



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 30, 2017 – 09:49 AM EDT

PDB ID : 3KZ4
Title : Crystal Structure of the Rotavirus Double Layered Particle
Authors : McClain, B.; Settembre, E.C.; Bellamy, A.R.; Harrison, S.C.
Deposited on : unknown
Resolution : 3.80 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

<http://wwpdb.org/validation/2016/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) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

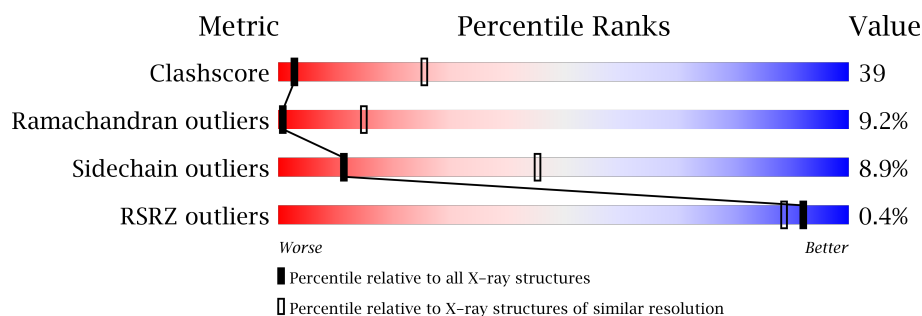
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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	112137	1030 (4.04-3.56)
Ramachandran outliers	110173	1011 (4.06-3.54)
Sidechain outliers	110143	1005 (4.06-3.54)
RSRZ outliers	101464	1032 (4.08-3.52)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	880	<div> <div>16%</div> <div>49%</div> <div>21%</div> <div>•</div> <div>11%</div> </div>
1	B	880	<div> <div>19%</div> <div>50%</div> <div>21%</div> <div>•</div> <div>8%</div> </div>
2	C	397	<div> <div>•</div> <div>60%</div> <div>31%</div> <div>8%</div> <div>•</div> </div>
2	D	397	<div> <div>57%</div> <div>32%</div> <div>9%</div> <div>•</div> </div>
2	E	397	<div> <div>58%</div> <div>33%</div> <div>8%</div> <div>•</div> </div>
2	F	397	<div> <div>•</div> <div>59%</div> <div>34%</div> <div>7%</div> <div>•</div> </div>
2	G	397	<div> <div>62%</div> <div>30%</div> <div>7%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
2	H	397	<div> <div></div> <div>60%</div> <div>32%</div> <div>7%</div> <div>.</div> </div>
2	I	397	<div> <div></div> <div>58%</div> <div>33%</div> <div>9%</div> <div>.</div> </div>
2	J	397	<div> <div></div> <div>58%</div> <div>34%</div> <div>8%</div> <div>.</div> </div>
2	K	397	<div> <div></div> <div>59%</div> <div>33%</div> <div>8%</div> <div>.</div> </div>
2	L	397	<div> <div>2%</div> <div></div> <div>57%</div> <div>35%</div> <div>7%</div> <div>.</div> </div>
2	M	397	<div> <div></div> <div>58%</div> <div>35%</div> <div>6%</div> <div>.</div> </div>
2	N	397	<div> <div></div> <div>56%</div> <div>34%</div> <div>9%</div> <div>.</div> </div>
2	O	397	<div> <div></div> <div>57%</div> <div>33%</div> <div>9%</div> <div>.</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 54109 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 Inner capsid protein VP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	781	Total	C	N	O	S	0	0	0
			6374	4049	1099	1190	36			
1	B	810	Total	C	N	O	S	0	0	0
			6624	4211	1138	1239	36			

- Molecule 2 is a protein called Intermediate capsid protein VP6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	D	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	E	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	F	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	G	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	H	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	I	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	J	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	K	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	L	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	M	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	N	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			

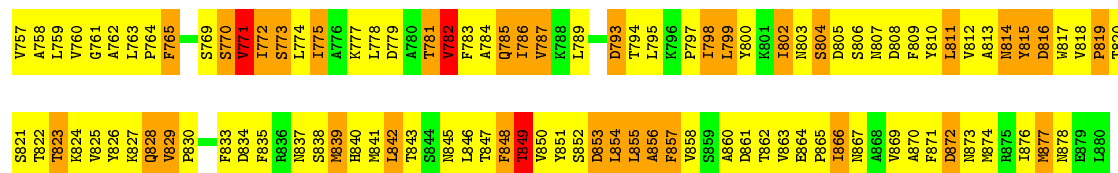
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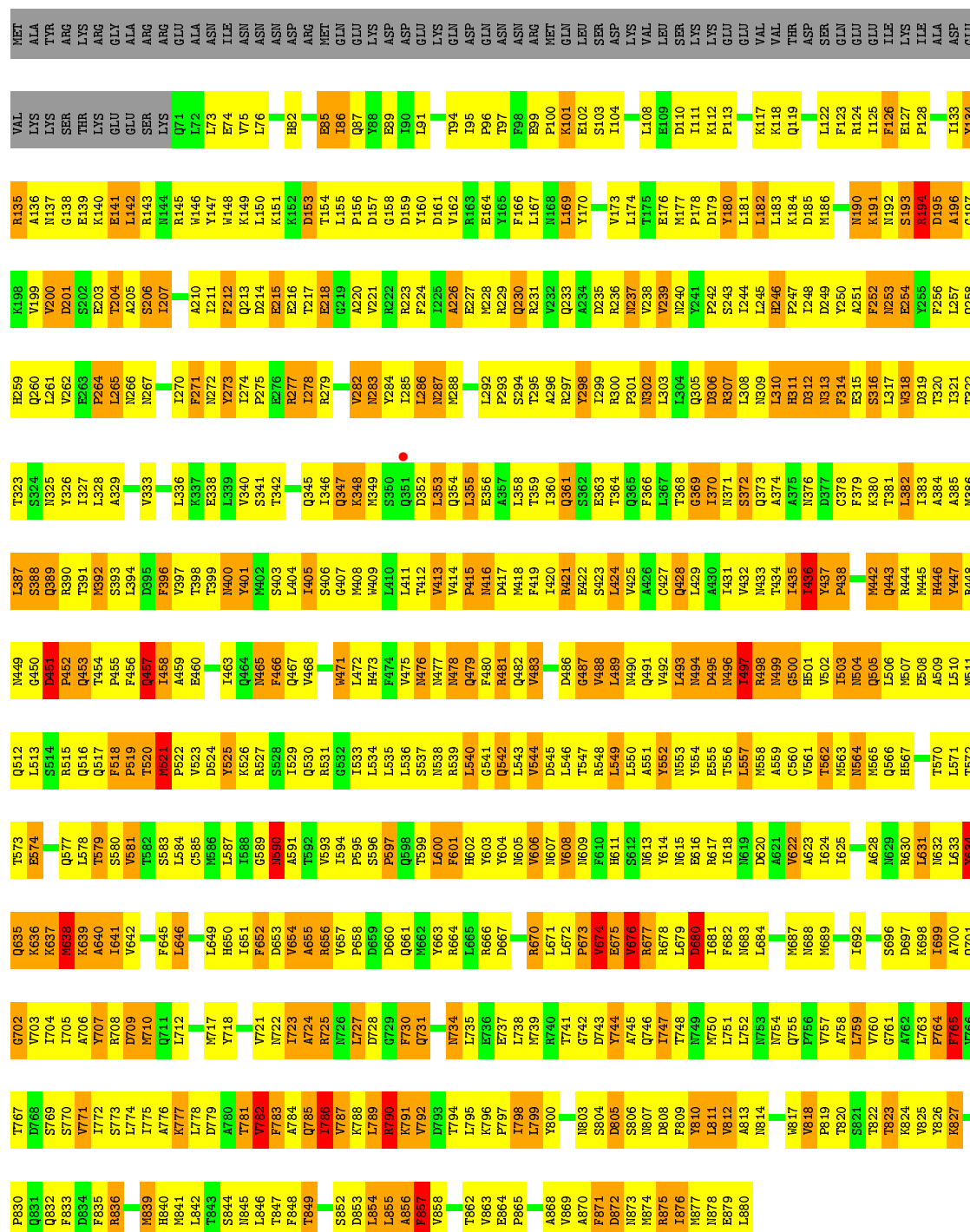
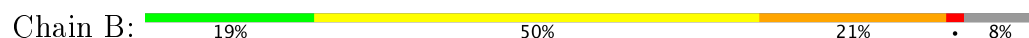
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

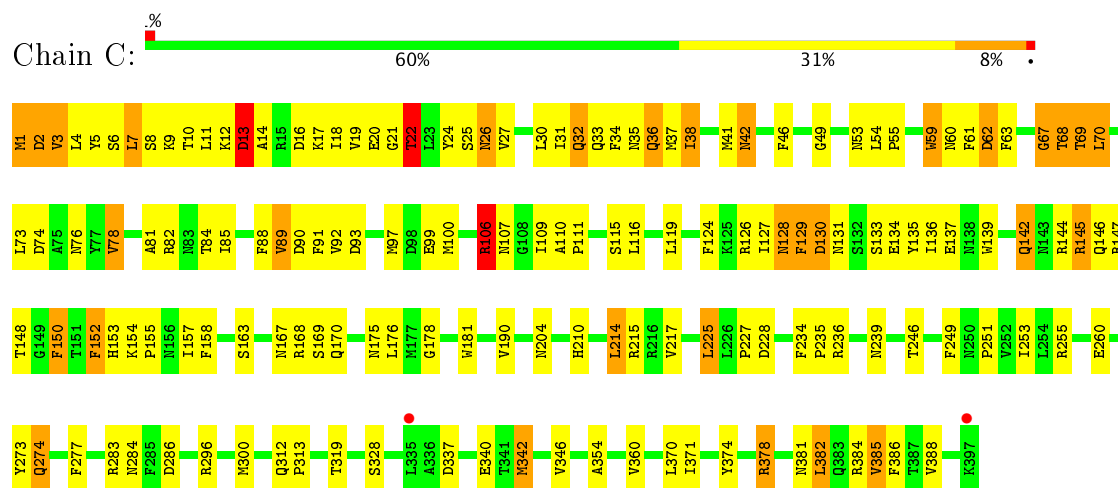
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	O	1	Total	Zn	0	0
			1	1		
3	I	1	Total	Zn	0	0
			1	1		
3	L	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	F	1	Total	Zn	0	0
			1	1		



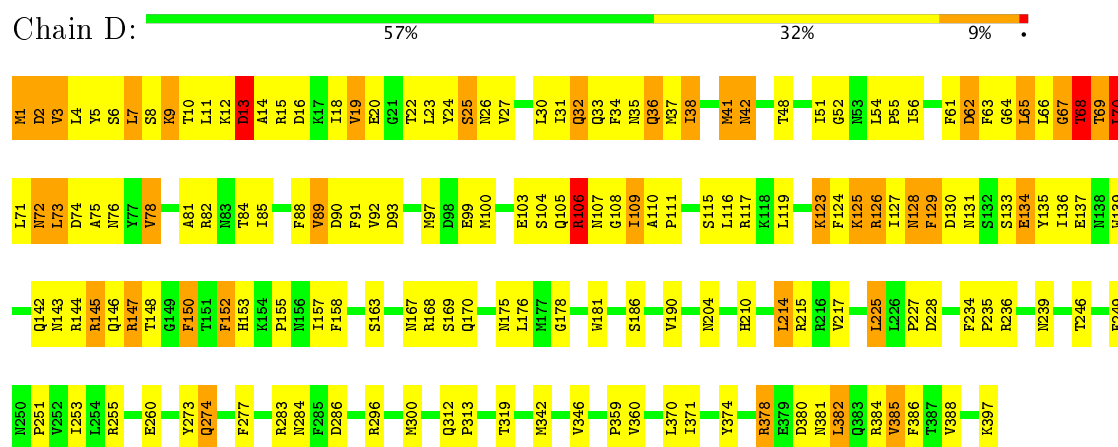
- Molecule 1: Inner capsid protein VP2



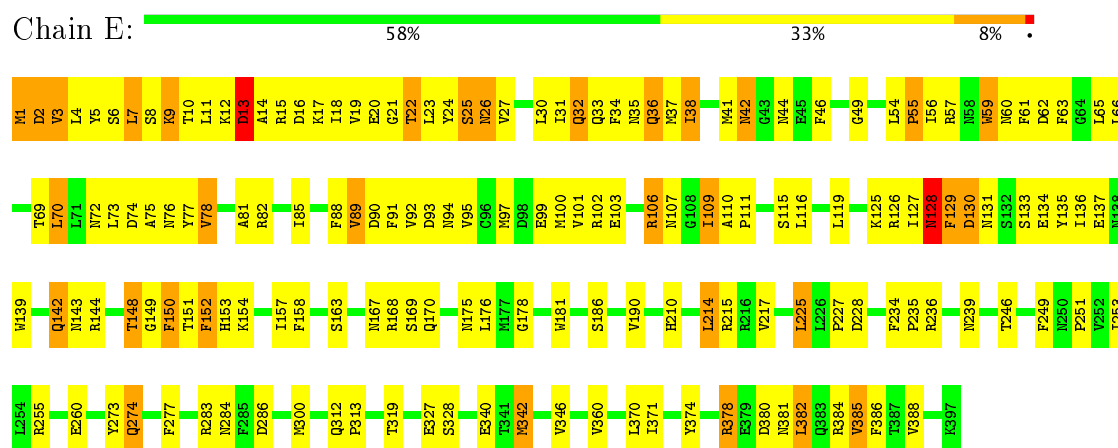
- Molecule 2: Intermediate capsid protein VP6



- Molecule 2: Intermediate capsid protein VP6

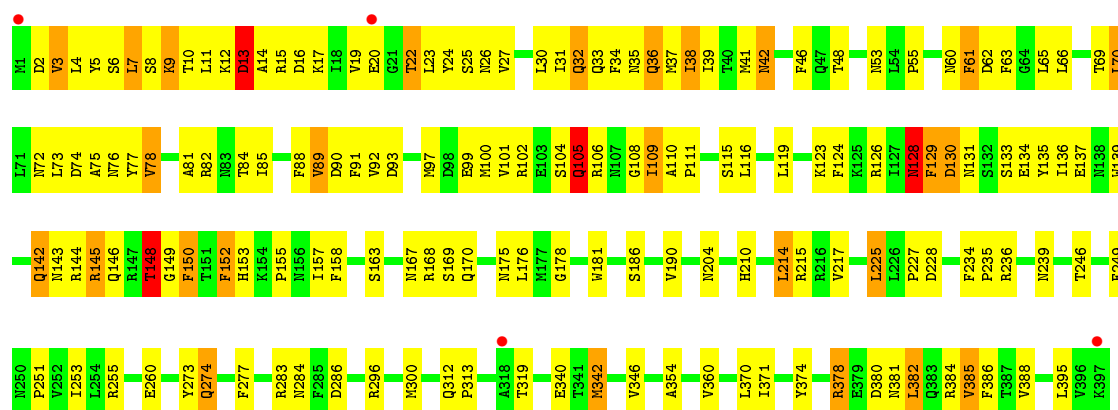


- Molecule 2: Intermediate capsid protein VP6

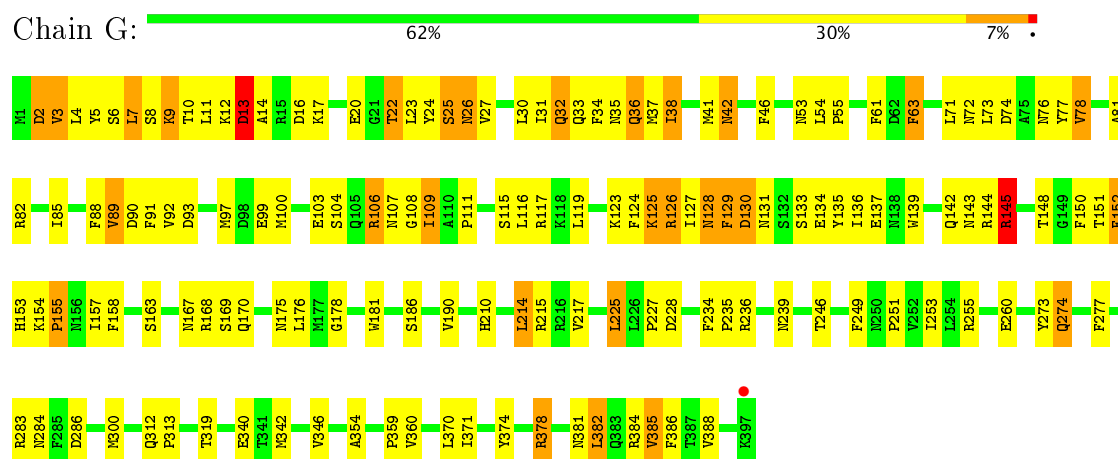


- Molecule 2: Intermediate capsid protein VP6

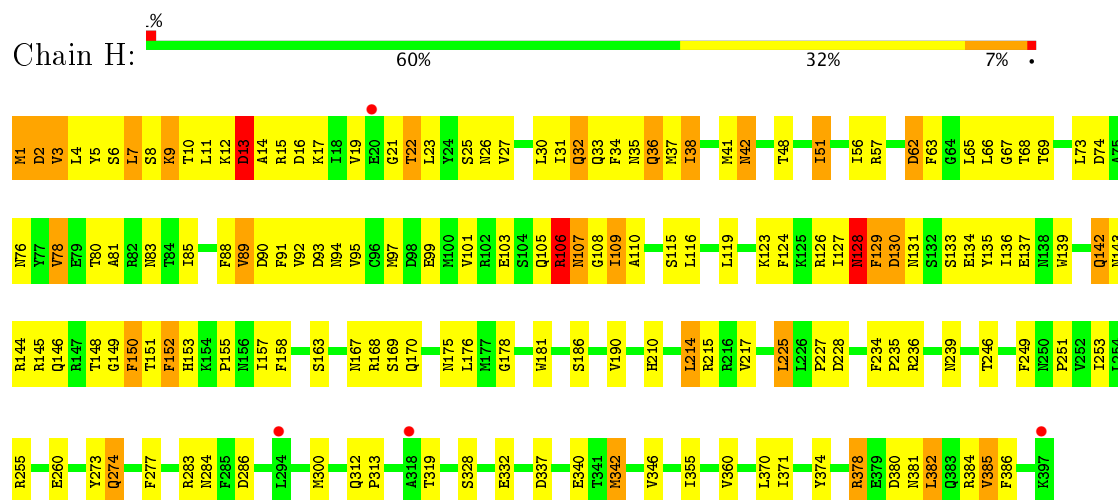




• Molecule 2: Intermediate capsid protein VP6

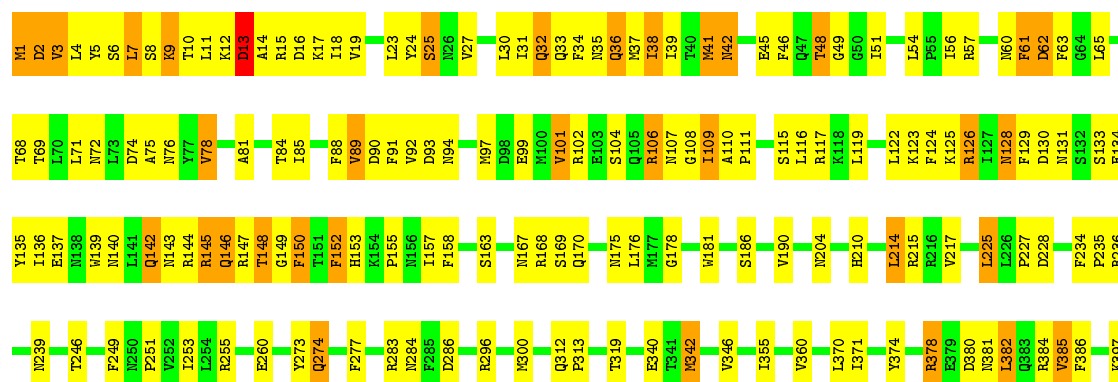


• Molecule 2: Intermediate capsid protein VP6

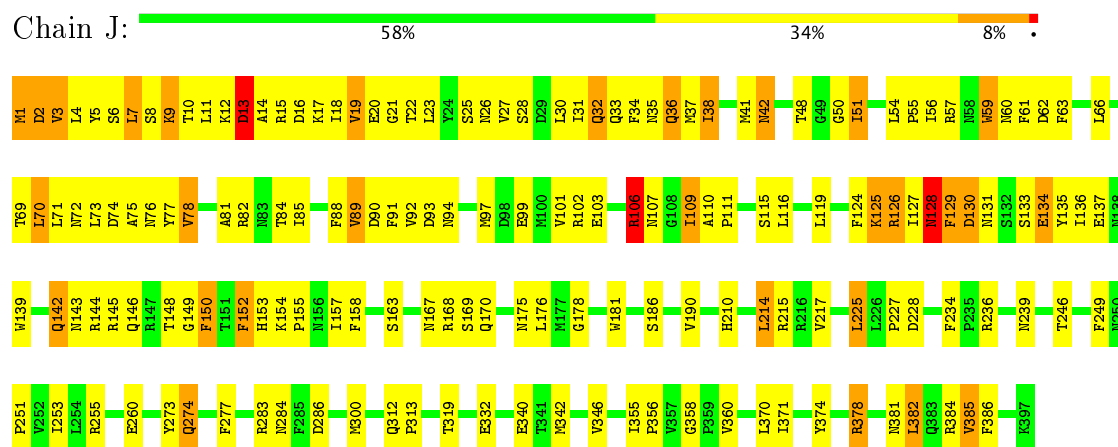


• Molecule 2: Intermediate capsid protein VP6

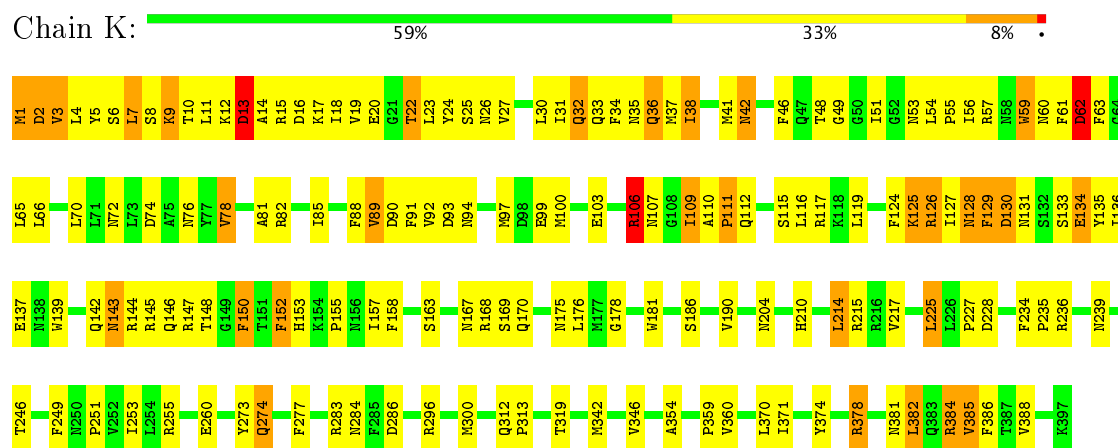




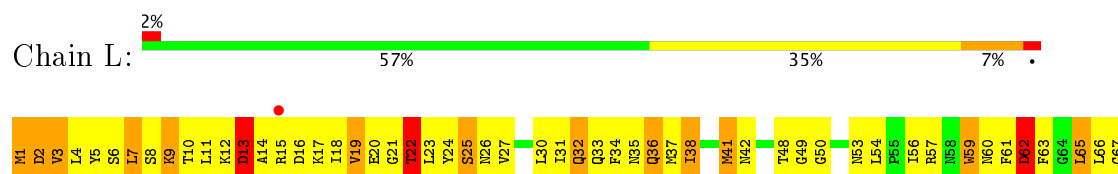
• Molecule 2: Intermediate capsid protein VP6

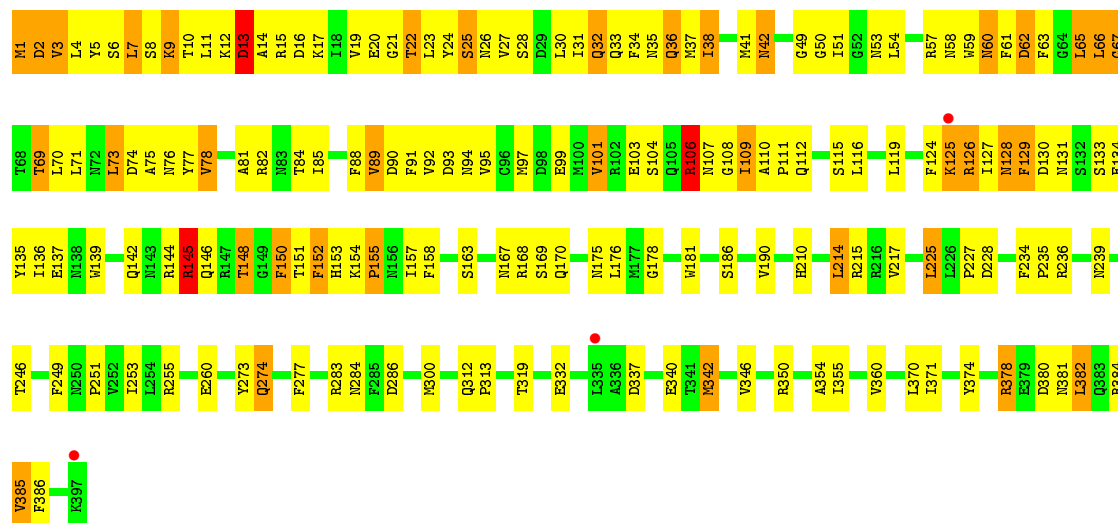


• Molecule 2: Intermediate capsid protein VP6

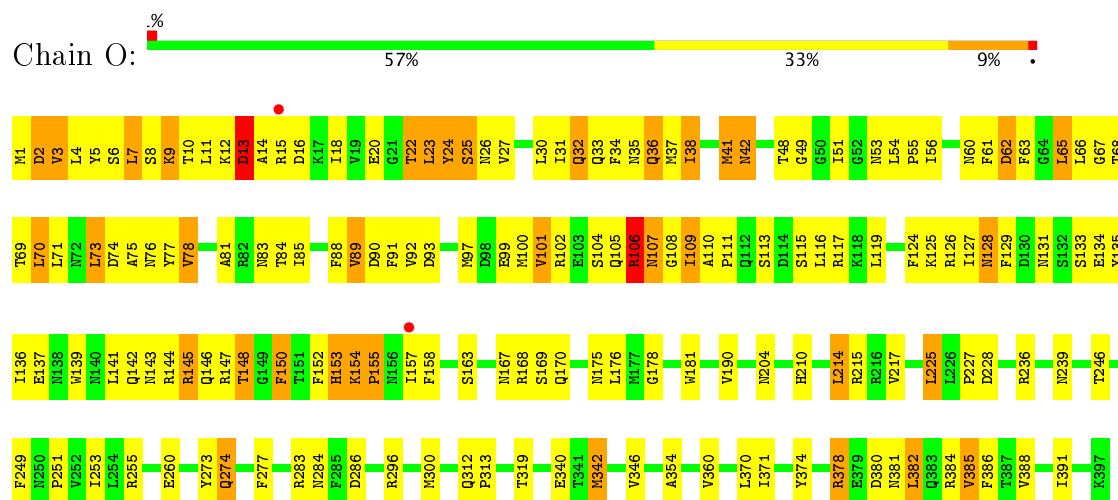


• Molecule 2: Intermediate capsid protein VP6





• Molecule 2: Intermediate capsid protein VP6



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	740.75Å 1198.07Å 1345.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.80 214.13 – 3.80	Depositor EDS
% Data completeness (in resolution range)	15.9 (30.00-3.80) 16.0 (214.13-3.80)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.49 (at 3.78Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.328 , 0.339 (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å ²)	167.1	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 164.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	54109	wwPDB-VP
Average B, all atoms (Å ²)	154.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.48	0/6491	0.84	9/8806 (0.1%)
1	B	0.50	0/6745	0.82	10/9149 (0.1%)
2	C	0.51	0/3232	0.78	5/4397 (0.1%)
2	D	0.51	0/3232	0.78	5/4397 (0.1%)
2	E	0.51	0/3232	0.77	5/4397 (0.1%)
2	F	0.50	0/3232	0.76	5/4397 (0.1%)
2	G	0.50	0/3232	0.77	5/4397 (0.1%)
2	H	0.50	0/3232	0.76	5/4397 (0.1%)
2	I	0.50	0/3232	0.77	5/4397 (0.1%)
2	J	0.51	0/3232	0.78	5/4397 (0.1%)
2	K	0.51	0/3232	0.77	5/4397 (0.1%)
2	L	0.51	0/3232	0.77	5/4397 (0.1%)
2	M	0.51	0/3232	0.77	5/4397 (0.1%)
2	N	0.51	0/3232	0.77	5/4397 (0.1%)
2	O	0.52	0/3232	0.79	7/4397 (0.2%)
All	All	0.50	0/55252	0.79	86/75116 (0.1%)

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

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

There are no bond length outliers.

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	TYR	CB-CG-CD2	10.70	127.42	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	TYR	CB-CG-CD1	-9.86	115.08	121.00
1	A	273	TYR	CA-CB-CG	9.85	132.12	113.40
1	B	273	TYR	CB-CG-CD1	9.85	126.91	121.00
1	B	273	TYR	CB-CG-CD2	-9.21	115.48	121.00
1	B	273	TYR	CA-CB-CG	9.02	130.53	113.40
1	A	367	LEU	N-CA-C	-7.59	90.51	111.00
1	A	298	TYR	N-CA-C	7.41	131.01	111.00
2	L	384	ARG	NE-CZ-NH2	7.00	123.80	120.30
2	H	384	ARG	NE-CZ-NH2	6.92	123.76	120.30
2	F	384	ARG	NE-CZ-NH2	6.86	123.73	120.30
2	I	384	ARG	NE-CZ-NH2	6.80	123.70	120.30
2	K	384	ARG	NE-CZ-NH2	6.75	123.67	120.30
1	A	639	LYS	N-CA-C	-6.67	92.98	111.00
2	D	236	ARG	NE-CZ-NH2	6.67	123.64	120.30
2	C	384	ARG	NE-CZ-NH2	6.67	123.64	120.30
2	O	384	ARG	NE-CZ-NH2	6.66	123.63	120.30
2	N	384	ARG	NE-CZ-NH2	6.62	123.61	120.30
2	E	384	ARG	NE-CZ-NH2	6.59	123.59	120.30
2	F	236	ARG	NE-CZ-NH2	6.57	123.58	120.30
2	D	384	ARG	NE-CZ-NH2	6.57	123.58	120.30
2	C	283	ARG	NE-CZ-NH2	6.51	123.56	120.30
2	L	236	ARG	NE-CZ-NH2	6.51	123.56	120.30
2	H	236	ARG	NE-CZ-NH2	6.51	123.55	120.30
2	M	283	ARG	NE-CZ-NH2	6.46	123.53	120.30
2	J	283	ARG	NE-CZ-NH2	6.42	123.51	120.30
2	M	236	ARG	NE-CZ-NH2	6.41	123.51	120.30
2	J	384	ARG	NE-CZ-NH2	6.40	123.50	120.30
2	M	384	ARG	NE-CZ-NH2	6.38	123.49	120.30
2	J	236	ARG	NE-CZ-NH2	6.38	123.49	120.30
2	I	236	ARG	NE-CZ-NH2	6.37	123.49	120.30
2	G	236	ARG	NE-CZ-NH2	6.35	123.47	120.30
2	N	236	ARG	NE-CZ-NH2	6.34	123.47	120.30
2	D	283	ARG	NE-CZ-NH2	6.30	123.45	120.30
2	O	283	ARG	NE-CZ-NH2	6.27	123.44	120.30
2	N	283	ARG	NE-CZ-NH2	6.26	123.43	120.30
2	G	384	ARG	NE-CZ-NH2	6.25	123.43	120.30
2	O	236	ARG	NE-CZ-NH2	6.25	123.42	120.30
2	E	236	ARG	NE-CZ-NH2	6.23	123.42	120.30
2	C	236	ARG	NE-CZ-NH2	6.23	123.42	120.30
2	K	236	ARG	NE-CZ-NH2	6.19	123.40	120.30
2	G	283	ARG	NE-CZ-NH2	6.17	123.39	120.30
2	E	283	ARG	NE-CZ-NH2	6.13	123.37	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	283	ARG	NE-CZ-NH2	6.12	123.36	120.30
1	B	636	LYS	N-CA-C	-6.10	94.53	111.00
2	K	283	ARG	NE-CZ-NH2	6.08	123.34	120.30
2	L	283	ARG	NE-CZ-NH2	6.08	123.34	120.30
2	H	283	ARG	NE-CZ-NH2	6.06	123.33	120.30
2	I	283	ARG	NE-CZ-NH2	6.03	123.31	120.30
2	O	154	LYS	N-CA-C	-5.98	94.86	111.00
2	O	300	MET	CG-SD-CE	5.80	109.48	100.20
2	C	300	MET	CG-SD-CE	5.80	109.47	100.20
2	F	300	MET	CG-SD-CE	5.79	109.47	100.20
2	I	300	MET	CG-SD-CE	5.78	109.44	100.20
2	N	300	MET	CG-SD-CE	5.76	109.42	100.20
2	L	300	MET	CG-SD-CE	5.76	109.41	100.20
1	B	497	ILE	N-CA-C	-5.75	95.47	111.00
2	M	300	MET	CG-SD-CE	5.75	109.41	100.20
2	D	300	MET	CG-SD-CE	5.75	109.39	100.20
2	J	300	MET	CG-SD-CE	5.74	109.39	100.20
2	G	300	MET	CG-SD-CE	5.73	109.37	100.20
2	H	300	MET	CG-SD-CE	5.72	109.36	100.20
2	K	300	MET	CG-SD-CE	5.70	109.31	100.20
1	B	76	LEU	CA-CB-CG	5.69	128.40	115.30
2	E	300	MET	CG-SD-CE	5.63	109.21	100.20
1	B	273	TYR	CB-CA-C	-5.50	99.39	110.40
1	B	811	LEU	N-CA-C	-5.48	96.21	111.00
2	M	342	MET	CG-SD-CE	5.35	108.75	100.20
2	D	342	MET	CG-SD-CE	5.32	108.70	100.20
2	G	342	MET	CG-SD-CE	5.29	108.67	100.20
1	A	317	LEU	CA-CB-CG	-5.27	103.18	115.30
2	J	342	MET	CG-SD-CE	5.27	108.63	100.20
1	B	317	LEU	CA-CB-CG	-5.25	103.24	115.30
2	L	342	MET	CG-SD-CE	5.23	108.57	100.20
2	O	153	HIS	N-CA-C	5.22	125.09	111.00
2	E	342	MET	CG-SD-CE	5.21	108.54	100.20
2	N	342	MET	CG-SD-CE	5.21	108.53	100.20
2	F	342	MET	CG-SD-CE	5.19	108.51	100.20
2	O	342	MET	CG-SD-CE	5.19	108.50	100.20
2	I	342	MET	CG-SD-CE	5.18	108.49	100.20
1	B	82	HIS	N-CA-C	-5.17	97.05	111.00
2	C	342	MET	CG-SD-CE	5.16	108.46	100.20
2	K	342	MET	CG-SD-CE	5.15	108.44	100.20
2	H	342	MET	CG-SD-CE	5.14	108.43	100.20
1	A	842	LEU	CA-CB-CG	-5.07	103.64	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	719	GLY	N-CA-C	-5.06	100.46	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	273	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6374	0	6394	992	0
1	B	6624	0	6652	1122	0
2	C	3162	0	3101	170	0
2	D	3162	0	3101	179	0
2	E	3162	0	3101	164	0
2	F	3162	0	3101	160	0
2	G	3162	0	3101	149	0
2	H	3162	0	3101	175	0
2	I	3162	0	3101	215	0
2	J	3162	0	3101	187	0
2	K	3162	0	3101	166	0
2	L	3162	0	3101	178	0
2	M	3162	0	3101	173	0
2	N	3162	0	3101	191	0
2	O	3162	0	3101	163	0
3	C	1	0	0	0	0
3	F	1	0	0	0	0
3	I	1	0	0	0	0
3	L	1	0	0	0	0
3	O	1	0	0	0	0
All	All	54109	0	53359	4148	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 39.

