



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 04:25 am BST

PDB ID : 1GFF
Title : THE ATOMIC STRUCTURE OF THE DEGRADED PROCAPSID PARTICLE OF THE BACTERIOPHAGE G4: INDUCED STRUCTURAL CHANGES IN THE PRESENCE OF CALCIUM IONS AND FUNCTIONAL IMPLICATIONS
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Deposited on : 1995-11-06
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

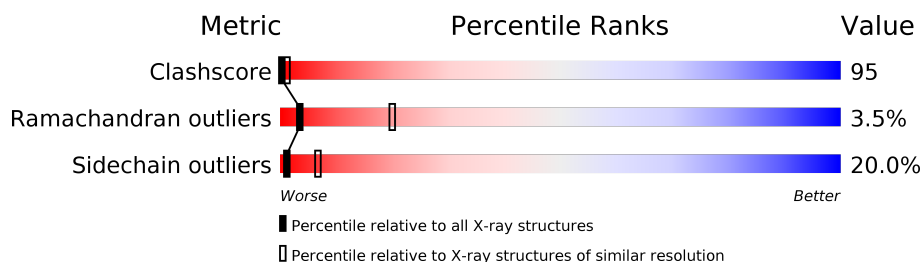
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	1	426	<div> <div>23%</div> <div>53%</div> <div>19%</div> <div>• •</div> </div>
2	2	177	<div> <div>10%</div> <div>61%</div> <div>27%</div> <div>•</div> </div>
3	3	25	<div> <div>12%</div> <div>28%</div> <div>• •</div> <div>52%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4779 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 BACTERIOPHAGE G4 CAPSID PROTEINS GPF, GPG, GPJ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	417	Total	C	N	O	S	0	0	0
			3357	2144	571	623	19			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	378	ASP	GLU	CONFLICT	UNP P03642

- Molecule 2 is a protein called BACTERIOPHAGE G4 CAPSID PROTEINS GPF, GPG, GPJ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	177	Total	C	N	O	S	0	0	0
			1325	840	229	252	4			

- Molecule 3 is a protein called BACTERIOPHAGE G4 CAPSID PROTEINS GPF, GPG, GPJ.

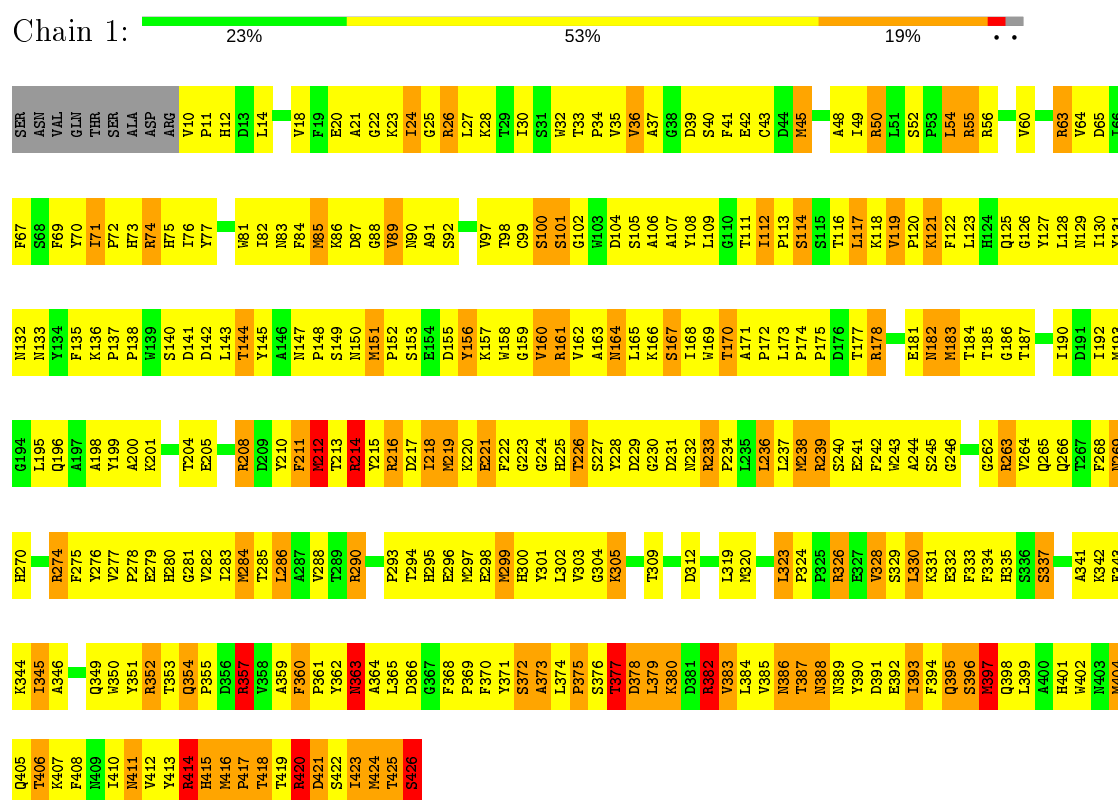
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	3	12	Total	C	N	O	0	0	0
			97	64	17	16			

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. 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. 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.

Note EDS was not executed.

- Molecule 1: BACTERIOPHAGE G4 CAPSID PROTEINS GPF, GPG, GPJ



- Molecule 2: BACTERIOPHAGE G4 CAPSID PROTEINS GPF, GPG, GPJ



● Molecule 3: BACTERIOPHAGE G4 CAPSID PROTEINS GPF, GPG, GPJ



MET	LYS	LYS	SER	ILE	ARG	ARG	SER	GLY	GLY	LYS	SER	LYS	G14	A15	R16	L17	W18	Y19	V20	G21	Q24	Y25
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4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	414.20 Å 414.20 Å 263.00 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	0.352 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4779	wwPDB-VP
Average B, all atoms (Å ²)	0.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.93	1/3461 (0.0%)	1.30	40/4713 (0.8%)
2	2	0.90	0/1354	1.40	10/1859 (0.5%)
3	3	1.23	0/100	1.47	1/135 (0.7%)
All	All	0.93	1/4915 (0.0%)	1.33	51/6707 (0.8%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	43	CYS	CB-SG	5.03	1.90	1.82

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	214	ARG	NE-CZ-NH2	7.91	124.26	120.30
1	1	357	ARG	NE-CZ-NH2	7.81	124.20	120.30
1	1	55	ARG	NE-CZ-NH2	7.78	124.19	120.30
2	2	61	ARG	NE-CZ-NH2	7.76	124.18	120.30
1	1	208	ARG	NE-CZ-NH2	7.75	124.17	120.30
1	1	414	ARG	NE-CZ-NH2	7.54	124.07	120.30
2	2	168	ARG	NE-CZ-NH2	7.50	124.05	120.30
1	1	326	ARG	NE-CZ-NH2	7.48	124.04	120.30
1	1	50	ARG	NE-CZ-NH2	7.45	124.02	120.30
2	2	38	ARG	NE-CZ-NH2	7.45	124.02	120.30
1	1	382	ARG	NE-CZ-NH2	7.44	124.02	120.30
1	1	216	ARG	NE-CZ-NH2	7.44	124.02	120.30
1	1	26	ARG	NE-CZ-NH2	7.44	124.02	120.30
2	2	135	ARG	NE-CZ-NH2	7.44	124.02	120.30
1	1	290	ARG	NE-CZ-NH2	7.43	124.02	120.30
3	3	16	ARG	NE-CZ-NH2	7.39	124.00	120.30
1	1	74	ARG	NE-CZ-NH2	7.37	123.98	120.30
1	1	161	ARG	NE-CZ-NH2	7.36	123.98	120.30
1	1	420	ARG	NE-CZ-NH2	7.36	123.98	120.30
1	1	63	ARG	NE-CZ-NH2	7.26	123.93	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	92	ARG	NE-CZ-NH2	7.25	123.92	120.30
1	1	274	ARG	NE-CZ-NH2	7.23	123.91	120.30
1	1	233	ARG	NE-CZ-NH2	7.22	123.91	120.30
1	1	178	ARG	NE-CZ-NH2	6.82	123.71	120.30
1	1	263	ARG	NE-CZ-NH2	6.79	123.69	120.30
1	1	239	ARG	NE-CZ-NH2	6.75	123.67	120.30
2	2	41	ILE	CB-CG1-CD1	-6.70	95.14	113.90
1	1	352	ARG	NE-CZ-NH2	6.52	123.56	120.30
1	1	284	MET	CG-SD-CE	6.33	110.32	100.20
1	1	56	ARG	NE-CZ-NH2	6.27	123.44	120.30
1	1	404	MET	CG-SD-CE	6.25	110.21	100.20
2	2	1	MET	CG-SD-CE	6.19	110.10	100.20
1	1	238	MET	CG-SD-CE	6.18	110.09	100.20
1	1	416	MET	CG-SD-CE	6.15	110.04	100.20
1	1	424	MET	CG-SD-CE	6.14	110.03	100.20
1	1	299	MET	CG-SD-CE	6.14	110.02	100.20
1	1	85	MET	CG-SD-CE	6.13	110.02	100.20
2	2	146	MET	CG-SD-CE	6.13	110.01	100.20
1	1	397	MET	CG-SD-CE	6.12	109.98	100.20
1	1	151	MET	CG-SD-CE	6.09	109.95	100.20
1	1	320	MET	CG-SD-CE	6.09	109.94	100.20
1	1	297	MET	CG-SD-CE	6.07	109.91	100.20
1	1	45	MET	CG-SD-CE	6.03	109.85	100.20
1	1	183	MET	CG-SD-CE	6.01	109.82	100.20
2	2	86	MET	CG-SD-CE	6.00	109.79	100.20
1	1	193	MET	CG-SD-CE	5.86	109.58	100.20
1	1	426	SER	CA-C-O	-5.70	108.14	120.10
1	1	219	MET	CG-SD-CE	5.67	109.27	100.20
1	1	212	MET	CG-SD-CE	5.63	109.20	100.20
2	2	64	GLU	CB-CA-C	-5.40	99.60	110.40
1	1	199	TYR	CB-CG-CD1	5.26	124.16	121.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	3357	0	3220	549	627
2	2	1325	0	1334	349	817
3	3	97	0	89	41	70
All	All	4779	0	4643	895	1437

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 95.

