2.05	0.57
1:B:350:LEU:HD12	1:B:984:LEU:O	2.03	0.57
1:B:986:VAL:HG12	1:B:990:VAL:HG23	1.85	0.57
1:C:844:MET:O	1:C:847:LEU:CD2	2.52	0.57
1:C:417:GLU:CB	1:C:973:ARG:HH12	2.16	0.57
1:A:193:LEU:HA	1:A:265:VAL:HG13	1.86	0.57
1:A:543:VAL:HG22	1:A:544:LEU:N	2.20	0.57
1:C:593:GLU:O	1:C:597:TYR:N	2.28	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:719:ASN:N	1:C:719:ASN:OD1	2.37	0.57
1:C:728:LYS:CG	1:C:729:ILE:N	2.68	0.57
1:C:190:PRO:CG	1:C:789:TRP:CZ2	2.83	0.57
1:C:897:ILE:HD13	1:C:950:LYS:HD2	1.86	0.57
1:A:947:GLU:O	1:A:950:LYS:O	2.22	0.57
1:B:330:THR:N	1:B:331:PRO:HD2	2.19	0.57
1:B:472:ILE:HG23	1:B:473:THR:H	1.69	0.57
1:B:729:ILE:O	1:B:730:ASP:HB2	2.04	0.57
1:B:84:SER:C	1:B:86:GLY:H	2.08	0.57
1:C:204:ILE:HG12	1:C:759:VAL:HG13	1.85	0.57
1:C:400:LEU:HG	1:C:929:VAL:HG12	1.85	0.57
1:C:997:SER:O	1:C:999:ALA:N	2.37	0.57
1:A:845:GLU:CD	1:A:859:TRP:HE1	2.08	0.57
1:B:280:GLU:CA	1:B:284:GLN:O	2.52	0.57
1:B:420:MET:HE2	1:B:425:LEU:HD23	1.87	0.57
1:B:602:GLU:C	1:B:604:ASN:N	2.58	0.57
1:B:836:SER:OG	1:B:838:GLY:N	2.38	0.57
1:B:873:ALA:HB3	1:B:874:PRO:CD	2.35	0.57
1:A:10:ILE:HG21	1:B:893:GLU:HB2	1.87	0.57
1:C:115:MET:N	1:C:116:PRO:CD	2.67	0.57
1:C:391:ASN:N	1:C:394:THR:CG2	2.67	0.57
1:C:520:PHE:O	1:C:523:SER:N	2.37	0.57
1:C:681:ASP:OD2	1:C:828:LEU:HD11	2.05	0.57
1:C:693:GLU:O	1:C:694:LYS:C	2.41	0.57
1:C:868:LEU:HD13	1:C:868:LEU:O	2.04	0.57
1:A:702:LEU:HD11	1:A:844:MET:CE	2.34	0.57
1:A:800:PRO:O	1:A:803:ALA:HB3	2.05	0.57
1:A:983:ILE:CD1	1:A:983:ILE:C	2.71	0.57
1:C:254:ASN:OD1	1:C:258:SER:O	2.22	0.57
1:A:330:THR:HG22	1:A:331:PRO:N	2.18	0.57
1:A:418:ARG:HH12	1:A:973:ARG:CB	2.18	0.57
1:B:24:GLY:CA	1:B:27:ILE:HG23	2.35	0.57
1:B:732:ASP:O	1:B:734:GLU:N	2.38	0.57
1:B:860:THR:CG2	1:B:861:GLY:N	2.67	0.57
1:B:92:LEU:N	1:B:92:LEU:HD22	2.19	0.57
1:C:484:VAL:HG13	1:C:488:LEU:HB3	1.87	0.57
1:C:764:ASP:OD2	1:C:765:ARG:HD2	2.05	0.57
1:C:894:SER:C	1:C:896:SER:H	2.07	0.57
1:A:993:THR:HG21	1:A:1000:GLN:OE1	2.05	0.57
1:A:445:ILE:HG22	1:A:943:ILE:HD13	1.86	0.57
1:A:489:THR:HB	1:A:490:PRO:HD3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:990:VAL:O	1:A:991:ILE:HB	2.05	0.57
1:B:356:TYR:CE2	1:B:365:THR:HG21	2.40	0.57
1:B:523:SER:O	1:B:526:HIS:HB2	2.05	0.57
1:B:543:VAL:HG12	1:B:543:VAL:O	2.04	0.57
1:B:560:PRO:CB	1:B:836:SER:HB3	2.33	0.57
1:C:203:VAL:O	1:C:204:ILE:C	2.42	0.57
1:C:76:MET:HE2	1:C:93:THR:HG22	1.86	0.57
1:C:8:ARG:HG2	1:C:8:ARG:HH21	1.70	0.57
1:A:172:VAL:HG23	1:A:172:VAL:O	2.05	0.56
1:A:356:TYR:C	1:A:358:PHE:H	2.08	0.56
1:A:522:LYS:N	1:A:522:LYS:HE2	2.20	0.56
1:A:971:ARG:HE	1:A:974:PRO:HG2	1.69	0.56
1:B:143:ILE:HD12	1:B:322:LYS:HB3	1.86	0.56
1:B:143:ILE:HG23	1:B:286:ALA:HB2	1.87	0.56
1:B:219:LEU:CD1	1:B:234:ILE:HG12	2.29	0.56
1:B:4:PHE:O	1:B:5:PHE:HB2	2.05	0.56
1:B:546:LEU:O	1:B:550:VAL:HB	2.04	0.56
1:A:729:ILE:HD13	1:C:234:ILE:HG23	1.86	0.56
1:C:131:LYS:HB2	1:C:295:THR:HG21	1.86	0.56
1:C:418:ARG:CD	1:C:970:MET:CE	2.81	0.56
1:C:463:THR:O	1:C:466:ILE:HD12	2.05	0.56
1:C:758:TYR:CG	1:C:758:TYR:O	2.57	0.56
1:C:777:ALA:O	1:C:779:TYR:N	2.38	0.56
1:C:965:LEU:HG	1:C:966:ASP:N	2.20	0.56
1:A:133:SER:HB3	1:A:136:PHE:CD1	2.40	0.56
1:A:55:LYS:HD3	1:A:816:LEU:HD11	1.87	0.56
1:A:736:ALA:HA	1:A:741:VAL:CG1	2.35	0.56
1:B:174:ASP:OD1	1:B:175:VAL:N	2.38	0.56
1:B:204:ILE:O	1:B:205:THR:C	2.42	0.56
1:B:439:GLN:NE2	1:B:486:LEU:HD11	2.21	0.56
1:C:576:VAL:HG21	1:C:591:LEU:HD22	1.87	0.56
1:C:615:PHE:CD2	1:C:615:PHE:O	2.58	0.56
1:C:713:LEU:CD1	1:C:835:LYS:H	2.16	0.56
1:A:999:ALA:HA	1:A:1002:ALA:HB3	1.88	0.56
1:A:391:ASN:H	1:A:394:THR:HG22	1.70	0.56
1:B:1017:LEU:H	1:B:1017:LEU:CD1	2.18	0.56
1:B:413:VAL:CG1	1:B:414:GLU:H	2.18	0.56
1:B:945:ILE:CG1	1:B:1026:PHE:CE2	2.87	0.56
1:A:200:PRO:HG2	1:A:749:THR:CA	2.29	0.56
1:A:171:GLY:O	1:A:294:ALA:HB2	2.05	0.56
1:A:455:PRO:HB2	1:A:877:TYR:HE1	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:ARG:H	1:A:536:ARG:HD2	1.70	0.56
1:A:607:GLU:HG2	1:A:632:LYS:HG2	1.87	0.56
1:A:223:PRO:CD	1:B:275:TYR:CD2	2.85	0.56
1:B:431:THR:OG1	1:B:494:ALA:HB2	2.05	0.56
1:B:589:LYS:O	1:B:592:ASN:HB2	2.05	0.56
1:B:792:ARG:CB	1:B:798:MET:HE2	2.34	0.56
1:B:986:VAL:HG12	1:B:990:VAL:CG2	2.34	0.56
1:A:113:LEU:CD1	1:C:108:GLN:HE22	2.18	0.56
1:C:568:ASP:OD1	1:C:634:TRP:CD1	2.58	0.56
1:C:663:VAL:O	1:C:664:PHE:HB3	2.05	0.56
1:C:680:PHE:HB3	1:C:841:MET:HE2	1.86	0.56
1:A:991:ILE:CD1	1:A:1008:MET:CG	2.83	0.56
1:A:282:ASN:ND2	1:A:599:LEU:HD11	2.20	0.56
1:A:596:HIS:C	1:A:598:TYR:N	2.59	0.56
1:B:25:LEU:C	1:B:27:ILE:H	2.07	0.56
1:B:358:PHE:HZ	1:B:976:LEU:HD12	1.71	0.56
1:B:989:LEU:HA	1:B:992:SER:HB2	1.87	0.56
1:C:220:GLY:CA	1:C:231:ASN:HD22	2.16	0.56
1:C:695:LEU:O	1:C:696:THR:O	2.24	0.56
1:A:255:GLN:O	1:A:256:ASP:OD1	2.23	0.56
1:A:370:ILE:CG2	1:A:370:ILE:O	2.54	0.56
1:A:455:PRO:O	1:A:458:PHE:HB2	2.05	0.56
1:B:25:LEU:O	1:B:28:LEU:HG	2.05	0.56
1:B:310:LEU:O	1:B:314:GLU:HG3	2.05	0.56
1:B:538:THR:C	1:B:540:ARG:H	2.09	0.56
1:B:671:ILE:O	1:B:673:GLU:HB2	2.05	0.56
1:B:699:ARG:HB3	1:B:699:ARG:HH11	1.71	0.56
1:C:146:ASP:HB2	1:C:148:THR:OG1	2.05	0.56
1:C:181:GLN:OE1	1:C:767:ARG:NE	2.38	0.56
1:C:456:MET:O	1:C:457:ALA:C	2.41	0.56
1:C:56:THR:O	1:C:60:THR:HB	2.06	0.56
1:C:277:ILE:CD1	1:C:620:ARG:NH2	2.66	0.56
1:A:199:THR:HB	1:A:200:PRO:HD2	1.88	0.56
1:A:443:VAL:CG1	1:A:444:GLY:H	2.02	0.56
1:A:481:SER:O	1:A:484:VAL:N	2.38	0.56
1:A:583:THR:O	1:A:584:GLN:C	2.44	0.56
1:B:235:ILE:CD1	1:B:235:ILE:H	2.08	0.56
1:B:378:GLY:O	1:B:381:ALA:HB3	2.06	0.56
1:B:775:SER:CB	1:B:780:ARG:HG3	2.35	0.56
1:B:907:LEU:O	1:B:909:VAL:N	2.38	0.56
1:B:960:LEU:CD1	1:B:961:ILE:N	2.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:983:ILE:CG2	1:C:1008:MET:HG3	2.34	0.56
1:C:34:GLN:HA	1:C:333:VAL:HG11	1.86	0.56
1:C:644:VAL:HG12	1:C:667:ASN:HB2	1.86	0.56
1:C:4:PHE:CD2	1:C:8:ARG:NH1	2.73	0.56
1:A:527:TYR:O	1:A:530:SER:OG	2.17	0.56
1:A:10:ILE:HG12	1:B:893:GLU:O	2.05	0.56
1:A:223:PRO:HD3	1:B:275:TYR:CB	2.36	0.56
1:B:179:GLY:N	1:B:277:ILE:HG21	2.21	0.56
1:B:349:ILE:HG22	1:B:350:LEU:HD23	1.88	0.56
1:C:5:PHE:CE2	1:C:11:PHE:HD2	2.23	0.56
1:C:308:ALA:O	1:C:311:ALA:HB3	2.05	0.56
1:C:34:GLN:O	1:C:35:TYR:CD2	2.59	0.56
1:C:39:ALA:HB2	1:C:673:GLU:CB	2.36	0.56
1:C:726:GLN:CD	1:C:812:GLY:HA3	2.26	0.56
1:C:204:ILE:HG13	1:C:773:VAL:HG11	1.86	0.56
1:C:197:GLN:HB3	1:C:798:MET:HE3	1.86	0.56
1:A:11:PHE:CE1	1:B:890:ALA:HB1	2.40	0.56
1:A:72:ILE:HD12	1:A:72:ILE:N	2.20	0.56
1:B:105:VAL:O	1:B:109:ASN:N	2.32	0.56
1:B:49:TYR:CD1	1:B:122:VAL:HG22	2.41	0.56
1:C:409:ALA:O	1:C:413:VAL:HG12	2.05	0.56
1:C:924:ASP:O	1:C:925:VAL:O	2.23	0.56
1:C:948:PHE:O	1:C:952:LEU:HB2	2.06	0.56
1:A:1:MET:H3	1:A:2:PRO:HD2	1.70	0.56
1:A:741:VAL:HG13	1:A:741:VAL:O	2.05	0.56
1:A:818:ARG:HD3	1:A:821:GLY:C	2.26	0.56
1:B:541:TYR:C	1:B:543:VAL:H	2.08	0.56
1:B:844:MET:C	1:B:846:GLN:H	2.09	0.56
1:B:99:ASP:OD2	1:B:99:ASP:C	2.42	0.56
1:C:166:ILE:CG2	1:C:166:ILE:CA	2.77	0.56
1:C:355:MET:HE2	1:C:355:MET:HA	1.88	0.56
1:C:577:GLN:HB3	1:C:624:THR:CG2	2.36	0.56
1:A:400:LEU:HD11	1:A:1003:VAL:HG13	1.84	0.55
1:A:113:LEU:CD2	1:C:127:VAL:O	2.54	0.55
1:A:298:ASN:HD22	1:A:300:LEU:N	2.04	0.55
1:A:481:SER:OG	1:A:482:VAL:N	2.38	0.55
1:A:982:PHE:O	1:A:985:GLY:N	2.39	0.55
1:B:1026:PHE:HB3	1:B:1030:ARG:NE	2.20	0.55
1:B:355:MET:CE	1:B:369:THR:CG2	2.84	0.55
1:B:405:LEU:HD12	1:B:405:LEU:C	2.26	0.55
1:C:546:LEU:O	1:C:550:VAL:HG12	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:598:TYR:HD2	1:C:606:VAL:HG21	1.71	0.55
1:A:572:PHE:CD1	1:A:572:PHE:N	2.74	0.55
1:A:58:GLN:HE22	1:A:816:LEU:HD13	1.71	0.55
1:A:753:ALA:O	1:A:774:MET:HG2	2.07	0.55
1:A:758:TYR:CG	1:A:758:TYR:O	2.55	0.55
1:B:341:VAL:HG23	1:B:395:MET:CE	2.36	0.55
1:B:435:MET:HA	1:B:435:MET:CE	2.36	0.55
1:B:937:LEU:O	1:B:940:LYS:HB3	2.06	0.55
1:B:969:ARG:HH11	1:B:969:ARG:HG2	1.70	0.55
1:C:247:GLY:HA3	1:C:263:ARG:HE	1.68	0.55
1:C:57:VAL:HB	1:C:58:GLN:HE21	1.70	0.55
1:A:999:ALA:HA	1:A:1002:ALA:CB	2.36	0.55
1:A:9:PRO:HD2	1:A:10:ILE:H	1.72	0.55
1:A:375:VAL:HG21	1:A:481:SER:HA	1.88	0.55
1:A:818:ARG:HB2	1:A:823:PRO:HA	1.88	0.55
1:A:841:MET:O	1:A:845:GLU:HG3	2.07	0.55
1:A:963:ALA:O	1:A:964:THR:C	2.45	0.55
1:B:115:MET:HE1	1:B:118:LEU:HD22	1.88	0.55
1:B:399:VAL:HG12	1:B:400:LEU:N	2.20	0.55
1:B:964:THR:O	1:B:968:VAL:HG23	2.05	0.55
1:C:997:SER:HA	1:C:1000:GLN:OE1	2.07	0.55
1:C:391:ASN:H	1:C:394:THR:CG2	2.18	0.55
1:C:418:ARG:C	1:C:420:MET:N	2.54	0.55
1:C:672:VAL:HG12	1:C:672:VAL:O	2.05	0.55
1:A:214:VAL:HG23	1:A:237:GLN:HB3	1.87	0.55
1:A:726:GLN:HG2	1:A:810:GLU:O	2.07	0.55
1:B:314:GLU:O	1:B:316:PHE:N	2.40	0.55
1:B:674:LEU:HD13	1:B:860:THR:HG22	1.84	0.55
1:B:896:SER:HA	1:B:899:PHE:HD2	1.71	0.55
1:C:545:TYR:OH	1:C:1021:PHE:HB3	2.05	0.55
1:C:34:GLN:HA	1:C:333:VAL:CG1	2.36	0.55
1:C:572:PHE:CZ	1:C:629:VAL:HG11	2.41	0.55
1:A:425:LEU:HB3	1:A:426:PRO:HD2	1.88	0.55
1:B:1007:VAL:HG22	1:B:1007:VAL:O	2.06	0.55
1:B:36:PRO:HD2	1:B:38:ILE:HD11	1.88	0.55
1:C:379:THR:CG2	1:C:477:ALA:HB2	2.35	0.55
1:C:428:LYS:O	1:C:432:ARG:HB2	2.06	0.55
1:C:530:SER:O	1:C:534:ILE:CG2	2.54	0.55
1:C:657:GLN:C	1:C:659:LYS:H	2.09	0.55
1:A:309:GLU:O	1:A:313:MET:HG2	2.06	0.55
1:A:44:THR:HA	1:A:91:THR:HA	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:756:GLY:CA	1:A:774:MET:HG3	2.37	0.55
1:A:973:ARG:N	1:A:974:PRO:CD	2.69	0.55
1:B:452:VAL:O	1:B:453:PHE:CB	2.55	0.55
1:B:7:ASP:O	1:B:8:ARG:CB	2.55	0.55
1:B:990:VAL:HG13	1:B:1005:THR:HG1	1.69	0.55
1:C:177:LEU:HD13	1:C:179:GLY:C	2.27	0.55
1:C:545:TYR:CZ	1:C:1025:PHE:CZ	2.94	0.55
1:C:204:ILE:HG12	1:C:759:VAL:CG1	2.37	0.55
1:A:298:ASN:O	1:A:299:ALA:C	2.44	0.55
1:A:425:LEU:H	1:A:425:LEU:CD1	2.18	0.55
1:B:1022:VAL:CG2	1:B:1023:PRO:CD	2.83	0.55
1:B:207:ILE:CG2	1:B:759:VAL:HG11	2.37	0.55
1:B:224:PRO:O	1:B:224:PRO:CD	2.54	0.55
1:B:404:LEU:HD13	1:B:449:LEU:CD1	2.31	0.55
1:B:68:ASN:O	1:B:70:ASN:N	2.37	0.55
1:C:536:ARG:HH21	1:C:536:ARG:HG2	1.71	0.55
1:C:703:LEU:O	1:C:706:ALA:HB3	2.06	0.55
1:C:758:TYR:HD1	1:C:758:TYR:N	2.02	0.55
1:C:758:TYR:HD2	1:C:770:LYS:HE2	1.70	0.55
1:A:106:GLN:O	1:A:107:VAL:C	2.42	0.55
1:A:298:ASN:HD21	1:A:300:LEU:H	1.54	0.55
1:A:621:GLY:C	1:A:623:ASN:H	2.10	0.55
1:A:764:ASP:HB3	1:A:769:LYS:HD2	1.88	0.55
1:A:455:PRO:HB2	1:A:877:TYR:CE1	2.42	0.55
1:B:177:LEU:C	1:B:177:LEU:HD12	2.27	0.55
1:B:191:ASN:O	1:B:194:ASN:HB3	2.06	0.55
1:B:330:THR:N	1:B:331:PRO:CD	2.70	0.55
1:B:472:ILE:HG23	1:B:473:THR:N	2.21	0.55
1:B:946:VAL:HG22	1:B:1026:PHE:HZ	1.55	0.55
1:B:983:ILE:HG23	1:B:1008:MET:HG2	1.88	0.55
1:C:291:ILE:HG22	1:C:291:ILE:O	1.99	0.55
1:A:280:GLU:HB2	1:A:284:GLN:O	2.07	0.55
1:A:405:LEU:O	1:A:406:VAL:C	2.46	0.55
1:A:542:LEU:CD2	1:A:1028:VAL:HG11	2.37	0.55
1:B:470:PHE:CE2	1:B:929:VAL:HG21	2.41	0.55
1:B:762:PHE:HE1	1:B:764:ASP:HB2	1.72	0.55
1:B:927:PHE:CZ	1:B:931:LEU:HD21	2.41	0.55
1:B:988:PRO:C	1:B:990:VAL:H	2.10	0.55
1:C:26:ALA:O	1:C:30:LEU:CG	2.53	0.55
1:A:255:GLN:N	1:A:255:GLN:OE1	2.40	0.55
1:A:528:THR:HG21	1:A:969:ARG:NE	2.17	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:TRP:O	1:B:17:ILE:HG12	2.06	0.55
1:B:547:ILE:O	1:B:550:VAL:O	2.25	0.55
1:B:638:PRO:HG2	1:B:639:GLY:H	1.72	0.55
1:B:6:ILE:HA	1:B:491:ALA:CA	2.37	0.55
1:B:350:LEU:HD13	1:B:984:LEU:CD1	2.37	0.55
1:C:166:ILE:C	1:C:167:SER:CA	2.65	0.55
1:C:355:MET:CE	1:C:355:MET:HA	2.37	0.55
1:C:598:TYR:CD2	1:C:606:VAL:HG21	2.42	0.55
1:C:717:ARG:HH12	1:C:829:GLY:HA2	1.71	0.55
1:A:644:VAL:O	1:A:646:ALA:N	2.40	0.54
1:B:226:LYS:CA	1:B:226:LYS:HE3	2.19	0.54
1:B:410:ILE:C	1:B:412:VAL:H	2.10	0.54
1:B:429:GLU:HA	1:B:432:ARG:HB3	1.87	0.54
1:B:425:LEU:HB3	1:B:498:LYS:O	2.06	0.54
1:B:961:ILE:O	1:B:965:LEU:HB2	2.07	0.54
1:C:326:PRO:O	1:C:327:TYR:C	2.43	0.54
1:A:228:GLN:HG2	1:B:781:MET:CG	2.32	0.54
1:A:307:ARG:NH1	1:A:325:TYR:CE2	2.75	0.54
1:A:309:GLU:O	1:A:311:ALA:O	2.25	0.54
1:A:886:LEU:O	1:A:887:CYS:C	2.46	0.54
1:B:602:GLU:CD	1:B:650:ARG:HH21	2.11	0.54
1:B:921:LEU:H	1:B:921:LEU:CD1	2.19	0.54
1:C:166:ILE:CG1	1:C:166:ILE:CA	2.77	0.54
1:C:448:VAL:O	1:C:448:VAL:HG12	2.07	0.54
1:C:688:ALA:O	1:C:690:LEU:N	2.40	0.54
1:C:939:ALA:O	1:C:943:ILE:CG1	2.55	0.54
1:A:300:LEU:HD22	1:A:334:LYS:HG3	1.88	0.54
1:A:445:ILE:HD13	1:A:940:LYS:CE	2.37	0.54
1:B:218:GLN:HA	1:B:234:ILE:HG13	1.88	0.54
1:B:367:ILE:HG12	1:B:492:LEU:HD13	1.90	0.54
1:B:639:GLY:O	1:B:641:GLU:HG3	2.07	0.54
1:B:70:ASN:N	1:B:70:ASN:ND2	2.56	0.54
1:C:331:PRO:O	1:C:335:ILE:HD12	2.08	0.54
1:C:485:ALA:O	1:C:490:PRO:HD3	2.08	0.54
1:C:637:ARG:HB3	1:C:642:ASN:CB	2.37	0.54
1:C:666:PHE:CD2	1:C:666:PHE:N	2.75	0.54
1:C:858:ASP:OD1	1:C:859:TRP:N	2.39	0.54
1:A:171:GLY:O	1:A:173:GLY:N	2.41	0.54
1:A:284:GLN:HE21	1:A:284:GLN:HA	1.73	0.54
1:A:281:PHE:N	1:A:284:GLN:O	2.38	0.54
1:A:818:ARG:HA	1:A:824:SER:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:892:TYR:C	1:B:894:SER:H	2.09	0.54
1:B:976:LEU:O	1:B:980:LEU:HD12	2.07	0.54
1:B:987:MET:N	1:B:988:PRO:CD	2.70	0.54
1:C:92:LEU:CD1	1:C:92:LEU:N	2.68	0.54
1:C:946:VAL:O	1:C:946:VAL:CG1	2.56	0.54
1:A:185:ARG:C	1:A:186:ILE:HG13	2.27	0.54
1:A:28:LEU:H	1:A:28:LEU:CD1	2.20	0.54
1:A:544:LEU:O	1:A:547:ILE:HB	2.06	0.54
1:A:759:VAL:HG12	1:A:760:ASN:N	2.21	0.54
1:B:493:CYS:O	1:B:494:ALA:CB	2.54	0.54
1:B:605:ASN:HD21	1:B:642:ASN:ND2	2.05	0.54
1:B:911:GLY:HA3	1:B:1013:THR:CG2	2.22	0.54
1:B:438:ILE:CD1	1:B:971:ARG:NH1	2.70	0.54
1:A:781:MET:HE3	1:C:228:GLN:OE1	2.08	0.54
1:C:337:ILE:HD13	1:C:337:ILE:C	2.27	0.54
1:C:49:TYR:HB3	1:C:52:ALA:HB3	1.89	0.54
1:C:758:TYR:HB3	1:C:772:TYR:CD2	2.42	0.54
1:A:342:LYS:O	1:A:343:THR:C	2.45	0.54
1:A:190:PRO:HG3	1:A:789:TRP:CZ2	2.43	0.54
1:A:911:GLY:N	1:A:914:LEU:HD13	2.23	0.54
1:A:904:VAL:HG21	1:A:942:ALA:HB2	1.88	0.54
1:A:418:ARG:NH2	1:A:970:MET:HA	2.23	0.54
1:B:325:TYR:O	1:B:326:PRO:O	2.25	0.54
1:B:960:LEU:C	1:B:960:LEU:HD13	2.27	0.54
1:C:945:ILE:HG23	1:C:1022:VAL:HG11	1.90	0.54
1:C:189:ASN:HD22	1:C:189:ASN:C	2.11	0.54
1:C:346:GLU:O	1:C:349:ILE:HB	2.08	0.54
1:C:419:VAL:HA	1:C:422:GLU:HB3	1.89	0.54
1:C:801:PHE:HA	1:C:804:PHE:CZ	2.43	0.54
1:C:850:LYS:O	1:C:851:LEU:O	2.25	0.54
1:A:277:ILE:C	1:A:277:ILE:HD13	2.28	0.54
1:A:66:GLU:O	1:A:68:ASN:N	2.40	0.54
1:B:146:ASP:O	1:B:147:GLY:C	2.44	0.54
1:C:1017:LEU:CD2	1:C:1017:LEU:O	2.49	0.54
1:C:118:LEU:CD1	1:C:118:LEU:N	2.69	0.54
1:C:685:ILE:O	1:C:685:ILE:HG13	2.05	0.54
1:C:687:GLN:HG2	1:C:856:GLY:H	1.72	0.54
1:C:4:PHE:CB	1:C:8:ARG:NH2	2.68	0.54
1:A:5:PHE:HD1	1:A:12:ALA:HB2	1.61	0.54
1:A:18:ILE:O	1:A:21:LEU:N	2.40	0.54
1:A:28:LEU:HD13	1:A:28:LEU:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:VAL:CG1	1:A:444:GLY:N	2.64	0.54
1:A:534:ILE:HD12	1:A:540:ARG:NH2	2.23	0.54
1:B:762:PHE:CE1	1:B:764:ASP:HB2	2.42	0.54
1:B:897:ILE:HG13	1:B:898:PRO:CD	2.37	0.54
1:C:354:VAL:C	1:C:356:TYR:H	2.11	0.54
1:C:578:LEU:HB3	1:C:579:PRO:CD	2.35	0.54
1:A:568:ASP:OD1	1:A:634:TRP:CZ3	2.61	0.54
1:A:635:ALA:C	1:A:637:ARG:N	2.60	0.54
1:B:104:GLN:O	1:B:107:VAL:N	2.41	0.54
1:B:735:LYS:O	1:B:738:ALA:HB3	2.08	0.54
1:B:850:LYS:CA	1:B:852:PRO:HD3	2.38	0.54
1:B:873:ALA:C	1:B:875:SER:H	2.10	0.54
1:A:781:MET:HE1	1:C:228:GLN:CG	2.38	0.54
1:C:331:PRO:C	1:C:335:ILE:HD12	2.29	0.54
1:C:5:PHE:HA	1:C:8:ARG:O	2.07	0.54
1:C:634:TRP:O	1:C:637:ARG:N	2.29	0.54
1:C:832:ALA:HB1	1:C:833:PRO:HD2	1.90	0.54
1:C:909:VAL:HG12	1:C:931:LEU:CD1	2.38	0.54
1:C:950:LYS:N	1:C:953:MET:HE2	2.14	0.54
1:C:988:PRO:O	1:C:989:LEU:C	2.45	0.54
1:A:42:ALA:O	1:A:43:VAL:HG23	2.08	0.54
1:A:574:THR:HG22	1:A:665:ALA:HB2	1.90	0.54
1:A:925:VAL:HA	1:A:928:GLN:NE2	2.23	0.54
1:B:140:VAL:CG1	1:B:291:ILE:HD12	2.38	0.54
1:B:317:PHE:CD1	1:B:321:LEU:HD23	2.43	0.54
1:B:533:GLY:O	1:B:537:SER:OG	2.24	0.54
1:B:680:PHE:C	1:B:680:PHE:CD1	2.82	0.54
1:B:43:VAL:HG23	1:B:94:PHE:HE2	1.72	0.54
1:C:423:GLU:HB3	1:C:426:PRO:HG3	1.88	0.54
1:A:46:SER:HA	1:A:88:VAL:O	2.08	0.53
1:B:146:ASP:O	1:B:148:THR:N	2.41	0.53
1:B:58:GLN:HB2	1:B:82:SER:CB	2.38	0.53
1:B:646:ALA:O	1:B:647:ILE:C	2.47	0.53
1:B:737:GLN:HG2	1:B:737:GLN:O	2.07	0.53
1:B:7:ASP:CG	1:B:8:ARG:HH21	2.12	0.53
1:B:888:LEU:HB2	1:B:898:PRO:HB3	1.90	0.53
1:C:169:THR:O	1:C:170:SER:C	2.41	0.53
1:C:245:GLU:O	1:C:246:PHE:C	2.47	0.53
1:C:457:ALA:CB	1:C:468:ARG:CA	2.86	0.53
1:C:578:LEU:HD21	1:C:590:VAL:HG21	1.89	0.53
1:C:643:LYS:O	1:C:647:ILE:CG1	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:713:LEU:HD12	1:C:834:GLY:HA3	1.89	0.53
1:A:164:ASP:OD1	1:A:164:ASP:N	2.41	0.53
1:A:533:GLY:O	1:A:535:LEU:HB2	2.08	0.53
1:A:568:ASP:CB	1:A:634:TRP:HZ3	2.15	0.53
1:A:699:ARG:NH2	1:A:722:GLU:OE1	2.38	0.53
1:A:729:ILE:HD13	1:C:234:ILE:CG2	2.39	0.53
1:B:231:ASN:C	1:B:231:ASN:ND2	2.59	0.53
1:B:280:GLU:HB2	1:B:284:GLN:C	2.29	0.53
1:B:701:GLN:OE1	1:B:851:LEU:HD11	2.08	0.53
1:B:899:PHE:O	1:B:903:LEU:HG	2.08	0.53
1:B:901:VAL:HG13	1:B:942:ALA:CB	2.39	0.53
1:B:95:GLU:O	1:B:98:THR:HB	2.08	0.53
1:C:952:LEU:HD11	1:C:966:ASP:HB2	1.90	0.53
1:A:1015:THR:O	1:A:1017:LEU:N	2.41	0.53
1:A:61:VAL:C	1:A:65:ILE:CG2	2.75	0.53
1:A:87:THR:HG22	1:A:88:VAL:N	2.24	0.53
1:A:991:ILE:HD11	1:A:1008:MET:HB2	1.89	0.53
1:B:566:ASP:O	1:B:567:GLU:O	2.25	0.53
1:B:644:VAL:O	1:B:645:GLU:C	2.45	0.53
1:B:65:ILE:CG2	1:B:90:ILE:HD12	2.38	0.53
1:B:692:HIS:C	1:B:692:HIS:ND1	2.57	0.53
1:B:905:VAL:N	1:B:906:PRO:HD2	2.24	0.53
1:A:113:LEU:HD23	1:C:127:VAL:O	2.08	0.53
1:A:128:SER:CB	1:B:113:LEU:HD22	2.39	0.53
1:A:173:GLY:O	1:A:174:ASP:HB2	2.09	0.53
1:A:559:LEU:HD12	1:A:560:PRO:CD	2.37	0.53
1:A:568:ASP:CG	1:A:637:ARG:HH12	2.10	0.53
1:A:884:VAL:O	1:A:888:LEU:HB2	2.09	0.53
1:A:108:GLN:OE1	1:B:112:GLN:NE2	2.41	0.53
1:C:1014:ALA:O	1:C:1018:ALA:HB3	2.09	0.53
1:C:158:VAL:HG12	1:C:159:ALA:N	2.23	0.53
1:A:1015:THR:C	1:A:1017:LEU:H	2.11	0.53
1:A:348:ILE:O	1:A:351:VAL:N	2.42	0.53
1:A:371:ALA:O	1:A:372:VAL:O	2.27	0.53
1:A:282:ASN:ND2	1:A:609:VAL:H	2.07	0.53
1:A:576:VAL:HB	1:A:663:VAL:HG22	1.89	0.53
1:A:740:GLY:O	1:A:794:ALA:N	2.32	0.53
1:A:988:PRO:O	1:A:990:VAL:N	2.42	0.53
1:B:16:ALA:HB1	1:B:374:VAL:HG21	1.90	0.53
1:B:210:GLN:HG3	1:B:249:ILE:CG2	2.36	0.53
1:B:545:TYR:C	1:B:547:ILE:N	2.59	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:945:ILE:CG2	1:C:1022:VAL:HG11	2.39	0.53
1:C:591:LEU:HD23	1:C:613:ASN:HB2	1.91	0.53
1:C:666:PHE:HD2	1:C:666:PHE:N	2.07	0.53
1:A:1011:MET:CE	1:A:1011:MET:HA	2.39	0.53
1:A:107:VAL:O	1:A:110:LYS:HB3	2.08	0.53
1:A:145:THR:HG23	1:A:145:THR:O	2.09	0.53
1:A:294:ALA:HB3	1:A:297:ALA:HB3	1.91	0.53
1:A:515:TRP:HD1	1:A:516:PHE:HB2	1.74	0.53
1:A:685:ILE:HD11	1:A:819:TYR:HD1	1.73	0.53
1:A:532:GLY:HA2	1:A:965:LEU:HD11	1.91	0.53
1:B:13:TRP:CE3	1:B:488:LEU:HD21	2.43	0.53
1:B:328:ASP:C	1:B:328:ASP:OD2	2.46	0.53
1:B:525:HIS:O	1:B:529:ASP:OD2	2.27	0.53
1:B:579:PRO:HD3	1:B:660:ASP:O	2.09	0.53
1:B:690:LEU:HB2	1:B:694:LYS:HB2	1.89	0.53
1:B:844:MET:O	1:B:846:GLN:N	2.41	0.53
1:C:989:LEU:HD12	1:C:1000:GLN:CB	2.39	0.53
1:C:92:LEU:HD22	1:C:107:VAL:HG21	1.91	0.53
1:C:2:PRO:C	1:C:6:ILE:HG13	2.28	0.53
1:C:305:ALA:O	1:C:309:GLU:N	2.41	0.53
1:C:451:ALA:O	1:C:455:PRO:CD	2.57	0.53
1:C:989:LEU:HB3	1:C:1004:GLY:HA3	1.91	0.53
1:A:965:LEU:O	1:A:969:ARG:CG	2.39	0.53
1:B:188:MET:HB2	1:B:775:SER:HA	1.89	0.53
1:B:199:THR:N	1:B:202:ASP:OD2	2.40	0.53
1:B:314:GLU:N	1:B:315:PRO:CD	2.72	0.53
1:B:317:PHE:CE2	1:B:323:ILE:HD11	2.44	0.53
1:B:317:PHE:HE2	1:B:323:ILE:HD11	1.74	0.53
1:B:357:LEU:O	1:B:357:LEU:HD12	2.08	0.53
1:C:754:TRP:CZ2	1:C:786:ILE:HG13	2.44	0.53
1:C:966:ASP:HA	1:C:969:ARG:HB2	1.91	0.53
1:A:185:ARG:O	1:A:186:ILE:HG12	2.08	0.53
1:A:230:LEU:HD23	1:A:230:LEU:H	1.73	0.53
1:A:307:ARG:NH1	1:A:325:TYR:CD2	2.76	0.53
1:A:633:ASP:O	1:A:635:ALA:N	2.42	0.53
1:A:783:PRO:C	1:A:784:ASP:O	2.46	0.53
1:A:935:ILE:O	1:A:935:ILE:CG2	2.57	0.53
1:B:763:ILE:HD11	1:C:59:ASP:CB	2.37	0.53
1:C:2:PRO:O	1:C:6:ILE:HG13	2.09	0.53
1:C:396:PHE:CE1	1:C:999:ALA:HB1	2.44	0.53
1:C:533:GLY:O	1:C:536:ARG:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:658:ILE:HD12	1:C:658:ILE:H	1.74	0.53
1:C:713:LEU:HB2	1:C:832:ALA:CB	2.37	0.53
1:C:847:LEU:N	1:C:847:LEU:CD2	2.70	0.53
1:C:868:LEU:O	1:C:869:SER:CB	2.56	0.53
1:A:180:SER:O	1:A:181:GLN:HB2	2.09	0.53
1:A:467:TYR:HE1	1:A:925:VAL:HG22	1.73	0.53
1:B:1025:PHE:H	1:B:1028:VAL:HG21	1.74	0.53
1:B:228:GLN:NE2	1:C:781:MET:HE3	2.24	0.53
1:B:187:TRP:HZ3	1:B:774:MET:HE3	1.73	0.53
1:C:894:SER:O	1:C:896:SER:N	2.42	0.53
1:A:222:THR:HG22	1:A:223:PRO:HD2	1.91	0.53
1:A:405:LEU:HD22	1:A:406:VAL:CA	2.38	0.53
1:B:111:LEU:O	1:B:113:LEU:N	2.42	0.53
1:B:518:ARG:HA	1:B:521:GLU:CG	2.39	0.53
1:C:1029:VAL:O	1:C:1033:PHE:CD2	2.62	0.53
1:A:780:ARG:NH2	1:C:223:PRO:HD2	2.24	0.53
1:A:166:ILE:O	1:A:169:THR:HG23	2.09	0.52
1:A:189:ASN:ND2	1:A:192:GLU:HB2	2.22	0.52
1:A:379:THR:HG21	1:A:477:ALA:HA	1.91	0.52
1:B:251:LEU:HD11	1:B:262:LEU:HG	1.91	0.52
1:B:448:VAL:O	1:B:452:VAL:CG2	2.57	0.52
1:B:705:GLU:C	1:B:707:ALA:O	2.47	0.52
1:B:703:LEU:O	1:B:705:GLU:HB2	2.09	0.52
1:C:280:GLU:HB3	1:C:284:GLN:O	2.09	0.52
1:C:287:SER:OG	1:C:288:GLY:N	2.42	0.52
1:B:225:VAL:N	1:C:781:MET:HE2	2.17	0.52
1:A:578:LEU:HD21	1:A:587:THR:HA	1.91	0.52
1:A:593:GLU:O	1:A:596:HIS:N	2.42	0.52
1:B:262:LEU:CD2	1:B:266:ALA:HB3	2.38	0.52
1:B:776:GLU:CG	1:B:777:ALA:N	2.72	0.52
1:B:972:LEU:O	1:B:976:LEU:HD23	2.08	0.52
1:C:156:ASP:O	1:C:157:TYR:C	2.47	0.52
1:C:50:PRO:HD3	1:C:125:GLN:HG3	1.91	0.52
1:C:57:VAL:HG12	1:C:88:VAL:HG22	1.90	0.52
1:A:541:TYR:O	1:A:543:VAL:O	2.26	0.52
1:A:706:ALA:HB3	1:A:716:VAL:HG21	1.92	0.52
1:A:775:SER:HB2	1:A:789:TRP:CZ2	2.45	0.52
1:A:820:ASN:O	1:A:822:LEU:HD22	2.10	0.52
1:B:114:ALA:O	1:B:115:MET:C	2.47	0.52
1:B:578:LEU:HD12	1:B:586:ARG:CZ	2.39	0.52
1:B:791:VAL:HG21	1:B:801:PHE:HE2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:849:SER:O	1:B:850:LYS:HE2	2.09	0.52
1:B:936:GLY:O	1:B:937:LEU:C	2.47	0.52
1:C:102:ILE:N	1:C:102:ILE:HD13	2.23	0.52
1:C:14:VAL:HG13	1:C:15:ILE:N	2.23	0.52
1:C:491:ALA:O	1:C:493:CYS:N	2.34	0.52
1:A:138:MET:CE	1:A:306:ILE:HD13	2.32	0.52
1:A:727:PHE:CE2	1:A:729:ILE:HD11	2.45	0.52
1:A:813:SER:CB	1:A:816:LEU:CD2	2.87	0.52
1:C:545:TYR:CZ	1:C:1021:PHE:CG	2.97	0.52
1:C:528:THR:O	1:C:528:THR:HG22	2.09	0.52
1:C:699:ARG:O	1:C:700:ASN:C	2.48	0.52
1:A:144:ASN:ND2	1:A:320:GLY:O	2.42	0.52
1:A:14:VAL:HG11	1:B:886:LEU:O	2.10	0.52
1:A:325:TYR:CD1	1:A:325:TYR:N	2.75	0.52
1:A:354:VAL:O	1:A:355:MET:HB3	2.09	0.52
1:A:344:LEU:HD22	1:A:376:LEU:HD11	1.92	0.52
1:A:600:THR:O	1:A:601:LYS:CB	2.57	0.52
1:A:644:VAL:C	1:A:646:ALA:N	2.60	0.52
1:B:439:GLN:HA	1:B:442:LEU:CD1	2.38	0.52
1:B:566:ASP:N	1:B:566:ASP:OD1	2.42	0.52
1:B:136:PHE:CE1	1:B:617:PHE:CZ	2.86	0.52
1:B:697:GLN:O	1:B:698:ALA:C	2.47	0.52
1:B:801:PHE:HA	1:B:804:PHE:CE1	2.44	0.52
1:B:889:ALA:O	1:B:892:TYR:O	2.27	0.52
1:C:536:ARG:C	1:C:538:THR:H	2.13	0.52
1:C:697:GLN:O	1:C:698:ALA:C	2.44	0.52
1:C:997:SER:O	1:C:1000:GLN:N	2.42	0.52
1:A:49:TYR:CE2	1:A:121:GLU:HG2	2.40	0.52
1:A:780:ARG:CG	1:A:780:ARG:NH1	2.69	0.52
1:A:822:LEU:O	1:A:823:PRO:C	2.48	0.52
1:B:190:PRO:CG	1:B:779:TYR:CG	2.93	0.52
1:C:950:LYS:NZ	1:C:1030:ARG:NE	2.57	0.52
1:C:218:GLN:HG2	1:C:232:ALA:O	2.08	0.52
1:C:367:ILE:O	1:C:367:ILE:HD12	2.10	0.52
1:C:532:GLY:O	1:C:534:ILE:HD12	2.09	0.52
1:C:554:TYR:CD1	1:C:558:ARG:NH2	2.68	0.52
1:C:827:ILE:HG22	1:C:827:ILE:O	2.09	0.52
1:B:129:VAL:O	1:B:129:VAL:CG1	2.51	0.52
1:B:238:THR:OG1	1:B:239:ARG:N	2.42	0.52
1:B:525:HIS:O	1:B:529:ASP:HB2	2.10	0.52
1:A:219:LEU:HD22	1:B:781:MET:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:402:ILE:O	1:C:406:VAL:CG2	2.56	0.52
1:C:485:ALA:HA	1:C:489:THR:OG1	2.09	0.52
1:A:514:GLY:O	1:A:518:ARG:HB2	2.08	0.52
1:B:921:LEU:HD22	1:B:1005:THR:HG22	1.91	0.52
1:B:160:ALA:HB2	1:B:181:GLN:OE1	2.09	0.52
1:B:578:LEU:HB2	1:B:623:ASN:HB2	1.92	0.52
1:C:1024:VAL:CG1	1:C:1028:VAL:CG2	2.88	0.52
1:C:552:MET:O	1:C:554:TYR:N	2.43	0.52
1:C:327:TYR:CB	1:C:628:PHE:HB3	2.39	0.52
1:A:313:MET:C	1:A:315:PRO:CD	2.77	0.52
1:A:643:LYS:O	1:A:647:ILE:HG13	2.10	0.52
1:A:671:ILE:O	1:A:672:VAL:C	2.47	0.52
1:A:978:THR:CG2	1:A:979:SER:N	2.72	0.52
1:B:157:TYR:CE1	1:B:318:PRO:HD3	2.44	0.52
1:B:224:PRO:O	1:B:224:PRO:HD2	2.09	0.52
1:B:831:ALA:HB2	1:B:840:ALA:CB	2.39	0.52
1:C:1022:VAL:O	1:C:1023:PRO:C	2.47	0.52
1:C:167:SER:N	1:C:167:SER:CB	2.65	0.52
1:C:409:ALA:O	1:C:410:ILE:O	2.28	0.52
1:A:183:ALA:N	1:A:271:GLY:O	2.41	0.52
1:A:1:MET:H3	1:A:2:PRO:CD	2.23	0.52
1:A:325:TYR:HD1	1:A:325:TYR:N	2.08	0.52
1:A:449:LEU:O	1:A:453:PHE:HD1	1.92	0.52
1:A:516:PHE:O	1:A:518:ARG:N	2.33	0.52
1:A:594:VAL:HA	1:A:655:PHE:HE2	1.69	0.52
1:B:1012:VAL:HG22	1:B:1013:THR:H	1.75	0.52
1:B:396:PHE:CD2	1:B:1003:VAL:HG21	2.45	0.52
1:B:59:ASP:HA	1:B:63:GLN:HB2	1.92	0.52
1:B:659:LYS:HD3	1:B:659:LYS:C	2.30	0.52