All (4148) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:771:VAL:HB	1:B:809:PHE:HB3	1.23	1.18
1:A:333:VAL:HG11	1:A:380:LYS:HA	1.27	1.15
1:A:428:GLN:OE1	1:A:456:PHE:HB2	1.46	1.13
1:A:563:MET:HA	1:A:563:MET:HE3	1.22	1.12
2:G:145:ARG:HB3	2:G:145:ARG:HH11	1.10	1.12
2:H:83:ASN:ND2	2:I:122:LEU:HB2	1.65	1.11
1:A:451:ASP:HB3	1:A:452:PRO:HD2	1.14	1.11
1:B:432:VAL:HA	1:B:436:ILE:HD11	1.18	1.11
1:B:734:ASN:HB3	1:B:737:GLU:HB2	1.28	1.10
1:B:718:TYR:HB3	1:B:721:VAL:HG21	1.33	1.10
1:A:270:ILE:HD11	1:A:292:LEU:HD11	1.31	1.09
1:B:548:ARG:NH1	1:B:878:ASN:H	1.50	1.09
2:L:22:THR:HG23	2:L:73:LEU:HD12	1.35	1.08
1:A:699:ILE:HG12	1:A:700:ALA:H	1.18	1.07
2:G:145:ARG:HD2	2:I:143:ASN:HA	1.34	1.07
1:B:200:VAL:HG21	1:B:243:SER:HB3	1.13	1.07
1:A:318:TRP:HA	1:A:321:ILE:HD12	1.34	1.07
2:N:106:ARG:H	2:N:106:ARG:HD3	1.17	1.06
1:B:790:ARG:HA	1:B:790:ARG:HE	0.98	1.06
1:B:318:TRP:HA	1:B:321:ILE:HD12	1.37	1.06
1:A:658:PRO:HG2	1:B:348:LYS:HG2	1.38	1.05
1:B:498:ARG:HB2	2:I:32:GLN:HE22	1.15	1.05
1:A:721:VAL:HG12	1:A:722:ASN:H	1.18	1.04
1:B:510:LEU:HD11	1:B:537:SER:HA	1.36	1.04
1:A:199:VAL:HG12	1:A:200:VAL:H	1.20	1.04
1:B:457:GLN:HG3	1:B:458:ILE:H	1.22	1.03
1:B:646:LEU:HA	1:B:649:LEU:HD12	1.40	1.03
1:A:428:GLN:NE2	1:A:455:PRO:HB2	1.73	1.03
1:A:451:ASP:CB	1:A:452:PRO:HD2	1.84	1.03
1:B:274:ILE:HG23	1:B:278:ILE:HD11	1.40	1.03
1:A:510:LEU:HD22	1:A:540:LEU:HD13	1.39	1.02
1:B:444:ARG:HH21	1:B:520:THR:HG23	1.20	1.02
1:A:310:LEU:HD12	1:A:310:LEU:H	1.21	1.02
1:B:457:GLN:HB2	1:B:476:ASN:ND2	1.75	1.02
1:A:513:LEU:HA	1:A:516:GLN:NE2	1.75	1.01
1:B:224:PHE:O	1:B:228:MET:HG2	1.61	1.01
1:B:573:THR:HG22	1:B:574:GLU:H	0.88	1.01
1:A:521:MET:HB3	1:A:522:PRO:HD3	1.39	1.01
1:B:790:ARG:HE	1:B:790:ARG:CA	1.70	1.00
1:A:506:LEU:HD23	1:A:544:VAL:HA	1.40	1.00
2:C:106:ARG:HD3	2:C:106:ARG:H	1.26	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:573:THR:HG22	1:B:574:GLU:N	1.71	0.99
1:A:705:ILE:HA	1:A:823:THR:HG22	1.43	0.99
1:B:674:VAL:HG21	1:B:679:LEU:HD13	1.44	0.99
1:B:510:LEU:HD22	1:B:540:LEU:HD13	1.42	0.99
1:B:573:THR:CG2	1:B:574:GLU:H	1.71	0.99
1:B:473:HIS:HB2	2:I:126:ARG:HH22	1.21	0.99
2:L:42:ASN:HA	2:L:61:PHE:HB2	1.43	0.98
1:B:371:ASN:HD22	1:B:583:SER:HB3	1.28	0.98
1:B:204:THR:HG23	1:B:244:ILE:HG22	1.44	0.98
2:H:106:ARG:H	2:H:106:ARG:HD3	1.26	0.98
1:A:275:PRO:HB2	1:A:278:ILE:HD11	1.45	0.98
1:B:265:LEU:HB3	1:B:296:ALA:HB1	1.46	0.98
1:B:435:ILE:HG22	1:B:436:ILE:H	1.29	0.98
2:J:106:ARG:HD3	2:J:106:ARG:H	1.23	0.97
1:B:743:ASP:C	1:B:744:TYR:HD2	1.67	0.97
1:B:700:ALA:HB2	1:B:827:LYS:HB2	1.45	0.97
1:B:700:ALA:CB	1:B:827:LYS:HB2	1.95	0.97
1:A:540:LEU:O	1:A:544:VAL:HG23	1.64	0.97
1:A:270:ILE:HG23	1:A:854:LEU:HD21	1.46	0.96
1:A:192:ASN:O	1:A:193:SER:HB3	1.65	0.96
1:B:200:VAL:HG21	1:B:243:SER:CB	1.96	0.96
2:H:83:ASN:HD21	2:I:122:LEU:HB2	1.30	0.96
1:A:660:ASP:HB3	1:B:539:ARG:HD2	1.43	0.96
1:A:588:ILE:HG22	1:A:589:GLY:H	1.28	0.96
1:B:717:MET:HE1	1:B:830:PRO:HD2	1.48	0.95
1:B:458:ILE:HD12	1:B:459:ALA:N	1.81	0.95
1:B:435:ILE:O	1:B:438:PRO:HD2	1.67	0.95
2:I:145:ARG:NH1	2:I:145:ARG:HB3	1.82	0.95
1:A:563:MET:HA	1:A:563:MET:CE	1.98	0.94
1:A:510:LEU:HD11	1:A:537:SER:HA	1.46	0.94
1:A:779:ASP:HA	1:A:798:ILE:CD1	1.98	0.93
1:B:446:HIS:O	1:B:447:TYR:HB2	1.68	0.93
2:O:27:VAL:O	2:O:31:ILE:HG12	1.66	0.93
1:B:764:PRO:O	1:B:765:PHE:HB3	1.65	0.93
1:B:518:PHE:HB3	1:B:519:PRO:HD2	1.49	0.93
1:B:790:ARG:HA	1:B:790:ARG:NE	1.84	0.92
1:A:428:GLN:HE21	1:A:455:PRO:HB2	1.30	0.92
2:G:145:ARG:HB3	2:G:145:ARG:NH1	1.84	0.92
1:B:126:PHE:HD2	1:B:126:PHE:H	1.09	0.92
1:B:190:ASN:HD21	1:B:193:SER:HB3	1.31	0.92
1:B:722:ASN:HD22	1:B:824:LYS:HA	1.35	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:6:SER:OG	2:G:128:ASN:HA	1.70	0.92
1:A:779:ASP:HA	1:A:798:ILE:HD12	1.50	0.91
1:B:428:GLN:HB2	1:B:456:PHE:CD1	2.05	0.91
1:B:513:LEU:HA	1:B:516:GLN:NE2	1.85	0.91
1:B:803:ASN:H	1:B:807:ASN:HD21	1.17	0.91
1:A:661:GLN:HE21	1:B:348:LYS:NZ	1.67	0.91
1:B:454:THR:HG21	1:B:476:ASN:ND2	1.86	0.91
1:B:166:PHE:HE2	1:B:689:MET:HA	1.34	0.91
1:B:459:ALA:HB1	1:B:463:ILE:HD11	1.51	0.90
1:A:588:ILE:HG22	1:A:589:GLY:N	1.85	0.90
2:L:88:PHE:O	2:L:92:VAL:HG23	1.72	0.90
1:A:126:PHE:HD2	1:A:126:PHE:N	1.68	0.90
1:A:339:LEU:HD22	1:A:588:ILE:HA	1.53	0.90
2:L:106:ARG:H	2:L:106:ARG:HD3	1.37	0.90
2:N:145:ARG:O	2:N:146:GLN:HG3	1.71	0.90
2:C:88:PHE:O	2:C:92:VAL:HG23	1.72	0.89
1:B:509:ALA:O	1:B:513:LEU:HG	1.71	0.89
1:A:169:LEU:O	1:A:173:VAL:HG23	1.73	0.89
1:A:244:ILE:HD13	1:A:835:PHE:HE1	1.38	0.89
1:A:660:ASP:HB3	1:B:539:ARG:HH11	1.38	0.89
2:K:106:ARG:H	2:K:106:ARG:HD3	1.37	0.89
1:A:855:LEU:O	1:A:857:PHE:N	2.06	0.88
1:B:457:GLN:O	1:B:459:ALA:N	2.05	0.88
1:A:371:ASN:C	1:A:373:GLN:H	1.71	0.88
1:A:486:ASP:HB2	1:A:490:ASN:HD22	1.38	0.88
1:B:99:GLU:HB3	1:B:100:PRO:HD3	1.54	0.88
1:B:658:PRO:HB2	1:B:661:GLN:HG2	1.56	0.88
1:B:874:MET:O	1:B:875:ARG:HB2	1.73	0.88
2:M:88:PHE:O	2:M:92:VAL:HG23	1.74	0.88
1:A:194:ARG:HH11	1:A:229:ARG:HG2	1.39	0.88
2:J:106:ARG:HD3	2:J:106:ARG:N	1.87	0.88
1:B:803:ASN:H	1:B:807:ASN:ND2	1.72	0.87
1:B:182:LEU:HD11	1:B:847:THR:H	1.38	0.87
1:B:297:ARG:HG3	1:B:848:PHE:HD2	1.40	0.87
1:A:428:GLN:HB2	1:A:456:PHE:CD1	2.09	0.86
1:A:509:ALA:O	1:A:513:LEU:HG	1.75	0.86
1:B:447:TYR:O	1:B:448:ARG:HG2	1.73	0.86
2:D:88:PHE:O	2:D:92:VAL:HG23	1.73	0.86
2:O:88:PHE:O	2:O:92:VAL:HG23	1.72	0.86
2:I:76:ASN:H	2:M:76:ASN:HB2	1.37	0.86
1:B:451:ASP:H	1:B:452:PRO:HD3	1.39	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:513:LEU:HA	1:B:516:GLN:CD	1.95	0.86
1:B:413:VAL:HG12	1:B:414:VAL:N	1.88	0.86
2:N:88:PHE:O	2:N:92:VAL:HG23	1.74	0.86
1:B:473:HIS:HB2	2:I:126:ARG:NH2	1.91	0.86
1:B:745:ALA:HB1	1:B:748:THR:HB	1.57	0.86
2:H:88:PHE:O	2:H:92:VAL:HG23	1.73	0.86
2:I:24:TYR:O	2:I:27:VAL:HG22	1.74	0.86
1:B:540:LEU:O	1:B:544:VAL:HG23	1.75	0.86
1:B:182:LEU:HD23	1:B:183:LEU:H	1.40	0.86
1:A:150:LEU:HD12	1:A:696:SER:HB2	1.58	0.86
1:A:275:PRO:HB2	1:A:278:ILE:CD1	2.04	0.86
2:E:88:PHE:O	2:E:92:VAL:HG23	1.75	0.86
2:J:88:PHE:O	2:J:92:VAL:HG23	1.75	0.85
1:A:451:ASP:HB3	1:A:452:PRO:CD	2.03	0.85
2:I:88:PHE:O	2:I:92:VAL:HG23	1.76	0.85
1:B:590:ASN:HD22	1:B:590:ASN:N	1.74	0.85
1:B:366:PHE:C	1:B:368:THR:H	1.76	0.85
2:C:150:PHE:HB2	2:C:152:PHE:CE1	2.11	0.85
1:A:366:PHE:C	1:A:368:THR:H	1.76	0.85
2:F:88:PHE:O	2:F:92:VAL:HG23	1.75	0.85
2:M:106:ARG:H	2:M:106:ARG:HD3	1.40	0.85
1:B:126:PHE:HD2	1:B:126:PHE:N	1.73	0.85
2:G:88:PHE:O	2:G:92:VAL:HG23	1.75	0.85
2:H:6:SER:OG	2:H:128:ASN:HA	1.77	0.85
2:M:6:SER:OG	2:M:128:ASN:HA	1.76	0.85
1:A:239:VAL:HG22	1:A:846:LEU:HG	1.58	0.84
1:B:723:ILE:HG22	1:B:724:ALA:H	1.40	0.84
1:B:306:ASP:O	1:B:308:LEU:N	2.10	0.84
1:B:518:PHE:HD2	2:H:69:THR:HB	1.40	0.84
2:K:88:PHE:O	2:K:92:VAL:HG23	1.76	0.84
1:A:660:ASP:HB3	1:B:539:ARG:CD	2.05	0.84
1:B:415:PRO:HG2	1:B:480:PHE:HD1	1.42	0.84
1:B:825:VAL:HG12	1:B:826:TYR:N	1.91	0.84
1:B:701:GLN:HB2	1:B:826:TYR:HD2	1.40	0.84
2:L:144:ARG:O	2:L:145:ARG:HB2	1.74	0.84
1:A:125:ILE:HD12	1:A:125:ILE:N	1.92	0.84
1:A:570:THR:HG22	1:A:571:LEU:H	1.42	0.84
1:B:200:VAL:CG2	1:B:243:SER:HB3	2.05	0.84
1:B:735:LEU:HG	1:B:760:VAL:O	1.78	0.84
1:B:498:ARG:NH1	2:J:25:SER:HB3	1.92	0.84
1:B:471:TRP:HB2	1:B:512:GLN:OE1	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:PHE:CD2	1:A:126:PHE:N	2.42	0.84
1:B:503:ILE:HD11	1:B:548:ARG:HG2	1.58	0.84
2:F:82:ARG:NH1	2:H:144:ARG:HD2	1.93	0.84
2:I:76:ASN:HB2	2:M:76:ASN:HB2	1.57	0.84
1:A:771:VAL:HG13	1:A:772:ILE:H	1.43	0.84
1:A:361:GLN:HB2	1:A:528:SER:OG	1.78	0.83
1:B:428:GLN:HG2	1:B:429:LEU:N	1.92	0.83
1:B:435:ILE:HG22	1:B:436:ILE:N	1.93	0.83
2:L:23:LEU:HD21	2:N:36:GLN:OE1	1.76	0.83
1:A:158:GLY:H	1:A:762:ALA:HB3	1.43	0.83
1:B:454:THR:HG21	1:B:476:ASN:HD21	1.39	0.83
2:I:23:LEU:HD23	2:I:24:TYR:N	1.94	0.83
1:A:216:GLU:CD	1:A:216:GLU:H	1.81	0.83
1:A:474:PHE:O	1:A:478:ASN:HB2	1.77	0.83
1:B:126:PHE:N	1:B:126:PHE:CD2	2.43	0.83
1:B:457:GLN:HB2	1:B:476:ASN:CG	1.98	0.83
1:B:799:LEU:HD22	1:B:800:TYR:N	1.93	0.83
1:A:471:TRP:HB2	1:A:512:GLN:OE1	1.79	0.83
1:A:524:ASP:O	1:A:526:LYS:N	2.10	0.83
1:A:647:LYS:HG3	1:A:654:VAL:HG21	1.59	0.83
2:O:6:SER:OG	2:O:128:ASN:HA	1.80	0.82
2:I:38:ILE:HG22	2:I:42:ASN:HD21	1.42	0.82
1:B:516:GLN:HA	1:B:518:PHE:HE1	1.41	0.82
1:B:590:ASN:H	1:B:590:ASN:HD22	1.25	0.82
1:A:461:GLN:HA	2:F:32:GLN:HE22	1.43	0.82
1:B:428:GLN:HA	1:B:431:ILE:HD12	1.61	0.82
2:F:150:PHE:HB2	2:F:152:PHE:CE1	2.15	0.82
1:A:486:ASP:HB2	1:A:490:ASN:ND2	1.94	0.81
1:A:734:ASN:HB3	1:A:737:GLU:HG2	1.61	0.81
1:B:722:ASN:HB2	1:B:824:LYS:HB3	1.62	0.81
2:H:109:ILE:HG13	2:H:109:ILE:O	1.79	0.81
1:B:454:THR:CG2	1:B:476:ASN:HD21	1.92	0.81
1:A:406:SER:O	1:A:409:TRP:HB3	1.81	0.81
2:L:22:THR:HB	2:N:128:ASN:O	1.79	0.81
1:B:494:ASN:ND2	1:B:495:ASP:H	1.79	0.81
1:B:769:SER:HB3	1:B:807:ASN:OD1	1.80	0.81
1:A:712:LEU:HB3	1:A:721:VAL:O	1.79	0.81
1:B:218:GLU:HG3	1:B:221:VAL:HG23	1.62	0.81
1:B:193:SER:HB2	1:B:226:ALA:HA	1.62	0.81
1:B:725:ARG:H	1:B:725:ARG:HD2	1.44	0.81
1:B:537:SER:O	1:B:540:LEU:HB3	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:76:ASN:HB2	2:J:76:ASN:HB2	1.60	0.81
1:B:498:ARG:HB2	2:I:32:GLN:NE2	1.94	0.81
1:B:511:MET:CE	2:J:70:LEU:HG	2.09	0.81
1:A:459:ALA:O	1:A:462:GLN:HB2	1.81	0.81
1:B:118:LYS:HG2	1:B:119:GLN:H	1.46	0.81
2:I:76:ASN:CB	2:M:76:ASN:HB2	2.11	0.81
1:A:712:LEU:HG	1:A:819:PRO:HB2	1.61	0.81
1:B:315:GLU:HB3	1:B:571:LEU:HD11	1.61	0.80
2:D:128:ASN:O	2:E:22:THR:HB	1.82	0.80
2:E:24:TYR:O	2:E:27:VAL:HG22	1.82	0.80
2:O:67:GLY:O	2:O:69:THR:N	2.14	0.80
1:A:660:ASP:O	1:A:662:MET:N	2.14	0.80
1:B:510:LEU:CD1	1:B:537:SER:HA	2.11	0.80
1:A:362:SER:HB2	1:A:365:GLN:NE2	1.97	0.80
1:A:699:ILE:HG12	1:A:700:ALA:N	1.97	0.80
2:L:150:PHE:HB2	2:L:152:PHE:CE1	2.17	0.80
1:A:546:LEU:HD21	1:A:588:ILE:CD1	2.12	0.80
1:A:126:PHE:H	1:A:126:PHE:HD2	1.26	0.80
1:A:270:ILE:CD1	1:A:292:LEU:HD11	2.10	0.80
1:B:239:VAL:HG23	1:B:844:SER:O	1.81	0.80
1:A:769:SER:HB3	1:A:807:ASN:OD1	1.82	0.80
2:N:144:ARG:O	2:N:145:ARG:HB2	1.81	0.80
1:B:869:VAL:CG1	1:B:873:ASN:HA	2.11	0.80
1:A:437:TYR:N	1:A:438:PRO:HD2	1.97	0.79
1:B:393:SER:O	1:B:394:LEU:HD23	1.82	0.79
1:B:506:LEU:HD23	1:B:544:VAL:HA	1.62	0.79
1:B:743:ASP:CG	1:B:745:ALA:H	1.85	0.79
1:A:199:VAL:HG12	1:A:200:VAL:N	1.97	0.79
1:A:303:LEU:HA	1:A:615:ASN:ND2	1.97	0.79
1:A:694:ARG:HG2	1:A:701:GLN:HE22	1.46	0.79
1:B:790:ARG:HG3	1:B:791:LYS:H	1.48	0.79
2:L:104:SER:O	2:L:108:GLY:HA3	1.82	0.79
1:A:869:VAL:HG11	1:A:873:ASN:HA	1.64	0.79
2:I:57:ARG:HH11	2:I:94:ASN:HD21	1.31	0.79
1:B:744:TYR:CD2	1:B:744:TYR:N	2.38	0.79
1:A:721:VAL:HG12	1:A:722:ASN:N	1.98	0.79
2:K:6:SER:OG	2:K:128:ASN:HA	1.82	0.79
1:B:457:GLN:HG3	1:B:458:ILE:N	1.98	0.79
1:B:465:ASN:HD22	1:B:468:VAL:HG23	1.47	0.79
1:A:480:PHE:CD2	1:A:493:LEU:HB3	2.18	0.79
1:A:606:VAL:HG23	1:A:607:ASN:H	1.46	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:673:PRO:O	1:B:674:VAL:HG13	1.83	0.79
2:H:2:ASP:HB2	2:H:128:ASN:HD21	1.46	0.79
1:B:124:ARG:C	1:B:125:ILE:HD12	2.02	0.79
2:N:50:GLY:O	2:N:51:ILE:HG23	1.83	0.79
1:A:869:VAL:CG1	1:A:873:ASN:HA	2.12	0.79
1:B:277:ARG:O	1:B:278:ILE:HG12	1.83	0.79
1:B:272:ASN:C	1:B:274:ILE:H	1.87	0.78
1:B:743:ASP:C	1:B:744:TYR:CD2	2.54	0.78
1:B:548:ARG:HH11	1:B:878:ASN:H	1.28	0.78
2:J:128:ASN:O	2:K:22:THR:HB	1.83	0.78
1:A:445:MET:C	1:A:447:TYR:H	1.84	0.78
2:M:145:ARG:O	2:M:146:GLN:HG3	1.83	0.78
1:A:305:GLN:O	1:A:307:ARG:HG3	1.82	0.78
1:A:428:GLN:HG2	1:A:429:LEU:N	1.98	0.78
1:B:523:VAL:C	1:B:525:TYR:H	1.85	0.78
1:A:118:LYS:HG2	1:A:119:GLN:N	1.98	0.78
1:A:480:PHE:HD2	1:A:493:LEU:HB3	1.49	0.78
1:B:606:VAL:HG23	1:B:607:ASN:H	1.46	0.78
1:B:549:LEU:HD13	1:B:877:MET:HE1	1.64	0.78
1:A:639:LYS:O	1:A:643:GLU:HG3	1.84	0.78
2:I:42:ASN:HA	2:I:61:PHE:HB2	1.66	0.78
1:B:702:GLY:HA3	1:B:759:LEU:O	1.84	0.77
1:B:717:MET:CE	1:B:830:PRO:HD2	2.15	0.77
2:N:144:ARG:NH2	2:N:146:GLN:HE22	1.81	0.77
1:B:374:ALA:HB1	1:B:580:SER:HB3	1.66	0.77
1:B:562:THR:HB	1:B:611:HIS:CD2	2.20	0.77
1:B:779:ASP:HA	1:B:798:ILE:CD1	2.14	0.77
1:B:406:SER:O	1:B:409:TRP:HB3	1.84	0.77
2:E:93:ASP:O	2:E:97:MET:HG3	1.84	0.77
2:H:106:ARG:CD	2:H:106:ARG:H	1.98	0.77
2:I:128:ASN:HD22	2:J:19:VAL:HB	1.49	0.77
2:K:93:ASP:O	2:K:97:MET:HG3	1.85	0.77
2:M:22:THR:HG23	2:M:73:LEU:HD12	1.66	0.77
1:B:764:PRO:O	1:B:765:PHE:CB	2.33	0.77
1:A:471:TRP:O	1:A:475:VAL:HG23	1.85	0.77
1:B:169:LEU:O	1:B:173:VAL:HG23	1.84	0.77
1:B:855:LEU:O	1:B:857:PHE:N	2.17	0.77
1:B:204:THR:CG2	1:B:244:ILE:HG22	2.14	0.77
2:H:93:ASP:O	2:H:97:MET:HG3	1.85	0.77
1:A:371:ASN:C	1:A:373:GLN:N	2.37	0.76
1:B:218:GLU:HG3	1:B:221:VAL:CG2	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:503:ILE:O	1:B:505:GLN:HG2	1.85	0.76
1:B:573:THR:O	1:B:574:GLU:HG2	1.84	0.76
1:B:166:PHE:CE2	1:B:689:MET:HA	2.20	0.76
1:B:744:TYR:HD2	1:B:744:TYR:N	1.77	0.76
2:F:17:LYS:HG2	2:H:130:ASP:HA	1.67	0.76
1:A:405:ILE:HG21	1:A:536:LEU:HG	1.67	0.76
1:A:614:TYR:O	1:A:618:ILE:HG12	1.85	0.76
1:B:200:VAL:HG23	1:B:242:PRO:O	1.86	0.76
1:B:731:GLN:HG2	2:D:62:ASP:HB2	1.67	0.76
1:A:548:ARG:HH12	1:A:878:ASN:H	1.34	0.76
1:A:122:LEU:HG	1:A:201:ASP:OD2	1.84	0.76
1:A:588:ILE:CG2	1:A:589:GLY:H	1.99	0.76
1:B:133:ILE:HD12	1:B:145:ARG:HB2	1.66	0.76
1:A:461:GLN:HA	2:F:32:GLN:NE2	2.00	0.76
1:B:678:ARG:O	1:B:681:ILE:HG22	1.85	0.76
2:C:24:TYR:O	2:C:27:VAL:HG22	1.86	0.76
2:D:67:GLY:O	2:D:68:THR:HG23	1.85	0.76
2:I:110:ALA:HB1	2:I:111:PRO:CD	2.16	0.76
1:A:678:ARG:O	1:A:681:ILE:HG22	1.86	0.76
1:A:158:GLY:H	1:A:762:ALA:CB	1.99	0.76
1:B:199:VAL:HG12	1:B:200:VAL:N	2.00	0.76
1:B:701:GLN:HA	1:B:761:GLY:O	1.85	0.76
2:G:93:ASP:O	2:G:97:MET:HG3	1.85	0.76
1:A:503:ILE:HD13	1:A:547:THR:HB	1.68	0.76
1:B:675:GLU:HB3	1:B:678:ARG:HG2	1.68	0.76
1:A:428:GLN:HA	1:A:431:ILE:HD12	1.68	0.76
1:A:244:ILE:HD13	1:A:835:PHE:CE1	2.21	0.76
1:B:96:PRO:O	1:B:652:PHE:HB3	1.84	0.76
2:I:93:ASP:O	2:I:97:MET:HG3	1.86	0.76
1:A:310:LEU:CD1	1:A:310:LEU:H	1.97	0.75
1:B:518:PHE:CB	1:B:519:PRO:HD2	2.14	0.75
2:C:145:ARG:HB3	2:C:145:ARG:NH1	2.02	0.75
2:F:104:SER:HB3	2:F:108:GLY:CA	2.16	0.75
1:B:781:THR:O	1:B:783:PHE:N	2.19	0.75
1:A:371:ASN:HA	1:A:374:ALA:HB3	1.68	0.75
1:A:457:GLN:HB2	1:A:476:ASN:HD21	1.52	0.75
2:L:19:VAL:HG23	2:N:128:ASN:HB3	1.69	0.75
2:J:93:ASP:O	2:J:97:MET:HG3	1.87	0.75
1:B:498:ARG:CB	2:I:32:GLN:HE22	1.97	0.75
1:B:251:ALA:HA	2:N:69:THR:HG21	1.69	0.75
1:A:694:ARG:HG2	1:A:701:GLN:NE2	2.01	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:38:ILE:HG22	2:C:42:ASN:HD21	1.51	0.74
1:B:698:LYS:O	1:B:699:ILE:HB	1.86	0.74
2:I:76:ASN:HB2	2:M:76:ASN:CB	2.17	0.74
1:A:148:TRP:CZ3	1:A:246:HIS:HB2	2.22	0.74
1:A:537:SER:O	1:A:540:LEU:HB3	1.87	0.74
1:B:491:GLN:HG3	1:B:565:MET:H	1.50	0.74
2:J:128:ASN:HB3	2:K:19:VAL:HG23	1.69	0.74
2:N:57:ARG:HH11	2:N:94:ASN:HD21	1.33	0.74
1:A:492:VAL:HG13	1:A:558:MET:SD	2.27	0.74
1:A:647:LYS:CG	1:A:654:VAL:HG21	2.17	0.74
1:B:482:GLN:HB2	1:B:493:LEU:HD22	1.70	0.74
1:B:675:GLU:HB3	1:B:678:ARG:CG	2.17	0.74
1:B:688:ASN:O	1:B:692:ILE:HD12	1.87	0.74
1:B:614:TYR:O	1:B:618:ILE:HG12	1.87	0.74
2:O:150:PHE:HB2	2:O:152:PHE:CE1	2.23	0.74
1:B:293:PRO:C	1:B:295:THR:H	1.90	0.74
2:D:23:LEU:HD23	2:D:24:TYR:N	2.03	0.74
2:D:93:ASP:O	2:D:97:MET:HG3	1.87	0.74
2:I:75:ALA:HB3	2:M:76:ASN:HA	1.68	0.74
2:L:93:ASP:O	2:L:97:MET:HG3	1.88	0.74
1:A:286:LEU:HD23	1:A:286:LEU:H	1.52	0.74
1:A:784:ALA:O	1:A:787:VAL:HG23	1.88	0.74
1:A:802:ILE:HA	1:A:807:ASN:HD21	1.52	0.74
1:B:190:ASN:ND2	1:B:193:SER:HB3	2.03	0.74
1:B:783:PHE:HD1	1:B:783:PHE:H	1.33	0.74
2:D:24:TYR:O	2:D:27:VAL:HG22	1.88	0.74
2:C:82:ARG:CZ	2:E:144:ARG:HD2	2.18	0.74
2:H:105:GLN:C	2:H:107:ASN:H	1.91	0.74
1:A:428:GLN:HB2	1:A:456:PHE:HD1	1.51	0.74
1:A:405:ILE:CG2	1:A:536:LEU:HG	2.18	0.74
2:E:54:LEU:HD12	2:E:55:PRO:HD2	1.70	0.74
1:A:164:GLU:O	1:A:167:LEU:HB3	1.87	0.74
1:A:301:PRO:O	1:A:303:LEU:HD23	1.87	0.74
1:A:252:PHE:HD2	1:A:684:LEU:HD21	1.52	0.74
1:B:510:LEU:HD11	1:B:537:SER:CA	2.15	0.74
2:D:6:SER:OG	2:D:128:ASN:HA	1.87	0.74
1:B:368:THR:HG22	1:B:371:ASN:HD21	1.51	0.73
1:B:433:ASN:ND2	1:B:446:HIS:HB3	2.02	0.73
2:J:150:PHE:HB2	2:J:152:PHE:CE1	2.22	0.73
1:A:117:LYS:O	1:A:179:ASP:HB2	1.88	0.73
1:A:275:PRO:CB	1:A:278:ILE:HD11	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:106:ARG:H	2:G:106:ARG:HD3	1.53	0.73
1:B:254:GLU:HG2	2:N:69:THR:HB	1.68	0.73
1:A:711:GLN:C	1:A:712:LEU:HD23	2.08	0.73
2:M:144:ARG:HD2	2:N:82:ARG:NH1	2.02	0.73
1:A:277:ARG:HD3	1:A:559:ALA:HB2	1.71	0.73
1:A:660:ASP:CB	1:B:539:ARG:HD2	2.19	0.73
1:B:257:LEU:O	1:B:260:GLN:HG3	1.88	0.73
2:C:93:ASP:O	2:C:97:MET:HG3	1.87	0.73
2:F:42:ASN:HA	2:F:61:PHE:HB2	1.70	0.73
2:H:109:ILE:HB	2:H:380:ASP:HB3	1.68	0.73
1:A:310:LEU:HD12	1:A:310:LEU:N	2.00	0.73
1:B:457:GLN:C	1:B:459:ALA:H	1.91	0.73
1:B:540:LEU:HD23	1:B:541:GLY:N	2.03	0.73
2:N:93:ASP:O	2:N:97:MET:HG3	1.87	0.73
1:A:499:ASN:HA	1:A:505:GLN:NE2	2.04	0.73
1:B:111:ILE:C	1:B:113:PRO:HD3	2.09	0.73
1:B:265:LEU:HB3	1:B:296:ALA:CB	2.17	0.73
2:I:145:ARG:HH11	2:I:145:ARG:HB3	1.50	0.73
2:N:24:TYR:O	2:N:27:VAL:HG22	1.89	0.73
1:A:245:LEU:HB3	1:A:249:ASP:HB2	1.71	0.73
1:A:286:LEU:HD23	1:A:286:LEU:N	2.04	0.73
1:B:703:VAL:HG13	1:B:824:LYS:O	1.89	0.73
2:F:93:ASP:O	2:F:97:MET:HG3	1.87	0.73
2:M:93:ASP:O	2:M:97:MET:HG3	1.88	0.73
1:A:631:LEU:HB3	1:A:633:LEU:HD13	1.69	0.73
1:A:661:GLN:HE21	1:B:348:LYS:HZ1	1.37	0.73
1:B:503:ILE:O	1:B:505:GLN:N	2.22	0.73
1:B:491:GLN:CD	1:B:564:ASN:HB3	2.08	0.73
1:B:674:VAL:HG23	1:B:679:LEU:HD22	1.69	0.73
1:B:771:VAL:HB	1:B:809:PHE:CB	2.11	0.73
1:B:770:SER:HB2	1:B:773:SER:OG	1.88	0.73
2:F:145:ARG:O	2:F:146:GLN:HG2	1.89	0.73
2:J:11:LEU:O	2:J:14:ALA:HB3	1.89	0.73
1:B:277:ARG:O	1:B:279:ARG:N	2.20	0.73
1:B:701:GLN:O	1:B:826:TYR:HB3	1.89	0.73
2:D:63:PHE:CD2	2:D:84:THR:HG23	2.24	0.73
2:H:27:VAL:O	2:H:31:ILE:HG12	1.88	0.73
2:F:23:LEU:HD21	2:H:36:GLN:OE1	1.89	0.73
1:B:436:ILE:HG13	1:B:437:TYR:H	1.54	0.72
1:B:471:TRP:O	1:B:475:VAL:HG23	1.88	0.72
2:H:106:ARG:N	2:H:106:ARG:HD3	2.03	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:643:GLU:HG2	1:A:662:MET:HE3	1.72	0.72
1:B:442:MET:CE	1:B:463:ILE:HG12	2.19	0.72
1:B:498:ARG:HH12	2:J:25:SER:HB3	1.52	0.72
1:B:521:MET:HB2	1:B:522:PRO:CD	2.19	0.72
1:B:712:LEU:CD1	1:B:722:ASN:HB3	2.18	0.72
1:A:510:LEU:CD1	1:A:537:SER:HA	2.20	0.72
1:B:435:ILE:C	1:B:436:ILE:HG12	2.08	0.72
1:B:516:GLN:HA	1:B:518:PHE:CE1	2.25	0.72
1:B:492:VAL:HG11	1:B:558:MET:HG2	1.71	0.72
1:B:630:ARG:O	1:B:631:LEU:HG	1.90	0.72
1:B:799:LEU:HD22	1:B:800:TYR:H	1.52	0.72
2:J:106:ARG:HG2	2:J:107:ASN:H	1.54	0.72
1:A:420:ILE:HG12	1:A:423:SER:HB2	1.69	0.72
1:A:496:ASN:HD22	1:A:498:ARG:HB2	1.53	0.72
1:A:629:ASN:O	1:A:631:LEU:N	2.17	0.72
1:B:615:ASN:O	1:B:618:ILE:HB	1.90	0.72
2:J:144:ARG:HD2	2:K:82:ARG:NH1	2.05	0.72
2:M:122:LEU:HB2	2:O:83:ASN:ND2	2.04	0.72
2:F:22:THR:HB	2:H:128:ASN:O	1.89	0.72
1:B:156:PRO:HB2	1:B:161:ASP:HB3	1.72	0.72
1:B:444:ARG:NH2	1:B:520:THR:HG23	2.03	0.72
1:A:239:VAL:CG2	1:A:846:LEU:HG	2.19	0.72
1:A:613:ASN:HD22	1:A:649:LEU:CD2	2.03	0.72
1:A:605:ASN:O	1:A:608:VAL:HB	1.90	0.72
1:A:146:TRP:O	1:A:833:PHE:HB3	1.89	0.72
1:A:721:VAL:CG1	1:A:722:ASN:H	2.01	0.72
1:B:551:ALA:O	1:B:555:GLU:HB2	1.90	0.72
1:B:825:VAL:HG12	1:B:826:TYR:H	1.53	0.72
2:D:145:ARG:O	2:D:146:GLN:HG3	1.90	0.72
2:I:135:TYR:OH	2:I:340:GLU:OE1	2.06	0.72
1:A:445:MET:O	1:A:447:TYR:N	2.23	0.71
1:B:355:LEU:HG	1:B:356:GLU:N	2.05	0.71
1:B:473:HIS:HB3	2:I:126:ARG:HH12	1.54	0.71
2:D:11:LEU:O	2:D:14:ALA:HB3	1.90	0.71
1:A:735:LEU:HG	1:A:760:VAL:O	1.89	0.71
1:A:764:PRO:O	1:A:797:PRO:HD2	1.91	0.71
1:B:422:GLU:HA	1:B:425:VAL:HG23	1.72	0.71
1:B:442:MET:HE1	1:B:463:ILE:HG12	1.71	0.71
1:B:480:PHE:CE2	1:B:493:LEU:HB2	2.24	0.71
2:J:130:ASP:HA	2:K:17:LYS:HG2	1.71	0.71
2:O:93:ASP:O	2:O:97:MET:HG3	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:PRO:CB	1:B:161:ASP:HB3	2.20	0.71
2:C:144:ARG:HD2	2:D:82:ARG:CZ	2.20	0.71
2:L:6:SER:OG	2:L:128:ASN:HA	1.91	0.71
1:A:246:HIS:HB3	1:A:249:ASP:OD2	1.90	0.71
1:A:709:ASP:HB3	1:A:820:THR:HG23	1.73	0.71
1:B:194:ARG:O	1:B:196:ALA:N	2.23	0.71
1:B:428:GLN:OE1	1:B:456:PHE:HB2	1.90	0.71
2:I:11:LEU:O	2:I:14:ALA:HB3	1.91	0.71
2:I:150:PHE:HB2	2:I:152:PHE:CE1	2.25	0.71
1:A:236:ARG:HB2	1:A:238:VAL:HG23	1.72	0.71
1:B:166:PHE:CE2	1:B:689:MET:HG3	2.24	0.71
1:B:791:LYS:O	1:B:792:VAL:HG22	1.91	0.71
2:K:11:LEU:O	2:K:14:ALA:HB3	1.91	0.71
1:A:530:GLN:HA	1:A:533:ILE:HD12	1.71	0.71
1:B:605:ASN:O	1:B:608:VAL:HB	1.91	0.71
2:K:38:ILE:HG22	2:K:42:ASN:HD21	1.56	0.71
1:A:194:ARG:NH1	1:A:229:ARG:HG2	2.05	0.71
2:N:11:LEU:O	2:N:14:ALA:HB3	1.91	0.71
2:N:38:ILE:HG22	2:N:42:ASN:HD21	1.56	0.71
1:B:277:ARG:HG2	1:B:278:ILE:H	1.54	0.71
2:H:116:LEU:HD12	2:H:119:LEU:HB2	1.73	0.71
2:O:11:LEU:O	2:O:14:ALA:HB3	1.90	0.71
1:A:283:ASN:O	1:A:863:VAL:HG23	1.91	0.71
2:G:36:GLN:OE1	2:H:23:LEU:HD21	1.91	0.71
1:A:496:ASN:ND2	1:A:498:ARG:HB2	2.06	0.71
1:A:510:LEU:HD11	1:A:537:SER:CA	2.21	0.71
1:B:712:LEU:HD12	1:B:722:ASN:HB3	1.72	0.71
1:B:548:ARG:HH12	1:B:878:ASN:H	1.35	0.71
2:G:4:LEU:HA	2:G:7:LEU:HD12	1.73	0.71
2:K:53:ASN:HD22	2:K:354:ALA:HB3	1.56	0.71
2:M:11:LEU:O	2:M:14:ALA:HB3	1.91	0.71
1:A:312:ASP:O	1:A:313:ASN:HB3	1.90	0.70
1:A:415:PRO:HG2	1:A:480:PHE:CD1	2.26	0.70
1:A:501:HIS:C	1:A:503:ILE:HG13	2.11	0.70
1:B:374:ALA:HB1	1:B:580:SER:HA	1.71	0.70
2:L:82:ARG:CZ	2:N:144:ARG:HD2	2.21	0.70
1:B:164:GLU:O	1:B:167:LEU:HB3	1.90	0.70
2:D:4:LEU:HA	2:D:7:LEU:HD12	1.73	0.70
2:M:150:PHE:HB2	2:M:152:PHE:CE1	2.26	0.70
1:A:615:ASN:O	1:A:618:ILE:HB	1.89	0.70
1:B:518:PHE:CD2	2:H:69:THR:HB	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:477:ASN:ND2	2:I:39:ILE:HG21	2.06	0.70
2:J:106:ARG:H	2:J:106:ARG:CD	2.03	0.70
2:J:109:ILE:HD12	2:J:109:ILE:O	1.91	0.70
1:B:259:HIS:CD2	1:B:677:ARG:HG3	2.25	0.70
2:C:11:LEU:O	2:C:14:ALA:HB3	1.90	0.70
2:J:12:LYS:C	2:J:14:ALA:H	1.94	0.70
1:B:511:MET:HE1	2:J:70:LEU:HG	1.72	0.70
2:K:54:LEU:HD12	2:K:55:PRO:HD2	1.71	0.70
2:N:4:LEU:HA	2:N:7:LEU:HD12	1.73	0.70
1:A:506:LEU:CD2	1:A:544:VAL:HA	2.18	0.70
1:A:551:ALA:O	1:A:555:GLU:HB2	1.92	0.70
1:B:230:GLN:HA	1:B:242:PRO:HD3	1.73	0.70
1:A:131:LEU:HD12	1:A:132:PRO:HD2	1.74	0.70