All (895) 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)
2:2:18:LEU:CB	2:2:43:ILE:HG22	1.19	1.64
2:2:18:LEU:HD23	2:2:41:ILE:CD1	1.26	1.63
1:1:138:PRO:HG2	3:3:20:VAL:CG1	1.20	1.60
1:1:138:PRO:CG	3:3:20:VAL:HG12	1.13	1.58
2:2:18:LEU:CD2	2:2:41:ILE:HD11	1.32	1.51
2:2:82:VAL:CG1	2:2:86:MET:SD	2.05	1.45
2:2:26:VAL:CA	2:2:54:SER:OG	1.70	1.39
2:2:26:VAL:N	2:2:54:SER:OG	1.58	1.37
1:1:419:THR:O	1:1:423:ILE:CD1	1.73	1.37
1:1:108:TYR:CE1	1:1:109:LEU:HD21	1.60	1.35
2:2:82:VAL:HG11	2:2:86:MET:SD	1.61	1.35
2:2:21:THR:HA	2:2:46:THR:CG2	1.56	1.34
1:1:138:PRO:CD	3:3:20:VAL:HG11	1.59	1.33
1:1:138:PRO:CD	3:3:20:VAL:CG1	2.06	1.32
1:1:138:PRO:CG	3:3:20:VAL:CG1	1.79	1.31
1:1:328:VAL:HG12	1:1:332:GLU:OE1	1.23	1.29
2:2:49:ALA:HA	2:2:152:TRP:O	1.21	1.29
2:2:21:THR:CA	2:2:46:THR:HG22	1.63	1.28
2:2:118:ASN:CG	2:2:119:GLY:H	1.22	1.27
2:2:18:LEU:CB	2:2:43:ILE:CG2	2.10	1.26
1:1:296:GLU:OE1	1:1:363:ASN:HA	1.33	1.24
1:1:419:THR:O	1:1:423:ILE:HD12	1.19	1.23
2:2:40:THR:HG23	2:2:162:SER:OG	1.11	1.22
2:2:43:ILE:O	2:2:45:ALA:N	1.72	1.21
2:2:164:ASN:OD1	2:2:165:GLN:N	1.73	1.20
2:2:18:LEU:HB3	2:2:43:ILE:CG2	1.71	1.20
2:2:40:THR:CG2	2:2:162:SER:OG	1.90	1.18
2:2:43:ILE:O	2:2:43:ILE:HG12	1.42	1.18
1:1:390:TYR:O	1:1:393:ILE:HG23	1.44	1.17
2:2:94:GLU:OE2	2:2:135:ARG:N	1.76	1.17
1:1:420:ARG:CA	1:1:423:ILE:HD11	1.73	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:295:HIS:NE2	1:1:373:ALA:O	1.76	1.16
1:1:18:VAL:CG1	1:1:406:THR:HG23	1.74	1.16
2:2:32:SER:HB2	2:2:41:ILE:HD11	1.24	1.16
1:1:357:ARG:HH11	1:1:357:ARG:CG	1.57	1.16
1:1:10:VAL:O	1:1:12:HIS:HD2	1.28	1.15
2:2:21:THR:HB	2:2:46:THR:CG2	1.77	1.15
2:2:49:ALA:CA	2:2:152:TRP:O	1.93	1.15
1:1:145:TYR:CD2	1:1:151:MET:HG2	1.82	1.14
2:2:21:THR:CA	2:2:46:THR:CG2	2.23	1.13
1:1:175:PRO:HG3	1:1:379:LEU:HD23	1.24	1.13
2:2:18:LEU:HB2	2:2:43:ILE:HG22	1.13	1.12
1:1:213:THR:HG22	3:3:21:GLY:O	1.49	1.12
2:2:118:ASN:ND2	2:2:119:GLY:H	1.49	1.11
1:1:418:THR:HG22	1:1:421:ASP:HB2	1.32	1.11
2:2:40:THR:CG2	2:2:162:SER:CB	2.28	1.10
2:2:82:VAL:HG13	2:2:86:MET:SD	1.85	1.10
1:1:108:TYR:CE1	1:1:109:LEU:CD2	2.32	1.10
2:2:21:THR:CB	2:2:46:THR:CG2	2.31	1.09
2:2:18:LEU:CD2	2:2:32:SER:HB2	1.82	1.09
1:1:138:PRO:HD2	3:3:20:VAL:CG1	1.75	1.09
1:1:368:PHE:HB3	1:1:370:PHE:CD2	1.87	1.08
1:1:63:ARG:NE	1:1:241:GLU:OE2	1.83	1.08
1:1:269:ASN:HD22	1:1:270:HIS:N	1.49	1.08
1:1:424:MET:O	1:1:426:SER:OG	1.68	1.08
2:2:42:LEU:O	2:2:42:LEU:HG	1.42	1.08
2:2:18:LEU:CG	2:2:43:ILE:HG22	1.83	1.08
1:1:418:THR:CG2	1:1:421:ASP:HB2	1.82	1.07
2:2:18:LEU:HB3	2:2:43:ILE:HG22	1.15	1.07
2:2:12:PRO:HG3	2:2:38:ARG:HB2	1.31	1.07
1:1:18:VAL:HG13	1:1:406:THR:HG23	1.35	1.07
2:2:26:VAL:N	2:2:54:SER:CB	2.17	1.07
2:2:94:GLU:HG2	2:2:141:VAL:HG12	1.33	1.06
2:2:40:THR:HG23	2:2:162:SER:CB	1.84	1.06
1:1:359:ALA:C	1:1:361:PRO:HD2	1.77	1.05
1:1:10:VAL:CG2	1:1:11:PRO:HD2	1.85	1.05
2:2:18:LEU:HB3	2:2:43:ILE:CB	1.85	1.05
1:1:386:ASN:ND2	1:1:386:ASN:O	1.87	1.05
1:1:420:ARG:HA	1:1:423:ILE:CD1	1.86	1.05
2:2:118:ASN:CG	2:2:119:GLY:N	1.99	1.05
1:1:357:ARG:HG2	1:1:357:ARG:NH1	1.58	1.04
1:1:386:ASN:C	1:1:386:ASN:HD22	1.60	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:10:VAL:O	1:1:12:HIS:CD2	2.10	1.04
2:2:21:THR:CB	2:2:46:THR:HG21	1.87	1.04
1:1:300:HIS:O	1:1:303:VAL:HG12	1.57	1.04
1:1:71:ILE:CD1	1:1:126:GLY:HA2	1.88	1.04
2:2:21:THR:HB	2:2:46:THR:HG21	1.04	1.03
2:2:18:LEU:HD21	2:2:32:SER:HB2	1.40	1.03
1:1:10:VAL:HG23	1:1:11:PRO:HD2	1.39	1.03
2:2:26:VAL:CB	2:2:54:SER:OG	2.07	1.02
1:1:63:ARG:CZ	1:1:241:GLU:OE2	2.06	1.02
1:1:175:PRO:HG3	1:1:379:LEU:CD2	1.89	1.02
1:1:242:PHE:CZ	1:1:268:PHE:HB3	1.94	1.02
2:2:31:LEU:HG	2:2:57:CYS:O	1.59	1.02
1:1:71:ILE:CD1	1:1:76:ILE:HD11	1.89	1.00
2:2:50:VAL:HG12	2:2:152:TRP:HB2	1.44	0.99
1:1:390:TYR:O	1:1:393:ILE:CG2	2.09	0.99
1:1:319:LEU:O	1:1:323:LEU:CD2	2.11	0.98
1:1:49:ILE:CG2	1:1:266:GLN:HB3	1.92	0.98
2:2:28:ALA:CB	2:2:55:GLY:O	2.12	0.98
1:1:319:LEU:O	1:1:323:LEU:HD22	1.64	0.97
1:1:178:ARG:HH22	1:1:205:GLU:CD	1.52	0.96
1:1:70:TYR:HB2	1:1:237:LEU:HD11	1.46	0.96
1:1:133:ASN:O	1:1:214:ARG:NH2	1.98	0.96
2:2:25:ALA:C	2:2:54:SER:HB3	1.86	0.96
1:1:18:VAL:HG12	1:1:406:THR:O	1.65	0.96
1:1:244:ALA:HA	1:1:266:GLN:HG2	1.47	0.95
1:1:357:ARG:HH11	1:1:357:ARG:HG2	0.79	0.95
1:1:416:MET:SD	1:1:417:PRO:HD2	2.07	0.95
1:1:98:THR:HG22	1:1:147:ASN:ND2	1.82	0.95
1:1:363:ASN:O	1:1:363:ASN:ND2	1.99	0.95
2:2:32:SER:HB2	2:2:41:ILE:CD1	1.96	0.94
1:1:108:TYR:HE1	1:1:109:LEU:HD21	1.22	0.94
2:2:86:MET:CE	2:2:147:LEU:HD22	1.97	0.94
2:2:36:LEU:HD13	2:2:61:ARG:HH21	1.32	0.93
2:2:9:HIS:CE1	2:2:162:SER:HB3	2.03	0.93
1:1:71:ILE:HD11	1:1:76:ILE:HD11	1.50	0.93
1:1:269:ASN:HD22	1:1:270:HIS:H	1.06	0.93
2:2:57:CYS:SG	2:2:91:ILE:HD11	2.09	0.93
2:2:136:THR:HB	2:2:139:ASN:HD21	1.34	0.93
1:1:363:ASN:C	1:1:363:ASN:HD22	1.72	0.92
2:2:82:VAL:CG1	2:2:86:MET:CG	2.47	0.92
2:2:94:GLU:OE1	2:2:135:ARG:HB2	1.68	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:132:ASN:ND2	1:1:143:LEU:H	1.67	0.92
2:2:59:VAL:HG23	2:2:143:ALA:O	1.69	0.92
1:1:132:ASN:HD21	1:1:143:LEU:H	0.98	0.92
2:2:18:LEU:HD12	2:2:19:ALA:H	1.35	0.92
1:1:178:ARG:NH2	1:1:205:GLU:CD	2.21	0.92
2:2:26:VAL:HB	2:2:54:SER:OG	1.68	0.91
2:2:40:THR:HG22	2:2:162:SER:HB2	1.53	0.91
2:2:40:THR:CG2	2:2:162:SER:HB2	2.00	0.91
2:2:136:THR:O	2:2:139:ASN:OD1	1.88	0.91
1:1:239:ARG:NH1	3:3:25:TYR:HE1	1.68	0.91
2:2:18:LEU:HB2	2:2:41:ILE:HG12	1.52	0.91
1:1:238:MET:HE3	1:1:239:ARG:H	1.36	0.91
2:2:18:LEU:CG	2:2:43:ILE:CG2	2.46	0.91
2:2:79:LEU:HD23	2:2:159:GLY:HA3	1.52	0.91
2:2:69:ASN:HD22	2:2:69:ASN:C	1.74	0.91
2:2:95:VAL:O	2:2:139:ASN:HB2	1.70	0.90
1:1:138:PRO:CG	3:3:20:VAL:HG11	1.83	0.90
1:1:323:LEU:N	1:1:323:LEU:HD22	1.86	0.90
1:1:328:VAL:CG1	1:1:332:GLU:OE1	2.17	0.90
2:2:43:ILE:O	2:2:44:ASN:C	2.03	0.90
1:1:420:ARG:HA	1:1:423:ILE:HD11	0.92	0.90
1:1:242:PHE:CZ	1:1:268:PHE:CB	2.54	0.90
1:1:323:LEU:H	1:1:323:LEU:CD2	1.84	0.90
2:2:28:ALA:HA	2:2:55:GLY:O	1.72	0.90
2:2:92:ARG:HD2	2:2:130:ILE:HG13	1.54	0.90
2:2:50:VAL:N	2:2:152:TRP:O	2.04	0.90
1:1:296:GLU:OE1	1:1:363:ASN:CA	2.20	0.89
2:2:153:THR:HG23	2:2:154:ALA:N	1.87	0.89
1:1:99:CYS:SG	1:1:148:PRO:HG2	2.12	0.89
1:1:108:TYR:CZ	1:1:151:MET:HE1	2.07	0.89
2:2:64:GLU:OE2	2:2:140:ASP:OD1	1.90	0.89
1:1:323:LEU:N	1:1:323:LEU:CD2	2.34	0.89
1:1:104:ASP:OD2	1:1:157:LYS:HE2	1.73	0.89
2:2:79:LEU:O	2:2:121:ALA:HA	1.74	0.88
2:2:97:ASP:CB	2:2:138:GLY:O	2.21	0.88
2:2:97:ASP:N	2:2:139:ASN:HA	1.87	0.88
1:1:30:ILE:HD12	1:1:45:MET:HE3	1.53	0.88
1:1:18:VAL:HG11	1:1:406:THR:HG23	1.56	0.88
1:1:49:ILE:HG22	1:1:266:GLN:HB3	1.55	0.88
2:2:9:HIS:HE1	2:2:162:SER:HB3	1.39	0.88
1:1:368:PHE:HB3	1:1:370:PHE:CE2	2.08	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:18:LEU:HD23	2:2:41:ILE:CG1	2.04	0.87
2:2:61:ARG:HG3	2:2:142:TYR:CE1	2.09	0.87
2:2:56:LEU:HD12	2:2:56:LEU:O	1.73	0.87
2:2:26:VAL:HA	2:2:54:SER:OG	1.72	0.87
2:2:118:ASN:ND2	2:2:121:ALA:H	1.71	0.86
2:2:52:THR:O	2:2:52:THR:CG2	2.23	0.86
1:1:420:ARG:O	1:1:424:MET:HG2	1.75	0.86
2:2:37:SER:C	2:2:38:ARG:HD3	1.95	0.86
1:1:221:GLU:HG3	1:1:221:GLU:O	1.74	0.86
1:1:128:LEU:HD22	1:1:143:LEU:O	1.75	0.85
1:1:245:SER:H	1:1:266:GLN:HE21	1.20	0.85
1:1:21:ALA:O	1:1:28:LYS:NZ	2.09	0.85
1:1:172:PRO:HG2	1:1:379:LEU:HD11	1.58	0.85
2:2:41:ILE:HG23	2:2:43:ILE:HG23	1.56	0.85
1:1:377:THR:O	1:1:382:ARG:NH1	2.09	0.85
2:2:28:ALA:CA	2:2:55:GLY:O	2.24	0.85
2:2:97:ASP:HB3	2:2:138:GLY:O	1.76	0.85
2:2:44:ASN:HD22	2:2:158:SER:HB2	1.42	0.85
1:1:167:SER:H	1:1:170:THR:HG22	1.41	0.85
2:2:86:MET:HE1	2:2:147:LEU:HD22	1.57	0.85
1:1:161:ARG:O	1:1:384:LEU:HD22	1.75	0.85
2:2:69:ASN:HD21	2:2:131:ASP:HB2	1.40	0.84
1:1:18:VAL:HG22	1:1:20:GLU:CG	2.07	0.84
2:2:40:THR:HG23	2:2:162:SER:HG	0.88	0.84
1:1:120:PRO:HG2	1:1:123:LEU:HD12	1.58	0.84
1:1:145:TYR:CG	1:1:151:MET:HG2	2.13	0.84
2:2:73:LEU:HD12	2:2:164:ASN:O	1.78	0.84
1:1:144:THR:O	1:1:144:THR:HG23	1.78	0.84
1:1:353:THR:HG22	1:1:354:GLN:N	1.93	0.84
2:2:95:VAL:O	2:2:139:ASN:CB	2.27	0.83
1:1:138:PRO:HD2	3:3:20:VAL:HG13	1.59	0.83
1:1:368:PHE:HB3	1:1:370:PHE:HD2	1.42	0.83
1:1:360:PHE:N	1:1:361:PRO:CD	2.42	0.83
1:1:423:ILE:HD13	1:1:423:ILE:H	1.43	0.83
1:1:163:ALA:O	1:1:290:ARG:NH1	2.12	0.82
1:1:372:SER:H	1:1:389:ASN:HD21	1.28	0.82
1:1:52:SER:HB2	1:1:394:PHE:CD2	2.15	0.81
2:2:36:LEU:O	2:2:61:ARG:O	1.98	0.81
2:2:82:VAL:HG12	2:2:86:MET:HG3	1.59	0.81
1:1:108:TYR:CD1	1:1:109:LEU:CD2	2.64	0.81
2:2:18:LEU:HD21	2:2:41:ILE:HD11	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:23:THR:HA	2:2:48:THR:CG2	2.10	0.81
2:2:153:THR:CG2	2:2:154:ALA:N	2.42	0.80
1:1:71:ILE:HD13	1:1:126:GLY:HA2	1.62	0.80
1:1:239:ARG:NH1	3:3:25:TYR:CE1	2.50	0.80
1:1:269:ASN:ND2	1:1:270:HIS:N	2.28	0.80
2:2:9:HIS:HB3	2:2:125:LYS:HE2	1.63	0.80
1:1:360:PHE:N	1:1:361:PRO:HD2	1.95	0.80
1:1:387:THR:HG22	1:1:388:ASN:N	1.96	0.80
2:2:37:SER:HB3	2:2:38:ARG:CD	2.12	0.80
1:1:363:ASN:C	1:1:363:ASN:ND2	2.31	0.80
1:1:372:SER:N	1:1:389:ASN:HD21	1.79	0.79
2:2:52:THR:O	2:2:52:THR:HG23	1.81	0.79
2:2:157:ILE:O	2:2:157:ILE:HG13	1.83	0.79
2:2:63:ASP:OD1	2:2:65:THR:HG23	1.82	0.79
1:1:133:ASN:C	1:1:214:ARG:NH2	2.36	0.79
1:1:238:MET:CE	1:1:239:ARG:H	1.96	0.79
1:1:120:PRO:HG2	1:1:123:LEU:CD1	2.11	0.79
2:2:95:VAL:CG1	2:2:142:TYR:HE2	1.94	0.79
2:2:26:VAL:N	2:2:54:SER:HB3	1.94	0.79
2:2:77:GLY:O	2:2:123:SER:HA	1.83	0.78
1:1:164:ASN:ND2	1:1:385:VAL:HB	1.98	0.78
1:1:210:TYR:O	3:3:21:GLY:HA2	1.82	0.78
2:2:101:PRO:HD3	2:2:142:TYR:CZ	2.19	0.78
1:1:162:VAL:C	1:1:384:LEU:HD23	2.03	0.78
2:2:130:ILE:HG12	2:2:131:ASP:N	1.98	0.78
2:2:101:PRO:CD	2:2:142:TYR:CZ	2.67	0.78
1:1:30:ILE:CD1	1:1:45:MET:HE3	2.12	0.78
2:2:37:SER:HB3	2:2:38:ARG:NH1	1.99	0.78
1:1:387:THR:CG2	1:1:388:ASN:N	2.46	0.78
1:1:345:ILE:HD11	1:1:349:GLN:HB3	1.66	0.77
1:1:416:MET:SD	1:1:417:PRO:CD	2.73	0.77
1:1:216:ARG:HA	1:1:226:THR:HG21	1.66	0.77
1:1:71:ILE:HD13	1:1:126:GLY:CA	2.15	0.77
2:2:36:LEU:HD13	2:2:61:ARG:NH2	2.00	0.77
2:2:165:GLN:OE1	2:2:167:ASN:OD1	2.02	0.77
2:2:118:ASN:ND2	2:2:119:GLY:N	2.23	0.77
2:2:18:LEU:HB3	2:2:43:ILE:CA	2.15	0.77
1:1:417:PRO:O	1:1:418:THR:HB	1.84	0.77
1:1:97:VAL:CG2	1:1:121:LYS:HA	2.15	0.77
2:2:18:LEU:HD21	2:2:32:SER:CB	2.15	0.76
1:1:136:LYS:HG3	1:1:136:LYS:O	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:23:THR:HA	2:2:48:THR:HG22	1.64	0.76
2:2:26:VAL:C	2:2:28:ALA:H	1.88	0.76
1:1:166:LYS:CD	3:3:18:TRP:CD1	2.69	0.76
1:1:319:LEU:O	1:1:323:LEU:HD21	1.84	0.76
2:2:153:THR:HG23	2:2:154:ALA:H	1.50	0.76
1:1:125:GLN:OE1	1:1:129:ASN:ND2	2.18	0.76
2:2:82:VAL:HG12	2:2:86:MET:CG	2.14	0.76
2:2:49:ALA:CB	2:2:153:THR:HA	2.15	0.76
2:2:44:ASN:HD22	2:2:158:SER:CB	1.98	0.76
1:1:10:VAL:HG22	1:1:11:PRO:HD2	1.67	0.76
2:2:94:GLU:OE2	2:2:135:ARG:CB	2.34	0.76
2:2:137:VAL:HG13	2:2:138:GLY:N	2.01	0.76
1:1:132:ASN:HD21	1:1:143:LEU:N	1.81	0.75
2:2:18:LEU:HG	2:2:43:ILE:CG2	2.15	0.75
1:1:170:THR:HG23	1:1:170:THR:O	1.85	0.75
2:2:21:THR:HA	2:2:46:THR:HG22	0.78	0.75
2:2:43:ILE:O	2:2:43:ILE:CG1	2.21	0.75
2:2:118:ASN:HD21	2:2:121:ALA:H	1.34	0.74
2:2:38:ARG:N	2:2:38:ARG:HD3	2.02	0.74
2:2:69:ASN:HA	2:2:133:HIS:CE1	2.22	0.74
1:1:71:ILE:CD1	1:1:126:GLY:CA	2.65	0.74
1:1:162:VAL:CG1	1:1:290:ARG:HD3	2.17	0.74
1:1:268:PHE:CZ	1:1:404:MET:CE	2.71	0.73
2:2:95:VAL:HG11	2:2:142:TYR:HE2	1.53	0.73
2:2:40:THR:HG22	2:2:162:SER:CB	2.09	0.73
2:2:28:ALA:HB1	2:2:55:GLY:O	1.89	0.73
1:1:166:LYS:HD3	3:3:18:TRP:CD1	2.23	0.73
1:1:18:VAL:HG21	1:1:20:GLU:OE2	1.89	0.73
1:1:231:ASP:CG	1:1:233:ARG:HH11	1.91	0.73
1:1:323:LEU:H	1:1:323:LEU:HD23	1.54	0.73
1:1:108:TYR:CZ	1:1:151:MET:CE	2.71	0.73
1:1:387:THR:HG22	1:1:388:ASN:HD22	1.53	0.72
2:2:32:SER:CB	2:2:41:ILE:HD11	2.14	0.72
1:1:156:TYR:C	1:1:156:TYR:CD1	2.62	0.72
2:2:86:MET:HE2	2:2:147:LEU:HB3	1.70	0.72
2:2:29:PRO:HA	2:2:103:ALA:HB2	1.72	0.72
2:2:24:PRO:HB3	2:2:56:LEU:HG	1.72	0.72
1:1:145:TYR:CD2	1:1:151:MET:CG	2.68	0.72
1:1:299:MET:SD	1:1:304:GLY:HA3	2.30	0.72
1:1:55:ARG:NH1	1:1:392:GLU:O	2.23	0.72
2:2:165:GLN:CD	2:2:167:ASN:OD1	2.28	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:30:ILE:HD12	1:1:45:MET:CE	2.19	0.71
1:1:49:ILE:HG23	1:1:266:GLN:HB3	1.72	0.71
1:1:420:ARG:CA	1:1:423:ILE:CD1	2.55	0.71
1:1:379:LEU:O	1:1:383:VAL:HG13	1.89	0.71
1:1:63:ARG:NH2	1:1:241:GLU:CD	2.43	0.71
1:1:63:ARG:NE	1:1:241:GLU:CD	2.44	0.71
2:2:94:GLU:CD	2:2:135:ARG:HB2	2.10	0.71
1:1:164:ASN:HD21	1:1:385:VAL:HB	1.55	0.71
1:1:329:SER:C	1:1:331:LYS:H	1.94	0.71
1:1:71:ILE:CG1	1:1:76:ILE:HD11	2.21	0.71
2:2:90:ALA:O	2:2:91:ILE:CG2	2.39	0.71
1:1:108:TYR:CD1	1:1:109:LEU:HD23	2.25	0.71
1:1:240:SER:OG	1:1:270:HIS:ND1	1.89	0.71
1:1:72:PRO:O	1:1:75:HIS:HB2	1.90	0.71
2:2:115:THR:OG1	2:2:122:ILE:HD11	1.90	0.71
2:2:32:SER:CB	2:2:41:ILE:CD1	2.69	0.71
1:1:98:THR:HG22	1:1:147:ASN:HD22	1.54	0.71
1:1:387:THR:HG22	1:1:388:ASN:H	1.56	0.71
1:1:397:MET:O	2:2:68:THR:OG1	2.08	0.71
2:2:81:ASN:O	2:2:157:ILE:HG22	1.91	0.71
1:1:353:THR:CG2	1:1:354:GLN:N	2.54	0.71
1:1:359:ALA:CB	1:1:361:PRO:HD2	2.20	0.70
1:1:100:SER:O	1:1:105:SER:CB	2.39	0.70
2:2:137:VAL:HG13	2:2:138:GLY:H	1.56	0.70
1:1:10:VAL:CG2	1:1:11:PRO:CD	2.69	0.70
1:1:63:ARG:HH21	1:1:241:GLU:CD	1.94	0.70
1:1:12:HIS:CE1	1:1:416:MET:HG3	2.27	0.70
1:1:144:THR:O	1:1:144:THR:CG2	2.40	0.70
1:1:63:ARG:HE	1:1:241:GLU:CD	1.95	0.70
2:2:89:PHE:CE1	2:2:110:VAL:HG12	2.27	0.70
2:2:26:VAL:HG13	2:2:27:ALA:H	1.57	0.70
2:2:37:SER:C	2:2:38:ARG:CD	2.60	0.70
1:1:65:ASP:HB2	1:1:288:VAL:CG1	2.22	0.69
1:1:24:ILE:HG12	1:1:401:HIS:HD2	1.57	0.69
2:2:9:HIS:HE1	2:2:162:SER:CB	2.03	0.69
1:1:116:THR:HB	1:1:118:LYS:NZ	2.08	0.69
1:1:196:GLN:NE2	1:1:196:GLN:HA	2.07	0.69
1:1:133:ASN:C	1:1:214:ARG:HH21	1.95	0.69
1:1:246:GLY:HA3	1:1:263:ARG:O	1.92	0.69
2:2:37:SER:HB3	2:2:38:ARG:HD3	1.74	0.68
2:2:49:ALA:HA	2:2:152:TRP:C	2.13	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:30:ILE:CD1	1:1:45:MET:CE	2.70	0.68
2:2:36:LEU:CD1	2:2:61:ARG:HH21	2.03	0.68
2:2:69:ASN:C	2:2:69:ASN:ND2	2.45	0.68
1:1:138:PRO:HD3	3:3:20:VAL:HG11	1.70	0.68
2:2:59:VAL:HA	2:2:144:GLY:HA3	1.74	0.68
1:1:335:HIS:CG	1:1:335:HIS:O	2.45	0.68
1:1:368:PHE:CD1	1:1:370:PHE:HE2	2.12	0.68
2:2:82:VAL:CG1	2:2:86:MET:HG3	2.16	0.68
1:1:301:TYR:HE1	1:1:332:GLU:OE1	1.76	0.68
1:1:98:THR:O	1:1:148:PRO:HD2	1.93	0.68
1:1:18:VAL:CG1	1:1:406:THR:CG2	2.64	0.67
1:1:300:HIS:O	1:1:303:VAL:CG1	2.38	0.67
1:1:295:HIS:CE1	1:1:373:ALA:O	2.45	0.67
1:1:97:VAL:HG23	1:1:121:LYS:HA	1.75	0.67
1:1:300:HIS:CD2	1:1:302:LEU:HB2	2.29	0.67
1:1:182:ASN:HD22	1:1:182:ASN:N	1.92	0.67
1:1:18:VAL:HG22	1:1:20:GLU:HG2	1.74	0.67
1:1:240:SER:CB	1:1:270:HIS:HD1	2.06	0.67
1:1:213:THR:CG2	3:3:21:GLY:O	2.34	0.67
1:1:323:LEU:HB2	1:1:324:PRO:HD2	1.75	0.67
1:1:349:GLN:HE21	1:1:349:GLN:HA	1.59	0.67
2:2:172:VAL:HG23	2:2:173:LEU:N	2.08	0.67
1:1:156:TYR:O	1:1:156:TYR:HD1	1.78	0.67
1:1:108:TYR:CE2	1:1:151:MET:HE1	2.29	0.67
1:1:386:ASN:C	1:1:386:ASN:ND2	2.31	0.67
1:1:127:TYR:N	1:1:284:MET:HE1	2.10	0.67
1:1:268:PHE:CE2	1:1:404:MET:SD	2.89	0.67
2:2:18:LEU:CD2	2:2:41:ILE:CD1	2.17	0.67
2:2:50:VAL:HG12	2:2:152:TRP:CB	2.23	0.67
1:1:208:ARG:NH1	1:1:218:ILE:HD12	2.10	0.66
1:1:240:SER:HG	1:1:270:HIS:CE1	2.06	0.66
2:2:86:MET:HB2	2:2:117:ASN:HD22	1.60	0.66
1:1:100:SER:O	1:1:105:SER:OG	2.14	0.66
1:1:22:GLY:HA2	1:1:158:TRP:CE3	2.30	0.66
1:1:97:VAL:HG23	1:1:121:LYS:CA	2.26	0.66
1:1:167:SER:HB3	1:1:170:THR:HB	1.77	0.66
1:1:227:SER:C	1:1:229:ASP:H	1.99	0.66
1:1:162:VAL:O	1:1:385:VAL:HG13	1.95	0.66
1:1:387:THR:HG22	1:1:388:ASN:ND2	2.10	0.66
2:2:41:ILE:CG2	2:2:43:ILE:HG23	2.24	0.66
1:1:45:MET:HE3	1:1:408:PHE:CZ	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:162:VAL:HG13	1:1:290:ARG:HD3	1.78	0.66
2:2:90:ALA:O	2:2:91:ILE:HG23	1.95	0.66
1:1:108:TYR:CE2	1:1:151:MET:CE	2.79	0.66
1:1:70:TYR:OH	1:1:277:VAL:HG13	1.97	0.65
2:2:18:LEU:HB2	2:2:43:ILE:CG2	2.04	0.65
1:1:101:SER:HA	1:1:117:LEU:HD21	1.77	0.65
1:1:268:PHE:HZ	1:1:404:MET:CE	2.08	0.65
1:1:353:THR:CG2	1:1:354:GLN:H	2.09	0.65
1:1:360:PHE:CD1	1:1:360:PHE:C	2.70	0.65
2:2:65:THR:OG1	2:2:65:THR:O	2.09	0.65
2:2:37:SER:HB3	2:2:38:ARG:HH11	1.60	0.65
1:1:98:THR:H	1:1:147:ASN:HD22	1.44	0.65
1:1:242:PHE:HE2	1:1:266:GLN:HG3	1.62	0.65
2:2:49:ALA:C	2:2:152:TRP:O	2.34	0.65
1:1:376:SER:O	1:1:378:ASP:N	2.30	0.65
1:1:63:ARG:HE	1:1:241:GLU:HG3	1.62	0.64
1:1:70:TYR:CE1	1:1:277:VAL:HG13	2.32	0.64
2:2:85:ASP:C	2:2:85:ASP:OD1	2.35	0.64
1:1:153:SER:O	1:1:157:LYS:HG3	1.97	0.64
1:1:24:ILE:HG12	1:1:401:HIS:CD2	2.32	0.64
2:2:18:LEU:CD2	2:2:32:SER:CB	2.69	0.64
1:1:138:PRO:HD2	3:3:20:VAL:HG11	1.41	0.64
1:1:26:ARG:NE	1:1:159:GLY:O	2.31	0.64
2:2:78:SER:HA	2:2:122:ILE:O	1.98	0.64
1:1:116:THR:CB	1:1:118:LYS:HZ3	2.11	0.64
2:2:59:VAL:CG2	2:2:60:VAL:N	2.61	0.64
1:1:239:ARG:HH11	3:3:25:TYR:HE1	1.43	0.63
1:1:116:THR:CB	1:1:118:LYS:NZ	2.62	0.63
1:1:45:MET:HE3	1:1:408:PHE:HZ	1.62	0.63
1:1:63:ARG:HE	1:1:241:GLU:CG	2.11	0.63
2:2:94:GLU:OE2	2:2:135:ARG:CA	2.46	0.63
1:1:70:TYR:CZ	1:1:277:VAL:HG13	2.33	0.63
2:2:89:PHE:CD1	2:2:110:VAL:HG12	2.33	0.63
1:1:82:ILE:O	1:1:86:LYS:HG3	1.98	0.63
1:1:389:ASN:O	1:1:389:ASN:OD1	2.17	0.63
1:1:63:ARG:CZ	1:1:241:GLU:CD	2.66	0.63
1:1:238:MET:HE2	1:1:239:ARG:O	1.98	0.63
1:1:77:TYR:HB2	1:1:81:TRP:HB2	1.81	0.63
2:2:87:ILE:HG22	2:2:148:TRP:O	1.98	0.63
1:1:238:MET:CE	1:1:239:ARG:O	2.47	0.62
1:1:420:ARG:O	1:1:424:MET:HB2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:49:ALA:HB2	2:2:153:THR:HA	1.80	0.62
1:1:167:SER:OG	1:1:168:ILE:N	2.30	0.62
1:1:214:ARG:O	1:1:217:ASP:HB2	1.99	0.62
1:1:156:TYR:C	1:1:156:TYR:HD1	2.01	0.62
1:1:67:PHE:HB3	1:1:69:PHE:CE2	2.34	0.62
2:2:50:VAL:CG1	2:2:50:VAL:O	2.47	0.62
1:1:102:GLY:O	1:1:105:SER:HB3	2.00	0.62
2:2:26:VAL:HG13	2:2:27:ALA:N	2.15	0.62
2:2:18:LEU:HD23	2:2:41:ILE:HD11	0.63	0.62
1:1:166:LYS:CG	3:3:18:TRP:CD1	2.82	0.62
2:2:94:GLU:OE1	2:2:135:ARG:CB	2.45	0.62
2:2:86:MET:HE2	2:2:147:LEU:HD22	1.82	0.62
2:2:51:THR:HG23	2:2:51:THR:O	2.00	0.61
2:2:59:VAL:HB	2:2:144:GLY:HA3	1.81	0.61
1:1:294:THR:CG2	1:1:370:PHE:HD1	2.13	0.61
1:1:294:THR:HG21	1:1:370:PHE:CD1	2.35	0.61
1:1:133:ASN:CA	1:1:214:ARG:HH21	2.13	0.61
1:1:242:PHE:CE1	1:1:268:PHE:HB2	2.36	0.61
1:1:420:ARG:O	1:1:424:MET:CG	2.47	0.61
1:1:414:ARG:CG	1:1:415:HIS:H	2.13	0.61
1:1:97:VAL:HG21	1:1:121:LYS:HA	1.80	0.61
1:1:133:ASN:HA	1:1:214:ARG:HH21	1.66	0.61
2:2:12:PRO:CG	2:2:38:ARG:HB2	2.19	0.61
1:1:418:THR:HG22	1:1:421:ASP:CB	2.20	0.61
2:2:94:GLU:OE2	2:2:135:ARG:HB2	1.99	0.61
2:2:26:VAL:C	2:2:28:ALA:N	2.53	0.61
2:2:37:SER:CB	2:2:38:ARG:HD3	2.30	0.61
1:1:71:ILE:HG13	1:1:76:ILE:HD11	1.82	0.61
1:1:18:VAL:HG11	1:1:406:THR:CG2	2.31	0.60
1:1:359:ALA:HB1	1:1:361:PRO:HD2	1.82	0.60
1:1:23:LYS:O	1:1:402:TRP:CD1	2.53	0.60
1:1:419:THR:C	1:1:423:ILE:CD1	2.65	0.60
1:1:295:HIS:HA	1:1:371:TYR:HB2	1.82	0.60
1:1:137:PRO:O	1:1:140:SER:HB3	2.01	0.60
1:1:166:LYS:CD	3:3:18:TRP:HD1	2.15	0.60
1:1:204:THR:O	1:1:208:ARG:HG3	2.02	0.60
1:1:300:HIS:HD2	1:1:302:LEU:HB2	1.65	0.60
2:2:92:ARG:HG2	2:2:92:ARG:HH11	1.65	0.60
2:2:97:ASP:HB2	2:2:138:GLY:O	2.02	0.60
1:1:305:LYS:O	1:1:305:LYS:HG3	2.01	0.60
1:1:102:GLY:O	1:1:105:SER:CB	2.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:126:GLY:C	1:1:284:MET:HE3	2.22	0.60
2:2:36:LEU:CD1	2:2:61:ARG:NH2	2.63	0.60
1:1:329:SER:C	1:1:331:LYS:N	2.55	0.60
1:1:231:ASP:OD1	1:1:233:ARG:NH1	2.35	0.60
1:1:50:ARG:NH1	1:1:265:GLN:OE1	2.35	0.60
1:1:383:VAL:CG2	1:1:384:LEU:N	2.64	0.60
2:2:18:LEU:CD2	2:2:41:ILE:CG1	2.70	0.60
1:1:162:VAL:C	1:1:384:LEU:CD2	2.71	0.59
1:1:357:ARG:NH1	1:1:357:ARG:CG	2.29	0.59
2:2:26:VAL:O	2:2:28:ALA:N	2.25	0.59
1:1:185:THR:HG23	1:1:186:GLY:O	2.02	0.59
1:1:163:ALA:N	1:1:384:LEU:HD23	2.17	0.59
1:1:60:VAL:HG13	1:1:369:PRO:HG2	1.83	0.59
1:1:153:SER:HA	1:1:156:TYR:CE2	2.37	0.59
1:1:165:LEU:HB2	1:1:293:PRO:HD3	1.85	0.59
1:1:11:PRO:HG3	1:1:413:TYR:CE1	2.38	0.59
2:2:118:ASN:HD21	2:2:120:LYS:H	1.50	0.59
1:1:397:MET:HG2	2:2:68:THR:OG1	2.03	0.59
1:1:26:ARG:HB3	1:1:159:GLY:O	2.03	0.59
2:2:23:THR:O	2:2:23:THR:OG1	2.21	0.58
1:1:138:PRO:HG3	3:3:20:VAL:CG1	2.19	0.58
1:1:382:ARG:HG2	1:1:382:ARG:O	2.02	0.58
2:2:137:VAL:CG1	2:2:138:GLY:H	2.17	0.58
2:2:94:GLU:CD	2:2:135:ARG:HG3	2.23	0.58
1:1:167:SER:O	3:3:18:TRP:CH2	2.57	0.58
1:1:383:VAL:CG2	1:1:384:LEU:H	2.17	0.58
2:2:90:ALA:C	2:2:91:ILE:HG23	2.24	0.58
1:1:106:ALA:O	1:1:109:LEU:N	2.29	0.58
1:1:69:PHE:CE1	1:1:236:LEU:HG	2.37	0.58
2:2:95:VAL:HG12	2:2:142:TYR:CE2	2.39	0.58
2:2:95:VAL:HG12	2:2:142:TYR:HE2	1.67	0.58
2:2:79:LEU:HD23	2:2:159:GLY:CA	2.29	0.58
1:1:70:TYR:OH	1:1:279:GLU:O	2.21	0.58
1:1:353:THR:HG22	1:1:354:GLN:H	1.64	0.58
1:1:18:VAL:HG22	1:1:20:GLU:HG3	1.83	0.58
1:1:166:LYS:HB3	3:3:18:TRP:NE1	2.19	0.58
2:2:95:VAL:CG1	2:2:142:TYR:CE2	2.82	0.58
1:1:245:SER:N	1:1:266:GLN:HE21	1.96	0.57
1:1:173:LEU:HB2	1:1:344:LYS:O	2.03	0.57
1:1:349:GLN:NE2	1:1:349:GLN:HA	2.19	0.57
2:2:101:PRO:HD3	2:2:142:TYR:OH	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:170:THR:CG2	1:1:170:THR:O	2.52	0.57
1:1:27:LEU:O	1:1:159:GLY:HA3	2.05	0.57
1:1:164:ASN:ND2	1:1:385:VAL:CB	2.67	0.57
1:1:268:PHE:HZ	1:1:404:MET:HE3	1.67	0.57
2:2:165:GLN:O	2:2:167:ASN:N	2.37	0.57
1:1:335:HIS:CD2	1:1:335:HIS:O	2.57	0.57
1:1:155:ASP:O	1:1:159:GLY:HA2	2.04	0.57
1:1:166:LYS:HG2	3:3:18:TRP:CG	2.39	0.57
1:1:227:SER:C	1:1:229:ASP:N	2.58	0.57
2:2:30:VAL:HG23	2:2:103:ALA:HA	1.86	0.57
2:2:94:GLU:OE1	2:2:135:ARG:HG3	2.05	0.57
1:1:63:ARG:NH2	1:1:241:GLU:OE1	2.37	0.57
2:2:156:THR:HG22	2:2:156:THR:O	2.04	0.57
2:2:26:VAL:CA	2:2:54:SER:CB	2.76	0.57
1:1:14:LEU:HD12	1:1:412:VAL:HG21	1.86	0.57
1:1:226:THR:O	1:1:233:ARG:NH2	2.26	0.57
1:1:120:PRO:CG	1:1:123:LEU:HD12	2.31	0.56
1:1:378:ASP:O	1:1:382:ARG:HD2	2.05	0.56
1:1:10:VAL:HG23	1:1:11:PRO:CD	2.26	0.56
1:1:40:SER:OG	1:1:413:TYR:HB2	2.06	0.56
2:2:101:PRO:HG3	2:2:142:TYR:CE2	2.40	0.56
1:1:397:MET:HG2	2:2:68:THR:HG1	1.70	0.56
2:2:156:THR:CG2	2:2:156:THR:O	2.53	0.56
1:1:300:HIS:HB3	1:1:303:VAL:HG12	1.87	0.56
2:2:94:GLU:CD	2:2:135:ARG:CB	2.74	0.56
1:1:166:LYS:HB3	3:3:18:TRP:CD1	2.41	0.56
1:1:174:PRO:O	1:1:177:THR:OG1	2.22	0.56
1:1:277:VAL:HG12	1:1:279:GLU:O	2.05	0.56
1:1:372:SER:H	1:1:389:ASN:ND2	2.02	0.56
1:1:387:THR:CG2	1:1:388:ASN:HD22	2.19	0.56
2:2:37:SER:HB3	2:2:38:ARG:CZ	2.36	0.56
1:1:128:LEU:CD2	1:1:143:LEU:O	2.51	0.56
2:2:98:GLY:N	2:2:140:ASP:OD2	2.27	0.56
2:2:59:VAL:HG23	2:2:143:ALA:C	2.26	0.56
1:1:12:HIS:CE1	1:1:416:MET:HB2	2.41	0.56
1:1:276:TYR:O	1:1:278:PRO:HD3	2.06	0.56
1:1:268:PHE:CZ	1:1:404:MET:SD	2.98	0.56
1:1:63:ARG:NH2	1:1:241:GLU:OE2	2.39	0.56
1:1:135:PHE:CE1	3:3:25:TYR:HB3	2.40	0.56
1:1:362:TYR:O	1:1:364:ALA:N	2.39	0.56
2:2:12:PRO:HG3	2:2:38:ARG:CB	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:178:ARG:HD3	1:1:181:GLU:OE1	2.06	0.55
1:1:167:SER:O	3:3:18:TRP:CZ3	2.59	0.55
2:2:69:ASN:HD21	2:2:131:ASP:CB	2.17	0.55
1:1:14:LEU:HD12	1:1:412:VAL:CG2	2.36	0.55
1:1:359:ALA:C	1:1:361:PRO:CD	2.61	0.55
2:2:50:VAL:O	2:2:50:VAL:HG13	2.05	0.55
2:2:101:PRO:HD3	2:2:142:TYR:CE2	2.42	0.55
2:2:117:ASN:OD1	2:2:118:ASN:N	2.40	0.55
2:2:97:ASP:OD1	2:2:140:ASP:OD1	2.24	0.55
1:1:171:ALA:N	1:1:172:PRO:HD3	2.22	0.55
1:1:69:PHE:CD1	1:1:236:LEU:HA	2.41	0.55
1:1:242:PHE:CE1	1:1:268:PHE:CB	2.89	0.55
2:2:18:LEU:HG	2:2:43:ILE:HG21	1.87	0.55
1:1:119:VAL:HG13	1:1:120:PRO:HD2	1.89	0.55
1:1:323:LEU:H	1:1:323:LEU:HD22	1.50	0.55
1:1:376:SER:O	1:1:377:THR:C	2.44	0.55
2:2:40:THR:HA	2:2:161:LEU:O	2.06	0.55
1:1:419:THR:O	1:1:423:ILE:HD13	1.96	0.54
2:2:38:ARG:N	2:2:38:ARG:CD	2.65	0.54
2:2:84:ALA:HB2	2:2:119:GLY:O	2.08	0.54
2:2:59:VAL:HG23	2:2:60:VAL:N	2.21	0.54
1:1:166:LYS:HD3	3:3:18:TRP:HD1	1.69	0.54
1:1:299:MET:SD	1:1:304:GLY:CA	2.96	0.54
1:1:45:MET:SD	1:1:408:PHE:CE1	3.00	0.54
1:1:108:TYR:CE1	1:1:109:LEU:CG	2.91	0.54
1:1:97:VAL:HG12	1:1:148:PRO:HD2	1.89	0.54
1:1:70:TYR:OH	1:1:277:VAL:CG1	2.55	0.54
2:2:160:VAL:HG22	2:2:161:LEU:N	2.22	0.54
2:2:41:ILE:HG12	2:2:43:ILE:CG2	2.37	0.54
2:2:92:ARG:HH22	2:2:141:VAL:HG11	1.70	0.54
1:1:135:PHE:CE1	3:3:25:TYR:CB	2.90	0.54
1:1:25:GLY:HA3	1:1:385:VAL:HG21	1.90	0.54
1:1:11:PRO:HG3	1:1:413:TYR:HE1	1.72	0.54
1:1:71:ILE:HD11	1:1:76:ILE:CD1	2.31	0.54
1:1:55:ARG:HH11	1:1:366:ASP:HB3	1.73	0.53
1:1:294:THR:CG2	1:1:370:PHE:CD1	2.91	0.53
2:2:96:ALA:C	2:2:139:ASN:HA	2.29	0.53
1:1:35:VAL:HG22	1:1:281:GLY:O	2.07	0.53
1:1:65:ASP:HB2	1:1:288:VAL:HG12	1.90	0.53
1:1:152:PRO:HG2	1:1:155:ASP:OD2	2.08	0.53
2:2:111:TYR:CD1	2:2:111:TYR:N	2.77	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:63:ASP:H	2:2:165:GLN:HE22	1.57	0.53
2:2:80:SER:HA	2:2:120:LYS:O	2.09	0.53
1:1:216:ARG:HD3	1:1:231:ASP:OD2	2.08	0.53
1:1:326:ARG:O	1:1:345:ILE:HG22	2.08	0.53
1:1:18:VAL:CG2	1:1:20:GLU:HG2	2.38	0.53
1:1:231:ASP:OD1	1:1:233:ARG:HG2	2.09	0.53
1:1:331:LYS:HG3	1:1:337:SER:O	2.08	0.53
1:1:242:PHE:CE2	1:1:266:GLN:HG3	2.41	0.53
1:1:60:VAL:CG1	1:1:369:PRO:HG2	2.38	0.53
1:1:383:VAL:HG22	1:1:384:LEU:H	1.72	0.53
2:2:94:GLU:CD	2:2:135:ARG:CG	2.78	0.53
1:1:120:PRO:HD2	1:1:123:LEU:HD12	1.92	0.52
1:1:359:ALA:CA	1:1:361:PRO:HD2	2.38	0.52
1:1:398:GLN:HB2	2:2:66:ASN:HD21	1.74	0.52
2:2:44:ASN:HA	2:2:158:SER:HA	1.91	0.52
1:1:238:MET:HG3	1:1:270:HIS:CE1	2.43	0.52
1:1:418:THR:HG23	1:1:421:ASP:H	1.74	0.52
2:2:59:VAL:CG2	2:2:60:VAL:O	2.57	0.52
1:1:127:TYR:N	1:1:284:MET:CE	2.72	0.52
1:1:182:ASN:N	1:1:182:ASN:ND2	2.55	0.52
1:1:420:ARG:O	1:1:424:MET:CB	2.57	0.52
2:2:59:VAL:HB	2:2:144:GLY:CA	2.39	0.52
2:2:44:ASN:ND2	2:2:158:SER:OG	2.42	0.52
2:2:57:CYS:SG	2:2:91:ILE:CD1	2.92	0.52
1:1:67:PHE:O	1:1:285:THR:HA	2.10	0.52
1:1:362:TYR:C	1:1:364:ALA:H	2.13	0.52
1:1:345:ILE:CD1	1:1:349:GLN:HB3	2.38	0.52
1:1:386:ASN:CG	1:1:386:ASN:O	2.47	0.52
1:1:101:SER:HA	1:1:117:LEU:CD2	2.39	0.51
1:1:18:VAL:CG2	1:1:20:GLU:OE2	2.56	0.51
2:2:25:ALA:CA	2:2:54:SER:HB3	2.40	0.51
2:2:26:VAL:CG1	2:2:27:ALA:H	2.23	0.51
1:1:359:ALA:HB1	1:1:361:PRO:CD	2.40	0.51
1:1:161:ARG:C	1:1:384:LEU:HD22	2.31	0.51
2:2:97:ASP:N	2:2:138:GLY:O	2.40	0.51
1:1:48:ALA:HA	1:1:266:GLN:O	2.11	0.51
2:2:108:TYR:C	2:2:108:TYR:CD1	2.84	0.51
2:2:59:VAL:CG2	2:2:143:ALA:O	2.51	0.51
2:2:160:VAL:CG2	2:2:161:LEU:N	2.73	0.51
2:2:41:ILE:HG12	2:2:43:ILE:HG22	1.93	0.51
1:1:21:ALA:HA	1:1:402:TRP:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:32:SER:CB	2:2:41:ILE:HD12	2.41	0.51
2:2:69:ASN:O	2:2:132:SER:HB3	2.11	0.51
1:1:404:MET:HG2	1:1:406:THR:HG22	1.93	0.51
1:1:63:ARG:HB2	1:1:243:TRP:CZ3	2.45	0.51
1:1:163:ALA:HA	1:1:384:LEU:HA	1.92	0.50
1:1:268:PHE:CZ	1:1:404:MET:HE1	2.44	0.50
2:2:59:VAL:CA	2:2:144:GLY:HA3	2.41	0.50
1:1:210:TYR:C	3:3:21:GLY:HA2	2.31	0.50
1:1:301:TYR:CE1	1:1:332:GLU:OE1	2.63	0.50
1:1:55:ARG:NH1	1:1:366:ASP:HB3	2.26	0.50
1:1:50:ARG:HA	1:1:264:VAL:O	2.11	0.50
2:2:59:VAL:HG23	2:2:60:VAL:O	2.11	0.50
1:1:208:ARG:HG2	1:1:212:MET:CE	2.41	0.50
2:2:59:VAL:CG2	2:2:143:ALA:C	2.80	0.50
1:1:166:LYS:HD3	3:3:18:TRP:HB2	1.93	0.50
1:1:12:HIS:CE1	1:1:416:MET:CB	2.95	0.50
1:1:71:ILE:HG13	1:1:76:ILE:CD1	2.40	0.50
1:1:414:ARG:HG2	1:1:415:HIS:H	1.77	0.50
1:1:67:PHE:CE2	3:3:25:TYR:CE2	2.99	0.50
1:1:156:TYR:O	1:1:156:TYR:CD1	2.61	0.50
1:1:131:TYR:CE2	1:1:136:LYS:HB3	2.46	0.50
1:1:237:LEU:HD22	1:1:275:PHE:CD1	2.47	0.50
2:2:30:VAL:HG23	2:2:103:ALA:N	2.27	0.50
2:2:110:VAL:C	2:2:111:TYR:CD1	2.85	0.50
2:2:37:SER:CA	2:2:38:ARG:HD3	2.41	0.50
2:2:18:LEU:HB3	2:2:43:ILE:HA	1.89	0.50
1:1:127:TYR:OH	1:1:160:VAL:HG12	2.12	0.50
1:1:390:TYR:O	1:1:393:ILE:HG22	2.07	0.50
1:1:23:LYS:O	1:1:402:TRP:NE1	2.45	0.50
2:2:79:LEU:HB2	2:2:82:VAL:HG21	1.94	0.50
2:2:118:ASN:HD21	2:2:121:ALA:N	2.06	0.49
2:2:85:ASP:O	2:2:85:ASP:OD1	2.29	0.49
1:1:380:LYS:O	1:1:383:VAL:HG22	2.11	0.49
1:1:76:ILE:CG2	1:1:121:LYS:HG2	2.43	0.49
1:1:126:GLY:HA3	1:1:284:MET:HE3	1.95	0.49
2:2:59:VAL:HB	2:2:144:GLY:N	2.27	0.49
1:1:133:ASN:HA	1:1:214:ARG:NH2	2.28	0.49
1:1:30:ILE:HD11	1:1:45:MET:CE	2.42	0.49
1:1:50:ARG:NH1	1:1:265:GLN:HG2	2.27	0.49
2:2:85:ASP:OD2	2:2:150:ASN:N	2.45	0.49
1:1:167:SER:N	1:1:170:THR:HG22	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:215:TYR:HA	1:1:218:ILE:HG23	1.94	0.49
1:1:329:SER:O	1:1:331:LYS:N	2.46	0.49
1:1:45:MET:SD	1:1:408:PHE:CZ	3.06	0.49
1:1:71:ILE:HD13	1:1:126:GLY:HA3	1.95	0.49
2:2:145:ILE:CD1	2:2:163:VAL:HG23	2.43	0.49
2:2:52:THR:O	2:2:52:THR:HG22	2.07	0.49
1:1:410:ILE:HG22	1:1:411:ASN:N	2.28	0.49
1:1:70:TYR:CE2	1:1:278:PRO:HD2	2.47	0.49
2:2:9:HIS:CE1	2:2:162:SER:CB	2.84	0.49
1:1:168:ILE:HG23	1:1:169:TRP:N	2.28	0.49
1:1:360:PHE:O	1:1:360:PHE:CD1	2.66	0.49
1:1:397:MET:CG	1:1:397:MET:O	2.61	0.49
2:2:76:ALA:HA	2:2:124:PHE:O	2.13	0.49
1:1:300:HIS:HB3	1:1:303:VAL:CG1	2.43	0.48
2:2:86:MET:SD	2:2:122:ILE:HG21	2.53	0.48
2:2:92:ARG:CD	2:2:130:ILE:HG13	2.33	0.48
2:2:18:LEU:CG	2:2:43:ILE:HG21	2.36	0.48
2:2:86:MET:CE	2:2:147:LEU:HD13	2.43	0.48
2:2:96:ALA:HA	2:2:139:ASN:HB3	1.95	0.48
1:1:18:VAL:CG2	1:1:20:GLU:CG	2.86	0.48
1:1:210:TYR:O	3:3:21:GLY:CA	2.58	0.48
1:1:120:PRO:HG2	1:1:123:LEU:CG	2.43	0.48
1:1:300:HIS:C	1:1:303:VAL:HG12	2.29	0.48
2:2:18:LEU:HB3	2:2:43:ILE:HB	1.84	0.48
2:2:157:ILE:O	2:2:157:ILE:CG1	2.58	0.48
2:2:94:GLU:OE2	2:2:135:ARG:CG	2.62	0.48
2:2:97:ASP:HA	2:2:140:ASP:OD2	2.14	0.48
1:1:69:PHE:CE1	1:1:236:LEU:CG	2.96	0.48
1:1:299:MET:CE	1:1:335:HIS:HA	2.44	0.48
1:1:383:VAL:HG23	1:1:384:LEU:N	2.28	0.48
2:2:137:VAL:CG1	2:2:138:GLY:N	2.68	0.48
2:2:102:THR:O	2:2:103:ALA:HB2	2.14	0.48
2:2:136:THR:CB	2:2:139:ASN:HD21	2.17	0.48
1:1:382:ARG:O	1:1:382:ARG:CG	2.62	0.48
2:2:85:ASP:OD1	2:2:149:SER:CA	2.34	0.48
1:1:208:ARG:HG2	1:1:212:MET:HE2	1.95	0.47
2:2:75:ILE:HG22	2:2:163:VAL:HG22	1.96	0.47
1:1:172:PRO:HG2	1:1:379:LEU:CD1	2.37	0.47
2:2:30:VAL:HG23	2:2:103:ALA:CA	2.43	0.47
2:2:45:ALA:HB3	2:2:157:ILE:HG13	1.97	0.47
1:1:113:PRO:O	1:1:114:SER:O	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:240:SER:OG	1:1:270:HIS:CE1	2.62	0.47
1:1:237:LEU:HD21	1:1:275:PHE:CE1	2.49	0.47
1:1:162:VAL:HG11	1:1:290:ARG:HD3	1.95	0.47
2:2:85:ASP:OD1	2:2:149:SER:HA	2.09	0.47
2:2:89:PHE:HD1	2:2:90:ALA:O	1.97	0.47
1:1:195:LEU:O	1:1:198:ALA:HB3	2.14	0.47
1:1:219:MET:O	1:1:222:PHE:HB2	2.14	0.47
1:1:40:SER:HA	1:1:275:PHE:O	2.13	0.47
1:1:218:ILE:O	1:1:222:PHE:HD2	1.98	0.47
1:1:171:ALA:N	1:1:172:PRO:CD	2.77	0.47
2:2:68:THR:O	2:2:71:HIS:CE1	2.67	0.47
1:1:208:ARG:HH12	1:1:218:ILE:HD12	1.78	0.47
1:1:379:LEU:O	1:1:380:LYS:C	2.52	0.47
1:1:416:MET:SD	1:1:417:PRO:HD3	2.54	0.47
1:1:394:PHE:HE1	1:1:401:HIS:CD2	2.33	0.47
2:2:66:ASN:C	2:2:68:THR:H	2.18	0.47
2:2:95:VAL:O	2:2:139:ASN:HB3	2.13	0.47
2:2:49:ALA:HB1	2:2:153:THR:HA	1.97	0.47
1:1:130:ILE:O	1:1:130:ILE:HG22	2.13	0.47
1:1:130:ILE:HA	1:1:234:PRO:HG2	1.97	0.47
2:2:118:ASN:HD21	2:2:120:LYS:N	2.12	0.47
1:1:108:TYR:OH	1:1:151:MET:HE2	2.15	0.46
1:1:165:LEU:O	1:1:170:THR:HG21	2.15	0.46
1:1:330:LEU:HB3	1:1:337:SER:OG	2.15	0.46
1:1:126:GLY:CA	1:1:284:MET:HE3	2.45	0.46
1:1:175:PRO:O	1:1:344:LYS:NZ	2.40	0.46
1:1:391:ASP:OD1	1:1:401:HIS:HE1	1.98	0.46
2:2:56:LEU:O	2:2:56:LEU:CD1	2.56	0.46
1:1:242:PHE:CE2	1:1:268:PHE:HB3	2.46	0.46
1:1:296:GLU:CD	1:1:363:ASN:HA	2.24	0.46
1:1:98:THR:HG22	1:1:147:ASN:CG	2.34	0.46
2:2:61:ARG:HG3	2:2:142:TYR:CD1	2.49	0.46
1:1:379:LEU:HA	1:1:382:ARG:HD3	1.96	0.46
2:2:37:SER:CB	2:2:38:ARG:NH1	2.74	0.46
2:2:73:LEU:CD2	2:2:143:ALA:HB1	2.45	0.46
1:1:166:LYS:CB	3:3:18:TRP:CD1	2.99	0.46
1:1:423:ILE:CD1	1:1:423:ILE:H	2.21	0.46
1:1:106:ALA:HB3	1:1:111:THR:O	2.16	0.46
1:1:24:ILE:HG22	1:1:25:GLY:N	2.31	0.46
1:1:377:THR:CG2	1:1:378:ASP:N	2.78	0.46
1:1:390:TYR:C	1:1:393:ILE:CG2	2.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:10:VAL:HG22	1:1:11:PRO:CD	2.42	0.46
1:1:155:ASP:O	1:1:159:GLY:CA	2.64	0.46
1:1:305:LYS:HB2	1:1:305:LYS:HE2	1.39	0.46
1:1:30:ILE:CD1	1:1:45:MET:HE1	2.46	0.46
1:1:330:LEU:HD13	1:1:341:ALA:CB	2.46	0.46
2:2:117:ASN:HB2	2:2:122:ILE:HG13	1.98	0.45
2:2:86:MET:HB2	2:2:117:ASN:ND2	2.31	0.45
1:1:135:PHE:CD1	3:3:25:TYR:HB2	2.50	0.45
1:1:120:PRO:O	1:1:123:LEU:HB2	2.16	0.45
1:1:97:VAL:CG2	1:1:121:LYS:HB2	2.47	0.45
2:2:41:ILE:CD1	2:2:43:ILE:CG2	2.95	0.45
2:2:63:ASP:H	2:2:165:GLN:NE2	2.14	0.45
2:2:96:ALA:HB3	2:2:99:VAL:HG21	1.98	0.45
1:1:200:ALA:O	1:1:204:THR:HG23	2.16	0.45
1:1:242:PHE:HE2	1:1:266:GLN:CG	2.30	0.45
1:1:163:ALA:HB1	3:3:24:GLN:NE2	2.31	0.45
3:3:16:ARG:O	3:3:17:LEU:HD23	2.16	0.45
1:1:67:PHE:HE2	3:3:25:TYR:CZ	2.35	0.45
2:2:90:ALA:O	2:2:91:ILE:HG22	2.17	0.45
1:1:120:PRO:CD	1:1:123:LEU:HD12	2.47	0.45
1:1:149:SER:C	1:1:150:ASN:HD22	2.20	0.45
1:1:242:PHE:CZ	1:1:268:PHE:CG	3.04	0.45
2:2:95:VAL:HG11	2:2:142:TYR:CE2	2.41	0.45
2:2:72:ALA:O	2:2:166:VAL:HG23	2.17	0.45
2:2:18:LEU:HD12	2:2:19:ALA:N	2.16	0.45
1:1:150:ASN:HD22	1:1:150:ASN:N	2.14	0.45
1:1:394:PHE:CE1	1:1:401:HIS:CD2	3.05	0.45
1:1:12:HIS:CE1	1:1:416:MET:CG	2.98	0.45
2:2:104:VAL:HG23	2:2:104:VAL:O	2.16	0.45
1:1:126:GLY:C	1:1:284:MET:CE	2.86	0.45
1:1:329:SER:OG	1:1:331:LYS:CB	2.65	0.45
1:1:323:LEU:HB2	1:1:324:PRO:CD	2.43	0.44
2:2:16:THR:O	2:2:16:THR:HG23	2.16	0.44
1:1:244:ALA:HA	1:1:266:GLN:CG	2.32	0.44
1:1:392:GLU:H	1:1:392:GLU:HG2	1.56	0.44
2:2:73:LEU:CD2	2:2:143:ALA:CB	2.95	0.44
2:2:61:ARG:HB3	2:2:61:ARG:HE	1.56	0.44
2:2:90:ALA:C	2:2:91:ILE:CG2	2.83	0.44
1:1:330:LEU:HD13	1:1:341:ALA:O	2.17	0.44
1:1:420:ARG:C	1:1:423:ILE:CD1	2.86	0.44
2:2:83:PRO:C	2:2:85:ASP:H	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:86:MET:HE1	2:2:147:LEU:HD13	1.99	0.44
2:2:94:GLU:OE1	2:2:135:ARG:CG	2.64	0.44
2:2:18:LEU:CD2	2:2:43:ILE:CG2	2.95	0.44
1:1:399:LEU:HA	1:1:399:LEU:HD23	1.78	0.44
2:2:77:GLY:N	2:2:124:PHE:CE1	2.85	0.44
1:1:71:ILE:HD12	1:1:126:GLY:HA2	1.87	0.44
1:1:416:MET:CB	1:1:417:PRO:HD2	2.47	0.44
1:1:45:MET:CE	1:1:408:PHE:CZ	2.98	0.44
1:1:165:LEU:O	1:1:293:PRO:CG	2.66	0.44
1:1:18:VAL:O	1:1:18:VAL:HG13	2.18	0.44
1:1:286:LEU:N	1:1:286:LEU:HD12	2.33	0.44
2:2:69:ASN:O	2:2:132:SER:N	2.36	0.44
2:2:101:PRO:HG3	2:2:142:TYR:CD2	2.53	0.44
1:1:334:PHE:CD2	1:1:375:PRO:HG3	2.53	0.43
1:1:388:ASN:C	1:1:390:TYR:H	2.20	0.43
1:1:64:VAL:O	1:1:241:GLU:HA	2.18	0.43
1:1:116:THR:O	1:1:117:LEU:HB2	2.18	0.43
1:1:133:ASN:CA	1:1:214:ARG:NH2	2.77	0.43
1:1:298:GLU:HB2	1:1:334:PHE:CE1	2.53	0.43
1:1:76:ILE:N	1:1:76:ILE:HD12	2.33	0.43
2:2:42:LEU:CG	2:2:42:LEU:O	2.33	0.43
1:1:137:PRO:O	1:1:140:SER:CB	2.66	0.43
2:2:164:ASN:OD1	2:2:164:ASN:C	2.46	0.43
1:1:100:SER:O	1:1:105:SER:HB2	2.17	0.43
1:1:137:PRO:HA	1:1:138:PRO:HD3	1.78	0.43
1:1:97:VAL:HG11	1:1:148:PRO:HD3	2.01	0.43
2:2:22:LYS:HD2	2:2:29:PRO:HB2	2.00	0.43
2:2:29:PRO:HA	2:2:103:ALA:CB	2.46	0.43
1:1:97:VAL:HG13	1:1:147:ASN:ND2	2.33	0.43
1:1:288:VAL:HG13	1:1:288:VAL:O	2.18	0.43
1:1:368:PHE:CB	1:1:370:PHE:HD2	2.20	0.43
1:1:162:VAL:HG11	1:1:288:VAL:CG2	2.49	0.43
1:1:238:MET:HE3	1:1:239:ARG:N	2.18	0.43
1:1:323:LEU:CB	1:1:324:PRO:HD2	2.45	0.43
1:1:11:PRO:CG	1:1:413:TYR:CE1	3.01	0.43
1:1:54:LEU:HD11	1:1:262:GLY:HA3	2.01	0.43
1:1:71:ILE:CG1	1:1:71:ILE:O	2.67	0.43
1:1:330:LEU:HD22	1:1:341:ALA:CB	2.49	0.43
1:1:65:ASP:HB2	1:1:288:VAL:HG13	2.01	0.43
2:2:91:ILE:HD13	2:2:146:MET:HB2	2.01	0.43
1:1:133:ASN:C	1:1:214:ARG:HH22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:41:PHE:CD1	1:1:41:PHE:C	2.93	0.42
1:1:67:PHE:HE2	3:3:25:TYR:CE2	2.37	0.42
1:1:374:LEU:O	1:1:375:PRO:O	2.37	0.42
2:2:92:ARG:HH11	2:2:92:ARG:CG	2.31	0.42
2:2:107:LEU:HD12	2:2:107:LEU:HA	1.82	0.42
2:2:41:ILE:HD13	2:2:41:ILE:HG21	1.35	0.42
1:1:128:LEU:HD21	1:1:143:LEU:HB3	2.02	0.42
1:1:45:MET:CG	1:1:408:PHE:CE1	3.03	0.42
1:1:12:HIS:HE1	1:1:416:MET:CB	2.33	0.42
1:1:107:ALA:CB	1:1:157:LYS:O	2.67	0.42
1:1:309:THR:OG1	1:1:312:ASP:OD2	2.25	0.42
1:1:36:VAL:HG13	1:1:414:ARG:HH11	1.84	0.42
2:2:145:ILE:CD1	2:2:163:VAL:CG2	2.98	0.42
2:2:32:SER:HB3	2:2:41:ILE:HD12	2.01	0.42
2:2:41:ILE:HD13	2:2:43:ILE:HG21	2.00	0.42
2:2:93:PHE:CZ	2:2:142:TYR:HB2	2.55	0.42
1:1:63:ARG:NH2	1:1:239:ARG:NH2	2.67	0.42
1:1:32:TRP:CE3	1:1:34:PRO:HD3	2.55	0.42
2:2:92:ARG:HH12	2:2:94:GLU:CG	2.33	0.42
1:1:298:GLU:OE2	1:1:355:PRO:HB3	2.20	0.42
1:1:368:PHE:O	1:1:370:PHE:N	2.49	0.42
1:1:71:ILE:HG12	1:1:71:ILE:O	2.20	0.42
2:2:101:PRO:CD	2:2:142:TYR:OH	2.65	0.42
1:1:242:PHE:CZ	1:1:268:PHE:HB2	2.48	0.41
1:1:97:VAL:HG12	1:1:98:THR:N	2.35	0.41
1:1:135:PHE:CZ	3:3:25:TYR:CD2	3.08	0.41
1:1:328:VAL:HG23	1:1:343:PHE:O	2.19	0.41
1:1:12:HIS:NE2	1:1:416:MET:HB2	2.35	0.41
2:2:101:PRO:CG	2:2:142:TYR:CE2	3.03	0.41
1:1:42:GLU:HB3	1:1:274:ARG:HA	2.02	0.41
2:2:118:ASN:ND2	2:2:120:LYS:H	2.18	0.41
1:1:109:LEU:HD22	1:1:123:LEU:O	2.20	0.41
1:1:323:LEU:CB	1:1:324:PRO:CD	2.98	0.41
1:1:397:MET:HG2	1:1:397:MET:O	2.19	0.41
2:2:18:LEU:HD23	2:2:43:ILE:CG2	2.50	0.41
2:2:41:ILE:CG1	2:2:43:ILE:CG2	2.98	0.41
1:1:122:PHE:O	1:1:126:GLY:HA3	2.20	0.41
2:2:13:ILE:HD13	2:2:13:ILE:HG21	1.83	0.41
2:2:23:THR:HA	2:2:48:THR:HG21	1.97	0.41
2:2:66:ASN:O	2:2:68:THR:N	2.53	0.41
1:1:130:ILE:O	1:1:130:ILE:CG2	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:135:PHE:CD1	3:3:25:TYR:CB	3.04	0.41
2:2:18:LEU:CD2	2:2:43:ILE:HG22	2.46	0.41
1:1:231:ASP:CG	1:1:233:ARG:NH1	2.68	0.41
2:2:94:GLU:HA	2:2:140:ASP:O	2.21	0.41
2:2:41:ILE:HD13	2:2:43:ILE:CG2	2.51	0.41
2:2:82:VAL:HG13	2:2:86:MET:CE	2.49	0.41
2:2:89:PHE:CE1	2:2:110:VAL:CG1	3.00	0.41
1:1:183:MET:SD	1:1:195:LEU:HA	2.61	0.41
1:1:18:VAL:HG12	1:1:406:THR:C	2.37	0.41
1:1:22:GLY:HA2	1:1:158:TRP:HE3	1.81	0.41
1:1:354:GLN:HB2	1:1:354:GLN:HE21	1.61	0.41
1:1:362:TYR:C	1:1:364:ALA:N	2.74	0.41
2:2:92:ARG:NH2	2:2:141:VAL:HG11	2.35	0.41
2:2:66:ASN:ND2	2:2:67:PRO:HD2	2.36	0.41
2:2:80:SER:C	2:2:82:VAL:N	2.73	0.41
1:1:22:GLY:HA2	1:1:158:TRP:CZ3	2.55	0.41
2:2:18:LEU:HA	2:2:18:LEU:HD13	1.78	0.41
1:1:328:VAL:O	1:1:342:LYS:HA	2.20	0.41
2:2:118:ASN:OD1	2:2:119:GLY:N	2.42	0.41
2:2:89:PHE:HE1	2:2:91:ILE:CG2	2.34	0.41
1:1:165:LEU:O	1:1:293:PRO:HG3	2.21	0.41
1:1:36:VAL:HB	1:1:280:HIS:CD2	2.56	0.41
1:1:410:ILE:CG2	1:1:411:ASN:N	2.84	0.41
1:1:97:VAL:HG23	1:1:121:LYS:CB	2.51	0.41
2:2:47:THR:HG21	2:2:152:TRP:HZ3	1.86	0.41
2:2:21:THR:CB	2:2:46:THR:HG23	2.37	0.41
1:1:174:PRO:HA	1:1:175:PRO:HD3	1.94	0.40
1:1:377:THR:HG22	1:1:378:ASP:N	2.36	0.40
1:1:81:TRP:O	1:1:84:PHE:HB3	2.22	0.40
2:2:45:ALA:O	2:2:157:ILE:N	2.54	0.40
1:1:196:GLN:NE2	1:1:196:GLN:CA	2.76	0.40
1:1:74:ARG:HB3	1:1:74:ARG:CZ	2.51	0.40
2:2:40:THR:HG23	2:2:162:SER:CA	2.48	0.40
1:1:237:LEU:CD2	1:1:275:PHE:CE1	3.04	0.40
1:1:162:VAL:HG11	1:1:288:VAL:HG21	2.03	0.40
1:1:50:ARG:NH2	1:1:265:GLN:OE1	2.49	0.40
1:1:45:MET:HG3	1:1:408:PHE:CE1	2.57	0.40
2:2:123:SER:OG	2:2:124:PHE:N	2.53	0.40
2:2:50:VAL:HG12	2:2:152:TRP:CG	2.56	0.40
1:1:330:LEU:HD12	1:1:343:PHE:CE1	2.56	0.40
2:2:92:ARG:NE	2:2:131:ASP:OD1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:31:LEU:HD23	2:2:31:LEU:HA	1.91	0.40
2:2:78:SER:O	2:2:79:LEU:HD23	2.21	0.40
2:2:88:ALA:O	2:2:113:ILE:HD11	2.20	0.40