1:B:867:ARG:HG2	1:B:867:ARG:HH11	1.75	0.52
1:B:970:MET:HA	1:B:970:MET:CE	2.40	0.52
1:B:940:LYS:NZ	1:B:978:THR:CG2	2.72	0.52
1:C:885:PHE:CD1	1:C:886:LEU:N	2.78	0.52
1:C:893:GLU:HG3	1:C:893:GLU:O	2.10	0.52
1:A:426:PRO:CB	1:A:427:PRO:HD2	2.40	0.51
1:A:682:PHE:CZ	1:A:857:TYR:HB2	2.44	0.51
1:A:924:ASP:O	1:A:927:PHE:N	2.36	0.51
1:B:1017:LEU:H	1:B:1017:LEU:HD12	1.75	0.51
1:B:287:SER:OG	1:B:288:GLY:N	2.41	0.51
1:B:2:PRO:C	1:B:4:PHE:H	2.13	0.51
1:B:578:LEU:CD1	1:B:586:ARG:NH2	2.68	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:493:CYS:SG	1:C:493:CYS:O	2.68	0.51
1:C:710:PRO:O	1:C:712:MET:O	2.28	0.51
1:C:950:LYS:O	1:C:954:ASP:HB2	2.09	0.51
1:A:189:ASN:O	1:A:189:ASN:OD1	2.29	0.51
1:A:330:THR:O	1:A:331:PRO:C	2.49	0.51
1:A:418:ARG:HH11	1:A:973:ARG:NE	2.09	0.51
1:A:536:ARG:C	1:A:538:THR:H	2.14	0.51
1:B:339:GLU:HB3	1:B:1000:GLN:HE22	1.75	0.51
1:B:219:LEU:HD23	1:C:783:PRO:CG	2.39	0.51
1:B:372:VAL:HB	1:B:402:ILE:CD1	2.40	0.51
1:B:485:ALA:HA	1:B:489:THR:CB	2.39	0.51
1:B:605:ASN:O	1:B:632:LYS:HG2	2.10	0.51
1:B:652:THR:O	1:B:656:SER:HB3	2.10	0.51
1:C:146:ASP:CB	1:C:148:THR:HG23	2.40	0.51
1:C:167:SER:N	1:C:175:VAL:HG21	2.20	0.51
1:C:909:VAL:HG12	1:C:931:LEU:HD11	1.93	0.51
1:A:11:PHE:C	1:A:13:TRP:H	2.14	0.51
1:A:330:THR:HG23	1:A:334:LYS:HE2	1.93	0.51
1:A:428:LYS:CE	1:A:429:GLU:OE2	2.58	0.51
1:A:47:ALA:HB3	1:A:88:VAL:HG21	1.92	0.51
1:B:211:ASN:ND2	1:B:246:PHE:HZ	2.09	0.51
1:B:395:MET:O	1:B:396:PHE:C	2.49	0.51
1:B:563:PHE:HB2	1:B:866:GLU:HG2	1.92	0.51
1:B:714:THR:HG22	1:B:831:ALA:HA	1.92	0.51
1:C:189:ASN:HD22	1:C:190:PRO:N	2.07	0.51
1:C:183:ALA:N	1:C:271:GLY:O	2.43	0.51
1:C:310:LEU:O	1:C:313:MET:HB2	2.10	0.51
1:C:396:PHE:O	1:C:400:LEU:HD23	2.10	0.51
1:C:379:THR:HB	1:C:398:MET:HE3	1.91	0.51
1:C:483:LEU:HD22	1:C:487:ILE:HD11	1.92	0.51
1:C:547:ILE:O	1:C:551:GLY:N	2.42	0.51
1:C:643:LYS:O	1:C:647:ILE:HG13	2.10	0.51
1:A:348:ILE:O	1:A:349:ILE:C	2.47	0.51
1:A:399:VAL:C	1:A:401:ALA:N	2.62	0.51
1:A:952:LEU:C	1:A:952:LEU:HD12	2.31	0.51
1:B:234:ILE:O	1:B:234:ILE:HG22	2.10	0.51
1:B:262:LEU:CD2	1:B:266:ALA:CB	2.89	0.51
1:B:307:ARG:HB2	1:B:307:ARG:HH11	1.75	0.51
1:B:785:ASP:O	1:B:788:ASP:N	2.40	0.51
1:B:792:ARG:HG3	1:B:798:MET:CE	2.40	0.51
1:B:685:ILE:HD11	1:B:858:ASP:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:925:VAL:HA	1:B:928:GLN:OE1	2.11	0.51
1:C:907:LEU:HD23	1:C:1018:ALA:HA	1.93	0.51
1:C:211:ASN:C	1:C:211:ASN:HD22	2.13	0.51
1:C:554:TYR:O	1:C:555:LEU:HB2	2.10	0.51
1:C:925:VAL:C	1:C:927:PHE:N	2.59	0.51
1:A:141:GLY:HA2	1:A:288:GLY:HA2	1.91	0.51
1:A:329:THR:O	1:A:329:THR:HG23	2.10	0.51
1:A:831:ALA:HB2	1:A:837:THR:HA	1.92	0.51
1:A:888:LEU:HD21	1:A:901:VAL:CB	2.39	0.51
1:B:1:MET:CB	1:B:2:PRO:CD	2.76	0.51
1:B:538:THR:HG23	1:B:540:ARG:NH2	2.26	0.51
1:B:5:PHE:N	1:B:7:ASP:O	2.43	0.51
1:B:842:GLU:O	1:B:846:GLN:HG3	2.11	0.51
1:C:214:VAL:HG23	1:C:237:GLN:HB2	1.91	0.51
1:C:324:VAL:HG23	1:C:325:TYR:N	2.25	0.51
1:C:344:LEU:CD2	1:C:399:VAL:CG2	2.89	0.51
1:C:540:ARG:NE	1:C:541:TYR:CE1	2.68	0.51
1:C:527:TYR:OH	1:C:968:VAL:CG1	2.58	0.51
1:A:169:THR:OG1	1:A:172:VAL:HG11	2.10	0.51
1:A:252:LYS:HB3	1:A:260:VAL:HG21	1.93	0.51
1:A:73:ASP:HB3	1:A:106:GLN:HE22	1.75	0.51
1:B:445:ILE:HG23	1:B:940:LYS:CG	2.29	0.51
1:B:457:ALA:C	1:B:459:PHE:H	2.13	0.51
1:B:518:ARG:HA	1:B:521:GLU:CB	2.40	0.51
1:B:700:ASN:O	1:B:704:ALA:CB	2.59	0.51
1:B:920:GLY:O	1:B:921:LEU:O	2.28	0.51
1:C:907:LEU:HG	1:C:1017:LEU:HD23	1.92	0.51
1:A:324:VAL:CG1	1:A:325:TYR:N	2.74	0.51
1:A:563:PHE:O	1:A:564:LEU:HD12	2.11	0.51
1:A:778:LYS:HG2	1:A:779:TYR:CE1	2.45	0.51
1:B:255:GLN:HG3	1:B:256:ASP:H	1.75	0.51
1:B:26:ALA:O	1:B:30:LEU:CB	2.59	0.51
1:B:314:GLU:H	1:B:315:PRO:HD2	1.75	0.51
1:B:369:THR:O	1:B:373:PRO:HD3	2.11	0.51
1:B:600:THR:CB	1:B:601:LYS:HZ1	2.21	0.51
1:C:911:GLY:N	1:C:1013:THR:HG21	2.25	0.51
1:C:685:ILE:CG1	1:C:687:GLN:OE1	2.56	0.51
1:C:774:MET:HG2	1:C:775:SER:N	2.25	0.51
1:C:912:ALA:O	1:C:914:LEU:O	2.28	0.51
1:A:401:ALA:HB2	1:A:474:ILE:HG12	1.92	0.51
1:A:844:MET:HE3	1:A:844:MET:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:GLN:HB3	1:A:854:GLY:O	2.11	0.51
1:B:351:VAL:O	1:B:351:VAL:HG12	2.11	0.51
1:B:605:ASN:O	1:B:632:LYS:N	2.40	0.51
1:B:648:THR:HG21	1:B:666:PHE:HA	1.93	0.51
1:B:699:ARG:CG	1:B:700:ASN:H	2.23	0.51
1:B:706:ALA:HA	1:B:713:LEU:HD22	1.93	0.51
1:B:701:GLN:HG3	1:B:851:LEU:CD2	2.41	0.51
1:C:18:ILE:O	1:C:20:MET:N	2.44	0.51
1:A:263:ARG:HH21	1:A:263:ARG:CB	2.13	0.51
1:A:308:ALA:O	1:A:311:ALA:HB3	2.11	0.51
1:A:574:THR:HG21	1:A:598:TYR:HE1	1.75	0.51
1:B:136:PHE:HA	1:B:292:LYS:HG3	1.93	0.51
1:B:460:GLY:HA2	1:B:872:GLN:HE22	1.76	0.51
1:C:218:GLN:HE21	1:C:231:ASN:HD21	1.57	0.51
1:C:321:LEU:C	1:C:321:LEU:HD13	2.31	0.51
1:C:393:LEU:HD13	1:C:466:ILE:CG2	2.37	0.51
1:C:410:ILE:O	1:C:412:VAL:N	2.43	0.51
1:C:681:ASP:OD2	1:C:828:LEU:CD1	2.59	0.51
1:C:792:ARG:HG3	1:C:793:ALA:O	2.11	0.51
1:C:905:VAL:CB	1:C:906:PRO:HD3	2.41	0.51
1:C:912:ALA:C	1:C:914:LEU:N	2.65	0.51
1:A:1024:VAL:CG1	1:A:1025:PHE:H	2.13	0.51
1:A:225:VAL:CG1	1:A:226:LYS:N	2.74	0.51
1:A:418:ARG:O	1:A:421:ALA:HB3	2.11	0.51
1:A:616:GLY:CA	1:A:624:THR:OG1	2.59	0.51
1:A:713:LEU:CG	1:A:714:THR:H	2.22	0.51
1:C:158:VAL:O	1:C:162:MET:N	2.39	0.51
1:C:222:THR:CB	1:C:223:PRO:HD3	2.35	0.51
1:C:248:LYS:O	1:C:249:ILE:C	2.48	0.51
1:C:305:ALA:O	1:C:306:ILE:C	2.48	0.51
1:C:3:ASN:HD21	1:C:432:ARG:CD	2.24	0.51
1:C:407:ASP:OD2	1:C:940:LYS:NZ	2.41	0.51
1:C:600:THR:OG1	1:C:601:LYS:N	2.44	0.51
1:C:934:THR:HG22	1:C:1011:MET:SD	2.51	0.51
1:A:456:MET:O	1:A:457:ALA:CB	2.48	0.50
1:A:901:VAL:CG1	1:A:943:ILE:HG13	2.40	0.50
1:A:902:MET:O	1:A:904:VAL:N	2.43	0.50
1:A:966:ASP:O	1:A:969:ARG:HB2	2.11	0.50
1:B:213:GLN:C	1:B:214:VAL:HG23	2.31	0.50
1:B:355:MET:SD	1:B:368:PRO:HB2	2.50	0.50
1:B:6:ILE:HD12	1:B:491:ALA:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:702:LEU:HD13	1:B:702:LEU:O	2.11	0.50
1:B:891:LEU:HD12	1:B:892:TYR:CE1	2.46	0.50
1:B:92:LEU:N	1:B:92:LEU:CD2	2.74	0.50
1:C:1016:VAL:HA	1:C:1019:ILE:HG22	1.92	0.50
1:A:890:ALA:HB1	1:C:11:PHE:CD1	2.46	0.50
1:C:260:VAL:O	1:C:260:VAL:CG1	2.59	0.50
1:C:6:ILE:HA	1:C:491:ALA:HB2	1.93	0.50
1:C:759:VAL:HG23	1:C:771:VAL:O	2.11	0.50
1:C:969:ARG:HG2	1:C:969:ARG:HH21	1.76	0.50
1:A:311:ALA:O	1:A:312:LYS:CB	2.59	0.50
1:A:344:LEU:HD22	1:A:402:ILE:CD1	2.40	0.50
1:A:402:ILE:CG2	1:A:403:GLY:N	2.73	0.50
1:A:45:ILE:HB	1:A:90:ILE:HB	1.93	0.50
1:A:562:SER:HB3	1:A:924:ASP:HB3	1.93	0.50
1:A:573:MET:SD	1:A:628:PHE:CD1	3.04	0.50
1:B:118:LEU:O	1:B:119:PRO:C	2.50	0.50
1:B:125:GLN:HG2	1:B:125:GLN:O	2.11	0.50
1:B:185:ARG:CG	1:B:185:ARG:HH11	2.17	0.50
1:B:702:LEU:C	1:B:703:LEU:O	2.50	0.50
1:B:960:LEU:HD12	1:B:961:ILE:N	2.25	0.50
1:C:1010:GLY:HA2	1:C:1013:THR:HG22	1.93	0.50
1:C:166:ILE:CA	1:C:166:ILE:CD1	2.88	0.50
1:A:108:GLN:O	1:A:110:LYS:N	2.45	0.50
1:A:57:VAL:HG13	1:A:57:VAL:O	2.11	0.50
1:A:593:GLU:O	1:A:594:VAL:C	2.46	0.50
1:A:746:ILE:HD13	1:A:804:PHE:CD1	2.46	0.50
1:B:200:PRO:O	1:B:203:VAL:HB	2.12	0.50
1:B:38:ILE:O	1:B:462:SER:HB2	2.12	0.50
1:B:380:PHE:CZ	1:B:398:MET:HE2	2.46	0.50
1:B:690:LEU:CB	1:B:694:LYS:HB2	2.41	0.50
1:B:701:GLN:HB3	1:B:851:LEU:HD13	1.93	0.50
1:C:449:LEU:O	1:C:452:VAL:N	2.35	0.50
1:C:327:TYR:HB3	1:C:628:PHE:HB3	1.93	0.50
1:C:57:VAL:HG12	1:C:88:VAL:CG2	2.40	0.50
1:C:889:ALA:O	1:C:890:ALA:C	2.50	0.50
1:C:897:ILE:HD13	1:C:950:LYS:CD	2.42	0.50
1:C:966:ASP:HA	1:C:969:ARG:CB	2.41	0.50
1:A:1026:PHE:O	1:A:1029:VAL:O	2.30	0.50
1:A:27:ILE:HG22	1:A:28:LEU:HD12	1.93	0.50
1:A:211:ASN:ND2	1:A:760:ASN:OD1	2.44	0.50
1:B:418:ARG:CZ	1:B:970:MET:SD	3.00	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:941:ASN:OD1	1:B:979:SER:OG	2.27	0.50
1:C:146:ASP:HB3	1:C:148:THR:HG23	1.94	0.50
1:A:275:TYR:CB	1:C:222:THR:HG22	2.41	0.50
1:C:247:GLY:O	1:C:263:ARG:HB2	2.11	0.50
1:C:332:PHE:CE1	1:C:569:GLN:HG2	2.46	0.50
1:C:54:ALA:N	1:C:57:VAL:HG23	2.27	0.50
1:C:897:ILE:N	1:C:898:PRO:HD2	2.27	0.50
1:A:355:MET:HE3	1:A:977:MET:CE	2.41	0.50
1:A:540:ARG:HD2	1:A:541:TYR:CD2	2.46	0.50
1:A:569:GLN:HA	1:A:634:TRP:CH2	2.47	0.50
1:A:946:VAL:O	1:A:946:VAL:CG1	2.59	0.50
1:B:545:TYR:HD2	1:B:546:LEU:HD23	1.77	0.50
1:B:72:ILE:N	1:B:72:ILE:HD13	2.25	0.50
1:B:799:VAL:HG23	1:B:800:PRO:HD2	1.94	0.50
1:B:915:ALA:O	1:B:917:THR:N	2.37	0.50
1:C:317:PHE:CB	1:C:318:PRO:CD	2.84	0.50
1:C:355:MET:N	1:C:355:MET:HE3	2.27	0.50
1:C:389:SER:HG	1:C:391:ASN:HD22	1.57	0.50
1:C:545:TYR:HA	1:C:548:ILE:HG13	1.92	0.50
1:A:114:ALA:O	1:A:115:MET:C	2.48	0.50
1:A:418:ARG:CG	1:A:970:MET:CE	2.90	0.50
1:B:143:ILE:O	1:B:322:LYS:N	2.38	0.50
1:B:18:ILE:O	1:B:19:ILE:C	2.49	0.50
1:B:585:GLU:O	1:B:588:GLN:N	2.43	0.50
1:B:930:GLY:O	1:B:934:THR:CG2	2.58	0.50
1:C:159:ALA:O	1:C:160:ALA:C	2.44	0.50
1:C:412:VAL:O	1:C:416:VAL:HG13	2.12	0.50
1:B:14:VAL:CG1	1:C:890:ALA:HB2	2.27	0.50
1:C:972:LEU:H	1:C:974:PRO:CD	2.22	0.50
1:A:405:LEU:HD13	1:A:405:LEU:H	1.76	0.50
1:A:463:THR:C	1:A:465:ALA:N	2.65	0.50
1:A:515:TRP:C	1:A:515:TRP:CD1	2.85	0.50
1:A:552:MET:SD	1:A:909:VAL:CG1	2.99	0.50
1:B:144:ASN:HA	1:B:321:LEU:HA	1.93	0.50
1:B:188:MET:SD	1:B:200:PRO:HB3	2.51	0.50
1:B:279:ALA:HA	1:B:611:ALA:O	2.11	0.50
1:B:841:MET:O	1:B:845:GLU:HB2	2.11	0.50
1:B:85:THR:CG2	1:B:87:THR:HB	2.42	0.50
1:B:975:ILE:H	1:B:975:ILE:HD12	1.76	0.50
1:C:141:GLY:HA3	1:C:324:VAL:CG2	2.36	0.50
1:C:166:ILE:CA	1:C:166:ILE:HD13	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:436:GLY:C	1:C:438:ILE:H	2.15	0.50
1:C:945:ILE:HB	1:C:971:ARG:HG3	1.93	0.50
1:A:220:GLY:H	1:A:231:ASN:HD22	1.60	0.50
1:A:912:ALA:HB2	1:A:1010:GLY:HA3	1.93	0.50
1:B:157:TYR:C	1:B:161:ASN:HD22	2.15	0.50
1:C:188:MET:HE1	1:C:200:PRO:HA	1.94	0.50
1:C:192:GLU:C	1:C:194:ASN:N	2.64	0.50
1:C:674:LEU:CD1	1:C:674:LEU:C	2.79	0.50
1:C:713:LEU:N	1:C:713:LEU:HD13	2.21	0.50
1:C:692:HIS:CE1	1:C:721:LEU:HD21	2.39	0.50
1:C:729:ILE:CD1	1:C:786:ILE:HD13	2.24	0.50
1:A:150:THR:O	1:A:151:GLN:C	2.50	0.50
1:A:1:MET:H2	1:A:2:PRO:HD2	1.77	0.50
1:A:16:ALA:HB2	1:A:488:LEU:HD13	1.94	0.50
1:A:884:VAL:HG12	1:A:902:MET:CE	2.42	0.50
1:B:348:ILE:HG23	1:B:372:VAL:HG21	1.94	0.50
1:B:602:GLU:HB2	1:B:606:VAL:HG23	1.93	0.50
1:C:11:PHE:O	1:C:11:PHE:CD2	2.65	0.50
1:C:752:ALA:O	1:C:774:MET:HA	2.11	0.50
1:C:774:MET:HG2	1:C:775:SER:H	1.76	0.50
1:C:861:GLY:O	1:C:864:TYR:N	2.44	0.50
1:A:198:LEU:HD22	1:A:202:ASP:CB	2.42	0.49
1:A:709:HIS:N	1:A:710:PRO:HD3	2.27	0.49
1:A:58:GLN:HE22	1:A:816:LEU:CD1	2.23	0.49
1:A:950:LYS:O	1:A:951:ASP:CB	2.59	0.49
1:B:115:MET:HE2	1:B:115:MET:HA	1.88	0.49
1:B:401:ALA:O	1:B:404:LEU:N	2.36	0.49
1:B:560:PRO:O	1:B:923:ASN:HB3	2.12	0.49
1:B:606:VAL:HA	1:B:631:LEU:HD23	1.92	0.49
1:B:659:LYS:CD	1:B:660:ASP:OD2	2.59	0.49
1:B:864:TYR:CD1	1:B:864:TYR:C	2.85	0.49
1:B:915:ALA:C	1:B:917:THR:H	2.15	0.49
1:B:968:VAL:O	1:B:972:LEU:HB2	2.11	0.49
1:C:35:TYR:HB3	1:C:36:PRO:HD2	1.93	0.49
1:C:568:ASP:O	1:C:568:ASP:OD1	2.29	0.49
1:C:713:LEU:HG	1:C:832:ALA:C	2.30	0.49
1:C:98:THR:HG22	1:C:99:ASP:N	2.26	0.49
1:A:281:PHE:O	1:A:284:GLN:HG2	2.13	0.49
1:A:337:ILE:O	1:A:339:GLU:O	2.30	0.49
1:B:148:THR:O	1:B:148:THR:HG22	2.12	0.49
1:B:399:VAL:O	1:B:400:LEU:C	2.50	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:THR:HG23	1:B:87:THR:H	1.76	0.49
1:C:1024:VAL:CG1	1:C:1028:VAL:HG21	2.42	0.49
1:C:448:VAL:HG22	1:C:887:CYS:HB3	1.94	0.49
1:C:633:ASP:O	1:C:634:TRP:HB2	2.12	0.49
1:C:713:LEU:HD12	1:C:833:PRO:O	2.12	0.49
1:C:754:TRP:CH2	1:C:780:ARG:HA	2.47	0.49
1:B:17:ILE:HG13	1:C:886:LEU:HD22	1.94	0.49
1:C:925:VAL:HG23	1:C:926:TYR:N	2.28	0.49
1:C:527:TYR:CZ	1:C:968:VAL:HG12	2.47	0.49
1:A:11:PHE:O	1:A:14:VAL:N	2.44	0.49
1:A:445:ILE:CD1	1:A:940:LYS:HE3	2.43	0.49
1:B:572:PHE:CZ	1:B:629:VAL:HG21	2.48	0.49
1:C:137:LEU:N	1:C:291:ILE:O	2.45	0.49
1:C:185:ARG:HG3	1:C:271:GLY:HA3	1.94	0.49
1:C:768:VAL:C	1:C:769:LYS:HG2	2.30	0.49
1:C:844:MET:HA	1:C:847:LEU:CD2	2.36	0.49
1:C:847:LEU:O	1:C:850:LYS:CG	2.55	0.49
1:C:680:PHE:HB2	1:C:859:TRP:HZ3	1.77	0.49
1:A:1031:ARG:O	1:A:1035:ARG:NH1	2.44	0.49
1:A:367:ILE:HG12	1:A:413:VAL:CG2	2.41	0.49
1:A:605:ASN:O	1:A:631:LEU:HA	2.12	0.49
1:C:1026:PHE:O	1:C:1029:VAL:HB	2.12	0.49
1:C:185:ARG:CG	1:C:271:GLY:HA3	2.42	0.49
1:C:321:LEU:C	1:C:321:LEU:CD1	2.79	0.49
1:C:432:ARG:CG	1:C:432:ARG:NH1	2.40	0.49
1:C:641:GLU:O	1:C:650:ARG:NH1	2.45	0.49
1:A:216:ALA:O	1:A:217:GLY:O	2.31	0.49
1:A:253:VAL:CG2	1:A:258:SER:O	2.42	0.49
1:A:540:ARG:HD2	1:A:541:TYR:CE2	2.48	0.49
1:A:61:VAL:C	1:A:65:ILE:HG22	2.25	0.49
1:A:73:ASP:O	1:A:75:LEU:N	2.43	0.49
1:A:971:ARG:C	1:A:974:PRO:CD	2.78	0.49
1:B:42:ALA:CB	1:B:93:THR:CG2	2.85	0.49
1:B:456:MET:CG	1:B:467:TYR:HB3	2.29	0.49
1:B:990:VAL:HG12	1:B:990:VAL:O	2.12	0.49
1:C:111:LEU:HD13	1:C:111:LEU:C	2.32	0.49
1:C:108:GLN:HG2	1:C:129:VAL:HG21	1.93	0.49
1:B:316:PHE:CZ	1:C:687:GLN:HG3	2.48	0.49
1:C:950:LYS:HZ1	1:C:1030:ARG:NE	2.09	0.49
1:A:394:THR:HG23	1:A:395:MET:HE2	1.95	0.49
1:A:599:LEU:O	1:A:600:THR:HB	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:832:ALA:O	1:A:833:PRO:C	2.49	0.49
1:A:911:GLY:H	1:A:914:LEU:CD1	2.25	0.49
1:B:941:ASN:HD21	1:B:1015:THR:HG23	1.77	0.49
1:B:178:PHE:C	1:B:277:ILE:HG21	2.32	0.49
1:B:281:PHE:CZ	1:B:608:SER:HB2	2.48	0.49
1:B:790:TYR:HD1	1:B:800:PRO:N	2.10	0.49
1:B:945:ILE:HD11	1:B:1022:VAL:HB	1.93	0.49
1:B:418:ARG:CG	1:B:970:MET:HE3	2.43	0.49
1:C:18:ILE:HG22	1:C:19:ILE:N	2.27	0.49
1:C:356:TYR:C	1:C:358:PHE:H	2.16	0.49
1:C:705:GLU:O	1:C:706:ALA:C	2.51	0.49
1:A:1004:GLY:O	1:A:1007:VAL:N	2.46	0.49
1:A:105:VAL:HG22	1:B:105:VAL:HG13	1.93	0.49
1:A:340:VAL:CG1	1:A:399:VAL:HG23	2.43	0.49
1:B:941:ASN:HD22	1:B:1015:THR:HA	1.77	0.49
1:B:1024:VAL:HG12	1:B:1028:VAL:HG21	1.94	0.49
1:B:545:TYR:OH	1:B:906:PRO:CG	2.56	0.49
1:B:655:PHE:CA	1:B:658:ILE:HG12	2.42	0.49
1:A:228:GLN:CG	1:B:781:MET:HG2	2.38	0.49
1:B:972:LEU:CD1	1:B:976:LEU:HD21	2.41	0.49
1:B:982:PHE:O	1:B:986:VAL:HG23	2.12	0.49
1:C:1032:ARG:O	1:C:1032:ARG:HG2	2.11	0.49
1:C:666:PHE:HD2	1:C:666:PHE:H	1.60	0.49
1:C:644:VAL:HG11	1:C:667:ASN:ND2	2.27	0.49
1:C:695:LEU:O	1:C:696:THR:C	2.51	0.49
1:A:198:LEU:HD22	1:A:202:ASP:HB3	1.95	0.49
1:A:1:MET:HG2	1:A:2:PRO:HD3	1.94	0.49
1:A:57:VAL:CG1	1:A:57:VAL:O	2.56	0.49
1:A:857:TYR:CD1	1:A:857:TYR:C	2.86	0.49
1:B:369:THR:O	1:B:372:VAL:HG13	2.13	0.49
1:B:2:PRO:CD	1:B:486:LEU:HD12	2.42	0.49
1:B:638:PRO:HG2	1:B:639:GLY:N	2.28	0.49
1:B:892:TYR:HB3	1:B:897:ILE:CD1	2.43	0.49
1:B:975:ILE:N	1:B:975:ILE:HD12	2.27	0.49
1:C:1010:GLY:C	1:C:1013:THR:HG22	2.33	0.49
1:C:115:MET:HB2	1:C:116:PRO:HD3	1.95	0.49
1:C:144:ASN:HD21	1:C:148:THR:N	2.10	0.49
1:C:158:VAL:HG11	1:C:177:LEU:CD2	2.42	0.49
1:C:371:ALA:O	1:C:375:VAL:HG23	2.12	0.49
1:C:578:LEU:CD2	1:C:661:ALA:CB	2.83	0.49
1:C:685:ILE:HD11	1:C:687:GLN:CA	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:418:ARG:NE	1:C:970:MET:HE2	2.27	0.49
1:A:478:MET:SD	1:A:478:MET:C	2.91	0.49
1:A:779:TYR:CD1	1:A:779:TYR:N	2.81	0.49
1:A:984:LEU:O	1:A:988:PRO:HD3	2.13	0.49
1:B:110:LYS:HD3	1:B:110:LYS:HA	1.57	0.49
1:B:115:MET:SD	1:B:127:VAL:HG11	2.53	0.49
1:B:150:THR:O	1:B:151:GLN:C	2.50	0.49
1:B:723:ASP:HA	1:B:814:PRO:HD3	1.95	0.49
1:C:277:ILE:HD11	1:C:620:ARG:HH21	1.75	0.49
1:C:422:GLU:OE2	1:C:423:GLU:HG3	2.13	0.49
1:C:476:SER:O	1:C:477:ALA:HB3	2.12	0.49
1:C:492:LEU:HA	1:C:495:THR:HB	1.95	0.49
1:C:536:ARG:O	1:C:538:THR:N	2.46	0.49
1:C:666:PHE:O	1:C:666:PHE:CD2	2.66	0.49
1:A:1017:LEU:HG	1:A:1017:LEU:O	2.13	0.49
1:A:445:ILE:HG13	1:A:446:ALA:N	2.27	0.49
1:A:575:MET:HB2	1:A:664:PHE:HB2	1.95	0.49
1:A:719:ASN:ND2	1:A:719:ASN:O	2.45	0.49
1:A:83:ASP:C	1:A:83:ASP:OD1	2.52	0.49
1:B:344:LEU:O	1:B:345:VAL:C	2.50	0.49
1:B:467:TYR:O	1:B:470:PHE:HB2	2.12	0.49
1:B:49:TYR:CG	1:B:122:VAL:CA	2.86	0.49
1:B:548:ILE:HD13	1:B:1017:LEU:HD23	1.94	0.49
1:C:211:ASN:HD21	1:C:239:ARG:HG3	1.78	0.49
1:A:275:TYR:HB2	1:C:222:THR:HG22	1.94	0.49
1:A:1022:VAL:HG22	1:A:1023:PRO:HD3	1.96	0.48
1:A:330:THR:HG22	1:A:331:PRO:CD	2.43	0.48
1:A:638:PRO:HG2	1:A:639:GLY:N	2.24	0.48
1:A:686:ASP:HB2	1:A:823:PRO:HB2	1.94	0.48
1:A:973:ARG:O	1:A:977:MET:HB2	2.13	0.48
1:B:213:GLN:O	1:B:214:VAL:HG23	2.12	0.48
1:B:339:GLU:O	1:B:343:THR:HG23	2.13	0.48
1:B:2:PRO:HG3	1:B:435:MET:HG2	1.94	0.48
1:B:967:ALA:O	1:B:968:VAL:C	2.52	0.48
1:A:886:LEU:HD21	1:C:17:ILE:CG2	2.43	0.48
1:C:445:ILE:HB	1:C:940:LYS:HG3	1.95	0.48
1:C:815:ARG:HH11	1:C:815:ARG:HG3	1.78	0.48
1:C:912:ALA:C	1:C:914:LEU:H	2.17	0.48
1:C:942:ALA:HA	1:C:945:ILE:HG22	1.94	0.48
1:A:406:VAL:O	1:A:407:ASP:C	2.49	0.48
1:A:454:VAL:N	1:A:455:PRO:HD2	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1024:VAL:O	1:B:1025:PHE:CB	2.57	0.48
1:B:130:GLU:C	1:B:131:LYS:O	2.49	0.48
1:B:30:LEU:HD23	1:B:390:ILE:CD1	2.44	0.48
1:B:363:ARG:NH1	1:B:498:LYS:HD2	2.28	0.48
1:B:51:GLY:C	1:B:53:ASP:OD2	2.51	0.48
1:B:776:GLU:O	1:B:777:ALA:O	2.30	0.48
1:B:679:GLY:CA	1:B:830:GLN:HB3	2.42	0.48
1:C:18:ILE:O	1:C:19:ILE:C	2.51	0.48
1:C:363:ARG:O	1:C:367:ILE:HG22	2.13	0.48
1:C:663:VAL:CG1	1:C:664:PHE:N	2.76	0.48
1:B:219:LEU:HD23	1:C:783:PRO:CD	2.42	0.48
1:C:94:PHE:O	1:C:95:GLU:O	2.31	0.48
1:A:111:LEU:HD11	1:A:127:VAL:CG1	2.43	0.48
1:A:182:TYR:CB	1:A:270:LEU:HD12	2.43	0.48
1:A:988:PRO:C	1:A:990:VAL:N	2.62	0.48
1:B:1017:LEU:N	1:B:1017:LEU:CD1	2.76	0.48
1:B:110:LYS:O	1:B:111:LEU:C	2.51	0.48
1:B:115:MET:O	1:B:123:GLN:NE2	2.47	0.48
1:B:410:ILE:CG2	1:B:414:GLU:OE2	2.49	0.48
1:B:6:ILE:N	1:B:491:ALA:HB2	2.28	0.48
1:B:545:TYR:C	1:B:547:ILE:H	2.15	0.48
1:B:791:VAL:HG23	1:B:801:PHE:HE2	1.77	0.48
1:B:885:PHE:CE2	1:B:898:PRO:HB2	2.48	0.48
1:C:911:GLY:HA3	1:C:1010:GLY:HA2	1.95	0.48
1:C:192:GLU:O	1:C:195:LYS:N	2.46	0.48
1:C:355:MET:CE	1:C:355:MET:CA	2.91	0.48
1:C:544:LEU:HD12	1:C:1021:PHE:HZ	1.78	0.48
1:C:872:GLN:HB2	1:C:875:SER:CB	2.37	0.48
1:C:945:ILE:O	1:C:946:VAL:CG2	2.59	0.48
1:A:193:LEU:CB	1:A:265:VAL:HG13	2.43	0.48
1:A:959:GLY:HA3	1:A:962:GLU:CB	2.24	0.48
1:B:443:VAL:O	1:B:444:GLY:C	2.50	0.48
1:B:462:SER:O	1:B:465:ALA:HB3	2.12	0.48
1:B:641:GLU:HA	1:B:650:ARG:HH11	1.77	0.48
1:B:84:SER:O	1:B:86:GLY:N	2.46	0.48
1:B:905:VAL:N	1:B:906:PRO:CD	2.76	0.48
1:B:941:ASN:HA	1:B:944:LEU:HD12	1.94	0.48
1:C:276:ASP:O	1:C:614:GLY:HA3	2.14	0.48
1:C:524:THR:O	1:C:527:TYR:HB3	2.14	0.48
1:C:72:ILE:HG22	1:C:94:PHE:CE2	2.45	0.48
1:A:219:LEU:HD12	1:A:232:ALA:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:676:THR:O	1:A:677:ALA:O	2.31	0.48
1:A:754:TRP:CZ3	1:A:780:ARG:HA	2.48	0.48
1:A:983:ILE:CG1	1:A:984:LEU:N	2.76	0.48
1:B:1029:VAL:HA	1:B:1032:ARG:HB3	1.96	0.48
1:B:82:SER:HA	1:B:88:VAL:HG13	1.95	0.48
1:C:391:ASN:H	1:C:394:THR:HG23	1.77	0.48
1:C:64:VAL:HG12	1:C:65:ILE:N	2.29	0.48
1:C:831:ALA:HB2	1:C:840:ALA:HB2	1.93	0.48
1:C:950:LYS:HE2	1:C:1026:PHE:CZ	2.48	0.48
1:A:13:TRP:CZ2	1:A:492:LEU:HD11	2.49	0.48
1:A:284:GLN:HE21	1:A:284:GLN:CA	2.27	0.48
1:A:519:MET:N	1:A:522:LYS:HE3	2.29	0.48
1:B:423:GLU:O	1:B:424:GLY:O	2.32	0.48
1:B:767:ARG:HD3	1:B:769:LYS:CE	2.37	0.48
1:A:276:ASP:CB	1:C:222:THR:HG23	2.21	0.48
1:A:781:MET:HE1	1:C:228:GLN:CD	2.34	0.48
1:C:420:MET:SD	1:C:498:LYS:HG2	2.54	0.48
1:C:566:ASP:OD1	1:C:669:PRO:HA	2.14	0.48
1:C:762:PHE:CE1	1:C:769:LYS:HB2	2.49	0.48
1:A:166:ILE:O	1:A:168:ARG:N	2.47	0.48
1:A:431:THR:O	1:A:432:ARG:C	2.51	0.48
1:A:467:TYR:CE1	1:A:925:VAL:HG22	2.48	0.48
1:A:56:THR:O	1:A:56:THR:CG2	2.59	0.48
1:A:909:VAL:O	1:A:912:ALA:HB3	2.14	0.48
1:A:418:ARG:NH1	1:A:973:ARG:HE	2.09	0.48
1:A:983:ILE:O	1:A:986:VAL:HG12	2.13	0.48
1:B:680:PHE:C	1:B:680:PHE:HD1	2.16	0.48
1:B:714:THR:O	1:B:715:SER:CB	2.61	0.48
1:C:389:SER:O	1:C:394:THR:HG21	2.14	0.48
1:C:55:LYS:HE2	1:C:59:ASP:OD1	2.14	0.48
1:C:84:SER:C	1:C:86:GLY:N	2.66	0.48
1:C:866:GLU:C	1:C:868:LEU:H	2.17	0.48
1:C:894:SER:OG	1:C:897:ILE:HG13	2.14	0.48
1:C:949:ALA:C	1:C:951:ASP:H	2.17	0.48
1:A:270:LEU:CD2	1:A:270:LEU:N	2.77	0.48
1:A:33:ALA:HA	1:A:299:ALA:HB2	1.96	0.48
1:A:687:GLN:HE21	1:A:856:GLY:HA3	1.78	0.48
1:A:990:VAL:O	1:A:991:ILE:CB	2.62	0.48
1:A:128:SER:HB3	1:B:113:LEU:HD22	1.94	0.48
1:B:30:LEU:HD23	1:B:390:ILE:HD11	1.96	0.48
1:B:483:LEU:O	1:B:485:ALA:O	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:682:PHE:HD1	1:B:859:TRP:CZ3	2.31	0.48
1:B:901:VAL:HG13	1:B:942:ALA:HB3	1.95	0.48
1:C:1016:VAL:HA	1:C:1019:ILE:CG2	2.43	0.48
1:C:66:GLU:HG2	1:C:78:MET:HE2	1.96	0.48
1:A:575:MET:O	1:A:663:VAL:HA	2.14	0.48
1:A:695:LEU:HA	1:A:695:LEU:HD12	1.38	0.48
1:A:445:ILE:HD13	1:A:940:LYS:HE3	1.95	0.48
1:B:133:SER:HB3	1:B:292:LYS:HD2	1.96	0.48
1:B:474:ILE:HG22	1:B:475:VAL:N	2.29	0.48
1:B:643:LYS:O	1:B:644:VAL:C	2.52	0.48
1:C:989:LEU:HD12	1:C:1000:GLN:HB3	1.94	0.48
1:C:457:ALA:N	1:C:459:PHE:CE2	2.78	0.48
1:C:375:VAL:HG13	1:C:480:LEU:HB2	1.95	0.48
1:C:601:LYS:O	1:C:603:LYS:N	2.42	0.48
1:C:613:ASN:C	1:C:613:ASN:OD1	2.52	0.48
1:C:701:GLN:O	1:C:704:ALA:N	2.46	0.48
1:C:839:GLU:HA	1:C:839:GLU:OE1	2.14	0.48
1:A:36:PRO:CD	1:A:393:LEU:HD12	2.44	0.48
1:A:399:VAL:C	1:A:401:ALA:H	2.16	0.48
1:A:926:TYR:HE1	1:A:999:ALA:HB2	1.70	0.48
1:B:1021:PHE:O	1:B:1024:VAL:HB	2.14	0.48
1:B:193:LEU:HD23	1:B:265:VAL:HG21	1.96	0.48
1:B:908:GLY:C	1:B:910:ILE:N	2.68	0.48
1:B:953:MET:O	1:B:953:MET:CG	2.61	0.48
1:C:213:GLN:HE22	1:C:238:THR:HA	1.76	0.48
1:C:184:MET:CE	1:C:270:LEU:HA	2.44	0.48
1:C:733:GLN:O	1:C:737:GLN:HG2	2.13	0.48
1:C:760:ASN:O	1:C:771:VAL:HG23	2.13	0.48
1:C:928:GLN:O	1:C:932:LEU:HG	2.13	0.48
1:A:214:VAL:CG1	1:A:215:ALA:N	2.51	0.47
1:A:379:THR:HG22	1:A:477:ALA:HA	1.96	0.47
1:A:413:VAL:HG23	1:A:493:CYS:CB	2.44	0.47
1:A:589:LYS:HA	1:A:592:ASN:ND2	2.29	0.47
1:A:818:ARG:CD	1:A:818:ARG:CB	2.82	0.47
1:A:907:LEU:O	1:A:910:ILE:HG13	2.13	0.47
1:B:10:ILE:HG13	1:C:893:GLU:HG3	1.96	0.47
1:B:183:ALA:N	1:B:271:GLY:O	2.46	0.47
1:B:47:ALA:CB	1:B:61:VAL:HG21	2.44	0.47
1:B:56:THR:O	1:B:60:THR:CB	2.62	0.47
1:C:344:LEU:HD23	1:C:399:VAL:CG2	2.43	0.47
1:C:389:SER:OG	1:C:391:ASN:ND2	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:696:THR:O	1:C:697:GLN:C	2.52	0.47
1:A:351:VAL:CG1	1:A:410:ILE:HD11	2.45	0.47
1:A:573:MET:SD	1:A:628:PHE:CE1	3.08	0.47
1:A:569:GLN:HA	1:A:634:TRP:HH2	1.78	0.47
1:B:102:ILE:O	1:B:105:VAL:HB	2.14	0.47
1:B:530:SER:O	1:B:534:ILE:HG12	2.13	0.47
1:B:84:SER:C	1:B:86:GLY:N	2.68	0.47
1:B:912:ALA:HB1	1:B:1006:GLY:O	2.14	0.47
1:C:45:ILE:CA	1:C:45:ILE:HD13	2.43	0.47
1:C:549:VAL:O	1:C:551:GLY:N	2.47	0.47
1:A:116:PRO:HB2	1:A:117:LEU:HD22	1.97	0.47
1:A:402:ILE:O	1:A:405:LEU:HD13	2.15	0.47
1:A:540:ARG:O	1:A:543:VAL:HG12	2.14	0.47
1:A:644:VAL:C	1:A:646:ALA:H	2.17	0.47
1:A:65:ILE:HG13	1:A:66:GLU:N	2.29	0.47
1:A:54:ALA:CB	1:A:816:LEU:HG	2.20	0.47
1:A:820:ASN:O	1:A:822:LEU:HD23	2.13	0.47
1:A:843:LEU:HD23	1:A:846:GLN:NE2	2.29	0.47
1:A:965:LEU:C	1:A:969:ARG:HG3	2.27	0.47
1:B:339:GLU:HB3	1:B:1000:GLN:NE2	2.29	0.47
1:B:1031:ARG:H	1:B:1034:SER:HG	1.56	0.47
1:B:187:TRP:CZ3	1:B:774:MET:CE	2.98	0.47
1:B:199:THR:C	1:B:201:VAL:N	2.65	0.47
1:B:413:VAL:HG13	1:B:414:GLU:H	1.76	0.47
1:B:472:ILE:O	1:B:473:THR:C	2.52	0.47
1:B:6:ILE:HA	1:B:491:ALA:CB	2.44	0.47
1:B:531:VAL:O	1:B:535:LEU:HD23	2.14	0.47
1:B:6:ILE:HD13	1:B:6:ILE:N	2.29	0.47
1:B:712:MET:HG2	1:B:843:LEU:HD12	1.96	0.47
1:B:876:LEU:O	1:B:880:SER:HB2	2.14	0.47
1:B:905:VAL:O	1:B:909:VAL:HG22	2.15	0.47
1:C:989:LEU:HD12	1:C:1000:GLN:CA	2.44	0.47
1:C:117:LEU:O	1:C:118:LEU:C	2.50	0.47
1:C:352:PHE:CE1	1:C:365:THR:HG22	2.49	0.47
1:C:414:GLU:O	1:C:414:GLU:HG3	2.14	0.47
1:C:709:HIS:C	1:C:711:ASP:H	2.17	0.47
1:C:865:GLN:O	1:C:868:LEU:O	2.33	0.47
1:A:268:ILE:N	1:A:268:ILE:HD12	2.28	0.47
1:A:410:ILE:HG22	1:A:411:VAL:N	2.29	0.47
1:A:466:ILE:O	1:A:469:GLN:N	2.46	0.47
1:A:809:TRP:O	1:A:810:GLU:HB3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:952:LEU:HD11	1:A:963:ALA:CB	2.44	0.47
1:B:219:LEU:HD12	1:B:234:ILE:CD1	2.44	0.47
1:B:25:LEU:C	1:B:27:ILE:N	2.67	0.47
1:B:271:GLY:HA3	1:B:275:TYR:OH	2.15	0.47
1:B:314:GLU:C	1:B:316:PHE:H	2.17	0.47
1:B:960:LEU:C	1:B:960:LEU:CD1	2.82	0.47
1:C:427:PRO:N	1:C:498:LYS:HE3	2.29	0.47
1:C:591:LEU:HA	1:C:591:LEU:HD13	1.44	0.47
1:C:66:GLU:HG2	1:C:78:MET:CE	2.45	0.47
1:C:878:ALA:C	1:C:880:SER:N	2.65	0.47
1:A:140:VAL:HG11	1:A:310:LEU:HD11	1.95	0.47
1:A:456:MET:HB2	1:A:471:SER:HB2	1.97	0.47
1:A:841:MET:O	1:A:844:MET:HB3	2.15	0.47
1:B:136:PHE:HE1	1:B:617:PHE:CE1	2.32	0.47
1:B:184:MET:HB2	1:B:762:PHE:CE2	2.49	0.47
1:B:407:ASP:O	1:B:408:ASP:C	2.51	0.47
1:B:49:TYR:CD1	1:B:122:VAL:CG1	2.83	0.47
1:B:690:LEU:HB2	1:B:694:LYS:HB3	1.97	0.47
1:B:703:LEU:HA	1:B:706:ALA:HB3	1.96	0.47
1:B:978:THR:HG22	1:B:979:SER:N	2.29	0.47
1:C:65:ILE:HD13	1:C:111:LEU:CD2	2.42	0.47
1:C:225:VAL:O	1:C:226:LYS:C	2.52	0.47
1:C:251:LEU:HD11	1:C:262:LEU:HA	1.95	0.47