1:A:467:GLN:HB2	1:A:515:ARG:HD2	1.72	0.70
1:A:762:ALA:O	1:A:763:LEU:HG	1.92	0.70
1:B:508:GLU:HG2	1:B:512:GLN:NE2	2.07	0.70
1:B:790:ARG:HG3	1:B:791:LYS:N	2.05	0.70
2:J:116:LEU:HD12	2:J:119:LEU:HB2	1.74	0.70
2:N:167:ASN:HD22	2:N:178:GLY:HA2	1.57	0.70
1:A:783:PHE:H	1:A:783:PHE:HD1	1.38	0.70
2:C:167:ASN:HD22	2:C:178:GLY:HA2	1.57	0.70
2:D:153:HIS:NE2	2:E:153:HIS:NE2	2.39	0.70
2:G:167:ASN:HD22	2:G:178:GLY:HA2	1.57	0.70
1:A:482:GLN:OE1	1:A:493:LEU:HD22	1.90	0.70
1:A:560:CYS:HB2	1:A:603:TYR:HD2	1.57	0.70
1:B:262:VAL:CG1	1:B:297:ARG:HB3	2.21	0.70
1:B:786:ILE:HG13	1:B:787:VAL:H	1.56	0.70
2:I:12:LYS:C	2:I:14:ALA:H	1.95	0.70
2:K:167:ASN:HD22	2:K:178:GLY:HA2	1.57	0.70
2:O:154:LYS:N	2:O:155:PRO:CD	2.54	0.70
1:B:393:SER:N	1:B:573:THR:HG23	2.06	0.70
1:B:857:PHE:HD1	1:B:857:PHE:H	1.40	0.70
2:C:4:LEU:HA	2:C:7:LEU:HD12	1.74	0.70
2:J:167:ASN:HD22	2:J:178:GLY:HA2	1.57	0.70
2:J:38:ILE:HG22	2:J:42:ASN:HD21	1.56	0.70
2:O:167:ASN:HD22	2:O:178:GLY:HA2	1.57	0.70
1:A:396:PHE:HB3	1:A:578:LEU:CD1	2.22	0.70
1:A:401:TYR:HA	1:A:404:LEU:HD13	1.73	0.70
1:A:436:ILE:HD11	1:A:437:TYR:CD1	2.27	0.70
1:B:721:VAL:CG1	1:B:799:LEU:HD21	2.22	0.70
2:C:6:SER:OG	2:C:128:ASN:HA	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:38:ILE:HG22	2:E:42:ASN:HD21	1.57	0.70
1:A:781:THR:O	1:A:783:PHE:N	2.24	0.69
1:B:318:TRP:CA	1:B:321:ILE:HD12	2.19	0.69
1:B:670:ARG:O	1:B:671:LEU:HD23	1.92	0.69
1:B:791:LYS:O	1:B:792:VAL:HG13	1.91	0.69
2:D:239:ASN:HD22	2:D:246:THR:HG22	1.57	0.69
2:O:4:LEU:HA	2:O:7:LEU:HD12	1.74	0.69
1:B:590:ASN:H	1:B:590:ASN:ND2	1.90	0.69
2:C:22:THR:OG1	2:C:26:ASN:ND2	2.25	0.69
2:F:104:SER:HB3	2:F:108:GLY:HA2	1.74	0.69
2:O:106:ARG:HD3	2:O:106:ARG:H	1.56	0.69
1:A:437:TYR:H	1:A:438:PRO:HD2	1.56	0.69
1:A:548:ARG:HH11	1:A:877:MET:HA	1.56	0.69
1:B:182:LEU:HD11	1:B:847:THR:N	2.07	0.69
2:C:239:ASN:HD22	2:C:246:THR:HG22	1.58	0.69
2:D:150:PHE:HB2	2:D:152:PHE:CE1	2.27	0.69
2:K:150:PHE:HB2	2:K:152:PHE:CE1	2.27	0.69
2:L:11:LEU:O	2:L:14:ALA:HB3	1.93	0.69
2:L:239:ASN:HD22	2:L:246:THR:HG22	1.58	0.69
2:N:106:ARG:N	2:N:106:ARG:HD3	2.01	0.69
1:A:275:PRO:HB2	1:A:278:ILE:CG1	2.22	0.69
1:A:306:ASP:C	1:A:308:LEU:H	1.95	0.69
2:F:110:ALA:HB1	2:F:111:PRO:CD	2.22	0.69
2:H:12:LYS:C	2:H:14:ALA:H	1.95	0.69
2:I:109:ILE:HD12	2:I:109:ILE:O	1.90	0.69
2:I:167:ASN:HD22	2:I:178:GLY:HA2	1.57	0.69
2:J:22:THR:O	2:J:72:ASN:HA	1.92	0.69
2:E:11:LEU:O	2:E:14:ALA:HB3	1.91	0.69
2:G:11:LEU:O	2:G:14:ALA:HB3	1.92	0.69
2:M:167:ASN:HD22	2:M:178:GLY:HA2	1.57	0.69
1:B:366:PHE:C	1:B:368:THR:N	2.46	0.69
1:B:374:ALA:HB1	1:B:580:SER:CB	2.23	0.69
1:A:634:TYR:HB2	1:B:875:ARG:HH22	1.57	0.69
2:E:5:TYR:CE2	2:E:131:ASN:HA	2.27	0.69
2:F:167:ASN:HD22	2:F:178:GLY:HA2	1.57	0.69
2:N:116:LEU:HD12	2:N:119:LEU:HB2	1.74	0.69
1:A:540:LEU:HD23	1:A:541:GLY:N	2.08	0.69
1:A:588:ILE:CG2	1:A:589:GLY:N	2.56	0.69
1:A:666:ARG:CG	1:A:667:ASP:N	2.55	0.69
1:A:803:ASN:HD22	1:A:805:ASP:HB3	1.58	0.69
1:B:772:ILE:HG23	1:B:773:SER:N	2.06	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:THR:HA	1:B:579:THR:HG23	1.75	0.69
1:A:664:ARG:HD3	1:B:538:ASN:OD1	1.92	0.69
1:B:563:MET:HA	1:B:563:MET:HE3	1.73	0.69
1:B:783:PHE:N	1:B:783:PHE:CD1	2.60	0.69
2:D:106:ARG:H	2:D:106:ARG:HD3	1.58	0.69
1:A:322:THR:HG22	1:A:390:ARG:HB2	1.75	0.69
1:A:451:ASP:CB	1:A:452:PRO:CD	2.68	0.69
1:A:689:MET:HA	1:A:692:ILE:HD13	1.73	0.69
2:E:150:PHE:HB2	2:E:152:PHE:CE1	2.27	0.69
2:E:109:ILE:HB	2:E:380:ASP:HB3	1.74	0.69
1:A:118:LYS:HG2	1:A:119:GLN:H	1.57	0.69
1:A:546:LEU:HD21	1:A:588:ILE:HD13	1.73	0.69
1:A:757:VAL:HG12	1:A:758:ALA:H	1.57	0.69
1:B:118:LYS:HG2	1:B:119:GLN:N	2.08	0.69
1:B:594:ILE:HD12	1:B:594:ILE:C	2.13	0.69
1:B:752:LEU:C	1:B:754:ASN:H	1.95	0.69
1:B:812:VAL:HG13	1:B:813:ALA:H	1.57	0.69
2:E:116:LEU:HD12	2:E:119:LEU:HB2	1.73	0.69
2:F:11:LEU:O	2:F:14:ALA:HB3	1.93	0.69
2:G:12:LYS:C	2:G:14:ALA:H	1.96	0.69
1:B:457:GLN:CG	1:B:458:ILE:H	1.89	0.69
1:B:633:LEU:O	1:B:633:LEU:HD23	1.92	0.69
2:H:239:ASN:HD22	2:H:246:THR:HG22	1.58	0.69
2:I:6:SER:OG	2:I:128:ASN:HA	1.92	0.69
2:K:106:ARG:HG2	2:K:107:ASN:H	1.56	0.69
2:K:144:ARG:O	2:K:145:ARG:HB2	1.92	0.69
2:L:167:ASN:HD22	2:L:178:GLY:HA2	1.57	0.69
2:M:116:LEU:HD12	2:M:119:LEU:HB2	1.75	0.69
2:M:12:LYS:C	2:M:14:ALA:H	1.96	0.69
2:O:109:ILE:O	2:O:109:ILE:HD12	1.92	0.69
1:A:306:ASP:O	1:A:308:LEU:N	2.25	0.68
1:A:570:THR:HG22	1:A:571:LEU:N	2.07	0.68
1:B:166:PHE:O	1:B:169:LEU:HB2	1.93	0.68
1:A:658:PRO:HG3	1:B:345:GLN:HA	1.75	0.68
1:B:805:ASP:O	1:B:807:ASN:N	2.26	0.68
2:E:12:LYS:C	2:E:14:ALA:H	1.96	0.68
1:A:366:PHE:CD1	1:A:366:PHE:N	2.60	0.68
1:A:661:GLN:NE2	1:B:348:LYS:NZ	2.39	0.68
1:A:807:ASN:O	1:A:809:PHE:N	2.26	0.68
1:B:264:PRO:O	1:B:265:LEU:HB2	1.92	0.68
2:F:6:SER:OG	2:F:128:ASN:HA	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:106:ARG:O	2:H:107:ASN:HB2	1.93	0.68
2:J:4:LEU:HA	2:J:7:LEU:HD12	1.75	0.68
2:L:116:LEU:HD12	2:L:119:LEU:HB2	1.75	0.68
2:D:12:LYS:C	2:D:14:ALA:H	1.95	0.68
2:E:167:ASN:HD22	2:E:178:GLY:HA2	1.57	0.68
2:F:4:LEU:HA	2:F:7:LEU:HD12	1.75	0.68
2:L:110:ALA:HB1	2:L:111:PRO:CD	2.23	0.68
2:N:12:LYS:C	2:N:14:ALA:H	1.94	0.68
1:B:548:ARG:NH1	1:B:878:ASN:N	2.35	0.68
2:C:116:LEU:HD12	2:C:119:LEU:HB2	1.75	0.68
2:D:116:LEU:HD12	2:D:119:LEU:HB2	1.75	0.68
2:F:116:LEU:HD12	2:F:119:LEU:HB2	1.75	0.68
2:F:153:HIS:NE2	2:H:153:HIS:NE2	2.41	0.68
2:H:11:LEU:O	2:H:14:ALA:HB3	1.93	0.68
2:N:239:ASN:HD22	2:N:246:THR:HG22	1.58	0.68
1:A:318:TRP:CA	1:A:321:ILE:HD12	2.19	0.68
2:I:116:LEU:HD12	2:I:119:LEU:HB2	1.75	0.68
1:B:180:TYR:HD1	1:B:181:LEU:N	1.91	0.68
2:I:239:ASN:HD22	2:I:246:THR:HG22	1.59	0.68
2:M:153:HIS:NE2	2:N:153:HIS:NE2	2.40	0.68
1:A:396:PHE:HB3	1:A:578:LEU:HD12	1.76	0.68
1:A:660:ASP:CB	1:B:539:ARG:HH11	2.04	0.68
1:B:431:ILE:HA	1:B:435:ILE:HD12	1.76	0.68
1:B:545:ASP:HB3	1:B:877:MET:SD	2.34	0.68
1:B:855:LEU:O	1:B:858:VAL:HG23	1.94	0.68
2:M:4:LEU:HA	2:M:7:LEU:HD12	1.75	0.68
1:A:659:ASP:O	1:A:662:MET:HB2	1.94	0.68
2:H:4:LEU:HA	2:H:7:LEU:HD12	1.76	0.68
2:I:4:LEU:HA	2:I:7:LEU:HD12	1.74	0.68
2:N:65:LEU:O	2:N:66:LEU:HD23	1.94	0.68
1:B:498:ARG:HB3	1:B:505:GLN:HE22	1.59	0.68
1:B:869:VAL:HG11	1:B:873:ASN:HA	1.74	0.68
2:H:167:ASN:HD22	2:H:178:GLY:HA2	1.57	0.68
2:I:135:TYR:CZ	2:I:342:MET:HE3	2.28	0.68
2:J:239:ASN:HD22	2:J:246:THR:HG22	1.58	0.68
2:O:12:LYS:C	2:O:14:ALA:H	1.96	0.68
1:A:136:ALA:O	1:A:137:ASN:HB3	1.94	0.68
1:A:587:LEU:HD13	1:A:587:LEU:O	1.94	0.68
1:B:143:ARG:HG3	1:B:216:GLU:OE2	1.92	0.68
1:B:246:HIS:CD2	1:B:248:ILE:H	2.11	0.68
1:B:530:GLN:HA	1:B:533:ILE:HD12	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:492:VAL:HG11	1:B:558:MET:CG	2.22	0.68
2:D:167:ASN:HD22	2:D:178:GLY:HA2	1.57	0.68
2:K:12:LYS:C	2:K:14:ALA:H	1.96	0.68
2:M:239:ASN:HD22	2:M:246:THR:HG22	1.59	0.68
1:A:589:GLY:O	1:A:591:ALA:N	2.26	0.67
1:B:499:ASN:O	1:B:500:GLY:C	2.33	0.67
2:I:9:LYS:O	2:I:13:ASP:HB2	1.94	0.67
2:H:76:ASN:HB2	2:J:76:ASN:CB	2.23	0.67
1:A:188:VAL:O	1:A:198:LYS:HA	1.93	0.67
1:B:125:ILE:N	1:B:125:ILE:HD12	2.10	0.67
1:B:721:VAL:HG12	1:B:722:ASN:N	2.08	0.67
2:C:12:LYS:C	2:C:14:ALA:H	1.96	0.67
2:D:144:ARG:O	2:D:145:ARG:HB2	1.94	0.67
2:F:12:LYS:C	2:F:14:ALA:H	1.96	0.67
2:G:239:ASN:HD22	2:G:246:THR:HG22	1.58	0.67
2:K:117:ARG:HH21	2:M:57:ARG:NH1	1.90	0.67
1:B:258:GLN:HB3	2:N:71:LEU:HB2	1.76	0.67
1:A:270:ILE:HG23	1:A:854:LEU:CD2	2.22	0.67
1:A:306:ASP:HB3	1:A:310:LEU:CD1	2.24	0.67
1:B:605:ASN:HD21	1:B:855:LEU:HD12	1.58	0.67
1:B:745:ALA:O	1:B:748:THR:N	2.28	0.67
2:D:38:ILE:HD12	2:D:65:LEU:HD23	1.75	0.67
2:E:4:LEU:HA	2:E:7:LEU:HD12	1.75	0.67
2:F:19:VAL:HG23	2:H:128:ASN:HB3	1.77	0.67
2:H:76:ASN:H	2:J:76:ASN:HB2	1.60	0.67
2:I:104:SER:O	2:I:108:GLY:HA3	1.94	0.67
2:K:116:LEU:HD12	2:K:119:LEU:HB2	1.76	0.67
2:L:4:LEU:HA	2:L:7:LEU:HD12	1.75	0.67
2:N:73:LEU:HD23	2:N:73:LEU:N	2.09	0.67
1:A:136:ALA:O	1:A:137:ASN:CB	2.43	0.67
1:A:310:LEU:O	1:A:318:TRP:HD1	1.76	0.67
1:B:183:LEU:HD12	1:B:844:SER:HB3	1.77	0.67
2:I:63:PHE:CD2	2:I:84:THR:HG23	2.28	0.67
2:O:239:ASN:HD22	2:O:246:THR:HG22	1.58	0.67
1:A:571:LEU:O	1:A:571:LEU:HD13	1.94	0.67
1:B:869:VAL:HG22	1:B:875:ARG:HA	1.76	0.67
2:F:239:ASN:HD22	2:F:246:THR:HG22	1.58	0.67
2:K:239:ASN:HD22	2:K:246:THR:HG22	1.58	0.67
1:B:666:ARG:CG	1:B:667:ASP:N	2.57	0.67
1:B:782:VAL:HG11	1:B:796:LYS:O	1.94	0.67
2:O:9:LYS:O	2:O:13:ASP:HB2	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:LEU:N	1:B:108:LEU:HD22	2.10	0.67
1:B:154:THR:O	1:B:155:LEU:HD23	1.94	0.67
2:K:4:LEU:HA	2:K:7:LEU:HD12	1.75	0.67
2:I:76:ASN:N	2:M:76:ASN:HB2	2.09	0.67
1:A:219:GLY:O	1:A:221:VAL:N	2.28	0.67
1:A:223:ARG:O	1:A:226:ALA:HB3	1.95	0.67
1:A:839:MET:HG2	1:A:840:HIS:H	1.60	0.67
1:B:371:ASN:ND2	1:B:583:SER:HB3	2.06	0.67
2:G:116:LEU:HD12	2:G:119:LEU:HB2	1.76	0.67
2:K:9:LYS:O	2:K:13:ASP:HB2	1.95	0.67
1:A:503:ILE:C	1:A:505:GLN:H	1.98	0.67
1:A:521:MET:HB3	1:A:522:PRO:CD	2.22	0.67
1:A:650:HIS:O	1:A:651:ILE:HB	1.94	0.67
1:B:200:VAL:HG12	1:B:201:ASP:N	2.08	0.67
1:B:700:ALA:HB1	1:B:827:LYS:HB2	1.75	0.67
1:B:771:VAL:HG12	1:B:772:ILE:N	2.09	0.67
1:A:252:PHE:CD2	1:A:684:LEU:HD21	2.30	0.66
1:B:523:VAL:C	1:B:525:TYR:N	2.47	0.66
2:O:116:LEU:HD12	2:O:119:LEU:HB2	1.76	0.66
1:A:524:ASP:OD1	1:A:525:TYR:N	2.27	0.66
1:B:229:ARG:HD2	1:B:230:GLN:HE22	1.60	0.66
1:B:672:LEU:HB3	1:B:673:PRO:HD2	1.77	0.66
2:D:99:GLU:OE1	2:D:116:LEU:HD22	1.94	0.66
2:D:99:GLU:HG2	2:D:99:GLU:O	1.94	0.66
2:O:49:GLY:HA2	2:O:54:LEU:HD23	1.77	0.66
1:A:563:MET:CA	1:A:563:MET:HE3	2.14	0.66
1:B:825:VAL:CG1	1:B:826:TYR:N	2.57	0.66
2:E:239:ASN:HD22	2:E:246:THR:HG22	1.59	0.66
1:A:246:HIS:CD2	1:A:248:ILE:H	2.14	0.66
1:A:508:GLU:HG2	1:A:512:GLN:NE2	2.10	0.66
1:B:724:ALA:HB2	1:B:824:LYS:HE3	1.77	0.66
2:C:153:HIS:NE2	2:E:153:HIS:NE2	2.43	0.66
2:E:14:ALA:O	2:E:18:ILE:HD12	1.95	0.66
1:A:701:GLN:HG2	1:A:826:TYR:CD2	2.31	0.66
1:B:374:ALA:HB1	1:B:580:SER:CA	2.25	0.66
2:L:153:HIS:NE2	2:M:153:HIS:NE2	2.44	0.66
1:A:454:THR:HB	1:A:457:GLN:HB3	1.78	0.66
1:A:513:LEU:O	1:A:516:GLN:OE1	2.14	0.66
1:A:653:ASP:HB3	1:A:656:ARG:HB2	1.77	0.66
1:B:396:PHE:HB2	1:B:578:LEU:HD11	1.77	0.66
2:E:23:LEU:HD23	2:E:24:TYR:N	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:9:LYS:O	2:N:13:ASP:HB2	1.96	0.66
2:N:150:PHE:HB2	2:N:152:PHE:CE1	2.30	0.66
1:A:277:ARG:HD3	1:A:559:ALA:CB	2.25	0.66
1:B:594:ILE:HB	1:B:595:PRO:CD	2.26	0.66
1:B:825:VAL:CG1	1:B:826:TYR:H	2.08	0.66
1:A:729:GLY:C	1:A:730:PHE:HD1	1.98	0.66
1:B:349:MET:O	1:B:353:LEU:HB2	1.94	0.66
2:C:2:ASP:HB2	2:C:128:ASN:HD21	1.60	0.66
2:J:5:TYR:CE2	2:J:131:ASN:HA	2.31	0.66
2:L:12:LYS:C	2:L:14:ALA:H	1.96	0.66
2:M:9:LYS:O	2:M:13:ASP:HB2	1.96	0.66
2:N:4:LEU:HA	2:N:7:LEU:CD1	2.26	0.66
1:A:521:MET:CE	1:A:521:MET:HA	2.26	0.66
1:B:140:LYS:O	1:B:142:LEU:N	2.29	0.66
1:B:445:MET:O	1:B:447:TYR:N	2.23	0.66
1:B:504:ASN:O	1:B:507:MET:N	2.29	0.66
2:C:22:THR:HG23	2:C:73:LEU:HD12	1.78	0.66
2:G:145:ARG:CB	2:G:145:ARG:HH11	2.00	0.66
2:I:110:ALA:HB1	2:I:111:PRO:HD2	1.77	0.66
1:B:170:TYR:HE1	1:B:681:ILE:HG23	1.60	0.66
1:B:194:ARG:HA	1:B:194:ARG:NE	2.11	0.66
2:O:4:LEU:HA	2:O:7:LEU:CD1	2.26	0.66
1:A:166:PHE:O	1:A:169:LEU:HB2	1.96	0.65
2:C:150:PHE:HB2	2:C:152:PHE:HE1	1.61	0.65
2:D:9:LYS:O	2:D:13:ASP:HB2	1.94	0.65
2:F:26:ASN:OD1	2:H:33:GLN:HB2	1.97	0.65
2:I:109:ILE:HB	2:I:380:ASP:HB3	1.79	0.65
2:N:150:PHE:HB2	2:N:152:PHE:HE1	1.61	0.65
1:A:603:TYR:O	1:A:606:VAL:HG22	1.96	0.65
2:C:54:LEU:HD12	2:C:55:PRO:HD2	1.77	0.65
2:C:4:LEU:HA	2:C:7:LEU:CD1	2.27	0.65
2:G:128:ASN:O	2:H:22:THR:HB	1.95	0.65
1:A:508:GLU:C	1:A:512:GLN:HE21	2.00	0.65
1:A:755:GLN:O	1:A:757:VAL:HG23	1.96	0.65
1:A:849:THR:HB	1:A:851:TYR:HE1	1.61	0.65
1:B:322:THR:HB	1:B:390:ARG:HH11	1.61	0.65
1:B:396:PHE:HE1	1:B:398:THR:HA	1.60	0.65
1:B:642:VAL:O	1:B:646:LEU:HG	1.96	0.65
2:D:109:ILE:HB	2:D:380:ASP:HB3	1.78	0.65
2:G:9:LYS:O	2:G:13:ASP:HB2	1.96	0.65
2:J:12:LYS:HG2	2:J:16:ASP:OD2	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:46:PHE:HE2	2:K:119:LEU:HD21	1.62	0.65
2:M:144:ARG:HD2	2:N:82:ARG:CZ	2.27	0.65
2:C:9:LYS:O	2:C:13:ASP:HB2	1.96	0.65
1:A:711:GLN:O	1:A:712:LEU:HD23	1.96	0.65
1:A:871:PHE:O	1:A:871:PHE:HD1	1.80	0.65
1:B:708:ARG:O	1:B:709:ASP:C	2.35	0.65
1:A:501:HIS:O	1:A:503:ILE:HG13	1.97	0.65
2:D:22:THR:O	2:D:72:ASN:HA	1.95	0.65
2:G:4:LEU:HA	2:G:7:LEU:CD1	2.26	0.65
2:I:150:PHE:HB2	2:I:152:PHE:CZ	2.32	0.65
1:A:516:GLN:N	1:A:516:GLN:OE1	2.28	0.65
1:A:622:VAL:HG11	1:A:673:PRO:O	1.97	0.65
1:A:642:VAL:O	1:A:646:LEU:HG	1.96	0.65
1:B:805:ASP:C	1:B:807:ASN:H	1.99	0.65
2:H:9:LYS:O	2:H:13:ASP:HB2	1.97	0.65
2:I:130:ASP:HA	2:J:17:LYS:HG2	1.78	0.65
2:I:153:HIS:NE2	2:K:153:HIS:NE2	2.45	0.65
1:A:142:LEU:O	1:A:144:ASN:N	2.28	0.65
1:A:589:GLY:C	1:A:591:ALA:H	1.99	0.65
1:A:782:VAL:O	1:A:785:GLN:HG2	1.97	0.65
1:A:658:PRO:CG	1:B:348:LYS:HG2	2.23	0.65
1:B:401:TYR:HA	1:B:404:LEU:HD13	1.79	0.65
1:B:170:TYR:CE1	1:B:681:ILE:HG23	2.31	0.65
1:A:779:ASP:CA	1:A:798:ILE:HD12	2.26	0.65
1:B:236:ARG:O	1:B:237:ASN:HB2	1.97	0.65
1:B:315:GLU:CB	1:B:571:LEU:HD11	2.25	0.65
1:A:271:PHE:HA	1:A:274:ILE:HD12	1.79	0.65
1:B:298:TYR:HD1	1:B:299:ILE:N	1.94	0.65
1:B:96:PRO:HG2	1:B:657:VAL:HG22	1.79	0.65
2:N:12:LYS:HG2	2:N:16:ASP:OD2	1.96	0.65
1:B:378:CYS:HB2	1:B:580:SER:HB2	1.79	0.64
2:E:9:LYS:O	2:E:13:ASP:HB2	1.97	0.64
2:F:9:LYS:O	2:F:13:ASP:HB2	1.97	0.64
2:I:4:LEU:HA	2:I:7:LEU:CD1	2.27	0.64
2:J:57:ARG:HH11	2:J:94:ASN:HD21	1.46	0.64
1:A:793:ASP:C	1:A:795:LEU:H	2.00	0.64
1:B:603:TYR:O	1:B:606:VAL:HG22	1.97	0.64
1:B:314:PHE:CZ	1:B:664:ARG:HG2	2.32	0.64
2:D:106:ARG:HG2	2:D:107:ASN:H	1.62	0.64
2:D:4:LEU:HA	2:D:7:LEU:CD1	2.27	0.64
2:L:9:LYS:O	2:L:13:ASP:HB2	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:802:ILE:HA	1:A:807:ASN:ND2	2.12	0.64
2:O:104:SER:HB3	2:O:108:GLY:HA2	1.79	0.64
1:A:714:ARG:HA	1:A:720:TYR:HB3	1.78	0.64
1:A:863:VAL:HG12	1:A:864:GLU:H	1.61	0.64
2:D:110:ALA:HB1	2:D:111:PRO:CD	2.28	0.64
2:L:27:VAL:O	2:L:31:ILE:HG12	1.97	0.64
1:A:414:VAL:HB	1:A:419:PHE:HE1	1.62	0.64
1:A:834:ASP:O	1:A:838:SER:HB2	1.97	0.64
1:B:182:LEU:CD2	1:B:183:LEU:H	2.08	0.64
1:B:457:GLN:CG	1:B:458:ILE:N	2.53	0.64
1:B:491:GLN:NE2	1:B:566:GLN:HG2	2.12	0.64
1:B:606:VAL:HG23	1:B:607:ASN:N	2.11	0.64
2:J:144:ARG:NH2	2:J:146:GLN:HE22	1.96	0.64
1:A:246:HIS:O	1:A:249:ASP:N	2.31	0.64
1:A:548:ARG:HB3	1:A:876:ILE:HG23	1.78	0.64
1:B:645:PHE:HD2	1:B:646:LEU:HD23	1.62	0.64
1:B:718:TYR:HB3	1:B:721:VAL:CG2	2.18	0.64
2:F:109:ILE:HB	2:F:380:ASP:HB3	1.79	0.64
2:J:9:LYS:O	2:J:13:ASP:HB2	1.98	0.64
2:J:4:LEU:HA	2:J:7:LEU:CD1	2.28	0.64
2:K:12:LYS:HG2	2:K:16:ASP:OD2	1.97	0.64
2:M:139:TRP:NE1	2:M:143:ASN:ND2	2.46	0.64
1:A:246:HIS:HD2	1:A:248:ILE:HB	1.63	0.64
1:A:378:CYS:SG	1:A:584:LEU:HD13	2.38	0.64
1:B:703:VAL:HG22	1:B:825:VAL:HG22	1.78	0.64
2:F:38:ILE:HG22	2:F:42:ASN:HD21	1.62	0.64
2:M:42:ASN:HA	2:M:61:PHE:HB3	1.80	0.64
2:N:128:ASN:O	2:N:129:PHE:HB3	1.98	0.64
1:A:606:VAL:HG23	1:A:607:ASN:N	2.13	0.64
1:B:182:LEU:HD11	1:B:847:THR:HA	1.78	0.64
1:B:389:GLN:OE1	1:B:389:GLN:HA	1.98	0.64
1:B:492:VAL:HG13	1:B:565:MET:SD	2.38	0.64
1:B:721:VAL:HG12	1:B:722:ASN:H	1.63	0.64
2:M:12:LYS:HG2	2:M:16:ASP:OD2	1.98	0.64
1:A:360:ILE:HG23	1:A:363:GLU:HB2	1.78	0.64
2:D:54:LEU:HD12	2:D:55:PRO:HD2	1.79	0.64
2:G:106:ARG:HG2	2:G:107:ASN:H	1.62	0.64
2:D:12:LYS:HG2	2:D:16:ASP:OD2	1.98	0.64
2:E:4:LEU:HA	2:E:7:LEU:CD1	2.28	0.64
2:H:57:ARG:HH11	2:H:94:ASN:HD21	1.44	0.64
2:K:4:LEU:HA	2:K:7:LEU:CD1	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:14:ALA:O	2:O:18:ILE:HD12	1.97	0.64
1:A:371:ASN:HB3	1:A:583:SER:HB2	1.80	0.63
1:A:158:GLY:N	1:A:762:ALA:HB3	2.13	0.63
1:B:491:GLN:HE22	1:B:566:GLN:HG2	1.63	0.63
1:B:498:ARG:CB	1:B:505:GLN:HE22	2.10	0.63
2:J:110:ALA:HB1	2:J:111:PRO:CD	2.28	0.63
2:I:19:VAL:CG2	2:K:128:ASN:HB3	2.27	0.63
2:L:12:LYS:HG2	2:L:16:ASP:OD2	1.98	0.63
2:M:27:VAL:O	2:M:31:ILE:HG12	1.97	0.63
1:A:772:ILE:O	1:A:775:ILE:HG13	1.98	0.63
1:B:346:ILE:O	1:B:349:MET:HB3	1.97	0.63
1:B:442:MET:HG2	1:B:443:GLN:H	1.63	0.63
1:B:645:PHE:CD2	1:B:646:LEU:HD23	2.33	0.63
2:F:4:LEU:HA	2:F:7:LEU:CD1	2.29	0.63
2:J:71:LEU:HG	2:J:72:ASN:OD1	1.98	0.63
2:M:4:LEU:HA	2:M:7:LEU:CD1	2.28	0.63
1:A:491:GLN:OE1	1:A:564:ASN:HB3	1.99	0.63
1:B:396:PHE:CE1	1:B:398:THR:HA	2.33	0.63
1:B:730:PHE:N	1:B:730:PHE:CD1	2.67	0.63
1:B:772:ILE:O	1:B:775:ILE:HB	1.98	0.63
2:F:110:ALA:HB1	2:F:111:PRO:HD2	1.80	0.63
2:I:145:ARG:HH11	2:I:145:ARG:CB	2.12	0.63
1:A:560:CYS:HB2	1:A:603:TYR:CD2	2.33	0.63
1:A:721:VAL:HG11	1:A:799:LEU:HD22	1.81	0.63
1:A:839:MET:HE2	1:A:839:MET:C	2.19	0.63
1:B:415:PRO:CB	1:B:480:PHE:HB2	2.28	0.63
1:B:503:ILE:HD11	1:B:548:ARG:CG	2.26	0.63
1:B:305:GLN:HG3	1:B:564:ASN:HD21	1.62	0.63
1:B:722:ASN:ND2	1:B:824:LYS:HA	2.10	0.63
2:D:109:ILE:HD12	2:D:109:ILE:O	1.99	0.63
2:F:12:LYS:HG2	2:F:16:ASP:OD2	1.99	0.63
2:O:141:LEU:HD12	2:O:148:THR:HG21	1.80	0.63
1:A:262:VAL:HG12	1:A:297:ARG:HB3	1.80	0.63
2:F:104:SER:O	2:F:105:GLN:HB2	1.98	0.63
1:B:498:ARG:HD3	2:I:32:GLN:HE21	1.63	0.63
2:L:346:VAL:HG21	2:L:385:VAL:HG13	1.81	0.63
1:B:231:ARG:HB3	1:B:240:ASN:HB2	1.80	0.63
1:B:422:GLU:HA	1:B:425:VAL:CG2	2.29	0.63
1:B:492:VAL:HG11	1:B:558:MET:SD	2.38	0.63
1:B:587:LEU:HG	1:B:587:LEU:O	1.97	0.63
1:B:701:GLN:HB2	1:B:826:TYR:CD2	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:735:LEU:HD21	1:B:759:LEU:HB3	1.80	0.63
1:A:513:LEU:HA	1:A:516:GLN:HE22	1.64	0.63
2:C:12:LYS:HG2	2:C:16:ASP:OD2	1.99	0.63
2:L:24:TYR:O	2:L:27:VAL:HG22	1.98	0.63
2:L:85:ILE:O	2:L:89:VAL:HG23	1.99	0.63
2:O:12:LYS:HG2	2:O:16:ASP:OD2	1.99	0.63
2:O:85:ILE:O	2:O:89:VAL:HG23	1.99	0.63
1:A:795:LEU:O	1:A:797:PRO:HD3	1.98	0.63
1:B:127:GLU:OE1	1:B:151:LYS:HE2	1.98	0.63
1:B:549:LEU:HD13	1:B:877:MET:CE	2.28	0.63
1:B:818:VAL:HG12	1:B:819:PRO:HD2	1.80	0.63
2:K:346:VAL:HG21	2:K:385:VAL:HG13	1.81	0.63
2:N:106:ARG:H	2:N:106:ARG:CD	1.99	0.63
2:O:147:ARG:HG2	2:O:148:THR:N	2.13	0.63
1:A:436:ILE:HD12	1:A:436:ILE:C	2.18	0.63
1:A:601:PHE:HD1	1:A:601:PHE:H	1.46	0.63
1:A:416:ASN:HB3	1:A:424:LEU:CD2	2.29	0.62
1:A:328:LEU:HD11	1:A:606:VAL:HG21	1.80	0.62
1:B:274:ILE:HG23	1:B:278:ILE:CD1	2.24	0.62
2:I:12:LYS:HG2	2:I:16:ASP:OD2	1.99	0.62
2:I:85:ILE:O	2:I:89:VAL:HG23	1.99	0.62
2:N:346:VAL:HG21	2:N:385:VAL:HG13	1.81	0.62
2:N:49:GLY:HA2	2:N:54:LEU:HD23	1.81	0.62
1:A:721:VAL:HG13	1:A:800:TYR:O	1.98	0.62
1:A:810:TYR:O	1:A:812:VAL:N	2.32	0.62
1:B:199:VAL:CG1	1:B:200:VAL:N	2.62	0.62
1:B:451:ASP:N	1:B:452:PRO:HD3	2.13	0.62
1:B:494:ASN:ND2	1:B:495:ASP:N	2.46	0.62
1:B:305:GLN:HE21	1:B:564:ASN:CG	2.03	0.62
1:B:704:ILE:O	1:B:823:THR:OG1	2.17	0.62
1:B:812:VAL:HG22	1:B:813:ALA:N	2.13	0.62
1:B:95:ILE:HG22	1:B:97:THR:OG1	1.99	0.62
2:J:346:VAL:HG21	2:J:385:VAL:HG13	1.81	0.62
2:O:346:VAL:HG21	2:O:385:VAL:HG13	1.81	0.62
1:A:360:ILE:CG2	1:A:363:GLU:HB2	2.29	0.62
1:A:472:LEU:O	1:A:476:ASN:HB2	1.99	0.62
1:A:545:ASP:HA	1:A:548:ARG:HD2	1.80	0.62
1:B:596:SER:HB2	1:B:599:THR:OG1	1.99	0.62
2:H:346:VAL:HG21	2:H:385:VAL:HG13	1.81	0.62
2:K:48:THR:HG22	2:K:115:SER:OG	1.98	0.62
2:J:144:ARG:HD2	2:K:82:ARG:CZ	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:135:TYR:OH	2:O:340:GLU:OE1	2.17	0.62
1:A:503:ILE:CD1	1:A:547:THR:HB	2.29	0.62
1:B:122:LEU:HD11	1:B:200:VAL:CG1	2.29	0.62
1:B:681:ILE:O	1:B:684:LEU:HB3	1.99	0.62
1:B:723:ILE:O	1:B:824:LYS:HD2	2.00	0.62
2:C:21:GLY:O	2:C:22:THR:O	2.17	0.62
1:B:497:ILE:HG12	2:I:68:THR:HG23	1.82	0.62
1:B:394:LEU:C	1:B:396:PHE:H	2.02	0.62
1:B:791:LYS:C	1:B:792:VAL:HG13	2.20	0.62
2:C:8:SER:O	2:C:11:LEU:N	2.33	0.62
2:E:116:LEU:HA	2:E:119:LEU:HD12	1.81	0.62
2:H:109:ILE:CG1	2:H:109:ILE:O	2.48	0.62
2:I:346:VAL:HG21	2:I:385:VAL:HG13	1.81	0.62
2:L:4:LEU:HA	2:L:7:LEU:CD1	2.28	0.62
1:A:763:LEU:HD23	1:A:764:PRO:HD3	1.80	0.62
1:B:432:VAL:HA	1:B:436:ILE:CD1	2.12	0.62
1:B:692:ILE:HD12	1:B:692:ILE:H	1.63	0.62
2:J:85:ILE:O	2:J:89:VAL:HG23	1.99	0.62
1:A:738:LEU:C	1:A:740:ARG:H	2.02	0.62
1:B:371:ASN:HA	1:B:374:ALA:HB3	1.82	0.62
1:B:435:ILE:O	1:B:436:ILE:HG12	2.00	0.62
1:A:556:THR:O	1:A:557:LEU:C	2.38	0.62
1:A:596:SER:O	1:A:600:LEU:HD12	1.99	0.62
2:F:346:VAL:HG21	2:F:385:VAL:HG13	1.81	0.62
2:H:4:LEU:HA	2:H:7:LEU:CD1	2.28	0.62
2:H:76:ASN:CB	2:J:76:ASN:HB2	2.30	0.62
2:I:23:LEU:HD23	2:I:24:TYR:H	1.65	0.62
2:J:22:THR:HG22	2:J:73:LEU:HD12	1.81	0.62
2:L:38:ILE:HD12	2:L:65:LEU:CD2	2.29	0.62
2:N:8:SER:O	2:N:11:LEU:N	2.33	0.62
1:B:634:TYR:O	1:B:635:GLN:HG2	1.99	0.62
2:G:46:PHE:HE2	2:G:119:LEU:HD21	1.63	0.62
2:H:12:LYS:HG2	2:H:16:ASP:OD2	2.00	0.62
2:L:62:ASP:CG	2:L:62:ASP:O	2.37	0.62
2:M:346:VAL:HG21	2:M:385:VAL:HG13	1.81	0.62
2:O:23:LEU:HD23	2:O:24:TYR:N	2.14	0.62
1:A:692:ILE:H	1:A:692:ILE:HD12	1.64	0.62
1:B:722:ASN:O	1:B:824:LYS:HB2	1.99	0.62
1:B:240:ASN:HA	1:B:842:LEU:O	2.00	0.62
2:D:27:VAL:O	2:D:31:ILE:HG12	1.99	0.62
2:L:109:ILE:HD12	2:L:109:ILE:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:503:ILE:HG21	1:B:544:VAL:HG13	1.80	0.61
2:E:12:LYS:HG2	2:E:16:ASP:OD2	1.99	0.61
1:A:568:VAL:HG12	1:A:569:GLN:N	2.14	0.61
1:B:863:VAL:HG12	1:B:864:GLU:H	1.65	0.61
2:G:27:VAL:O	2:G:31:ILE:HG12	2.01	0.61
1:B:508:GLU:CD	2:J:71:LEU:HB3	2.20	0.61
2:L:22:THR:HG23	2:L:73:LEU:CD1	2.23	0.61
2:M:116:LEU:HA	2:M:119:LEU:HD12	1.82	0.61
2:M:145:ARG:CZ	2:M:145:ARG:HB3	2.31	0.61
2:N:66:LEU:HD13	2:N:77:TYR:OH	2.00	0.61
1:A:225:ILE:HA	1:A:228:MET:HE1	1.83	0.61
1:A:362:SER:CB	1:A:365:GLN:NE2	2.63	0.61
1:A:447:TYR:OH	1:A:458:ILE:HG23	2.01	0.61
1:B:194:ARG:HA	1:B:194:ARG:CZ	2.30	0.61
1:B:94:THR:O	1:B:316:SER:HB3	2.01	0.61
1:B:415:PRO:HG2	1:B:480:PHE:CD1	2.30	0.61
1:B:428:GLN:HB2	1:B:456:PHE:HD1	1.61	0.61
1:B:182:LEU:HD21	1:B:846:LEU:HA	1.82	0.61
2:D:23:LEU:HD23	2:D:24:TYR:H	1.62	0.61
2:D:346:VAL:HG21	2:D:385:VAL:HG13	1.81	0.61
2:E:8:SER:O	2:E:11:LEU:N	2.34	0.61
2:E:346:VAL:HG21	2:E:385:VAL:HG13	1.81	0.61
1:B:744:TYR:O	1:B:745:ALA:HB3	2.00	0.61
2:G:12:LYS:HG2	2:G:16:ASP:OD2	1.99	0.61
2:J:116:LEU:HA	2:J:119:LEU:HD12	1.82	0.61
2:K:8:SER:O	2:K:11:LEU:N	2.34	0.61
2:O:38:ILE:HG22	2:O:42:ASN:HD21	1.64	0.61
1:A:389:GLN:O	1:A:389:GLN:HG3	2.00	0.61
1:B:521:MET:HB2	1:B:522:PRO:HD2	1.81	0.61
2:G:128:ASN:HB3	2:H:19:VAL:HG23	1.81	0.61