All (1437) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:112:ILE:CA	1:1:201:LYS:CD[2_555]	0.12	2.08
1:1:91:ALA:CA	1:1:141:ASP:CA[2_555]	0.25	1.95
1:1:349:GLN:CA	1:1:423:ILE:CG1[3_555]	0.27	1.93
2:2:8:LYS:O	2:2:89:PHE:CZ[8_556]	0.30	1.90
1:1:74:ARG:CZ	1:1:231:ASP:N[2_555]	0.30	1.90
1:1:87:ASP:CG	1:1:142:ASP:C[2_555]	0.35	1.85
1:1:349:GLN:CB	1:1:423:ILE:CB[3_555]	0.40	1.80
2:2:67:PRO:O	2:2:99:VAL:CB[8_556]	0.41	1.79
1:1:87:ASP:OD2	1:1:142:ASP:O[2_555]	0.43	1.77
2:2:107:LEU:CA	2:2:168:ARG:N[8_556]	0.47	1.73
2:2:73:LEU:CB	2:2:91:ILE:O[8_556]	0.48	1.72
2:2:64:GLU:CD	2:2:134:PRO:CD[8_556]	0.48	1.72
2:2:127:ALA:C	2:2:145:ILE:C[8_556]	0.50	1.70
2:2:113:ILE:CA	2:2:124:PHE:CE1[8_556]	0.51	1.69
1:1:352:ARG:CB	1:1:420:ARG:CB[3_555]	0.51	1.69
1:1:34:PRO:CA	1:1:212:MET:SD[2_555]	0.51	1.69
2:2:59:VAL:CG2	2:2:130:ILE:N[8_556]	0.51	1.69
2:2:127:ALA:CB	2:2:146:MET:CB[8_556]	0.52	1.68
2:2:68:THR:O	2:2:95:VAL:CG1[8_556]	0.53	1.67
2:2:114:GLU:N	2:2:124:PHE:CD2[8_556]	0.53	1.67
1:1:84:PHE:N	1:1:142:ASP:OD2[2_555]	0.54	1.66
2:2:76:ALA:O	2:2:112:PRO:CB[8_556]	0.55	1.65
1:1:220:LYS:CG	1:1:277:VAL:CG2[3_555]	0.56	1.64
2:2:116:PHE:CA	2:2:116:PHE:CG[8_556]	0.56	1.64
2:2:8:LYS:NZ	2:2:147:LEU:CA[8_556]	0.57	1.63
1:1:39:ASP:O	1:1:220:LYS:CE[2_555]	0.57	1.63
1:1:74:ARG:NE	1:1:231:ASP:CA[2_555]	0.57	1.63
2:2:69:ASN:C	2:2:142:TYR:CZ[8_556]	0.58	1.62
2:2:61:ARG:CB	2:2:131:ASP:CB[8_556]	0.58	1.62
2:2:108:TYR:CB	2:2:166:VAL:CA[8_556]	0.58	1.62
1:1:87:ASP:OD1	1:1:143:LEU:N[2_555]	0.59	1.61
2:2:67:PRO:CD	2:2:96:ALA:CB[8_556]	0.59	1.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:71:ILE:N	1:1:219:MET:SD[2_555]	0.64	1.56
1:1:85:MET:CE	1:1:214:ARG:CZ[2_555]	0.65	1.55
2:2:62:ILE:CA	2:2:92:ARG:CZ[8_556]	0.66	1.54
1:1:222:PHE:CE1	1:1:284:MET:CA[3_555]	0.67	1.53
2:2:59:VAL:C	2:2:129:THR:O[8_556]	0.67	1.53
2:2:111:TYR:CG	2:2:163:VAL:CB[8_556]	0.67	1.53
1:1:87:ASP:N	1:1:132:ASN:ND2[2_555]	0.67	1.53
2:2:130:ILE:CG2	2:2:143:ALA:CA[8_556]	0.68	1.52
2:2:107:LEU:CD1	2:2:168:ARG:CG[8_556]	0.68	1.52
1:1:72:PRO:C	1:1:215:TYR:CG[2_555]	0.68	1.52
1:1:32:TRP:CZ2	1:1:204:THR:CB[2_555]	0.68	1.52
2:2:128:VAL:CB	2:2:145:ILE:N[8_556]	0.69	1.51
1:1:39:ASP:C	1:1:220:LYS:NZ[2_555]	0.70	1.50
2:2:65:THR:CA	2:2:139:ASN:CG[8_556]	0.70	1.50
2:2:4:LYS:NZ	2:2:150:ASN:N[8_556]	0.71	1.49
1:1:352:ARG:N	1:1:420:ARG:CG[3_555]	0.71	1.49
2:2:116:PHE:C	2:2:116:PHE:CD1[8_556]	0.72	1.48
2:2:87:ILE:C	2:2:125:LYS:O[8_556]	0.72	1.48
1:1:216:ARG:N	1:1:280:HIS:O[3_555]	0.73	1.47
2:2:71:HIS:C	2:2:93:PHE:CE2[8_556]	0.74	1.46
1:1:12:HIS:NE2	3:3:16:ARG:NH1[2_555]	0.74	1.46
2:2:64:GLU:CB	2:2:134:PRO:CB[8_556]	0.74	1.46
1:1:349:GLN:CG	1:1:423:ILE:N[3_555]	0.74	1.46
2:2:109:ASP:N	2:2:164:ASN:OD1[8_556]	0.76	1.44
2:2:107:LEU:O	2:2:167:ASN:N[8_556]	0.76	1.44
2:2:7:SER:C	2:2:148:TRP:CE2[8_556]	0.76	1.44
1:1:222:PHE:CD1	1:1:284:MET:N[3_555]	0.76	1.44
1:1:12:HIS:NE2	3:3:16:ARG:CZ[2_555]	0.77	1.43
1:1:168:ILE:CG2	1:1:425:THR:CA[3_555]	0.77	1.43
2:2:6:ILE:CG2	2:2:54:SER:N[8_556]	0.77	1.43
2:2:62:ILE:C	2:2:92:ARG:NH2[8_556]	0.77	1.43
1:1:85:MET:CE	1:1:214:ARG:NH2[2_555]	0.77	1.43
1:1:73:HIS:N	1:1:215:TYR:CB[2_555]	0.77	1.43
2:2:71:HIS:CA	2:2:93:PHE:CZ[8_556]	0.79	1.41
1:1:222:PHE:CA	1:1:283:ILE:CB[3_555]	0.79	1.41
2:2:61:ARG:C	2:2:131:ASP:OD1[8_556]	0.79	1.41
1:1:33:THR:CG2	1:1:221:GLU:CD[2_555]	0.79	1.41
1:1:421:ASP:O	3:3:18:TRP:CH2[2_555]	0.79	1.41
1:1:224:GLY:O	1:1:275:PHE:CE2[3_555]	0.80	1.40
2:2:8:LYS:CG	2:2:148:TRP:CB[8_556]	0.80	1.40
1:1:85:MET:C	1:1:132:ASN:O[2_555]	0.80	1.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:218:ILE:CA	1:1:281:GLY:O[3_555]	0.80	1.40
1:1:73:HIS:CA	1:1:215:TYR:CB[2_555]	0.80	1.40
2:2:87:ILE:CG1	2:2:125:LYS:CB[8_556]	0.80	1.40
1:1:416:MET:CB	3:3:16:ARG:CG[2_555]	0.81	1.39
1:1:349:GLN:OE1	1:1:422:SER:N[3_555]	0.81	1.39
2:2:106:ALA:O	2:2:168:ARG:C[8_556]	0.82	1.38
2:2:63:ASP:CB	2:2:94:GLU:OE1[8_556]	0.82	1.38
1:1:74:ARG:CD	1:1:231:ASP:C[2_555]	0.83	1.37
1:1:89:VAL:C	1:1:140:SER:OG[2_555]	0.84	1.36
1:1:72:PRO:C	1:1:215:TYR:CD2[2_555]	0.84	1.36
2:2:107:LEU:O	2:2:167:ASN:CA[8_556]	0.84	1.36
2:2:59:VAL:CB	2:2:129:THR:C[8_556]	0.84	1.36
2:2:60:VAL:O	2:2:130:ILE:C[8_556]	0.84	1.36
2:2:114:GLU:O	2:2:115:THR:OG1[8_556]	0.85	1.35
2:2:6:ILE:CB	2:2:53:HIS:C[8_556]	0.85	1.35
1:1:90:ASN:ND2	1:1:380:LYS:CD[2_555]	0.85	1.35
2:2:88:ALA:N	2:2:125:LYS:O[8_556]	0.85	1.35
2:2:69:ASN:C	2:2:142:TYR:CE2[8_556]	0.85	1.35
2:2:74:SER:C	2:2:90:ALA:O[8_556]	0.86	1.34
2:2:89:PHE:N	2:2:126:ASP:N[8_556]	0.86	1.34
2:2:74:SER:CA	2:2:90:ALA:O[8_556]	0.87	1.33
2:2:65:THR:CA	2:2:139:ASN:OD1[8_556]	0.87	1.33
1:1:217:ASP:N	1:1:280:HIS:C[3_555]	0.87	1.33
1:1:90:ASN:CG	1:1:380:LYS:CE[2_555]	0.88	1.32
2:2:66:ASN:N	2:2:139:ASN:CB[8_556]	0.88	1.32
1:1:86:LYS:CA	1:1:132:ASN:CA[2_555]	0.88	1.32
2:2:8:LYS:C	2:2:89:PHE:CE2[8_556]	0.88	1.32
1:1:227:SER:OG	1:1:229:ASP:OD2[3_555]	0.88	1.32
1:1:231:ASP:CG	1:1:279:GLU:OE1[3_555]	0.90	1.30
2:2:109:ASP:C	2:2:164:ASN:CA[8_556]	0.90	1.30
2:2:59:VAL:CG1	2:2:129:THR:CA[8_556]	0.91	1.29
1:1:233:ARG:NH1	1:1:279:GLU:CD[3_555]	0.91	1.29
2:2:128:VAL:CA	2:2:145:ILE:N[8_556]	0.91	1.29
1:1:352:ARG:CA	1:1:420:ARG:CG[3_555]	0.92	1.28
2:2:67:PRO:N	2:2:96:ALA:CA[8_556]	0.92	1.28
2:2:7:SER:CA	2:2:148:TRP:NE1[8_556]	0.92	1.28
2:2:109:ASP:O	2:2:164:ASN:C[8_556]	0.92	1.28
1:1:417:PRO:CB	3:3:18:TRP:N[2_555]	0.92	1.28
1:1:86:LYS:CA	1:1:132:ASN:CB[2_555]	0.92	1.28
1:1:416:MET:CE	3:3:19:TYR:CE1[2_555]	0.93	1.27
2:2:127:ALA:C	2:2:146:MET:N[8_556]	0.93	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:133:HIS:CD2	2:2:140:ASP:CG[8_556]	0.93	1.27
2:2:88:ALA:C	2:2:126:ASP:N[8_556]	0.93	1.27
1:1:222:PHE:CG	1:1:283:ILE:C[3_555]	0.94	1.26
2:2:76:ALA:C	2:2:112:PRO:CB[8_556]	0.94	1.26
1:1:418:THR:N	3:3:17:LEU:N[2_555]	0.94	1.26
2:2:65:THR:C	2:2:139:ASN:CB[8_556]	0.94	1.26
1:1:90:ASN:N	1:1:140:SER:OG[2_555]	0.94	1.26
1:1:222:PHE:CG	1:1:283:ILE:CA[3_555]	0.95	1.25
2:2:8:LYS:CE	2:2:148:TRP:N[8_556]	0.95	1.25
2:2:133:HIS:CG	2:2:140:ASP:CG[8_556]	0.95	1.25
1:1:222:PHE:N	1:1:283:ILE:CG1[3_555]	0.95	1.25
2:2:69:ASN:CB	2:2:142:TYR:OH[8_556]	0.95	1.25
2:2:109:ASP:O	2:2:164:ASN:O[8_556]	0.95	1.25
2:2:60:VAL:O	2:2:131:ASP:N[8_556]	0.96	1.24
1:1:112:ILE:N	1:1:201:LYS:CG[2_555]	0.96	1.24
2:2:127:ALA:CA	2:2:146:MET:N[8_556]	0.96	1.24
1:1:418:THR:CG2	3:3:17:LEU:CG[2_555]	0.96	1.24
2:2:7:SER:CA	2:2:148:TRP:CE2[8_556]	0.97	1.23
1:1:87:ASP:OD1	1:1:143:LEU:CA[2_555]	0.97	1.23
1:1:84:PHE:N	1:1:142:ASP:CG[2_555]	0.97	1.23
1:1:222:PHE:CA	1:1:283:ILE:CG2[3_555]	0.97	1.23
1:1:349:GLN:CG	1:1:423:ILE:CA[3_555]	0.98	1.22
2:2:133:HIS:CD2	2:2:140:ASP:CB[8_556]	0.98	1.22
2:2:6:ILE:CG2	2:2:53:HIS:C[8_556]	0.98	1.22
1:1:83:ASN:C	1:1:142:ASP:CG[2_555]	0.98	1.22
2:2:8:LYS:CE	2:2:147:LEU:C[8_556]	0.98	1.22
2:2:4:LYS:NZ	2:2:150:ASN:CA[8_556]	0.98	1.22
1:1:418:THR:N	3:3:17:LEU:CA[2_555]	0.99	1.21
2:2:36:LEU:O	2:2:135:ARG:NH2[8_556]	0.99	1.21
2:2:107:LEU:C	2:2:167:ASN:N[8_556]	1.00	1.20
2:2:66:ASN:O	2:2:96:ALA:O[8_556]	1.00	1.20
2:2:63:ASP:CB	2:2:94:GLU:CD[8_556]	1.00	1.20
2:2:60:VAL:CG2	2:2:111:TYR:OH[8_556]	1.00	1.20
2:2:66:ASN:C	2:2:96:ALA:CA[8_556]	1.00	1.20
2:2:113:ILE:N	2:2:124:PHE:CE1[8_556]	1.01	1.19
2:2:127:ALA:O	2:2:145:ILE:C[8_556]	1.01	1.19
2:2:110:VAL:N	2:2:164:ASN:CB[8_556]	1.02	1.18
1:1:218:ILE:N	1:1:281:GLY:O[3_555]	1.02	1.18
2:2:108:TYR:CB	2:2:166:VAL:N[8_556]	1.02	1.18
2:2:111:TYR:CG	2:2:163:VAL:CG1[8_556]	1.03	1.17
2:2:38:ARG:CD	2:2:109:ASP:OD1[8_556]	1.03	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:109:ASP:CA	2:2:164:ASN:OD1[8_556]	1.03	1.17
2:2:64:GLU:CG	2:2:134:PRO:N[8_556]	1.03	1.17
1:1:34:PRO:CB	1:1:212:MET:SD[2_555]	1.03	1.17
2:2:62:ILE:CA	2:2:92:ARG:NH2[8_556]	1.04	1.16
1:1:87:ASP:CG	1:1:143:LEU:N[2_555]	1.04	1.16
1:1:231:ASP:OD2	1:1:279:GLU:OE1[3_555]	1.04	1.16
2:2:111:TYR:CB	2:2:163:VAL:CG2[8_556]	1.04	1.16
1:1:352:ARG:CB	1:1:420:ARG:CA[3_555]	1.04	1.16
1:1:73:HIS:ND1	1:1:214:ARG:C[2_555]	1.04	1.16
2:2:89:PHE:O	2:2:126:ASP:O[8_556]	1.04	1.16
2:2:61:ARG:CA	2:2:131:ASP:CB[8_556]	1.05	1.15
2:2:6:ILE:CA	2:2:53:HIS:O[8_556]	1.05	1.15
2:2:37:SER:O	2:2:109:ASP:CG[8_556]	1.05	1.15
2:2:107:LEU:CB	2:2:168:ARG:N[8_556]	1.06	1.14
1:1:91:ALA:N	1:1:141:ASP:N[2_555]	1.06	1.14
2:2:113:ILE:CA	2:2:124:PHE:CZ[8_556]	1.07	1.13
2:2:66:ASN:C	2:2:96:ALA:N[8_556]	1.07	1.13
1:1:74:ARG:NH1	1:1:230:GLY:C[2_555]	1.07	1.13
2:2:65:THR:O	2:2:139:ASN:ND2[8_556]	1.08	1.12
1:1:233:ARG:NH1	1:1:279:GLU:CG[3_555]	1.08	1.12
2:2:110:VAL:N	2:2:164:ASN:CA[8_556]	1.08	1.12
1:1:39:ASP:CA	1:1:220:LYS:NZ[2_555]	1.08	1.12
1:1:87:ASP:OD2	1:1:142:ASP:C[2_555]	1.08	1.12
1:1:350:TRP:O	1:1:424:MET:CE[3_555]	1.09	1.11
1:1:73:HIS:N	1:1:215:TYR:CG[2_555]	1.09	1.11
1:1:418:THR:CG2	3:3:17:LEU:CD1[2_555]	1.09	1.11
2:2:114:GLU:CB	2:2:122:ILE:CD1[8_556]	1.09	1.11
2:2:59:VAL:CA	2:2:129:THR:C[8_556]	1.09	1.11
2:2:87:ILE:CD1	2:2:125:LYS:CD[8_556]	1.09	1.11
2:2:111:TYR:CD1	2:2:163:VAL:CG1[8_556]	1.10	1.10
2:2:130:ILE:CG2	2:2:143:ALA:N[8_556]	1.10	1.10
2:2:65:THR:C	2:2:139:ASN:CG[8_556]	1.10	1.10
2:2:63:ASP:CA	2:2:94:GLU:OE2[8_556]	1.10	1.10
1:1:74:ARG:NH1	1:1:230:GLY:O[2_555]	1.10	1.10
2:2:114:GLU:CD	2:2:122:ILE:CG2[8_556]	1.11	1.09
1:1:33:THR:CG2	1:1:221:GLU:OE2[2_555]	1.11	1.09
2:2:65:THR:CG2	2:2:136:THR:O[8_556]	1.11	1.09
2:2:128:VAL:CB	2:2:144:GLY:C[8_556]	1.11	1.09
2:2:127:ALA:CB	2:2:146:MET:CA[8_556]	1.11	1.09
1:1:12:HIS:CD2	3:3:16:ARG:NH1[2_555]	1.11	1.09
2:2:132:SER:O	2:2:141:VAL:N[8_556]	1.11	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:150:ASN:OD1	1:1:150:ASN:OD1[8_556]	1.11	1.09
2:2:106:ALA:O	2:2:169:GLU:N[8_556]	1.12	1.08
2:2:65:THR:OG1	2:2:139:ASN:ND2[8_556]	1.12	1.08
2:2:113:ILE:C	2:2:124:PHE:CD2[8_556]	1.12	1.08
2:2:36:LEU:O	2:2:135:ARG:CZ[8_556]	1.12	1.08
1:1:416:MET:CE	3:3:19:TYR:CD1[2_555]	1.12	1.08
2:2:64:GLU:CG	2:2:134:PRO:CD[8_556]	1.13	1.07
2:2:72:ALA:N	2:2:93:PHE:CE2[8_556]	1.13	1.07
2:2:68:THR:CB	2:2:95:VAL:CG2[8_556]	1.13	1.07
2:2:116:PHE:O	2:2:116:PHE:CE1[8_556]	1.13	1.07
2:2:59:VAL:CA	2:2:129:THR:O[8_556]	1.13	1.07
1:1:74:ARG:CZ	1:1:230:GLY:C[2_555]	1.13	1.07
1:1:218:ILE:CA	1:1:281:GLY:C[3_555]	1.13	1.07
2:2:92:ARG:O	2:2:165:GLN:CA[8_556]	1.13	1.07
2:2:109:ASP:C	2:2:164:ASN:C[8_556]	1.14	1.06
1:1:217:ASP:OD2	1:1:280:HIS:CD2[3_555]	1.14	1.06
2:2:132:SER:CA	2:2:141:VAL:C[8_556]	1.14	1.06
1:1:85:MET:CA	1:1:132:ASN:O[2_555]	1.15	1.05
1:1:70:TYR:C	1:1:219:MET:CE[2_555]	1.15	1.05
1:1:218:ILE:O	1:1:282:VAL:CA[3_555]	1.15	1.05
1:1:352:ARG:CA	1:1:420:ARG:CB[3_555]	1.16	1.04
1:1:71:ILE:N	1:1:219:MET:CE[2_555]	1.16	1.04
2:2:114:GLU:N	2:2:124:PHE:CE2[8_556]	1.16	1.04
1:1:215:TYR:O	1:1:281:GLY:CA[3_555]	1.16	1.04
2:2:65:THR:CB	2:2:139:ASN:OD1[8_556]	1.17	1.03
2:2:111:TYR:C	2:2:162:SER:O[8_556]	1.17	1.03
2:2:36:LEU:C	2:2:135:ARG:CZ[8_556]	1.17	1.03
2:2:67:PRO:O	2:2:99:VAL:CG2[8_556]	1.18	1.02
2:2:7:SER:C	2:2:148:TRP:CD2[8_556]	1.18	1.02
1:1:91:ALA:O	1:1:141:ASP:OD1[2_555]	1.18	1.02
1:1:39:ASP:C	1:1:220:LYS:CE[2_555]	1.18	1.02
2:2:75:ILE:O	2:2:89:PHE:CB[8_556]	1.18	1.02
1:1:86:LYS:N	1:1:132:ASN:CB[2_555]	1.19	1.01
1:1:222:PHE:CE1	1:1:284:MET:N[3_555]	1.19	1.01
2:2:116:PHE:C	2:2:116:PHE:CG[8_556]	1.19	1.01
2:2:113:ILE:C	2:2:124:PHE:CE2[8_556]	1.20	1.00
1:1:85:MET:C	1:1:132:ASN:C[2_555]	1.20	1.00
2:2:59:VAL:CB	2:2:129:THR:CA[8_556]	1.20	1.00
2:2:6:ILE:CB	2:2:53:HIS:O[8_556]	1.20	1.00
2:2:73:LEU:C	2:2:91:ILE:N[8_556]	1.21	0.99
2:2:8:LYS:O	2:2:89:PHE:CE2[8_556]	1.21	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:116:PHE:CB	2:2:116:PHE:CB[8_556]	1.21	0.99
1:1:168:ILE:CD1	1:1:424:MET:CA[3_555]	1.21	0.99
2:2:67:PRO:N	2:2:96:ALA:CB[8_556]	1.21	0.99
2:2:106:ALA:C	2:2:168:ARG:C[8_556]	1.21	0.99
1:1:74:ARG:NH2	1:1:231:ASP:N[2_555]	1.21	0.99
2:2:59:VAL:CB	2:2:130:ILE:N[8_556]	1.22	0.98
2:2:73:LEU:CG	2:2:91:ILE:O[8_556]	1.22	0.98
1:1:217:ASP:N	1:1:281:GLY:N[3_555]	1.22	0.98
2:2:68:THR:C	2:2:95:VAL:CG1[8_556]	1.22	0.98
1:1:168:ILE:CG2	1:1:425:THR:C[3_555]	1.22	0.98
1:1:216:ARG:O	1:1:279:GLU:O[3_555]	1.23	0.97
1:1:349:GLN:CB	1:1:423:ILE:CA[3_555]	1.23	0.97
2:2:106:ALA:O	2:2:168:ARG:O[8_556]	1.23	0.97
2:2:36:LEU:C	2:2:135:ARG:NH2[8_556]	1.24	0.96
1:1:91:ALA:C	1:1:141:ASP:CB[2_555]	1.24	0.96
2:2:69:ASN:CA	2:2:142:TYR:OH[8_556]	1.24	0.96
1:1:222:PHE:N	1:1:283:ILE:CD1[3_555]	1.24	0.96
1:1:74:ARG:CD	1:1:231:ASP:CA[2_555]	1.24	0.96
2:2:130:ILE:CB	2:2:143:ALA:O[8_556]	1.24	0.96
2:2:70:HIS:N	2:2:142:TYR:CZ[8_556]	1.24	0.96
2:2:73:LEU:CB	2:2:91:ILE:C[8_556]	1.25	0.95
2:2:116:PHE:C	2:2:116:PHE:CE1[8_556]	1.25	0.95
2:2:110:VAL:O	2:2:163:VAL:C[8_556]	1.25	0.95
1:1:84:PHE:O	1:1:136:LYS:NZ[2_555]	1.25	0.95
1:1:74:ARG:NE	1:1:231:ASP:N[2_555]	1.25	0.95
2:2:107:LEU:CB	2:2:167:ASN:C[8_556]	1.26	0.94
2:2:61:ARG:O	2:2:131:ASP:OD1[8_556]	1.26	0.94
2:2:73:LEU:CA	2:2:91:ILE:C[8_556]	1.26	0.94
2:2:8:LYS:CD	2:2:148:TRP:N[8_556]	1.26	0.94
1:1:222:PHE:CD1	1:1:283:ILE:C[3_555]	1.26	0.94
2:2:73:LEU:N	2:2:91:ILE:CG1[8_556]	1.27	0.93
1:1:231:ASP:OD1	1:1:279:GLU:OE1[3_555]	1.27	0.93
1:1:12:HIS:CG	3:3:16:ARG:NH2[2_555]	1.27	0.93
2:2:63:ASP:C	2:2:94:GLU:OE2[8_556]	1.27	0.93
1:1:222:PHE:CD2	1:1:283:ILE:N[3_555]	1.27	0.93
1:1:349:GLN:CD	1:1:423:ILE:N[3_555]	1.27	0.93
2:2:128:VAL:N	2:2:145:ILE:C[8_556]	1.27	0.93
2:2:8:LYS:NZ	2:2:147:LEU:CB[8_556]	1.27	0.93
1:1:35:VAL:CG2	1:1:217:ASP:O[2_555]	1.28	0.92
1:1:72:PRO:O	1:1:215:TYR:CG[2_555]	1.28	0.92
1:1:222:PHE:CD2	1:1:283:ILE:CA[3_555]	1.28	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:109:ASP:C	2:2:164:ASN:CB[8_556]	1.28	0.92
2:2:75:ILE:N	2:2:90:ALA:N[8_556]	1.28	0.92
2:2:37:SER:O	2:2:109:ASP:CB[8_556]	1.28	0.92
2:2:112:PRO:N	2:2:162:SER:O[8_556]	1.29	0.91
1:1:218:ILE:C	1:1:282:VAL:N[3_555]	1.29	0.91
1:1:216:ARG:CG	1:1:280:HIS:N[3_555]	1.29	0.91
2:2:71:HIS:CG	2:2:93:PHE:CD1[8_556]	1.29	0.91
2:2:111:TYR:CD2	2:2:163:VAL:CB[8_556]	1.29	0.91
1:1:218:ILE:O	1:1:282:VAL:C[3_555]	1.29	0.91
2:2:108:TYR:CD2	2:2:166:VAL:CG1[8_556]	1.29	0.91
2:2:66:ASN:CB	2:2:95:VAL:C[8_556]	1.29	0.91
2:2:128:VAL:CG2	2:2:145:ILE:CG1[8_556]	1.29	0.91
1:1:86:LYS:CB	1:1:132:ASN:CB[2_555]	1.29	0.91
2:2:67:PRO:CG	2:2:96:ALA:CB[8_556]	1.29	0.91
2:2:69:ASN:N	2:2:99:VAL:O[8_556]	1.30	0.90
2:2:74:SER:N	2:2:91:ILE:CG2[8_556]	1.30	0.90
1:1:86:LYS:C	1:1:132:ASN:ND2[2_555]	1.30	0.90
2:2:92:ARG:C	2:2:165:GLN:CG[8_556]	1.30	0.90
2:2:73:LEU:C	2:2:91:ILE:CA[8_556]	1.30	0.90
2:2:7:SER:N	2:2:148:TRP:CZ2[8_556]	1.30	0.90
2:2:71:HIS:CA	2:2:93:PHE:CE2[8_556]	1.30	0.90
2:2:63:ASP:O	2:2:94:GLU:CG[8_556]	1.30	0.90
2:2:8:LYS:N	2:2:148:TRP:CG[8_556]	1.31	0.89
1:1:91:ALA:C	1:1:141:ASP:CG[2_555]	1.31	0.89
1:1:90:ASN:ND2	1:1:380:LYS:CE[2_555]	1.31	0.89
1:1:222:PHE:CB	1:1:283:ILE:CB[3_555]	1.32	0.88
2:2:61:ARG:CA	2:2:131:ASP:CG[8_556]	1.32	0.88
2:2:76:ALA:N	2:2:112:PRO:CA[8_556]	1.32	0.88
2:2:4:LYS:CE	2:2:150:ASN:CA[8_556]	1.32	0.88
2:2:61:ARG:CA	2:2:131:ASP:CA[8_556]	1.32	0.88
2:2:61:ARG:C	2:2:131:ASP:CG[8_556]	1.32	0.88
1:1:218:ILE:N	1:1:281:GLY:C[3_555]	1.33	0.87
2:2:132:SER:CA	2:2:141:VAL:O[8_556]	1.33	0.87
2:2:62:ILE:CA	2:2:92:ARG:NE[8_556]	1.33	0.87
1:1:352:ARG:C	1:1:420:ARG:NE[3_555]	1.33	0.87
1:1:84:PHE:C	1:1:142:ASP:OD1[2_555]	1.33	0.87
2:2:65:THR:CG2	2:2:136:THR:C[8_556]	1.33	0.87
2:2:88:ALA:CB	2:2:126:ASP:CB[8_556]	1.33	0.87
1:1:12:HIS:CD2	3:3:16:ARG:CZ[2_555]	1.33	0.87
2:2:64:GLU:CB	2:2:134:PRO:CG[8_556]	1.33	0.87
1:1:92:SER:N	1:1:141:ASP:CG[2_555]	1.33	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:116:PHE:O	2:2:116:PHE:CD1[8_556]	1.34	0.86
1:1:86:LYS:N	1:1:132:ASN:CA[2_555]	1.34	0.86
2:2:65:THR:N	2:2:139:ASN:OD1[8_556]	1.34	0.86
2:2:76:ALA:O	2:2:112:PRO:CG[8_556]	1.34	0.86
1:1:416:MET:CE	3:3:19:TYR:CZ[2_555]	1.34	0.86
1:1:73:HIS:ND1	1:1:215:TYR:N[2_555]	1.34	0.86
2:2:133:HIS:CG	2:2:140:ASP:CB[8_556]	1.35	0.85
1:1:91:ALA:CA	1:1:141:ASP:C[2_555]	1.35	0.85
1:1:349:GLN:NE2	1:1:423:ILE:CD1[3_555]	1.35	0.85
2:2:116:PHE:CA	2:2:116:PHE:CB[8_556]	1.35	0.85
1:1:222:PHE:CB	1:1:283:ILE:CA[3_555]	1.35	0.85
1:1:222:PHE:C	1:1:283:ILE:CG2[3_555]	1.35	0.85
1:1:72:PRO:O	1:1:215:TYR:CD2[2_555]	1.36	0.84
1:1:85:MET:SD	1:1:214:ARG:CZ[2_555]	1.36	0.84
2:2:59:VAL:O	2:2:129:THR:O[8_556]	1.36	0.84
1:1:87:ASP:CG	1:1:142:ASP:O[2_555]	1.36	0.84
1:1:85:MET:SD	1:1:214:ARG:NE[2_555]	1.36	0.84
1:1:74:ARG:NH2	1:1:230:GLY:C[2_555]	1.36	0.84
1:1:35:VAL:CG1	1:1:221:GLU:N[2_555]	1.36	0.84
1:1:34:PRO:CB	1:1:212:MET:CE[2_555]	1.36	0.84
2:2:73:LEU:CA	2:2:91:ILE:CA[8_556]	1.36	0.84
2:2:71:HIS:NE2	2:2:95:VAL:N[8_556]	1.37	0.83
2:2:111:TYR:CA	2:2:162:SER:O[8_556]	1.38	0.82
1:1:416:MET:CA	3:3:16:ARG:CG[2_555]	1.38	0.82
1:1:91:ALA:C	1:1:141:ASP:CA[2_555]	1.38	0.82
1:1:418:THR:C	3:3:17:LEU:CD2[2_555]	1.38	0.82
2:2:87:ILE:CD1	2:2:125:LYS:CG[8_556]	1.38	0.82
2:2:6:ILE:CD1	2:2:52:THR:CG2[8_556]	1.39	0.81
1:1:350:TRP:CA	1:1:424:MET:SD[3_555]	1.39	0.81
2:2:75:ILE:CA	2:2:111:TYR:O[8_556]	1.39	0.81
2:2:71:HIS:CA	2:2:93:PHE:CE1[8_556]	1.39	0.81
1:1:352:ARG:CZ	1:1:419:THR:CG2[3_555]	1.39	0.81
1:1:37:ALA:N	1:1:217:ASP:OD1[2_555]	1.39	0.81
2:2:108:TYR:CG	2:2:166:VAL:CG2[8_556]	1.39	0.81
2:2:61:ARG:O	2:2:131:ASP:CG[8_556]	1.39	0.81
1:1:352:ARG:CA	1:1:420:ARG:CD[3_555]	1.40	0.80
1:1:12:HIS:CE1	3:3:16:ARG:CZ[2_555]	1.40	0.80
2:2:74:SER:CB	2:2:89:PHE:CE1[8_556]	1.40	0.80
1:1:215:TYR:C	1:1:280:HIS:O[3_555]	1.40	0.80
2:2:66:ASN:C	2:2:96:ALA:C[8_556]	1.40	0.80