1:C:398:MET:O	1:C:401:ALA:HB3	2.14	0.47
1:C:705:GLU:C	1:C:707:ALA:N	2.66	0.47
1:C:713:LEU:HD11	1:C:834:GLY:C	2.34	0.47
1:A:191:ASN:O	1:A:192:GLU:C	2.51	0.47
1:A:922:THR:O	1:A:924:ASP:N	2.42	0.47
1:A:104:GLN:HE22	1:B:109:ASN:HB3	1.78	0.47
1:B:12:ALA:O	1:B:14:VAL:N	2.48	0.47
1:B:904:VAL:C	1:B:906:PRO:HD2	2.35	0.47
1:C:114:ALA:O	1:C:115:MET:O	2.32	0.47
1:C:392:THR:O	1:C:393:LEU:C	2.53	0.47
1:C:66:GLU:OE2	1:C:80:SER:OG	2.26	0.47
1:C:899:PHE:H	1:C:899:PHE:HD1	1.54	0.47
1:A:154:ILE:HG22	1:A:287:SER:HB3	1.97	0.47
1:A:583:THR:HG23	1:A:622:GLN:HE21	1.80	0.47
1:B:49:TYR:CD1	1:B:122:VAL:HA	2.48	0.47
1:B:156:ASP:CG	1:B:182:TYR:CD2	2.88	0.47
1:B:449:LEU:HB2	1:B:478:MET:HG3	1.97	0.47
1:B:560:PRO:O	1:B:923:ASN:CB	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:578:LEU:HD12	1:B:586:ARG:HH21	1.70	0.47
1:B:640:GLU:N	1:B:643:LYS:HG3	2.29	0.47
1:C:767:ARG:HG2	1:C:769:LYS:HD3	1.96	0.47
1:C:698:ALA:O	1:C:851:LEU:HD23	2.14	0.47
1:A:453:PHE:CZ	1:A:474:ILE:HG21	2.49	0.47
1:A:691:GLY:O	1:A:692:HIS:C	2.53	0.47
1:A:736:ALA:O	1:A:741:VAL:HG13	2.13	0.47
1:B:633:ASP:CG	1:B:634:TRP:N	2.68	0.47
1:B:732:ASP:O	1:B:733:GLN:C	2.53	0.47
1:A:225:VAL:HG22	1:B:778:LYS:NZ	2.30	0.47
1:C:344:LEU:CD2	1:C:399:VAL:HG23	2.44	0.47
1:C:423:GLU:HB3	1:C:426:PRO:CD	2.43	0.47
1:C:655:PHE:C	1:C:657:GLN:H	2.17	0.47
1:C:904:VAL:O	1:C:906:PRO:N	2.48	0.47
1:A:26:ALA:O	1:A:30:LEU:HG	2.15	0.47
1:A:689:GLY:O	1:A:690:LEU:O	2.33	0.47
1:B:568:ASP:OD2	1:B:634:TRP:HZ3	1.98	0.47
1:B:867:ARG:O	1:B:871:ASN:ND2	2.48	0.47
1:B:8:ARG:HD2	1:B:8:ARG:N	2.29	0.47
1:B:918:PHE:O	1:B:919:ARG:O	2.32	0.47
1:C:34:GLN:HG2	1:C:333:VAL:HG21	1.96	0.47
1:C:338:HIS:C	1:C:338:HIS:ND1	2.68	0.47
1:C:476:SER:C	1:C:478:MET:N	2.67	0.47
1:C:657:GLN:C	1:C:659:LYS:N	2.68	0.47
1:C:445:ILE:CD1	1:C:940:LYS:HE3	2.44	0.47
1:A:146:ASP:O	1:A:148:THR:N	2.48	0.47
1:A:592:ASN:O	1:A:595:THR:HB	2.15	0.47
1:A:574:THR:OG1	1:A:627:ALA:HB3	2.14	0.47
1:A:948:PHE:CD2	1:A:948:PHE:N	2.81	0.47
1:B:1004:GLY:O	1:B:1007:VAL:HG12	2.14	0.47
1:B:1017:LEU:O	1:B:1021:PHE:HB2	2.15	0.47
1:B:121:GLU:O	1:B:125:GLN:HB3	2.14	0.47
1:B:210:GLN:CG	1:B:249:ILE:HG23	2.41	0.47
1:B:419:VAL:O	1:B:426:PRO:CG	2.59	0.47
1:B:404:LEU:HD21	1:B:937:LEU:HD21	1.97	0.47
1:B:960:LEU:HD11	1:B:1027:VAL:HG11	1.96	0.47
1:C:586:ARG:O	1:C:589:LYS:HB2	2.15	0.47
1:C:830:GLN:OE1	1:C:832:ALA:HA	2.14	0.47
1:C:972:LEU:O	1:C:973:ARG:C	2.52	0.47
1:A:395:MET:CE	1:A:395:MET:HA	2.45	0.47
1:A:434:SER:O	1:A:436:GLY:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:ALA:O	1:B:13:TRP:C	2.53	0.47
1:B:249:ILE:HD12	1:B:262:LEU:HD12	1.97	0.47
1:B:374:VAL:HG13	1:B:484:VAL:HG21	1.96	0.47
1:C:244:GLU:CA	1:C:263:ARG:HH22	2.21	0.47
1:C:54:ALA:H	1:C:57:VAL:HG23	1.80	0.47
1:C:699:ARG:NH2	1:C:722:GLU:OE1	2.44	0.47
1:C:750:LEU:HA	1:C:750:LEU:HD23	1.51	0.47
1:C:713:LEU:CD2	1:C:832:ALA:O	2.62	0.47
1:C:949:ALA:C	1:C:951:ASP:N	2.68	0.47
1:A:520:PHE:O	1:A:522:LYS:N	2.48	0.46
1:A:583:THR:CG2	1:A:584:GLN:N	2.78	0.46
1:A:615:PHE:HE1	1:A:628:PHE:HZ	1.63	0.46
1:A:623:ASN:C	1:A:623:ASN:ND2	2.68	0.46
1:B:391:ASN:OD1	1:B:394:THR:N	2.47	0.46
1:B:410:ILE:O	1:B:414:GLU:HG2	2.15	0.46
1:B:778:LYS:NZ	1:B:778:LYS:H	2.10	0.46
1:C:1030:ARG:HA	1:C:1033:PHE:HD2	1.79	0.46
1:C:266:ALA:O	1:C:267:LYS:C	2.53	0.46
1:C:449:LEU:O	1:C:452:VAL:HG23	2.15	0.46
1:C:599:LEU:O	1:C:603:LYS:HB2	2.15	0.46
1:C:76:MET:CE	1:C:93:THR:HG22	2.45	0.46
1:A:45:ILE:HG12	1:A:129:VAL:HG22	1.97	0.46
1:A:190:PRO:HD3	1:A:789:TRP:CZ2	2.50	0.46
1:A:247:GLY:O	1:A:263:ARG:HB2	2.15	0.46
1:A:292:LYS:O	1:A:293:LEU:O	2.33	0.46
1:A:335:ILE:O	1:A:339:GLU:HG2	2.15	0.46
1:A:813:SER:OG	1:A:816:LEU:HD23	2.15	0.46
1:A:930:GLY:O	1:A:932:LEU:N	2.48	0.46
1:A:945:ILE:O	1:A:949:ALA:HB2	2.15	0.46
1:B:1022:VAL:N	1:B:1023:PRO:HD2	2.29	0.46
1:B:814:PRO:O	1:B:815:ARG:HG2	2.14	0.46
1:A:10:ILE:HD11	1:B:895:TRP:CD1	2.49	0.46
1:C:545:TYR:CE1	1:C:1021:PHE:CD1	3.03	0.46
1:C:552:MET:HE1	1:C:909:VAL:HG21	1.96	0.46
1:A:199:THR:CB	1:A:200:PRO:CD	2.93	0.46
1:A:568:ASP:OD2	1:A:644:VAL:HG23	2.15	0.46
1:A:872:GLN:O	1:A:873:ALA:C	2.53	0.46
1:B:1024:VAL:CG1	1:B:1028:VAL:HG21	2.45	0.46
1:B:862:MET:O	1:B:865:GLN:HB3	2.15	0.46
1:B:909:VAL:HG12	1:B:931:LEU:HD22	1.97	0.46
1:A:819:TYR:O	1:A:820:ASN:C	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:699:ARG:NH2	1:B:722:GLU:OE1	2.49	0.46
1:B:705:GLU:C	1:B:707:ALA:N	2.69	0.46
1:C:547:ILE:O	1:C:550:VAL:HG12	2.15	0.46
1:C:874:PRO:HG2	1:C:875:SER:H	1.81	0.46
1:A:1004:GLY:O	1:A:1006:GLY:N	2.49	0.46
1:A:11:PHE:O	1:A:13:TRP:N	2.49	0.46
1:A:162:MET:HB2	1:A:313:MET:SD	2.56	0.46
1:A:243:THR:HG21	1:A:269:GLU:HA	1.97	0.46
1:A:690:LEU:CD1	1:A:854:GLY:CA	2.71	0.46
1:B:118:LEU:HD23	1:B:122:VAL:HG11	1.97	0.46
1:B:455:PRO:O	1:B:456:MET:C	2.53	0.46
1:B:708:LYS:HD2	1:B:709:HIS:NE2	2.30	0.46
1:B:781:MET:HE2	1:B:781:MET:N	2.31	0.46
1:B:8:ARG:H	1:B:9:PRO:HD3	1.80	0.46
1:C:1035:ARG:HA	1:C:1035:ARG:NE	2.26	0.46
1:C:193:LEU:HB3	1:C:198:LEU:O	2.15	0.46
1:C:243:THR:OG1	1:C:244:GLU:N	2.49	0.46
1:C:360:GLN:OE1	1:C:516:PHE:HE2	1.99	0.46
1:C:391:ASN:O	1:C:394:THR:HG22	2.16	0.46
1:C:445:ILE:HD12	1:C:446:ALA:N	2.30	0.46
1:C:74:ASN:HB3	1:C:95:GLU:CB	2.44	0.46
1:A:264:ASP:O	1:A:266:ALA:N	2.49	0.46
1:A:534:ILE:HD12	1:A:540:ARG:HH22	1.81	0.46
1:A:621:GLY:C	1:A:623:ASN:N	2.68	0.46
1:A:655:PHE:O	1:A:658:ILE:HG12	2.16	0.46
1:A:678:THR:O	1:A:837:THR:OG1	2.25	0.46
1:B:199:THR:HB	1:B:200:PRO:HD2	1.98	0.46
1:B:49:TYR:CG	1:B:122:VAL:HG22	2.50	0.46
1:B:555:LEU:CD2	1:B:555:LEU:H	2.23	0.46
1:C:188:MET:CE	1:C:200:PRO:HB3	2.46	0.46
1:C:23:GLY:HA3	1:C:377:LEU:O	2.16	0.46
1:C:368:PRO:HG3	1:C:413:VAL:HG11	1.96	0.46
1:C:657:GLN:HB3	1:C:658:ILE:HD12	1.98	0.46
1:C:699:ARG:HD2	1:C:703:LEU:HD11	1.98	0.46
1:C:790:TYR:C	1:C:791:VAL:CG2	2.84	0.46
1:A:102:ILE:HA	1:A:105:VAL:HG23	1.98	0.46
1:A:298:ASN:CB	1:A:301:ASP:OD1	2.61	0.46
1:A:324:VAL:CG1	1:A:325:TYR:H	2.21	0.46
1:A:572:PHE:N	1:A:572:PHE:HD1	2.13	0.46
1:A:701:GLN:OE1	1:A:852:PRO:HD3	2.15	0.46
1:A:713:LEU:O	1:A:714:THR:CB	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1016:VAL:C	1:B:1018:ALA:H	2.18	0.46
1:B:120:GLN:CG	1:B:124:GLN:HG2	2.43	0.46
1:B:309:GLU:O	1:B:312:LYS:HB2	2.15	0.46
1:B:355:MET:HG2	1:B:410:ILE:HD11	1.98	0.46
1:B:776:GLU:O	1:B:777:ALA:C	2.54	0.46
1:C:303:ALA:O	1:C:304:ALA:C	2.53	0.46
1:C:162:MET:HE3	1:C:313:MET:HE2	1.98	0.46
1:C:376:LEU:O	1:C:377:LEU:C	2.52	0.46
1:A:1021:PHE:HB3	1:A:1025:PHE:CE1	2.51	0.46
1:A:133:SER:HB3	1:A:136:PHE:HD1	1.79	0.46
1:A:133:SER:HG	1:A:136:PHE:HE1	1.62	0.46
1:A:279:ALA:HA	1:A:612:VAL:HG12	1.97	0.46
1:B:49:TYR:OH	1:B:127:VAL:N	2.49	0.46
1:B:193:LEU:HA	1:B:265:VAL:HG21	1.98	0.46
1:B:335:ILE:C	1:B:337:ILE:N	2.68	0.46
1:B:514:GLY:HA2	1:B:517:ASN:HD22	1.81	0.46
1:B:655:PHE:HA	1:B:658:ILE:HG12	1.97	0.46
1:C:35:TYR:CG	1:C:671:ILE:HG12	2.50	0.46
1:C:452:VAL:CG1	1:C:935:ILE:HG22	2.46	0.46
1:C:536:ARG:HH11	1:C:961:ILE:CD1	2.07	0.46
1:C:592:ASN:ND2	1:C:592:ASN:H	2.14	0.46
1:C:44:THR:HG22	1:C:91:THR:HA	1.98	0.46
1:A:269:GLU:HG2	1:A:269:GLU:O	2.16	0.46
1:A:443:VAL:O	1:A:444:GLY:C	2.52	0.46
1:A:537:SER:O	1:A:539:GLY:N	2.48	0.46
1:A:600:THR:CG2	1:A:600:THR:O	2.62	0.46
1:A:600:THR:O	1:A:601:LYS:HB2	2.16	0.46
1:A:621:GLY:O	1:A:623:ASN:N	2.49	0.46
1:A:884:VAL:HG12	1:A:902:MET:HE3	1.97	0.46
1:A:897:ILE:HG21	1:A:950:LYS:NZ	2.31	0.46
1:B:189:ASN:HD22	1:B:190:PRO:CD	2.28	0.46
1:B:722:GLU:O	1:B:814:PRO:CG	2.64	0.46
1:B:686:ASP:CB	1:B:823:PRO:O	2.63	0.46
1:B:882:ILE:HG22	1:B:886:LEU:HD11	1.98	0.46
1:C:211:ASN:C	1:C:211:ASN:ND2	2.69	0.46
1:C:236:ALA:O	1:C:237:GLN:C	2.54	0.46
1:C:467:TYR:CZ	1:C:925:VAL:HG12	2.51	0.46
1:C:545:TYR:O	1:C:546:LEU:C	2.54	0.46
1:C:730:ASP:O	1:C:730:ASP:OD1	2.34	0.46
1:A:111:LEU:HD11	1:A:127:VAL:HG11	1.98	0.46
1:A:421:ALA:O	1:A:423:GLU:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:ILE:O	1:A:469:GLN:CB	2.61	0.46
1:A:515:TRP:CA	1:A:519:MET:SD	2.97	0.46
1:A:83:ASP:HA	1:A:815:ARG:HA	1.98	0.46
1:B:613:ASN:O	1:B:625:GLY:HA2	2.16	0.46
1:B:646:ALA:O	1:B:648:THR:N	2.48	0.46
1:B:701:GLN:HG3	1:B:851:LEU:HD22	1.98	0.46
1:C:1010:GLY:CA	1:C:1013:THR:HG22	2.46	0.46
1:B:129:VAL:H	1:C:109:ASN:HD21	1.63	0.46
1:C:155:SER:HB3	1:C:180:SER:H	1.79	0.46
1:C:384:ALA:O	1:C:385:ALA:C	2.53	0.46
1:C:598:TYR:HB3	1:C:606:VAL:HG11	1.98	0.46
1:C:818:ARG:HA	1:C:824:SER:H	1.81	0.46
1:C:841:MET:O	1:C:842:GLU:C	2.54	0.46
1:C:452:VAL:HG11	1:C:935:ILE:HG22	1.98	0.46
1:A:342:LYS:HG3	1:A:343:THR:N	2.32	0.45
1:A:376:LEU:C	1:A:377:LEU:O	2.54	0.45
1:A:427:PRO:HG3	1:A:497:LEU:O	2.15	0.45
1:A:530:SER:O	1:A:534:ILE:HG12	2.16	0.45
1:B:1012:VAL:C	1:B:1014:ALA:H	2.19	0.45
1:B:347:ALA:HB1	1:B:402:ILE:HG21	1.97	0.45
1:B:535:LEU:O	1:B:536:ARG:C	2.55	0.45
1:B:771:VAL:O	1:B:771:VAL:CG1	2.37	0.45
1:B:870:GLY:O	1:B:872:GLN:N	2.49	0.45
1:B:900:SER:O	1:B:903:LEU:HB2	2.16	0.45
1:C:218:GLN:CG	1:C:232:ALA:O	2.65	0.45
1:C:353:LEU:O	1:C:356:TYR:CB	2.65	0.45
1:C:45:ILE:HG23	1:C:45:ILE:HD12	1.71	0.45
1:C:379:THR:HG23	1:C:477:ALA:HB2	1.96	0.45
1:C:560:PRO:O	1:C:922:THR:HG22	2.13	0.45
1:C:938:SER:O	1:C:941:ASN:ND2	2.49	0.45
1:A:868:LEU:HB3	1:A:869:SER:H	1.61	0.45
1:B:419:VAL:HG12	1:B:419:VAL:O	2.16	0.45
1:B:489:THR:N	1:B:490:PRO:HD2	2.30	0.45
1:B:534:ILE:HG23	1:B:541:TYR:CE1	2.51	0.45
1:C:445:ILE:O	1:C:448:VAL:N	2.47	0.45
1:C:907:LEU:O	1:C:910:ILE:CG2	2.61	0.45
1:C:915:ALA:O	1:C:919:ARG:N	2.44	0.45
1:A:1004:GLY:O	1:A:1005:THR:C	2.54	0.45
1:A:105:VAL:HB	1:A:106:GLN:H	1.56	0.45
1:A:189:ASN:HB2	1:A:779:TYR:CE2	2.52	0.45
1:A:42:ALA:C	1:A:43:VAL:HG23	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:THR:C	1:A:540:ARG:H	2.20	0.45
1:A:758:TYR:HB2	1:A:772:TYR:CE2	2.52	0.45
1:A:774:MET:HE3	1:A:774:MET:HB3	1.77	0.45
1:A:892:TYR:O	1:A:893:GLU:HG3	2.15	0.45
1:B:663:VAL:O	1:B:663:VAL:HG12	2.16	0.45
1:B:843:LEU:O	1:B:844:MET:C	2.53	0.45
1:C:1028:VAL:O	1:C:1032:ARG:HB3	2.17	0.45
1:C:34:GLN:C	1:C:35:TYR:CG	2.88	0.45
1:C:696:THR:O	1:C:699:ARG:N	2.49	0.45
1:C:69:MET:CE	1:C:92:LEU:HD21	2.45	0.45
1:C:705:GLU:O	1:C:708:LYS:N	2.45	0.45
1:C:897:ILE:HG12	1:C:950:LYS:CE	2.47	0.45
1:A:200:PRO:O	1:A:203:VAL:HB	2.16	0.45
1:A:218:GLN:HB3	1:A:231:ASN:HD21	1.81	0.45
1:A:49:TYR:O	1:A:50:PRO:C	2.54	0.45
1:A:729:ILE:CG2	1:A:730:ASP:N	2.50	0.45
1:A:354:VAL:HG13	1:A:980:LEU:HD23	1.97	0.45
1:B:125:GLN:O	1:B:125:GLN:HG3	2.16	0.45
1:B:240:LEU:HB2	1:B:246:PHE:CE2	2.52	0.45
1:B:549:VAL:O	1:B:550:VAL:C	2.54	0.45
1:B:199:THR:HB	1:B:749:THR:HG22	1.98	0.45
1:B:714:THR:HG22	1:B:831:ALA:N	2.31	0.45
1:B:847:LEU:CD2	1:B:847:LEU:N	2.73	0.45
1:C:1015:THR:O	1:C:1019:ILE:HB	2.16	0.45
1:C:545:TYR:CZ	1:C:1021:PHE:CD2	3.05	0.45
1:C:900:SER:HA	1:C:1029:VAL:HG21	1.98	0.45
1:C:925:VAL:O	1:C:926:TYR:HB2	2.17	0.45
1:A:1019:ILE:O	1:A:1023:PRO:HG3	2.16	0.45
1:A:541:TYR:HD2	1:A:541:TYR:N	2.15	0.45
1:A:846:GLN:HB2	1:A:846:GLN:HE21	1.48	0.45
1:B:1022:VAL:CG2	1:B:1023:PRO:HD3	2.35	0.45
1:B:149:MET:HB2	1:B:154:ILE:HG23	1.99	0.45
1:B:539:GLY:C	1:B:541:TYR:H	2.19	0.45
1:B:558:ARG:NH2	1:B:917:THR:OG1	2.48	0.45
1:B:927:PHE:O	1:B:930:GLY:N	2.50	0.45
1:C:29:LYS:HE2	1:C:29:LYS:HB3	1.73	0.45
1:C:314:GLU:HA	1:C:317:PHE:CZ	2.51	0.45
1:C:372:VAL:CG1	1:C:373:PRO:HD3	2.28	0.45
1:C:417:GLU:HB3	1:C:973:ARG:NH1	2.26	0.45
1:C:748:THR:O	1:C:752:ALA:HB2	2.16	0.45
1:C:910:ILE:HG22	1:C:911:GLY:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:986:VAL:HG12	1:C:986:VAL:O	2.17	0.45
1:A:17:ILE:HG22	1:A:21:LEU:CD2	2.46	0.45
1:A:235:ILE:O	1:A:235:ILE:HG22	2.16	0.45
1:A:193:LEU:HD12	1:A:265:VAL:CG1	2.47	0.45
1:A:2:PRO:O	1:A:6:ILE:N	2.48	0.45
1:A:355:MET:HA	1:A:977:MET:CE	2.41	0.45
1:A:488:LEU:HG	1:A:492:LEU:HD22	1.99	0.45
1:A:532:GLY:HA2	1:A:965:LEU:CD1	2.46	0.45
1:A:548:ILE:O	1:A:551:GLY:N	2.49	0.45
1:A:643:LYS:NZ	1:A:995:ALA:HB2	2.31	0.45
1:B:100:ALA:HA	1:B:103:ALA:HB3	1.99	0.45
1:B:189:ASN:O	1:B:193:LEU:HB2	2.16	0.45
1:B:228:GLN:NE2	1:C:781:MET:CE	2.79	0.45
1:B:314:GLU:HB2	1:B:315:PRO:HD3	1.98	0.45
1:B:66:GLU:HG3	1:B:78:MET:SD	2.57	0.45
1:C:184:MET:HE3	1:C:270:LEU:HD12	1.99	0.45
1:C:162:MET:CB	1:C:313:MET:HE1	2.18	0.45
1:C:424:GLY:C	1:C:425:LEU:HD22	2.37	0.45
1:C:454:VAL:O	1:C:456:MET:O	2.35	0.45
1:C:527:TYR:O	1:C:529:ASP:N	2.50	0.45
1:C:801:PHE:CD1	1:C:804:PHE:HE1	2.34	0.45
1:A:14:VAL:CG1	1:B:886:LEU:HB3	2.46	0.45
1:A:758:TYR:CE1	1:A:770:LYS:HG2	2.52	0.45
1:A:819:TYR:O	1:A:822:LEU:N	2.42	0.45
1:A:8:ARG:HG3	1:A:8:ARG:O	2.16	0.45
1:A:979:SER:O	1:A:983:ILE:CG2	2.65	0.45
1:B:609:VAL:HG12	1:B:609:VAL:O	2.17	0.45
1:B:671:ILE:HG12	1:B:671:ILE:H	1.51	0.45
1:B:70:ASN:ND2	1:B:70:ASN:O	2.50	0.45
1:B:531:VAL:CG1	1:B:965:LEU:HD11	2.47	0.45
1:C:527:TYR:CZ	1:C:1019:ILE:HG13	2.52	0.45
1:C:1030:ARG:HB3	1:C:1030:ARG:HE	1.32	0.45
1:C:443:VAL:O	1:C:447:MET:HB2	2.17	0.45
1:C:49:TYR:CD2	1:C:52:ALA:HB2	2.51	0.45
1:C:559:LEU:HD13	1:C:917:THR:CG2	2.46	0.45
1:A:1015:THR:C	1:A:1017:LEU:N	2.70	0.45
1:A:308:ALA:HB1	1:A:312:LYS:HE3	1.99	0.45
1:A:200:PRO:HG2	1:A:749:THR:HG23	1.98	0.45
1:B:111:LEU:HD21	1:B:127:VAL:CG1	2.47	0.45
1:B:130:GLU:O	1:B:131:LYS:O	2.35	0.45
1:B:42:ALA:HA	1:B:93:THR:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:714:THR:HG22	1:B:831:ALA:CA	2.47	0.45
1:B:78:MET:HG3	1:B:92:LEU:HD13	1.99	0.45
1:A:780:ARG:NH2	1:C:223:PRO:O	2.48	0.45
1:C:380:PHE:CZ	1:C:398:MET:SD	3.10	0.45
1:C:401:ALA:HB2	1:C:474:ILE:HG12	1.98	0.45
1:C:470:PHE:O	1:C:471:SER:C	2.55	0.45
1:C:643:LYS:C	1:C:647:ILE:HG13	2.37	0.45
1:C:663:VAL:HG12	1:C:664:PHE:N	2.32	0.45
1:C:742:SER:OG	1:C:745:ASP:HB2	2.17	0.45
1:C:753:ALA:O	1:C:775:SER:CB	2.65	0.45
1:C:81:ASN:OD1	1:C:815:ARG:HD2	2.17	0.45
1:C:871:ASN:O	1:C:872:GLN:O	2.35	0.45
1:A:106:GLN:O	1:A:107:VAL:O	2.35	0.45
1:A:305:ALA:O	1:A:308:ALA:HB3	2.17	0.45
1:A:676:THR:OG1	1:A:677:ALA:N	2.46	0.45
1:A:750:LEU:HD22	1:A:750:LEU:O	2.17	0.45
1:A:843:LEU:C	1:A:845:GLU:N	2.69	0.45
1:A:897:ILE:O	1:A:900:SER:OG	2.23	0.45
1:A:902:MET:C	1:A:904:VAL:H	2.20	0.45
1:B:921:LEU:HD21	1:B:1005:THR:CG2	2.45	0.45
1:B:198:LEU:HD23	1:B:792:ARG:NH2	2.31	0.45
1:B:371:ALA:O	1:B:372:VAL:C	2.55	0.45
1:B:543:VAL:O	1:B:547:ILE:HD11	2.14	0.45
1:B:640:GLU:H	1:B:643:LYS:HG3	1.81	0.45
1:B:76:MET:HG2	1:B:95:GLU:HG3	1.99	0.45
1:C:313:MET:O	1:C:316:PHE:HD1	2.00	0.45
1:C:395:MET:O	1:C:396:PHE:C	2.55	0.45
1:C:484:VAL:O	1:C:488:LEU:N	2.50	0.45
1:C:758:TYR:HA	1:C:772:TYR:HA	1.98	0.45
1:C:778:LYS:O	1:C:779:TYR:HD2	1.99	0.45
1:C:819:TYR:CE1	1:C:820:ASN:ND2	2.85	0.45
1:C:712:MET:CB	1:C:835:LYS:HG3	2.26	0.45
1:C:888:LEU:HB3	1:C:898:PRO:CB	2.41	0.45
1:C:82:SER:HB2	1:C:88:VAL:HA	1.97	0.45
1:A:991:ILE:HG13	1:A:1004:GLY:HA3	1.98	0.45
1:A:10:ILE:HD11	1:B:895:TRP:CG	2.52	0.45
1:A:115:MET:C	1:A:117:LEU:N	2.71	0.45
1:A:344:LEU:HD13	1:A:376:LEU:HD12	1.99	0.45
1:A:549:VAL:HG13	1:A:550:VAL:N	2.32	0.45
1:A:923:ASN:OD1	1:A:923:ASN:O	2.36	0.45
1:A:991:ILE:HD13	1:A:1008:MET:CG	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:TYR:O	1:B:161:ASN:N	2.48	0.45
1:B:221:GLY:HA3	1:C:780:ARG:HH11	1.82	0.45
1:B:223:PRO:HG2	1:C:780:ARG:HH22	1.81	0.45
1:B:330:THR:H	1:B:331:PRO:CD	2.29	0.45
1:B:404:LEU:C	1:B:406:VAL:N	2.70	0.45
1:B:410:ILE:C	1:B:412:VAL:N	2.70	0.45
1:B:570:GLY:N	1:B:634:TRP:CH2	2.85	0.45
1:B:638:PRO:CG	1:B:639:GLY:N	2.80	0.45
1:C:115:MET:SD	1:C:127:VAL:HG11	2.57	0.45
1:C:372:VAL:HG21	1:C:402:ILE:HG23	1.99	0.45
1:C:69:MET:HE3	1:C:72:ILE:CD1	2.47	0.45
1:C:873:ALA:N	1:C:874:PRO:HD2	2.32	0.45
1:A:775:SER:OG	1:A:780:ARG:HG2	2.17	0.44
1:B:124:GLN:O	1:B:125:GLN:CB	2.63	0.44
1:B:49:TYR:CE2	1:B:125:GLN:HB3	2.52	0.44
1:B:126:GLY:C	1:B:127:VAL:HG23	2.38	0.44
1:B:564:LEU:HD23	1:B:565:PRO:HD2	1.99	0.44
1:B:862:MET:O	1:B:863:SER:C	2.54	0.44
1:B:418:ARG:NH2	1:B:970:MET:CG	2.78	0.44
1:B:944:LEU:CB	1:B:975:ILE:HD11	2.47	0.44
1:C:1016:VAL:C	1:C:1018:ALA:H	2.16	0.44
1:C:332:PHE:O	1:C:333:VAL:C	2.56	0.44
1:C:730:ASP:C	1:C:730:ASP:OD1	2.55	0.44
1:B:219:LEU:HD21	1:C:783:PRO:HG3	1.93	0.44
1:A:128:SER:HB2	1:B:113:LEU:CD2	2.48	0.44
1:A:173:GLY:O	1:A:174:ASP:CB	2.65	0.44
1:A:180:SER:O	1:A:181:GLN:CB	2.65	0.44
1:A:344:LEU:O	1:A:345:VAL:C	2.52	0.44
1:A:595:THR:HA	1:A:609:VAL:HG21	1.99	0.44
1:A:991:ILE:CG2	1:A:991:ILE:O	2.65	0.44
1:A:995:ALA:O	1:A:996:GLY:C	2.54	0.44
1:B:198:LEU:HD11	1:B:252:LYS:HB2	1.99	0.44
1:B:34:GLN:HB2	1:B:333:VAL:HG22	1.98	0.44
1:B:531:VAL:O	1:B:535:LEU:CD2	2.65	0.44
1:B:535:LEU:O	1:B:538:THR:N	2.50	0.44
1:B:600:THR:OG1	1:B:601:LYS:CE	2.65	0.44
1:B:613:ASN:ND2	1:B:613:ASN:C	2.70	0.44
1:B:691:GLY:O	1:B:693:GLU:N	2.50	0.44
1:B:78:MET:HB3	1:B:78:MET:HE3	1.80	0.44
1:B:888:LEU:O	1:B:889:ALA:C	2.55	0.44
1:B:97:GLY:O	1:B:98:THR:O	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:SER:H	1:C:175:VAL:CG2	2.22	0.44
1:C:263:ARG:HA	1:C:268:ILE:HD12	1.99	0.44
1:C:267:LYS:HE3	1:C:267:LYS:HB2	1.91	0.44
1:C:143:ILE:HD13	1:C:286:ALA:HB2	1.92	0.44
1:C:748:THR:O	1:C:752:ALA:CB	2.65	0.44
1:A:133:SER:O	1:A:292:LYS:HE2	2.17	0.44
1:A:428:LYS:HG3	1:A:429:GLU:HG3	1.97	0.44
1:A:56:THR:HG23	1:C:213:GLN:CG	2.46	0.44
1:A:683:GLU:CD	1:A:826:GLU:HB2	2.38	0.44
1:A:813:SER:OG	1:A:816:LEU:CD2	2.66	0.44
1:A:930:GLY:C	1:A:932:LEU:N	2.69	0.44
1:A:944:LEU:O	1:A:947:GLU:HB3	2.18	0.44
1:A:953:MET:HE2	1:A:959:GLY:O	2.17	0.44
1:B:983:ILE:HG23	1:B:1008:MET:CG	2.47	0.44
1:A:128:SER:CB	1:B:113:LEU:CD2	2.96	0.44
1:B:195:LYS:NZ	1:B:196:PHE:CZ	2.83	0.44
1:B:314:GLU:C	1:B:316:PHE:N	2.70	0.44
1:B:356:TYR:CD2	1:B:365:THR:HG21	2.52	0.44
1:B:577:GLN:C	1:B:578:LEU:O	2.55	0.44
1:B:860:THR:O	1:B:863:SER:HB2	2.17	0.44
1:B:873:ALA:HB3	1:B:874:PRO:HD3	1.99	0.44
1:C:103:ALA:O	1:C:104:GLN:C	2.55	0.44
1:C:393:LEU:HG	1:C:393:LEU:H	1.60	0.44
1:C:394:THR:O	1:C:395:MET:HE2	2.17	0.44
1:C:547:ILE:HA	1:C:550:VAL:HG12	1.99	0.44
1:C:601:LYS:C	1:C:603:LYS:H	2.21	0.44
1:C:688:ALA:C	1:C:690:LEU:N	2.69	0.44
1:C:894:SER:C	1:C:896:SER:N	2.70	0.44
1:C:904:VAL:O	1:C:906:PRO:HD2	2.18	0.44
1:A:254:ASN:O	1:A:256:ASP:N	2.50	0.44
1:A:391:ASN:O	1:A:392:THR:C	2.54	0.44
1:A:463:THR:C	1:A:465:ALA:H	2.19	0.44
1:A:773:VAL:O	1:A:773:VAL:HG13	2.16	0.44
1:A:80:SER:HB2	1:A:90:ILE:HG12	1.98	0.44
1:A:843:LEU:O	1:A:845:GLU:N	2.51	0.44
1:A:989:LEU:O	1:A:993:THR:OG1	2.31	0.44
1:B:115:MET:HE3	1:B:118:LEU:HD13	1.99	0.44
1:B:190:PRO:CD	1:B:779:TYR:CD2	3.01	0.44
1:B:48:SER:N	1:B:49:TYR:CE1	2.73	0.44
1:B:873:ALA:C	1:B:875:SER:N	2.71	0.44
1:C:121:GLU:O	1:C:758:TYR:OH	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:321:LEU:HA	1:C:321:LEU:HD22	1.67	0.44
1:C:393:LEU:HD11	1:C:466:ILE:HG23	1.98	0.44
1:C:545:TYR:O	1:C:547:ILE:N	2.50	0.44
1:B:217:GLY:HA3	1:C:754:TRP:O	2.17	0.44
1:B:228:GLN:CG	1:C:781:MET:HE1	2.47	0.44
1:C:461:GLY:HA3	1:C:869:SER:OG	2.18	0.44
1:A:968:VAL:HG22	1:A:1023:PRO:HB3	1.87	0.44
1:A:25:LEU:C	1:A:25:LEU:HD13	2.38	0.44
1:A:336:SER:O	1:A:337:ILE:C	2.55	0.44
1:A:635:ALA:O	1:A:637:ARG:N	2.51	0.44
1:A:70:ASN:ND2	1:A:70:ASN:N	2.66	0.44
1:A:768:VAL:HG23	1:A:768:VAL:O	2.17	0.44
1:B:170:SER:O	1:B:172:VAL:HG23	2.18	0.44
1:B:609:VAL:HG22	1:B:629:VAL:HB	1.99	0.44
1:B:654:ALA:O	1:B:656:SER:N	2.50	0.44
1:C:314:GLU:O	1:C:317:PHE:CE2	2.71	0.44
1:C:680:PHE:HB2	1:C:859:TRP:CZ3	2.52	0.44
1:C:721:LEU:HD11	1:C:815:ARG:O	2.16	0.44
1:A:187:TRP:O	1:A:266:ALA:HB1	2.18	0.44
1:A:516:PHE:C	1:A:518:ARG:H	2.20	0.44
1:B:947:GLU:O	1:B:951:ASP:HB2	2.18	0.44
1:C:115:MET:CE	1:C:118:LEU:HD21	2.36	0.44
1:C:228:GLN:NE2	1:C:230:LEU:O	2.51	0.44
1:C:399:VAL:C	1:C:401:ALA:N	2.71	0.44
1:C:463:THR:HA	1:C:466:ILE:CD1	2.38	0.44
1:C:457:ALA:HB2	1:C:468:ARG:HA	1.98	0.44
1:C:790:TYR:O	1:C:791:VAL:HG23	2.17	0.44
1:A:151:GLN:HE22	1:A:278:ILE:HG23	1.82	0.44
1:A:355:MET:HG2	1:A:365:THR:HG22	1.98	0.44
1:A:658:ILE:O	1:A:659:LYS:O	2.34	0.44
1:A:925:VAL:N	1:A:928:GLN:HE21	2.16	0.44
1:B:459:PHE:HB3	1:B:460:GLY:H	1.64	0.44
1:B:490:PRO:O	1:B:492:LEU:N	2.51	0.44
1:B:833:PRO:CG	1:B:834:GLY:H	2.26	0.44
1:B:844:MET:C	1:B:846:GLN:N	2.70	0.44
1:B:87:THR:HG21	1:B:620:ARG:CZ	2.48	0.44
1:B:885:PHE:CD2	1:B:898:PRO:HB2	2.53	0.44
1:B:904:VAL:O	1:B:905:VAL:C	2.56	0.44
1:B:956:GLU:CD	1:B:956:GLU:H	2.21	0.44
1:B:987:MET:HE2	1:B:990:VAL:HB	1.99	0.44
1:C:21:LEU:O	1:C:25:LEU:HG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:GLY:CA	1:C:268:ILE:HD13	2.45	0.44
1:C:434:SER:O	1:C:438:ILE:HB	2.17	0.44
1:A:24:GLY:O	1:A:27:ILE:HB	2.18	0.44
1:A:702:LEU:HB2	1:A:851:LEU:HD21	2.00	0.44
1:B:104:GLN:NE2	1:B:108:GLN:HE21	2.16	0.44
1:B:5:PHE:C	1:B:491:ALA:HB2	2.37	0.44
1:B:729:ILE:CG1	1:B:730:ASP:N	2.66	0.44
1:B:753:ALA:HB3	1:B:754:TRP:HD1	1.83	0.44
1:B:859:TRP:HB3	1:B:863:SER:CB	2.31	0.44
1:B:937:LEU:HD11	1:B:982:PHE:CE2	2.52	0.44
1:B:9:PRO:HD2	1:C:893:GLU:OE1	2.17	0.44
1:C:249:ILE:HD13	1:C:249:ILE:HG21	1.68	0.44
1:C:1:MET:HE2	1:C:439:GLN:HE22	1.77	0.44
1:C:544:LEU:HD12	1:C:1021:PHE:CZ	2.52	0.44
1:C:850:LYS:O	1:C:851:LEU:C	2.56	0.44
1:C:860:THR:HG23	1:C:860:THR:O	2.17	0.44
1:C:950:LYS:HE2	1:C:1026:PHE:HZ	1.83	0.44
1:A:652:THR:HG22	1:A:653:ARG:HD3	1.98	0.44
1:A:756:GLY:CA	1:A:774:MET:HB2	2.48	0.44
1:A:752:ALA:O	1:A:756:GLY:HA2	2.17	0.44
1:B:120:GLN:HA	1:B:123:GLN:HB2	2.00	0.44
1:B:197:GLN:HA	1:B:798:MET:SD	2.58	0.44
1:B:515:TRP:O	1:B:519:MET:HB2	2.17	0.44
1:B:907:LEU:C	1:B:910:ILE:HG22	2.38	0.44
1:C:930:GLY:HA3	1:C:1007:VAL:HG23	2.00	0.44
1:C:242:SER:O	1:C:243:THR:C	2.55	0.44
1:C:328:ASP:OD1	1:C:330:THR:HB	2.18	0.44
1:C:45:ILE:CA	1:C:45:ILE:CD1	2.95	0.44
1:C:463:THR:CA	1:C:466:ILE:HD13	2.38	0.44
1:C:561:SER:HA	1:C:923:ASN:CB	2.48	0.44
1:C:66:GLU:O	1:C:67:GLN:C	2.55	0.44
1:C:866:GLU:O	1:C:868:LEU:N	2.51	0.44
1:C:975:ILE:CG2	1:C:976:LEU:N	2.77	0.44
1:A:9:PRO:CD	1:A:10:ILE:H	2.28	0.43
1:A:29:LYS:O	1:A:29:LYS:CG	2.66	0.43
1:A:572:PHE:CE1	1:A:629:VAL:HG13	2.53	0.43
1:A:583:THR:HG22	1:A:584:GLN:N	2.32	0.43
1:A:646:ALA:O	1:A:649:MET:HB2	2.17	0.43
1:A:680:PHE:CD1	1:A:680:PHE:C	2.91	0.43
1:A:801:PHE:CG	1:A:802:SER:N	2.86	0.43
1:A:108:GLN:OE1	1:B:112:GLN:CD	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:TYR:CE2	1:B:125:GLN:HG2	2.53	0.43
1:B:247:GLY:CA	1:B:268:ILE:CD1	2.47	0.43
1:B:462:SER:CB	1:B:865:GLN:NE2	2.81	0.43
1:B:201:VAL:HG22	1:B:748:THR:HB	1.99	0.43
1:B:75:LEU:HD12	1:B:93:THR:O	2.17	0.43
1:B:781:MET:HB2	1:B:781:MET:HE3	1.73	0.43
1:B:892:TYR:O	1:B:894:SER:N	2.51	0.43
1:C:420:MET:SD	1:C:498:LYS:CG	3.06	0.43
1:C:708:LYS:O	1:C:710:PRO:CD	2.65	0.43
1:A:106:GLN:O	1:A:110:LYS:CB	2.62	0.43
1:A:253:VAL:HA	1:A:258:SER:O	2.18	0.43
1:A:393:LEU:HD22	1:A:466:ILE:HG23	2.00	0.43
1:A:72:ILE:CG2	1:A:94:PHE:HE2	2.31	0.43
1:B:111:LEU:HD21	1:B:127:VAL:HG12	2.00	0.43
1:B:154:ILE:O	1:B:155:SER:C	2.57	0.43
1:B:261:LEU:CD1	1:B:261:LEU:N	2.71	0.43
1:B:418:ARG:HH21	1:B:970:MET:HG3	1.83	0.43
1:B:425:LEU:HA	1:B:426:PRO:HD3	1.61	0.43
1:B:568:ASP:O	1:B:634:TRP:CH2	2.71	0.43
1:B:597:TYR:CD2	1:B:655:PHE:CE1	3.06	0.43
1:B:760:ASN:HD22	1:B:761:ASP:N	2.09	0.43
1:A:225:VAL:HG22	1:B:778:LYS:HZ1	1.83	0.43
1:B:418:ARG:NH2	1:B:970:MET:HG3	2.33	0.43
1:C:1007:VAL:O	1:C:1008:MET:C	2.56	0.43
1:C:352:PHE:HA	1:C:369:THR:CG2	2.32	0.43
1:C:541:TYR:N	1:C:541:TYR:CD1	2.86	0.43
1:A:102:ILE:O	1:A:102:ILE:HG23	2.14	0.43
1:A:101:ASP:O	1:A:105:VAL:HG23	2.18	0.43
1:A:173:GLY:HA3	1:A:294:ALA:HA	1.98	0.43
1:A:435:MET:HA	1:A:438:ILE:CD1	2.49	0.43
1:A:549:VAL:HG13	1:A:550:VAL:H	1.83	0.43
1:A:66:GLU:OE2	1:A:818:ARG:HD2	2.18	0.43
1:A:69:MET:HA	1:A:69:MET:CE	2.46	0.43
1:A:714:THR:O	1:A:715:SER:HB2	2.17	0.43
1:A:699:ARG:NH1	1:A:722:GLU:OE1	2.49	0.43
1:A:947:GLU:C	1:A:949:ALA:N	2.69	0.43
1:A:971:ARG:HA	1:A:971:ARG:HE	1.81	0.43
1:B:179:GLY:N	1:B:277:ILE:CG2	2.81	0.43
1:B:490:PRO:O	1:B:493:CYS:O	2.36	0.43
1:B:543:VAL:O	1:B:547:ILE:HD12	2.19	0.43
1:C:259:ARG:HB2	1:C:259:ARG:HH11	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:418:ARG:HG3	1:C:419:VAL:N	2.33	0.43
1:C:454:VAL:O	1:C:454:VAL:CG2	2.65	0.43
1:C:549:VAL:O	1:C:550:VAL:C	2.56	0.43
1:C:935:ILE:HG22	1:C:936:GLY:N	2.33	0.43
1:A:1020:PHE:C	1:A:1023:PRO:HD2	2.39	0.43
1:A:171:GLY:O	1:A:294:ALA:CB	2.65	0.43
1:A:435:MET:SD	1:A:490:PRO:HG3	2.58	0.43
1:A:541:TYR:CD2	1:A:541:TYR:N	2.84	0.43
1:A:577:GLN:HB2	1:A:577:GLN:HE21	1.54	0.43
1:A:620:ARG:HD2	1:A:620:ARG:N	2.34	0.43
1:A:711:ASP:OD2	1:A:711:ASP:N	2.50	0.43
1:A:447:MET:CB	1:A:887:CYS:SG	2.96	0.43
1:B:309:GLU:O	1:B:312:LYS:N	2.49	0.43
1:B:570:GLY:N	1:B:634:TRP:HH2	2.16	0.43
1:B:592:ASN:HA	1:B:595:THR:HG23	1.99	0.43
1:B:607:GLU:HG2	1:B:632:LYS:HD3	2.00	0.43
1:B:701:GLN:HA	1:B:704:ALA:CB	2.44	0.43
1:B:757:SER:O	1:B:759:VAL:HG23	2.18	0.43
1:B:986:VAL:O	1:B:986:VAL:HG12	2.18	0.43
1:C:524:THR:O	1:C:527:TYR:N	2.51	0.43