2:G:38:ILE:HG22	2:G:42:ASN:HD21	1.64	0.61
2:I:116:LEU:HA	2:I:119:LEU:HD12	1.82	0.61
2:L:8:SER:O	2:L:11:LEU:N	2.33	0.61
2:M:63:PHE:CD2	2:M:84:THR:HG23	2.35	0.61
2:O:8:SER:O	2:O:11:LEU:N	2.34	0.61
1:A:506:LEU:HD21	1:A:543:LEU:C	2.20	0.61
1:B:297:ARG:HG3	1:B:848:PHE:CD2	2.29	0.61
2:D:85:ILE:O	2:D:89:VAL:HG23	2.01	0.61
1:A:443:GLN:CD	1:A:521:MET:HG2	2.21	0.61
1:B:545:ASP:HA	1:B:548:ARG:HD2	1.82	0.61
1:A:282:VAL:O	1:A:284:TYR:N	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:GLN:O	1:A:445:MET:N	2.34	0.61
1:A:450:GLY:O	1:A:451:ASP:HB2	2.01	0.61
1:A:257:LEU:HD13	1:A:843:THR:O	2.01	0.61
1:B:496:ASN:HB3	1:B:498:ARG:HB3	1.83	0.61
2:O:147:ARG:O	2:O:148:THR:HB	1.99	0.61
2:O:150:PHE:CD1	2:O:150:PHE:N	2.69	0.61
1:A:125:ILE:HD13	1:A:126:PHE:HE2	1.66	0.61
2:J:6:SER:OG	2:J:128:ASN:HA	2.00	0.61
2:L:72:ASN:ND2	2:N:126:ARG:HH11	1.99	0.61
2:O:116:LEU:HA	2:O:119:LEU:HD12	1.82	0.61
1:A:701:GLN:HB3	1:A:826:TYR:HD2	1.66	0.61
1:B:523:VAL:O	1:B:525:TYR:N	2.34	0.61
1:B:96:PRO:O	1:B:320:THR:HG21	1.99	0.61
2:E:135:TYR:CZ	2:E:342:MET:HE3	2.36	0.61
2:G:346:VAL:HG21	2:G:385:VAL:HG13	1.81	0.61
2:I:19:VAL:HG23	2:K:128:ASN:HB3	1.83	0.61
2:J:8:SER:O	2:J:11:LEU:N	2.34	0.61
2:K:152:PHE:N	2:K:152:PHE:CD1	2.69	0.61
2:N:116:LEU:HA	2:N:119:LEU:HD12	1.82	0.61
1:A:434:THR:HG22	1:A:434:THR:O	2.00	0.60
1:A:570:THR:CG2	1:A:571:LEU:H	2.12	0.60
1:A:660:ASP:O	1:A:661:GLN:C	2.38	0.60
1:A:817:TRP:CG	1:A:818:VAL:N	2.65	0.60
1:B:133:ILE:CD1	1:B:145:ARG:HB2	2.31	0.60
1:B:180:TYR:CD1	1:B:181:LEU:N	2.68	0.60
1:B:333:VAL:HG11	1:B:380:LYS:HA	1.83	0.60
1:B:482:GLN:CB	1:B:493:LEU:HD22	2.30	0.60
2:E:150:PHE:HB2	2:E:152:PHE:CZ	2.37	0.60
2:N:109:ILE:HB	2:N:380:ASP:HB3	1.82	0.60
1:A:319:ASP:OD2	1:A:571:LEU:HB3	2.00	0.60
1:A:403:SER:HA	1:A:582:THR:OG1	2.00	0.60
1:A:631:LEU:HB3	1:A:633:LEU:CD1	2.31	0.60
1:A:817:TRP:CH2	1:A:819:PRO:HA	2.36	0.60
1:B:156:PRO:HB2	1:B:161:ASP:CB	2.30	0.60
1:B:527:ARG:O	1:B:531:ARG:CG	2.49	0.60
1:B:503:ILE:HD13	1:B:544:VAL:CG1	2.31	0.60
1:B:779:ASP:HA	1:B:798:ILE:HD11	1.82	0.60
2:C:346:VAL:HG21	2:C:385:VAL:HG13	1.81	0.60
2:F:109:ILE:O	2:F:109:ILE:HD12	2.01	0.60
2:H:142:GLN:HE21	2:H:143:ASN:N	1.98	0.60
2:L:150:PHE:HB2	2:L:152:PHE:HE1	1.60	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:49:GLY:HA2	2:M:54:LEU:CD2	2.31	0.60
1:A:122:LEU:HD11	1:A:200:VAL:HG12	1.82	0.60
1:A:308:LEU:O	1:A:309:ASN:C	2.39	0.60
1:A:625:ILE:O	1:A:628:ALA:HB3	2.00	0.60
1:A:757:VAL:HG12	1:A:758:ALA:N	2.17	0.60
1:A:779:ASP:HA	1:A:798:ILE:HD11	1.80	0.60
1:B:118:LYS:CG	1:B:119:GLN:H	2.13	0.60
1:B:684:LEU:O	1:B:687:MET:HG2	2.02	0.60
2:D:133:SER:O	2:D:135:TYR:N	2.35	0.60
1:A:355:LEU:HD13	1:A:363:GLU:HG2	1.83	0.60
1:B:424:LEU:O	1:B:424:LEU:HD12	2.01	0.60
2:E:57:ARG:HH11	2:E:94:ASN:HD21	1.49	0.60
2:I:153:HIS:NE2	2:J:153:HIS:NE2	2.50	0.60
2:M:8:SER:O	2:M:11:LEU:N	2.34	0.60
2:M:5:TYR:CE2	2:M:131:ASN:HA	2.37	0.60
2:N:12:LYS:C	2:N:14:ALA:N	2.54	0.60
1:B:275:PRO:HD2	1:B:278:ILE:HD11	1.83	0.60
1:B:492:VAL:O	1:B:493:LEU:C	2.40	0.60
1:B:875:ARG:HD3	1:B:878:ASN:HD22	1.66	0.60
2:E:133:SER:O	2:E:135:TYR:N	2.35	0.60
2:L:116:LEU:HA	2:L:119:LEU:HD12	1.83	0.60
2:O:24:TYR:HB2	2:O:71:LEU:HD12	1.83	0.60
1:A:437:TYR:CD2	1:A:442:MET:HG3	2.36	0.60
1:A:803:ASN:C	1:A:805:ASP:H	2.05	0.60
1:B:389:GLN:NE2	1:B:567:HIS:HA	2.17	0.60
1:B:604:TYR:O	1:B:608:VAL:HG23	2.00	0.60
2:D:8:SER:O	2:D:11:LEU:N	2.34	0.60
2:H:8:SER:O	2:H:11:LEU:N	2.34	0.60
2:N:157:ILE:HG12	2:N:214:LEU:HD13	1.84	0.60
2:N:27:VAL:O	2:N:30:LEU:N	2.34	0.60
1:A:203:GLU:O	1:A:207:ILE:HG13	2.02	0.60
1:B:371:ASN:HD22	1:B:583:SER:CB	2.10	0.60
1:B:674:VAL:CG2	1:B:679:LEU:HD13	2.27	0.60
1:B:745:ALA:O	1:B:746:GLN:C	2.40	0.60
1:B:874:MET:O	1:B:875:ARG:CB	2.50	0.60
2:E:85:ILE:O	2:E:89:VAL:HG23	2.01	0.60
2:F:104:SER:HB3	2:F:108:GLY:HA3	1.84	0.60
2:H:23:LEU:H	2:H:26:ASN:ND2	2.00	0.60
2:I:68:THR:HG22	2:I:69:THR:N	2.16	0.60
2:L:73:LEU:HD22	2:L:77:TYR:CD2	2.36	0.60
2:M:145:ARG:NH1	2:M:145:ARG:HB3	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ILE:HA	1:A:228:MET:CE	2.32	0.60
1:A:237:ASN:O	1:A:237:ASN:OD1	2.20	0.60
1:A:326:TYR:CD1	1:A:384:ALA:HB1	2.36	0.60
1:A:492:VAL:CG1	1:A:558:MET:SD	2.90	0.60
1:A:546:LEU:CD1	1:A:584:LEU:HD23	2.32	0.60
1:A:666:ARG:HG3	1:A:667:ASP:N	2.14	0.60
1:A:727:LEU:O	1:A:727:LEU:HD12	2.02	0.60
1:B:274:ILE:CG2	1:B:278:ILE:HD11	2.25	0.60
1:B:371:ASN:C	1:B:373:GLN:N	2.52	0.60
1:B:387:LEU:HD23	1:B:554:TYR:CE1	2.36	0.60
1:B:508:GLU:C	1:B:512:GLN:HE21	2.05	0.60
1:B:743:ASP:OD2	1:B:745:ALA:HA	2.01	0.60
2:C:133:SER:O	2:C:135:TYR:N	2.34	0.60
2:D:116:LEU:HA	2:D:119:LEU:HD12	1.82	0.60
2:F:133:SER:O	2:F:135:TYR:N	2.35	0.60
2:G:157:ILE:HG12	2:G:214:LEU:HD13	1.84	0.60
2:J:110:ALA:HB1	2:J:111:PRO:HD2	1.83	0.60
2:K:116:LEU:HA	2:K:119:LEU:HD12	1.84	0.60
2:K:5:TYR:CE2	2:K:131:ASN:HA	2.37	0.60
2:M:274:GLN:N	2:M:274:GLN:HE21	2.00	0.60
1:B:180:TYR:CD1	1:B:180:TYR:C	2.75	0.60
1:B:435:ILE:CG2	1:B:436:ILE:H	2.09	0.60
1:B:502:VAL:O	1:B:504:ASN:N	2.35	0.60
1:B:723:ILE:O	1:B:724:ALA:HB2	2.01	0.60
2:D:38:ILE:HG22	2:D:42:ASN:HD21	1.67	0.60
2:E:157:ILE:HG12	2:E:214:LEU:HD13	1.84	0.60
2:J:133:SER:O	2:J:135:TYR:N	2.35	0.60
2:J:274:GLN:N	2:J:274:GLN:HE21	2.00	0.60
1:A:535:LEU:O	1:A:539:ARG:HG2	2.02	0.60
1:B:555:GLU:OE2	1:B:871:PHE:HE2	1.85	0.60
1:B:601:PHE:H	1:B:601:PHE:HD1	1.47	0.60
2:F:157:ILE:HG12	2:F:214:LEU:HD13	1.84	0.60
2:G:73:LEU:HD22	2:G:77:TYR:CD2	2.37	0.60
2:H:5:TYR:CE2	2:H:131:ASN:HA	2.37	0.60
2:K:133:SER:O	2:K:135:TYR:N	2.35	0.60
2:M:152:PHE:CD1	2:M:152:PHE:N	2.70	0.60
2:O:8:SER:C	2:O:10:THR:N	2.55	0.60
1:A:445:MET:C	1:A:447:TYR:N	2.54	0.59
1:A:604:TYR:O	1:A:608:VAL:HG23	2.01	0.59
1:B:482:GLN:O	1:B:482:GLN:HG3	2.02	0.59
1:B:535:LEU:O	1:B:539:ARG:HG2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:274:GLN:HE21	2:C:274:GLN:N	2.00	0.59
2:C:85:ILE:O	2:C:89:VAL:HG23	2.01	0.59
2:D:128:ASN:ND2	2:E:19:VAL:HG21	2.17	0.59
2:G:111:PRO:HB3	2:G:116:LEU:HD23	1.83	0.59
2:H:133:SER:O	2:H:135:TYR:N	2.35	0.59
1:B:508:GLU:OE2	2:J:71:LEU:HB3	2.02	0.59
1:A:366:PHE:C	1:A:368:THR:N	2.48	0.59
1:A:577:GLN:O	1:A:581:VAL:HG23	2.01	0.59
1:B:513:LEU:HA	1:B:516:GLN:OE1	2.01	0.59
2:H:152:PHE:N	2:H:152:PHE:CD1	2.69	0.59
2:I:157:ILE:HG12	2:I:214:LEU:HD13	1.84	0.59
2:D:76:ASN:HB2	2:L:76:ASN:HB2	1.83	0.59
2:M:24:TYR:O	2:M:27:VAL:HG22	2.02	0.59
2:L:19:VAL:CG2	2:N:128:ASN:HB3	2.32	0.59
1:A:246:HIS:CD2	1:A:248:ILE:HB	2.36	0.59
1:A:548:ARG:HH11	1:A:877:MET:CA	2.14	0.59
1:A:744:TYR:O	1:A:746:GLN:N	2.35	0.59
1:A:747:ILE:HD11	1:A:786:ILE:HG21	1.85	0.59
1:B:112:LYS:N	1:B:113:PRO:HD3	2.18	0.59
1:B:124:ARG:HB2	1:B:249:ASP:CG	2.22	0.59
1:B:363:GLU:HA	1:B:363:GLU:OE1	2.02	0.59
1:B:401:TYR:O	1:B:404:LEU:HB2	2.02	0.59
1:B:863:VAL:HG12	1:B:864:GLU:N	2.17	0.59
2:C:131:ASN:HD22	2:C:131:ASN:N	1.99	0.59
2:G:85:ILE:O	2:G:89:VAL:HG23	2.01	0.59
2:H:274:GLN:HE21	2:H:274:GLN:N	2.00	0.59
2:M:133:SER:O	2:M:135:TYR:N	2.35	0.59
2:N:274:GLN:HE21	2:N:274:GLN:N	2.00	0.59
2:N:85:ILE:O	2:N:89:VAL:HG23	2.02	0.59
1:A:703:VAL:HG21	1:A:797:PRO:HB3	1.84	0.59
1:B:543:LEU:HD23	1:B:546:LEU:HD12	1.84	0.59
2:F:23:LEU:HD11	2:H:36:GLN:HB2	1.85	0.59
2:J:8:SER:C	2:J:10:THR:N	2.55	0.59
1:A:415:PRO:HB3	1:A:479:GLN:HA	1.84	0.59
1:A:521:MET:HA	1:A:521:MET:HE2	1.84	0.59
1:A:545:ASP:O	1:A:548:ARG:N	2.35	0.59
1:A:700:ALA:O	1:A:701:GLN:HB2	2.02	0.59
1:A:839:MET:HG2	1:A:840:HIS:N	2.16	0.59
1:B:383:ILE:HD11	1:B:550:LEU:CD2	2.32	0.59
2:D:70:LEU:HD12	2:D:71:LEU:N	2.17	0.59
2:L:157:ILE:HG12	2:L:214:LEU:HD13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:53:ASN:HD22	2:L:354:ALA:HB3	1.66	0.59
1:A:371:ASN:O	1:A:373:GLN:N	2.36	0.59
1:A:548:ARG:NH1	1:A:877:MET:HA	2.17	0.59
1:A:770:SER:O	1:A:771:VAL:C	2.40	0.59
1:B:141:GLU:O	1:B:142:LEU:HB2	2.03	0.59
1:B:368:THR:O	1:B:371:ASN:ND2	2.36	0.59
1:B:393:SER:HB3	1:B:573:THR:HG21	1.84	0.59
2:C:8:SER:C	2:C:10:THR:N	2.55	0.59
2:D:104:SER:O	2:D:108:GLY:HA3	2.02	0.59
2:H:135:TYR:CZ	2:H:342:MET:HE3	2.38	0.59
2:M:135:TYR:OH	2:M:340:GLU:OE1	2.20	0.59
2:M:74:ASP:OD2	2:M:76:ASN:HB3	2.03	0.59
2:O:274:GLN:N	2:O:274:GLN:HE21	2.00	0.59
1:A:160:TYR:CZ	1:A:635:GLN:HB2	2.38	0.59
1:A:803:ASN:H	1:A:807:ASN:ND2	2.00	0.59
1:B:190:ASN:HD21	1:B:193:SER:CB	2.10	0.59
1:B:498:ARG:HH22	2:J:25:SER:H	1.49	0.59
2:C:5:TYR:CE2	2:C:131:ASN:HA	2.36	0.59
2:D:157:ILE:HG12	2:D:214:LEU:HD13	1.84	0.59
2:J:157:ILE:HG12	2:J:214:LEU:HD13	1.84	0.59
2:K:157:ILE:HG12	2:K:214:LEU:HD13	1.84	0.59
2:L:130:ASP:HA	2:M:17:LYS:HG2	1.83	0.59
1:A:413:VAL:HG12	1:A:414:VAL:N	2.17	0.59
1:A:464:GLN:HG3	2:F:39:ILE:HD11	1.84	0.59
1:A:368:THR:HG21	1:A:582:THR:HB	1.83	0.59
2:E:274:GLN:HE21	2:E:274:GLN:N	2.00	0.59
2:G:8:SER:C	2:G:10:THR:N	2.56	0.59
2:H:157:ILE:HG12	2:H:214:LEU:HD13	1.84	0.59
2:J:124:PHE:O	2:J:127:ILE:HG13	2.03	0.59
2:D:76:ASN:H	2:L:76:ASN:HB2	1.67	0.59
1:A:216:GLU:CD	1:A:216:GLU:N	2.55	0.59
1:A:322:THR:HG21	1:A:390:ARG:HA	1.83	0.59
1:A:467:GLN:HE21	1:A:511:MET:HG2	1.67	0.59
1:A:520:THR:HG21	1:A:526:LYS:HD3	1.85	0.59
1:A:409:TRP:HH2	1:A:547:THR:HG1	1.50	0.59
1:A:545:ASP:HA	1:A:548:ARG:CD	2.33	0.59
1:A:771:VAL:HG22	1:A:772:ILE:N	2.18	0.59
1:A:784:ALA:O	1:A:785:GLN:C	2.41	0.59
1:B:833:PHE:CZ	1:B:835:PHE:HA	2.38	0.59
2:F:274:GLN:N	2:F:274:GLN:HE21	2.00	0.59
2:F:8:SER:O	2:F:11:LEU:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:152:PHE:N	2:G:152:PHE:CD1	2.71	0.59
2:G:71:LEU:HG	2:G:72:ASN:N	2.17	0.59
2:H:85:ILE:O	2:H:89:VAL:HG23	2.03	0.59
2:J:12:LYS:C	2:J:14:ALA:N	2.55	0.59
2:L:274:GLN:HE21	2:L:274:GLN:N	2.00	0.59
2:O:4:LEU:HG	2:O:391:ILE:HG21	1.85	0.59
1:A:242:PRO:HA	1:A:841:MET:SD	2.42	0.59
1:A:401:TYR:O	1:A:404:LEU:HB2	2.02	0.59
1:A:546:LEU:HD11	1:A:588:ILE:HD12	1.83	0.59
1:A:629:ASN:C	1:A:631:LEU:H	2.02	0.59
1:A:722:ASN:HD22	1:A:824:LYS:HA	1.68	0.59
1:A:810:TYR:CD1	1:A:811:LEU:N	2.71	0.59
1:B:803:ASN:N	1:B:807:ASN:ND2	2.48	0.59
2:I:152:PHE:N	2:I:152:PHE:CD1	2.70	0.59
2:K:8:SER:C	2:K:10:THR:N	2.55	0.59
2:M:135:TYR:CZ	2:M:342:MET:HE3	2.37	0.59
2:M:38:ILE:HG22	2:M:42:ASN:HD21	1.67	0.59
2:N:109:ILE:O	2:N:109:ILE:HD12	2.03	0.59
2:O:12:LYS:C	2:O:14:ALA:N	2.57	0.59
2:O:100:MET:HG3	2:O:388:VAL:HG11	1.85	0.59
1:A:437:TYR:CE2	1:A:442:MET:HG3	2.37	0.58
1:A:484:VAL:HG12	1:A:485:ILE:H	1.68	0.58
1:A:571:LEU:HD23	1:B:531:ARG:NH2	2.17	0.58
1:A:803:ASN:O	1:A:805:ASP:N	2.36	0.58
1:B:285:ILE:C	1:B:286:LEU:HD13	2.22	0.58
1:B:326:TYR:CD1	1:B:384:ALA:HB1	2.37	0.58
1:B:745:ALA:HB1	1:B:748:THR:CB	2.31	0.58
2:F:116:LEU:HA	2:F:119:LEU:HD12	1.85	0.58
2:G:153:HIS:NE2	2:H:153:HIS:NE2	2.51	0.58
2:H:116:LEU:HA	2:H:119:LEU:HD12	1.84	0.58
1:A:428:GLN:NE2	1:A:455:PRO:CB	2.59	0.58
1:A:508:GLU:O	1:A:512:GLN:HG3	2.02	0.58
1:B:437:TYR:CD2	1:B:443:GLN:HB3	2.38	0.58
1:B:463:ILE:HG21	1:B:468:VAL:HG11	1.84	0.58
1:A:571:LEU:HD23	1:B:531:ARG:CZ	2.32	0.58
1:B:875:ARG:HD3	1:B:878:ASN:ND2	2.18	0.58
2:C:12:LYS:C	2:C:14:ALA:N	2.56	0.58
2:C:157:ILE:HG12	2:C:214:LEU:HD13	1.84	0.58
2:G:274:GLN:HE21	2:G:274:GLN:N	2.00	0.58
2:H:22:THR:HG23	2:H:73:LEU:HD12	1.83	0.58
1:A:420:ILE:CD1	1:A:422:GLU:HG3	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:ILE:C	1:A:505:GLN:N	2.55	0.58
1:B:111:ILE:HG22	1:B:113:PRO:HD3	1.84	0.58
1:B:190:ASN:O	1:B:192:ASN:N	2.37	0.58
1:B:223:ARG:O	1:B:226:ALA:HB3	2.03	0.58
1:A:661:GLN:HG3	1:B:348:LYS:HZ1	1.67	0.58
1:B:421:ARG:O	1:B:425:VAL:HG23	2.02	0.58
2:D:274:GLN:N	2:D:274:GLN:HE21	2.00	0.58
2:E:152:PHE:N	2:E:152:PHE:CD1	2.71	0.58
2:K:260:GLU:HG2	2:K:274:GLN:HG3	1.85	0.58
2:L:5:TYR:CE2	2:L:131:ASN:HA	2.37	0.58
2:M:157:ILE:HG12	2:M:214:LEU:HD13	1.84	0.58
2:M:85:ILE:O	2:M:89:VAL:HG23	2.02	0.58
1:A:197:GLY:O	1:A:198:LYS:C	2.42	0.58
2:D:130:ASP:HA	2:E:17:LYS:HG2	1.84	0.58
2:F:5:TYR:CE2	2:F:131:ASN:HA	2.38	0.58
2:G:133:SER:O	2:G:135:TYR:N	2.35	0.58
2:I:10:THR:O	2:I:14:ALA:HB2	2.04	0.58
2:K:145:ARG:O	2:K:146:GLN:HG2	2.02	0.58
2:L:17:LYS:HG2	2:N:130:ASP:HA	1.84	0.58
1:A:244:ILE:O	1:A:245:LEU:HD23	2.03	0.58
1:A:259:HIS:CD2	1:A:677:ARG:HG3	2.38	0.58
1:B:218:GLU:O	1:B:221:VAL:HG23	2.03	0.58
2:G:116:LEU:HA	2:G:119:LEU:HD12	1.84	0.58
2:G:12:LYS:C	2:G:14:ALA:N	2.57	0.58
2:F:130:ASP:HA	2:G:17:LYS:HG2	1.85	0.58
2:L:74:ASP:OD2	2:L:76:ASN:HB3	2.03	0.58
2:O:157:ILE:HG12	2:O:214:LEU:HD13	1.84	0.58
1:A:160:TYR:OH	1:A:635:GLN:HB2	2.04	0.58
1:A:180:TYR:CD1	1:A:180:TYR:C	2.75	0.58
1:A:188:VAL:HG12	1:A:189:GLU:N	2.17	0.58
1:B:508:GLU:O	1:B:512:GLN:HG3	2.04	0.58
2:E:22:THR:HG23	2:E:73:LEU:HD12	1.86	0.58
2:H:8:SER:C	2:H:10:THR:N	2.56	0.58
2:K:49:GLY:HA3	2:K:55:PRO:O	2.03	0.58
2:M:128:ASN:O	2:N:22:THR:HB	2.03	0.58
2:N:133:SER:O	2:N:135:TYR:N	2.36	0.58
1:A:744:TYR:C	1:A:746:GLN:H	2.07	0.58
1:B:371:ASN:HB3	1:B:583:SER:HB2	1.86	0.58
1:B:772:ILE:CG2	1:B:773:SER:N	2.66	0.58
2:C:116:LEU:HA	2:C:119:LEU:HD12	1.84	0.58
2:F:85:ILE:O	2:F:89:VAL:HG23	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:260:GLU:HG2	2:I:274:GLN:HG3	1.86	0.58
2:J:5:TYR:HE2	2:J:131:ASN:HA	1.69	0.58
2:K:85:ILE:O	2:K:89:VAL:HG23	2.02	0.58
2:O:260:GLU:HG2	2:O:274:GLN:HG3	1.86	0.58
1:A:613:ASN:HD22	1:A:649:LEU:HD23	1.69	0.58
1:B:416:ASN:O	1:B:418:MET:N	2.36	0.58
1:B:340:VAL:HB	1:B:587:LEU:HD12	1.84	0.58
2:E:8:SER:C	2:E:10:THR:N	2.55	0.58
2:F:260:GLU:HG2	2:F:274:GLN:HG3	1.86	0.58
2:G:8:SER:O	2:G:11:LEU:N	2.36	0.58
2:J:116:LEU:HD12	2:J:119:LEU:HD12	1.86	0.58
2:L:133:SER:O	2:L:135:TYR:N	2.36	0.58
2:M:12:LYS:C	2:M:14:ALA:N	2.57	0.58
2:N:116:LEU:HD12	2:N:119:LEU:HD12	1.86	0.58
1:A:303:LEU:HA	1:A:615:ASN:HD22	1.67	0.58
1:A:304:LEU:N	1:A:615:ASN:HD21	2.02	0.58
1:A:365:GLN:HB2	1:A:366:PHE:CZ	2.39	0.58
1:A:420:ILE:CG1	1:A:423:SER:HB2	2.32	0.58
1:A:568:VAL:HG12	1:A:569:GLN:H	1.68	0.58
1:B:190:ASN:HB2	1:B:199:VAL:HG23	1.85	0.58
1:B:459:ALA:O	1:B:463:ILE:HG13	2.03	0.58
1:B:696:SER:O	1:B:827:LYS:HE3	2.04	0.58
2:C:260:GLU:HG2	2:C:274:GLN:HG3	1.86	0.58
2:C:7:LEU:O	2:C:11:LEU:HG	2.04	0.58
2:D:68:THR:O	2:D:69:THR:C	2.41	0.58
2:J:10:THR:O	2:J:14:ALA:HB2	2.04	0.58
2:K:12:LYS:C	2:K:14:ALA:N	2.56	0.58
2:O:133:SER:O	2:O:135:TYR:N	2.36	0.58
1:A:390:ARG:HD2	1:A:570:THR:HG21	1.84	0.58
1:A:803:ASN:H	1:A:807:ASN:HD22	1.50	0.58
1:B:491:GLN:HE22	1:B:566:GLN:CG	2.16	0.58
2:I:274:GLN:HE21	2:I:274:GLN:N	2.00	0.57
2:I:38:ILE:HG22	2:I:42:ASN:ND2	2.16	0.57
2:K:274:GLN:HE21	2:K:274:GLN:N	2.01	0.57
2:K:53:ASN:HD22	2:K:354:ALA:CB	2.17	0.57
2:L:104:SER:HB3	2:L:108:GLY:HA2	1.86	0.57
2:L:12:LYS:C	2:L:14:ALA:N	2.56	0.57
1:A:527:ARG:O	1:A:531:ARG:CG	2.51	0.57
1:A:681:ILE:O	1:A:684:LEU:HB3	2.03	0.57
1:B:140:LYS:C	1:B:142:LEU:H	2.06	0.57
1:B:199:VAL:CG1	1:B:200:VAL:H	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:260:GLU:HG2	2:D:274:GLN:HG3	1.86	0.57
2:F:12:LYS:C	2:F:14:ALA:N	2.56	0.57
2:I:8:SER:O	2:I:11:LEU:N	2.36	0.57
2:I:133:SER:O	2:I:135:TYR:N	2.36	0.57
2:M:260:GLU:HG2	2:M:274:GLN:HG3	1.86	0.57
1:A:548:ARG:NH1	1:A:878:ASN:H	2.01	0.57
1:B:434:THR:HG22	1:B:434:THR:O	2.04	0.57
1:B:472:LEU:O	1:B:476:ASN:HB2	2.04	0.57
1:B:415:PRO:HB2	1:B:480:PHE:HB2	1.86	0.57
1:B:494:ASN:CG	1:B:495:ASP:H	2.07	0.57
2:E:260:GLU:HG2	2:E:274:GLN:HG3	1.86	0.57
2:G:10:THR:O	2:G:14:ALA:HB2	2.05	0.57
2:F:144:ARG:HD2	2:G:82:ARG:NH1	2.19	0.57
2:I:12:LYS:C	2:I:14:ALA:N	2.56	0.57
2:K:8:SER:O	2:K:10:THR:N	2.38	0.57
2:K:10:THR:O	2:K:14:ALA:HB2	2.05	0.57
2:K:62:ASP:O	2:K:62:ASP:CG	2.42	0.57
2:M:8:SER:C	2:M:10:THR:N	2.55	0.57
1:B:254:GLU:HG2	2:N:69:THR:CB	2.34	0.57
2:N:76:ASN:HB2	2:O:76:ASN:H	1.69	0.57
2:F:8:SER:C	2:F:10:THR:N	2.55	0.57
2:I:8:SER:C	2:I:10:THR:N	2.56	0.57
2:L:144:ARG:O	2:L:145:ARG:CB	2.48	0.57
1:A:127:GLU:OE2	1:A:151:LYS:HG2	2.03	0.57
1:A:503:ILE:HG22	1:A:506:LEU:HB2	1.86	0.57
1:A:738:LEU:O	1:A:740:ARG:N	2.37	0.57
1:A:771:VAL:CG1	1:A:809:PHE:HB3	2.34	0.57
2:C:116:LEU:HD12	2:C:119:LEU:HD12	1.86	0.57
2:K:7:LEU:O	2:K:11:LEU:HG	2.04	0.57
2:L:145:ARG:O	2:L:146:GLN:HG3	2.04	0.57
2:L:7:LEU:O	2:L:11:LEU:HG	2.05	0.57
1:A:783:PHE:O	1:A:786:ILE:HD12	2.05	0.57
1:B:117:LYS:HB2	1:B:179:ASP:OD2	2.04	0.57
1:B:786:ILE:HG13	1:B:787:VAL:HG23	1.87	0.57
1:B:817:TRP:CD1	1:B:818:VAL:N	2.73	0.57
2:E:149:GLY:C	2:E:150:PHE:CD1	2.77	0.57
2:N:5:TYR:CE2	2:N:131:ASN:HA	2.39	0.57
1:A:131:LEU:HD12	1:A:132:PRO:CD	2.35	0.57
1:A:259:HIS:ND1	1:A:260:GLN:N	2.52	0.57
1:B:246:HIS:HB3	1:B:249:ASP:OD2	2.05	0.57
1:B:477:ASN:O	1:B:478:ASN:C	2.43	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:518:PHE:N	1:B:518:PHE:CD1	2.72	0.57
1:B:535:LEU:O	1:B:539:ARG:CG	2.52	0.57
1:B:703:VAL:HG12	1:B:704:ILE:N	2.20	0.57
2:C:128:ASN:HB3	2:D:19:VAL:CG2	2.35	0.57
2:G:116:LEU:HD12	2:G:119:LEU:HD12	1.87	0.57
2:G:260:GLU:HG2	2:G:274:GLN:HG3	1.86	0.57
1:A:163:ARG:HH22	1:A:736:GLU:CD	2.07	0.57
1:B:340:VAL:HB	1:B:587:LEU:CD1	2.35	0.57
1:B:701:GLN:O	1:B:702:GLY:O	2.23	0.57
1:B:839:MET:C	1:B:839:MET:SD	2.83	0.57
2:I:116:LEU:HD12	2:I:119:LEU:HD12	1.86	0.57
1:B:473:HIS:CB	2:I:126:ARG:HH22	2.08	0.57
2:I:145:ARG:O	2:I:146:GLN:HG3	2.04	0.57
2:M:106:ARG:H	2:M:106:ARG:CD	2.14	0.57
2:O:150:PHE:HB2	2:O:152:PHE:HE1	1.70	0.57
1:A:122:LEU:HD11	1:A:201:ASP:HB2	1.85	0.57
1:A:187:ALA:O	1:A:188:VAL:HG23	2.04	0.57
1:A:420:ILE:CD1	1:A:423:SER:HB2	2.35	0.57
1:A:512:GLN:O	1:A:516:GLN:HG3	2.05	0.57
1:A:710:MET:CE	1:A:824:LYS:HE2	2.35	0.57
1:B:277:ARG:C	1:B:278:ILE:HG12	2.23	0.57
1:B:492:VAL:CG1	1:B:558:MET:SD	2.93	0.57
2:J:260:GLU:HG2	2:J:274:GLN:HG3	1.86	0.57
2:N:260:GLU:HG2	2:N:274:GLN:HG3	1.85	0.57
1:B:271:PHE:O	1:B:274:ILE:HB	2.05	0.57
1:B:312:ASP:O	1:B:313:ASN:HB2	2.05	0.57
1:B:673:PRO:C	1:B:674:VAL:HG22	2.26	0.57
2:C:150:PHE:HB2	2:C:152:PHE:CZ	2.40	0.57
2:E:27:VAL:O	2:E:31:ILE:HG12	2.05	0.57
2:E:35:ASN:HA	2:E:38:ILE:HD12	1.87	0.57
2:G:5:TYR:CE2	2:G:131:ASN:HA	2.40	0.57
2:G:24:TYR:O	2:G:27:VAL:HG22	2.03	0.57
2:H:7:LEU:O	2:H:11:LEU:HG	2.05	0.57
2:L:144:ARG:HD2	2:M:82:ARG:NH1	2.20	0.57
1:A:180:TYR:HD1	1:A:181:LEU:N	2.03	0.56
1:A:597:PRO:HB3	1:A:860:ALA:CB	2.35	0.56
1:B:137:ASN:OD1	1:B:137:ASN:O	2.22	0.56
1:B:272:ASN:C	1:B:274:ILE:N	2.54	0.56
1:B:775:ILE:HD12	1:B:775:ILE:N	2.20	0.56
1:B:790:ARG:CA	1:B:790:ARG:NE	2.47	0.56
2:D:116:LEU:HD12	2:D:119:LEU:HD12	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:8:SER:C	2:D:10:THR:N	2.54	0.56
2:D:128:ASN:HB3	2:E:19:VAL:HG23	1.87	0.56
2:G:135:TYR:OH	2:G:340:GLU:OE1	2.23	0.56
2:G:61:PHE:HA	2:G:63:PHE:HE1	1.70	0.56
2:H:42:ASN:OD1	2:H:62:ASP:HA	2.05	0.56
2:K:14:ALA:O	2:K:18:ILE:HD12	2.05	0.56
1:B:254:GLU:CG	2:N:69:THR:HB	2.35	0.56
2:N:74:ASP:OD2	2:N:76:ASN:HB3	2.05	0.56
1:A:226:ALA:O	1:A:228:MET:N	2.32	0.56
1:A:332:VAL:HG13	1:A:599:THR:CG2	2.36	0.56
1:A:703:VAL:HG22	1:A:825:VAL:HG22	1.87	0.56
1:B:97:THR:HA	1:B:320:THR:HG23	1.86	0.56
2:E:12:LYS:C	2:E:14:ALA:N	2.56	0.56
2:M:139:TRP:HE1	2:M:143:ASN:HD21	1.52	0.56
2:O:110:ALA:HB1	2:O:111:PRO:CD	2.35	0.56
1:A:305:GLN:O	1:A:307:ARG:N	2.38	0.56
1:A:765:PHE:CD1	1:A:765:PHE:C	2.79	0.56
1:B:393:SER:N	1:B:573:THR:CG2	2.68	0.56
2:D:10:THR:O	2:D:14:ALA:HB2	2.05	0.56
2:D:8:SER:O	2:D:10:THR:N	2.38	0.56
2:I:116:LEU:CD1	2:I:119:LEU:HD12	2.36	0.56
2:J:152:PHE:CD1	2:J:152:PHE:N	2.71	0.56
2:K:35:ASN:HA	2:K:38:ILE:HD12	1.87	0.56
2:N:24:TYR:O	2:N:26:ASN:N	2.38	0.56
1:A:135:ARG:O	1:A:136:ALA:C	2.44	0.56
1:A:275:PRO:O	1:A:278:ILE:HG13	2.05	0.56
1:A:420:ILE:HD12	1:A:422:GLU:HG3	1.87	0.56
1:A:649:LEU:O	1:A:650:HIS:O	2.24	0.56
1:B:368:THR:O	1:B:369:GLY:O	2.23	0.56
1:B:390:ARG:HG3	1:B:391:THR:H	1.69	0.56
1:B:409:TRP:CH2	1:B:413:VAL:HG21	2.40	0.56
1:B:556:THR:O	1:B:557:LEU:C	2.44	0.56
2:H:260:GLU:HG2	2:H:274:GLN:HG3	1.85	0.56
1:A:209:ASP:O	1:A:213:GLN:HG3	2.05	0.56
1:A:308:LEU:HB2	1:A:614:TYR:OH	2.06	0.56
1:A:410:LEU:O	1:A:413:VAL:HB	2.05	0.56
1:A:587:LEU:C	1:A:588:ILE:HG13	2.24	0.56
1:A:729:GLY:C	1:A:730:PHE:CD1	2.78	0.56
1:B:153:ASP:OD1	1:B:153:ASP:O	2.22	0.56
1:B:870:ALA:C	1:B:872:ASP:N	2.56	0.56
2:D:12:LYS:C	2:D:14:ALA:N	2.56	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2:ASP:HB2	2:G:128:ASN:HD21	1.71	0.56
2:H:10:THR:O	2:H:14:ALA:HB2	2.06	0.56
2:H:27:VAL:CG2	2:H:31:ILE:HD11	2.35	0.56
2:J:74:ASP:OD2	2:J:76:ASN:HB3	2.04	0.56
2:M:110:ALA:HB1	2:M:111:PRO:CD	2.36	0.56
2:M:150:PHE:CD1	2:M:150:PHE:N	2.74	0.56
1:A:190:ASN:OD1	1:A:192:ASN:N	2.38	0.56
1:B:303:LEU:HD13	1:B:562:THR:HG21	1.88	0.56
1:B:618:ILE:O	1:B:622:VAL:HG23	2.06	0.56
2:H:108:GLY:C	2:H:110:ALA:H	2.09	0.56
2:L:38:ILE:HD12	2:L:65:LEU:HD23	1.86	0.56
2:M:10:THR:O	2:M:14:ALA:HB2	2.05	0.56
2:M:7:LEU:O	2:M:11:LEU:HG	2.06	0.56
2:N:144:ARG:O	2:N:145:ARG:CB	2.52	0.56
2:O:116:LEU:HD12	2:O:119:LEU:HD12	1.87	0.56
1:A:245:LEU:HB3	1:A:249:ASP:CB	2.34	0.56
1:B:203:GLU:O	1:B:207:ILE:HG13	2.05	0.56
1:B:246:HIS:ND1	1:B:247:PRO:HD2	2.20	0.56
2:E:109:ILE:O	2:E:109:ILE:HD12	2.05	0.56
2:E:5:TYR:HE2	2:E:131:ASN:HA	1.69	0.56
2:F:150:PHE:HB2	2:F:152:PHE:HE1	1.70	0.56
2:I:76:ASN:H	2:M:76:ASN:CB	2.13	0.56
2:L:8:SER:C	2:L:10:THR:N	2.55	0.56
2:L:260:GLU:HG2	2:L:274:GLN:HG3	1.86	0.56
1:B:392:MET:HA	1:B:573:THR:HG23	1.87	0.56
2:C:35:ASN:HA	2:C:38:ILE:HD12	1.88	0.56
2:D:38:ILE:HD12	2:D:65:LEU:CD2	2.35	0.56
2:E:8:SER:O	2:E:10:THR:N	2.39	0.56
2:F:116:LEU:HD12	2:F:119:LEU:HD12	1.88	0.56
2:F:7:LEU:O	2:F:11:LEU:HG	2.06	0.56
2:K:99:GLU:O	2:K:384:ARG:NH1	2.39	0.56
2:M:150:PHE:HB2	2:M:152:PHE:CZ	2.41	0.56
2:N:10:THR:O	2:N:14:ALA:HB2	2.06	0.56
1:A:319:ASP:OD2	1:A:571:LEU:CB	2.53	0.56
1:A:857:PHE:H	1:A:857:PHE:HD1	1.52	0.56
1:B:153:ASP:CG	1:B:153:ASP:O	2.43	0.56
1:B:496:ASN:HB3	1:B:498:ARG:CB	2.35	0.56
1:B:305:GLN:HE21	1:B:564:ASN:ND2	2.04	0.56
2:E:99:GLU:O	2:E:99:GLU:HG3	2.05	0.56
2:K:57:ARG:NH1	2:K:94:ASN:HD21	2.03	0.56
2:M:116:LEU:HD12	2:M:119:LEU:HD12	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:35:ASN:HA	2:M:38:ILE:HD12	1.86	0.56
2:O:35:ASN:HA	2:O:38:ILE:HD12	1.88	0.56
2:O:7:LEU:O	2:O:11:LEU:HG	2.06	0.56
1:A:389:GLN:O	1:A:389:GLN:CG	2.54	0.56
1:A:389:GLN:NE2	1:A:568:VAL:H	2.04	0.56
1:A:404:LEU:CD2	1:A:435:ILE:HD11	2.36	0.56
1:A:461:GLN:HB3	2:F:32:GLN:NE2	2.20	0.56
1:A:852:SER:O	1:A:853:ASP:HB3	2.04	0.56
2:D:128:ASN:HB3	2:E:19:VAL:CG2	2.36	0.56