2:2:109:ASP:CA	2:2:164:ASN:CG[8_556]	1.40	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:39:ASP:O	1:1:220:LYS:NZ[2_555]	1.40	0.80
2:2:75:ILE:CB	2:2:111:TYR:O[8_556]	1.40	0.80
2:2:63:ASP:CG	2:2:94:GLU:OE1[8_556]	1.40	0.80
1:1:217:ASP:OD2	1:1:280:HIS:CG[3_555]	1.41	0.79
2:2:62:ILE:N	2:2:131:ASP:O[8_556]	1.41	0.79
1:1:222:PHE:N	1:1:283:ILE:CB[3_555]	1.41	0.79
2:2:72:ALA:N	2:2:93:PHE:CD2[8_556]	1.41	0.79
1:1:74:ARG:CD	1:1:231:ASP:O[2_555]	1.41	0.79
2:2:60:VAL:C	2:2:131:ASP:N[8_556]	1.41	0.79
1:1:220:LYS:CB	1:1:277:VAL:CG2[3_555]	1.41	0.79
2:2:64:GLU:O	2:2:139:ASN:O[8_556]	1.42	0.78
2:2:109:ASP:N	2:2:165:GLN:N[8_556]	1.42	0.78
1:1:89:VAL:CA	1:1:140:SER:CB[2_555]	1.42	0.78
1:1:222:PHE:CD2	1:1:283:ILE:C[3_555]	1.42	0.78
1:1:72:PRO:CA	1:1:215:TYR:CD2[2_555]	1.42	0.78
1:1:73:HIS:CG	1:1:215:TYR:N[2_555]	1.42	0.78
2:2:74:SER:N	2:2:91:ILE:CB[8_556]	1.42	0.78
1:1:217:ASP:N	1:1:280:HIS:CA[3_555]	1.42	0.78
2:2:34:PRO:CB	2:2:70:HIS:NE2[8_556]	1.43	0.77
1:1:87:ASP:CB	1:1:142:ASP:CA[2_555]	1.43	0.77
2:2:69:ASN:O	2:2:142:TYR:CE2[8_556]	1.43	0.77
2:2:127:ALA:CA	2:2:146:MET:CA[8_556]	1.43	0.77
1:1:222:PHE:CG	1:1:284:MET:N[3_555]	1.43	0.77
2:2:67:PRO:C	2:2:99:VAL:CB[8_556]	1.43	0.77
1:1:417:PRO:CG	3:3:18:TRP:O[2_555]	1.43	0.77
2:2:8:LYS:CG	2:2:148:TRP:CA[8_556]	1.44	0.76
1:1:74:ARG:NE	1:1:231:ASP:C[2_555]	1.44	0.76
2:2:114:GLU:CG	2:2:122:ILE:CD1[8_556]	1.44	0.76
2:2:64:GLU:OE1	2:2:134:PRO:CD[8_556]	1.44	0.76
1:1:218:ILE:C	1:1:281:GLY:C[3_555]	1.44	0.76
1:1:90:ASN:CB	1:1:380:LYS:CE[2_555]	1.44	0.76
1:1:214:ARG:CB	1:1:280:HIS:CB[3_555]	1.44	0.76
2:2:73:LEU:C	2:2:91:ILE:CB[8_556]	1.44	0.76
2:2:8:LYS:N	2:2:148:TRP:CD2[8_556]	1.44	0.76
2:2:113:ILE:CA	2:2:124:PHE:CD1[8_556]	1.45	0.75
2:2:34:PRO:CB	2:2:70:HIS:CD2[8_556]	1.45	0.75
2:2:63:ASP:CA	2:2:94:GLU:CD[8_556]	1.45	0.75
1:1:83:ASN:C	1:1:142:ASP:OD2[2_555]	1.45	0.75
2:2:8:LYS:CB	2:2:148:TRP:CB[8_556]	1.45	0.75
1:1:74:ARG:CZ	1:1:231:ASP:CA[2_555]	1.45	0.75
1:1:91:ALA:CB	1:1:141:ASP:CA[2_555]	1.46	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:130:ILE:CG2	2:2:143:ALA:C[8_556]	1.46	0.74
1:1:83:ASN:O	1:1:142:ASP:CG[2_555]	1.46	0.74
2:2:114:GLU:CG	2:2:122:ILE:CG2[8_556]	1.46	0.74
2:2:127:ALA:O	2:2:145:ILE:O[8_556]	1.46	0.74
1:1:112:ILE:N	1:1:201:LYS:CD[2_555]	1.46	0.74
2:2:113:ILE:N	2:2:124:PHE:CD1[8_556]	1.46	0.74
1:1:86:LYS:CB	1:1:132:ASN:CG[2_555]	1.46	0.74
1:1:418:THR:CB	3:3:17:LEU:CG[2_555]	1.46	0.74
2:2:59:VAL:CG2	2:2:130:ILE:CA[8_556]	1.46	0.74
2:2:59:VAL:CG1	2:2:129:THR:CB[8_556]	1.47	0.73
2:2:88:ALA:CA	2:2:126:ASP:CA[8_556]	1.47	0.73
2:2:112:PRO:CD	2:2:162:SER:N[8_556]	1.47	0.73
1:1:168:ILE:CD1	1:1:424:MET:N[3_555]	1.47	0.73
2:2:115:THR:N	2:2:123:SER:O[8_556]	1.47	0.73
2:2:108:TYR:O	2:2:164:ASN:ND2[8_556]	1.47	0.73
2:2:88:ALA:N	2:2:125:LYS:C[8_556]	1.47	0.73
2:2:8:LYS:C	2:2:89:PHE:CZ[8_556]	1.48	0.72
1:1:35:VAL:O	1:1:217:ASP:CB[2_555]	1.48	0.72
2:2:116:PHE:CE1	2:2:117:ASN:N[8_556]	1.48	0.72
1:1:81:TRP:CZ2	1:1:214:ARG:CG[2_555]	1.48	0.72
1:1:91:ALA:C	1:1:141:ASP:OD1[2_555]	1.48	0.72
2:2:113:ILE:C	2:2:124:PHE:CG[8_556]	1.48	0.72
1:1:226:THR:CA	1:1:228:TYR:OH[3_555]	1.48	0.72
1:1:70:TYR:O	1:1:219:MET:CE[2_555]	1.48	0.72
1:1:416:MET:SD	3:3:19:TYR:CE1[2_555]	1.48	0.72
2:2:108:TYR:CA	2:2:166:VAL:CA[8_556]	1.48	0.72
2:2:65:THR:CB	2:2:139:ASN:CG[8_556]	1.48	0.72
1:1:33:THR:CG2	1:1:221:GLU:CG[2_555]	1.48	0.72
2:2:64:GLU:CB	2:2:134:PRO:CA[8_556]	1.49	0.71
1:1:352:ARG:N	1:1:420:ARG:CD[3_555]	1.49	0.71
2:2:114:GLU:CA	2:2:124:PHE:CD2[8_556]	1.49	0.71
1:1:91:ALA:CA	1:1:141:ASP:CB[2_555]	1.49	0.71
1:1:417:PRO:C	3:3:17:LEU:N[2_555]	1.49	0.71
1:1:86:LYS:CD	1:1:129:ASN:CA[2_555]	1.49	0.71
2:2:66:ASN:CA	2:2:96:ALA:N[8_556]	1.49	0.71
1:1:224:GLY:O	1:1:275:PHE:CZ[3_555]	1.49	0.71
2:2:114:GLU:O	2:2:115:THR:CB[8_556]	1.49	0.71
1:1:85:MET:O	1:1:132:ASN:C[2_555]	1.49	0.71
1:1:112:ILE:CB	1:1:201:LYS:CD[2_555]	1.50	0.70
2:2:6:ILE:O	2:2:53:HIS:CG[8_556]	1.50	0.70
2:2:4:LYS:NZ	2:2:149:SER:C[8_556]	1.50	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:349:GLN:CA	1:1:423:ILE:CB[3_555]	1.50	0.70
1:1:72:PRO:O	1:1:215:TYR:CD1[2_555]	1.50	0.70
2:2:93:PHE:N	2:2:165:GLN:CG[8_556]	1.50	0.70
2:2:93:PHE:C	2:2:165:GLN:OE1[8_556]	1.50	0.70
2:2:114:GLU:OE2	2:2:122:ILE:CG2[8_556]	1.50	0.70
2:2:108:TYR:C	2:2:164:ASN:OD1[8_556]	1.51	0.69
2:2:109:ASP:CA	2:2:165:GLN:N[8_556]	1.51	0.69
1:1:224:GLY:C	1:1:275:PHE:CZ[3_555]	1.51	0.69
2:2:127:ALA:O	2:2:146:MET:N[8_556]	1.51	0.69
1:1:73:HIS:NE2	1:1:218:ILE:CG2[2_555]	1.51	0.69
1:1:349:GLN:CB	1:1:423:ILE:CG1[3_555]	1.51	0.69
1:1:89:VAL:C	1:1:140:SER:CB[2_555]	1.51	0.69
2:2:66:ASN:O	2:2:96:ALA:C[8_556]	1.51	0.69
2:2:7:SER:O	2:2:148:TRP:CH2[8_556]	1.51	0.69
1:1:34:PRO:N	1:1:212:MET:SD[2_555]	1.51	0.69
2:2:74:SER:N	2:2:91:ILE:CA[8_556]	1.51	0.69
2:2:7:SER:O	2:2:148:TRP:CZ3[8_556]	1.51	0.69
2:2:60:VAL:O	2:2:130:ILE:CA[8_556]	1.51	0.69
2:2:107:LEU:CA	2:2:168:ARG:CA[8_556]	1.51	0.69
2:2:71:HIS:N	2:2:93:PHE:CZ[8_556]	1.51	0.69
2:2:107:LEU:N	2:2:168:ARG:CA[8_556]	1.52	0.68
2:2:37:SER:N	2:2:135:ARG:NH2[8_556]	1.52	0.68
2:2:62:ILE:O	2:2:92:ARG:NH2[8_556]	1.52	0.68
2:2:127:ALA:C	2:2:145:ILE:O[8_556]	1.52	0.68
1:1:168:ILE:CD1	1:1:424:MET:C[3_555]	1.52	0.68
1:1:91:ALA:N	1:1:141:ASP:CA[2_555]	1.52	0.68
2:2:73:LEU:O	2:2:91:ILE:N[8_556]	1.53	0.67
1:1:349:GLN:NE2	1:1:419:THR:O[3_555]	1.53	0.67
2:2:110:VAL:N	2:2:164:ASN:N[8_556]	1.53	0.67
2:2:70:HIS:N	2:2:142:TYR:CE2[8_556]	1.53	0.67
1:1:85:MET:CE	1:1:214:ARG:NH1[2_555]	1.53	0.67
2:2:116:PHE:CA	2:2:116:PHE:CD2[8_556]	1.53	0.67
1:1:216:ARG:CB	1:1:279:GLU:CB[3_555]	1.53	0.67
2:2:111:TYR:CD2	2:2:163:VAL:CG1[8_556]	1.53	0.67
1:1:418:THR:CA	3:3:16:ARG:O[2_555]	1.54	0.66
2:2:116:PHE:CD1	2:2:117:ASN:N[8_556]	1.54	0.66
2:2:65:THR:CA	2:2:139:ASN:CB[8_556]	1.54	0.66
1:1:218:ILE:CG1	1:1:282:VAL:CB[3_555]	1.54	0.66
1:1:87:ASP:CB	1:1:142:ASP:C[2_555]	1.54	0.66
2:2:62:ILE:CB	2:2:92:ARG:CZ[8_556]	1.54	0.66
1:1:417:PRO:CG	3:3:18:TRP:N[2_555]	1.54	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:218:ILE:C	1:1:282:VAL:CA[3_555]	1.54	0.66
2:2:106:ALA:C	2:2:169:GLU:N[8_556]	1.54	0.66
1:1:418:THR:N	3:3:17:LEU:CB[2_555]	1.54	0.66
2:2:92:ARG:O	2:2:165:GLN:CB[8_556]	1.54	0.66
2:2:8:LYS:CE	2:2:147:LEU:CA[8_556]	1.54	0.66
1:1:88:GLY:CA	1:1:136:LYS:CB[2_555]	1.55	0.65
2:2:71:HIS:NE2	2:2:94:GLU:C[8_556]	1.55	0.65
2:2:66:ASN:CA	2:2:95:VAL:C[8_556]	1.55	0.65
2:2:69:ASN:O	2:2:142:TYR:CZ[8_556]	1.55	0.65
1:1:417:PRO:CG	3:3:18:TRP:C[2_555]	1.55	0.65
2:2:128:VAL:N	2:2:145:ILE:CA[8_556]	1.55	0.65
2:2:127:ALA:N	2:2:146:MET:N[8_556]	1.55	0.65
2:2:110:VAL:CA	2:2:164:ASN:N[8_556]	1.55	0.65
2:2:92:ARG:O	2:2:165:GLN:C[8_556]	1.56	0.64
2:2:127:ALA:N	2:2:146:MET:O[8_556]	1.56	0.64
2:2:37:SER:N	2:2:135:ARG:NH1[8_556]	1.56	0.64
1:1:168:ILE:CG1	1:1:425:THR:N[3_555]	1.56	0.64
2:2:88:ALA:CA	2:2:126:ASP:N[8_556]	1.56	0.64
2:2:6:ILE:CD1	2:2:52:THR:O[8_556]	1.56	0.64
1:1:112:ILE:CA	1:1:201:LYS:CG[2_555]	1.56	0.64
2:2:108:TYR:CD2	2:2:166:VAL:CB[8_556]	1.56	0.64
2:2:73:LEU:CA	2:2:91:ILE:CB[8_556]	1.56	0.64
1:1:222:PHE:CA	1:1:283:ILE:CG1[3_555]	1.56	0.64
2:2:108:TYR:CD2	2:2:166:VAL:CG2[8_556]	1.57	0.63
2:2:133:HIS:CE1	2:2:140:ASP:OD2[8_556]	1.57	0.63
2:2:108:TYR:CB	2:2:166:VAL:CB[8_556]	1.57	0.63
2:2:36:LEU:O	2:2:135:ARG:NE[8_556]	1.57	0.63
2:2:75:ILE:CG2	2:2:90:ALA:CB[8_556]	1.57	0.63
1:1:85:MET:O	1:1:132:ASN:O[2_555]	1.57	0.63
2:2:64:GLU:N	2:2:134:PRO:CA[8_556]	1.58	0.62
1:1:12:HIS:CD2	3:3:16:ARG:NH2[2_555]	1.58	0.62
2:2:88:ALA:CA	2:2:126:ASP:CB[8_556]	1.58	0.62
1:1:87:ASP:OD1	1:1:142:ASP:C[2_555]	1.58	0.62
1:1:91:ALA:O	1:1:141:ASP:CG[2_555]	1.58	0.62
2:2:71:HIS:CD2	2:2:93:PHE:C[8_556]	1.58	0.62
1:1:12:HIS:ND1	3:3:16:ARG:NH2[2_555]	1.58	0.62
2:2:110:VAL:C	2:2:163:VAL:C[8_556]	1.58	0.62
1:1:83:ASN:O	1:1:142:ASP:CB[2_555]	1.58	0.62
2:2:111:TYR:CG	2:2:163:VAL:CG2[8_556]	1.58	0.62
2:2:133:HIS:ND1	2:2:140:ASP:OD2[8_556]	1.58	0.62
2:2:67:PRO:CD	2:2:96:ALA:CA[8_556]	1.59	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:132:SER:OG	2:2:140:ASP:O[8_556]	1.59	0.61
1:1:220:LYS:CB	1:1:277:VAL:CG1[3_555]	1.59	0.61
1:1:70:TYR:CE1	1:1:220:LYS:N[2_555]	1.59	0.61
2:2:59:VAL:CG2	2:2:129:THR:C[8_556]	1.59	0.61
2:2:108:TYR:CG	2:2:166:VAL:CB[8_556]	1.59	0.61
1:1:349:GLN:OE1	1:1:422:SER:CA[3_555]	1.59	0.61
1:1:352:ARG:C	1:1:420:ARG:CD[3_555]	1.59	0.61
2:2:6:ILE:CG2	2:2:54:SER:CA[8_556]	1.59	0.61
1:1:86:LYS:N	1:1:132:ASN:C[2_555]	1.59	0.61
2:2:7:SER:O	2:2:148:TRP:CZ2[8_556]	1.59	0.61
1:1:421:ASP:O	3:3:18:TRP:CZ3[2_555]	1.59	0.61
2:2:72:ALA:CB	2:2:104:VAL:CG1[8_556]	1.59	0.61
1:1:233:ARG:NH1	1:1:279:GLU:OE2[3_555]	1.60	0.60
2:2:108:TYR:CA	2:2:166:VAL:N[8_556]	1.60	0.60
2:2:113:ILE:C	2:2:124:PHE:CZ[8_556]	1.60	0.60
1:1:352:ARG:CG	1:1:420:ARG:CA[3_555]	1.60	0.60
2:2:112:PRO:CD	2:2:162:SER:O[8_556]	1.60	0.60
1:1:74:ARG:NH2	1:1:230:GLY:CA[2_555]	1.60	0.60
2:2:114:GLU:CG	2:2:122:ILE:CG1[8_556]	1.60	0.60
2:2:67:PRO:C	2:2:99:VAL:CG2[8_556]	1.60	0.60
1:1:91:ALA:CA	1:1:141:ASP:N[2_555]	1.60	0.60
2:2:73:LEU:CG	2:2:91:ILE:C[8_556]	1.60	0.60
1:1:84:PHE:CA	1:1:142:ASP:CG[2_555]	1.60	0.60
1:1:84:PHE:CA	1:1:142:ASP:OD1[2_555]	1.60	0.60
2:2:65:THR:C	2:2:139:ASN:ND2[8_556]	1.60	0.60
2:2:61:ARG:O	2:2:131:ASP:OD2[8_556]	1.61	0.59
2:2:76:ALA:CA	2:2:112:PRO:CA[8_556]	1.61	0.59
1:1:150:ASN:CG	1:1:150:ASN:CG[8_556]	1.61	0.59
1:1:416:MET:CE	3:3:19:TYR:CG[2_555]	1.61	0.59
2:2:111:TYR:CB	2:2:163:VAL:CB[8_556]	1.61	0.59
2:2:74:SER:CA	2:2:90:ALA:C[8_556]	1.61	0.59
2:2:7:SER:O	2:2:148:TRP:CE2[8_556]	1.61	0.59
2:2:7:SER:CA	2:2:148:TRP:CZ2[8_556]	1.61	0.59
2:2:66:ASN:CA	2:2:95:VAL:O[8_556]	1.61	0.59
2:2:66:ASN:N	2:2:95:VAL:O[8_556]	1.62	0.58
1:1:123:LEU:CD2	1:1:208:ARG:NH2[2_555]	1.62	0.58
1:1:70:TYR:C	1:1:219:MET:SD[2_555]	1.62	0.58
1:1:224:GLY:N	1:1:237:LEU:CD1[3_555]	1.62	0.58
1:1:233:ARG:CZ	1:1:279:GLU:CG[3_555]	1.62	0.58
2:2:64:GLU:CA	2:2:134:PRO:CB[8_556]	1.62	0.58
1:1:73:HIS:ND1	1:1:214:ARG:O[2_555]	1.62	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:69:ASN:CA	2:2:142:TYR:CZ[8_556]	1.62	0.58
2:2:69:ASN:O	2:2:142:TYR:CD2[8_556]	1.62	0.58
1:1:395:GLN:C	2:2:102:THR:OG1[8_556]	1.62	0.58
1:1:349:GLN:C	1:1:423:ILE:CG1[3_555]	1.62	0.58
2:2:132:SER:OG	2:2:141:VAL:N[8_556]	1.62	0.58
2:2:62:ILE:CG2	2:2:141:VAL:CB[8_556]	1.62	0.58
2:2:7:SER:O	2:2:148:TRP:CE3[8_556]	1.62	0.58
1:1:350:TRP:C	1:1:424:MET:SD[3_555]	1.62	0.58
2:2:37:SER:C	2:2:109:ASP:CG[8_556]	1.62	0.58
1:1:90:ASN:CG	1:1:380:LYS:CD[2_555]	1.62	0.58
2:2:132:SER:OG	2:2:141:VAL:CA[8_556]	1.62	0.58
1:1:86:LYS:CE	1:1:128:LEU:C[2_555]	1.62	0.58
2:2:89:PHE:O	2:2:126:ASP:C[8_556]	1.62	0.58
2:2:71:HIS:CB	2:2:93:PHE:CD1[8_556]	1.62	0.58
1:1:352:ARG:CG	1:1:420:ARG:CB[3_555]	1.62	0.58
2:2:128:VAL:CG1	2:2:144:GLY:CA[8_556]	1.63	0.57
2:2:107:LEU:N	2:2:168:ARG:N[8_556]	1.63	0.57
2:2:67:PRO:N	2:2:96:ALA:N[8_556]	1.63	0.57
1:1:86:LYS:CA	1:1:132:ASN:N[2_555]	1.63	0.57
2:2:74:SER:CB	2:2:89:PHE:CD1[8_556]	1.63	0.57
2:2:110:VAL:C	2:2:164:ASN:N[8_556]	1.63	0.57
2:2:74:SER:N	2:2:90:ALA:O[8_556]	1.63	0.57
1:1:73:HIS:CB	1:1:215:TYR:N[2_555]	1.63	0.57
1:1:74:ARG:NH1	1:1:231:ASP:N[2_555]	1.63	0.57
2:2:112:PRO:CD	2:2:162:SER:CA[8_556]	1.63	0.57
2:2:67:PRO:O	2:2:99:VAL:CA[8_556]	1.63	0.57
2:2:133:HIS:NE2	2:2:140:ASP:OD2[8_556]	1.63	0.57
2:2:116:PHE:CE1	2:2:117:ASN:CA[8_556]	1.63	0.57
1:1:112:ILE:C	1:1:201:LYS:CD[2_555]	1.64	0.56
2:2:71:HIS:CB	2:2:93:PHE:CG[8_556]	1.64	0.56
2:2:111:TYR:CE1	2:2:163:VAL:CG1[8_556]	1.64	0.56
1:1:218:ILE:CG1	1:1:282:VAL:N[3_555]	1.64	0.56
1:1:216:ARG:CA	1:1:280:HIS:O[3_555]	1.64	0.56
1:1:219:MET:N	1:1:281:GLY:C[3_555]	1.64	0.56
1:1:32:TRP:CH2	1:1:204:THR:CA[2_555]	1.64	0.56
2:2:61:ARG:CA	2:2:131:ASP:OD1[8_556]	1.64	0.56
2:2:6:ILE:CG2	2:2:53:HIS:O[8_556]	1.64	0.56
1:1:84:PHE:C	1:1:136:LYS:NZ[2_555]	1.64	0.56
1:1:112:ILE:CA	1:1:201:LYS:CE[2_555]	1.64	0.56
2:2:76:ALA:C	2:2:112:PRO:CA[8_556]	1.64	0.56
1:1:12:HIS:NE2	3:3:16:ARG:NE[2_555]	1.64	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:132:SER:OG	2:2:140:ASP:C[8_556]	1.65	0.55
1:1:35:VAL:CG1	1:1:221:GLU:CA[2_555]	1.65	0.55
2:2:37:SER:CA	2:2:109:ASP:OD2[8_556]	1.65	0.55
1:1:35:VAL:O	1:1:217:ASP:CA[2_555]	1.65	0.55
2:2:107:LEU:O	2:2:166:VAL:C[8_556]	1.65	0.55
1:1:352:ARG:O	1:1:420:ARG:NE[3_555]	1.65	0.55
2:2:7:SER:O	2:2:148:TRP:CD2[8_556]	1.65	0.55
2:2:116:PHE:N	2:2:116:PHE:N[8_556]	1.65	0.55
2:2:66:ASN:C	2:2:95:VAL:C[8_556]	1.65	0.55
2:2:67:PRO:N	2:2:96:ALA:C[8_556]	1.65	0.55
1:1:216:ARG:CD	1:1:279:GLU:CB[3_555]	1.65	0.55
2:2:107:LEU:CA	2:2:167:ASN:C[8_556]	1.65	0.55
2:2:63:ASP:CB	2:2:94:GLU:OE2[8_556]	1.65	0.55
1:1:122:PHE:CE1	1:1:208:ARG:NH1[2_555]	1.65	0.55
1:1:71:ILE:CA	1:1:219:MET:CE[2_555]	1.65	0.55
2:2:132:SER:C	2:2:141:VAL:N[8_556]	1.66	0.54
1:1:34:PRO:C	1:1:212:MET:CG[2_555]	1.66	0.54
1:1:227:SER:OG	1:1:229:ASP:CG[3_555]	1.66	0.54
1:1:91:ALA:CB	1:1:141:ASP:C[2_555]	1.66	0.54
1:1:168:ILE:CB	1:1:424:MET:O[3_555]	1.66	0.54
2:2:108:TYR:N	2:2:167:ASN:N[8_556]	1.66	0.54
1:1:222:PHE:CB	1:1:283:ILE:CG2[3_555]	1.66	0.54
1:1:216:ARG:C	1:1:279:GLU:O[3_555]	1.66	0.54
1:1:83:ASN:O	1:1:142:ASP:OD1[2_555]	1.66	0.54
1:1:217:ASP:C	1:1:281:GLY:O[3_555]	1.66	0.54
2:2:37:SER:CA	2:2:135:ARG:NH2[8_556]	1.66	0.54
1:1:417:PRO:CG	3:3:18:TRP:CA[2_555]	1.66	0.54
1:1:74:ARG:NE	1:1:231:ASP:CB[2_555]	1.66	0.54
1:1:73:HIS:CG	1:1:215:TYR:CA[2_555]	1.66	0.54
2:2:87:ILE:CD1	2:2:125:LYS:CB[8_556]	1.66	0.54
2:2:6:ILE:O	2:2:53:HIS:CB[8_556]	1.67	0.53
1:1:72:PRO:N	1:1:215:TYR:CE2[2_555]	1.67	0.53
1:1:168:ILE:CB	1:1:424:MET:C[3_555]	1.67	0.53
1:1:32:TRP:CZ2	1:1:204:THR:OG1[2_555]	1.67	0.53
2:2:62:ILE:O	2:2:133:HIS:O[8_556]	1.67	0.53
1:1:87:ASP:N	1:1:132:ASN:CG[2_555]	1.67	0.53
2:2:107:LEU:CG	2:2:168:ARG:CG[8_556]	1.67	0.53
2:2:111:TYR:N	2:2:163:VAL:CA[8_556]	1.67	0.53
2:2:87:ILE:O	2:2:125:LYS:O[8_556]	1.67	0.53
2:2:7:SER:C	2:2:148:TRP:NE1[8_556]	1.67	0.53
2:2:36:LEU:CD1	2:2:135:ARG:CD[8_556]	1.67	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:72:PRO:O	1:1:215:TYR:CE2[2_555]	1.67	0.53
2:2:8:LYS:O	2:2:89:PHE:CE1[8_556]	1.68	0.52
1:1:395:GLN:O	2:2:102:THR:CG2[8_556]	1.68	0.52
1:1:32:TRP:CZ2	1:1:204:THR:CA[2_555]	1.68	0.52
1:1:92:SER:N	1:1:141:ASP:OD1[2_555]	1.68	0.52
1:1:349:GLN:N	1:1:423:ILE:CG1[3_555]	1.68	0.52
1:1:33:THR:CB	1:1:221:GLU:CG[2_555]	1.68	0.52
2:2:6:ILE:C	2:2:53:HIS:O[8_556]	1.68	0.52
1:1:222:PHE:CD1	1:1:284:MET:CA[3_555]	1.68	0.52
2:2:107:LEU:C	2:2:168:ARG:N[8_556]	1.68	0.52
2:2:37:SER:CB	2:2:109:ASP:OD2[8_556]	1.68	0.52
2:2:8:LYS:N	2:2:148:TRP:CD1[8_556]	1.68	0.52
2:2:9:HIS:N	2:2:89:PHE:CE2[8_556]	1.68	0.52
2:2:59:VAL:C	2:2:129:THR:C[8_556]	1.68	0.52
2:2:64:GLU:OE2	2:2:134:PRO:CD[8_556]	1.68	0.52
1:1:221:GLU:C	1:1:283:ILE:CD1[3_555]	1.68	0.52
1:1:32:TRP:CE2	1:1:204:THR:CB[2_555]	1.68	0.52
2:2:128:VAL:CG2	2:2:145:ILE:CB[8_556]	1.69	0.51
1:1:92:SER:CA	1:1:141:ASP:OD1[2_555]	1.69	0.51
2:2:9:HIS:CD2	2:2:110:VAL:CB[8_556]	1.69	0.51
2:2:133:HIS:CG	2:2:140:ASP:OD2[8_556]	1.69	0.51
1:1:86:LYS:NZ	1:1:129:ASN:ND2[2_555]	1.69	0.51
2:2:66:ASN:CA	2:2:96:ALA:CA[8_556]	1.69	0.51
2:2:110:VAL:O	2:2:163:VAL:CA[8_556]	1.69	0.51
2:2:111:TYR:CA	2:2:163:VAL:CA[8_556]	1.69	0.51
1:1:32:TRP:CH2	1:1:204:THR:O[2_555]	1.69	0.51
2:2:141:VAL:CG2	2:2:141:VAL:CG2[8_556]	1.69	0.51
2:2:89:PHE:C	2:2:126:ASP:O[8_556]	1.69	0.51
2:2:113:ILE:CB	2:2:124:PHE:CE1[8_556]	1.69	0.51
1:1:351:TYR:C	1:1:420:ARG:CG[3_555]	1.69	0.51
2:2:74:SER:O	2:2:90:ALA:O[8_556]	1.69	0.51
2:2:37:SER:N	2:2:135:ARG:CZ[8_556]	1.70	0.50
2:2:62:ILE:N	2:2:92:ARG:NE[8_556]	1.70	0.50
1:1:32:TRP:CH2	1:1:204:THR:C[2_555]	1.70	0.50
2:2:110:VAL:C	2:2:163:VAL:CA[8_556]	1.70	0.50
1:1:168:ILE:CG2	1:1:425:THR:N[3_555]	1.70	0.50
1:1:89:VAL:CG2	1:1:137:PRO:CG[2_555]	1.70	0.50
1:1:216:ARG:C	1:1:280:HIS:C[3_555]	1.70	0.50
2:2:108:TYR:CA	2:2:165:GLN:C[8_556]	1.70	0.50
2:2:65:THR:CG2	2:2:136:THR:CA[8_556]	1.70	0.50
2:2:88:ALA:CB	2:2:126:ASP:CG[8_556]	1.70	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:39:ASP:O	1:1:220:LYS:CD[2_555]	1.70	0.50
2:2:62:ILE:C	2:2:92:ARG:CZ[8_556]	1.70	0.50
2:2:71:HIS:CD2	2:2:93:PHE:O[8_556]	1.70	0.50
1:1:34:PRO:CG	1:1:212:MET:CE[2_555]	1.70	0.50
1:1:89:VAL:CA	1:1:140:SER:OG[2_555]	1.70	0.50
2:2:71:HIS:ND1	2:2:93:PHE:CD1[8_556]	1.71	0.49
1:1:216:ARG:CG	1:1:279:GLU:C[3_555]	1.71	0.49
1:1:349:GLN:CB	1:1:423:ILE:CG2[3_555]	1.71	0.49
2:2:71:HIS:C	2:2:93:PHE:CZ[8_556]	1.71	0.49
1:1:36:VAL:C	1:1:217:ASP:OD1[2_555]	1.71	0.49
2:2:68:THR:CA	2:2:95:VAL:CG2[8_556]	1.71	0.49
1:1:157:LYS:NZ	2:2:138:GLY:CA[8_556]	1.71	0.49
1:1:222:PHE:O	1:1:283:ILE:CG2[3_555]	1.71	0.49
2:2:116:PHE:CA	2:2:116:PHE:CD1[8_556]	1.71	0.49
2:2:69:ASN:C	2:2:142:TYR:OH[8_556]	1.71	0.49
1:1:87:ASP:CA	1:1:132:ASN:ND2[2_555]	1.71	0.49
2:2:64:GLU:CA	2:2:134:PRO:CA[8_556]	1.72	0.48
2:2:6:ILE:O	2:2:53:HIS:CD2[8_556]	1.72	0.48
2:2:64:GLU:OE1	2:2:134:PRO:CG[8_556]	1.72	0.48
1:1:84:PHE:N	1:1:142:ASP:OD1[2_555]	1.72	0.48
2:2:133:HIS:CD2	2:2:140:ASP:OD2[8_556]	1.72	0.48
1:1:218:ILE:C	1:1:281:GLY:O[3_555]	1.72	0.48
2:2:128:VAL:CG2	2:2:145:ILE:N[8_556]	1.73	0.47
2:2:108:TYR:CA	2:2:165:GLN:O[8_556]	1.73	0.47
1:1:417:PRO:CD	3:3:18:TRP:O[2_555]	1.73	0.47
1:1:92:SER:N	1:1:141:ASP:CB[2_555]	1.73	0.47
2:2:65:THR:CG2	2:2:139:ASN:OD1[8_556]	1.73	0.47
2:2:74:SER:N	2:2:91:ILE:N[8_556]	1.73	0.47
2:2:6:ILE:CB	2:2:54:SER:N[8_556]	1.73	0.47
2:2:126:ASP:C	2:2:146:MET:O[8_556]	1.73	0.47
2:2:8:LYS:NZ	2:2:147:LEU:C[8_556]	1.73	0.47