1:C:527:TYR:OH	1:C:1019:ILE:HG13	2.18	0.43
1:A:108:GLN:HB3	1:A:109:ASN:H	1.49	0.43
1:A:223:PRO:HD3	1:B:275:TYR:HD2	1.72	0.43
1:A:193:LEU:CA	1:A:265:VAL:HG13	2.49	0.43
1:A:356:TYR:C	1:A:358:PHE:N	2.71	0.43
1:A:577:GLN:CD	1:A:624:THR:HG22	2.39	0.43
1:A:713:LEU:HB2	1:A:833:PRO:HD3	2.00	0.43
1:A:739:LEU:HD22	1:A:739:LEU:H	1.83	0.43
1:A:818:ARG:HD3	1:A:822:LEU:N	2.34	0.43
1:B:324:VAL:HG23	1:B:326:PRO:CD	2.48	0.43
1:B:736:ALA:C	1:B:738:ALA:H	2.20	0.43
1:B:792:ARG:CB	1:B:798:MET:HE1	2.45	0.43
1:C:338:HIS:C	1:C:338:HIS:HD1	2.21	0.43
1:C:246:PHE:HZ	1:C:762:PHE:CB	2.31	0.43
1:C:713:LEU:CB	1:C:832:ALA:HB3	2.43	0.43
1:A:246:PHE:O	1:A:249:ILE:HD13	2.14	0.43
1:A:348:ILE:HD11	1:A:372:VAL:HG11	1.99	0.43
1:A:340:VAL:CG1	1:A:399:VAL:HG21	2.35	0.43
1:A:541:TYR:C	1:A:543:VAL:O	2.57	0.43
1:A:713:LEU:CD2	1:A:714:THR:N	2.52	0.43
1:A:747:ASN:HD21	1:C:237:GLN:NE2	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:775:SER:OG	1:A:776:GLU:O	2.33	0.43
1:A:190:PRO:HD2	1:A:779:TYR:CD2	2.53	0.43
1:A:961:ILE:O	1:A:965:LEU:HD22	2.18	0.43
1:B:485:ALA:C	1:B:487:ILE:H	2.22	0.43
1:B:595:THR:HB	1:B:609:VAL:HG11	2.00	0.43
1:B:200:PRO:CG	1:B:749:THR:HG22	2.49	0.43
1:A:113:LEU:CD2	1:C:128:SER:HA	2.43	0.43
1:C:1:MET:CB	1:C:2:PRO:CD	2.87	0.43
1:C:242:SER:O	1:C:244:GLU:N	2.51	0.43
1:C:279:ALA:C	1:C:280:GLU:HG3	2.36	0.43
1:C:317:PHE:O	1:C:318:PRO:C	2.55	0.43
1:C:483:LEU:O	1:C:487:ILE:HD12	2.18	0.43
1:C:491:ALA:C	1:C:493:CYS:H	2.21	0.43
1:A:356:TYR:O	1:A:358:PHE:N	2.51	0.43
1:A:441:ALA:HB1	1:A:944:LEU:HD21	2.01	0.43
1:A:65:ILE:HD12	1:A:65:ILE:C	2.37	0.43
1:A:713:LEU:HB2	1:A:833:PRO:CD	2.49	0.43
1:A:8:ARG:CG	1:A:8:ARG:O	2.67	0.43
1:B:65:ILE:HG23	1:B:111:LEU:HD13	2.01	0.43
1:B:415:ASN:OD1	1:B:434:SER:OG	2.36	0.43
1:C:549:VAL:C	1:C:551:GLY:H	2.21	0.43
1:C:702:LEU:HD23	1:C:702:LEU:O	2.19	0.43
1:C:758:TYR:CD2	1:C:758:TYR:O	2.71	0.43
1:C:758:TYR:CD1	1:C:758:TYR:N	2.62	0.43
1:C:801:PHE:CD1	1:C:804:PHE:CE1	3.07	0.43
1:A:376:LEU:O	1:A:377:LEU:O	2.36	0.43
1:A:514:GLY:C	1:A:516:PHE:H	2.22	0.43
1:A:547:ILE:O	1:A:550:VAL:HB	2.19	0.43
1:B:518:ARG:HA	1:B:521:GLU:HG3	1.99	0.43
1:C:184:MET:HE3	1:C:270:LEU:HA	2.00	0.43
1:C:483:LEU:HA	1:C:483:LEU:HD23	1.81	0.43
1:C:633:ASP:O	1:C:635:ALA:N	2.44	0.43
1:C:847:LEU:CA	1:C:850:LYS:HD3	2.28	0.43
1:C:987:MET:N	1:C:988:PRO:HD2	2.34	0.43
1:A:21:LEU:HA	1:A:21:LEU:HD13	1.60	0.43
1:A:472:ILE:HA	1:A:475:VAL:HG12	2.01	0.43
1:A:649:MET:O	1:A:653:ARG:NE	2.52	0.43
1:A:689:GLY:O	1:A:690:LEU:C	2.56	0.43
1:A:901:VAL:HG11	1:A:943:ILE:CG1	2.47	0.43
1:A:128:SER:HB2	1:B:113:LEU:HD22	2.01	0.43
1:B:324:VAL:C	1:B:326:PRO:HD2	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:490:PRO:C	1:B:492:LEU:H	2.22	0.43
1:B:833:PRO:HG2	1:B:834:GLY:N	2.27	0.43
1:B:47:ALA:HB3	1:B:88:VAL:HB	2.01	0.43
1:B:891:LEU:HD12	1:B:892:TYR:CD1	2.53	0.43
1:B:975:ILE:H	1:B:975:ILE:CD1	2.32	0.43
1:C:345:VAL:O	1:C:348:ILE:CG1	2.62	0.43
1:C:490:PRO:O	1:C:491:ALA:O	2.37	0.43
1:C:576:VAL:HG21	1:C:591:LEU:CD2	2.49	0.43
1:C:688:ALA:HB3	1:C:690:LEU:HD13	2.01	0.43
1:C:69:MET:HE1	1:C:92:LEU:CD2	2.49	0.43
1:A:143:ILE:HG12	1:A:144:ASN:N	2.33	0.43
1:A:182:TYR:HA	1:A:271:GLY:O	2.18	0.43
1:A:225:VAL:HG12	1:A:226:LYS:N	2.34	0.43
1:A:270:LEU:HD22	1:A:270:LEU:N	2.33	0.43
1:A:332:PHE:O	1:A:332:PHE:CD2	2.72	0.43
1:A:578:LEU:H	1:A:578:LEU:CD2	2.32	0.43
1:A:713:LEU:CG	1:A:833:PRO:HD3	2.44	0.43
1:A:7:ASP:O	1:A:9:PRO:HD3	2.18	0.43
1:B:324:VAL:HG23	1:B:326:PRO:HD3	2.00	0.43
1:B:545:TYR:O	1:B:546:LEU:C	2.57	0.43
1:B:867:ARG:HG2	1:B:867:ARG:NH1	2.33	0.43
1:B:908:GLY:O	1:B:910:ILE:N	2.52	0.43
1:C:245:GLU:O	1:C:248:LYS:N	2.51	0.43
1:C:265:VAL:O	1:C:266:ALA:HB2	2.19	0.43
1:C:396:PHE:CD1	1:C:926:TYR:CE1	3.06	0.43
1:C:819:TYR:CE2	1:C:860:THR:HB	2.54	0.43
1:C:959:GLY:O	1:C:963:ALA:CB	2.67	0.43
1:A:112:GLN:HA	1:A:112:GLN:HE21	1.83	0.42
1:A:416:VAL:O	1:A:420:MET:HG3	2.18	0.42
1:A:731:ILE:CD1	1:A:731:ILE:H	2.28	0.42
1:B:655:PHE:HA	1:B:658:ILE:HG21	2.01	0.42
1:B:690:LEU:O	1:B:691:GLY:O	2.37	0.42
1:C:150:THR:OG1	1:C:153:ASP:OD1	2.36	0.42
1:C:193:LEU:O	1:C:198:LEU:N	2.41	0.42
1:C:497:LEU:HD12	1:C:498:LYS:H	1.80	0.42
1:C:628:PHE:N	1:C:628:PHE:CD1	2.87	0.42
1:A:354:VAL:HG12	1:A:355:MET:N	2.34	0.42
1:A:668:LEU:O	1:A:668:LEU:HD12	2.19	0.42
1:A:706:ALA:HB2	1:A:847:LEU:HD12	2.00	0.42
1:A:711:ASP:C	1:A:713:LEU:H	2.22	0.42
1:A:916:ALA:O	1:A:919:ARG:O	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:LYS:O	1:B:132:SER:HB3	2.19	0.42
1:B:139:VAL:O	1:B:140:VAL:O	2.36	0.42
1:C:94:PHE:CZ	1:C:103:ALA:HB1	2.54	0.42
1:A:781:MET:CE	1:C:228:GLN:CD	2.88	0.42
1:C:390:ILE:HD13	1:C:390:ILE:HG21	1.73	0.42
1:C:708:LYS:O	1:C:710:PRO:HD3	2.19	0.42
1:C:719:ASN:O	1:C:721:LEU:N	2.52	0.42
1:C:77:TYR:CE1	1:C:860:THR:OG1	2.65	0.42
1:A:1023:PRO:O	1:A:1027:VAL:CG2	2.63	0.42
1:A:107:VAL:HG12	1:A:108:GLN:N	2.35	0.42
1:A:185:ARG:NH2	1:A:774:MET:HE2	2.34	0.42
1:A:922:THR:C	1:A:924:ASP:H	2.22	0.42
1:A:978:THR:C	1:A:980:LEU:N	2.72	0.42
1:B:960:LEU:HD11	1:B:1027:VAL:CG1	2.48	0.42
1:B:255:GLN:HG3	1:B:256:ASP:N	2.35	0.42
1:B:405:LEU:C	1:B:405:LEU:CD1	2.86	0.42
1:B:908:GLY:O	1:B:911:GLY:N	2.52	0.42
1:C:103:ALA:O	1:C:105:VAL:N	2.52	0.42
1:C:143:ILE:HA	1:C:143:ILE:HD13	1.20	0.42
1:C:58:GLN:OE1	1:C:82:SER:CA	2.67	0.42
1:C:982:PHE:O	1:C:983:ILE:C	2.57	0.42
1:A:111:LEU:O	1:A:113:LEU:N	2.53	0.42
1:A:117:LEU:N	1:A:117:LEU:HD22	2.34	0.42
1:A:119:PRO:O	1:A:122:VAL:N	2.45	0.42
1:A:331:PRO:O	1:A:335:ILE:HG23	2.19	0.42
1:A:370:ILE:O	1:A:370:ILE:HG22	2.18	0.42
1:A:417:GLU:OE2	1:A:417:GLU:HA	2.19	0.42
1:A:426:PRO:HB3	1:A:427:PRO:HD2	2.01	0.42
1:A:545:TYR:HA	1:A:548:ILE:HG12	2.01	0.42
1:A:680:PHE:HB2	1:A:859:TRP:CZ3	2.54	0.42
1:B:1031:ARG:CA	1:B:1034:SER:OG	2.67	0.42
1:B:362:PHE:O	1:B:364:ALA:N	2.52	0.42
1:B:513:PHE:O	1:B:516:PHE:HB2	2.19	0.42
1:B:574:THR:HA	1:B:665:ALA:HA	2.02	0.42
1:B:638:PRO:CG	1:B:639:GLY:H	2.30	0.42
1:B:725:PRO:HB2	1:B:809:TRP:CZ3	2.55	0.42
1:C:997:SER:HB2	1:C:1001:ASN:OD1	2.20	0.42
1:C:104:GLN:HB3	1:C:104:GLN:HE21	1.57	0.42
1:A:113:LEU:CD1	1:C:108:GLN:NE2	2.81	0.42
1:C:139:VAL:HG12	1:C:140:VAL:N	2.33	0.42
1:C:34:GLN:HB3	1:C:333:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:743:ILE:CD1	1:C:743:ILE:H	2.20	0.42
1:A:119:PRO:HG2	1:A:122:VAL:CG2	2.48	0.42
1:A:254:ASN:N	1:A:258:SER:OG	2.34	0.42
1:A:323:ILE:O	1:A:323:ILE:HD13	2.18	0.42
1:A:614:GLY:O	1:A:620:ARG:HB3	2.19	0.42
1:A:190:PRO:HD3	1:A:789:TRP:CH2	2.54	0.42
1:A:924:ASP:O	1:A:925:VAL:C	2.58	0.42
1:A:350:LEU:HD12	1:A:981:ALA:HA	2.02	0.42
1:B:121:GLU:HG2	1:B:121:GLU:H	1.67	0.42
1:B:391:ASN:O	1:B:395:MET:HG2	2.19	0.42
1:B:469:GLN:O	1:B:472:ILE:HG22	2.19	0.42
1:B:538:THR:N	1:B:540:ARG:NH2	2.63	0.42
1:B:566:ASP:O	1:B:567:GLU:C	2.57	0.42
1:B:700:ASN:O	1:B:704:ALA:HB2	2.19	0.42
1:B:740:GLY:HA3	1:B:794:ALA:CB	2.49	0.42
1:C:1028:VAL:HG12	1:C:1032:ARG:NH1	2.34	0.42
1:C:192:GLU:O	1:C:194:ASN:N	2.53	0.42
1:C:220:GLY:CA	1:C:231:ASN:ND2	2.60	0.42
1:C:306:ILE:O	1:C:309:GLU:N	2.52	0.42
1:C:764:ASP:HB3	1:C:769:LYS:HZ2	1.84	0.42
1:C:778:LYS:CD	1:C:779:TYR:CE2	2.91	0.42
1:C:713:LEU:CD2	1:C:835:LYS:H	2.31	0.42
1:C:897:ILE:O	1:C:900:SER:OG	2.28	0.42
1:A:371:ALA:O	1:A:372:VAL:C	2.57	0.42
1:A:376:LEU:HD23	1:A:376:LEU:N	2.35	0.42
1:A:449:LEU:O	1:A:453:PHE:HB2	2.19	0.42
1:A:199:THR:HG21	1:A:792:ARG:H	1.84	0.42
1:A:909:VAL:HG13	1:A:931:LEU:HD11	2.02	0.42
1:A:972:LEU:HD13	1:A:976:LEU:HG	2.01	0.42
1:B:144:ASN:ND2	1:B:144:ASN:O	2.53	0.42
1:B:219:LEU:CD1	1:B:234:ILE:CD1	2.98	0.42
1:B:254:ASN:O	1:B:257:GLY:N	2.46	0.42
1:B:343:THR:HA	1:B:346:GLU:HB3	2.02	0.42
1:B:628:PHE:CD1	1:B:628:PHE:N	2.87	0.42
1:B:72:ILE:HD12	1:B:72:ILE:HG23	1.63	0.42
1:B:76:MET:CG	1:B:95:GLU:HG3	2.49	0.42
1:C:5:PHE:CD2	1:C:12:ALA:HB2	2.54	0.42
1:C:759:VAL:HG22	1:C:759:VAL:H	1.38	0.42
1:C:911:GLY:H	1:C:1013:THR:HG21	1.84	0.42
1:A:178:PHE:CD1	1:A:178:PHE:N	2.88	0.42
1:A:17:ILE:O	1:A:18:ILE:C	2.56	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:ARG:CD	1:A:970:MET:CG	2.97	0.42
1:A:946:VAL:O	1:A:949:ALA:HB3	2.20	0.42
1:B:1026:PHE:HB3	1:B:1030:ARG:HH21	1.84	0.42
1:B:10:ILE:HG12	1:B:10:ILE:H	1.69	0.42
1:B:193:LEU:HA	1:B:265:VAL:CG2	2.49	0.42
1:B:213:GLN:O	1:B:214:VAL:CG2	2.67	0.42
1:B:143:ILE:HG22	1:B:285:PRO:O	2.20	0.42
1:B:420:MET:HE2	1:B:425:LEU:HA	2.02	0.42
1:B:484:VAL:C	1:B:485:ALA:O	2.56	0.42
1:B:573:MET:HE1	1:B:617:PHE:HE2	1.85	0.42
1:B:655:PHE:C	1:B:658:ILE:CG1	2.88	0.42
1:B:659:LYS:HD2	1:B:660:ASP:OD2	2.20	0.42
1:B:799:VAL:HA	1:B:800:PRO:HD2	1.78	0.42
1:B:987:MET:CE	1:B:987:MET:O	2.64	0.42
1:C:210:GLN:OE1	1:C:250:LEU:N	2.47	0.42
1:C:525:HIS:O	1:C:529:ASP:N	2.52	0.42
1:C:622:GLN:O	1:C:622:GLN:HG2	2.19	0.42
1:A:911:GLY:C	1:A:1010:GLY:H	2.23	0.42
1:A:1027:VAL:O	1:A:1029:VAL:O	2.37	0.42
1:A:380:PHE:CZ	1:A:398:MET:HE1	2.55	0.42
1:A:425:LEU:N	1:A:425:LEU:CD1	2.71	0.42
1:A:44:THR:HG21	1:A:89:GLN:CG	2.50	0.42
1:A:750:LEU:C	1:A:750:LEU:HD13	2.40	0.42
1:A:876:LEU:HA	1:A:879:ILE:HD12	2.01	0.42
1:A:890:ALA:HB1	1:C:11:PHE:HA	2.02	0.42
1:A:897:ILE:HG12	1:A:950:LYS:HE2	2.02	0.42
1:B:921:LEU:HD21	1:B:1005:THR:HG22	1.94	0.42
1:B:1030:ARG:C	1:B:1032:ARG:H	2.22	0.42
1:B:443:VAL:HG12	1:B:444:GLY:N	2.34	0.42
1:B:714:THR:O	1:B:715:SER:OG	2.32	0.42
1:B:912:ALA:HB2	1:B:1010:GLY:HA3	2.00	0.42
1:C:1024:VAL:O	1:C:1025:PHE:C	2.56	0.42
1:C:516:PHE:CD2	1:C:517:ASN:N	2.88	0.42
1:C:355:MET:HE1	1:C:977:MET:HG2	2.01	0.42
1:A:207:ILE:HG22	1:A:207:ILE:O	2.19	0.42
1:A:359:LEU:HD11	1:A:417:GLU:HB3	2.02	0.42
1:A:531:VAL:HG22	1:A:1020:PHE:HD1	1.85	0.42
1:A:775:SER:HB2	1:A:789:TRP:HZ2	1.84	0.42
1:A:865:GLN:O	1:A:866:GLU:C	2.58	0.42
1:A:880:SER:O	1:A:882:ILE:N	2.53	0.42
1:A:975:ILE:O	1:A:976:LEU:C	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:GLN:HB2	1:C:781:MET:HE1	2.01	0.42
1:B:231:ASN:HD22	1:B:232:ALA:N	2.18	0.42
1:B:395:MET:HA	1:B:398:MET:HG2	2.00	0.42
1:B:408:ASP:C	1:B:410:ILE:N	2.68	0.42
1:B:410:ILE:O	1:B:413:VAL:HG12	2.20	0.42
1:B:428:LYS:O	1:B:432:ARG:HB2	2.20	0.42
1:B:514:GLY:HA2	1:B:517:ASN:ND2	2.35	0.42
1:B:857:TYR:O	1:B:858:ASP:HB2	2.20	0.42
1:C:185:ARG:HG2	1:C:271:GLY:CA	2.50	0.42
1:C:417:GLU:CA	1:C:417:GLU:OE2	2.56	0.42
1:C:513:PHE:HA	1:C:516:PHE:HB2	1.92	0.42
1:C:619:GLY:O	1:C:620:ARG:O	2.38	0.42
1:C:695:LEU:C	1:C:825:MET:HE2	2.40	0.42
1:C:3:ASN:HD22	1:C:6:ILE:HD12	1.85	0.42
1:C:914:LEU:O	1:C:915:ALA:CB	2.66	0.42
1:A:189:ASN:HB2	1:A:779:TYR:CZ	2.54	0.42
1:A:328:ASP:C	1:A:328:ASP:OD1	2.59	0.42
1:A:568:ASP:CB	1:A:634:TRP:CZ3	2.97	0.42
1:A:874:PRO:HB2	1:A:875:SER:H	1.50	0.42
1:B:20:MET:HG2	1:B:374:VAL:HA	2.02	0.42
1:B:476:SER:O	1:B:478:MET:N	2.53	0.42
1:B:578:LEU:HB3	1:B:579:PRO:CD	2.50	0.42
1:B:578:LEU:CD1	1:B:586:ARG:HH21	2.30	0.42
1:B:898:PRO:O	1:B:899:PHE:C	2.56	0.42
1:B:992:SER:CB	1:B:1000:GLN:OE1	2.67	0.42
1:C:137:LEU:CD2	1:C:137:LEU:C	2.87	0.42
1:C:159:ALA:CB	1:C:181:GLN:HB2	2.50	0.42
1:C:362:PHE:O	1:C:365:THR:N	2.43	0.42
1:C:446:ALA:C	1:C:448:VAL:H	2.23	0.42
1:C:715:SER:O	1:C:717:ARG:NH1	2.52	0.42
1:C:181:GLN:NE2	1:C:769:LYS:HD2	2.34	0.42
1:C:40:PRO:HB3	1:C:76:MET:HE1	2.02	0.42
1:A:99:ASP:HB3	1:A:102:ILE:HG22	2.02	0.41
1:A:115:MET:C	1:A:117:LEU:H	2.23	0.41
1:A:13:TRP:O	1:A:17:ILE:N	2.52	0.41
1:A:169:THR:OG1	1:A:172:VAL:CG1	2.68	0.41
1:A:189:ASN:O	1:A:189:ASN:CG	2.56	0.41
1:A:268:ILE:HD12	1:A:268:ILE:H	1.84	0.41
1:A:332:PHE:C	1:A:332:PHE:CD2	2.93	0.41
1:A:373:PRO:O	1:A:377:LEU:HB2	2.21	0.41
1:A:531:VAL:HG12	1:A:531:VAL:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:671:ILE:HG13	1:A:674:LEU:HD12	2.02	0.41
1:A:857:TYR:O	1:A:857:TYR:CG	2.73	0.41
1:A:418:ARG:HD2	1:A:970:MET:HE2	2.01	0.41
1:B:1030:ARG:H	1:B:1030:ARG:HG3	1.72	0.41
1:B:189:ASN:HB2	1:B:265:VAL:O	2.20	0.41
1:B:376:LEU:O	1:B:379:THR:N	2.50	0.41
1:B:415:ASN:HA	1:B:418:ARG:HB3	2.01	0.41
1:B:665:ALA:O	1:B:666:PHE:CD2	2.73	0.41
1:B:470:PHE:CE2	1:B:929:VAL:HG11	2.55	0.41
1:B:952:LEU:HA	1:B:956:GLU:OE2	2.20	0.41
1:C:344:LEU:O	1:C:348:ILE:HG23	2.19	0.41
1:C:449:LEU:CB	1:C:478:MET:HE1	2.50	0.41
1:C:49:TYR:CG	1:C:52:ALA:HB2	2.56	0.41
1:C:685:ILE:HD12	1:C:686:ASP:C	2.40	0.41
1:C:815:ARG:NH1	1:C:815:ARG:HG3	2.35	0.41
1:C:714:THR:HA	1:C:830:GLN:O	2.20	0.41
1:C:915:ALA:CA	1:C:918:PHE:HB3	2.40	0.41
1:A:139:VAL:O	1:A:139:VAL:CG2	2.63	0.41
1:A:407:ASP:O	1:A:409:ALA:N	2.53	0.41
1:A:631:LEU:HD11	1:A:644:VAL:HG22	2.02	0.41
1:A:886:LEU:HD21	1:C:17:ILE:HG21	2.01	0.41
1:A:43:VAL:O	1:A:91:THR:HA	2.21	0.41
1:B:1013:THR:HG23	1:B:1013:THR:O	2.20	0.41
1:B:115:MET:HE3	1:B:118:LEU:HD22	2.01	0.41
1:B:158:VAL:CA	1:B:162:MET:HG2	2.35	0.41
1:B:230:LEU:HD21	1:C:809:TRP:HH2	1.83	0.41
1:B:231:ASN:ND2	1:B:232:ALA:N	2.69	0.41
1:B:33:ALA:O	1:B:337:ILE:HD11	2.20	0.41
1:B:531:VAL:HG22	1:B:535:LEU:CD2	2.50	0.41
1:B:610:PHE:O	1:B:627:ALA:HB1	2.19	0.41
1:B:641:GLU:CA	1:B:650:ARG:NH1	2.81	0.41
1:B:713:LEU:HD21	1:B:844:MET:HG2	2.03	0.41
1:B:987:MET:CE	1:B:990:VAL:HB	2.50	0.41
1:C:414:GLU:OE1	1:C:977:MET:CE	2.55	0.41
1:C:15:ILE:HD12	1:C:487:ILE:HG21	2.02	0.41
1:C:574:THR:HG22	1:C:575:MET:O	2.20	0.41
1:C:790:TYR:O	1:C:791:VAL:CG2	2.68	0.41
1:A:187:TRP:CH2	1:C:223:PRO:HG2	2.56	0.41
1:A:274:ASN:HB2	2:A:2001:MIY:O8	2.20	0.41
1:A:138:MET:CE	1:A:306:ILE:HB	2.51	0.41
1:A:360:GLN:HB3	1:A:360:GLN:HE21	1.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:653:ARG:O	1:A:655:PHE:N	2.53	0.41
1:B:423:GLU:OE1	1:B:427:PRO:HD3	2.20	0.41
1:B:65:ILE:HG23	1:B:69:MET:HE2	2.03	0.41
1:B:668:LEU:HG	1:B:668:LEU:H	1.51	0.41
1:C:975:ILE:HG21	1:C:1019:ILE:HD13	2.02	0.41
1:C:290:GLY:O	1:C:291:ILE:HG13	2.20	0.41
1:C:375:VAL:HG22	1:C:484:VAL:HG21	2.01	0.41
1:C:396:PHE:HD1	1:C:926:TYR:HE1	1.68	0.41
1:C:402:ILE:HG21	1:C:402:ILE:HD13	1.84	0.41
1:C:578:LEU:HD22	1:C:661:ALA:HB1	1.96	0.41
1:C:713:LEU:HD21	1:C:835:LYS:N	2.33	0.41
1:A:65:ILE:HB	1:A:118:LEU:HD11	2.02	0.41
1:A:281:PHE:O	1:A:282:ASN:C	2.57	0.41
1:A:552:MET:HE1	1:A:906:PRO:CB	2.50	0.41
1:A:63:GLN:HB3	1:A:64:VAL:H	1.16	0.41
1:A:944:LEU:HD23	1:A:944:LEU:HA	1.66	0.41
1:A:991:ILE:HG12	1:A:1005:THR:H	1.85	0.41
1:B:1015:THR:O	1:B:1018:ALA:HB3	2.20	0.41
1:B:149:MET:CB	1:B:154:ILE:HG23	2.50	0.41
1:B:189:ASN:HB3	1:B:192:GLU:HB3	2.03	0.41
1:B:495:THR:O	1:B:498:LYS:HE3	2.20	0.41
1:B:605:ASN:OD1	1:B:642:ASN:CB	2.68	0.41
1:B:782:LEU:O	1:B:784:ASP:N	2.53	0.41
1:B:944:LEU:HB2	1:B:975:ILE:HD11	2.03	0.41
1:A:781:MET:CE	1:C:228:GLN:OE1	2.68	0.41
1:C:276:ASP:C	1:C:277:ILE:HG13	2.40	0.41
1:C:299:ALA:O	1:C:300:LEU:C	2.56	0.41
1:C:456:MET:O	1:C:457:ALA:HB3	2.21	0.41
1:C:577:GLN:HB3	1:C:624:THR:HG22	2.01	0.41
1:C:892:TYR:OH	1:C:943:ILE:HG23	2.20	0.41
1:C:904:VAL:C	1:C:906:PRO:HD2	2.40	0.41
1:A:1007:VAL:O	1:A:1011:MET:HB2	2.21	0.41
1:A:187:TRP:HA	1:A:774:MET:O	2.21	0.41
1:A:472:ILE:O	1:A:473:THR:C	2.59	0.41
1:A:598:TYR:O	1:A:602:GLU:HB2	2.20	0.41
1:A:780:ARG:O	1:A:780:ARG:HD2	2.21	0.41
1:A:905:VAL:O	1:A:909:VAL:CG2	2.49	0.41
1:B:109:ASN:HA	1:B:109:ASN:HD22	1.75	0.41
1:B:391:ASN:OD1	1:B:391:ASN:C	2.58	0.41
1:B:468:ARG:O	1:B:470:PHE:N	2.54	0.41
1:B:659:LYS:HD3	1:B:660:ASP:OD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:VAL:CG2	1:B:94:PHE:HE2	2.32	0.41
1:C:1018:ALA:HA	1:C:1021:PHE:HB2	2.02	0.41
1:C:246:PHE:O	1:C:249:ILE:HB	2.21	0.41
1:C:33:ALA:HB2	1:C:298:ASN:HD22	1.84	0.41
1:C:55:LYS:HG2	1:C:55:LYS:O	2.20	0.41
1:C:643:LYS:O	1:C:647:ILE:HG12	2.20	0.41
1:C:696:THR:HA	1:C:825:MET:HE1	2.02	0.41
1:C:961:ILE:O	1:C:961:ILE:HG22	2.19	0.41
1:C:974:PRO:O	1:C:975:ILE:C	2.59	0.41
1:A:277:ILE:CD1	1:A:277:ILE:C	2.88	0.41
1:A:55:LYS:O	1:A:58:GLN:N	2.53	0.41
1:A:605:ASN:O	1:A:632:LYS:N	2.54	0.41
1:B:34:GLN:OE1	1:B:35:TYR:CD2	2.74	0.41
1:B:2:PRO:O	1:B:3:ASN:HB2	2.20	0.41
1:B:411:VAL:H	1:B:411:VAL:HG22	1.55	0.41
1:B:659:LYS:HA	1:B:659:LYS:CE	2.48	0.41
1:B:200:PRO:HG2	1:B:749:THR:HA	2.03	0.41
1:B:764:ASP:OD1	1:B:764:ASP:C	2.59	0.41
1:B:790:TYR:HD1	1:B:800:PRO:CA	2.33	0.41
1:B:892:TYR:CB	1:B:897:ILE:CD1	2.80	0.41
1:B:989:LEU:CA	1:B:992:SER:HB2	2.49	0.41
1:C:196:PHE:O	1:C:197:GLN:HB2	2.21	0.41
1:C:351:VAL:HG12	1:C:369:THR:HG22	2.02	0.41
1:C:457:ALA:HB2	1:C:468:ARG:N	2.35	0.41
1:C:465:ALA:O	1:C:469:GLN:HG2	2.21	0.41
1:C:535:LEU:HG	1:C:535:LEU:O	2.19	0.41
1:C:680:PHE:CD2	1:C:829:GLY:O	2.73	0.41
1:C:54:ALA:HB2	1:C:84:SER:CA	2.51	0.41
1:C:964:THR:O	1:C:967:ALA:HB3	2.20	0.41
1:C:965:LEU:O	1:C:969:ARG:HB2	2.21	0.41
1:C:969:ARG:HG2	1:C:969:ARG:NH2	2.35	0.41
1:C:396:PHE:HE1	1:C:999:ALA:HB1	1.85	0.41
1:A:346:GLU:O	1:A:347:ALA:C	2.57	0.41
1:A:354:VAL:CG1	1:A:980:LEU:HD23	2.51	0.41
1:A:709:HIS:N	1:A:710:PRO:CD	2.83	0.41
1:A:904:VAL:O	1:A:905:VAL:C	2.59	0.41
1:A:928:GLN:H	1:A:928:GLN:HG3	1.38	0.41
1:A:930:GLY:O	1:A:931:LEU:C	2.57	0.41
1:B:177:LEU:HG	1:B:179:GLY:O	2.21	0.41
1:B:178:PHE:HE1	1:B:615:PHE:CE2	2.39	0.41
1:B:298:ASN:O	1:B:302:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:ILE:O	1:B:337:ILE:N	2.50	0.41
1:B:355:MET:SD	1:B:410:ILE:HD11	2.61	0.41
1:B:447:MET:SD	1:B:887:CYS:HB3	2.60	0.41
1:B:612:VAL:HG21	1:B:628:PHE:HE1	1.85	0.41
1:C:910:ILE:HG23	1:C:1013:THR:OG1	2.20	0.41
1:C:1014:ALA:O	1:C:1018:ALA:CB	2.69	0.41
1:C:351:VAL:O	1:C:355:MET:HB2	2.20	0.41
1:C:518:ARG:H	1:C:518:ARG:HG2	1.66	0.41
1:C:861:GLY:H	1:C:864:TYR:HB2	1.85	0.41
1:A:104:GLN:HB2	1:A:131:LYS:NZ	2.36	0.41
1:A:32:VAL:HA	1:A:390:ILE:O	2.21	0.41
1:A:461:GLY:O	1:A:462:SER:C	2.58	0.41
1:A:726:GLN:CG	1:A:810:GLU:O	2.69	0.41
1:A:817:GLU:HG3	1:A:824:SER:O	2.20	0.41
1:A:847:LEU:HD23	1:A:847:LEU:N	2.36	0.41
1:B:227:GLY:O	1:C:585:GLU:OE2	2.38	0.41
1:B:49:TYR:HE2	1:B:125:GLN:HG2	1.86	0.41
1:B:594:VAL:HG22	1:B:663:VAL:HG11	2.01	0.41
1:C:159:ALA:HB1	1:C:181:GLN:HB2	2.03	0.41
1:C:2:PRO:O	1:C:3:ASN:C	2.58	0.41
1:C:372:VAL:HG23	1:C:405:LEU:HD12	2.02	0.41
1:C:418:ARG:NH2	1:C:948:PHE:HZ	2.19	0.41
1:C:445:ILE:HD13	1:C:940:LYS:CE	2.49	0.41
1:C:532:GLY:O	1:C:534:ILE:N	2.54	0.41
1:C:713:LEU:N	1:C:713:LEU:HD22	2.35	0.41
1:C:774:MET:CG	1:C:775:SER:N	2.84	0.41
1:C:816:LEU:HA	1:C:816:LEU:HD23	1.70	0.41
1:C:898:PRO:HG2	1:C:899:PHE:CD1	2.56	0.41
1:C:932:LEU:HD23	1:C:932:LEU:HA	1.74	0.41
1:A:155:SER:OG	1:A:179:GLY:HA3	2.21	0.41
1:A:210:GLN:HG3	1:A:249:ILE:HG21	2.00	0.41
1:A:330:THR:HG22	1:A:331:PRO:HD3	2.03	0.41
1:A:531:VAL:O	1:A:534:ILE:HG13	2.20	0.41
1:A:844:MET:HA	1:A:844:MET:CE	2.51	0.41
1:A:358:PHE:CD2	1:A:973:ARG:HG3	2.56	0.41
1:A:989:LEU:HA	1:A:992:SER:O	2.21	0.41
1:B:219:LEU:HD12	1:B:219:LEU:H	1.86	0.41
1:B:416:VAL:O	1:B:426:PRO:HG2	2.20	0.41
1:B:47:ALA:HB3	1:B:88:VAL:CG2	2.51	0.41
1:B:943:ILE:HD12	1:B:943:ILE:HA	1.89	0.41
1:B:531:VAL:CG1	1:B:965:LEU:HD21	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:972:LEU:HD11	1:B:976:LEU:HD21	2.03	0.41
1:C:449:LEU:CB	1:C:478:MET:CE	2.98	0.41
1:C:527:TYR:C	1:C:529:ASP:H	2.24	0.41
1:C:631:LEU:HD11	1:C:644:VAL:HG22	2.03	0.41
1:C:58:GLN:CG	1:C:82:SER:OG	2.69	0.41
1:C:873:ALA:O	1:C:874:PRO:C	2.58	0.41
1:C:9:PRO:C	1:C:10:ILE:HG12	2.40	0.41
1:A:1018:ALA:HB1	1:A:1022:VAL:HG13	1.93	0.41
1:A:190:PRO:HG2	1:A:788:ASP:HB3	2.03	0.41
2:A:2001:MIY:O5	2:A:2001:MIY:O6	2.39	0.41
1:A:277:ILE:HA	1:A:613:ASN:O	2.21	0.41
1:A:310:LEU:C	1:A:311:ALA:O	2.56	0.41
1:A:601:LYS:O	1:A:602:GLU:HG2	2.21	0.41
1:A:952:LEU:CD1	1:A:963:ALA:HB1	2.50	0.41
1:B:167:SER:HA	1:B:175:VAL:HG21	2.02	0.41
1:B:199:THR:C	1:B:201:VAL:H	2.24	0.41
1:B:199:THR:O	1:B:202:ASP:N	2.53	0.41
1:B:354:VAL:C	1:B:356:TYR:H	2.24	0.41
1:B:525:HIS:O	1:B:529:ASP:CB	2.68	0.41
1:B:619:GLY:H	1:B:721:LEU:CD1	2.34	0.41
1:B:586:ARG:NH2	1:B:660:ASP:HB2	2.36	0.41
1:B:665:ALA:O	1:B:666:PHE:CG	2.74	0.41
1:B:71:GLY:O	1:B:72:ILE:C	2.60	0.41
1:B:828:LEU:HD23	1:B:828:LEU:HA	1.82	0.41
1:B:831:ALA:CB	1:B:840:ALA:CB	2.83	0.41
1:B:900:SER:O	1:B:903:LEU:N	2.36	0.41
1:C:279:ALA:C	1:C:280:GLU:CG	2.89	0.41
1:C:32:VAL:O	1:C:300:LEU:HD13	2.21	0.41
1:C:317:PHE:N	1:C:317:PHE:CD2	2.88	0.41
1:C:931:LEU:HD22	1:C:931:LEU:HA	1.77	0.41
1:A:143:ILE:HG21	1:A:281:PHE:HD2	1.83	0.41
1:A:281:PHE:CE1	1:A:608:SER:HB2	2.56	0.41
1:A:353:LEU:C	1:A:354:VAL:O	2.57	0.41
1:A:367:ILE:HG13	1:A:368:PRO:HD3	2.02	0.41
1:A:351:VAL:HG13	1:A:410:ILE:HD11	2.03	0.41
1:A:579:PRO:O	1:A:580:ALA:C	2.60	0.41
1:A:588:GLN:HG2	1:A:613:ASN:HD21	1.85	0.41
1:A:62:THR:O	1:A:63:GLN:C	2.57	0.41
1:A:740:GLY:O	1:A:793:ALA:CA	2.69	0.41
1:A:843:LEU:O	1:A:844:MET:C	2.59	0.41
1:A:958:LYS:HB3	1:A:959:GLY:H	1.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:888:LEU:O	1:B:892:TYR:N	2.54	0.41
1:C:226:LYS:HB3	1:C:227:GLY:H	1.69	0.41
1:C:25:LEU:H	1:C:25:LEU:HG	1.76	0.41
1:C:58:GLN:OE1	1:C:82:SER:CB	2.69	0.41
1:C:69:MET:HE1	1:C:92:LEU:HD21	2.02	0.41
1:C:687:GLN:HB2	1:C:854:GLY:O	2.20	0.41
1:C:949:ALA:O	1:C:951:ASP:N	2.54	0.41
1:A:1016:VAL:O	1:A:1016:VAL:CG1	2.69	0.40
1:A:134:SER:O	1:A:135:SER:HB3	2.21	0.40
1:A:347:ALA:O	1:A:350:LEU:HB2	2.21	0.40
1:A:399:VAL:O	1:A:401:ALA:N	2.54	0.40
1:A:753:ALA:HB3	1:A:754:TRP:CD1	2.56	0.40
1:B:462:SER:HB3	1:B:865:GLN:NE2	2.35	0.40
1:B:602:GLU:HG2	1:B:602:GLU:H	1.48	0.40
1:A:234:ILE:HG23	1:B:727:PHE:HD1	1.87	0.40
1:B:898:PRO:C	1:B:900:SER:N	2.74	0.40
1:C:102:ILE:CG2	1:C:106:GLN:CG	2.98	0.40
1:C:157:TYR:CE1	1:C:318:PRO:HD3	2.56	0.40
1:C:203:VAL:O	1:C:207:ILE:HG13	2.21	0.40
1:C:166:ILE:HG21	1:C:291:ILE:HD11	2.03	0.40
1:C:399:VAL:HA	1:C:402:ILE:HG13	2.03	0.40
1:C:410:ILE:O	1:C:411:VAL:C	2.59	0.40
1:C:405:LEU:HD21	1:C:477:ALA:O	2.21	0.40
1:C:545:TYR:OH	1:C:1021:PHE:O	2.39	0.40
1:C:615:PHE:HD2	1:C:615:PHE:O	2.04	0.40
1:C:732:ASP:OD2	1:C:735:LYS:HG3	2.20	0.40
1:C:548:ILE:HD13	1:C:907:LEU:HD12	2.01	0.40
1:A:157:TYR:CE2	1:A:321:LEU:HD22	2.56	0.40
1:A:590:VAL:HG23	1:A:590:VAL:H	1.70	0.40
1:B:1021:PHE:O	1:B:1025:PHE:CE1	2.74	0.40
1:B:103:ALA:O	1:B:104:GLN:O	2.39	0.40
1:B:410:ILE:O	1:B:412:VAL:N	2.54	0.40
1:B:587:THR:OG1	1:B:623:ASN:HA	2.21	0.40
1:B:58:GLN:O	1:B:59:ASP:OD2	2.39	0.40
1:B:714:THR:HG22	1:B:830:GLN:C	2.42	0.40
1:B:737:GLN:CG	1:B:737:GLN:O	2.70	0.40
1:C:186:ILE:HB	1:C:773:VAL:HA	2.03	0.40
1:C:367:ILE:HG13	1:C:368:PRO:N	2.36	0.40
1:C:425:LEU:H	1:C:426:PRO:HD3	1.86	0.40
1:C:444:GLY:O	1:C:445:ILE:C	2.59	0.40
1:C:662:MET:H	1:C:662:MET:HG2	1.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:808:ARG:O	1:C:809:TRP:C	2.58	0.40
1:A:287:SER:O	1:A:288:GLY:O	2.38	0.40
1:A:531:VAL:O	1:A:534:ILE:CG1	2.70	0.40
1:A:638:PRO:CG	1:A:639:GLY:H	2.27	0.40
1:A:797:GLN:O	1:A:799:VAL:HG23	2.21	0.40
1:B:24:GLY:HA2	1:B:27:ILE:HG21	2.02	0.40
1:B:518:ARG:C	1:B:520:PHE:N	2.75	0.40
1:B:541:TYR:C	1:B:543:VAL:N	2.73	0.40
1:A:219:LEU:HD23	1:B:754:TRP:HZ3	1.86	0.40
1:B:940:LYS:HZ1	1:B:978:THR:CG2	2.35	0.40
1:A:113:LEU:HD11	1:C:108:GLN:NE2	2.36	0.40
1:C:467:TYR:OH	1:C:925:VAL:HG12	2.21	0.40
1:C:557:VAL:HG12	1:C:557:VAL:O	2.21	0.40
1:C:762:PHE:CD2	1:C:763:ILE:N	2.89	0.40
1:A:205:THR:O	1:A:205:THR:CG2	2.49	0.40
1:B:10:ILE:O	1:B:11:PHE:C	2.60	0.40
1:B:173:GLY:H	1:B:294:ALA:H	1.68	0.40
1:B:58:GLN:HB2	1:B:82:SER:OG	2.22	0.40
1:B:655:PHE:O	1:B:658:ILE:CG1	2.69	0.40
1:B:187:TRP:HA	1:B:774:MET:O	2.22	0.40
1:B:961:ILE:HA	1:B:964:THR:HB	2.04	0.40
1:C:106:GLN:HG2	1:C:106:GLN:H	1.63	0.40
1:C:142:VAL:HG13	1:C:321:LEU:HD11	2.03	0.40
1:C:145:THR:N	1:C:320:GLY:O	2.53	0.40
1:C:251:LEU:HD11	1:C:262:LEU:HD12	2.03	0.40
1:C:25:LEU:O	1:C:27:ILE:N	2.54	0.40
1:C:34:GLN:HG3	1:C:34:GLN:H	1.76	0.40
1:C:760:ASN:C	1:C:760:ASN:OD1	2.59	0.40
1:C:713:LEU:HD23	1:C:831:ALA:CA	2.52	0.40
1:C:907:LEU:O	1:C:1013:THR:O	2.39	0.40
1:C:983:ILE:O	1:C:985:GLY:N	2.55	0.40
1:C:9:PRO:C	1:C:11:PHE:H	2.24	0.40
1:A:73:ASP:H	1:A:106:GLN:HE22	1.69	0.40
1:A:330:THR:HG23	1:A:334:LYS:CE	2.51	0.40
1:A:348:ILE:HD11	1:A:372:VAL:HG12	2.03	0.40
1:A:405:LEU:C	1:A:405:LEU:HD22	2.39	0.40
1:A:492:LEU:HD12	1:A:492:LEU:HA	1.89	0.40
1:A:576:VAL:HG11	1:A:591:LEU:HD23	2.03	0.40
1:A:879:ILE:H	1:A:879:ILE:HG13	1.71	0.40
1:B:104:GLN:NE2	1:B:108:GLN:NE2	2.70	0.40
1:B:122:VAL:O	1:B:123:GLN:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:PHE:N	1:B:386:PHE:CD1	2.89	0.40
1:B:344:LEU:HD13	1:B:398:MET:HB2	2.04	0.40
1:B:55:LYS:O	1:B:56:THR:C	2.59	0.40
1:B:759:VAL:HG12	1:B:760:ASN:HB2	2.04	0.40
1:B:863:SER:O	1:B:866:GLU:N	2.53	0.40
1:B:879:ILE:O	1:B:883:VAL:HG23	2.22	0.40
1:C:477:ALA:H	1:C:480:LEU:HD23	1.86	0.40
1:C:61:VAL:O	1:C:62:THR:C	2.60	0.40
1:C:653:ARG:HG3	1:C:654:ALA:N	2.36	0.40
1:B:11:PHE:HA	1:C:890:ALA:HA	2.04	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	1018/1053 (97%)	627 (62%)	225 (22%)	166 (16%)	0	0
1	B	1018/1053 (97%)	616 (60%)	246 (24%)	156 (15%)	0	0
1	C	1018/1053 (97%)	642 (63%)	236 (23%)	140 (14%)	0	1
All	All	3054/3159 (97%)	1885 (62%)	707 (23%)	462 (15%)	0	0