2:E:38:ILE:HG22	2:E:42:ASN:ND2	2.19	0.56
2:J:35:ASN:HA	2:J:38:ILE:HD12	1.87	0.56
2:J:50:GLY:O	2:J:51:ILE:HB	2.05	0.56
2:J:8:SER:O	2:J:10:THR:N	2.39	0.56
1:A:503:ILE:CG2	1:A:506:LEU:HB2	2.36	0.56
1:B:325:ASN:O	1:B:328:LEU:HB3	2.05	0.56
1:B:498:ARG:HG3	1:B:505:GLN:OE1	2.05	0.56
1:B:516:GLN:O	1:B:517:GLN:NE2	2.39	0.56
2:D:7:LEU:O	2:D:11:LEU:HG	2.06	0.56
2:N:7:LEU:O	2:N:11:LEU:HG	2.06	0.56
1:A:440:PHE:O	1:A:442:MET:N	2.38	0.55
1:A:490:ASN:HB3	1:A:492:VAL:HG23	1.88	0.55
1:A:332:VAL:HG13	1:A:599:THR:HG22	1.87	0.55
1:B:266:ASN:O	1:B:267:ASN:C	2.45	0.55
1:B:563:MET:SD	1:B:611:HIS:CD2	2.99	0.55
1:B:707:TYR:HE2	1:B:754:ASN:OD1	1.89	0.55
1:B:763:LEU:HD22	1:B:764:PRO:CD	2.36	0.55
1:B:712:LEU:CB	1:B:819:PRO:HB2	2.36	0.55
2:D:152:PHE:CD1	2:D:152:PHE:N	2.73	0.55
2:F:10:THR:O	2:F:14:ALA:HB2	2.05	0.55
2:I:145:ARG:CZ	2:I:145:ARG:HB3	2.35	0.55
2:I:57:ARG:NH1	2:I:94:ASN:HD21	2.02	0.55
1:A:314:PHE:O	1:A:316:SER:N	2.38	0.55
1:A:346:ILE:O	1:A:349:MET:HB3	2.06	0.55
1:A:414:VAL:O	1:A:416:ASN:N	2.38	0.55
1:A:738:LEU:HA	1:A:741:THR:HG22	1.88	0.55
1:B:260:GLN:O	1:B:262:VAL:N	2.39	0.55
1:B:363:GLU:O	1:B:363:GLU:HG3	2.05	0.55
2:E:129:PHE:C	2:E:129:PHE:CD1	2.80	0.55
2:F:53:ASN:HD22	2:F:354:ALA:HB3	1.71	0.55
1:A:396:PHE:CB	1:A:578:LEU:HD12	2.37	0.55
1:A:535:LEU:O	1:A:539:ARG:CG	2.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:GLU:HB3	1:B:151:LYS:HE3	1.87	0.55
1:B:433:ASN:HD21	1:B:446:HIS:HB3	1.71	0.55
2:C:153:HIS:CD2	2:E:153:HIS:NE2	2.75	0.55
2:F:144:ARG:O	2:F:145:ARG:HB2	2.06	0.55
2:N:116:LEU:CD1	2:N:119:LEU:HD12	2.36	0.55
2:N:8:SER:C	2:N:10:THR:N	2.55	0.55
2:N:99:GLU:O	2:N:99:GLU:HG3	2.06	0.55
2:O:8:SER:O	2:O:10:THR:N	2.40	0.55
1:A:275:PRO:HB2	1:A:278:ILE:HG13	1.87	0.55
1:A:725:ARG:HB3	1:A:828:GLN:OE1	2.06	0.55
1:A:804:SER:HB2	1:A:810:TYR:CB	2.35	0.55
1:B:428:GLN:HG3	1:B:456:PHE:HD1	1.70	0.55
2:C:99:GLU:HG3	2:C:99:GLU:O	2.07	0.55
2:H:12:LYS:C	2:H:14:ALA:N	2.56	0.55
2:I:35:ASN:HA	2:I:38:ILE:HD12	1.87	0.55
2:J:116:LEU:CD1	2:J:119:LEU:HD12	2.36	0.55
1:A:150:LEU:HD12	1:A:696:SER:CB	2.34	0.55
1:A:822:THR:C	1:A:823:THR:HG23	2.26	0.55
1:B:413:VAL:HG12	1:B:414:VAL:H	1.69	0.55
1:B:868:ALA:C	1:B:876:ILE:HG23	2.26	0.55
2:G:106:ARG:N	2:G:106:ARG:HD3	2.22	0.55
2:J:128:ASN:HB3	2:K:19:VAL:CG2	2.36	0.55
2:J:14:ALA:C	2:J:16:ASP:H	2.10	0.55
2:N:6:SER:OG	2:N:128:ASN:HA	2.05	0.55
1:A:383:ILE:HD11	1:A:550:LEU:HD23	1.89	0.55
1:A:744:TYR:C	1:A:746:GLN:N	2.60	0.55
1:B:508:GLU:HG2	1:B:512:GLN:HE21	1.71	0.55
1:B:625:ILE:O	1:B:628:ALA:HB3	2.06	0.55
1:B:650:HIS:O	1:B:652:PHE:N	2.39	0.55
1:B:675:GLU:HB3	1:B:678:ARG:HG3	1.88	0.55
1:B:675:GLU:O	1:B:676:VAL:C	2.44	0.55
1:B:723:ILE:HG22	1:B:724:ALA:N	2.16	0.55
1:B:804:SER:HA	1:B:810:TYR:CZ	2.42	0.55
2:C:144:ARG:HD2	2:D:82:ARG:NH1	2.20	0.55
2:C:145:ARG:O	2:C:146:GLN:HG3	2.06	0.55
2:D:116:LEU:CD1	2:D:119:LEU:HD12	2.36	0.55
2:F:8:SER:O	2:F:10:THR:N	2.39	0.55
2:G:63:PHE:N	2:G:63:PHE:CD1	2.74	0.55
2:H:116:LEU:HD12	2:H:119:LEU:HD12	1.89	0.55
2:L:116:LEU:HD12	2:L:119:LEU:HD12	1.87	0.55
2:L:35:ASN:HA	2:L:38:ILE:HD12	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:10:THR:O	2:O:14:ALA:HB2	2.06	0.55
2:O:144:ARG:O	2:O:145:ARG:HG2	2.07	0.55
1:A:732:GLN:O	1:A:733:ILE:HG23	2.06	0.55
1:B:371:ASN:O	1:B:373:GLN:N	2.39	0.55
1:B:784:ALA:O	1:B:785:GLN:O	2.25	0.55
2:C:10:THR:O	2:C:14:ALA:HB2	2.06	0.55
2:C:82:ARG:NH1	2:E:144:ARG:HD2	2.21	0.55
2:H:99:GLU:HG3	2:H:99:GLU:O	2.07	0.55
2:I:89:VAL:O	2:I:91:PHE:N	2.40	0.55
2:L:8:SER:O	2:L:10:THR:N	2.39	0.55
2:O:49:GLY:HA2	2:O:54:LEU:CD2	2.37	0.55
1:A:510:LEU:HD22	1:A:540:LEU:CD1	2.26	0.55
1:A:563:MET:O	1:A:565:MET:N	2.40	0.55
1:B:122:LEU:HG	1:B:201:ASP:CG	2.27	0.55
1:B:160:TYR:OH	1:B:635:GLN:HG3	2.07	0.55
1:B:113:PRO:HG2	1:B:609:ASN:HB3	1.89	0.55
1:B:763:LEU:O	1:B:764:PRO:O	2.25	0.55
2:C:152:PHE:N	2:C:152:PHE:CD1	2.74	0.55
2:H:8:SER:O	2:H:10:THR:N	2.40	0.55
2:I:101:VAL:HB	2:I:355:ILE:HG21	1.88	0.55
2:I:153:HIS:NE2	2:J:153:HIS:CD2	2.75	0.55
2:I:60:ASN:C	2:I:61:PHE:CD1	2.80	0.55
2:J:38:ILE:HG22	2:J:42:ASN:ND2	2.22	0.55
2:K:35:ASN:HA	2:K:38:ILE:CD1	2.37	0.55
1:B:787:VAL:O	1:B:788:LYS:C	2.46	0.55
2:G:8:SER:O	2:G:10:THR:N	2.40	0.55
2:L:10:THR:O	2:L:14:ALA:HB2	2.06	0.55
2:L:116:LEU:CD1	2:L:119:LEU:HD12	2.37	0.55
2:M:99:GLU:HG3	2:M:99:GLU:O	2.07	0.55
1:A:500:GLY:O	1:A:502:VAL:N	2.36	0.55
1:B:360:ILE:HD12	1:B:360:ILE:N	2.22	0.55
1:B:654:VAL:O	1:B:656:ARG:N	2.39	0.55
1:B:698:LYS:O	1:B:699:ILE:CB	2.53	0.55
2:C:109:ILE:HG23	2:C:110:ALA:H	1.70	0.55
2:C:116:LEU:CD1	2:C:119:LEU:HD12	2.36	0.55
2:C:167:ASN:ND2	2:C:178:GLY:HA2	2.23	0.55
2:E:7:LEU:O	2:E:11:LEU:HG	2.07	0.55
2:F:144:ARG:O	2:F:145:ARG:CB	2.55	0.55
2:F:152:PHE:CD1	2:F:152:PHE:N	2.74	0.55
2:N:35:ASN:HA	2:N:38:ILE:HD12	1.89	0.55
1:A:142:LEU:O	1:A:143:ARG:HG2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:TYR:O	1:A:529:ILE:HG13	2.05	0.54
1:A:705:ILE:HG22	1:A:757:VAL:O	2.07	0.54
1:A:717:MET:HE1	1:A:830:PRO:O	2.07	0.54
1:B:195:ASP:O	1:B:197:GLY:N	2.39	0.54
1:B:245:LEU:HD12	1:B:250:TYR:HA	1.89	0.54
2:E:116:LEU:HD12	2:E:119:LEU:HD12	1.88	0.54
2:J:131:ASN:N	2:J:131:ASN:HD22	2.04	0.54
2:L:82:ARG:NH1	2:N:144:ARG:HD2	2.22	0.54
2:N:8:SER:O	2:N:10:THR:N	2.40	0.54
1:A:742:GLY:HA3	1:B:285:ILE:HD11	1.89	0.54
1:B:388:SER:O	1:B:389:GLN:HB2	2.07	0.54
1:B:779:ASP:HA	1:B:798:ILE:HG13	1.89	0.54
2:C:135:TYR:OH	2:C:340:GLU:OE1	2.24	0.54
2:D:144:ARG:HD2	2:E:82:ARG:CZ	2.36	0.54
2:C:22:THR:HB	2:E:128:ASN:O	2.08	0.54
2:G:35:ASN:HA	2:G:38:ILE:HD12	1.89	0.54
2:I:124:PHE:O	2:I:126:ARG:N	2.39	0.54
2:I:153:HIS:CD2	2:K:153:HIS:NE2	2.75	0.54
2:I:8:SER:O	2:I:10:THR:N	2.40	0.54
2:J:35:ASN:HA	2:J:38:ILE:CD1	2.37	0.54
2:O:35:ASN:HA	2:O:38:ILE:CD1	2.37	0.54
1:A:120:THR:HA	1:A:186:MET:HE1	1.88	0.54
1:A:151:LYS:O	1:A:152:LYS:HB2	2.06	0.54
1:A:166:PHE:CE2	1:A:689:MET:HG3	2.42	0.54
1:A:393:SER:HB2	1:A:573:THR:HG21	1.90	0.54
1:A:730:PHE:CD1	1:A:730:PHE:N	2.75	0.54
1:A:717:MET:SD	1:A:829:VAL:HG22	2.47	0.54
1:A:863:VAL:HG12	1:A:864:GLU:N	2.22	0.54
1:A:871:PHE:O	1:A:871:PHE:CD1	2.60	0.54
2:E:35:ASN:HA	2:E:38:ILE:CD1	2.37	0.54
2:H:116:LEU:CD1	2:H:119:LEU:HD12	2.38	0.54
2:H:150:PHE:HB2	2:H:152:PHE:CE1	2.43	0.54
2:I:49:GLY:HA2	2:I:54:LEU:HD21	1.90	0.54
2:M:8:SER:O	2:M:10:THR:N	2.40	0.54
2:O:116:LEU:CD1	2:O:119:LEU:HD12	2.37	0.54
2:O:144:ARG:O	2:O:146:GLN:N	2.41	0.54
1:A:111:ILE:HG23	1:A:111:ILE:O	2.07	0.54
1:A:643:GLU:HG2	1:A:662:MET:CE	2.37	0.54
1:B:404:LEU:O	1:B:407:GLY:N	2.40	0.54
2:C:8:SER:O	2:C:10:THR:N	2.40	0.54
2:D:110:ALA:HB1	2:D:111:PRO:HD2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:16:ASP:HB3	2:E:131:ASN:O	2.06	0.54
2:F:65:LEU:O	2:F:66:LEU:HD23	2.08	0.54
2:N:42:ASN:HA	2:N:61:PHE:HB2	1.88	0.54
1:A:530:GLN:HA	1:A:533:ILE:CD1	2.37	0.54
1:A:633:LEU:C	1:A:635:GLN:H	2.11	0.54
1:A:663:TYR:O	1:A:666:ARG:HG2	2.08	0.54
1:B:323:THR:O	1:B:326:TYR:HB3	2.08	0.54
1:B:326:TYR:CD1	1:B:384:ALA:CB	2.91	0.54
1:B:370:ILE:O	1:B:373:GLN:HB3	2.08	0.54
1:B:506:LEU:HD21	1:B:543:LEU:C	2.27	0.54
2:E:10:THR:O	2:E:14:ALA:HB2	2.07	0.54
2:F:35:ASN:HA	2:F:38:ILE:HD12	1.90	0.54
2:H:74:ASP:OD2	2:H:76:ASN:HB3	2.07	0.54
1:B:481:ARG:HG2	2:I:65:LEU:HD12	1.89	0.54
1:B:666:ARG:HG3	1:B:667:ASP:N	2.20	0.54
2:E:116:LEU:CD1	2:E:119:LEU:HD12	2.38	0.54
2:E:167:ASN:ND2	2:E:178:GLY:HA2	2.22	0.54
2:I:167:ASN:ND2	2:I:178:GLY:HA2	2.22	0.54
2:J:7:LEU:O	2:J:11:LEU:HG	2.06	0.54
2:N:110:ALA:HB1	2:N:111:PRO:CD	2.37	0.54
2:O:158:PHE:HE2	2:O:214:LEU:HD22	1.73	0.54
1:A:217:THR:O	1:A:217:THR:HG22	2.07	0.54
1:A:501:HIS:C	1:A:503:ILE:H	2.09	0.54
1:B:428:GLN:HG2	1:B:429:LEU:H	1.71	0.54
1:B:875:ARG:CD	1:B:878:ASN:HD22	2.20	0.54
2:C:14:ALA:C	2:C:16:ASP:H	2.10	0.54
2:C:35:ASN:HA	2:C:38:ILE:CD1	2.38	0.54
2:D:14:ALA:C	2:D:16:ASP:H	2.11	0.54
2:H:35:ASN:HA	2:H:38:ILE:HD12	1.89	0.54
2:I:106:ARG:HD3	2:I:106:ARG:H	1.72	0.54
2:J:99:GLU:HG3	2:J:99:GLU:O	2.08	0.54
2:M:139:TRP:HE1	2:M:143:ASN:ND2	2.04	0.54
2:O:14:ALA:C	2:O:16:ASP:H	2.11	0.54
1:A:311:HIS:HB3	1:A:318:TRP:NE1	2.23	0.54
1:A:645:PHE:HD2	1:A:646:LEU:HD23	1.72	0.54
1:A:650:HIS:O	1:A:651:ILE:CB	2.56	0.54
1:A:738:LEU:C	1:A:740:ARG:N	2.62	0.54
1:A:701:GLN:HG2	1:A:826:TYR:CE2	2.43	0.54
1:B:501:HIS:C	1:B:503:ILE:N	2.60	0.54
2:F:158:PHE:HE2	2:F:214:LEU:HD22	1.73	0.54
2:K:14:ALA:C	2:K:16:ASP:H	2.11	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:167:ASN:ND2	2:M:178:GLY:HA2	2.23	0.54
1:A:178:PRO:HD2	1:A:256:PHE:CE2	2.43	0.54
1:B:427:CYS:O	1:B:431:ILE:HG13	2.08	0.54
1:B:771:VAL:CG1	1:B:772:ILE:N	2.71	0.54
2:D:167:ASN:ND2	2:D:178:GLY:HA2	2.23	0.54
2:G:116:LEU:CD1	2:G:119:LEU:HD12	2.38	0.54
2:K:158:PHE:HE2	2:K:214:LEU:HD22	1.73	0.54
2:L:128:ASN:O	2:M:22:THR:HB	2.08	0.54
2:L:72:ASN:ND2	2:N:126:ARG:NH1	2.56	0.54
1:A:273:TYR:O	1:A:273:TYR:CD2	2.61	0.54
1:A:298:TYR:O	1:A:299:ILE:HB	2.06	0.54
1:B:457:GLN:CB	1:B:476:ASN:ND2	2.63	0.54
1:B:653:ASP:O	1:B:654:VAL:C	2.46	0.54
2:C:67:GLY:C	2:C:69:THR:H	2.09	0.54
2:D:35:ASN:HA	2:D:38:ILE:HD12	1.89	0.54
2:I:7:LEU:O	2:I:11:LEU:HG	2.08	0.54
2:J:27:VAL:O	2:J:30:LEU:N	2.40	0.54
2:M:116:LEU:CD1	2:M:119:LEU:HD12	2.37	0.54
2:N:167:ASN:ND2	2:N:178:GLY:HA2	2.22	0.54
1:A:804:SER:HB2	1:A:810:TYR:HA	1.89	0.53
1:B:125:ILE:CD1	1:B:125:ILE:N	2.71	0.53
1:B:125:ILE:HB	1:B:126:PHE:CD2	2.43	0.53
1:B:393:SER:CB	1:B:573:THR:HG21	2.38	0.53
1:B:457:GLN:O	1:B:458:ILE:HG13	2.08	0.53
1:B:503:ILE:HD13	1:B:544:VAL:HG12	1.88	0.53
1:B:862:THR:HG22	1:B:863:VAL:O	2.09	0.53
2:E:74:ASP:OD2	2:E:76:ASN:HB3	2.08	0.53
2:F:116:LEU:CD1	2:F:119:LEU:HD12	2.38	0.53
2:G:150:PHE:HB2	2:G:152:PHE:CE1	2.43	0.53
2:G:22:THR:OG1	2:G:26:ASN:ND2	2.41	0.53
2:H:23:LEU:N	2:H:26:ASN:ND2	2.57	0.53
2:H:135:TYR:OH	2:H:340:GLU:OE1	2.25	0.53
2:I:158:PHE:HE2	2:I:214:LEU:HD22	1.73	0.53
2:K:116:LEU:HD12	2:K:119:LEU:HD12	1.89	0.53
2:M:35:ASN:HA	2:M:38:ILE:CD1	2.38	0.53
1:A:306:ASP:C	1:A:308:LEU:N	2.56	0.53
1:B:252:PHE:O	1:B:254:GLU:N	2.40	0.53
1:B:467:GLN:HB3	1:B:512:GLN:HG2	1.90	0.53
2:G:128:ASN:HB3	2:H:19:VAL:CG2	2.37	0.53
2:G:46:PHE:CE2	2:G:119:LEU:HD21	2.43	0.53
2:K:150:PHE:HB2	2:K:152:PHE:CZ	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:167:ASN:ND2	2:K:178:GLY:HA2	2.22	0.53
2:L:153:HIS:NE2	2:N:153:HIS:NE2	2.55	0.53
2:N:14:ALA:C	2:N:16:ASP:H	2.10	0.53
2:N:89:VAL:O	2:N:91:PHE:N	2.41	0.53
1:B:140:LYS:C	1:B:142:LEU:N	2.60	0.53
1:B:449:ASN:HD21	1:B:455:PRO:CG	2.21	0.53
2:C:158:PHE:HE2	2:C:214:LEU:HD22	1.73	0.53
2:D:70:LEU:HD12	2:D:71:LEU:H	1.74	0.53
2:G:130:ASP:HA	2:H:17:LYS:HG2	1.90	0.53
2:K:215:ARG:HG3	2:K:371:ILE:O	2.09	0.53
2:N:158:PHE:HE2	2:N:214:LEU:HD22	1.73	0.53
2:N:49:GLY:HA2	2:N:54:LEU:CD2	2.39	0.53
2:O:24:TYR:O	2:O:27:VAL:HG22	2.09	0.53
1:A:503:ILE:HG22	1:A:506:LEU:H	1.73	0.53
1:A:705:ILE:HG12	1:A:705:ILE:O	2.07	0.53
1:B:211:ILE:O	1:B:213:GLN:N	2.41	0.53
2:D:99:GLU:CD	2:D:116:LEU:HD22	2.28	0.53
2:E:116:LEU:HA	2:E:119:LEU:CD1	2.38	0.53
2:F:99:GLU:HG3	2:F:99:GLU:O	2.08	0.53
2:I:35:ASN:HA	2:I:38:ILE:CD1	2.38	0.53
2:J:150:PHE:HB2	2:J:152:PHE:CZ	2.42	0.53
2:L:38:ILE:O	2:L:42:ASN:OD1	2.27	0.53
2:O:215:ARG:HG3	2:O:371:ILE:O	2.09	0.53
1:A:542:GLN:O	1:A:545:ASP:HB2	2.08	0.53
1:A:771:VAL:O	1:A:772:ILE:C	2.46	0.53
1:B:122:LEU:HD11	1:B:200:VAL:HG12	1.88	0.53
1:B:170:TYR:CE1	1:B:681:ILE:CG2	2.92	0.53
1:B:182:LEU:HD23	1:B:183:LEU:N	2.15	0.53
1:B:199:VAL:HG12	1:B:200:VAL:H	1.70	0.53
1:B:246:HIS:CE1	1:B:247:PRO:HD2	2.44	0.53
1:B:497:ILE:HG23	2:I:68:THR:HG23	1.89	0.53
1:B:94:THR:HG23	1:B:658:PRO:HG3	1.90	0.53
2:D:144:ARG:HD2	2:E:82:ARG:NH1	2.23	0.53
2:G:99:GLU:O	2:G:99:GLU:HG3	2.09	0.53
2:H:158:PHE:HE2	2:H:214:LEU:HD22	1.73	0.53
2:I:215:ARG:HG3	2:I:371:ILE:O	2.09	0.53
2:J:116:LEU:HA	2:J:119:LEU:CD1	2.38	0.53
2:L:158:PHE:HE2	2:L:214:LEU:HD22	1.73	0.53
2:L:63:PHE:N	2:L:63:PHE:CD1	2.75	0.53
2:N:215:ARG:HG3	2:N:371:ILE:O	2.09	0.53
1:A:311:HIS:NE2	1:A:566:GLN:NE2	2.54	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:LEU:HD22	1:A:584:LEU:HD21	1.90	0.53
1:A:560:CYS:CB	1:A:603:TYR:HD2	2.21	0.53
1:B:133:ILE:HD11	1:B:147:TYR:CE1	2.43	0.53
1:B:200:VAL:HB	1:B:204:THR:HG21	1.89	0.53
1:B:298:TYR:CD1	1:B:299:ILE:N	2.75	0.53
1:B:428:GLN:CG	1:B:456:PHE:HD1	2.21	0.53
1:B:498:ARG:HG3	1:B:505:GLN:HE22	1.73	0.53
1:B:770:SER:HB3	1:B:772:ILE:HG22	1.90	0.53
1:A:642:VAL:HG13	1:A:665:LEU:HD23	1.90	0.53
2:D:116:LEU:HA	2:D:119:LEU:CD1	2.39	0.53
2:E:158:PHE:HE2	2:E:214:LEU:HD22	1.73	0.53
2:G:158:PHE:HE2	2:G:214:LEU:HD22	1.73	0.53
2:J:158:PHE:HE2	2:J:214:LEU:HD22	1.73	0.53
2:K:131:ASN:HD22	2:K:131:ASN:N	2.05	0.53
2:L:215:ARG:HG3	2:L:371:ILE:O	2.09	0.53
2:N:35:ASN:HA	2:N:38:ILE:CD1	2.38	0.53
2:O:167:ASN:ND2	2:O:178:GLY:HA2	2.22	0.53
1:A:238:VAL:HG12	1:A:239:VAL:N	2.24	0.53
1:A:487:GLY:O	1:A:488:VAL:HG23	2.08	0.53
1:A:491:GLN:HB3	1:A:564:ASN:HB3	1.90	0.53
1:A:647:LYS:C	1:A:649:LEU:H	2.12	0.53
1:B:400:ASN:ND2	1:B:403:SER:OG	2.41	0.53
1:B:436:ILE:O	1:B:438:PRO:N	2.42	0.53
1:B:458:ILE:HD12	1:B:458:ILE:C	2.29	0.53
1:B:498:ARG:CB	2:I:32:GLN:NE2	2.66	0.53
1:B:577:GLN:C	1:B:579:THR:N	2.60	0.53
2:E:110:ALA:HB1	2:E:111:PRO:CD	2.39	0.53
2:F:14:ALA:C	2:F:16:ASP:H	2.11	0.53
2:F:144:ARG:HD2	2:G:82:ARG:CZ	2.38	0.53
2:I:116:LEU:HA	2:I:119:LEU:CD1	2.38	0.53
2:I:99:GLU:O	2:I:99:GLU:HG3	2.09	0.53
2:I:144:ARG:HD2	2:J:82:ARG:NH1	2.24	0.53
2:O:74:ASP:OD2	2:O:76:ASN:HB3	2.09	0.53
1:A:271:PHE:O	1:A:274:ILE:HD12	2.08	0.53
1:A:325:ASN:O	1:A:328:LEU:HB3	2.09	0.53
1:A:550:LEU:O	1:A:551:ALA:C	2.47	0.53
1:A:771:VAL:HA	1:A:802:ILE:HD11	1.91	0.53
1:A:853:ASP:O	1:A:854:LEU:CB	2.56	0.53
1:A:876:ILE:HG22	1:A:877:MET:HG2	1.89	0.53
1:B:371:ASN:C	1:B:373:GLN:H	2.11	0.53
1:B:755:GLN:O	1:B:757:VAL:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:786:ILE:O	1:B:788:LYS:N	2.41	0.53
1:B:548:ARG:HD3	1:B:877:MET:H	1.73	0.53
2:C:215:ARG:HG3	2:C:371:ILE:O	2.09	0.53
2:H:167:ASN:ND2	2:H:178:GLY:HA2	2.23	0.53
2:H:215:ARG:HG3	2:H:371:ILE:O	2.09	0.53
2:K:116:LEU:CD1	2:K:119:LEU:HD12	2.39	0.53
2:K:46:PHE:CE2	2:K:119:LEU:HD21	2.41	0.53
2:K:65:LEU:C	2:K:66:LEU:HG	2.29	0.53
2:M:145:ARG:NH1	2:M:145:ARG:CB	2.71	0.53
2:M:158:PHE:HE2	2:M:214:LEU:HD22	1.74	0.53
2:N:31:ILE:O	2:N:34:PHE:HB3	2.09	0.53
2:O:89:VAL:O	2:O:91:PHE:N	2.42	0.53
1:A:661:GLN:NE2	1:B:348:LYS:HZ2	2.06	0.53
1:B:182:LEU:CD2	1:B:183:LEU:N	2.71	0.53
1:B:387:LEU:O	1:B:389:GLN:N	2.42	0.53
1:B:501:HIS:ND1	1:B:548:ARG:HG2	2.24	0.53
1:B:642:VAL:O	1:B:645:PHE:HB3	2.09	0.53
1:B:654:VAL:HG12	1:B:655:ALA:N	2.24	0.53
1:B:708:ARG:O	1:B:710:MET:N	2.42	0.53
2:D:35:ASN:HA	2:D:38:ILE:CD1	2.39	0.53
2:F:167:ASN:ND2	2:F:178:GLY:HA2	2.22	0.53
2:G:215:ARG:HG3	2:G:371:ILE:O	2.09	0.53
2:J:215:ARG:HG3	2:J:371:ILE:O	2.09	0.53
1:B:508:GLU:OE2	2:J:70:LEU:HD23	2.09	0.53
2:M:215:ARG:HG3	2:M:371:ILE:O	2.09	0.53
2:O:99:GLU:O	2:O:99:GLU:HG3	2.09	0.53
1:A:323:THR:O	1:A:326:TYR:HB3	2.08	0.52
1:A:401:TYR:N	1:A:401:TYR:CD1	2.75	0.52
1:A:428:GLN:CD	1:A:456:PHE:HB2	2.27	0.52
1:A:606:VAL:O	1:A:607:ASN:C	2.46	0.52
1:A:721:VAL:CG1	1:A:799:LEU:HD22	2.39	0.52
1:A:794:THR:HG22	1:A:794:THR:O	2.08	0.52
1:A:297:ARG:HG3	1:A:848:PHE:CE2	2.43	0.52
1:B:437:TYR:HD2	1:B:443:GLN:HB3	1.73	0.52
1:B:499:ASN:O	1:B:500:GLY:O	2.27	0.52
1:B:504:ASN:O	1:B:505:GLN:C	2.46	0.52
1:B:654:VAL:O	1:B:657:VAL:HG23	2.08	0.52
1:B:742:GLY:O	1:B:744:TYR:CE2	2.62	0.52
2:I:14:ALA:C	2:I:16:ASP:H	2.11	0.52
2:J:129:PHE:CD1	2:J:129:PHE:C	2.82	0.52
2:J:139:TRP:C	2:J:139:TRP:CD1	2.83	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:89:VAL:O	2:K:91:PHE:N	2.43	0.52
2:L:152:PHE:N	2:L:152:PHE:CD1	2.77	0.52
1:A:255:TYR:O	1:A:259:HIS:HB3	2.08	0.52
1:A:424:LEU:HD12	1:A:424:LEU:O	2.08	0.52
1:A:618:ILE:HD13	1:A:645:PHE:CZ	2.44	0.52
1:A:722:ASN:C	1:A:723:ILE:HG13	2.29	0.52
1:B:135:ARG:O	1:B:138:GLY:N	2.43	0.52
1:B:326:TYR:CE1	1:B:384:ALA:HB3	2.44	0.52
1:B:466:PHE:O	1:B:467:GLN:C	2.47	0.52
1:B:663:TYR:O	1:B:666:ARG:HG2	2.09	0.52
2:L:61:PHE:O	2:L:62:ASP:HB3	2.07	0.52
2:M:48:THR:O	2:M:56:ILE:HA	2.10	0.52
1:A:329:ALA:O	1:A:333:VAL:HG23	2.10	0.52
1:A:340:VAL:HB	1:A:587:LEU:CD2	2.39	0.52
1:A:658:PRO:HB2	1:A:660:ASP:OD1	2.09	0.52
1:B:525:TYR:O	1:B:529:ILE:HG13	2.08	0.52
1:B:311:HIS:CD2	1:B:566:GLN:OE1	2.62	0.52
2:C:381:ASN:O	2:C:385:VAL:HB	2.10	0.52
2:D:158:PHE:HE2	2:D:214:LEU:HD22	1.74	0.52
2:D:215:ARG:HG3	2:D:371:ILE:O	2.09	0.52
2:D:42:ASN:HA	2:D:61:PHE:HB2	1.92	0.52
2:E:14:ALA:C	2:E:16:ASP:H	2.11	0.52
2:H:150:PHE:HB2	2:H:152:PHE:CZ	2.44	0.52
2:M:101:VAL:HG23	2:M:102:ARG:N	2.24	0.52
2:M:116:LEU:HA	2:M:119:LEU:CD1	2.38	0.52
2:O:110:ALA:HB1	2:O:111:PRO:HD2	1.90	0.52
2:O:116:LEU:HA	2:O:119:LEU:CD1	2.39	0.52
1:A:200:VAL:O	1:A:204:THR:OG1	2.17	0.52
1:A:361:GLN:HG3	1:A:362:SER:H	1.75	0.52
1:A:326:TYR:CD1	1:A:384:ALA:CB	2.92	0.52
1:A:555:GLU:OE2	1:A:871:PHE:CE2	2.63	0.52
1:B:418:MET:HB3	1:B:567:HIS:NE2	2.24	0.52
1:B:431:ILE:O	1:B:435:ILE:HB	2.09	0.52
1:B:689:MET:HA	1:B:692:ILE:HD13	1.91	0.52
2:D:24:TYR:CZ	2:D:68:THR:HG22	2.44	0.52
2:G:35:ASN:HA	2:G:38:ILE:CD1	2.39	0.52
2:I:74:ASP:OD2	2:I:76:ASN:HB3	2.08	0.52
2:J:150:PHE:HB2	2:J:152:PHE:HE1	1.73	0.52
2:L:167:ASN:ND2	2:L:178:GLY:HA2	2.22	0.52
2:M:31:ILE:O	2:M:34:PHE:HB3	2.09	0.52
2:O:23:LEU:HB3	2:O:26:ASN:HD21	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:PHE:O	1:A:315:GLU:C	2.48	0.52
1:A:421:ARG:O	1:A:425:VAL:HG23	2.10	0.52
1:A:742:GLY:O	1:A:743:ASP:O	2.28	0.52
1:A:872:ASP:OD2	1:A:874:MET:HB2	2.10	0.52
1:B:340:VAL:O	1:B:587:LEU:HD11	2.09	0.52
1:B:277:ARG:NH1	1:B:559:ALA:HB2	2.25	0.52
2:D:74:ASP:OD2	2:D:76:ASN:HB3	2.09	0.52
2:F:150:PHE:HB2	2:F:152:PHE:CZ	2.44	0.52
2:F:381:ASN:O	2:F:385:VAL:HB	2.10	0.52
2:G:381:ASN:O	2:G:385:VAL:HB	2.10	0.52
2:K:53:ASN:ND2	2:K:354:ALA:HB3	2.25	0.52
2:L:8:SER:C	2:L:10:THR:H	2.13	0.52
2:N:116:LEU:HA	2:N:119:LEU:CD1	2.39	0.52
1:A:286:LEU:O	1:A:287:ASN:HB2	2.09	0.52
1:A:464:GLN:O	1:A:465:ASN:HB2	2.08	0.52
1:B:396:PHE:C	1:B:396:PHE:CD1	2.83	0.52
1:B:527:ARG:HH11	1:B:527:ARG:HG3	1.74	0.52
1:B:527:ARG:O	1:B:531:ARG:HG2	2.08	0.52
1:B:558:MET:O	1:B:561:VAL:HG23	2.09	0.52
1:B:763:LEU:HD22	1:B:764:PRO:HD2	1.92	0.52
1:B:811:LEU:HD23	1:B:811:LEU:N	2.24	0.52
2:E:215:ARG:HG3	2:E:371:ILE:O	2.09	0.52
2:F:215:ARG:HG3	2:F:371:ILE:O	2.09	0.52
2:G:7:LEU:O	2:G:11:LEU:HG	2.09	0.52
2:H:57:ARG:NH1	2:H:94:ASN:HD21	2.07	0.52
2:M:21:GLY:O	2:M:22:THR:O	2.28	0.52
2:O:107:ASN:CG	2:O:107:ASN:O	2.48	0.52
1:A:721:VAL:HG13	1:A:800:TYR:C	2.29	0.52
1:A:803:ASN:C	1:A:805:ASP:N	2.63	0.52
1:B:211:ILE:O	1:B:212:PHE:C	2.48	0.52
1:B:326:TYR:HD1	1:B:384:ALA:HB1	1.75	0.52
1:B:570:THR:HG22	1:B:571:LEU:H	1.75	0.52
1:B:632:ASN:O	1:B:634:TYR:N	2.38	0.52
2:D:8:SER:C	2:D:10:THR:H	2.13	0.52
2:F:129:PHE:C	2:F:129:PHE:CD1	2.83	0.52
2:F:5:TYR:HE2	2:F:131:ASN:HA	1.75	0.52
2:G:14:ALA:C	2:G:16:ASP:H	2.11	0.52
2:I:14:ALA:O	2:I:18:ILE:HD12	2.10	0.52
2:J:167:ASN:ND2	2:J:178:GLY:HA2	2.23	0.52
2:J:381:ASN:O	2:J:385:VAL:HB	2.10	0.52
2:K:381:ASN:O	2:K:385:VAL:HB	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:381:ASN:O	2:L:385:VAL:HB	2.10	0.52
2:N:12:LYS:O	2:N:14:ALA:N	2.43	0.52
2:N:381:ASN:O	2:N:385:VAL:HB	2.10	0.52
2:O:381:ASN:O	2:O:385:VAL:HB	2.10	0.52
1:A:786:ILE:O	1:A:789:LEU:N	2.43	0.52
1:B:550:LEU:O	1:B:551:ALA:C	2.49	0.52
1:B:812:VAL:HG23	1:B:817:TRP:CZ3	2.45	0.52
2:D:23:LEU:HD22	2:D:25:SER:OG	2.10	0.52
2:D:41:MET:O	2:D:42:ASN:C	2.47	0.52
2:L:31:ILE:O	2:L:34:PHE:HB3	2.10	0.52
2:M:89:VAL:O	2:M:91:PHE:N	2.43	0.52
1:A:323:THR:OG1	1:A:390:ARG:NH1	2.43	0.52
1:A:467:GLN:HB3	1:A:512:GLN:HG2	1.92	0.52
1:A:163:ARG:NH2	1:A:736:GLU:OE2	2.42	0.52
1:B:314:PHE:N	1:B:314:PHE:CD1	2.77	0.52
1:B:444:ARG:HH22	1:B:520:THR:HA	1.75	0.52
1:B:540:LEU:HA	1:B:543:LEU:HB2	1.92	0.52
1:B:723:ILE:CG2	1:B:724:ALA:H	2.13	0.52
2:H:139:TRP:CD1	2:H:139:TRP:C	2.83	0.52
2:H:14:ALA:C	2:H:16:ASP:H	2.11	0.52
2:K:99:GLU:O	2:K:99:GLU:HG3	2.10	0.52
2:L:106:ARG:N	2:L:106:ARG:HD3	2.17	0.52
2:L:110:ALA:HB1	2:L:111:PRO:HD2	1.92	0.52
2:L:35:ASN:HA	2:L:38:ILE:CD1	2.39	0.52
2:M:14:ALA:C	2:M:16:ASP:H	2.11	0.52
2:M:8:SER:C	2:M:10:THR:H	2.13	0.52
1:B:293:PRO:C	1:B:295:THR:N	2.60	0.52
2:F:135:TYR:OH	2:F:340:GLU:OE1	2.28	0.52
2:F:35:ASN:HA	2:F:38:ILE:CD1	2.40	0.52
2:H:128:ASN:O	2:H:129:PHE:HB3	2.09	0.52
2:M:131:ASN:N	2:M:131:ASN:HD22	2.07	0.52
1:A:310:LEU:O	1:A:318:TRP:CD1	2.62	0.51
1:A:540:LEU:C	1:A:540:LEU:HD23	2.30	0.51
1:A:769:SER:O	1:A:771:VAL:N	2.43	0.51
1:B:235:ASP:O	1:B:236:ARG:HB2	2.10	0.51
1:B:286:LEU:N	1:B:286:LEU:HD22	2.25	0.51
1:B:322:THR:O	1:B:323:THR:C	2.48	0.51
1:B:530:GLN:HA	1:B:533:ILE:CD1	2.40	0.51
1:B:563:MET:HA	1:B:563:MET:CE	2.39	0.51
1:B:606:VAL:O	1:B:607:ASN:C	2.47	0.51
2:C:116:LEU:HA	2:C:119:LEU:CD1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:89:VAL:O	2:J:91:PHE:N	2.43	0.51
2:M:27:VAL:CG2	2:M:31:ILE:HD11	2.40	0.51
2:O:133:SER:O	2:O:136:ILE:HG22	2.10	0.51
1:A:125:ILE:CD1	1:A:125:ILE:N	2.63	0.51
1:A:269:ILE:HG21	1:A:298:TYR:HE2	1.76	0.51
1:A:431:ILE:HG23	1:A:435:ILE:HD12	1.91	0.51
1:B:378:CYS:SG	1:B:581:VAL:HA	2.50	0.51
1:B:422:GLU:O	1:B:425:VAL:N	2.43	0.51
2:C:27:VAL:O	2:C:30:LEU:N	2.38	0.51
2:D:105:GLN:NE2	2:D:359:PRO:O	2.43	0.51
2:H:145:ARG:O	2:H:146:GLN:HG3	2.10	0.51
2:I:139:TRP:CD1	2:I:139:TRP:C	2.84	0.51
2:J:11:LEU:O	2:J:15:ARG:N	2.39	0.51
2:K:74:ASP:OD2	2:K:76:ASN:HB3	2.10	0.51
1:A:259:HIS:HD1	1:A:260:GLN:N	2.07	0.51
1:A:326:TYR:CE1	1:A:384:ALA:HB3	2.45	0.51
1:A:647:LYS:O	1:A:649:LEU:N	2.43	0.51
1:B:133:ILE:HD11	1:B:147:TYR:HE1	1.76	0.51
2:C:24:TYR:OH	2:C:68:THR:HG22	2.10	0.51
2:D:6:SER:O	2:D:8:SER:N	2.44	0.51
2:E:135:TYR:OH	2:E:340:GLU:OE1	2.28	0.51
2:G:6:SER:HG	2:G:128:ASN:HA	1.72	0.51
2:H:148:THR:OG1	2:H:332:GLU:HG2	2.10	0.51
2:I:128:ASN:HD22	2:J:19:VAL:CB	2.21	0.51
2:H:76:ASN:N	2:J:76:ASN:HB2	2.24	0.51
2:K:41:MET:O	2:K:42:ASN:C	2.49	0.51
2:L:116:LEU:HA	2:L:119:LEU:CD1	2.40	0.51
2:M:381:ASN:O	2:M:385:VAL:HB	2.10	0.51
1:A:420:ILE:HG12	1:A:423:SER:CB	2.38	0.51
1:A:519:PRO:O	1:A:520:THR:HG23	2.10	0.51
1:A:645:PHE:CD2	1:A:646:LEU:HD23	2.44	0.51
1:B:442:MET:SD	1:B:463:ILE:HA	2.49	0.51
1:B:460:GLU:HG3	1:B:473:HIS:HD2	1.76	0.51