2:2:58:HIS:N	2:2:129:THR:CG2[8_556]	1.73	0.47
2:2:64:GLU:CD	2:2:134:PRO:N[8_556]	1.73	0.47
2:2:7:SER:C	2:2:148:TRP:CZ2[8_556]	1.73	0.47
1:1:168:ILE:CD1	1:1:425:THR:N[3_555]	1.73	0.47
1:1:225:HIS:N	1:1:275:PHE:CZ[3_555]	1.74	0.46
2:2:110:VAL:O	2:2:163:VAL:O[8_556]	1.74	0.46
2:2:37:SER:O	2:2:109:ASP:OD2[8_556]	1.74	0.46
2:2:94:GLU:N	2:2:165:GLN:OE1[8_556]	1.74	0.46
2:2:93:PHE:CA	2:2:165:GLN:OE1[8_556]	1.74	0.46
2:2:70:HIS:O	2:2:101:PRO:CG[8_556]	1.74	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:352:ARG:CD	1:1:420:ARG:N[3_555]	1.74	0.46
1:1:231:ASP:OD1	1:1:279:GLU:CD[3_555]	1.74	0.46
2:2:116:PHE:CZ	2:2:117:ASN:N[8_556]	1.74	0.46
1:1:34:PRO:CB	1:1:212:MET:CG[2_555]	1.74	0.46
1:1:219:MET:N	1:1:282:VAL:N[3_555]	1.75	0.45
2:2:6:ILE:N	2:2:53:HIS:CB[8_556]	1.75	0.45
2:2:65:THR:O	2:2:139:ASN:CG[8_556]	1.75	0.45
1:1:421:ASP:CB	3:3:17:LEU:CD1[2_555]	1.75	0.45
2:2:61:ARG:CB	2:2:131:ASP:CG[8_556]	1.75	0.45
2:2:63:ASP:CG	2:2:94:GLU:CD[8_556]	1.75	0.45
2:2:112:PRO:CG	2:2:162:SER:N[8_556]	1.75	0.45
1:1:217:ASP:CA	1:1:281:GLY:N[3_555]	1.75	0.45
2:2:111:TYR:CA	2:2:162:SER:C[8_556]	1.75	0.45
1:1:86:LYS:CE	1:1:129:ASN:N[2_555]	1.75	0.45
2:2:88:ALA:C	2:2:125:LYS:C[8_556]	1.75	0.45
2:2:8:LYS:CD	2:2:147:LEU:C[8_556]	1.75	0.45
2:2:112:PRO:CD	2:2:162:SER:C[8_556]	1.75	0.45
2:2:69:ASN:C	2:2:142:TYR:CE1[8_556]	1.76	0.44
2:2:9:HIS:NE2	2:2:110:VAL:CB[8_556]	1.76	0.44
1:1:73:HIS:N	1:1:215:TYR:CA[2_555]	1.76	0.44
2:2:71:HIS:ND1	2:2:93:PHE:CE1[8_556]	1.76	0.44
1:1:352:ARG:NE	1:1:419:THR:CG2[3_555]	1.76	0.44
2:2:128:VAL:CG2	2:2:145:ILE:CA[8_556]	1.76	0.44
1:1:86:LYS:CB	1:1:132:ASN:OD1[2_555]	1.76	0.44
1:1:352:ARG:NH2	1:1:419:THR:CG2[3_555]	1.76	0.44
1:1:218:ILE:N	1:1:281:GLY:CA[3_555]	1.76	0.44
1:1:92:SER:CA	1:1:141:ASP:CG[2_555]	1.76	0.44
2:2:70:HIS:CA	2:2:101:PRO:CG[8_556]	1.76	0.44
2:2:128:VAL:CA	2:2:145:ILE:CA[8_556]	1.76	0.44
2:2:107:LEU:C	2:2:167:ASN:CA[8_556]	1.76	0.44
1:1:35:VAL:O	1:1:217:ASP:C[2_555]	1.76	0.44
1:1:73:HIS:CB	1:1:215:TYR:CB[2_555]	1.76	0.44
2:2:8:LYS:CG	2:2:148:TRP:N[8_556]	1.76	0.44
2:2:73:LEU:CA	2:2:91:ILE:CG1[8_556]	1.76	0.44
1:1:122:PHE:CZ	1:1:208:ARG:CD[2_555]	1.76	0.44
1:1:86:LYS:CA	1:1:132:ASN:CG[2_555]	1.76	0.44
2:2:34:PRO:CG	2:2:70:HIS:ND1[8_556]	1.76	0.44
2:2:74:SER:C	2:2:90:ALA:C[8_556]	1.76	0.44
2:2:116:PHE:CB	2:2:116:PHE:CG[8_556]	1.77	0.43
1:1:83:ASN:C	1:1:142:ASP:OD1[2_555]	1.77	0.43
2:2:92:ARG:O	2:2:165:GLN:CG[8_556]	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:128:VAL:CA	2:2:144:GLY:C[8_556]	1.77	0.43
2:2:71:HIS:CE1	2:2:95:VAL:N[8_556]	1.77	0.43
1:1:39:ASP:N	1:1:220:LYS:NZ[2_555]	1.77	0.43
1:1:220:LYS:CG	1:1:277:VAL:CB[3_555]	1.77	0.43
1:1:70:TYR:CD1	1:1:219:MET:C[2_555]	1.77	0.43
2:2:71:HIS:CD2	2:2:94:GLU:N[8_556]	1.77	0.43
2:2:74:SER:N	2:2:90:ALA:C[8_556]	1.77	0.43
1:1:85:MET:CB	1:1:132:ASN:O[2_555]	1.77	0.43
2:2:62:ILE:N	2:2:131:ASP:OD1[8_556]	1.77	0.43
2:2:114:GLU:N	2:2:124:PHE:CG[8_556]	1.77	0.43
2:2:87:ILE:CG1	2:2:125:LYS:CG[8_556]	1.77	0.43
2:2:61:ARG:N	2:2:131:ASP:N[8_556]	1.78	0.42
1:1:416:MET:CE	3:3:19:TYR:CE2[2_555]	1.78	0.42
2:2:114:GLU:CG	2:2:122:ILE:CB[8_556]	1.78	0.42
2:2:127:ALA:CA	2:2:146:MET:CB[8_556]	1.78	0.42
2:2:7:SER:N	2:2:148:TRP:CE2[8_556]	1.78	0.42
2:2:62:ILE:CB	2:2:92:ARG:NH2[8_556]	1.78	0.42
1:1:218:ILE:N	1:1:281:GLY:N[3_555]	1.78	0.42
1:1:168:ILE:CB	1:1:425:THR:N[3_555]	1.78	0.42
1:1:218:ILE:O	1:1:283:ILE:N[3_555]	1.78	0.42
1:1:34:PRO:C	1:1:212:MET:SD[2_555]	1.78	0.42
2:2:63:ASP:C	2:2:94:GLU:CD[8_556]	1.78	0.42
2:2:70:HIS:N	2:2:101:PRO:CD[8_556]	1.78	0.42
1:1:87:ASP:CG	1:1:142:ASP:CA[2_555]	1.78	0.42
1:1:73:HIS:CB	1:1:215:TYR:CA[2_555]	1.78	0.42
2:2:106:ALA:O	2:2:169:GLU:CA[8_556]	1.78	0.42
1:1:12:HIS:CE1	3:3:16:ARG:NH1[2_555]	1.79	0.41
2:2:109:ASP:CA	2:2:164:ASN:CA[8_556]	1.79	0.41
1:1:72:PRO:O	1:1:215:TYR:CE1[2_555]	1.79	0.41
1:1:333:PHE:CE1	1:1:425:THR:CB[3_555]	1.79	0.41
2:2:130:ILE:CB	2:2:143:ALA:C[8_556]	1.79	0.41
2:2:69:ASN:ND2	2:2:142:TYR:CE1[8_556]	1.79	0.41
1:1:346:ALA:O	1:1:423:ILE:CG2[3_555]	1.79	0.41
2:2:66:ASN:C	2:2:96:ALA:O[8_556]	1.79	0.41
1:1:349:GLN:CA	1:1:423:ILE:CD1[3_555]	1.79	0.41
2:2:74:SER:CA	2:2:91:ILE:CG2[8_556]	1.79	0.41
2:2:73:LEU:CD1	2:2:91:ILE:C[8_556]	1.79	0.41
1:1:419:THR:N	3:3:17:LEU:CD2[2_555]	1.79	0.41
1:1:72:PRO:C	1:1:215:TYR:CD1[2_555]	1.79	0.41
1:1:353:THR:N	1:1:420:ARG:CD[3_555]	1.79	0.41
1:1:86:LYS:C	1:1:132:ASN:CG[2_555]	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:218:ILE:CA	1:1:282:VAL:N[3_555]	1.79	0.41
1:1:70:TYR:OH	1:1:216:ARG:O[2_555]	1.79	0.41
2:2:64:GLU:CG	2:2:134:PRO:CG[8_556]	1.80	0.40
1:1:220:LYS:CB	1:1:277:VAL:CB[3_555]	1.80	0.40
2:2:34:PRO:CG	2:2:70:HIS:CG[8_556]	1.80	0.40
2:2:73:LEU:C	2:2:91:ILE:CG1[8_556]	1.80	0.40
1:1:150:ASN:CG	1:1:150:ASN:OD1[8_556]	1.80	0.40
1:1:168:ILE:CG1	1:1:424:MET:C[3_555]	1.80	0.40
2:2:88:ALA:C	2:2:126:ASP:CA[8_556]	1.80	0.40
2:2:68:THR:O	2:2:95:VAL:CB[8_556]	1.80	0.40
2:2:88:ALA:CA	2:2:125:LYS:C[8_556]	1.80	0.40
2:2:108:TYR:CG	2:2:166:VAL:CA[8_556]	1.80	0.40
2:2:36:LEU:CG	2:2:135:ARG:CD[8_556]	1.80	0.40
2:2:75:ILE:O	2:2:89:PHE:CA[8_556]	1.80	0.40
1:1:418:THR:CA	3:3:16:ARG:C[2_555]	1.80	0.40
2:2:110:VAL:O	2:2:163:VAL:N[8_556]	1.80	0.40
2:2:61:ARG:CG	2:2:69:ASN:ND2[8_556]	1.80	0.40
2:2:64:GLU:CG	2:2:134:PRO:CA[8_556]	1.80	0.40
1:1:231:ASP:CG	1:1:279:GLU:CD[3_555]	1.81	0.39
2:2:92:ARG:NH1	2:2:165:GLN:NE2[8_556]	1.81	0.39
2:2:127:ALA:C	2:2:145:ILE:CA[8_556]	1.81	0.39
1:1:352:ARG:CA	1:1:420:ARG:NE[3_555]	1.81	0.39
1:1:353:THR:CB	1:1:424:MET:CB[3_555]	1.81	0.39
2:2:74:SER:OG	2:2:110:VAL:CG1[8_556]	1.81	0.39
1:1:416:MET:CB	3:3:16:ARG:CB[2_555]	1.81	0.39
1:1:421:ASP:O	3:3:18:TRP:CZ2[2_555]	1.81	0.39
1:1:222:PHE:CZ	1:1:284:MET:CA[3_555]	1.81	0.39
2:2:64:GLU:OE2	2:2:133:HIS:CB[8_556]	1.81	0.39
2:2:128:VAL:N	2:2:145:ILE:O[8_556]	1.81	0.39
2:2:111:TYR:CG	2:2:163:VAL:CA[8_556]	1.82	0.38
2:2:65:THR:N	2:2:139:ASN:CG[8_556]	1.82	0.38
2:2:113:ILE:C	2:2:124:PHE:CD1[8_556]	1.82	0.38
2:2:107:LEU:CB	2:2:168:ARG:CA[8_556]	1.82	0.38
1:1:216:ARG:CG	1:1:279:GLU:CB[3_555]	1.82	0.38
1:1:217:ASP:OD2	1:1:280:HIS:NE2[3_555]	1.82	0.38
1:1:218:ILE:CG1	1:1:282:VAL:CA[3_555]	1.82	0.38
2:2:113:ILE:CG1	2:2:124:PHE:CD1[8_556]	1.82	0.38
1:1:83:ASN:C	1:1:142:ASP:CB[2_555]	1.82	0.38
1:1:416:MET:CB	3:3:16:ARG:CD[2_555]	1.82	0.38
2:2:63:ASP:OD1	2:2:94:GLU:OE2[8_556]	1.82	0.38
2:2:127:ALA:N	2:2:146:MET:C[8_556]	1.82	0.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:35:VAL:CB	1:1:217:ASP:O[2_555]	1.82	0.38
2:2:65:THR:CB	2:2:139:ASN:ND2[8_556]	1.82	0.38
2:2:37:SER:C	2:2:109:ASP:OD2[8_556]	1.82	0.38
1:1:227:SER:CB	1:1:229:ASP:OD2[3_555]	1.82	0.38
1:1:87:ASP:OD1	1:1:143:LEU:C[2_555]	1.82	0.38
1:1:86:LYS:C	1:1:132:ASN:CA[2_555]	1.82	0.38
1:1:73:HIS:CE1	1:1:214:ARG:O[2_555]	1.83	0.37
1:1:88:GLY:CA	1:1:136:LYS:CD[2_555]	1.83	0.37
1:1:219:MET:O	1:1:283:ILE:CG1[3_555]	1.83	0.37
1:1:220:LYS:CD	1:1:277:VAL:CB[3_555]	1.83	0.37
1:1:355:PRO:CB	1:1:426:SER:C[3_555]	1.83	0.37
2:2:6:ILE:CA	2:2:53:HIS:C[8_556]	1.83	0.37
2:2:67:PRO:O	2:2:99:VAL:CG1[8_556]	1.83	0.37
2:2:107:LEU:O	2:2:167:ASN:C[8_556]	1.83	0.37
2:2:70:HIS:O	2:2:101:PRO:CB[8_556]	1.83	0.37
2:2:64:GLU:OE2	2:2:133:HIS:CA[8_556]	1.83	0.37
2:2:69:ASN:O	2:2:142:TYR:CE1[8_556]	1.83	0.37
2:2:128:VAL:N	2:2:145:ILE:N[8_556]	1.83	0.37
1:1:85:MET:C	1:1:132:ASN:CA[2_555]	1.83	0.37
2:2:8:LYS:N	2:2:148:TRP:CE2[8_556]	1.84	0.36
1:1:395:GLN:O	2:2:102:THR:OG1[8_556]	1.84	0.36
2:2:66:ASN:CB	2:2:96:ALA:N[8_556]	1.84	0.36
2:2:109:ASP:CB	2:2:165:GLN:N[8_556]	1.84	0.36
2:2:66:ASN:CB	2:2:95:VAL:CA[8_556]	1.84	0.36
2:2:61:ARG:CA	2:2:131:ASP:N[8_556]	1.84	0.36
1:1:349:GLN:CG	1:1:423:ILE:C[3_555]	1.84	0.36
2:2:58:HIS:CA	2:2:129:THR:CG2[8_556]	1.84	0.36
1:1:88:GLY:O	1:1:140:SER:CB[2_555]	1.84	0.36
1:1:150:ASN:CB	1:1:150:ASN:CG[8_556]	1.84	0.36
1:1:333:PHE:CE1	1:1:425:THR:OG1[3_555]	1.84	0.36
1:1:418:THR:CA	3:3:17:LEU:CA[2_555]	1.84	0.36
2:2:116:PHE:C	2:2:116:PHE:CD2[8_556]	1.84	0.36
1:1:86:LYS:N	1:1:132:ASN:O[2_555]	1.84	0.36
2:2:111:TYR:CD1	2:2:163:VAL:CB[8_556]	1.84	0.36
1:1:220:LYS:CD	1:1:277:VAL:CG2[3_555]	1.84	0.36
1:1:34:PRO:CA	1:1:212:MET:CG[2_555]	1.85	0.35
2:2:59:VAL:N	2:2:129:THR:O[8_556]	1.85	0.35
2:2:127:ALA:CB	2:2:146:MET:CG[8_556]	1.85	0.35
2:2:70:HIS:N	2:2:101:PRO:CG[8_556]	1.85	0.35
2:2:133:HIS:CD2	2:2:140:ASP:CA[8_556]	1.85	0.35
2:2:71:HIS:C	2:2:93:PHE:CD2[8_556]	1.85	0.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:61:ARG:N	2:2:131:ASP:CG[8_556]	1.85	0.35
1:1:224:GLY:C	1:1:275:PHE:CE2[3_555]	1.85	0.35
1:1:349:GLN:OE1	1:1:421:ASP:C[3_555]	1.85	0.35
2:2:63:ASP:O	2:2:94:GLU:CB[8_556]	1.85	0.35
2:2:64:GLU:CD	2:2:134:PRO:CG[8_556]	1.86	0.34
1:1:12:HIS:CE1	3:3:19:TYR:OH[2_555]	1.86	0.34
1:1:352:ARG:CB	1:1:420:ARG:CG[3_555]	1.86	0.34
1:1:112:ILE:CB	1:1:201:LYS:CG[2_555]	1.86	0.34
2:2:107:LEU:N	2:2:168:ARG:C[8_556]	1.86	0.34
1:1:150:ASN:CB	1:1:150:ASN:ND2[8_556]	1.86	0.34
2:2:66:ASN:O	2:2:95:VAL:C[8_556]	1.86	0.34
1:1:72:PRO:CA	1:1:215:TYR:CE2[2_555]	1.86	0.34
1:1:222:PHE:CE1	1:1:283:ILE:C[3_555]	1.86	0.34
2:2:132:SER:C	2:2:141:VAL:O[8_556]	1.86	0.34
2:2:59:VAL:CG1	2:2:129:THR:C[8_556]	1.86	0.34
2:2:113:ILE:CB	2:2:124:PHE:CD1[8_556]	1.86	0.34
1:1:418:THR:CA	3:3:17:LEU:CD2[2_555]	1.86	0.34
1:1:418:THR:N	3:3:16:ARG:C[2_555]	1.86	0.34
1:1:216:ARG:CD	1:1:279:GLU:CA[3_555]	1.86	0.34
1:1:351:TYR:C	1:1:420:ARG:CD[3_555]	1.86	0.34
2:2:59:VAL:CA	2:2:129:THR:CA[8_556]	1.86	0.34
2:2:127:ALA:N	2:2:146:MET:CA[8_556]	1.86	0.34
2:2:133:HIS:CG	2:2:140:ASP:OD1[8_556]	1.86	0.34
2:2:87:ILE:CA	2:2:125:LYS:O[8_556]	1.87	0.33
2:2:113:ILE:C	2:2:124:PHE:CE1[8_556]	1.87	0.33
1:1:92:SER:C	1:1:141:ASP:OD1[2_555]	1.87	0.33
2:2:109:ASP:CA	2:2:164:ASN:CB[8_556]	1.87	0.33
1:1:122:PHE:CD1	1:1:218:ILE:CD1[2_555]	1.87	0.33
1:1:88:GLY:CA	1:1:136:LYS:CG[2_555]	1.87	0.33
2:2:130:ILE:CA	2:2:143:ALA:O[8_556]	1.87	0.33
1:1:84:PHE:CA	1:1:142:ASP:OD2[2_555]	1.87	0.33
1:1:88:GLY:N	1:1:136:LYS:CD[2_555]	1.87	0.33
1:1:72:PRO:O	1:1:215:TYR:CZ[2_555]	1.87	0.33
1:1:418:THR:CA	3:3:17:LEU:CG[2_555]	1.87	0.33
2:2:4:LYS:NZ	2:2:150:ASN:C[8_556]	1.87	0.33
2:2:111:TYR:CA	2:2:163:VAL:N[8_556]	1.88	0.32
2:2:116:PHE:C	2:2:116:PHE:CZ[8_556]	1.88	0.32
2:2:7:SER:CB	2:2:148:TRP:NE1[8_556]	1.88	0.32
2:2:74:SER:CB	2:2:91:ILE:CG2[8_556]	1.88	0.32
1:1:352:ARG:NE	1:1:419:THR:C[3_555]	1.88	0.32
2:2:36:LEU:C	2:2:135:ARG:NH1[8_556]	1.88	0.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:89:VAL:N	1:1:140:SER:CB[2_555]	1.88	0.32
2:2:109:ASP:CA	2:2:164:ASN:C[8_556]	1.88	0.32
2:2:73:LEU:CA	2:2:91:ILE:O[8_556]	1.88	0.32
2:2:109:ASP:O	2:2:164:ASN:CA[8_556]	1.88	0.32
2:2:60:VAL:N	2:2:129:THR:O[8_556]	1.88	0.32
1:1:71:ILE:CA	1:1:219:MET:SD[2_555]	1.88	0.32
1:1:417:PRO:CB	3:3:18:TRP:CA[2_555]	1.88	0.32
1:1:416:MET:CE	3:3:19:TYR:CD2[2_555]	1.89	0.31
1:1:418:THR:O	3:3:17:LEU:CA[2_555]	1.89	0.31
2:2:70:HIS:N	2:2:142:TYR:CE1[8_556]	1.89	0.31
1:1:89:VAL:CB	1:1:137:PRO:CG[2_555]	1.89	0.31
2:2:6:ILE:CB	2:2:53:HIS:CA[8_556]	1.89	0.31
2:2:69:ASN:CA	2:2:142:TYR:CE2[8_556]	1.89	0.31
2:2:116:PHE:N	2:2:116:PHE:CD2[8_556]	1.89	0.31
2:2:109:ASP:N	2:2:165:GLN:C[8_556]	1.89	0.31
1:1:86:LYS:CD	1:1:129:ASN:N[2_555]	1.89	0.31
1:1:349:GLN:O	1:1:420:ARG:O[3_555]	1.89	0.31
1:1:32:TRP:CH2	1:1:204:THR:CB[2_555]	1.89	0.31
2:2:59:VAL:N	2:2:129:THR:N[8_556]	1.89	0.31
2:2:65:THR:CB	2:2:136:THR:O[8_556]	1.89	0.31
2:2:133:HIS:NE2	2:2:140:ASP:CG[8_556]	1.89	0.31
2:2:69:ASN:O	2:2:142:TYR:CG[8_556]	1.89	0.31
1:1:35:VAL:CG1	1:1:221:GLU:CB[2_555]	1.89	0.31
1:1:418:THR:CG2	3:3:17:LEU:CD2[2_555]	1.90	0.30
2:2:66:ASN:O	2:2:95:VAL:O[8_556]	1.90	0.30
2:2:61:ARG:CB	2:2:131:ASP:CA[8_556]	1.90	0.30
2:2:109:ASP:N	2:2:164:ASN:CG[8_556]	1.90	0.30
2:2:73:LEU:CD1	2:2:92:ARG:N[8_556]	1.90	0.30
2:2:34:PRO:CG	2:2:70:HIS:CE1[8_556]	1.90	0.30
1:1:71:ILE:CG1	1:1:215:TYR:CE1[2_555]	1.90	0.30
2:2:73:LEU:O	2:2:144:GLY:O[8_556]	1.90	0.30
1:1:90:ASN:CB	1:1:380:LYS:NZ[2_555]	1.90	0.30
1:1:40:SER:N	1:1:220:LYS:NZ[2_555]	1.90	0.30
1:1:223:GLY:N	1:1:283:ILE:CD1[3_555]	1.90	0.30
2:2:4:LYS:CD	2:2:150:ASN:CA[8_556]	1.90	0.30
1:1:226:THR:N	1:1:228:TYR:OH[3_555]	1.91	0.29
2:2:76:ALA:N	2:2:112:PRO:N[8_556]	1.91	0.29
2:2:132:SER:CA	2:2:142:TYR:N[8_556]	1.91	0.29
1:1:85:MET:CE	1:1:214:ARG:NE[2_555]	1.91	0.29
2:2:68:THR:N	2:2:95:VAL:CG2[8_556]	1.91	0.29
2:2:89:PHE:N	2:2:126:ASP:CA[8_556]	1.91	0.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:333:PHE:CD1	1:1:425:THR:CB[3_555]	1.91	0.29
1:1:87:ASP:CB	1:1:143:LEU:N[2_555]	1.91	0.29
1:1:84:PHE:O	1:1:136:LYS:CE[2_555]	1.91	0.29
2:2:106:ALA:C	2:2:168:ARG:CA[8_556]	1.91	0.29
2:2:67:PRO:CA	2:2:99:VAL:CG2[8_556]	1.91	0.29
1:1:222:PHE:CE1	1:1:284:MET:C[3_555]	1.91	0.29
1:1:216:ARG:CG	1:1:279:GLU:CA[3_555]	1.91	0.29
2:2:113:ILE:O	2:2:124:PHE:CD2[8_556]	1.91	0.29
2:2:63:ASP:N	2:2:92:ARG:NH2[8_556]	1.91	0.29
2:2:88:ALA:CA	2:2:125:LYS:O[8_556]	1.92	0.28
2:2:59:VAL:N	2:2:129:THR:CA[8_556]	1.92	0.28
2:2:63:ASP:CG	2:2:94:GLU:OE2[8_556]	1.92	0.28
1:1:222:PHE:CZ	1:1:284:MET:N[3_555]	1.92	0.28
1:1:216:ARG:N	1:1:280:HIS:C[3_555]	1.92	0.28
2:2:132:SER:O	2:2:141:VAL:CA[8_556]	1.92	0.28
1:1:224:GLY:CA	1:1:237:LEU:CD1[3_555]	1.92	0.28
1:1:217:ASP:C	1:1:281:GLY:N[3_555]	1.92	0.28
2:2:87:ILE:C	2:2:125:LYS:C[8_556]	1.92	0.28
1:1:349:GLN:CG	1:1:423:ILE:CB[3_555]	1.92	0.28
2:2:71:HIS:N	2:2:93:PHE:CE1[8_556]	1.92	0.28
1:1:226:THR:C	1:1:228:TYR:OH[3_555]	1.92	0.28
2:2:75:ILE:N	2:2:90:ALA:O[8_556]	1.92	0.28
2:2:114:GLU:OE2	2:2:122:ILE:CB[8_556]	1.92	0.28
2:2:58:HIS:C	2:2:129:THR:N[8_556]	1.93	0.27
2:2:65:THR:OG1	2:2:139:ASN:CG[8_556]	1.93	0.27
1:1:73:HIS:CA	1:1:215:TYR:CG[2_555]	1.93	0.27
1:1:418:THR:CA	3:3:17:LEU:N[2_555]	1.93	0.27
1:1:85:MET:N	1:1:142:ASP:OD1[2_555]	1.93	0.27
2:2:60:VAL:C	2:2:130:ILE:C[8_556]	1.93	0.27
1:1:218:ILE:CB	1:1:282:VAL:N[3_555]	1.93	0.27
2:2:116:PHE:N	2:2:116:PHE:CG[8_556]	1.93	0.27
1:1:35:VAL:CA	1:1:217:ASP:O[2_555]	1.93	0.27
2:2:133:HIS:ND1	2:2:140:ASP:CG[8_556]	1.93	0.27
2:2:37:SER:OG	2:2:109:ASP:OD2[8_556]	1.93	0.27
2:2:66:ASN:N	2:2:139:ASN:CA[8_556]	1.93	0.27
2:2:65:THR:CG2	2:2:136:THR:N[8_556]	1.93	0.27
2:2:130:ILE:CB	2:2:143:ALA:N[8_556]	1.93	0.27
2:2:69:ASN:CG	2:2:142:TYR:OH[8_556]	1.93	0.27
2:2:66:ASN:CB	2:2:95:VAL:O[8_556]	1.93	0.27
2:2:64:GLU:N	2:2:94:GLU:OE2[8_556]	1.94	0.26
1:1:418:THR:CB	3:3:17:LEU:CD2[2_555]	1.94	0.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:128:VAL:CB	2:2:145:ILE:CA[8_556]	1.94	0.26
1:1:89:VAL:O	1:1:140:SER:OG[2_555]	1.94	0.26
1:1:224:GLY:O	1:1:275:PHE:CD2[3_555]	1.94	0.26
2:2:8:LYS:CA	2:2:148:TRP:CG[8_556]	1.94	0.26
2:2:112:PRO:O	2:2:145:ILE:CD1[8_556]	1.94	0.26
2:2:61:ARG:N	2:2:131:ASP:CB[8_556]	1.94	0.26
2:2:34:PRO:CG	2:2:70:HIS:CD2[8_556]	1.94	0.26
2:2:70:HIS:C	2:2:101:PRO:CG[8_556]	1.94	0.26
1:1:36:VAL:CA	1:1:217:ASP:OD1[2_555]	1.94	0.26
2:2:61:ARG:CG	2:2:131:ASP:CB[8_556]	1.94	0.26
1:1:349:GLN:OE1	1:1:423:ILE:N[3_555]	1.94	0.26
1:1:416:MET:SD	3:3:19:TYR:CD1[2_555]	1.94	0.26
2:2:62:ILE:CG1	2:2:92:ARG:CG[8_556]	1.94	0.26
2:2:109:ASP:C	2:2:165:GLN:N[8_556]	1.94	0.26
2:2:107:LEU:CB	2:2:167:ASN:O[8_556]	1.94	0.26
2:2:107:LEU:C	2:2:166:VAL:C[8_556]	1.95	0.25
2:2:112:PRO:C	2:2:124:PHE:CE1[8_556]	1.95	0.25
2:2:60:VAL:N	2:2:130:ILE:CA[8_556]	1.95	0.25
2:2:132:SER:CB	2:2:141:VAL:C[8_556]	1.95	0.25
1:1:214:ARG:CB	1:1:280:HIS:CG[3_555]	1.95	0.25
2:2:133:HIS:NE2	2:2:140:ASP:CB[8_556]	1.95	0.25
2:2:8:LYS:N	2:2:148:TRP:NE1[8_556]	1.95	0.25
2:2:89:PHE:N	2:2:125:LYS:C[8_556]	1.95	0.25
1:1:72:PRO:C	1:1:215:TYR:CE2[2_555]	1.95	0.25
1:1:12:HIS:NE2	3:3:16:ARG:NH2[2_555]	1.95	0.25
1:1:70:TYR:CE1	1:1:219:MET:C[2_555]	1.96	0.24
2:2:111:TYR:CE2	2:2:163:VAL:CG1[8_556]	1.96	0.24
2:2:107:LEU:C	2:2:167:ASN:C[8_556]	1.96	0.24
1:1:350:TRP:C	1:1:424:MET:CE[3_555]	1.96	0.24
1:1:90:ASN:OD1	1:1:380:LYS:CE[2_555]	1.96	0.24
2:2:109:ASP:N	2:2:165:GLN:CA[8_556]	1.96	0.24
2:2:108:TYR:O	2:2:164:ASN:CG[8_556]	1.96	0.24
1:1:223:GLY:C	1:1:237:LEU:CD1[3_555]	1.96	0.24
1:1:217:ASP:O	1:1:281:GLY:O[3_555]	1.96	0.24
2:2:111:TYR:CD2	2:2:163:VAL:CG2[8_556]	1.96	0.24
2:2:106:ALA:C	2:2:168:ARG:O[8_556]	1.96	0.24
2:2:113:ILE:CA	2:2:124:PHE:CE2[8_556]	1.96	0.24
2:2:71:HIS:O	2:2:93:PHE:CE2[8_556]	1.96	0.24
1:1:218:ILE:CB	1:1:281:GLY:C[3_555]	1.96	0.24
2:2:107:LEU:CD1	2:2:168:ARG:CD[8_556]	1.96	0.24
1:1:12:HIS:CE1	3:3:16:ARG:NH2[2_555]	1.97	0.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:73:HIS:N	1:1:215:TYR:CD2[2_555]	1.97	0.23
1:1:231:ASP:OD1	1:1:279:GLU:OE2[3_555]	1.97	0.23
1:1:72:PRO:CB	1:1:215:TYR:CD2[2_555]	1.97	0.23
2:2:69:ASN:C	2:2:142:TYR:CD2[8_556]	1.97	0.23
1:1:222:PHE:CE2	1:1:283:ILE:C[3_555]	1.97	0.23
1:1:231:ASP:OD2	1:1:279:GLU:CD[3_555]	1.97	0.23
2:2:71:HIS:N	2:2:142:TYR:CB[8_556]	1.97	0.23
2:2:71:HIS:NE2	2:2:94:GLU:CA[8_556]	1.97	0.23
2:2:92:ARG:C	2:2:165:GLN:CB[8_556]	1.97	0.23
2:2:8:LYS:CA	2:2:89:PHE:CE2[8_556]	1.97	0.23
2:2:66:ASN:C	2:2:95:VAL:O[8_556]	1.97	0.23
2:2:71:HIS:CB	2:2:93:PHE:CE1[8_556]	1.97	0.23
1:1:12:HIS:CG	3:3:16:ARG:CZ[2_555]	1.97	0.23
1:1:89:VAL:CG1	1:1:380:LYS:CG[2_555]	1.97	0.23
2:2:107:LEU:CD1	2:2:168:ARG:CB[8_556]	1.97	0.23
2:2:70:HIS:CA	2:2:142:TYR:CD1[8_556]	1.97	0.23
2:2:67:PRO:CB	2:2:99:VAL:CG2[8_556]	1.97	0.23
1:1:416:MET:N	3:3:16:ARG:CD[2_555]	1.97	0.23
2:2:64:GLU:N	2:2:135:ARG:N[8_556]	1.97	0.23
1:1:72:PRO:N	1:1:215:TYR:CZ[2_555]	1.97	0.23
2:2:62:ILE:CG2	2:2:141:VAL:CG1[8_556]	1.97	0.23