All (462) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	64	VAL
1	A	65	ILE
1	A	73	ASP
1	A	74	ASN
1	A	90	ILE
1	A	96	SER

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Mol	Chain	Res	Type
1	A	135	SER
1	A	137	LEU
1	A	147	GLY
1	A	167	SER
1	A	170	SER
1	A	172	VAL
1	A	174	ASP
1	A	181	GLN
1	A	218	GLN
1	A	221	GLY
1	A	255	GLN
1	A	288	GLY
1	A	293	LEU
1	A	294	ALA
1	A	318	PRO
1	A	376	LEU
1	A	422	GLU
1	A	435	MET
1	A	439	GLN
1	A	443	VAL
1	A	444	GLY
1	A	515	TRP
1	A	521	GLU
1	A	538	THR
1	A	580	ALA
1	A	597	TYR
1	A	601	LYS
1	A	659	LYS
1	A	660	ASP
1	A	672	VAL
1	A	676	THR
1	A	677	ALA
1	A	687	GLN
1	A	689	GLY
1	A	690	LEU
1	A	715	SER
1	A	759	VAL
1	A	775	SER
1	A	784	ASP
1	A	820	ASN
1	A	866	GLU
1	A	868	LEU

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Mol	Chain	Res	Type
1	A	991	ILE
1	A	1016	VAL
1	A	1024	VAL
1	A	1025	PHE
1	B	8	ARG
1	B	12	ALA
1	B	13	TRP
1	B	22	ALA
1	B	50	PRO
1	B	51	GLY
1	B	54	ALA
1	B	56	THR
1	B	85	THR
1	B	98	THR
1	B	112	GLN
1	B	147	GLY
1	B	173	GLY
1	B	228	GLN
1	B	258	SER
1	B	268	ILE
1	B	270	LEU
1	B	326	PRO
1	B	357	LEU
1	B	361	ASN
1	B	408	ASP
1	B	409	ALA
1	B	424	GLY
1	B	466	ILE
1	B	535	LEU
1	B	536	ARG
1	B	538	THR
1	B	549	VAL
1	B	567	GLU
1	B	602	GLU
1	B	606	VAL
1	B	613	ASN
1	B	638	PRO
1	B	644	VAL
1	B	647	ILE
1	B	655	PHE
1	B	671	ILE
1	B	693	GLU