1:B:498:ARG:CG	1:B:505:GLN:HE22	2.23	0.51
1:B:498:ARG:HG3	1:B:505:GLN:NE2	2.26	0.51
1:B:639:LYS:O	1:B:642:VAL:HG23	2.10	0.51
1:B:699:ILE:HG13	1:B:763:LEU:O	2.10	0.51
1:B:779:ASP:HA	1:B:798:ILE:CG1	2.39	0.51
1:B:89:GLU:C	1:B:91:LEU:N	2.61	0.51
2:C:74:ASP:OD2	2:C:76:ASN:HB3	2.11	0.51
2:D:381:ASN:O	2:D:385:VAL:HB	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:6:SER:O	2:E:8:SER:N	2.44	0.51
2:E:89:VAL:O	2:E:91:PHE:N	2.44	0.51
2:G:89:VAL:O	2:G:91:PHE:N	2.44	0.51
2:H:5:TYR:HE2	2:H:131:ASN:HA	1.75	0.51
1:A:631:LEU:O	1:A:633:LEU:HD12	2.10	0.51
1:A:773:SER:HB3	1:A:778:LEU:HD12	1.91	0.51
1:B:104:ILE:HD12	1:B:327:ILE:HD12	1.92	0.51
1:A:661:GLN:HG3	1:B:348:LYS:NZ	2.26	0.51
1:B:548:ARG:HH11	1:B:878:ASN:N	2.04	0.51
1:B:594:ILE:C	1:B:594:ILE:CD1	2.79	0.51
1:B:705:ILE:HG22	1:B:707:TYR:CE1	2.45	0.51
2:D:139:TRP:C	2:D:139:TRP:CD1	2.84	0.51
2:D:89:VAL:O	2:D:91:PHE:N	2.43	0.51
2:H:31:ILE:O	2:H:34:PHE:HB3	2.11	0.51
2:K:155:PRO:O	2:K:186:SER:HB3	2.10	0.51
2:M:253:ILE:HD13	2:M:319:THR:HB	1.93	0.51
2:N:133:SER:O	2:N:136:ILE:HG22	2.11	0.51
2:N:41:MET:O	2:N:42:ASN:C	2.49	0.51
2:O:106:ARG:HD3	2:O:106:ARG:N	2.23	0.51
1:A:252:PHE:O	1:A:254:GLU:N	2.44	0.51
1:A:427:CYS:O	1:A:431:ILE:HG13	2.11	0.51
1:A:496:ASN:O	1:A:497:ILE:C	2.49	0.51
1:A:443:GLN:NE2	1:A:521:MET:HB3	2.25	0.51
1:B:178:PRO:HD2	1:B:256:PHE:CE2	2.45	0.51
1:B:272:ASN:O	1:B:274:ILE:N	2.43	0.51
1:B:431:ILE:HG23	1:B:435:ILE:HD12	1.93	0.51
1:B:481:ARG:NH2	1:B:496:ASN:HD21	2.08	0.51
2:E:31:ILE:O	2:E:34:PHE:HB3	2.09	0.51
2:K:116:LEU:HA	2:K:119:LEU:CD1	2.41	0.51
2:L:89:VAL:O	2:L:91:PHE:N	2.43	0.51
1:A:158:GLY:O	1:A:162:VAL:HG23	2.09	0.51
1:A:159:ASP:O	1:A:162:VAL:HB	2.11	0.51
1:A:814:ASN:O	1:A:815:TYR:C	2.48	0.51
1:B:302:ASN:O	1:B:303:LEU:HD23	2.11	0.51
1:B:305:GLN:NE2	1:B:564:ASN:ND2	2.58	0.51
2:C:110:ALA:HB1	2:C:111:PRO:CD	2.41	0.51
2:D:360:VAL:O	2:D:378:ARG:HD3	2.11	0.51
2:F:8:SER:C	2:F:10:THR:H	2.14	0.51
2:F:109:ILE:CB	2:F:380:ASP:HB3	2.40	0.51
2:H:105:GLN:C	2:H:107:ASN:N	2.58	0.51
2:H:381:ASN:O	2:H:385:VAL:HB	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:253:ILE:HD13	2:J:319:THR:HB	1.92	0.51
2:K:106:ARG:HD3	2:K:106:ARG:N	2.17	0.51
2:K:253:ILE:HD13	2:K:319:THR:HB	1.93	0.51
2:O:253:ILE:HD13	2:O:319:THR:HB	1.93	0.51
2:O:31:ILE:O	2:O:34:PHE:HB3	2.11	0.51
2:O:54:LEU:HD12	2:O:55:PRO:HD2	1.93	0.51
1:A:326:TYR:HD1	1:A:384:ALA:HB1	1.75	0.51
1:A:793:ASP:C	1:A:795:LEU:N	2.63	0.51
1:B:481:ARG:CZ	1:B:496:ASN:OD1	2.59	0.51
1:B:491:GLN:O	1:B:491:GLN:HG3	2.10	0.51
1:B:658:PRO:HD2	1:B:661:GLN:HG3	1.93	0.51
2:C:139:TRP:CD1	2:C:139:TRP:C	2.83	0.51
2:C:42:ASN:HA	2:C:61:PHE:HB2	1.92	0.51
2:E:381:ASN:O	2:E:385:VAL:HB	2.10	0.51
2:F:23:LEU:HD11	2:H:36:GLN:OE1	2.10	0.51
2:F:360:VAL:O	2:F:378:ARG:HD3	2.11	0.51
2:G:111:PRO:HB3	2:G:116:LEU:CD2	2.41	0.51
2:H:35:ASN:HA	2:H:38:ILE:CD1	2.41	0.51
2:I:381:ASN:O	2:I:385:VAL:HB	2.10	0.51
2:J:12:LYS:O	2:J:14:ALA:N	2.43	0.51
2:J:360:VAL:O	2:J:378:ARG:HD3	2.11	0.51
2:L:14:ALA:C	2:L:16:ASP:H	2.12	0.51
2:L:99:GLU:HG3	2:L:99:GLU:O	2.10	0.51
2:M:106:ARG:HG2	2:M:107:ASN:H	1.75	0.51
2:M:24:TYR:O	2:M:26:ASN:N	2.44	0.51
2:M:360:VAL:O	2:M:378:ARG:HD3	2.11	0.51
2:M:109:ILE:HB	2:M:380:ASP:HB3	1.93	0.51
2:O:41:MET:O	2:O:42:ASN:C	2.49	0.51
1:A:130:GLN:O	1:A:131:LEU:HB3	2.10	0.51
1:A:368:THR:HG22	1:A:368:THR:O	2.09	0.51
1:A:631:LEU:CB	1:A:633:LEU:HD13	2.38	0.51
1:B:577:GLN:C	1:B:579:THR:H	2.14	0.51
1:B:712:LEU:HD11	1:B:722:ASN:HB3	1.93	0.51
1:B:869:VAL:N	1:B:876:ILE:HG23	2.26	0.51
2:C:17:LYS:HG2	2:E:130:ASP:HA	1.92	0.51
2:C:89:VAL:O	2:C:91:PHE:N	2.43	0.51
2:F:89:VAL:O	2:F:91:PHE:N	2.44	0.51
2:G:253:ILE:HD13	2:G:319:THR:HB	1.93	0.51
2:G:360:VAL:O	2:G:378:ARG:HD3	2.11	0.51
2:L:139:TRP:C	2:L:139:TRP:CD1	2.84	0.51
1:A:362:SER:HB2	1:A:365:GLN:HE22	1.72	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:HIS:C	1:A:503:ILE:N	2.62	0.51
1:A:527:ARG:O	1:A:531:ARG:HG2	2.10	0.51
1:A:546:LEU:HD11	1:A:584:LEU:HD23	1.93	0.51
1:A:618:ILE:O	1:A:622:VAL:HG23	2.11	0.51
1:A:701:GLN:O	1:A:761:GLY:O	2.29	0.51
1:B:140:LYS:HE2	1:B:805:ASP:OD2	2.10	0.51
2:C:128:ASN:HB3	2:D:19:VAL:HG23	1.93	0.51
2:F:74:ASP:OD2	2:F:76:ASN:HB3	2.11	0.51
2:F:63:PHE:CD2	2:F:84:THR:HG23	2.46	0.51
2:G:103:GLU:HG3	2:G:359:PRO:HD2	1.93	0.51
2:G:116:LEU:HA	2:G:119:LEU:CD1	2.40	0.51
2:J:153:HIS:NE2	2:K:153:HIS:NE2	2.59	0.51
2:N:60:ASN:C	2:N:61:PHE:CD1	2.84	0.51
2:O:8:SER:C	2:O:10:THR:H	2.14	0.51
2:O:23:LEU:C	2:O:23:LEU:HD23	2.31	0.51
1:A:508:GLU:O	1:A:512:GLN:NE2	2.45	0.50
1:A:555:GLU:OE1	1:A:871:PHE:HD2	1.93	0.50
1:A:676:VAL:O	1:A:680:ASP:HB2	2.10	0.50
1:B:178:PRO:HD2	1:B:256:PHE:CD2	2.45	0.50
1:B:509:ALA:O	1:B:513:LEU:CG	2.50	0.50
1:B:539:ARG:O	1:B:542:GLN:N	2.44	0.50
1:B:805:ASP:C	1:B:807:ASN:N	2.65	0.50
2:C:129:PHE:C	2:C:129:PHE:CD1	2.85	0.50
2:C:49:GLY:HA2	2:C:54:LEU:HD23	1.93	0.50
2:F:253:ILE:HD13	2:F:319:THR:HB	1.93	0.50
2:H:116:LEU:HA	2:H:119:LEU:CD1	2.40	0.50
2:H:12:LYS:O	2:H:14:ALA:N	2.44	0.50
2:K:11:LEU:O	2:K:15:ARG:N	2.38	0.50
2:L:135:TYR:CZ	2:L:342:MET:HE3	2.45	0.50
2:N:135:TYR:OH	2:N:340:GLU:OE1	2.25	0.50
1:A:452:PRO:O	1:A:453:GLN:CB	2.58	0.50
1:A:467:GLN:NE2	1:A:511:MET:HG2	2.25	0.50
1:B:182:LEU:HD11	1:B:847:THR:CA	2.40	0.50
1:B:392:MET:C	1:B:573:THR:HG23	2.32	0.50
1:B:449:ASN:ND2	1:B:455:PRO:CG	2.75	0.50
1:B:527:ARG:O	1:B:531:ARG:HG3	2.10	0.50
1:B:671:LEU:O	1:B:672:LEU:HD23	2.10	0.50
2:C:133:SER:O	2:C:136:ILE:HG22	2.12	0.50
2:D:155:PRO:O	2:D:186:SER:HB3	2.11	0.50
2:G:8:SER:C	2:G:10:THR:H	2.14	0.50
2:I:133:SER:O	2:I:136:ILE:HG22	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:360:VAL:O	2:K:378:ARG:HD3	2.11	0.50
2:L:23:LEU:HD11	2:N:36:GLN:HB2	1.92	0.50
1:A:520:THR:O	1:A:521:MET:HE3	2.11	0.50
1:B:298:TYR:HE1	1:B:300:ARG:HA	1.77	0.50
1:B:518:PHE:CB	1:B:519:PRO:CD	2.89	0.50
1:B:878:ASN:OD1	1:B:878:ASN:O	2.29	0.50
2:D:253:ILE:HD13	2:D:319:THR:HB	1.93	0.50
2:E:8:SER:C	2:E:10:THR:H	2.14	0.50
2:E:56:ILE:HG22	2:E:56:ILE:O	2.11	0.50
2:F:61:PHE:N	2:F:61:PHE:CD1	2.79	0.50
2:H:89:VAL:O	2:H:91:PHE:N	2.44	0.50
2:K:60:ASN:C	2:K:61:PHE:CD1	2.85	0.50
2:L:150:PHE:CD1	2:L:150:PHE:N	2.78	0.50
2:L:155:PRO:O	2:L:186:SER:HB3	2.11	0.50
2:L:6:SER:O	2:L:8:SER:N	2.44	0.50
2:N:8:SER:C	2:N:10:THR:H	2.14	0.50
2:N:23:LEU:O	2:N:26:ASN:ND2	2.43	0.50
1:A:199:VAL:CG1	1:A:200:VAL:H	2.07	0.50
1:A:436:ILE:CD1	1:A:437:TYR:CD1	2.94	0.50
1:A:822:THR:O	1:A:823:THR:HG23	2.12	0.50
1:A:545:ASP:OD1	1:A:877:MET:HA	2.11	0.50
1:B:457:GLN:C	1:B:458:ILE:HG13	2.31	0.50
1:B:596:SER:O	1:B:599:THR:HB	2.11	0.50
1:B:712:LEU:HB2	1:B:819:PRO:HB2	1.94	0.50
2:C:12:LYS:O	2:C:14:ALA:N	2.45	0.50
2:G:31:ILE:O	2:G:34:PHE:HB3	2.11	0.50
2:G:6:SER:O	2:G:8:SER:N	2.44	0.50
2:H:253:ILE:HD13	2:H:319:THR:HB	1.93	0.50
1:B:498:ARG:HD3	2:I:32:GLN:NE2	2.26	0.50
2:I:31:ILE:O	2:I:34:PHE:HB3	2.11	0.50
2:L:133:SER:O	2:L:136:ILE:HG22	2.12	0.50
2:L:253:ILE:HD13	2:L:319:THR:HB	1.93	0.50
2:N:106:ARG:HG2	2:N:107:ASN:H	1.77	0.50
2:N:139:TRP:C	2:N:139:TRP:CD1	2.84	0.50
2:N:66:LEU:HD13	2:N:77:TYR:CZ	2.46	0.50
1:A:389:GLN:OE1	1:A:567:HIS:HA	2.11	0.50
1:A:634:TYR:HD1	1:A:635:GLN:HG3	1.76	0.50
1:B:428:GLN:NE2	1:B:455:PRO:HB2	2.26	0.50
1:B:826:TYR:O	1:B:827:LYS:C	2.50	0.50
2:C:360:VAL:O	2:C:378:ARG:HD3	2.11	0.50
2:C:46:PHE:HE2	2:C:119:LEU:HD21	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:124:PHE:O	2:D:127:ILE:HG13	2.11	0.50
2:D:12:LYS:O	2:D:14:ALA:N	2.45	0.50
2:D:100:MET:HG3	2:D:388:VAL:HG11	1.93	0.50
2:F:139:TRP:C	2:F:139:TRP:CD1	2.85	0.50
2:G:124:PHE:O	2:G:127:ILE:HG13	2.11	0.50
2:I:124:PHE:C	2:I:126:ARG:H	2.14	0.50
2:J:8:SER:C	2:J:10:THR:H	2.14	0.50
2:L:125:LYS:O	2:L:127:ILE:N	2.42	0.50
2:L:360:VAL:O	2:L:378:ARG:HD3	2.11	0.50
1:A:214:ASP:O	1:A:215:GLU:C	2.50	0.50
1:B:176:GLU:O	1:B:178:PRO:HD3	2.11	0.50
1:B:387:LEU:HD23	1:B:554:TYR:HE1	1.74	0.50
1:B:578:LEU:HA	1:B:581:VAL:CG2	2.42	0.50
2:C:14:ALA:C	2:C:16:ASP:N	2.65	0.50
2:E:139:TRP:C	2:E:139:TRP:CD1	2.84	0.50
2:E:150:PHE:CD1	2:E:150:PHE:N	2.80	0.50
2:E:151:THR:C	2:E:152:PHE:CD1	2.84	0.50
2:E:253:ILE:HD13	2:E:319:THR:HB	1.93	0.50
2:F:73:LEU:HD22	2:F:77:TYR:CD2	2.46	0.50
2:G:139:TRP:C	2:G:139:TRP:CD1	2.85	0.50
2:G:167:ASN:ND2	2:G:178:GLY:HA2	2.22	0.50
2:I:6:SER:O	2:I:8:SER:N	2.44	0.50
2:J:6:SER:O	2:J:8:SER:N	2.45	0.50
2:L:11:LEU:O	2:L:15:ARG:N	2.39	0.50
2:O:11:LEU:O	2:O:15:ARG:N	2.40	0.50
1:A:229:ARG:O	1:A:242:PRO:CG	2.60	0.50
1:A:332:VAL:HG11	1:A:557:LEU:HD21	1.93	0.50
1:A:675:GLU:O	1:A:676:VAL:C	2.50	0.50
1:B:364:THR:O	1:B:364:THR:HG22	2.12	0.50
1:B:463:ILE:HG21	1:B:468:VAL:CG1	2.41	0.50
1:B:499:ASN:N	1:B:505:GLN:NE2	2.60	0.50
1:B:536:LEU:HD22	1:B:536:LEU:N	2.27	0.50
1:B:618:ILE:HD13	1:B:645:PHE:CZ	2.47	0.50
1:B:170:TYR:CE1	1:B:682:PHE:HB2	2.47	0.50
1:B:810:TYR:HA	1:B:812:VAL:HG12	1.92	0.50
2:C:31:ILE:O	2:C:34:PHE:HB3	2.12	0.50
2:D:133:SER:O	2:D:136:ILE:HG22	2.11	0.50
2:F:6:SER:O	2:F:8:SER:N	2.45	0.50
2:I:8:SER:C	2:I:10:THR:H	2.14	0.50
2:I:360:VAL:O	2:I:378:ARG:HD3	2.11	0.50
2:K:124:PHE:O	2:K:126:ARG:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:35:ASN:O	2:L:36:GLN:C	2.50	0.50
2:N:104:SER:O	2:N:108:GLY:HA3	2.12	0.50
1:A:289:ASP:C	1:A:290:ARG:HG2	2.32	0.50
1:A:297:ARG:HG3	1:A:848:PHE:CD2	2.46	0.50
1:A:309:ASN:HA	1:A:311:HIS:CE1	2.47	0.50
1:A:603:TYR:O	1:A:606:VAL:CG2	2.60	0.50
1:A:704:ILE:HG23	1:A:758:ALA:HB2	1.94	0.50
1:B:141:GLU:O	1:B:142:LEU:CB	2.60	0.50
1:B:477:ASN:O	1:B:479:GLN:N	2.44	0.50
1:B:510:LEU:HD12	1:B:513:LEU:HD12	1.94	0.50
1:A:660:ASP:CA	1:B:539:ARG:HH11	2.24	0.50
1:B:392:MET:HB3	1:B:574:GLU:O	2.10	0.50
1:B:113:PRO:HD2	1:B:609:ASN:HB3	1.94	0.50
2:E:101:VAL:HG23	2:E:102:ARG:N	2.27	0.50
2:I:12:LYS:O	2:I:14:ALA:N	2.45	0.50
2:I:150:PHE:N	2:I:150:PHE:CD1	2.79	0.50
2:J:23:LEU:O	2:J:26:ASN:ND2	2.45	0.50
2:N:360:VAL:O	2:N:378:ARG:HD3	2.11	0.50
1:A:369:GLY:O	1:A:370:ILE:C	2.49	0.50
1:A:503:ILE:O	1:A:503:ILE:HG22	2.12	0.50
1:A:613:ASN:HD22	1:A:649:LEU:HD21	1.75	0.50
1:B:306:ASP:C	1:B:308:LEU:H	2.08	0.50
1:B:436:ILE:CG1	1:B:437:TYR:H	2.21	0.50
1:B:444:ARG:HH21	1:B:520:THR:CG2	2.09	0.50
2:C:253:ILE:HD13	2:C:319:THR:HB	1.93	0.50
2:E:24:TYR:O	2:E:26:ASN:N	2.43	0.50
2:E:360:VAL:O	2:E:378:ARG:HD3	2.11	0.50
2:F:153:HIS:NE2	2:G:153:HIS:CD2	2.80	0.50
2:G:124:PHE:O	2:G:126:ARG:N	2.45	0.50
2:G:155:PRO:O	2:G:186:SER:HB3	2.12	0.50
2:G:74:ASP:OD2	2:G:76:ASN:HB3	2.12	0.50
2:J:144:ARG:O	2:J:145:ARG:HB2	2.12	0.50
2:J:63:PHE:CD1	2:J:63:PHE:N	2.80	0.50
2:K:8:SER:C	2:K:10:THR:H	2.14	0.50
2:N:253:ILE:HD13	2:N:319:THR:HB	1.93	0.50
2:O:30:LEU:O	2:O:31:ILE:C	2.51	0.50
1:A:310:LEU:CD1	1:A:310:LEU:N	2.69	0.49
1:A:311:HIS:HA	1:A:318:TRP:CD1	2.47	0.49
1:A:392:MET:O	1:A:420:ILE:HG23	2.11	0.49
1:A:465:ASN:HB3	1:A:468:VAL:HB	1.94	0.49
1:A:555:GLU:OE1	1:A:871:PHE:CD2	2.66	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:TYR:OH	1:A:594:ILE:HG23	2.12	0.49
1:A:674:VAL:HG12	1:A:678:ARG:HB2	1.93	0.49
1:A:774:LEU:HD12	1:A:774:LEU:O	2.11	0.49
1:B:394:LEU:C	1:B:396:PHE:N	2.65	0.49
1:B:305:GLN:NE2	1:B:564:ASN:CG	2.65	0.49
2:J:14:ALA:C	2:J:16:ASP:N	2.65	0.49
2:K:133:SER:O	2:K:136:ILE:HG22	2.12	0.49
2:O:6:SER:O	2:O:8:SER:N	2.45	0.49
1:A:141:GLU:O	1:A:142:LEU:HB2	2.11	0.49
1:A:230:GLN:NE2	1:A:230:GLN:O	2.45	0.49
1:A:390:ARG:HG3	1:A:391:THR:N	2.26	0.49
1:A:404:LEU:O	1:A:405:ILE:C	2.50	0.49
1:A:503:ILE:HG22	1:A:506:LEU:CB	2.42	0.49
1:A:779:ASP:N	1:A:779:ASP:OD1	2.43	0.49
1:B:267:ASN:N	1:B:292:LEU:HD12	2.27	0.49
1:B:322:THR:HG21	1:B:390:ARG:HA	1.94	0.49
1:B:639:LYS:O	1:B:642:VAL:N	2.44	0.49
1:B:134:TYR:CD2	1:B:803:ASN:HB2	2.47	0.49
2:C:106:ARG:HD3	2:C:106:ARG:N	2.10	0.49
2:C:60:ASN:C	2:C:61:PHE:CD1	2.85	0.49
2:F:116:LEU:HA	2:F:119:LEU:CD1	2.42	0.49
2:G:133:SER:O	2:G:136:ILE:HG22	2.12	0.49
2:H:101:VAL:HB	2:H:355:ILE:HG21	1.94	0.49
2:H:360:VAL:O	2:H:378:ARG:HD3	2.11	0.49
2:M:139:TRP:C	2:M:139:TRP:CD1	2.84	0.49
2:O:14:ALA:C	2:O:16:ASP:N	2.66	0.49
2:O:35:ASN:HD21	2:O:66:LEU:HD12	1.77	0.49
1:A:415:PRO:HD2	1:A:480:PHE:HE1	1.76	0.49
1:A:501:HIS:O	1:A:503:ILE:N	2.37	0.49
1:A:527:ARG:HH11	1:A:527:ARG:HG3	1.77	0.49
1:B:159:ASP:OD2	1:B:761:GLY:HA3	2.11	0.49
1:B:277:ARG:CB	1:B:277:ARG:NH1	2.75	0.49
1:B:428:GLN:HE22	1:B:455:PRO:HB2	1.77	0.49
1:B:480:PHE:O	1:B:481:ARG:C	2.49	0.49
1:B:501:HIS:C	1:B:503:ILE:H	2.15	0.49
1:B:590:ASN:ND2	1:B:590:ASN:N	2.46	0.49
1:B:735:LEU:CD2	1:B:759:LEU:HB3	2.42	0.49
2:C:8:SER:C	2:C:10:THR:H	2.14	0.49
2:E:12:LYS:O	2:E:14:ALA:N	2.45	0.49
2:E:22:THR:CG2	2:E:73:LEU:HD12	2.42	0.49
2:K:31:ILE:O	2:K:34:PHE:HB3	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:688:ASN:O	1:A:689:MET:C	2.51	0.49
1:A:149:LYS:NZ	1:A:697:ASP:OD1	2.45	0.49
1:A:771:VAL:HG12	1:A:809:PHE:HB3	1.93	0.49
1:B:450:GLY:O	1:B:451:ASP:HB2	2.11	0.49
1:B:428:GLN:CB	1:B:456:PHE:HD1	2.24	0.49
1:B:498:ARG:HH12	2:J:25:SER:CB	2.23	0.49
1:B:698:LYS:C	1:B:699:ILE:HD13	2.33	0.49
1:B:698:LYS:O	1:B:699:ILE:HD13	2.12	0.49
1:B:869:VAL:HG13	1:B:873:ASN:HA	1.92	0.49
2:G:14:ALA:C	2:G:16:ASP:N	2.66	0.49
2:H:8:SER:C	2:H:10:THR:H	2.14	0.49
2:M:133:SER:O	2:M:136:ILE:HG22	2.13	0.49
2:O:139:TRP:CD1	2:O:139:TRP:C	2.85	0.49
1:A:178:PRO:HD2	1:A:256:PHE:HE2	1.77	0.49
1:A:333:VAL:CG1	1:A:380:LYS:HA	2.19	0.49
1:A:415:PRO:HG2	1:A:480:PHE:HD1	1.73	0.49
1:A:718:TYR:CD1	1:A:718:TYR:N	2.80	0.49
1:B:122:LEU:O	1:B:123:PHE:HB3	2.12	0.49
1:B:174:LEU:O	1:B:177:MET:HB2	2.12	0.49
1:B:305:GLN:O	1:B:307:ARG:N	2.46	0.49
1:B:812:VAL:HA	1:B:817:TRP:HZ3	1.78	0.49
2:J:144:ARG:NH2	2:J:146:GLN:NE2	2.61	0.49
2:K:12:LYS:O	2:K:14:ALA:N	2.45	0.49
2:K:14:ALA:C	2:K:16:ASP:N	2.65	0.49
2:N:22:THR:OG1	2:N:26:ASN:ND2	2.40	0.49
2:O:63:PHE:CD1	2:O:63:PHE:N	2.81	0.49
1:B:150:LEU:HD12	1:B:696:SER:HA	1.93	0.49
1:B:603:TYR:O	1:B:606:VAL:CG2	2.61	0.49
1:B:856:ALA:C	1:B:858:VAL:H	2.14	0.49
2:C:153:HIS:CE1	2:D:153:HIS:CD2	3.01	0.49
2:C:6:SER:O	2:C:8:SER:N	2.45	0.49
2:F:12:LYS:O	2:F:14:ALA:N	2.45	0.49
2:H:155:PRO:O	2:H:186:SER:HB3	2.13	0.49
2:J:115:SER:O	2:J:119:LEU:HG	2.13	0.49
2:J:30:LEU:O	2:J:31:ILE:C	2.51	0.49
2:J:31:ILE:O	2:J:34:PHE:HB3	2.13	0.49
2:O:360:VAL:O	2:O:378:ARG:HD3	2.11	0.49
1:A:147:TYR:CD1	1:A:147:TYR:N	2.80	0.49
1:A:452:PRO:O	1:A:453:GLN:HB3	2.13	0.49
1:A:457:GLN:O	1:A:459:ALA:N	2.45	0.49
1:A:548:ARG:O	1:A:551:ALA:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:GLN:HE22	1:A:568:VAL:H	1.60	0.49
1:A:854:LEU:O	1:A:856:ALA:N	2.46	0.49
1:B:457:GLN:C	1:B:459:ALA:N	2.57	0.49
1:B:544:VAL:HG11	1:B:548:ARG:HH21	1.78	0.49
1:B:807:ASN:C	1:B:809:PHE:N	2.66	0.49
2:C:153:HIS:O	2:C:154:LYS:C	2.50	0.49
2:C:35:ASN:O	2:C:36:GLN:C	2.51	0.49
2:E:115:SER:O	2:E:119:LEU:HG	2.13	0.49
2:F:150:PHE:CD1	2:F:150:PHE:N	2.80	0.49
2:F:14:ALA:C	2:F:16:ASP:N	2.66	0.49
2:G:153:HIS:NE2	2:H:153:HIS:CD2	2.81	0.49
2:I:253:ILE:HD13	2:I:319:THR:HB	1.93	0.49
2:I:5:TYR:CE2	2:I:131:ASN:HA	2.47	0.49
2:L:139:TRP:HE1	2:L:143:ASN:HD22	1.61	0.49
2:M:5:TYR:HE2	2:M:131:ASN:HA	1.77	0.49
2:N:14:ALA:C	2:N:16:ASP:N	2.65	0.49
1:A:539:ARG:O	1:A:542:GLN:N	2.44	0.49
1:A:652:PHE:CD1	1:A:652:PHE:N	2.80	0.49
1:A:662:MET:O	1:A:665:LEU:CB	2.61	0.49
1:A:820:THR:O	1:A:820:THR:HG22	2.13	0.49
1:B:182:LEU:HD21	1:B:846:LEU:HD12	1.95	0.49
1:B:184:LYS:C	1:B:186:MET:H	2.15	0.49
1:B:288:MET:HA	1:B:288:MET:CE	2.42	0.49
1:B:487:GLY:O	1:B:488:VAL:HB	2.13	0.49
1:B:580:SER:O	1:B:581:VAL:C	2.51	0.49
1:B:854:LEU:CD2	1:B:855:LEU:N	2.76	0.49
2:E:110:ALA:HB1	2:E:111:PRO:HD2	1.95	0.49
2:E:21:GLY:O	2:E:22:THR:O	2.31	0.49
2:F:72:ASN:ND2	2:H:126:ARG:NH1	2.60	0.49
2:I:14:ALA:C	2:I:16:ASP:N	2.66	0.49
2:J:2:ASP:HB2	2:J:128:ASN:HD21	1.77	0.49
2:O:109:ILE:HB	2:O:380:ASP:HB3	1.94	0.49
1:A:192:ASN:O	1:A:193:SER:CB	2.49	0.49
1:B:139:GLU:O	1:B:141:GLU:N	2.46	0.49
1:B:428:GLN:O	1:B:432:VAL:HG23	2.13	0.49
1:B:501:HIS:O	1:B:503:ILE:HG13	2.12	0.49
1:B:676:VAL:O	1:B:680:ASP:HB2	2.13	0.49
1:B:845:ASN:HB3	1:B:848:PHE:HE1	1.77	0.49
2:D:35:ASN:O	2:D:36:GLN:C	2.51	0.49
2:F:101:VAL:HG23	2:F:102:ARG:N	2.27	0.49
2:F:46:PHE:CE2	2:F:119:LEU:HD21	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:42:ASN:HA	2:G:61:PHE:HB2	1.94	0.49
2:H:6:SER:O	2:H:8:SER:N	2.46	0.49
2:I:144:ARG:NH2	2:I:146:GLN:HE22	2.10	0.49
2:J:101:VAL:HG23	2:J:102:ARG:N	2.27	0.49
2:J:150:PHE:CD1	2:J:150:PHE:N	2.81	0.49
2:J:35:ASN:O	2:J:36:GLN:C	2.51	0.49
2:K:139:TRP:C	2:K:139:TRP:CD1	2.85	0.49
2:L:12:LYS:O	2:L:14:ALA:N	2.45	0.49
1:A:311:HIS:HE2	1:A:566:GLN:HE22	1.59	0.49
1:A:646:LEU:HD23	1:A:646:LEU:N	2.28	0.49
1:A:666:ARG:HG2	1:A:667:ASP:H	1.78	0.49
1:A:597:PRO:HB3	1:A:860:ALA:HB3	1.94	0.49
1:B:277:ARG:NH1	1:B:277:ARG:HB2	2.28	0.49
1:B:422:GLU:N	1:B:422:GLU:OE1	2.46	0.49
1:B:587:LEU:CG	1:B:587:LEU:O	2.60	0.49
2:C:106:ARG:HG2	2:C:107:ASN:H	1.77	0.49
2:G:12:LYS:O	2:G:14:ALA:N	2.46	0.49
1:B:473:HIS:CB	2:I:126:ARG:NH2	2.69	0.49
2:K:59:TRP:CD1	2:K:59:TRP:N	2.79	0.49
2:M:12:LYS:O	2:M:14:ALA:N	2.46	0.49
1:A:122:LEU:HD11	1:A:201:ASP:CB	2.43	0.48
1:A:271:PHE:CA	1:A:274:ILE:HD12	2.43	0.48
1:A:404:LEU:O	1:A:407:GLY:N	2.46	0.48
1:A:179:ASP:HA	1:A:677:ARG:NH2	2.27	0.48
1:B:302:ASN:ND2	1:B:615:ASN:HB3	2.27	0.48
1:B:785:GLN:O	1:B:787:VAL:N	2.46	0.48
2:E:14:ALA:C	2:E:16:ASP:N	2.66	0.48
2:G:115:SER:O	2:G:119:LEU:HG	2.13	0.48
2:G:129:PHE:C	2:G:129:PHE:CD1	2.86	0.48
2:I:49:GLY:HA2	2:I:54:LEU:CD2	2.43	0.48
2:L:41:MET:O	2:L:42:ASN:C	2.51	0.48
2:O:69:THR:O	2:O:70:LEU:O	2.31	0.48
1:A:322:THR:O	1:A:323:THR:C	2.50	0.48
1:A:529:ILE:O	1:A:533:ILE:HG13	2.12	0.48
1:B:436:ILE:O	1:B:437:TYR:C	2.51	0.48
1:B:473:HIS:O	1:B:477:ASN:ND2	2.46	0.48
1:B:583:SER:O	1:B:587:LEU:HB3	2.12	0.48
1:B:789:LEU:O	1:B:790:ARG:C	2.51	0.48
2:K:30:LEU:O	2:K:31:ILE:C	2.52	0.48
2:K:6:SER:O	2:K:8:SER:N	2.46	0.48
2:L:109:ILE:HB	2:L:380:ASP:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:14:ALA:C	2:L:16:ASP:N	2.67	0.48
2:L:135:TYR:OH	2:L:340:GLU:OE1	2.30	0.48
2:M:38:ILE:HG22	2:M:42:ASN:ND2	2.27	0.48
2:M:6:SER:O	2:M:8:SER:N	2.45	0.48
2:N:53:ASN:ND2	2:N:354:ALA:HB3	2.28	0.48
2:O:48:THR:O	2:O:56:ILE:HA	2.12	0.48
1:A:434:THR:O	1:A:434:THR:CG2	2.61	0.48
1:B:477:ASN:HD21	2:I:39:ILE:HG21	1.77	0.48
1:B:486:ASP:O	1:B:488:VAL:N	2.46	0.48
1:B:522:PRO:O	1:B:525:TYR:HB2	2.14	0.48
1:B:765:PHE:CZ	1:B:767:THR:HG23	2.48	0.48
2:C:130:ASP:C	2:C:131:ASN:HD22	2.17	0.48
2:G:144:ARG:O	2:G:145:ARG:HB2	2.14	0.48
2:H:149:GLY:C	2:H:150:PHE:CD1	2.87	0.48
2:H:14:ALA:C	2:H:16:ASP:N	2.66	0.48
2:I:19:VAL:HG21	2:K:128:ASN:HB3	1.94	0.48
2:J:135:TYR:OH	2:J:340:GLU:OE1	2.30	0.48
2:M:123:LYS:HG3	2:M:124:PHE:CE1	2.49	0.48
2:M:131:ASN:O	2:N:16:ASP:HB3	2.13	0.48
2:O:144:ARG:C	2:O:145:ARG:HG2	2.33	0.48
1:A:122:LEU:HD23	1:A:122:LEU:N	2.28	0.48
1:A:384:ALA:O	1:A:385:ALA:C	2.50	0.48
1:A:390:ARG:HE	1:A:574:GLU:HG2	1.78	0.48
1:A:704:ILE:O	1:A:823:THR:HB	2.14	0.48
1:B:228:MET:O	1:B:228:MET:HG3	2.12	0.48
1:B:231:ARG:CB	1:B:240:ASN:HB2	2.42	0.48
1:B:275:PRO:HD2	1:B:278:ILE:CD1	2.43	0.48
1:B:329:ALA:HB3	1:B:384:ALA:CB	2.43	0.48
1:B:422:GLU:O	1:B:425:VAL:HB	2.12	0.48
1:B:442:MET:O	1:B:443:GLN:C	2.50	0.48
2:E:133:SER:O	2:E:136:ILE:HG22	2.13	0.48
2:J:36:GLN:OE1	2:K:23:LEU:HD21	2.13	0.48
2:K:35:ASN:O	2:K:36:GLN:C	2.51	0.48
2:L:5:TYR:HE2	2:L:130:ASP:O	1.97	0.48
1:A:170:TYR:CE1	1:A:682:PHE:HB2	2.49	0.48
1:A:226:ALA:C	1:A:228:MET:H	2.15	0.48
1:A:305:GLN:OE1	1:A:564:ASN:ND2	2.44	0.48
1:A:484:VAL:CG1	1:A:485:ILE:H	2.25	0.48
1:A:486:ASP:OD2	1:A:490:ASN:HB2	2.13	0.48
1:A:545:ASP:OD1	1:A:548:ARG:NH1	2.46	0.48
1:A:545:ASP:O	1:A:546:LEU:C	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:LEU:C	1:B:110:ASP:N	2.67	0.48
1:B:113:PRO:CD	1:B:609:ASN:HB3	2.43	0.48
1:B:176:GLU:O	1:B:178:PRO:CD	2.61	0.48
1:B:521:MET:CB	1:B:522:PRO:CD	2.90	0.48
1:B:392:MET:CA	1:B:573:THR:HG23	2.43	0.48
2:D:125:LYS:O	2:D:127:ILE:N	2.46	0.48
2:E:6:SER:OG	2:E:128:ASN:HA	2.13	0.48
2:H:115:SER:O	2:H:119:LEU:HG	2.13	0.48
2:H:22:THR:OG1	2:H:26:ASN:ND2	2.46	0.48
2:H:35:ASN:O	2:H:36:GLN:C	2.51	0.48
2:I:48:THR:O	2:I:56:ILE:HA	2.13	0.48
2:J:155:PRO:O	2:J:186:SER:HB3	2.14	0.48
2:O:14:ALA:O	2:O:18:ILE:CD1	2.61	0.48
2:O:42:ASN:HA	2:O:61:PHE:HB2	1.95	0.48
1:A:118:LYS:CG	1:A:119:GLN:N	2.73	0.48
1:A:404:LEU:CB	1:A:435:ILE:HD11	2.43	0.48
1:A:428:GLN:CB	1:A:456:PHE:HD1	2.22	0.48
1:A:460:GLU:C	1:A:462:GLN:H	2.16	0.48
1:A:516:GLN:CD	1:A:516:GLN:H	2.11	0.48
1:A:659:ASP:O	1:A:660:ASP:O	2.32	0.48
1:A:822:THR:O	1:A:823:THR:OG1	2.22	0.48
1:A:865:PRO:O	1:A:867:ASN:N	2.47	0.48
1:B:104:ILE:HD12	1:B:327:ILE:CD1	2.44	0.48
1:B:782:VAL:O	1:B:785:GLN:HB2	2.14	0.48
2:C:150:PHE:CD1	2:C:150:PHE:N	2.82	0.48
2:D:150:PHE:HB2	2:D:152:PHE:HE1	1.77	0.48
2:D:24:TYR:CE1	2:D:68:THR:HG22	2.48	0.48
2:D:31:ILE:O	2:D:34:PHE:HB3	2.13	0.48
2:E:35:ASN:O	2:E:36:GLN:C	2.52	0.48
2:F:53:ASN:ND2	2:F:354:ALA:HB3	2.28	0.48
2:G:54:LEU:HD12	2:G:55:PRO:HD2	1.96	0.48
2:M:128:ASN:HD22	2:N:19:VAL:HB	1.79	0.48
2:N:35:ASN:O	2:N:36:GLN:C	2.51	0.48
2:O:32:GLN:O	2:O:33:GLN:C	2.52	0.48
1:A:363:GLU:C	1:A:366:PHE:HE1	2.16	0.48
1:A:458:ILE:O	1:A:462:GLN:HG2	2.13	0.48
1:A:627:ALA:O	1:A:631:LEU:HG	2.13	0.48
1:A:629:ASN:C	1:A:631:LEU:N	2.61	0.48
1:B:190:ASN:O	1:B:190:ASN:CG	2.52	0.48
1:B:220:ALA:O	1:B:223:ARG:HB2	2.14	0.48
1:B:415:PRO:O	1:B:416:ASN:C	2.52	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:459:ALA:HB1	1:B:463:ILE:CD1	2.36	0.48
1:B:305:GLN:CG	1:B:564:ASN:HD21	2.26	0.48
1:B:723:ILE:O	1:B:724:ALA:CB	2.61	0.48
1:B:785:GLN:O	1:B:786:ILE:C	2.51	0.48
2:C:30:LEU:O	2:C:31:ILE:C	2.52	0.48
2:C:63:PHE:N	2:C:63:PHE:CD1	2.81	0.48
2:E:23:LEU:O	2:E:26:ASN:ND2	2.47	0.48
2:F:144:ARG:O	2:F:145:ARG:HG3	2.14	0.48
2:G:23:LEU:HD23	2:G:24:TYR:N	2.28	0.48
2:I:45:GLU:C	2:I:46:PHE:CD1	2.87	0.48
2:K:150:PHE:CD1	2:K:150:PHE:N	2.82	0.48
2:L:30:LEU:O	2:L:31:ILE:C	2.52	0.48
2:N:6:SER:O	2:N:8:SER:N	2.47	0.48
1:A:145:ARG:HB3	1:A:147:TYR:CE1	2.49	0.48
1:A:589:GLY:C	1:A:591:ALA:N	2.66	0.48
1:B:233:GLN:HB2	1:B:238:VAL:HB	1.96	0.48
1:B:319:ASP:OD2	1:B:572:THR:N	2.46	0.48
1:B:452:PRO:O	1:B:453:GLN:OE1	2.32	0.48
1:B:594:ILE:HB	1:B:595:PRO:HD2	1.94	0.48
1:B:655:ALA:C	1:B:657:VAL:H	2.17	0.48