2:2:107:LEU:CG	2:2:168:ARG:CB[8_556]	1.97	0.23
2:2:8:LYS:NZ	2:2:147:LEU:N[8_556]	1.97	0.23
2:2:66:ASN:O	2:2:96:ALA:N[8_556]	1.98	0.22
1:1:350:TRP:O	1:1:424:MET:SD[3_555]	1.98	0.22
1:1:74:ARG:CG	1:1:231:ASP:CA[2_555]	1.98	0.22
1:1:34:PRO:CG	1:1:212:MET:SD[2_555]	1.98	0.22
2:2:126:ASP:CA	2:2:146:MET:O[8_556]	1.98	0.22
1:1:391:ASP:OD2	2:2:98:GLY:O[8_556]	1.98	0.22
2:2:60:VAL:CG1	2:2:111:TYR:CE2[8_556]	1.98	0.22
1:1:74:ARG:NH2	1:1:230:GLY:N[2_555]	1.98	0.22
1:1:86:LYS:CD	1:1:128:LEU:O[2_555]	1.98	0.22
1:1:86:LYS:O	1:1:131:TYR:CD2[2_555]	1.98	0.22
1:1:92:SER:CA	1:1:141:ASP:OD2[2_555]	1.98	0.22
2:2:62:ILE:CA	2:2:92:ARG:NH1[8_556]	1.98	0.22
2:2:70:HIS:CB	2:2:101:PRO:CG[8_556]	1.98	0.22
2:2:64:GLU:CB	2:2:134:PRO:N[8_556]	1.98	0.22
1:1:73:HIS:CA	1:1:215:TYR:CA[2_555]	1.98	0.22
1:1:12:HIS:ND1	3:3:16:ARG:CZ[2_555]	1.98	0.22
2:2:62:ILE:CB	2:2:92:ARG:NE[8_556]	1.98	0.22
2:2:130:ILE:CG2	2:2:143:ALA:CB[8_556]	1.99	0.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:32:TRP:NE1	1:1:204:THR:CG2[2_555]	1.99	0.21
2:2:63:ASP:CB	2:2:135:ARG:CG[8_556]	1.99	0.21
2:2:93:PHE:CB	2:2:166:VAL:O[8_556]	1.99	0.21
2:2:34:PRO:CG	2:2:70:HIS:NE2[8_556]	1.99	0.21
2:2:69:ASN:O	2:2:142:TYR:CD1[8_556]	1.99	0.21
1:1:349:GLN:CG	1:1:422:SER:C[3_555]	1.99	0.21
2:2:71:HIS:CB	2:2:93:PHE:CD2[8_556]	1.99	0.21
1:1:74:ARG:CB	1:1:231:ASP:CB[2_555]	1.99	0.21
1:1:74:ARG:CD	1:1:232:ASN:N[2_555]	1.99	0.21
1:1:85:MET:O	1:1:132:ASN:CA[2_555]	1.99	0.21
1:1:222:PHE:CD2	1:1:282:VAL:C[3_555]	1.99	0.21
2:2:67:PRO:CB	2:2:96:ALA:CB[8_556]	1.99	0.21
2:2:65:THR:CA	2:2:139:ASN:ND2[8_556]	1.99	0.21
2:2:109:ASP:O	2:2:165:GLN:N[8_556]	1.99	0.21
1:1:85:MET:SD	1:1:214:ARG:NH1[2_555]	1.99	0.21
1:1:168:ILE:CG2	1:1:425:THR:O[3_555]	1.99	0.21
2:2:63:ASP:CG	2:2:135:ARG:CB[8_556]	1.99	0.21
2:2:63:ASP:N	2:2:92:ARG:NH1[8_556]	2.00	0.20
1:1:74:ARG:CZ	1:1:230:GLY:O[2_555]	2.00	0.20
1:1:421:ASP:C	3:3:18:TRP:CH2[2_555]	2.00	0.20
1:1:349:GLN:O	1:1:424:MET:CG[3_555]	2.00	0.20
2:2:111:TYR:CZ	2:2:163:VAL:CG1[8_556]	2.00	0.20
2:2:132:SER:N	2:2:141:VAL:O[8_556]	2.00	0.20
1:1:33:THR:CG2	1:1:221:GLU:OE1[2_555]	2.00	0.20
2:2:63:ASP:CB	2:2:135:ARG:CB[8_556]	2.00	0.20
2:2:61:ARG:N	2:2:131:ASP:OD1[8_556]	2.00	0.20
1:1:217:ASP:N	1:1:280:HIS:O[3_555]	2.00	0.20
2:2:133:HIS:CD2	2:2:140:ASP:OD1[8_556]	2.00	0.20
2:2:67:PRO:CA	2:2:96:ALA:CB[8_556]	2.00	0.20
1:1:72:PRO:C	1:1:215:TYR:CB[2_555]	2.00	0.20
2:2:111:TYR:CB	2:2:163:VAL:CA[8_556]	2.00	0.20
2:2:63:ASP:CA	2:2:135:ARG:CG[8_556]	2.00	0.20
1:1:70:TYR:CG	1:1:219:MET:CG[2_555]	2.01	0.19
2:2:63:ASP:O	2:2:94:GLU:CD[8_556]	2.01	0.19
2:2:64:GLU:C	2:2:134:PRO:CB[8_556]	2.01	0.19
2:2:109:ASP:C	2:2:164:ASN:CG[8_556]	2.01	0.19
1:1:216:ARG:CB	1:1:279:GLU:C[3_555]	2.01	0.19
1:1:349:GLN:CD	1:1:422:SER:N[3_555]	2.01	0.19
2:2:75:ILE:C	2:2:111:TYR:O[8_556]	2.01	0.19
2:2:73:LEU:C	2:2:90:ALA:C[8_556]	2.01	0.19
2:2:37:SER:O	2:2:109:ASP:OD1[8_556]	2.01	0.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:73:HIS:CE1	1:1:218:ILE:CG2[2_555]	2.01	0.19
1:1:73:HIS:C	1:1:215:TYR:CB[2_555]	2.02	0.18
1:1:395:GLN:O	2:2:102:THR:CB[8_556]	2.02	0.18
1:1:217:ASP:CG	1:1:280:HIS:CG[3_555]	2.02	0.18
2:2:127:ALA:CA	2:2:145:ILE:C[8_556]	2.02	0.18
1:1:218:ILE:O	1:1:282:VAL:N[3_555]	2.02	0.18
1:1:71:ILE:C	1:1:215:TYR:CZ[2_555]	2.02	0.18
2:2:63:ASP:C	2:2:94:GLU:CG[8_556]	2.02	0.18
1:1:168:ILE:CB	1:1:425:THR:CA[3_555]	2.02	0.18
2:2:128:VAL:CB	2:2:144:GLY:CA[8_556]	2.02	0.18
1:1:90:ASN:O	1:1:141:ASP:CB[2_555]	2.02	0.18
2:2:108:TYR:CB	2:2:166:VAL:C[8_556]	2.02	0.18
1:1:70:TYR:CD1	1:1:219:MET:O[2_555]	2.02	0.18
1:1:168:ILE:CD1	1:1:423:ILE:C[3_555]	2.02	0.18
1:1:86:LYS:NZ	1:1:125:GLN:OE1[2_555]	2.02	0.18
2:2:71:HIS:CA	2:2:93:PHE:CD2[8_556]	2.02	0.18
2:2:60:VAL:CG2	2:2:111:TYR:CZ[8_556]	2.03	0.17
2:2:109:ASP:C	2:2:164:ASN:O[8_556]	2.03	0.17
2:2:62:ILE:N	2:2:92:ARG:NH2[8_556]	2.03	0.17
2:2:71:HIS:CG	2:2:93:PHE:CE1[8_556]	2.03	0.17
2:2:133:HIS:CB	2:2:140:ASP:OD1[8_556]	2.03	0.17
1:1:214:ARG:O	1:1:281:GLY:N[3_555]	2.03	0.17
2:2:114:GLU:CD	2:2:122:ILE:CD1[8_556]	2.03	0.17
1:1:333:PHE:CD1	1:1:425:THR:CG2[3_555]	2.03	0.17
1:1:353:THR:OG1	1:1:421:ASP:CA[3_555]	2.03	0.17
2:2:128:VAL:CG1	2:2:145:ILE:N[8_556]	2.03	0.17
1:1:91:ALA:CB	1:1:142:ASP:N[2_555]	2.03	0.17
1:1:349:GLN:OE1	1:1:422:SER:C[3_555]	2.03	0.17
1:1:225:HIS:CA	1:1:275:PHE:CZ[3_555]	2.03	0.17
1:1:12:HIS:CE1	3:3:16:ARG:NE[2_555]	2.04	0.16
1:1:233:ARG:NH1	1:1:279:GLU:OE1[3_555]	2.04	0.16
1:1:222:PHE:CB	1:1:283:ILE:CG1[3_555]	2.04	0.16
1:1:88:GLY:C	1:1:140:SER:CB[2_555]	2.04	0.16
2:2:37:SER:C	2:2:109:ASP:OD1[8_556]	2.04	0.16
2:2:76:ALA:O	2:2:112:PRO:CA[8_556]	2.04	0.16
2:2:63:ASP:OD2	2:2:94:GLU:OE1[8_556]	2.04	0.16
2:2:132:SER:CB	2:2:142:TYR:N[8_556]	2.04	0.16
1:1:417:PRO:CB	3:3:17:LEU:C[2_555]	2.04	0.16
1:1:352:ARG:CB	1:1:420:ARG:N[3_555]	2.04	0.16
1:1:73:HIS:CE1	1:1:214:ARG:C[2_555]	2.04	0.16
2:2:108:TYR:O	2:2:164:ASN:OD1[8_556]	2.04	0.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:352:ARG:NE	1:1:419:THR:O[3_555]	2.04	0.16
2:2:6:ILE:CA	2:2:53:HIS:CB[8_556]	2.04	0.16
2:2:115:THR:CG2	2:2:124:PHE:CA[8_556]	2.04	0.16
2:2:116:PHE:O	2:2:116:PHE:CZ[8_556]	2.04	0.16
1:1:418:THR:C	3:3:17:LEU:CA[2_555]	2.05	0.15
1:1:33:THR:O	1:1:221:GLU:CB[2_555]	2.05	0.15
2:2:75:ILE:N	2:2:90:ALA:CA[8_556]	2.05	0.15
2:2:128:VAL:CG1	2:2:144:GLY:C[8_556]	2.05	0.15
2:2:65:THR:OG1	2:2:136:THR:CB[8_556]	2.05	0.15
1:1:218:ILE:CD1	1:1:282:VAL:CB[3_555]	2.05	0.15
2:2:130:ILE:CG2	2:2:143:ALA:O[8_556]	2.05	0.15
2:2:64:GLU:CB	2:2:134:PRO:CD[8_556]	2.05	0.15
1:1:86:LYS:CE	1:1:128:LEU:O[2_555]	2.05	0.15
1:1:36:VAL:CG1	1:1:211:PHE:O[2_555]	2.05	0.15
2:2:58:HIS:O	2:2:129:THR:N[8_556]	2.05	0.15
2:2:113:ILE:O	2:2:124:PHE:CG[8_556]	2.05	0.15
2:2:62:ILE:N	2:2:92:ARG:CZ[8_556]	2.05	0.15
2:2:59:VAL:CB	2:2:129:THR:O[8_556]	2.05	0.15
1:1:113:PRO:CD	1:1:201:LYS:NZ[2_555]	2.05	0.15
2:2:4:LYS:NZ	2:2:149:SER:O[8_556]	2.05	0.15
1:1:88:GLY:O	1:1:140:SER:C[2_555]	2.05	0.15
2:2:77:GLY:N	2:2:112:PRO:CB[8_556]	2.06	0.14
2:2:110:VAL:O	2:2:164:ASN:N[8_556]	2.06	0.14
1:1:222:PHE:CG	1:1:283:ILE:CB[3_555]	2.06	0.14
1:1:35:VAL:N	1:1:217:ASP:O[2_555]	2.06	0.14
2:2:64:GLU:N	2:2:134:PRO:C[8_556]	2.06	0.14
1:1:87:ASP:CB	1:1:141:ASP:O[2_555]	2.06	0.14
2:2:107:LEU:CD2	2:2:168:ARG:CB[8_556]	2.06	0.14
2:2:69:ASN:CA	2:2:99:VAL:O[8_556]	2.06	0.14
2:2:6:ILE:C	2:2:53:HIS:CB[8_556]	2.06	0.14
1:1:352:ARG:CB	1:1:420:ARG:C[3_555]	2.06	0.14
1:1:84:PHE:O	1:1:142:ASP:OD1[2_555]	2.06	0.14
1:1:215:TYR:C	1:1:281:GLY:CA[3_555]	2.06	0.14
2:2:4:LYS:CE	2:2:150:ASN:C[8_556]	2.06	0.14
2:2:4:LYS:CE	2:2:150:ASN:N[8_556]	2.06	0.14
2:2:60:VAL:O	2:2:130:ILE:O[8_556]	2.06	0.14
2:2:108:TYR:N	2:2:166:VAL:CA[8_556]	2.06	0.14
1:1:353:THR:CG2	1:1:426:SER:OG[3_555]	2.06	0.14
1:1:32:TRP:CZ2	1:1:204:THR:CG2[2_555]	2.07	0.13
1:1:298:GLU:OE2	1:1:426:SER:C[3_555]	2.07	0.13
2:2:76:ALA:CA	2:2:112:PRO:CB[8_556]	2.07	0.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:70:TYR:CE1	1:1:219:MET:CB[2_555]	2.07	0.13
1:1:355:PRO:CA	1:1:426:SER:C[3_555]	2.07	0.13
1:1:352:ARG:CD	1:1:419:THR:C[3_555]	2.07	0.13
1:1:72:PRO:CD	1:1:215:TYR:CE2[2_555]	2.07	0.13
1:1:222:PHE:CE1	1:1:284:MET:CB[3_555]	2.07	0.13
1:1:81:TRP:CH2	1:1:214:ARG:CA[2_555]	2.07	0.13
1:1:351:TYR:O	1:1:420:ARG:CD[3_555]	2.07	0.13
1:1:122:PHE:CE1	1:1:208:ARG:CZ[2_555]	2.07	0.13
1:1:217:ASP:CA	1:1:280:HIS:CA[3_555]	2.07	0.13
1:1:333:PHE:CD1	1:1:425:THR:OG1[3_555]	2.07	0.13
1:1:222:PHE:CD2	1:1:284:MET:N[3_555]	2.07	0.13
2:2:59:VAL:CA	2:2:129:THR:N[8_556]	2.08	0.12
1:1:33:THR:O	1:1:221:GLU:CG[2_555]	2.08	0.12
1:1:32:TRP:CE2	1:1:204:THR:CG2[2_555]	2.08	0.12
1:1:86:LYS:CG	1:1:132:ASN:CB[2_555]	2.08	0.12
2:2:72:ALA:C	2:2:91:ILE:CG1[8_556]	2.08	0.12
2:2:73:LEU:O	2:2:90:ALA:C[8_556]	2.08	0.12
2:2:7:SER:C	2:2:148:TRP:CG[8_556]	2.08	0.12
1:1:86:LYS:CD	1:1:128:LEU:C[2_555]	2.08	0.12
2:2:127:ALA:CB	2:2:146:MET:N[8_556]	2.08	0.12
2:2:65:THR:OG1	2:2:136:THR:CG2[8_556]	2.08	0.12
2:2:71:HIS:CA	2:2:93:PHE:CD1[8_556]	2.08	0.12
2:2:133:HIS:CB	2:2:140:ASP:CG[8_556]	2.08	0.12
2:2:64:GLU:C	2:2:139:ASN:OD1[8_556]	2.08	0.12
2:2:67:PRO:CA	2:2:96:ALA:C[8_556]	2.08	0.12
1:1:215:TYR:O	1:1:281:GLY:N[3_555]	2.08	0.12
2:2:73:LEU:N	2:2:91:ILE:CB[8_556]	2.08	0.12
1:1:71:ILE:N	1:1:219:MET:CG[2_555]	2.09	0.11
2:2:64:GLU:O	2:2:134:PRO:CB[8_556]	2.09	0.11
1:1:349:GLN:CB	1:1:423:ILE:N[3_555]	2.09	0.11
2:2:74:SER:O	2:2:110:VAL:CA[8_556]	2.09	0.11
2:2:59:VAL:N	2:2:129:THR:C[8_556]	2.09	0.11
2:2:59:VAL:N	2:2:129:THR:CB[8_556]	2.09	0.11
2:2:76:ALA:N	2:2:111:TYR:O[8_556]	2.09	0.11
2:2:74:SER:OG	2:2:89:PHE:CE1[8_556]	2.09	0.11
2:2:130:ILE:CB	2:2:143:ALA:CA[8_556]	2.10	0.10
1:1:216:ARG:C	1:1:279:GLU:C[3_555]	2.10	0.10
2:2:37:SER:CB	2:2:135:ARG:NH1[8_556]	2.10	0.10
1:1:225:HIS:CD2	1:1:278:PRO:CG[3_555]	2.10	0.10
2:2:61:ARG:O	2:2:135:ARG:NE[8_556]	2.10	0.10
2:2:59:VAL:CB	2:2:129:THR:N[8_556]	2.10	0.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:37:SER:CA	2:2:135:ARG:NH1[8_556]	2.10	0.10
1:1:12:HIS:CG	3:3:16:ARG:NH1[2_555]	2.10	0.10
1:1:91:ALA:N	1:1:141:ASP:C[2_555]	2.10	0.10
2:2:114:GLU:CD	2:2:122:ILE:CB[8_556]	2.10	0.10
2:2:127:ALA:C	2:2:146:MET:CA[8_556]	2.10	0.10
2:2:115:THR:CA	2:2:115:THR:CA[8_556]	2.10	0.10
2:2:36:LEU:C	2:2:135:ARG:NE[8_556]	2.10	0.10
1:1:91:ALA:CB	1:1:141:ASP:N[2_555]	2.10	0.10
2:2:64:GLU:CG	2:2:133:HIS:C[8_556]	2.10	0.10
1:1:35:VAL:CG2	1:1:220:LYS:N[2_555]	2.10	0.10
1:1:91:ALA:CB	1:1:140:SER:O[2_555]	2.10	0.10
1:1:416:MET:N	3:3:16:ARG:CG[2_555]	2.10	0.10
2:2:128:VAL:CA	2:2:145:ILE:O[8_556]	2.10	0.10
1:1:73:HIS:N	1:1:215:TYR:C[2_555]	2.10	0.10
1:1:352:ARG:CG	1:1:420:ARG:N[3_555]	2.10	0.10
1:1:89:VAL:O	1:1:140:SER:CA[2_555]	2.10	0.10
2:2:108:TYR:CA	2:2:167:ASN:N[8_556]	2.10	0.10
2:2:108:TYR:CA	2:2:166:VAL:C[8_556]	2.11	0.09
2:2:111:TYR:CD1	2:2:163:VAL:CA[8_556]	2.11	0.09
2:2:116:PHE:CA	2:2:116:PHE:CA[8_556]	2.11	0.09
2:2:114:GLU:C	2:2:123:SER:O[8_556]	2.11	0.09
1:1:214:ARG:O	1:1:280:HIS:C[3_555]	2.11	0.09
1:1:349:GLN:CD	1:1:422:SER:C[3_555]	2.11	0.09
2:2:116:PHE:C	2:2:116:PHE:CE2[8_556]	2.11	0.09
2:2:131:ASP:O	2:2:141:VAL:O[8_556]	2.11	0.09
1:1:86:LYS:C	1:1:132:ASN:CB[2_555]	2.11	0.09
1:1:217:ASP:OD2	1:1:280:HIS:ND1[3_555]	2.11	0.09
1:1:215:TYR:C	1:1:280:HIS:C[3_555]	2.11	0.09
2:2:59:VAL:CG2	2:2:130:ILE:C[8_556]	2.11	0.09
1:1:418:THR:O	3:3:17:LEU:CD2[2_555]	2.11	0.09
2:2:109:ASP:C	2:2:164:ASN:N[8_556]	2.11	0.09
1:1:89:VAL:O	1:1:140:SER:CB[2_555]	2.11	0.09
1:1:112:ILE:N	1:1:201:LYS:CB[2_555]	2.12	0.08
2:2:70:HIS:N	2:2:142:TYR:OH[8_556]	2.12	0.08
1:1:85:MET:SD	1:1:214:ARG:CD[2_555]	2.12	0.08
2:2:64:GLU:CG	2:2:134:PRO:CB[8_556]	2.12	0.08
2:2:71:HIS:CD2	2:2:94:GLU:CA[8_556]	2.12	0.08
2:2:132:SER:CA	2:2:141:VAL:CA[8_556]	2.12	0.08
2:2:88:ALA:O	2:2:126:ASP:N[8_556]	2.12	0.08
1:1:222:PHE:CD1	1:1:283:ILE:O[3_555]	2.12	0.08
2:2:70:HIS:CA	2:2:142:TYR:CG[8_556]	2.12	0.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:128:VAL:CA	2:2:145:ILE:C[8_556]	2.12	0.08
1:1:222:PHE:CG	1:1:283:ILE:O[3_555]	2.12	0.08
1:1:85:MET:CG	1:1:214:ARG:NE[2_555]	2.12	0.08
1:1:34:PRO:CA	1:1:212:MET:CE[2_555]	2.12	0.08
2:2:73:LEU:CA	2:2:92:ARG:N[8_556]	2.12	0.08
2:2:70:HIS:CA	2:2:142:TYR:CE1[8_556]	2.12	0.08
2:2:108:TYR:C	2:2:165:GLN:C[8_556]	2.12	0.08
1:1:89:VAL:CG2	1:1:137:PRO:CB[2_555]	2.12	0.08
1:1:220:LYS:O	1:1:283:ILE:CD1[3_555]	2.12	0.08
2:2:116:PHE:CB	2:2:116:PHE:CD1[8_556]	2.13	0.07
1:1:36:VAL:CA	1:1:217:ASP:CG[2_555]	2.13	0.07
2:2:108:TYR:C	2:2:164:ASN:CG[8_556]	2.13	0.07
2:2:113:ILE:O	2:2:124:PHE:CE2[8_556]	2.13	0.07
2:2:128:VAL:N	2:2:146:MET:N[8_556]	2.13	0.07
1:1:70:TYR:CD1	1:1:219:MET:CB[2_555]	2.13	0.07
1:1:35:VAL:O	1:1:217:ASP:O[2_555]	2.13	0.07
1:1:91:ALA:O	1:1:141:ASP:CB[2_555]	2.13	0.07
1:1:87:ASP:CG	1:1:143:LEU:CA[2_555]	2.13	0.07
2:2:71:HIS:CG	2:2:93:PHE:O[8_556]	2.13	0.07
2:2:73:LEU:CD1	2:2:92:ARG:CB[8_556]	2.13	0.07
1:1:84:PHE:O	1:1:136:LYS:CD[2_555]	2.13	0.07
2:2:68:THR:OG1	2:2:95:VAL:CG2[8_556]	2.13	0.07
2:2:37:SER:CA	2:2:135:ARG:CZ[8_556]	2.13	0.07
1:1:216:ARG:C	1:1:280:HIS:O[3_555]	2.14	0.06
2:2:69:ASN:ND2	2:2:142:TYR:CZ[8_556]	2.14	0.06
2:2:132:SER:C	2:2:141:VAL:C[8_556]	2.14	0.06
2:2:68:THR:CB	2:2:95:VAL:CB[8_556]	2.14	0.06
2:2:7:SER:C	2:2:148:TRP:CE3[8_556]	2.14	0.06
1:1:87:ASP:OD2	1:1:142:ASP:CA[2_555]	2.14	0.06
2:2:107:LEU:CD2	2:2:168:ARG:CG[8_556]	2.14	0.06
1:1:416:MET:C	3:3:16:ARG:CG[2_555]	2.14	0.06
2:2:4:LYS:CD	2:2:150:ASN:ND2[8_556]	2.14	0.06
1:1:91:ALA:N	1:1:141:ASP:O[2_555]	2.14	0.06
2:2:8:LYS:CA	2:2:148:TRP:CB[8_556]	2.14	0.06
1:1:418:THR:OG1	3:3:15:ALA:O[2_555]	2.14	0.06
1:1:216:ARG:C	1:1:281:GLY:N[3_555]	2.14	0.06
1:1:91:ALA:N	1:1:141:ASP:CB[2_555]	2.14	0.06
1:1:222:PHE:CZ	1:1:283:ILE:C[3_555]	2.14	0.06
2:2:132:SER:CB	2:2:141:VAL:CA[8_556]	2.15	0.05
2:2:127:ALA:O	2:2:145:ILE:CA[8_556]	2.15	0.05
2:2:75:ILE:CA	2:2:90:ALA:N[8_556]	2.15	0.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:87:ASP:CB	1:1:142:ASP:N[2_555]	2.15	0.05
1:1:81:TRP:CZ2	1:1:214:ARG:CD[2_555]	2.15	0.05
2:2:68:THR:CA	2:2:95:VAL:CG1[8_556]	2.15	0.05
2:2:73:LEU:CD2	2:2:91:ILE:O[8_556]	2.15	0.05
2:2:88:ALA:C	2:2:126:ASP:CB[8_556]	2.15	0.05
1:1:89:VAL:N	1:1:140:SER:OG[2_555]	2.15	0.05
2:2:128:VAL:CB	2:2:144:GLY:O[8_556]	2.15	0.05
1:1:349:GLN:CG	1:1:424:MET:N[3_555]	2.15	0.05
1:1:216:ARG:CB	1:1:279:GLU:CA[3_555]	2.15	0.05
2:2:65:THR:CA	2:2:139:ASN:CA[8_556]	2.15	0.05
2:2:114:GLU:CB	2:2:122:ILE:CG1[8_556]	2.15	0.05
2:2:69:ASN:CB	2:2:142:TYR:CZ[8_556]	2.15	0.05
2:2:86:MET:SD	2:2:114:GLU:OE1[8_556]	2.15	0.05
2:2:66:ASN:O	2:2:96:ALA:CA[8_556]	2.15	0.05
2:2:69:ASN:N	2:2:142:TYR:OH[8_556]	2.15	0.05
2:2:108:TYR:CD1	2:2:166:VAL:CG2[8_556]	2.15	0.05
2:2:63:ASP:OD1	2:2:136:THR:N[8_556]	2.15	0.05
2:2:71:HIS:CG	2:2:93:PHE:CG[8_556]	2.16	0.04
2:2:62:ILE:CG1	2:2:92:ARG:NE[8_556]	2.16	0.04
1:1:74:ARG:NE	1:1:232:ASN:N[2_555]	2.16	0.04
2:2:70:HIS:C	2:2:93:PHE:CZ[8_556]	2.16	0.04
2:2:73:LEU:C	2:2:91:ILE:CG2[8_556]	2.16	0.04
1:1:417:PRO:C	3:3:17:LEU:CB[2_555]	2.16	0.04
2:2:59:VAL:CA	2:2:130:ILE:N[8_556]	2.16	0.04
2:2:115:THR:N	2:2:124:PHE:CB[8_556]	2.16	0.04
2:2:115:THR:O	2:2:123:SER:O[8_556]	2.16	0.04
2:2:108:TYR:N	2:2:166:VAL:C[8_556]	2.16	0.04
1:1:418:THR:CA	3:3:17:LEU:CB[2_555]	2.16	0.04
2:2:108:TYR:CB	2:2:165:GLN:C[8_556]	2.16	0.04
1:1:88:GLY:N	1:1:136:LYS:CB[2_555]	2.16	0.04
1:1:349:GLN:CD	1:1:423:ILE:CD1[3_555]	2.16	0.04
1:1:168:ILE:CG2	1:1:426:SER:N[3_555]	2.16	0.04
2:2:8:LYS:CA	2:2:148:TRP:CD2[8_556]	2.16	0.04
1:1:35:VAL:N	1:1:212:MET:CG[2_555]	2.16	0.04
2:2:74:SER:O	2:2:111:TYR:N[8_556]	2.16	0.04
2:2:71:HIS:N	2:2:142:TYR:CG[8_556]	2.17	0.03
2:2:74:SER:CB	2:2:90:ALA:O[8_556]	2.17	0.03
2:2:89:PHE:N	2:2:126:ASP:O[8_556]	2.17	0.03
2:2:106:ALA:CA	2:2:169:GLU:N[8_556]	2.17	0.03
2:2:4:LYS:CE	2:2:149:SER:O[8_556]	2.17	0.03
2:2:65:THR:O	2:2:139:ASN:CB[8_556]	2.17	0.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:417:PRO:C	3:3:17:LEU:CA[2_555]	2.17	0.03
2:2:64:GLU:OE2	2:2:134:PRO:N[8_556]	2.17	0.03
1:1:41:PHE:CE2	1:1:221:GLU:O[2_555]	2.17	0.03
1:1:72:PRO:CA	1:1:215:TYR:CG[2_555]	2.17	0.03
2:2:4:LYS:CD	2:2:150:ASN:CG[8_556]	2.17	0.03
2:2:38:ARG:CG	2:2:109:ASP:OD1[8_556]	2.17	0.03
2:2:92:ARG:C	2:2:165:GLN:CA[8_556]	2.17	0.03
2:2:60:VAL:CB	2:2:111:TYR:OH[8_556]	2.17	0.03
2:2:71:HIS:CE1	2:2:95:VAL:CB[8_556]	2.17	0.03
1:1:122:PHE:CZ	1:1:208:ARG:NE[2_555]	2.17	0.03
1:1:333:PHE:CZ	1:1:425:THR:OG1[3_555]	2.17	0.03
2:2:114:GLU:OE1	2:2:122:ILE:CG2[8_556]	2.18	0.02
2:2:130:ILE:N	2:2:143:ALA:O[8_556]	2.18	0.02
1:1:90:ASN:OD1	1:1:380:LYS:CD[2_555]	2.18	0.02
1:1:216:ARG:CA	1:1:280:HIS:C[3_555]	2.18	0.02
2:2:61:ARG:CA	2:2:131:ASP:C[8_556]	2.18	0.02
1:1:33:THR:CB	1:1:221:GLU:CD[2_555]	2.18	0.02
1:1:90:ASN:ND2	1:1:380:LYS:NZ[2_555]	2.18	0.02
2:2:107:LEU:O	2:2:167:ASN:CB[8_556]	2.18	0.02
1:1:227:SER:O	1:1:229:ASP:OD2[3_555]	2.18	0.02
2:2:8:LYS:CE	2:2:147:LEU:O[8_556]	2.18	0.02
2:2:107:LEU:CA	2:2:168:ARG:C[8_556]	2.18	0.02
2:2:63:ASP:OD1	2:2:94:GLU:CD[8_556]	2.18	0.02
1:1:353:THR:N	1:1:420:ARG:NE[3_555]	2.18	0.02
1:1:353:THR:OG1	1:1:420:ARG:O[3_555]	2.18	0.02
2:2:111:TYR:CD1	2:2:163:VAL:C[8_556]	2.18	0.02
2:2:93:PHE:CA	2:2:165:GLN:CD[8_556]	2.18	0.02
2:2:106:ALA:CA	2:2:169:GLU:CG[8_556]	2.18	0.02
1:1:224:GLY:CA	1:1:237:LEU:CD2[3_555]	2.18	0.02
1:1:352:ARG:N	1:1:420:ARG:CB[3_555]	2.18	0.02
2:2:63:ASP:N	2:2:92:ARG:CZ[8_556]	2.18	0.02
2:2:93:PHE:CA	2:2:165:GLN:CG[8_556]	2.18	0.02
1:1:40:SER:N	1:1:220:LYS:CE[2_555]	2.18	0.02
1:1:222:PHE:CD1	1:1:284:MET:C[3_555]	2.18	0.02
1:1:70:TYR:C	1:1:219:MET:CG[2_555]	2.19	0.01
2:2:87:ILE:CG1	2:2:125:LYS:CA[8_556]	2.19	0.01
1:1:70:TYR:CD1	1:1:219:MET:CG[2_555]	2.19	0.01
1:1:85:MET:O	1:1:136:LYS:CG[2_555]	2.19	0.01
2:2:128:VAL:C	2:2:145:ILE:N[8_556]	2.19	0.01
2:2:109:ASP:C	2:2:164:ASN:OD1[8_556]	2.19	0.01
1:1:352:ARG:NE	1:1:419:THR:CB[3_555]	2.19	0.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:396:SER:N	2:2:102:THR:OG1[8_556]	2.19	0.01
2:2:113:ILE:CG2	2:2:145:ILE:CG2[8_556]	2.19	0.01
1:1:35:VAL:C	1:1:217:ASP:O[2_555]	2.19	0.01
2:2:113:ILE:CA	2:2:124:PHE:CG[8_556]	2.19	0.01
1:1:233:ARG:CZ	1:1:279:GLU:CD[3_555]	2.19	0.01
1:1:90:ASN:C	1:1:141:ASP:N[2_555]	2.19	0.01
2:2:106:ALA:CB	2:2:169:GLU:N[8_556]	2.19	0.01
2:2:75:ILE:CA	2:2:111:TYR:C[8_556]	2.19	0.01
1:1:74:ARG:CB	1:1:231:ASP:CA[2_555]	2.19	0.01
1:1:217:ASP:CB	1:1:280:HIS:CA[3_555]	2.19	0.01
2:2:62:ILE:CG2	2:2:92:ARG:NH2[8_556]	2.19	0.01