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Mol	Chain	Res	Type
1	B	703	LEU
1	B	705	GLU
1	B	712	MET
1	B	715	SER
1	B	733	GLN
1	B	777	ALA
1	B	786	ILE
1	B	805	SER
1	B	851	LEU
1	B	871	ASN
1	B	907	LEU
1	B	908	GLY
1	B	921	LEU
1	B	1012	VAL
1	B	1034	SER
1	C	19	ILE
1	C	52	ALA
1	C	61	VAL
1	C	81	ASN
1	C	95	GLU
1	C	164	ASP
1	C	167	SER
1	C	187	TRP
1	C	226	LYS
1	C	258	SER
1	C	311	ALA
1	C	319	SER
1	C	336	SER
1	C	366	LEU
1	C	404	LEU
1	C	410	ILE
1	C	411	VAL
1	C	418	ARG
1	C	419	VAL
1	C	460	GLY
1	C	464	GLY
1	C	532	GLY
1	C	536	ARG
1	C	601	LYS
1	C	658	ILE
1	C	690	LEU
1	C	696	THR

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Mol	Chain	Res	Type
1	C	715	SER
1	C	720	GLY
1	C	778	LYS
1	C	869	SER
1	C	871	ASN
1	C	872	GLN
1	C	905	VAL
1	C	925	VAL
1	C	946	VAL
1	C	952	LEU
1	C	960	LEU
1	C	965	LEU
1	C	983	ILE
1	C	989	LEU
1	C	993	THR
1	C	1017	LEU
1	C	1035	ARG
1	A	18	ILE
1	A	53	ASP
1	A	67	GLN
1	A	105	VAL
1	A	109	ASN
1	A	146	ASP
1	A	192	GLU
1	A	206	ALA
1	A	217	GLY
1	A	256	ASP
1	A	317	PHE
1	A	353	LEU
1	A	357	LEU
1	A	372	VAL
1	A	411	VAL
1	A	428	LYS
1	A	459	PHE
1	A	496	MET
1	A	535	LEU
1	A	582	ALA
1	A	634	TRP
1	A	638	PRO
1	A	651	ALA
1	A	654	ALA
1	A	679	GLY