1:B:745:ALA:HA	1:B:748:THR:OG1	2.13	0.48
1:B:775:ILE:N	1:B:775:ILE:CD1	2.76	0.48
2:D:70:LEU:CG	2:D:71:LEU:N	2.76	0.48
2:I:128:ASN:O	2:J:22:THR:HB	2.14	0.48
2:M:22:THR:HG23	2:M:73:LEU:CD1	2.39	0.48
1:A:239:VAL:HG21	1:A:845:ASN:O	2.13	0.48
1:A:484:VAL:HG12	1:A:485:ILE:N	2.28	0.48
1:A:328:LEU:HG	1:A:603:TYR:HE1	1.79	0.48
1:A:769:SER:O	1:A:770:SER:C	2.51	0.48
1:A:817:TRP:CZ3	1:A:819:PRO:HA	2.49	0.48
1:B:214:ASP:O	1:B:216:GLU:N	2.47	0.48
1:B:283:ASN:O	1:B:863:VAL:HG23	2.13	0.48
1:B:517:GLN:N	1:B:518:PHE:CE1	2.79	0.48
1:B:536:LEU:CD2	1:B:536:LEU:N	2.77	0.48
1:B:811:LEU:HA	1:B:814:ASN:HD22	1.79	0.48
1:B:712:LEU:HB3	1:B:819:PRO:HB2	1.96	0.48
2:C:145:ARG:HB3	2:C:145:ARG:CZ	2.43	0.48
2:D:14:ALA:C	2:D:16:ASP:N	2.66	0.48
2:F:31:ILE:O	2:F:34:PHE:HB3	2.13	0.48
1:B:466:PHE:CD1	2:H:80:THR:HG22	2.48	0.48
2:I:37:MET:O	2:I:38:ILE:C	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:346:VAL:CG2	2:J:385:VAL:HG13	2.44	0.48
2:L:106:ARG:HG2	2:L:107:ASN:H	1.78	0.48
2:L:50:GLY:HA2	2:L:56:ILE:HD11	1.95	0.48
1:A:314:PHE:N	1:A:314:PHE:CD1	2.82	0.48
1:A:365:GLN:C	1:A:366:PHE:CG	2.88	0.48
1:A:436:ILE:HD11	1:A:437:TYR:CE1	2.49	0.48
1:A:527:ARG:O	1:A:531:ARG:HG3	2.13	0.48
1:A:660:ASP:C	1:A:662:MET:N	2.66	0.48
1:A:694:ARG:HD2	1:A:828:GLN:HG3	1.96	0.48
1:B:126:PHE:HB3	1:B:149:LYS:O	2.14	0.48
1:B:236:ARG:O	1:B:237:ASN:CB	2.61	0.48
1:B:384:ALA:O	1:B:385:ALA:C	2.50	0.48
1:B:447:TYR:OH	1:B:458:ILE:HD11	2.13	0.48
1:B:449:ASN:HD21	1:B:455:PRO:HG3	1.78	0.48
1:B:478:ASN:C	1:B:480:PHE:H	2.17	0.48
1:B:533:ILE:O	1:B:536:LEU:HB2	2.14	0.48
1:B:540:LEU:C	1:B:540:LEU:HD23	2.34	0.48
1:B:639:LYS:O	1:B:640:ALA:C	2.52	0.48
1:B:89:GLU:C	1:B:91:LEU:H	2.16	0.48
2:F:38:ILE:HG22	2:F:42:ASN:ND2	2.27	0.48
2:I:346:VAL:CG2	2:I:385:VAL:HG13	2.44	0.48
2:I:35:ASN:O	2:I:36:GLN:C	2.52	0.48
2:I:41:MET:O	2:I:42:ASN:C	2.52	0.48
2:J:133:SER:O	2:J:136:ILE:HG22	2.13	0.48
2:J:19:VAL:O	2:J:21:GLY:N	2.47	0.48
2:K:115:SER:O	2:K:119:LEU:HG	2.14	0.48
2:L:139:TRP:HE1	2:L:143:ASN:ND2	2.11	0.48
2:M:14:ALA:C	2:M:16:ASP:N	2.66	0.48
2:M:30:LEU:O	2:M:31:ILE:C	2.52	0.48
2:M:35:ASN:O	2:M:36:GLN:C	2.51	0.48
2:O:346:VAL:CG2	2:O:385:VAL:HG13	2.44	0.48
2:O:35:ASN:O	2:O:36:GLN:C	2.52	0.48
2:O:63:PHE:CD2	2:O:84:THR:HG23	2.49	0.48
1:B:122:LEU:HD11	1:B:200:VAL:HG11	1.94	0.47
1:B:405:ILE:O	1:B:408:MET:HB2	2.14	0.47
2:C:131:ASN:ND2	2:C:131:ASN:N	2.62	0.47
2:D:66:LEU:O	2:D:67:GLY:O	2.31	0.47
2:E:131:ASN:HD22	2:E:131:ASN:N	2.11	0.47
2:I:48:THR:HG21	2:I:94:ASN:HB3	1.96	0.47
2:J:48:THR:O	2:J:56:ILE:HA	2.13	0.47
2:L:346:VAL:CG2	2:L:385:VAL:HG13	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:41:MET:O	2:M:42:ASN:C	2.52	0.47
2:N:152:PHE:N	2:N:152:PHE:CD1	2.82	0.47
2:N:42:ASN:HA	2:N:61:PHE:CB	2.44	0.47
2:N:99:GLU:OE2	2:N:112:GLN:HG2	2.13	0.47
2:O:12:LYS:O	2:O:14:ALA:N	2.46	0.47
1:A:540:LEU:HA	1:A:543:LEU:HB2	1.96	0.47
1:B:822:THR:HG22	1:B:822:THR:O	2.14	0.47
2:C:5:TYR:HE2	2:C:131:ASN:HA	1.80	0.47
2:G:35:ASN:O	2:G:36:GLN:C	2.52	0.47
2:H:51:ILE:O	2:H:51:ILE:HG23	2.14	0.47
2:H:22:THR:HG23	2:H:73:LEU:CD1	2.43	0.47
2:M:115:SER:O	2:M:119:LEU:HG	2.14	0.47
1:A:306:ASP:HB3	1:A:310:LEU:HD11	1.95	0.47
1:A:383:ILE:O	1:A:384:ALA:C	2.53	0.47
1:A:437:TYR:N	1:A:438:PRO:CD	2.73	0.47
1:A:503:ILE:HG12	1:A:547:THR:HG21	1.96	0.47
1:A:539:ARG:NH2	1:A:588:ILE:O	2.47	0.47
1:A:636:LYS:O	1:A:637:LYS:C	2.52	0.47
1:A:660:ASP:O	1:A:663:TYR:N	2.47	0.47
1:A:701:GLN:HB3	1:A:826:TYR:CD2	2.46	0.47
1:B:295:THR:O	1:B:297:ARG:HG2	2.14	0.47
1:B:296:ALA:C	1:B:297:ARG:HG2	2.35	0.47
1:B:493:LEU:HD11	1:B:567:HIS:HB2	1.95	0.47
1:B:638:MET:HE1	1:B:666:ARG:HH12	1.78	0.47
2:D:32:GLN:O	2:D:33:GLN:C	2.52	0.47
2:F:30:LEU:O	2:F:31:ILE:C	2.53	0.47
2:F:35:ASN:O	2:F:36:GLN:C	2.53	0.47
2:H:133:SER:O	2:H:136:ILE:HG22	2.14	0.47
2:I:33:GLN:HA	2:J:23:LEU:HD12	1.95	0.47
1:B:511:MET:HE3	2:J:70:LEU:HG	1.94	0.47
2:M:11:LEU:O	2:M:15:ARG:N	2.41	0.47
1:A:714:ARG:HG2	1:A:720:TYR:HD2	1.79	0.47
1:A:710:MET:HE1	1:A:824:LYS:HE2	1.97	0.47
1:A:827:LYS:O	1:A:828:GLN:O	2.32	0.47
1:B:355:LEU:HG	1:B:356:GLU:H	1.76	0.47
1:B:460:GLU:HG3	1:B:473:HIS:CD2	2.49	0.47
1:B:513:LEU:HA	1:B:516:GLN:HE22	1.71	0.47
2:D:48:THR:O	2:D:56:ILE:HA	2.14	0.47
2:E:30:LEU:O	2:E:31:ILE:C	2.51	0.47
2:G:346:VAL:CG2	2:G:385:VAL:HG13	2.45	0.47
2:H:151:THR:C	2:H:152:PHE:CD1	2.88	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:37:MET:O	2:M:38:ILE:C	2.53	0.47
2:N:32:GLN:O	2:N:33:GLN:C	2.53	0.47
2:O:153:HIS:O	2:O:154:LYS:C	2.52	0.47
1:A:148:TRP:CH2	1:A:246:HIS:HB2	2.49	0.47
1:A:311:HIS:N	1:A:311:HIS:ND1	2.63	0.47
1:A:742:GLY:CA	1:B:285:ILE:HD11	2.44	0.47
1:B:513:LEU:O	1:B:516:GLN:OE1	2.32	0.47
1:B:666:ARG:HG2	1:B:667:ASP:H	1.79	0.47
1:B:735:LEU:HD21	1:B:759:LEU:CB	2.45	0.47
1:B:95:ILE:O	1:B:97:THR:N	2.46	0.47
2:C:115:SER:O	2:C:119:LEU:HG	2.15	0.47
2:E:32:GLN:O	2:E:33:GLN:C	2.52	0.47
2:F:133:SER:O	2:F:136:ILE:HG22	2.14	0.47
1:B:481:ARG:HG2	2:I:65:LEU:CD1	2.44	0.47
2:J:129:PHE:O	2:J:131:ASN:ND2	2.47	0.47
2:K:125:LYS:O	2:K:127:ILE:N	2.45	0.47
2:N:23:LEU:HD23	2:N:24:TYR:N	2.29	0.47
2:O:115:SER:O	2:O:119:LEU:HG	2.14	0.47
1:A:338:GLU:O	1:A:338:GLU:HG3	2.14	0.47
1:A:527:ARG:HH11	1:A:531:ARG:HH21	1.63	0.47
1:A:596:SER:HB3	1:A:599:THR:OG1	2.15	0.47
1:A:723:ILE:O	1:A:824:LYS:HD2	2.14	0.47
1:B:593:VAL:HG12	1:B:594:ILE:N	2.30	0.47
2:E:346:VAL:CG2	2:E:385:VAL:HG13	2.44	0.47
2:F:78:VAL:O	2:F:81:ALA:HB3	2.14	0.47
2:G:153:HIS:O	2:G:154:LYS:C	2.53	0.47
2:I:144:ARG:O	2:I:145:ARG:HB2	2.15	0.47
2:K:100:MET:HG3	2:K:388:VAL:HG11	1.95	0.47
2:M:53:ASN:O	2:M:353:TYR:HD2	1.97	0.47
2:N:152:PHE:HD2	2:N:337:ASP:HB3	1.78	0.47
1:A:248:ILE:O	1:A:251:ALA:HB3	2.14	0.47
1:A:454:THR:HB	1:A:457:GLN:CB	2.44	0.47
1:A:772:ILE:HA	1:A:775:ILE:CD1	2.45	0.47
1:B:308:LEU:HA	1:B:308:LEU:HD23	1.73	0.47
1:B:583:SER:O	1:B:584:LEU:C	2.53	0.47
2:F:142:GLN:HE21	2:F:143:ASN:N	2.12	0.47
2:F:72:ASN:ND2	2:H:126:ARG:HH11	2.12	0.47
2:H:23:LEU:N	2:H:26:ASN:HD22	2.12	0.47
2:I:124:PHE:C	2:I:126:ARG:N	2.68	0.47
2:I:139:TRP:HE1	2:I:143:ASN:HD22	1.62	0.47
2:J:63:PHE:CD2	2:J:84:THR:HG23	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:32:GLN:O	2:K:33:GLN:C	2.53	0.47
2:M:27:VAL:HG21	2:M:31:ILE:HD11	1.97	0.47
2:N:115:SER:O	2:N:119:LEU:HG	2.15	0.47
2:N:11:LEU:O	2:N:15:ARG:N	2.39	0.47
2:N:124:PHE:O	2:N:127:ILE:HG13	2.15	0.47
1:A:133:ILE:O	1:A:134:TYR:HD2	1.97	0.47
1:A:205:ALA:O	1:A:206:SER:C	2.52	0.47
1:A:450:GLY:O	1:A:451:ASP:CB	2.62	0.47
1:A:494:ASN:CG	1:A:495:ASP:N	2.67	0.47
1:A:508:GLU:HG2	1:A:512:GLN:HE21	1.75	0.47
1:A:516:GLN:C	1:A:518:PHE:H	2.18	0.47
1:A:699:ILE:HA	1:A:763:LEU:O	2.14	0.47
1:B:211:ILE:C	1:B:213:GLN:N	2.67	0.47
1:B:122:LEU:O	1:B:253:ASN:OD1	2.32	0.47
1:B:548:ARG:O	1:B:551:ALA:HB3	2.15	0.47
1:B:721:VAL:CG1	1:B:722:ASN:N	2.77	0.47
1:B:725:ARG:H	1:B:725:ARG:CD	2.22	0.47
1:B:852:SER:O	1:B:854:LEU:N	2.46	0.47
2:I:102:ARG:HG2	2:I:102:ARG:HH11	1.80	0.47
2:L:32:GLN:O	2:L:33:GLN:C	2.52	0.47
2:L:37:MET:O	2:L:38:ILE:C	2.53	0.47
2:L:128:ASN:ND2	2:M:19:VAL:HG21	2.30	0.47
1:A:428:GLN:CD	1:A:456:PHE:N	2.67	0.47
1:A:510:LEU:HD12	1:A:513:LEU:HD12	1.96	0.47
1:A:510:LEU:CD2	1:A:540:LEU:HD13	2.29	0.47
1:A:578:LEU:HA	1:A:581:VAL:CG2	2.44	0.47
1:A:594:ILE:HG12	1:A:595:PRO:HD2	1.95	0.47
1:A:647:LYS:C	1:A:649:LEU:N	2.68	0.47
1:A:763:LEU:HD23	1:A:764:PRO:CD	2.44	0.47
1:B:360:ILE:O	1:B:361:GLN:HB2	2.15	0.47
1:B:458:ILE:HD12	1:B:459:ALA:CA	2.45	0.47
1:B:480:PHE:CE2	1:B:493:LEU:CB	2.96	0.47
1:B:549:LEU:HA	1:B:549:LEU:HD12	1.64	0.47
2:D:115:SER:O	2:D:119:LEU:HG	2.15	0.47
2:D:346:VAL:CG2	2:D:385:VAL:HG13	2.44	0.47
2:F:46:PHE:HE2	2:F:119:LEU:HD21	1.80	0.47
2:G:30:LEU:O	2:G:31:ILE:C	2.52	0.47
2:I:115:SER:O	2:I:119:LEU:HG	2.14	0.47
2:K:103:GLU:HG3	2:K:359:PRO:HD2	1.95	0.47
2:L:100:MET:HG3	2:L:388:VAL:HG11	1.95	0.47
2:N:346:VAL:CG2	2:N:385:VAL:HG13	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:104:SER:O	2:O:108:GLY:HA3	2.15	0.47
2:O:73:LEU:HD22	2:O:77:TYR:CD2	2.50	0.47
1:A:217:THR:O	1:A:218:GLU:HB2	2.13	0.47
1:A:332:VAL:O	1:A:333:VAL:C	2.53	0.47
1:A:277:ARG:CD	1:A:559:ALA:HB2	2.43	0.47
1:A:663:TYR:O	1:A:666:ARG:N	2.47	0.47
1:A:803:ASN:ND2	1:A:806:SER:H	2.13	0.47
1:B:653:ASP:O	1:B:653:ASP:CG	2.52	0.47
1:B:845:ASN:HB3	1:B:848:PHE:CE1	2.49	0.47
1:B:854:LEU:O	1:B:856:ALA:N	2.47	0.47
2:C:106:ARG:H	2:C:106:ARG:CD	2.10	0.47
2:E:5:TYR:HE2	2:E:130:ASP:O	1.98	0.47
2:F:53:ASN:HD22	2:F:354:ALA:CB	2.26	0.47
2:I:23:LEU:HD22	2:I:25:SER:OG	2.14	0.47
2:J:27:VAL:HG21	2:J:31:ILE:HD11	1.96	0.47
2:K:27:VAL:O	2:K:31:ILE:HG12	2.15	0.47
2:M:32:GLN:O	2:M:33:GLN:C	2.52	0.47
2:O:135:TYR:CZ	2:O:342:MET:HE3	2.50	0.47
1:A:122:LEU:CD1	1:A:201:ASP:HB2	2.45	0.47
1:A:356:GLU:HB3	1:A:357:ALA:H	1.30	0.47
1:B:112:LYS:N	1:B:113:PRO:CD	2.78	0.47
1:B:354:GLN:HA	1:B:354:GLN:OE1	2.15	0.47
1:B:503:ILE:O	1:B:504:ASN:C	2.54	0.47
1:B:519:PRO:O	1:B:520:THR:OG1	2.32	0.47
1:B:383:ILE:HD11	1:B:550:LEU:HD23	1.97	0.47
1:B:645:PHE:HD2	1:B:646:LEU:CD2	2.25	0.47
1:B:752:LEU:C	1:B:754:ASN:N	2.63	0.47
1:B:87:GLN:C	1:B:89:GLU:N	2.68	0.47
2:C:150:PHE:HA	2:D:397:LYS:NZ	2.30	0.47
1:A:461:GLN:CA	2:F:32:GLN:NE2	2.75	0.47
2:G:32:GLN:O	2:G:33:GLN:C	2.53	0.47
2:H:11:LEU:O	2:H:15:ARG:N	2.39	0.47
2:H:346:VAL:CG2	2:H:385:VAL:HG13	2.44	0.47
2:K:109:ILE:HG13	2:K:110:ALA:N	2.29	0.47
2:N:37:MET:O	2:N:38:ILE:C	2.53	0.47
2:O:65:LEU:O	2:O:66:LEU:HD23	2.15	0.47
1:A:169:LEU:HA	1:A:169:LEU:HD12	1.62	0.46
1:A:180:TYR:CD1	1:A:181:LEU:N	2.83	0.46
1:A:286:LEU:H	1:A:286:LEU:CD2	2.10	0.46
1:B:409:TRP:O	1:B:412:THR:HB	2.16	0.46
1:B:479:GLN:O	1:B:480:PHE:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:129:PHE:CE1	2:C:130:ASP:HB2	2.50	0.46
2:D:128:ASN:HD22	2:E:19:VAL:HG21	1.80	0.46
2:E:41:MET:O	2:E:42:ASN:C	2.52	0.46
2:F:106:ARG:NH1	2:F:106:ARG:HB2	2.30	0.46
2:F:27:VAL:O	2:F:30:LEU:N	2.47	0.46
2:I:36:GLN:HE22	2:I:126:ARG:HD3	1.80	0.46
2:I:42:ASN:OD1	2:I:62:ASP:N	2.48	0.46
2:L:27:VAL:CG2	2:L:31:ILE:HD11	2.45	0.46
2:L:57:ARG:HB3	2:L:59:TRP:CZ2	2.49	0.46
2:N:124:PHE:O	2:N:126:ARG:N	2.49	0.46
2:N:30:LEU:O	2:N:31:ILE:C	2.54	0.46
1:A:419:PHE:CD1	1:A:419:PHE:N	2.82	0.46
1:A:746:GLN:O	1:A:750:MET:HG3	2.14	0.46
1:A:760:VAL:HG12	1:A:761:GLY:N	2.30	0.46
2:D:150:PHE:N	2:D:150:PHE:CD1	2.83	0.46
2:E:54:LEU:HD12	2:E:55:PRO:CD	2.42	0.46
2:I:128:ASN:HB3	2:J:19:VAL:CG2	2.44	0.46
2:I:144:ARG:O	2:I:145:ARG:CB	2.64	0.46
2:M:14:ALA:O	2:M:18:ILE:HD12	2.16	0.46
1:A:250:TYR:HB2	1:A:840:HIS:CD2	2.50	0.46
1:A:253:ASN:O	1:A:256:PHE:HB2	2.14	0.46
1:A:386:MET:HE3	1:A:414:VAL:HG13	1.96	0.46
1:A:499:ASN:CA	1:A:505:GLN:NE2	2.77	0.46
1:A:854:LEU:CD2	1:A:855:LEU:N	2.78	0.46
1:A:856:ALA:O	1:A:858:VAL:N	2.41	0.46
1:B:282:VAL:O	1:B:284:TYR:N	2.48	0.46
1:B:369:GLY:C	1:B:371:ASN:N	2.69	0.46
1:B:420:ILE:O	1:B:422:GLU:N	2.48	0.46
1:B:75:VAL:HG12	1:B:75:VAL:O	2.16	0.46
1:B:820:THR:O	1:B:820:THR:HG22	2.15	0.46
2:C:110:ALA:HB1	2:C:111:PRO:HD2	1.97	0.46
2:C:62:ASP:H	2:C:63:PHE:HD1	1.62	0.46
2:E:73:LEU:HD22	2:E:77:TYR:CD2	2.50	0.46
2:F:100:MET:HG3	2:F:388:VAL:HG11	1.97	0.46
2:I:32:GLN:O	2:I:33:GLN:C	2.54	0.46
2:L:153:HIS:O	2:L:154:LYS:C	2.54	0.46
2:N:66:LEU:O	2:N:67:GLY:C	2.53	0.46
2:N:76:ASN:HB2	2:O:76:ASN:HB2	1.97	0.46
1:A:363:GLU:HA	1:A:366:PHE:HE1	1.80	0.46
1:A:428:GLN:HG3	1:A:456:PHE:HA	1.97	0.46
1:A:722:ASN:HB3	1:A:824:LYS:HA	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:818:VAL:HA	1:B:819:PRO:HD3	1.75	0.46
1:B:500:GLY:HA3	1:B:871:PHE:HZ	1.80	0.46
2:C:19:VAL:HG23	2:E:128:ASN:HB3	1.98	0.46
2:D:38:ILE:HG22	2:D:42:ASN:ND2	2.30	0.46
2:F:115:SER:O	2:F:119:LEU:HG	2.14	0.46
2:H:150:PHE:N	2:H:150:PHE:CD1	2.84	0.46
2:H:27:VAL:HG21	2:H:31:ILE:HD11	1.96	0.46
2:I:1:MET:C	2:I:3:VAL:N	2.67	0.46
2:J:32:GLN:O	2:J:33:GLN:C	2.54	0.46
2:K:63:PHE:N	2:K:63:PHE:CD1	2.82	0.46
2:L:153:HIS:NE2	2:M:153:HIS:CD2	2.84	0.46
2:M:128:ASN:HB3	2:N:19:VAL:HG23	1.97	0.46
1:A:145:ARG:HB3	1:A:147:TYR:HE1	1.79	0.46
1:A:151:LYS:O	1:A:152:LYS:CB	2.63	0.46
1:A:405:ILE:HG21	1:A:536:LEU:CG	2.43	0.46
1:A:775:ILE:C	1:A:777:LYS:H	2.19	0.46
1:A:548:ARG:HB2	1:A:877:MET:HE2	1.98	0.46
1:B:298:TYR:C	1:B:298:TYR:CD1	2.88	0.46
1:B:739:MET:C	1:B:741:THR:H	2.19	0.46
2:D:14:ALA:O	2:D:18:ILE:HD12	2.16	0.46
2:J:153:HIS:O	2:J:154:LYS:C	2.53	0.46
2:J:148:THR:OG1	2:J:332:GLU:HG2	2.15	0.46
2:K:54:LEU:HD12	2:K:55:PRO:CD	2.41	0.46
2:N:150:PHE:N	2:N:150:PHE:CD1	2.84	0.46
2:O:141:LEU:CD1	2:O:148:THR:HG21	2.46	0.46
2:O:1:MET:O	2:O:2:ASP:C	2.53	0.46
2:O:60:ASN:C	2:O:61:PHE:CD1	2.89	0.46
1:A:122:LEU:CG	1:A:201:ASP:HB2	2.46	0.46
1:A:197:GLY:O	1:A:198:LYS:O	2.34	0.46
1:A:454:THR:HG22	1:A:457:GLN:H	1.80	0.46
1:A:639:LYS:HE3	1:A:659:ASP:OD1	2.15	0.46
1:A:772:ILE:O	1:A:773:SER:C	2.54	0.46
1:B:366:PHE:O	1:B:368:THR:N	2.48	0.46
1:B:490:ASN:O	1:B:492:VAL:HG23	2.15	0.46
1:B:605:ASN:ND2	1:B:855:LEU:HD12	2.30	0.46
2:I:61:PHE:N	2:I:61:PHE:CD1	2.83	0.46
2:O:139:TRP:NE1	2:O:143:ASN:ND2	2.63	0.46
1:A:299:ILE:O	1:A:301:PRO:HD3	2.15	0.46
1:A:329:ALA:HB3	1:A:384:ALA:CB	2.46	0.46
1:A:601:PHE:O	1:A:602:HIS:C	2.54	0.46
1:A:620:ASP:O	1:A:624:ILE:HG13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:PHE:CZ	1:A:664:ARG:HG2	2.51	0.46
1:B:413:VAL:CG1	1:B:414:VAL:H	2.26	0.46
1:B:608:VAL:O	1:B:609:ASN:C	2.54	0.46
1:B:857:PHE:CD1	1:B:857:PHE:N	2.72	0.46
2:D:123:LYS:HG3	2:D:124:PHE:CE1	2.50	0.46
2:D:61:PHE:N	2:D:61:PHE:CD1	2.84	0.46
2:F:346:VAL:CG2	2:F:385:VAL:HG13	2.44	0.46
2:F:22:THR:CG2	2:F:73:LEU:HD12	2.45	0.46
2:K:129:PHE:C	2:K:129:PHE:CD1	2.89	0.46
2:L:49:GLY:HA2	2:L:54:LEU:HD23	1.98	0.46
1:A:404:LEU:HB3	1:A:435:ILE:HD11	1.98	0.46
1:A:506:LEU:HD23	1:A:544:VAL:CA	2.29	0.46
1:A:660:ASP:HB3	1:B:539:ARG:NH1	2.20	0.46
1:A:706:ALA:C	1:A:708:ARG:H	2.19	0.46
1:A:708:ARG:HD2	1:A:708:ARG:HA	1.80	0.46
1:B:373:GLN:O	1:B:376:ASN:N	2.49	0.46
1:B:478:ASN:O	1:B:480:PHE:N	2.45	0.46
1:B:601:PHE:HB3	1:B:855:LEU:HD13	1.98	0.46
1:B:770:SER:O	1:B:773:SER:HB2	2.15	0.46
1:B:854:LEU:O	1:B:855:LEU:C	2.54	0.46
2:C:346:VAL:CG2	2:C:385:VAL:HG13	2.44	0.46
2:C:41:MET:O	2:C:42:ASN:C	2.53	0.46
2:F:22:THR:HG23	2:F:73:LEU:HD12	1.98	0.46
2:G:41:MET:O	2:G:42:ASN:C	2.54	0.46
2:M:346:VAL:CG2	2:M:385:VAL:HG13	2.45	0.46
2:L:153:HIS:CD2	2:N:153:HIS:NE2	2.83	0.46
2:N:61:PHE:N	2:N:61:PHE:CD1	2.84	0.46
1:A:779:ASP:OD2	1:A:822:THR:O	2.34	0.46
1:A:846:LEU:HA	1:A:846:LEU:HD23	1.65	0.46
1:A:867:ASN:CG	1:A:867:ASN:O	2.54	0.46
1:B:118:LYS:CG	1:B:119:GLN:N	2.73	0.46
1:B:239:VAL:CG2	1:B:845:ASN:O	2.63	0.46
1:B:345:GLN:HG3	1:B:349:MET:CE	2.46	0.46
1:B:510:LEU:HD13	1:B:540:LEU:HB2	1.98	0.46
1:B:383:ILE:HD11	1:B:550:LEU:HD22	1.97	0.46
1:B:314:PHE:HZ	1:B:664:ARG:HG2	1.78	0.46
1:B:727:LEU:HG	1:B:727:LEU:O	2.15	0.46
1:B:783:PHE:O	1:B:784:ALA:C	2.54	0.46
1:B:848:PHE:O	1:B:849:THR:OG1	2.28	0.46
1:A:461:GLN:CB	2:F:32:GLN:NE2	2.79	0.46
2:I:155:PRO:O	2:I:186:SER:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:382:LEU:HD22	2:I:386:PHE:CE2	2.51	0.46
2:J:142:GLN:HE21	2:J:143:ASN:N	2.13	0.46
2:J:27:VAL:CG2	2:J:31:ILE:HD11	2.45	0.46
2:L:104:SER:HB3	2:L:108:GLY:CA	2.46	0.46
2:O:22:THR:CG2	2:O:73:LEU:HD12	2.46	0.46
2:O:37:MET:O	2:O:38:ILE:C	2.54	0.46
1:A:245:LEU:O	1:A:246:HIS:HB2	2.16	0.46
1:A:428:GLN:OE1	1:A:456:PHE:CB	2.38	0.46
1:A:509:ALA:O	1:A:513:LEU:CG	2.55	0.46
1:A:821:SER:OG	1:A:822:THR:N	2.46	0.46
1:B:340:VAL:O	1:B:341:SER:C	2.54	0.46
1:B:613:ASN:O	1:B:617:ARG:HG2	2.16	0.46
1:B:94:THR:O	1:B:94:THR:HG22	2.16	0.46
2:D:30:LEU:O	2:D:31:ILE:C	2.53	0.46
2:F:239:ASN:ND2	2:F:246:THR:HG22	2.29	0.46
2:H:106:ARG:O	2:H:107:ASN:CB	2.62	0.46
2:H:239:ASN:ND2	2:H:246:THR:HG22	2.30	0.46
2:I:135:TYR:CE1	2:I:342:MET:HE3	2.51	0.46
2:K:346:VAL:CG2	2:K:385:VAL:HG13	2.44	0.46
1:A:549:LEU:HA	1:A:549:LEU:HD12	1.65	0.45
1:B:137:ASN:CG	1:B:137:ASN:O	2.55	0.45
1:B:170:TYR:CZ	1:B:682:PHE:HB2	2.52	0.45
1:B:637:LYS:HA	1:B:641:ILE:HD11	1.97	0.45
1:B:675:GLU:O	1:B:677:ARG:N	2.49	0.45
2:G:5:TYR:HE2	2:G:131:ASN:HA	1.80	0.45
2:H:62:ASP:H	2:H:63:PHE:HD1	1.63	0.45
2:J:382:LEU:HD22	2:J:386:PHE:CE2	2.52	0.45
2:J:37:MET:O	2:J:38:ILE:C	2.54	0.45
2:K:382:LEU:HD22	2:K:386:PHE:CE2	2.51	0.45
2:N:1:MET:C	2:N:3:VAL:N	2.69	0.45
2:N:1:MET:O	2:N:2:ASP:C	2.55	0.45
1:A:416:ASN:C	1:A:418:MET:N	2.70	0.45
1:B:282:VAL:HG13	1:B:283:ASN:N	2.31	0.45
1:B:583:SER:OG	1:B:584:LEU:N	2.48	0.45
1:B:772:ILE:HG22	1:B:809:PHE:CE2	2.51	0.45
2:C:135:TYR:CZ	2:C:342:MET:HE3	2.52	0.45
2:G:109:ILE:O	2:G:109:ILE:HD12	2.17	0.45
2:F:17:LYS:HE2	2:H:130:ASP:OD2	2.16	0.45
2:H:21:GLY:O	2:H:22:THR:O	2.34	0.45
2:I:136:ILE:HG23	2:I:137:GLU:N	2.31	0.45
2:I:1:MET:O	2:I:2:ASP:C	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:30:LEU:O	2:I:31:ILE:C	2.52	0.45
2:I:36:GLN:HB2	2:J:23:LEU:HD11	1.97	0.45
2:I:89:VAL:C	2:I:91:PHE:H	2.19	0.45
1:B:508:GLU:OE2	2:J:70:LEU:CD2	2.65	0.45
2:L:115:SER:O	2:L:119:LEU:HG	2.15	0.45
2:L:73:LEU:HD22	2:L:77:TYR:HD2	1.77	0.45
2:M:382:LEU:HD22	2:M:386:PHE:CE2	2.52	0.45
1:A:353:LEU:HD22	1:A:531:ARG:HB3	1.98	0.45
1:A:526:LYS:HG3	1:A:527:ARG:N	2.31	0.45
1:A:608:VAL:O	1:A:609:ASN:C	2.55	0.45
1:A:688:ASN:O	1:A:691:GLN:N	2.49	0.45
1:A:706:ALA:O	1:A:708:ARG:N	2.45	0.45
1:B:542:GLN:OE1	1:B:542:GLN:N	2.49	0.45
1:B:594:ILE:HD12	1:B:594:ILE:O	2.17	0.45
1:B:633:LEU:O	1:B:635:GLN:N	2.48	0.45
1:B:872:ASP:CG	1:B:874:MET:H	2.20	0.45
2:C:124:PHE:O	2:C:127:ILE:HG13	2.16	0.45
2:C:59:TRP:N	2:C:59:TRP:CD1	2.83	0.45
2:E:190:VAL:HG21	2:E:210:HIS:HB2	1.99	0.45
2:F:32:GLN:O	2:F:33:GLN:C	2.54	0.45
2:H:382:LEU:HD22	2:H:386:PHE:CE2	2.51	0.45
1:B:498:ARG:CZ	2:J:25:SER:HB3	2.47	0.45
2:J:78:VAL:O	2:J:81:ALA:N	2.40	0.45
2:K:24:TYR:O	2:K:27:VAL:HG22	2.16	0.45
2:L:239:ASN:ND2	2:L:246:THR:HG22	2.29	0.45
2:L:22:THR:CG2	2:L:73:LEU:HD12	2.24	0.45
2:M:53:ASN:HD22	2:M:354:ALA:HB3	1.81	0.45
2:N:24:TYR:CE1	2:N:31:ILE:HG13	2.51	0.45
1:A:266:ASN:C	1:A:292:LEU:HD12	2.36	0.45
1:A:466:PHE:O	1:A:467:GLN:C	2.54	0.45
1:A:518:PHE:CB	1:A:519:PRO:CD	2.94	0.45
1:A:688:ASN:O	1:A:690:ASP:N	2.50	0.45
1:B:119:GLN:CG	1:B:181:LEU:HD11	2.46	0.45
1:B:159:ASP:O	1:B:162:VAL:HB	2.16	0.45
1:B:420:ILE:O	1:B:421:ARG:C	2.54	0.45
1:B:589:GLY:C	1:B:591:ALA:H	2.20	0.45
2:C:37:MET:O	2:C:38:ILE:C	2.55	0.45
2:D:1:MET:C	2:D:3:VAL:N	2.70	0.45
2:D:37:MET:O	2:D:38:ILE:C	2.55	0.45
2:J:1:MET:C	2:J:3:VAL:N	2.68	0.45
2:L:89:VAL:C	2:L:91:PHE:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:144:ARG:O	2:M:145:ARG:HB2	2.17	0.45
1:A:857:PHE:CD1	1:A:857:PHE:N	2.83	0.45
1:B:205:ALA:O	1:B:206:SER:C	2.55	0.45
1:B:434:THR:O	1:B:435:ILE:CG1	2.65	0.45
1:B:854:LEU:HD22	1:B:855:LEU:H	1.82	0.45
2:C:382:LEU:HD22	2:C:386:PHE:CE2	2.51	0.45
2:D:190:VAL:HG21	2:D:210:HIS:HB2	1.99	0.45
2:D:382:LEU:HD22	2:D:386:PHE:CE2	2.52	0.45
2:I:225:LEU:HD13	2:I:277:PHE:HD2	1.82	0.45
2:M:130:ASP:HA	2:N:17:LYS:HG2	1.98	0.45
2:N:110:ALA:HB1	2:N:111:PRO:HD2	1.99	0.45
1:A:246:HIS:O	1:A:247:PRO:C	2.54	0.45
1:A:482:GLN:OE1	1:A:493:LEU:CD2	2.64	0.45
1:A:804:SER:HB2	1:A:810:TYR:CA	2.47	0.45
1:A:712:LEU:CG	1:A:819:PRO:HB2	2.40	0.45
1:A:822:THR:O	1:A:823:THR:CB	2.64	0.45
1:B:646:LEU:N	1:B:646:LEU:HD23	2.32	0.45
1:B:852:SER:O	1:B:853:ASP:HB3	2.16	0.45
2:C:128:ASN:O	2:D:22:THR:HB	2.17	0.45
2:C:190:VAL:HG21	2:C:210:HIS:HB2	1.99	0.45
2:D:24:TYR:O	2:D:26:ASN:N	2.50	0.45
2:D:78:VAL:O	2:D:81:ALA:HB3	2.17	0.45
2:E:312:GLN:HB3	2:E:313:PRO:HA	1.99	0.45
2:H:107:ASN:ND2	2:H:109:ILE:HG23	2.32	0.45
2:H:190:VAL:HG21	2:H:210:HIS:HB2	1.99	0.45
2:H:32:GLN:O	2:H:33:GLN:C	2.54	0.45
2:L:190:VAL:HG21	2:L:210:HIS:HB2	1.99	0.45
2:M:155:PRO:HA	2:M:337:ASP:HB2	1.99	0.45
1:A:155:LEU:HA	1:A:156:PRO:HD3	1.55	0.45
1:A:319:ASP:OD2	1:A:571:LEU:N	2.49	0.45
1:A:546:LEU:HD13	1:A:584:LEU:HD23	1.97	0.45
1:B:419:PHE:O	1:B:420:ILE:C	2.54	0.45
1:B:554:TYR:O	1:B:558:MET:HB2	2.17	0.45
1:B:577:GLN:O	1:B:579:THR:N	2.50	0.45
1:B:601:PHE:CD1	1:B:601:PHE:N	2.80	0.45
1:B:742:GLY:O	1:B:744:TYR:HE2	1.98	0.45
1:B:772:ILE:O	1:B:773:SER:C	2.54	0.45
1:B:85:GLU:O	1:B:86:ILE:C	2.54	0.45
2:D:54:LEU:HD12	2:D:55:PRO:CD	2.46	0.45
2:E:11:LEU:O	2:E:15:ARG:N	2.41	0.45
2:E:382:LEU:HD22	2:E:386:PHE:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:190:VAL:HG21	2:F:210:HIS:HB2	1.99	0.45
2:G:150:PHE:HB2	2:G:152:PHE:CZ	2.51	0.45
2:H:105:GLN:O	2:H:107:ASN:N	2.50	0.45
2:H:312:GLN:HB3	2:H:313:PRO:HA	1.99	0.45
2:J:60:ASN:C	2:J:61:PHE:CD1	2.90	0.45
2:L:382:LEU:HD22	2:L:386:PHE:CE2	2.52	0.45
2:M:110:ALA:HB1	2:M:111:PRO:HD2	1.99	0.45
2:N:23:LEU:HD22	2:N:25:SER:OG	2.17	0.45
1:A:252:PHE:CD2	1:A:684:LEU:CD2	3.00	0.45
1:A:339:LEU:O	1:A:340:VAL:C	2.55	0.45
1:A:452:PRO:O	1:A:453:GLN:OE1	2.35	0.45
1:A:454:THR:O	1:A:457:GLN:HB3	2.17	0.45
1:A:503:ILE:O	1:A:505:GLN:N	2.50	0.45
1:A:506:LEU:CD2	1:A:544:VAL:CA	2.94	0.45
1:A:580:SER:O	1:A:581:VAL:C	2.55	0.45
1:B:400:ASN:O	1:B:404:LEU:CD1	2.65	0.45
1:B:601:PHE:O	1:B:602:HIS:C	2.53	0.45
2:D:225:LEU:HD13	2:D:277:PHE:HD2	1.82	0.45
2:E:154:LYS:N	2:E:327:GLU:O	2.42	0.45
2:E:37:MET:O	2:E:38:ILE:C	2.54	0.45
2:F:312:GLN:HB3	2:F:313:PRO:HA	1.99	0.45
2:G:382:LEU:HD22	2:G:386:PHE:CE2	2.51	0.45
2:H:48:THR:O	2:H:56:ILE:HA	2.17	0.45
2:I:145:ARG:O	2:I:146:GLN:CG	2.65	0.45
2:I:42:ASN:OD1	2:I:61:PHE:HB3	2.16	0.45
2:J:225:LEU:HD13	2:J:277:PHE:HD2	1.82	0.45
2:J:41:MET:O	2:J:42:ASN:C	2.54	0.45
2:M:225:LEU:HD13	2:M:277:PHE:HD2	1.82	0.45
2:O:217:VAL:HG22	2:O:286:ASP:HB3	1.99	0.45
1:A:186:MET:HG3	1:A:200:VAL:HG13	1.98	0.45
1:A:583:SER:OG	1:A:584:LEU:N	2.50	0.45
1:A:762:ALA:C	1:A:763:LEU:HG	2.37	0.45
1:A:783:PHE:N	1:A:783:PHE:CD1	2.72	0.45
1:B:119:GLN:NE2	1:B:181:LEU:HD11	2.32	0.45
1:B:277:ARG:HH11	1:B:277:ARG:HB3	1.80	0.45
1:B:496:ASN:HB3	1:B:499:ASN:H	1.82	0.45
1:B:573:THR:CG2	1:B:574:GLU:N	2.45	0.45
1:B:786:ILE:HG22	1:B:792:VAL:HG12	1.98	0.45
1:B:771:VAL:HG21	1:B:809:PHE:O	2.17	0.45
2:C:127:ILE:O	2:C:127:ILE:HG22	2.15	0.45
2:C:136:ILE:HG23	2:C:137:GLU:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:225:LEU:HD13	2:E:277:PHE:HD2	1.82	0.45
2:F:225:LEU:HD13	2:F:277:PHE:HD2	1.82	0.45
2:F:382:LEU:HD22	2:F:386:PHE:CE2	2.52	0.45
2:H:30:LEU:O	2:H:31:ILE:C	2.53	0.45