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	1	415/426 (97%)	362 (87%)	40 (10%)	13 (3%)	4	23
2	2	175/177 (99%)	137 (78%)	30 (17%)	8 (5%)	2	14
3	3	10/25 (40%)	7 (70%)	3 (30%)	0	100	100
All	All	600/628 (96%)	506 (84%)	73 (12%)	21 (4%)	3	20

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	114	SER
1	1	377	THR
1	1	417	PRO
2	2	44	ASN
2	2	166	VAL
1	1	101	SER
1	1	363	ASN
1	1	380	LYS

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Mol	Chain	Res	Type
1	1	418	THR
2	2	27	ALA
2	2	103	ALA
1	1	373	ALA
1	1	379	LEU
2	2	76	ALA
1	1	330	LEU
1	1	388	ASN
1	1	395	GLN
1	1	375	PRO
2	2	67	PRO
2	2	113	ILE
2	2	137	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	1	369/377 (98%)	308 (84%)	61 (16%)	2	11
2	2	148/148 (100%)	106 (72%)	42 (28%)	0	2
3	3	8/19 (42%)	6 (75%)	2 (25%)	0	3
All	All	525/544 (96%)	420 (80%)	105 (20%)	1	7

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	24	ILE
1	1	36	VAL
1	1	54	LEU
1	1	71	ILE
1	1	89	VAL
1	1	100	SER
1	1	112	ILE
1	1	117	LEU
1	1	119	VAL