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Mol	Chain	Res	Type
1	A	713	LEU
1	A	730	ASP
1	A	752	ALA
1	A	753	ALA
1	A	794	ALA
1	A	881	LEU
1	A	903	LEU
1	A	925	VAL
1	A	931	LEU
1	A	951	ASP
1	A	957	GLY
1	A	958	LYS
1	A	964	THR
1	A	971	ARG
1	A	1004	GLY
1	A	1005	THR
1	A	1010	GLY
1	A	1034	SER
1	B	2	PRO
1	B	48	SER
1	B	69	MET
1	B	104	GLN
1	B	110	LYS
1	B	125	GLN
1	B	131	LYS
1	B	171	GLY
1	B	175	VAL
1	B	265	VAL
1	B	319	SER
1	B	327	TYR
1	B	363	ARG
1	B	461	GLY
1	B	491	ALA
1	B	495	THR
1	B	519	MET
1	B	539	GLY
1	B	601	LYS
1	B	603	LYS
1	B	618	ALA
1	B	621	GLY
1	B	659	LYS
1	B	669	PRO

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Mol	Chain	Res	Type
1	B	675	GLY
1	B	711	ASP
1	B	730	ASP
1	B	820	ASN
1	B	821	GLY
1	B	831	ALA
1	B	834	GLY
1	B	852	PRO
1	B	863	SER
1	B	919	ARG
1	B	942	ALA
1	B	943	ILE
1	B	959	GLY
1	B	966	ASP
1	B	1011	MET
1	B	1013	THR
1	C	10	ILE
1	C	51	GLY
1	C	54	ALA
1	C	67	GLN
1	C	160	ALA
1	C	255	GLN
1	C	394	THR
1	C	447	MET
1	C	451	ALA
1	C	535	LEU
1	C	537	SER
1	C	540	ARG
1	C	546	LEU
1	C	576	VAL
1	C	577	GLN
1	C	593	GLU
1	C	620	ARG
1	C	671	ILE
1	C	673	GLU
1	C	697	GLN
1	C	706	ALA
1	C	716	VAL
1	C	837	THR
1	C	867	ARG
1	C	890	ALA
1	C	895	TRP

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Mol	Chain	Res	Type
1	C	935	ILE
1	C	950	LYS
1	C	975	ILE
1	C	984	LEU
1	C	998	GLY
1	C	1029	VAL
1	A	12	ALA
1	A	54	ALA
1	A	69	MET
1	A	116	PRO
1	A	265	VAL
1	A	319	SER
1	A	330	THR
1	A	354	VAL
1	A	362	PHE
1	A	400	LEU
1	A	421	ALA
1	A	446	ALA
1	A	539	GLY
1	A	566	ASP
1	A	600	THR
1	A	692	HIS
1	A	714	THR
1	A	751	GLY
1	A	844	MET
1	A	869	SER
1	A	887	CYS
1	A	892	TYR
1	A	950	LYS
1	A	988	PRO
1	B	31	PRO
1	B	140	VAL
1	B	254	ASN
1	B	400	LEU
1	B	471	SER
1	B	677	ALA
1	B	689	GLY
1	B	692	HIS
1	B	783	PRO
1	B	891	LEU
1	B	909	VAL
1	B	918	PHE

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Mol	Chain	Res	Type
1	B	1026	PHE
1	C	18	ILE
1	C	257	GLY
1	C	327	TYR
1	C	357	LEU
1	C	438	ILE
1	C	468	ARG
1	C	491	ALA
1	C	519	MET
1	C	530	SER
1	C	550	VAL
1	C	664	PHE
1	C	675	GLY
1	C	678	THR
1	C	852	PRO
1	C	926	TYR
1	C	994	GLY
1	C	1010	GLY
1	A	15	ILE
1	A	19	ILE
1	A	191	ASN
1	A	301	ASP
1	A	377	LEU
1	A	407	ASP
1	A	436	GLY
1	A	458	PHE
1	A	517	ASN
1	A	537	SER
1	A	544	LEU
1	A	675	GLY
1	A	688	ALA
1	A	795	ASP
1	A	886	LEU
1	A	907	LEU
1	A	923	ASN
1	A	960	LEU
1	A	989	LEU
1	A	1031	ARG
1	B	55	LYS
1	B	59	ASP
1	B	72	ILE
1	B	103	ALA