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Mol	Chain	Res	Type
1	1	121	LYS
1	1	144	THR
1	1	156	TYR
1	1	160	VAL
1	1	164	ASN
1	1	167	SER
1	1	170	THR
1	1	182	ASN
1	1	184	THR
1	1	187	THR
1	1	190	ILE
1	1	192	ILE
1	1	211	PHE
1	1	212	MET
1	1	214	ARG
1	1	218	ILE
1	1	221	GLU
1	1	226	THR
1	1	236	LEU
1	1	269	ASN
1	1	286	LEU
1	1	305	LYS
1	1	323	LEU
1	1	328	VAL
1	1	337	SER
1	1	345	ILE
1	1	354	GLN
1	1	357	ARG
1	1	360	PHE
1	1	363	ASN
1	1	365	LEU
1	1	372	SER
1	1	377	THR
1	1	378	ASP
1	1	382	ARG
1	1	383	VAL
1	1	386	ASN
1	1	387	THR
1	1	393	ILE
1	1	396	SER
1	1	397	MET
1	1	405	GLN

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Mol	Chain	Res	Type
1	1	406	THR
1	1	407	LYS
1	1	411	ASN
1	1	414	ARG
1	1	415	HIS
1	1	420	ARG
1	1	421	ASP
1	1	423	ILE
1	1	425	THR
1	1	426	SER
2	2	6	ILE
2	2	14	ASN
2	2	18	LEU
2	2	21	THR
2	2	23	THR
2	2	35	ASN
2	2	37	SER
2	2	38	ARG
2	2	40	THR
2	2	42	LEU
2	2	43	ILE
2	2	50	VAL
2	2	52	THR
2	2	53	HIS
2	2	54	SER
2	2	56	LEU
2	2	57	CYS
2	2	59	VAL
2	2	61	ARG
2	2	62	ILE
2	2	65	THR
2	2	69	ASN
2	2	81	ASN
2	2	85	ASP
2	2	86	MET
2	2	107	LEU
2	2	111	TYR
2	2	114	GLU
2	2	118	ASN
2	2	122	ILE
2	2	123	SER
2	2	129	THR

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Mol	Chain	Res	Type
2	2	130	ILE
2	2	150	ASN
2	2	153	THR
2	2	155	SER
2	2	156	THR
2	2	165	GLN
2	2	168	ARG
2	2	172	VAL
2	2	173	LEU
2	2	176	LEU
3	3	16	ARG
3	3	25	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	12	HIS
1	1	16	HIS
1	1	79	GLN
1	1	80	GLN
1	1	83	ASN
1	1	125	GLN
1	1	129	ASN
1	1	132	ASN
1	1	147	ASN
1	1	150	ASN
1	1	164	ASN
1	1	182	ASN
1	1	196	GLN
1	1	266	GLN
1	1	269	ASN
1	1	300	HIS
1	1	335	HIS
1	1	349	GLN
1	1	354	GLN
1	1	386	ASN
1	1	388	ASN
1	1	389	ASN
1	1	395	GLN
1	1	401	HIS
1	1	411	ASN
2	2	9	HIS

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Mol	Chain	Res	Type
2	2	35	ASN
2	2	44	ASN
2	2	69	ASN
2	2	71	HIS
2	2	81	ASN
2	2	118	ASN
2	2	139	ASN
2	2	165	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.