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Mol	Chain	Res	Type
1	B	105	VAL
1	B	414	GLU
1	B	422	GLU
1	B	444	GLY
1	B	465	ALA
1	B	473	THR
1	B	517	ASN
1	B	640	GLU
1	B	688	ALA
1	B	708	LYS
1	B	729	ILE
1	B	835	LYS
1	B	937	LEU
1	B	941	ASN
1	B	954	ASP
1	B	1014	ALA
1	C	34	GLN
1	C	85	THR
1	C	104	GLN
1	C	146	ASP
1	C	190	PRO
1	C	252	LYS
1	C	355	MET
1	C	422	GLU
1	C	427	PRO
1	C	492	LEU
1	C	520	PHE
1	C	521	GLU
1	C	545	TYR
1	C	639	GLY
1	C	709	HIS
1	C	851	LEU
1	C	976	LEU
1	C	990	VAL
1	A	361	ASN
1	A	408	ASP
1	A	434	SER
1	A	453	PHE
1	A	548	ILE
1	A	656	SER
1	A	896	SER
1	A	996	GLY

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Mol	Chain	Res	Type
1	B	19	ILE
1	B	109	ASN
1	B	115	MET
1	B	127	VAL
1	B	157	TYR
1	B	381	ALA
1	B	407	ASP
1	B	427	PRO
1	B	656	SER
1	B	781	MET
1	B	845	GLU
1	C	3	ASN
1	C	32	VAL
1	C	163	LYS
1	C	223	PRO
1	C	345	VAL
1	C	424	GLY
1	C	425	LEU
1	C	426	PRO
1	C	490	PRO
1	C	582	ALA
1	C	592	ASN
1	C	602	GLU
1	C	777	ALA
1	C	967	ALA
1	C	988	PRO
1	A	277	ILE
1	A	455	PRO
1	A	650	ARG
1	A	874	PRO
1	B	224	PRO
1	B	428	LYS
1	B	460	GLY
1	B	870	GLY
1	B	874	PRO
1	C	50	PRO
1	C	306	ILE
1	C	477	ALA
1	A	36	PRO
1	A	43	VAL
1	A	224	PRO
1	A	320	GLY

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Mol	Chain	Res	Type
1	A	570	GLY
1	A	729	ILE
1	B	315	PRO
1	B	672	VAL
1	C	15	ILE
1	C	166	ILE
1	C	172	VAL
1	C	220	GLY
1	C	717	ARG
1	C	786	ILE
1	C	1007	VAL
1	A	186	ILE
1	A	549	VAL
1	B	223	PRO
1	B	402	ILE
1	B	550	VAL
1	B	796	GLY
1	B	1016	VAL
1	C	644	VAL
1	A	50	PRO
1	A	345	VAL
1	A	773	VAL
1	A	1012	VAL
1	B	36	PRO
1	B	253	VAL
1	B	578	LEU
1	B	901	VAL
1	A	207	ILE
1	A	452	VAL
1	B	222	THR
1	B	833	PRO
1	C	9	PRO
1	C	315	PRO
1	B	107	VAL
1	C	1028	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	833/859 (97%)	661 (79%)	172 (21%)	1	5
1	B	833/859 (97%)	665 (80%)	168 (20%)	1	5
1	C	833/859 (97%)	665 (80%)	168 (20%)	1	5
All	All	2499/2577 (97%)	1991 (80%)	508 (20%)	1	5

All (508) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	4	PHE
1	A	5	PHE
1	A	6	ILE
1	A	14	VAL
1	A	21	LEU
1	A	38	ILE
1	A	45	ILE
1	A	49	TYR
1	A	53	ASP
1	A	55	LYS
1	A	63	GLN
1	A	65	ILE
1	A	66	GLU
1	A	69	MET
1	A	78	MET
1	A	79	SER
1	A	80	SER
1	A	84	SER
1	A	88	VAL
1	A	89	GLN
1	A	91	THR
1	A	92	LEU
1	A	93	THR
1	A	98	THR
1	A	106	GLN
1	A	109	ASN
1	A	110	LYS
1	A	112	GLN
1	A	115	MET
1	A	117	LEU
1	A	120	GLN

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Mol	Chain	Res	Type
1	A	121	GLU
1	A	123	GLN
1	A	130	GLU
1	A	137	LEU
1	A	139	VAL
1	A	143	ILE
1	A	150	THR
1	A	164	ASP
1	A	166	ILE
1	A	180	SER
1	A	193	LEU
1	A	202	ASP
1	A	213	GLN
1	A	222	THR
1	A	226	LYS
1	A	233	SER
1	A	243	THR
1	A	254	ASN
1	A	260	VAL
1	A	273	GLU
1	A	277	ILE
1	A	284	GLN
1	A	298	ASN
1	A	302	THR
1	A	310	LEU
1	A	321	LEU
1	A	323	ILE
1	A	330	THR
1	A	335	ILE
1	A	337	ILE
1	A	339	GLU
1	A	342	LYS
1	A	349	ILE
1	A	351	VAL
1	A	356	TYR
1	A	357	LEU
1	A	361	ASN
1	A	363	ARG
1	A	367	ILE
1	A	376	LEU
1	A	389	SER
1	A	390	ILE

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Mol	Chain	Res	Type
1	A	394	THR
1	A	400	LEU
1	A	404	LEU
1	A	405	LEU
1	A	406	VAL
1	A	408	ASP
1	A	414	GLU
1	A	417	GLU
1	A	420	MET
1	A	425	LEU
1	A	429	GLU
1	A	433	LYS
1	A	438	ILE
1	A	442	LEU
1	A	445	ILE
1	A	447	MET
1	A	453	PHE
1	A	480	LEU
1	A	481	SER
1	A	484	VAL
1	A	498	LYS
1	A	513	PHE
1	A	515	TRP
1	A	518	ARG
1	A	522	LYS
1	A	536	ARG
1	A	546	LEU
1	A	556	PHE
1	A	557	VAL
1	A	572	PHE
1	A	573	MET
1	A	577	GLN
1	A	578	LEU
1	A	588	GLN
1	A	603	LYS
1	A	610	PHE
1	A	617	PHE
1	A	620	ARG
1	A	623	ASN
1	A	636	ASP
1	A	641	GLU
1	A	643	LYS

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Mol	Chain	Res	Type
1	A	653	ARG
1	A	659	LYS
1	A	666	PHE
1	A	668	LEU
1	A	671	ILE
1	A	672	VAL
1	A	676	THR
1	A	687	GLN
1	A	693	GLU
1	A	701	GLN
1	A	705	GLU
1	A	711	ASP
1	A	713	LEU
1	A	717	ARG
1	A	719	ASN
1	A	722	GLU
1	A	731	ILE
1	A	745	ASP
1	A	750	LEU
1	A	758	TYR
1	A	768	VAL
1	A	774	MET
1	A	775	SER
1	A	780	ARG
1	A	786	ILE
1	A	788	ASP
1	A	795	ASP
1	A	801	PHE
1	A	807	SER
1	A	815	ARG
1	A	818	ARG
1	A	828	LEU
1	A	843	LEU
1	A	846	GLN
1	A	887	CYS
1	A	899	PHE
1	A	917	THR
1	A	919	ARG
1	A	952	LEU
1	A	954	ASP
1	A	955	LYS
1	A	960	LEU

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Mol	Chain	Res	Type
1	A	971	ARG
1	A	976	LEU
1	A	978	THR
1	A	979	SER
1	A	982	PHE
1	A	983	ILE
1	A	986	VAL
1	A	992	SER
1	A	993	THR
1	A	1013	THR
1	A	1022	VAL
1	A	1030	ARG
1	A	1035	ARG
1	A	1036	LYS
1	B	6	ILE
1	B	8	ARG
1	B	11	PHE
1	B	13	TRP
1	B	21	LEU
1	B	50	PRO
1	B	59	ASP
1	B	61	VAL
1	B	67	GLN
1	B	70	ASN
1	B	72	ILE
1	B	73	ASP
1	B	74	ASN
1	B	78	MET
1	B	81	ASN
1	B	88	VAL
1	B	92	LEU
1	B	93	THR
1	B	102	ILE
1	B	104	GLN
1	B	115	MET
1	B	121	GLU
1	B	136	PHE
1	B	140	VAL
1	B	144	ASN
1	B	145	THR
1	B	150	THR
1	B	153	ASP

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Mol	Chain	Res	Type
1	B	166	ILE
1	B	174	ASP
1	B	176	GLN
1	B	180	SER
1	B	182	TYR
1	B	185	ARG
1	B	189	ASN
1	B	191	ASN
1	B	193	LEU
1	B	202	ASP
1	B	219	LEU
1	B	223	PRO
1	B	224	PRO
1	B	226	LYS
1	B	234	ILE
1	B	235	ILE
1	B	237	GLN
1	B	243	THR
1	B	253	VAL
1	B	256	ASP
1	B	261	LEU
1	B	267	LYS
1	B	269	GLU
1	B	270	LEU
1	B	289	LEU
1	B	292	LYS
1	B	293	LEU
1	B	298	ASN
1	B	319	SER
1	B	323	ILE
1	B	330	THR
1	B	336	SER
1	B	341	VAL
1	B	342	LYS
1	B	343	THR
1	B	356	TYR
1	B	357	LEU
1	B	365	THR
1	B	379	THR
1	B	386	PHE
1	B	394	THR
1	B	398	MET

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Mol	Chain	Res	Type
1	B	405	LEU
1	B	410	ILE
1	B	411	VAL
1	B	416	VAL
1	B	417	GLU
1	B	428	LYS
1	B	435	MET
1	B	437	GLN
1	B	452	VAL
1	B	466	ILE
1	B	473	THR
1	B	480	LEU
1	B	496	MET
1	B	497	LEU
1	B	513	PHE
1	B	516	PHE
1	B	523	SER
1	B	538	THR
1	B	540	ARG
1	B	549	VAL
1	B	554	TYR
1	B	555	LEU
1	B	558	ARG
1	B	566	ASP
1	B	574	THR
1	B	591	LEU
1	B	595	THR
1	B	601	LYS
1	B	607	GLU
1	B	612	VAL
1	B	623	ASN
1	B	624	THR
1	B	629	VAL
1	B	641	GLU
1	B	648	THR
1	B	652	THR
1	B	653	ARG
1	B	655	PHE
1	B	656	SER
1	B	659	LYS
1	B	662	MET
1	B	668	LEU

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Mol	Chain	Res	Type
1	B	671	ILE
1	B	680	PHE
1	B	692	HIS
1	B	694	LYS
1	B	696	THR
1	B	703	LEU
1	B	711	ASP
1	B	712	MET
1	B	735	LYS
1	B	743	ILE
1	B	744	ASN
1	B	758	TYR
1	B	760	ASN
1	B	764	ASP
1	B	770	LYS
1	B	778	LYS
1	B	781	MET
1	B	782	LEU
1	B	788	ASP
1	B	808	ARG
1	B	813	SER
1	B	828	LEU
1	B	830	GLN
1	B	836	SER
1	B	847	LEU
1	B	864	TYR
1	B	871	ASN
1	B	875	SER
1	B	876	LEU
1	B	879	ILE
1	B	880	SER
1	B	895	TRP
1	B	900	SER
1	B	921	LEU
1	B	922	THR
1	B	940	LYS
1	B	943	ILE
1	B	946	VAL
1	B	951	ASP
1	B	953	MET
1	B	956	GLU
1	B	965	LEU

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Mol	Chain	Res	Type
1	B	966	ASP
1	B	970	MET
1	B	972	LEU
1	B	977	MET
1	B	978	THR
1	B	984	LEU
1	B	987	MET
1	B	989	LEU
1	B	992	SER
1	B	993	THR
1	B	1017	LEU
1	B	1019	ILE
1	B	1027	VAL
1	B	1036	LYS
1	C	4	PHE
1	C	10	ILE
1	C	13	TRP
1	C	17	ILE
1	C	19	ILE
1	C	29	LYS
1	C	37	THR
1	C	48	SER
1	C	49	TYR
1	C	50	PRO
1	C	58	GLN
1	C	60	THR
1	C	63	GLN
1	C	64	VAL
1	C	70	ASN
1	C	75	LEU
1	C	77	TYR
1	C	83	ASP
1	C	89	GLN
1	C	91	THR
1	C	92	LEU
1	C	104	GLN
1	C	110	LYS
1	C	111	LEU
1	C	118	LEU
1	C	137	LEU
1	C	138	MET
1	C	143	ILE

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Mol	Chain	Res	Type
1	C	148	THR
1	C	149	MET
1	C	152	GLU
1	C	153	ASP
1	C	158	VAL
1	C	162	MET
1	C	163	LYS
1	C	164	ASP
1	C	170	SER
1	C	177	LEU
1	C	189	ASN
1	C	191	ASN
1	C	192	GLU
1	C	194	ASN
1	C	204	ILE
1	C	210	GLN
1	C	211	ASN
1	C	228	GLN
1	C	231	ASN
1	C	235	ILE
1	C	239	ARG
1	C	245	GLU
1	C	252	LYS
1	C	253	VAL
1	C	258	SER
1	C	259	ARG
1	C	265	VAL
1	C	268	ILE
1	C	269	GLU
1	C	274	ASN
1	C	293	LEU
1	C	295	THR
1	C	300	LEU
1	C	313	MET
1	C	316	PHE
1	C	317	PHE
1	C	321	LEU
1	C	324	VAL
1	C	337	ILE
1	C	355	MET
1	C	367	ILE
1	C	372	VAL

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Mol	Chain	Res	Type
1	C	406	VAL
1	C	417	GLU
1	C	419	VAL
1	C	425	LEU
1	C	432	ARG
1	C	437	GLN
1	C	438	ILE
1	C	458	PHE
1	C	459	PHE
1	C	468	ARG
1	C	475	VAL
1	C	481	SER
1	C	492	LEU
1	C	493	CYS
1	C	496	MET
1	C	497	LEU
1	C	521	GLU
1	C	523	SER
1	C	535	LEU
1	C	536	ARG
1	C	544	LEU
1	C	546	LEU
1	C	564	LEU
1	C	568	ASP
1	C	571	VAL
1	C	575	MET
1	C	576	VAL
1	C	577	GLN
1	C	588	GLN
1	C	591	LEU
1	C	608	SER
1	C	613	ASN
1	C	617	PHE
1	C	624	THR
1	C	626	ILE
1	C	630	SER
1	C	647	ILE
1	C	648	THR
1	C	650	ARG
1	C	659	LYS
1	C	662	MET
1	C	666	PHE

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Mol	Chain	Res	Type
1	C	668	LEU
1	C	674	LEU
1	C	676	THR
1	C	685	ILE
1	C	695	LEU
1	C	696	THR
1	C	699	ARG
1	C	713	LEU
1	C	719	ASN
1	C	728	LYS
1	C	730	ASP
1	C	733	GLN
1	C	745	ASP
1	C	750	LEU
1	C	758	TYR
1	C	759	VAL
1	C	765	ARG
1	C	768	VAL
1	C	769	LYS
1	C	770	LYS
1	C	782	LEU
1	C	783	PRO
1	C	792	ARG
1	C	799	VAL
1	C	805	SER
1	C	808	ARG
1	C	813	SER
1	C	828	LEU
1	C	837	THR
1	C	847	LEU
1	C	850	LYS
1	C	860	THR
1	C	868	LEU
1	C	872	GLN
1	C	876	LEU
1	C	885	PHE
1	C	899	PHE
1	C	904	VAL
1	C	919	ARG
1	C	921	LEU
1	C	923	ASN
1	C	931	LEU

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Mol	Chain	Res	Type
1	C	935	ILE
1	C	938	SER
1	C	941	ASN
1	C	945	ILE
1	C	952	LEU
1	C	958	LYS
1	C	979	SER
1	C	982	PHE
1	C	984	LEU
1	C	989	LEU
1	C	991	ILE
1	C	1021	PHE
1	C	1030	ARG
1	C	1035	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	67	GLN
1	A	68	ASN
1	A	70	ASN
1	A	106	GLN
1	A	108	GLN
1	A	109	ASN
1	A	123	GLN
1	A	124	GLN
1	A	144	ASN
1	A	151	GLN
1	A	191	ASN
1	A	231	ASN
1	A	274	ASN
1	A	282	ASN
1	A	284	GLN
1	A	298	ASN
1	A	360	GLN
1	A	361	ASN
1	A	517	ASN
1	A	577	GLN
1	A	622	GLN
1	A	687	GLN
1	A	719	ASN

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Mol	Chain	Res	Type
1	A	846	GLN
1	A	865	GLN
1	A	928	GLN
1	A	1001	ASN
1	B	68	ASN
1	B	70	ASN
1	B	104	GLN
1	B	108	GLN
1	B	109	ASN
1	B	112	GLN
1	B	123	GLN
1	B	125	GLN
1	B	151	GLN
1	B	161	ASN
1	B	189	ASN
1	B	194	ASN
1	B	210	GLN
1	B	213	GLN
1	B	218	GLN
1	B	228	GLN
1	B	231	ASN
1	B	237	GLN
1	B	254	ASN
1	B	415	ASN
1	B	437	GLN
1	B	439	GLN
1	B	469	GLN
1	B	517	ASN
1	B	526	HIS
1	B	577	GLN
1	B	584	GLN
1	B	613	ASN
1	B	623	ASN
1	B	642	ASN
1	B	726	GLN
1	B	744	ASN
1	B	760	ASN
1	B	830	GLN
1	B	846	GLN
1	B	865	GLN
1	B	871	ASN
1	B	872	GLN

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Mol	Chain	Res	Type
1	C	3	ASN
1	C	63	GLN
1	C	104	GLN
1	C	108	GLN
1	C	120	GLN
1	C	123	GLN
1	C	124	GLN
1	C	144	ASN
1	C	176	GLN
1	C	189	ASN
1	C	191	ASN
1	C	197	GLN
1	C	211	ASN
1	C	213	GLN
1	C	231	ASN
1	C	237	GLN
1	C	284	GLN
1	C	415	ASN
1	C	439	GLN
1	C	577	GLN
1	C	584	GLN
1	C	588	GLN
1	C	592	ASN
1	C	605	ASN
1	C	622	GLN
1	C	667	ASN
1	C	846	GLN
1	C	941	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MIY	A	2001	-	35,36,36	1.27	3 (8%)	41,58,58	2.61	17 (41%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MIY	A	2001	-	-	5/12/70/70	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	MIY	C4-N1	4.03	1.56	1.47
2	A	2001	MIY	C18-C17	3.08	1.54	1.52
2	A	2001	MIY	C4-C3	2.33	1.56	1.51

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	MIY	C1-C18-C17	8.44	119.78	109.88
2	A	2001	MIY	O6-C17-C16	-5.94	115.77	123.90
2	A	2001	MIY	O7-C18-C17	-4.52	102.92	110.14
2	A	2001	MIY	C18-C17-C16	4.14	127.27	123.06
2	A	2001	MIY	CN7-N7-C10	-3.93	102.99	115.17
2	A	2001	MIY	C13-C14-C9	3.91	123.45	119.05
2	A	2001	MIY	O5-C15-C14	-3.14	116.06	121.99
2	A	2001	MIY	C71-N7-CN7	-3.04	106.33	116.12
2	A	2001	MIY	C13-C14-C15	-3.03	117.03	121.47
2	A	2001	MIY	O2-C3-C2	-2.89	117.89	122.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	MIY	C18-C1-C2	2.85	120.28	115.75
2	A	2001	MIY	O5-C15-C16	2.57	124.72	120.78
2	A	2001	MIY	O6-C17-C18	2.37	116.80	113.37
2	A	2001	MIY	O1-C1-C2	-2.18	118.97	123.55
2	A	2001	MIY	C11-C10-N7	-2.15	118.55	121.59
2	A	2001	MIY	C19-N1-C4	2.09	119.00	114.09
2	A	2001	MIY	C9-C10-N7	2.00	121.36	118.91

There are no chirality outliers.

All (5) torsion outliers are listed below:

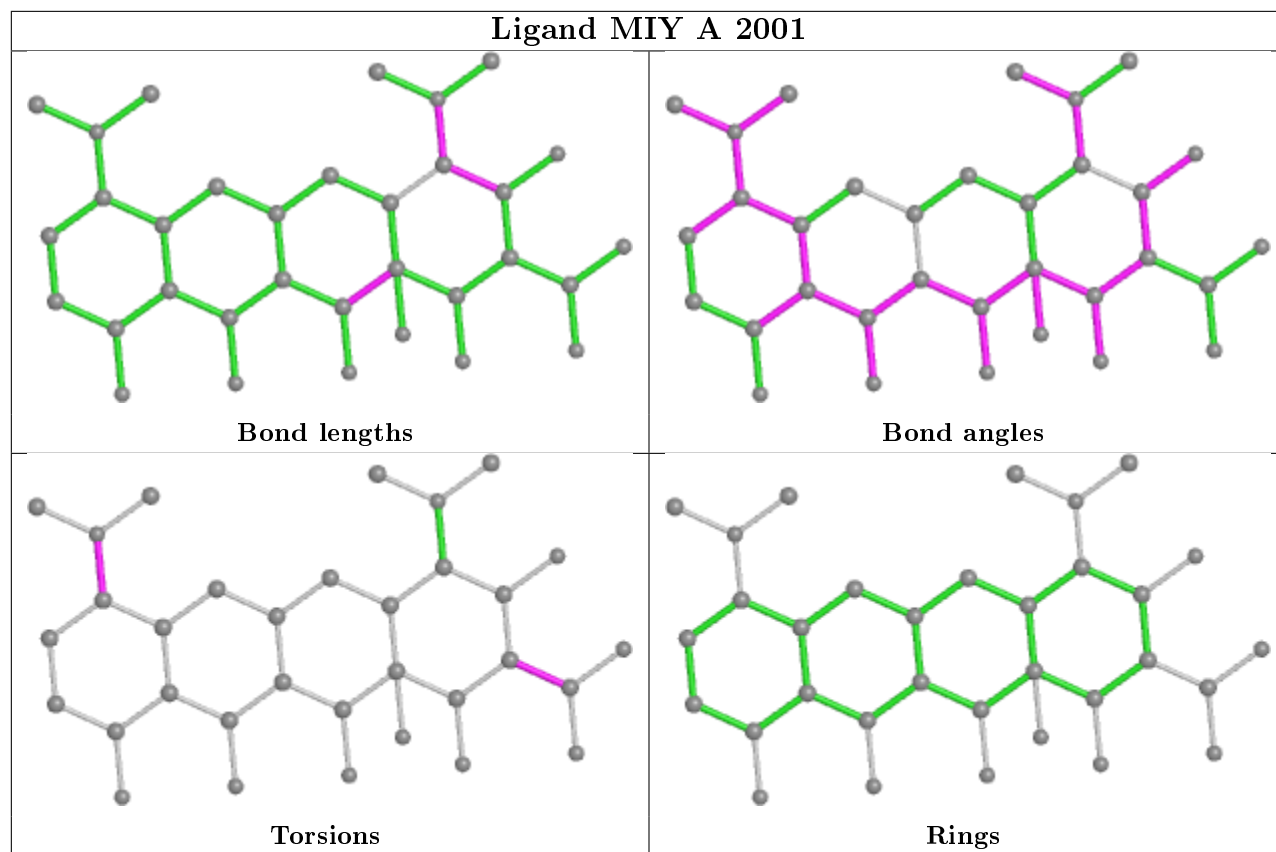
Mol	Chain	Res	Type	Atoms
2	A	2001	MIY	C1-C2-C21-O8
2	A	2001	MIY	C1-C2-C21-N2
2	A	2001	MIY	C3-C2-C21-N2
2	A	2001	MIY	C3-C2-C21-O8
2	A	2001	MIY	C9-C10-N7-CN7

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	MIY	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	1022/1053 (97%)	-0.46	8 (0%) 86 72	3, 87, 108, 120	0
1	B	1022/1053 (97%)	-0.32	12 (1%) 79 61	42, 93, 108, 120	0
1	C	1022/1053 (97%)	-0.47	18 (1%) 68 47	5, 84, 109, 120	0
All	All	3066/3159 (97%)	-0.42	38 (1%) 79 61	3, 88, 108, 120	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1034	SER	4.9
1	C	870	GLY	4.7
1	C	514	GLY	3.7
1	C	538	THR	3.5
1	C	656	SER	3.5
1	C	539	GLY	3.4
1	A	871	ASN	3.2
1	C	513	PHE	3.2
1	A	253	VAL	3.2
1	B	957	GLY	3.1
1	C	515	TRP	3.1
1	B	529	ASP	3.1
1	C	869	SER	2.9
1	B	1036	LYS	2.9
1	C	437	GLN	2.8
1	C	436	GLY	2.8
1	C	536	ARG	2.7
1	B	832	ALA	2.7
1	B	526	HIS	2.7
1	C	424	GLY	2.7
1	A	145	THR	2.7
1	C	1034	SER	2.6
1	A	526	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	318	PRO	2.5
1	C	521	GLU	2.4
1	B	951	ASP	2.3
1	B	515	TRP	2.3
1	C	676	THR	2.3
1	C	951	ASP	2.2
1	C	920	GLY	2.2
1	B	521	GLU	2.2
1	B	652	THR	2.2
1	B	304	ALA	2.2
1	A	134	SER	2.1
1	A	538	THR	2.1
1	B	554	TYR	2.1
1	A	518	ARG	2.0
1	C	526	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

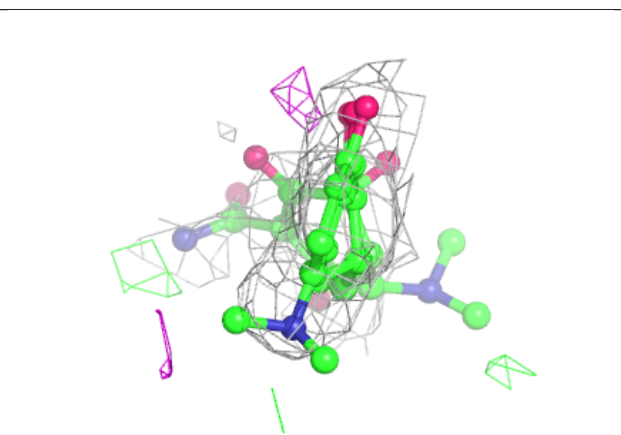
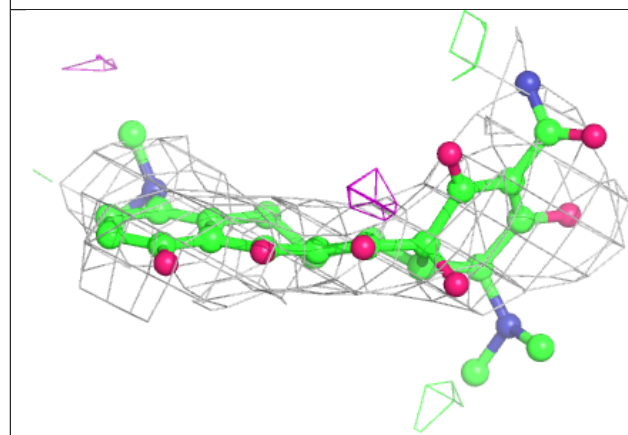
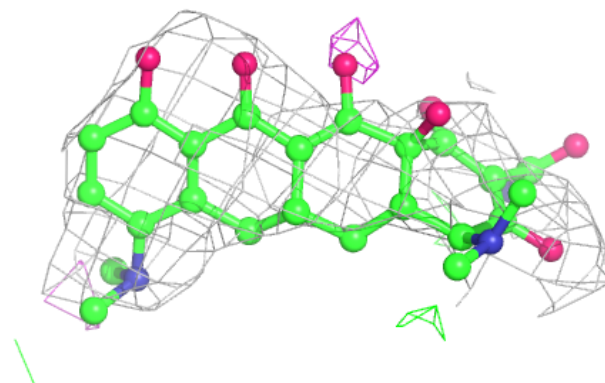
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MIY	A	2001	33/33	0.82	0.32	112,122,129,131	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around MIY A 2001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.