2:I:273:TYR:C	2:I:274:GLN:HE21	2.20	0.45
2:I:217:VAL:HG22	2:I:286:ASP:HB3	1.99	0.45
2:J:70:LEU:HD22	2:J:72:ASN:O	2.16	0.45
2:J:89:VAL:C	2:J:91:PHE:H	2.21	0.45
2:M:312:GLN:HB3	2:M:313:PRO:HA	1.99	0.45
2:N:89:VAL:C	2:N:91:PHE:H	2.21	0.45
2:O:131:ASN:HD22	2:O:131:ASN:N	2.14	0.45
2:O:190:VAL:HG21	2:O:210:HIS:HB2	1.99	0.45
2:O:225:LEU:HD13	2:O:277:PHE:HD2	1.82	0.45
2:O:273:TYR:C	2:O:274:GLN:HE21	2.21	0.45
1:A:224:PHE:O	1:A:225:ILE:C	2.55	0.45
1:A:269:ILE:HG21	1:A:298:TYR:CE2	2.51	0.45
1:A:428:GLN:HG2	1:A:429:LEU:H	1.79	0.45
1:A:866:ILE:HG22	1:A:866:ILE:O	2.17	0.45
1:B:467:GLN:HE21	1:B:511:MET:HG2	1.82	0.45
1:B:596:SER:O	1:B:597:PRO:C	2.55	0.45
1:B:772:ILE:CG2	1:B:809:PHE:HE2	2.29	0.45
1:B:846:LEU:HD12	1:B:847:THR:N	2.32	0.45
2:C:217:VAL:HG22	2:C:286:ASP:HB3	1.99	0.45
2:C:32:GLN:O	2:C:33:GLN:C	2.54	0.45
2:G:190:VAL:HG21	2:G:210:HIS:HB2	1.99	0.45
2:H:126:ARG:C	2:H:127:ILE:HG13	2.37	0.45
2:J:217:VAL:HG22	2:J:286:ASP:HB3	1.99	0.45
2:J:312:GLN:HB3	2:J:313:PRO:HA	1.99	0.45
2:K:190:VAL:HG21	2:K:210:HIS:HB2	1.99	0.45
2:M:42:ASN:HA	2:M:61:PHE:CB	2.46	0.45
2:N:135:TYR:CZ	2:N:342:MET:HE3	2.53	0.45
2:N:382:LEU:HD22	2:N:386:PHE:CE2	2.52	0.45
1:A:117:LYS:HB2	1:A:179:ASP:CG	2.37	0.44
1:A:118:LYS:CG	1:A:119:GLN:H	2.29	0.44
1:A:420:ILE:HD11	1:A:423:SER:HB2	1.99	0.44
1:A:587:LEU:O	1:A:587:LEU:HD22	2.17	0.44
1:A:680:ASP:HA	1:A:683:ASN:HD22	1.81	0.44
1:B:428:GLN:CB	1:B:456:PHE:CD1	2.90	0.44
1:B:763:LEU:HD22	1:B:764:PRO:HD3	1.99	0.44
2:C:1:MET:C	2:C:3:VAL:N	2.70	0.44
2:D:136:ILE:HG23	2:D:137:GLU:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:217:VAL:HG22	2:D:286:ASP:HB3	1.99	0.44
2:E:44:ASN:HB3	2:E:46:PHE:HE1	1.81	0.44
2:G:273:TYR:C	2:G:274:GLN:HE21	2.20	0.44
2:G:312:GLN:HB3	2:G:313:PRO:HA	1.99	0.44
2:G:78:VAL:O	2:G:81:ALA:HB3	2.18	0.44
2:I:190:VAL:HG21	2:I:210:HIS:HB2	1.99	0.44
2:J:153:HIS:NE2	2:K:153:HIS:CD2	2.84	0.44
2:K:225:LEU:HD13	2:K:277:PHE:HD2	1.82	0.44
2:K:37:MET:O	2:K:38:ILE:C	2.55	0.44
2:L:225:LEU:HD13	2:L:277:PHE:HD2	1.82	0.44
2:L:312:GLN:HB3	2:L:313:PRO:HA	1.99	0.44
2:L:60:ASN:C	2:L:61:PHE:CD1	2.91	0.44
1:A:101:LYS:C	1:A:103:SER:H	2.20	0.44
1:A:270:ILE:HD11	1:A:292:LEU:CD1	2.23	0.44
1:A:286:LEU:O	1:A:287:ASN:CB	2.65	0.44
1:A:296:ALA:C	1:A:297:ARG:HG2	2.38	0.44
1:A:348:LYS:O	1:A:351:GLN:HB2	2.17	0.44
1:B:148:TRP:HE1	1:B:833:PHE:HD1	1.64	0.44
1:B:226:ALA:O	1:B:228:MET:N	2.50	0.44
1:B:248:ILE:O	1:B:251:ALA:HB3	2.17	0.44
1:B:420:ILE:O	1:B:420:ILE:HG23	2.18	0.44
1:B:463:ILE:HD12	1:B:472:LEU:CD1	2.47	0.44
1:B:374:ALA:O	1:B:580:SER:HB2	2.17	0.44
2:C:22:THR:HG23	2:C:73:LEU:CD1	2.46	0.44
2:C:54:LEU:HD12	2:C:55:PRO:CD	2.44	0.44
2:F:273:TYR:C	2:F:274:GLN:HE21	2.21	0.44
2:F:78:VAL:O	2:F:81:ALA:N	2.43	0.44
2:I:140:ASN:O	2:I:143:ASN:N	2.50	0.44
2:J:1:MET:O	2:J:2:ASP:C	2.54	0.44
2:M:239:ASN:ND2	2:M:246:THR:HG22	2.30	0.44
2:N:225:LEU:HD13	2:N:277:PHE:HD2	1.82	0.44
2:O:382:LEU:HD22	2:O:386:PHE:CE2	2.51	0.44
2:O:1:MET:C	2:O:3:VAL:N	2.68	0.44
1:A:229:ARG:O	1:A:242:PRO:HG3	2.18	0.44
1:A:556:THR:O	1:A:558:MET:N	2.51	0.44
1:A:660:ASP:OD1	1:A:661:GLN:N	2.50	0.44
1:A:674:VAL:HB	1:A:679:LEU:HB2	1.99	0.44
1:B:183:LEU:HD12	1:B:844:SER:CB	2.47	0.44
1:B:368:THR:HG22	1:B:371:ASN:ND2	2.26	0.44
1:B:382:LEU:HA	1:B:382:LEU:HD12	1.62	0.44
1:B:447:TYR:C	1:B:448:ARG:HG2	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:674:VAL:O	1:B:675:GLU:C	2.54	0.44
1:B:757:VAL:HG12	1:B:758:ALA:N	2.32	0.44
2:C:27:VAL:O	2:C:30:LEU:HB3	2.17	0.44
2:C:69:THR:OG1	2:C:70:LEU:N	2.49	0.44
2:C:89:VAL:C	2:C:91:PHE:H	2.21	0.44
2:F:153:HIS:CD2	2:H:153:HIS:NE2	2.86	0.44
2:K:111:PRO:O	2:K:112:GLN:HG2	2.17	0.44
2:K:239:ASN:ND2	2:K:246:THR:HG22	2.29	0.44
2:K:78:VAL:O	2:K:81:ALA:N	2.40	0.44
2:L:136:ILE:HG23	2:L:137:GLU:N	2.32	0.44
1:A:597:PRO:HB3	1:A:860:ALA:HB1	1.99	0.44
1:A:804:SER:CB	1:A:810:TYR:HA	2.48	0.44
1:B:158:GLY:O	1:B:159:ASP:C	2.56	0.44
1:B:630:ARG:O	1:B:631:LEU:CG	2.62	0.44
1:B:751:LEU:O	1:B:754:ASN:HA	2.16	0.44
1:B:790:ARG:CG	1:B:791:LYS:N	2.71	0.44
1:B:250:TYR:HB2	1:B:840:HIS:CD2	2.53	0.44
2:C:145:ARG:HH11	2:C:145:ARG:CB	2.30	0.44
2:C:152:PHE:O	2:C:328:SER:HA	2.17	0.44
2:C:63:PHE:CD2	2:C:84:THR:HG23	2.52	0.44
2:E:1:MET:C	2:E:3:VAL:N	2.68	0.44
2:E:66:LEU:HB3	2:E:77:TYR:OH	2.16	0.44
2:E:78:VAL:O	2:E:81:ALA:HB3	2.17	0.44
2:F:48:THR:HG22	2:F:115:SER:OG	2.18	0.44
2:J:225:LEU:HD13	2:J:277:PHE:CD2	2.53	0.44
2:J:89:VAL:C	2:J:91:PHE:N	2.71	0.44
2:K:27:VAL:CG2	2:K:31:ILE:HD11	2.48	0.44
2:L:34:PHE:O	2:L:37:MET:HB3	2.17	0.44
2:N:190:VAL:HG21	2:N:210:HIS:HB2	1.99	0.44
2:O:89:VAL:C	2:O:91:PHE:H	2.21	0.44
1:A:130:GLN:NE2	1:A:146:TRP:CZ2	2.85	0.44
1:A:513:LEU:CA	1:A:516:GLN:NE2	2.65	0.44
1:A:557:LEU:O	1:A:558:MET:C	2.55	0.44
1:A:870:ALA:C	1:A:872:ASP:H	2.20	0.44
1:B:277:ARG:CB	1:B:277:ARG:HH11	2.30	0.44
1:B:446:HIS:O	1:B:447:TYR:CB	2.49	0.44
1:B:498:ARG:HH11	1:B:502:VAL:HG11	1.83	0.44
1:B:707:TYR:N	1:B:707:TYR:CD1	2.85	0.44
2:G:239:ASN:ND2	2:G:246:THR:HG22	2.29	0.44
2:F:82:ARG:CZ	2:H:144:ARG:HD2	2.47	0.44
2:H:37:MET:O	2:H:38:ILE:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:101:VAL:HG11	2:I:355:ILE:HG13	1.99	0.44
2:J:273:TYR:C	2:J:274:GLN:HE21	2.20	0.44
2:K:136:ILE:HG23	2:K:137:GLU:N	2.32	0.44
2:K:1:MET:O	2:K:2:ASP:C	2.54	0.44
2:K:1:MET:C	2:K:3:VAL:N	2.68	0.44
2:L:273:TYR:C	2:L:274:GLN:HE21	2.21	0.44
2:D:75:ALA:HB3	2:L:76:ASN:HA	2.00	0.44
2:M:136:ILE:HG23	2:M:137:GLU:N	2.33	0.44
2:M:150:PHE:O	2:M:330:VAL:HG13	2.17	0.44
2:N:38:ILE:HG22	2:N:42:ASN:ND2	2.29	0.44
2:N:78:VAL:O	2:N:81:ALA:HB3	2.17	0.44
1:A:488:VAL:O	1:A:490:ASN:N	2.51	0.44
1:A:516:GLN:OE1	1:A:517:GLN:N	2.50	0.44
1:A:727:LEU:O	1:A:727:LEU:CD1	2.65	0.44
1:A:771:VAL:HG13	1:A:772:ILE:N	2.22	0.44
1:A:701:GLN:CG	1:A:826:TYR:CD2	3.00	0.44
1:B:393:SER:HA	1:B:423:SER:CB	2.47	0.44
1:B:449:ASN:ND2	1:B:455:PRO:HG3	2.33	0.44
1:B:680:ASP:HA	1:B:683:ASN:HD22	1.82	0.44
1:B:727:LEU:HD23	1:B:826:TYR:CE1	2.53	0.44
2:E:225:LEU:HD13	2:E:277:PHE:CD2	2.53	0.44
2:E:273:TYR:C	2:E:274:GLN:HE21	2.21	0.44
2:F:11:LEU:O	2:F:15:ARG:N	2.40	0.44
2:F:249:PHE:CE2	2:F:251:PRO:HG3	2.53	0.44
2:F:37:MET:O	2:F:38:ILE:C	2.56	0.44
2:F:41:MET:O	2:F:42:ASN:C	2.56	0.44
2:G:104:SER:O	2:G:108:GLY:CA	2.66	0.44
2:G:33:GLN:HB2	2:H:26:ASN:OD1	2.16	0.44
2:H:67:GLY:O	2:H:69:THR:N	2.51	0.44
2:I:24:TYR:N	2:I:71:LEU:O	2.51	0.44
2:K:273:TYR:C	2:K:274:GLN:HE21	2.21	0.44
2:M:225:LEU:HD13	2:M:277:PHE:CD2	2.53	0.44
2:M:273:TYR:C	2:M:274:GLN:HE21	2.20	0.44
2:N:63:PHE:N	2:N:63:PHE:CD1	2.85	0.44
2:O:125:LYS:C	2:O:127:ILE:H	2.21	0.44
2:O:136:ILE:HG23	2:O:137:GLU:N	2.32	0.44
1:A:312:ASP:O	1:A:313:ASN:CB	2.63	0.44
1:A:795:LEU:HA	1:A:795:LEU:HD12	1.74	0.44
1:B:428:GLN:HA	1:B:431:ILE:CD1	2.42	0.44
1:B:519:PRO:O	1:B:520:THR:CB	2.66	0.44
1:B:738:LEU:HD12	1:B:738:LEU:HA	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:3:VAL:O	2:C:4:LEU:C	2.56	0.44
2:D:249:PHE:CE2	2:D:251:PRO:HG3	2.53	0.44
2:D:73:LEU:N	2:D:73:LEU:HD23	2.33	0.44
2:G:23:LEU:C	2:G:23:LEU:HD23	2.38	0.44
2:H:142:GLN:NE2	2:H:143:ASN:N	2.65	0.44
2:H:217:VAL:HG22	2:H:286:ASP:HB3	2.00	0.44
2:H:249:PHE:CE2	2:H:251:PRO:HG3	2.53	0.44
2:I:225:LEU:HD13	2:I:277:PHE:CD2	2.53	0.44
2:I:46:PHE:HE2	2:I:119:LEU:HD21	1.83	0.44
2:J:78:VAL:O	2:J:81:ALA:HB3	2.17	0.44
2:K:110:ALA:HB1	2:K:111:PRO:HD2	2.00	0.44
2:K:14:ALA:O	2:K:16:ASP:N	2.51	0.44
2:K:312:GLN:HB3	2:K:313:PRO:HA	1.99	0.44
2:M:151:THR:C	2:M:152:PHE:CD1	2.91	0.44
2:M:249:PHE:CE2	2:M:251:PRO:HG3	2.53	0.44
2:N:217:VAL:HG22	2:N:286:ASP:HB3	2.00	0.44
2:O:153:HIS:CD2	2:O:154:LYS:N	2.86	0.44
2:O:169:SER:HA	2:O:176:LEU:HD23	2.00	0.44
2:O:225:LEU:HD13	2:O:277:PHE:CD2	2.53	0.44
1:A:625:ILE:H	1:A:625:ILE:HG13	1.62	0.44
1:B:108:LEU:CD2	1:B:108:LEU:N	2.79	0.44
1:B:155:LEU:HA	1:B:156:PRO:HD3	1.81	0.44
1:B:282:VAL:HG13	1:B:283:ASN:H	1.83	0.44
1:B:305:GLN:OE1	1:B:305:GLN:HA	2.18	0.44
1:B:404:LEU:O	1:B:405:ILE:C	2.55	0.44
1:B:487:GLY:O	1:B:488:VAL:CB	2.66	0.44
1:B:508:GLU:O	1:B:512:GLN:NE2	2.48	0.44
2:C:249:PHE:CE2	2:C:251:PRO:HG3	2.53	0.44
2:D:66:LEU:HD23	2:D:66:LEU:HA	1.72	0.44
2:E:217:VAL:HG22	2:E:286:ASP:HB3	2.00	0.44
2:F:169:SER:HA	2:F:176:LEU:HD23	2.00	0.44
2:G:169:SER:HA	2:G:176:LEU:HD23	2.00	0.44
2:I:122:LEU:C	2:I:124:PHE:H	2.21	0.44
2:J:103:GLU:OE1	2:J:358:GLY:HA3	2.18	0.44
2:K:14:ALA:C	2:K:18:ILE:HD12	2.39	0.44
2:K:227:PRO:HD3	2:K:277:PHE:CG	2.53	0.44
2:L:225:LEU:HD13	2:L:277:PHE:CD2	2.53	0.44
2:M:217:VAL:HG22	2:M:286:ASP:HB3	1.99	0.44
2:O:312:GLN:HB3	2:O:313:PRO:HA	1.99	0.44
1:A:160:TYR:HE1	1:A:633:LEU:HA	1.83	0.44
1:A:245:LEU:O	1:A:246:HIS:CB	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:LEU:H	1:A:260:GLN:HE21	1.65	0.44
1:A:618:ILE:HD13	1:A:645:PHE:HZ	1.83	0.44
1:A:799:LEU:HD22	1:A:800:TYR:H	1.82	0.44
1:B:101:LYS:HB2	1:B:102:GLU:H	1.68	0.44
1:B:111:ILE:HG22	1:B:113:PRO:CD	2.48	0.44
1:B:122:LEU:HD12	1:B:124:ARG:HH22	1.82	0.44
1:B:207:ILE:O	1:B:210:ALA:HB3	2.18	0.44
1:B:353:LEU:HD23	1:B:353:LEU:O	2.18	0.44
1:B:473:HIS:HB3	2:I:126:ARG:NH1	2.26	0.44
1:B:496:ASN:HD22	1:B:498:ARG:HB2	1.83	0.44
1:B:543:LEU:O	1:B:546:LEU:HB2	2.18	0.44
1:B:675:GLU:O	1:B:678:ARG:N	2.51	0.44
1:B:790:ARG:CG	1:B:791:LYS:H	2.18	0.44
1:B:870:ALA:O	1:B:871:PHE:C	2.55	0.44
2:C:273:TYR:C	2:C:274:GLN:HE21	2.21	0.44
2:D:169:SER:HA	2:D:176:LEU:HD23	2.00	0.44
2:D:5:TYR:CE2	2:D:131:ASN:HA	2.52	0.44
2:E:125:LYS:C	2:E:127:ILE:H	2.21	0.44
2:E:249:PHE:CE2	2:E:251:PRO:HG3	2.53	0.44
2:G:150:PHE:N	2:G:150:PHE:CD1	2.86	0.44
2:G:100:MET:HG3	2:G:388:VAL:HG11	1.99	0.44
2:G:37:MET:O	2:G:38:ILE:C	2.55	0.44
2:H:78:VAL:O	2:H:81:ALA:HB3	2.17	0.44
2:I:63:PHE:N	2:I:63:PHE:CD1	2.86	0.44
2:K:49:GLY:HA2	2:K:54:LEU:HD23	1.99	0.44
2:K:89:VAL:C	2:K:91:PHE:N	2.71	0.44
2:L:63:PHE:CD2	2:L:84:THR:HG23	2.53	0.44
2:M:190:VAL:HG21	2:M:210:HIS:HB2	1.99	0.44
2:N:169:SER:HA	2:N:176:LEU:HD23	2.00	0.44
2:N:21:GLY:O	2:N:22:THR:C	2.56	0.44
2:O:106:ARG:HG2	2:O:107:ASN:H	1.83	0.44
2:O:78:VAL:O	2:O:81:ALA:HB3	2.18	0.44
1:A:119:GLN:NE2	1:A:178:PRO:HG2	2.33	0.43
1:A:428:GLN:HE22	1:A:455:PRO:HB2	1.74	0.43
1:B:293:PRO:O	1:B:295:THR:N	2.50	0.43
1:B:321:ILE:O	1:B:322:THR:C	2.57	0.43
1:B:510:LEU:O	1:B:513:LEU:N	2.51	0.43
1:B:529:ILE:O	1:B:533:ILE:HG13	2.18	0.43
1:B:506:LEU:CD2	1:B:544:VAL:HA	2.39	0.43
2:C:225:LEU:HD13	2:C:277:PHE:HD2	1.82	0.43
2:D:273:TYR:C	2:D:274:GLN:HE21	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:312:GLN:HB3	2:D:313:PRO:HA	1.99	0.43
2:E:89:VAL:C	2:E:91:PHE:H	2.22	0.43
2:G:225:LEU:HD13	2:G:277:PHE:CD2	2.53	0.43
2:H:225:LEU:HD13	2:H:277:PHE:CD2	2.53	0.43
2:H:225:LEU:HD13	2:H:277:PHE:HD2	1.82	0.43
2:H:41:MET:O	2:H:42:ASN:C	2.56	0.43
2:I:89:VAL:C	2:I:91:PHE:N	2.70	0.43
2:J:125:LYS:O	2:J:127:ILE:N	2.42	0.43
2:L:217:VAL:HG22	2:L:286:ASP:HB3	2.00	0.43
2:L:3:VAL:O	2:L:4:LEU:C	2.56	0.43
2:M:89:VAL:C	2:M:91:PHE:H	2.21	0.43
2:N:2:ASP:HB2	2:N:128:ASN:HD21	1.83	0.43
2:N:151:THR:C	2:N:152:PHE:CD1	2.91	0.43
2:N:155:PRO:O	2:N:186:SER:HB3	2.17	0.43
2:N:62:ASP:H	2:N:63:PHE:HD1	1.66	0.43
2:O:227:PRO:HD3	2:O:277:PHE:CG	2.53	0.43
2:O:3:VAL:O	2:O:4:LEU:C	2.56	0.43
1:A:141:GLU:O	1:A:142:LEU:CB	2.65	0.43
1:A:187:ALA:O	1:A:188:VAL:CG2	2.66	0.43
1:A:333:VAL:HB	1:A:380:LYS:HG2	2.00	0.43
1:A:416:ASN:C	1:A:418:MET:H	2.21	0.43
1:A:810:TYR:C	1:A:812:VAL:N	2.71	0.43
1:A:722:ASN:ND2	1:A:823:THR:O	2.51	0.43
1:A:854:LEU:O	1:A:855:LEU:C	2.56	0.43
1:B:138:GLY:O	1:B:804:SER:HB3	2.18	0.43
1:B:190:ASN:O	1:B:192:ASN:O	2.35	0.43
1:B:341:SER:O	1:B:342:THR:C	2.57	0.43
1:B:498:ARG:CD	2:I:32:GLN:NE2	2.82	0.43
1:B:503:ILE:HG12	1:B:547:THR:HB	2.00	0.43
1:B:491:GLN:CG	1:B:564:ASN:HB3	2.48	0.43
1:B:374:ALA:CB	1:B:580:SER:HB3	2.44	0.43
1:B:635:GLN:C	1:B:636:LYS:O	2.50	0.43
2:C:153:HIS:NE2	2:D:153:HIS:NE2	2.66	0.43
2:C:227:PRO:HD3	2:C:277:PHE:CG	2.53	0.43
2:C:239:ASN:ND2	2:C:246:THR:HG22	2.29	0.43
2:C:312:GLN:HB3	2:C:313:PRO:HA	1.99	0.43
2:D:99:GLU:CD	2:D:116:LEU:CD2	2.86	0.43
2:E:1:MET:O	2:E:2:ASP:C	2.56	0.43
2:G:61:PHE:N	2:G:61:PHE:CD1	2.86	0.43
2:I:36:GLN:CB	2:J:23:LEU:HD11	2.48	0.43
2:K:217:VAL:HG22	2:K:286:ASP:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:14:ALA:O	2:L:18:ILE:HD12	2.18	0.43
2:L:35:ASN:O	2:L:37:MET:N	2.51	0.43
2:M:169:SER:HA	2:M:176:LEU:HD23	2.00	0.43
2:M:22:THR:OG1	2:M:26:ASN:ND2	2.45	0.43
2:O:249:PHE:CE2	2:O:251:PRO:HG3	2.53	0.43
1:A:143:ARG:HG3	1:A:144:ASN:N	2.34	0.43
1:A:181:LEU:N	1:A:260:GLN:HE21	2.16	0.43
1:A:215:GLU:CD	1:A:215:GLU:H	2.21	0.43
1:A:396:PHE:HD2	1:A:578:LEU:HD11	1.84	0.43
1:A:501:HIS:CA	1:A:503:ILE:HG13	2.48	0.43
1:A:591:ALA:O	1:A:877:MET:SD	2.76	0.43
1:A:772:ILE:O	1:A:774:LEU:N	2.51	0.43
1:A:751:LEU:HD21	1:A:783:PHE:O	2.18	0.43
1:A:769:SER:CB	1:A:807:ASN:OD1	2.60	0.43
1:B:309:ASN:HA	1:B:311:HIS:CE1	2.54	0.43
1:B:791:LYS:HB3	1:B:792:VAL:H	1.59	0.43
2:D:63:PHE:N	2:D:63:PHE:CD1	2.86	0.43
2:E:78:VAL:O	2:E:81:ALA:N	2.41	0.43
2:F:217:VAL:HG22	2:F:286:ASP:HB3	1.99	0.43
2:G:225:LEU:HD13	2:G:277:PHE:HD2	1.82	0.43
2:G:53:ASN:ND2	2:G:354:ALA:HB3	2.33	0.43
2:H:227:PRO:HD3	2:H:277:PHE:CG	2.53	0.43
2:I:169:SER:HA	2:I:176:LEU:HD23	2.00	0.43
2:J:3:VAL:O	2:J:4:LEU:C	2.56	0.43
2:K:5:TYR:HE2	2:K:131:ASN:HA	1.79	0.43
2:K:3:VAL:O	2:K:4:LEU:C	2.56	0.43
2:N:136:ILE:HG23	2:N:137:GLU:N	2.33	0.43
2:M:128:ASN:HB3	2:N:19:VAL:CG2	2.48	0.43
2:N:227:PRO:HD3	2:N:277:PHE:CG	2.53	0.43
1:A:383:ILE:O	1:A:386:MET:N	2.52	0.43
1:A:750:MET:CE	1:A:757:VAL:HG21	2.48	0.43
1:A:781:THR:HG22	1:A:782:VAL:N	2.34	0.43
1:B:312:ASP:CG	1:B:312:ASP:O	2.56	0.43
1:B:510:LEU:HA	1:B:513:LEU:HD12	1.99	0.43
1:B:510:LEU:HD22	1:B:540:LEU:CD1	2.30	0.43
1:B:542:GLN:O	1:B:543:LEU:C	2.57	0.43
1:B:595:PRO:HB2	1:B:600:LEU:HD11	2.00	0.43
2:C:1:MET:O	2:C:2:ASP:C	2.56	0.43
2:E:142:GLN:HE21	2:E:143:ASN:N	2.16	0.43
2:E:227:PRO:HD3	2:E:277:PHE:CG	2.53	0.43
2:F:227:PRO:HD3	2:F:277:PHE:CG	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:249:PHE:CE2	2:G:251:PRO:HG3	2.53	0.43
2:G:6:SER:C	2:G:8:SER:N	2.72	0.43
2:H:169:SER:HA	2:H:176:LEU:HD23	2.00	0.43
2:I:146:GLN:O	2:I:148:THR:HG23	2.19	0.43
2:I:227:PRO:HD3	2:I:277:PHE:CG	2.53	0.43
2:I:312:GLN:HB3	2:I:313:PRO:HA	1.99	0.43
2:K:225:LEU:HD13	2:K:277:PHE:CD2	2.53	0.43
2:L:42:ASN:CA	2:L:61:PHE:HB2	2.30	0.43
2:L:89:VAL:C	2:L:91:PHE:N	2.71	0.43
2:M:24:TYR:N	2:M:71:LEU:O	2.49	0.43
2:N:153:HIS:O	2:N:154:LYS:C	2.57	0.43
2:N:225:LEU:HD13	2:N:277:PHE:CD2	2.53	0.43
2:N:101:VAL:HG11	2:N:355:ILE:HG13	2.01	0.43
1:A:243:SER:O	1:A:839:MET:HG2	2.19	0.43
1:A:408:MET:HG2	1:A:471:TRP:CH2	2.53	0.43
1:A:415:PRO:O	1:A:417:ASP:N	2.43	0.43
1:A:546:LEU:HD23	1:A:546:LEU:HA	1.86	0.43
1:A:583:SER:O	1:A:584:LEU:C	2.56	0.43
1:A:714:ARG:HG2	1:A:720:TYR:CD2	2.54	0.43
1:A:717:MET:HE3	1:A:829:VAL:HG13	2.01	0.43
1:A:799:LEU:HD23	1:A:799:LEU:HA	1.68	0.43
1:A:548:ARG:HH11	1:A:877:MET:H	1.67	0.43
1:B:309:ASN:HA	1:B:311:HIS:NE2	2.33	0.43
1:B:451:ASP:H	1:B:452:PRO:CD	2.20	0.43
1:B:540:LEU:HD23	1:B:541:GLY:CA	2.48	0.43
1:B:703:VAL:CG1	1:B:704:ILE:N	2.81	0.43
1:B:706:ALA:C	1:B:708:ARG:N	2.72	0.43
1:B:772:ILE:O	1:B:775:ILE:N	2.51	0.43
2:C:78:VAL:O	2:C:81:ALA:HB3	2.17	0.43
2:E:125:LYS:O	2:E:127:ILE:N	2.51	0.43
2:E:136:ILE:HG23	2:E:137:GLU:N	2.34	0.43
2:E:24:TYR:HE1	2:E:31:ILE:HG13	1.83	0.43
2:E:60:ASN:C	2:E:61:PHE:CD1	2.91	0.43
2:F:225:LEU:HD13	2:F:277:PHE:CD2	2.53	0.43
2:F:3:VAL:O	2:F:4:LEU:C	2.56	0.43
2:G:217:VAL:HG22	2:G:286:ASP:HB3	1.99	0.43
2:G:38:ILE:H	2:G:38:ILE:HG13	1.59	0.43
2:H:1:MET:O	2:H:2:ASP:C	2.57	0.43
2:I:34:PHE:O	2:I:37:MET:HB3	2.18	0.43
2:J:169:SER:HA	2:J:176:LEU:HD23	2.00	0.43
2:K:89:VAL:C	2:K:91:PHE:H	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:169:SER:HA	2:L:176:LEU:HD23	2.00	0.43
2:L:249:PHE:CE2	2:L:251:PRO:HG3	2.53	0.43
2:M:123:LYS:HG3	2:M:124:PHE:CD1	2.53	0.43
2:M:155:PRO:HA	2:M:337:ASP:CB	2.49	0.43
2:M:63:PHE:HD2	2:M:84:THR:HG23	1.81	0.43
2:N:145:ARG:HE	2:N:145:ARG:HA	1.83	0.43
2:N:312:GLN:HB3	2:N:313:PRO:HA	1.99	0.43
2:N:24:TYR:HE1	2:N:31:ILE:HG13	1.83	0.43
2:N:63:PHE:CD2	2:N:84:THR:HG23	2.54	0.43
1:A:298:TYR:CD1	1:A:298:TYR:C	2.91	0.43
1:A:353:LEU:C	1:A:354:GLN:HG2	2.37	0.43
1:A:501:HIS:HA	1:A:503:ILE:HG13	2.01	0.43
1:A:521:MET:CB	1:A:522:PRO:HD3	2.26	0.43
1:A:563:MET:O	1:A:564:ASN:C	2.56	0.43
1:A:675:GLU:HB3	1:A:678:ARG:HG2	2.01	0.43
1:B:224:PHE:CD1	2:O:71:LEU:HD13	2.54	0.43
1:B:231:ARG:HA	1:B:231:ARG:HD2	1.77	0.43
1:B:383:ILE:O	1:B:386:MET:N	2.51	0.43
1:B:772:ILE:CG2	1:B:773:SER:H	2.29	0.43
2:E:152:PHE:O	2:E:328:SER:HA	2.19	0.43
2:F:163:SER:HB3	2:F:181:TRP:CZ2	2.54	0.43
2:G:151:THR:C	2:G:152:PHE:CD1	2.92	0.43
2:G:89:VAL:C	2:G:91:PHE:H	2.22	0.43
2:O:62:ASP:H	2:O:63:PHE:HD1	1.66	0.43
1:A:428:GLN:O	1:A:432:VAL:HG23	2.19	0.43
1:A:387:LEU:HD23	1:A:554:TYR:CE1	2.54	0.43
1:A:693:GLU:O	1:A:695:ALA:O	2.37	0.43
1:B:434:THR:C	1:B:435:ILE:HG13	2.37	0.43
1:B:620:ASP:O	1:B:624:ILE:HG13	2.19	0.43
1:B:666:ARG:HG2	1:B:667:ASP:N	2.32	0.43
1:B:743:ASP:CG	1:B:744:TYR:N	2.72	0.43
1:B:770:SER:O	1:B:771:VAL:C	2.57	0.43
2:C:78:VAL:O	2:C:81:ALA:N	2.40	0.43
2:D:11:LEU:O	2:D:15:ARG:N	2.40	0.43
2:D:89:VAL:C	2:D:91:PHE:H	2.22	0.43
2:E:169:SER:HA	2:E:176:LEU:HD23	2.00	0.43
2:G:145:ARG:HE	2:I:142:GLN:NE2	2.17	0.43
2:H:273:TYR:C	2:H:274:GLN:HE21	2.21	0.43
2:H:35:ASN:O	2:H:37:MET:N	2.52	0.43
2:J:136:ILE:HG23	2:J:137:GLU:N	2.33	0.43
2:J:14:ALA:O	2:J:16:ASP:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:508:GLU:OE1	2:J:71:LEU:HB3	2.18	0.43
2:L:78:VAL:O	2:L:81:ALA:HB3	2.18	0.43
2:N:154:LYS:N	2:N:155:PRO:CD	2.82	0.43
1:A:370:ILE:O	1:A:374:ALA:HB2	2.19	0.43
1:A:393:SER:C	1:A:394:LEU:HG	2.38	0.43
1:A:571:LEU:HD22	1:A:571:LEU:HA	1.74	0.43
1:A:709:ASP:O	1:A:710:MET:HB3	2.18	0.43
1:A:785:GLN:O	1:A:786:ILE:C	2.57	0.43
1:B:433:ASN:C	1:B:435:ILE:H	2.22	0.43
1:B:658:PRO:HB2	1:B:661:GLN:CG	2.39	0.43
1:B:776:ALA:O	1:B:778:LEU:N	2.52	0.43
1:B:871:PHE:CD1	1:B:872:ASP:N	2.87	0.43
2:C:53:ASN:HD22	2:C:354:ALA:HB3	1.83	0.43
2:I:11:LEU:O	2:I:15:ARG:N	2.38	0.43
2:I:4:LEU:O	2:I:5:TYR:C	2.57	0.43
2:J:190:VAL:HG21	2:J:210:HIS:HB2	1.99	0.43
2:M:74:ASP:O	2:M:75:ALA:C	2.57	0.43
2:N:125:LYS:C	2:N:127:ILE:H	2.22	0.43
2:N:249:PHE:CE2	2:N:251:PRO:HG3	2.53	0.43
2:N:3:VAL:O	2:N:4:LEU:C	2.56	0.43
1:A:396:PHE:HB3	1:A:578:LEU:HG	2.00	0.43
1:A:420:ILE:HD12	1:A:422:GLU:CG	2.49	0.43
1:A:481:ARG:HH12	1:A:497:ILE:CD1	2.32	0.43
1:A:510:LEU:HD13	1:A:540:LEU:HB2	2.01	0.43
1:A:393:SER:HB2	1:A:573:THR:CG2	2.48	0.43
1:A:815:TYR:HD1	1:A:815:TYR:H	1.62	0.43
1:B:218:GLU:OE1	1:B:836:ARG:NH2	2.51	0.43
1:B:409:TRP:CZ3	1:B:413:VAL:HG23	2.54	0.43
1:B:625:ILE:H	1:B:625:ILE:HG13	1.60	0.43
1:B:870:ALA:O	1:B:872:ASP:N	2.52	0.43
2:C:14:ALA:O	2:C:16:ASP:N	2.52	0.43
2:C:35:ASN:O	2:C:37:MET:N	2.52	0.43
2:C:89:VAL:C	2:C:91:PHE:N	2.72	0.43
2:D:89:VAL:C	2:D:91:PHE:N	2.72	0.43
2:E:70:LEU:HB3	2:E:72:ASN:O	2.19	0.43
2:G:3:VAL:O	2:G:4:LEU:C	2.56	0.43
2:H:135:TYR:CE1	2:H:342:MET:HE3	2.54	0.43
2:H:89:VAL:C	2:H:91:PHE:N	2.73	0.43
2:I:27:VAL:O	2:I:30:LEU:HB3	2.19	0.43
2:J:66:LEU:HD23	2:J:66:LEU:HA	1.81	0.43
2:I:16:ASP:HB3	2:K:131:ASN:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:163:SER:HB3	2:K:181:TRP:CZ2	2.54	0.43
2:M:1:MET:C	2:M:3:VAL:N	2.71	0.43
2:N:50:GLY:O	2:N:51:ILE:CG2	2.61	0.43
2:O:89:VAL:C	2:O:91:PHE:N	2.71	0.43
1:A:319:ASP:OD2	1:A:572:THR:N	2.52	0.43
1:A:339:LEU:HD13	1:A:588:ILE:HG12	2.00	0.43
1:A:396:PHE:HB3	1:A:578:LEU:CG	2.47	0.43
1:A:496:ASN:O	1:A:498:ARG:N	2.51	0.43
1:A:598:GLN:HG3	1:A:598:GLN:H	1.61	0.43
1:A:656:ARG:HB3	1:B:347:GLN:NE2	2.34	0.43
1:B:134:TYR:N	1:B:134:TYR:CD1	2.86	0.43
1:B:126:PHE:CB	1:B:149:LYS:O	2.67	0.43
1:B:477:ASN:ND2	2:I:39:ILE:CG2	2.81	0.43
1:B:810:TYR:C	1:B:812:VAL:HG12	2.38	0.43
1:B:89:GLU:O	1:B:91:LEU:N	2.52	0.43
2:D:225:LEU:HD13	2:D:277:PHE:CD2	2.53	0.43
2:E:49:GLY:HA2	2:E:54:LEU:HD23	2.01	0.43
2:F:89:VAL:C	2:F:91:PHE:H	2.22	0.43
2:I:149:GLY:C	2:I:150:PHE:CD1	2.92	0.43
2:J:34:PHE:O	2:J:37:MET:HB3	2.18	0.43
2:J:35:ASN:O	2:J:37:MET:N	2.52	0.43
2:K:27:VAL:O	2:K:30:LEU:N	2.52	0.43
2:M:34:PHE:O	2:M:37:MET:HB3	2.19	0.43
2:M:56:ILE:O	2:M:56:ILE:HG22	2.19	0.43
2:O:163:SER:HB3	2:O:181:TRP:CZ2	2.54	0.43
1:A:355:LEU:HA	1:A:355:LEU:HD23	1.79	0.42
1:B:249:ASP:O	1:B:250:TYR:C	2.58	0.42
1:B:251:ALA:HA	2:N:69:THR:CG2	2.42	0.42
1:B:305:GLN:HG3	1:B:489:LEU:CD2	2.49	0.42
1:B:698:LYS:C	1:B:699:ILE:CD1	2.87	0.42
1:B:795:LEU:O	1:B:797:PRO:HD3	2.18	0.42
1:B:548:ARG:CD	1:B:877:MET:H	2.31	0.42
1:B:99:GLU:HB3	1:B:100:PRO:CD	2.35	0.42
2:C:34:PHE:O	2:C:37:MET:HB3	2.19	0.42
2:C:38:ILE:H	2:C:38:ILE:HG13	1.58	0.42
2:D:150:PHE:HB2	2:D:152:PHE:CZ	2.53	0.42
2:D:227:PRO:HD3	2:D:277:PHE:CG	2.53	0.42
2:E:154:LYS:HG2	2:E:186:SER:OG	2.19	0.42
2:F:148:THR:HB	2:F:149:GLY:H	1.64	0.42
2:F:89:VAL:C	2:F:91:PHE:N	2.72	0.42
2:H:89:VAL:C	2:H:91:PHE:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:163:SER:HB3	2:I:181:TRP:CZ2	2.54	0.42
2:I:249:PHE:CE2	2:I:251:PRO:HG3	2.53	0.42
2:J:227:PRO:HD3	2:J:277:PHE:CG	2.53	0.42
2:J:249:PHE:CE2	2:J:251:PRO:HG3	2.53	0.42
2:K:125:LYS:C	2:K:127:ILE:H	2.22	0.42
2:L:38:ILE:H	2:L:38:ILE:HG13	1.55	0.42
2:N:27:VAL:O	2:N:28:SER:C	2.58	0.42
2:N:35:ASN:O	2:N:37:MET:N	2.52	0.42
2:O:23:LEU:CD2	2:O:24:TYR:N	2.82	0.42
1:A:124:ARG:C	1:A:125:ILE:HD12	2.37	0.42
1:A:273:TYR:O	1:A:273:TYR:HD2	2.01	0.42
1:A:587:LEU:HD22	1:A:587:LEU:C	2.39	0.42
1:A:613:ASN:O	1:A:617:ARG:HG2	2.19	0.42
1:A:633:LEU:C	1:A:635:GLN:N	2.72	0.42
1:B:308:LEU:HB3	1:B:310:LEU:CD2	2.49	0.42
1:B:346:ILE:HA	1:B:349:MET:HB2	2.01	0.42
1:B:393:SER:H	1:B:573:THR:CG2	2.31	0.42
1:B:413:VAL:O	1:B:414:VAL:C	2.58	0.42
1:B:491:GLN:NE2	1:B:566:GLN:CG	2.79	0.42
1:B:701:GLN:N	1:B:701:GLN:CD	2.72	0.42
2:C:163:SER:HB3	2:C:181:TRP:CZ2	2.54	0.42
2:C:169:SER:HA	2:C:176:LEU:HD23	2.00	0.42
2:C:225:LEU:HD13	2:C:277:PHE:CD2	2.53	0.42
2:C:4:LEU:O	2:C:5:TYR:C	2.58	0.42
2:D:14:ALA:O	2:D:16:ASP:N	2.52	0.42
2:D:3:VAL:O	2:D:4:LEU:C	2.57	0.42
2:E:150:PHE:HB2	2:E:152:PHE:HE1	1.81	0.42
2:E:6:SER:C	2:E:8:SER:N	2.73	0.42
2:G:227:PRO:HD3	2:G:277:PHE:CG	2.54	0.42
2:I:14:ALA:C	2:I:18:ILE:HD12	2.39	0.42
1:B:498:ARG:CD	2:I:32:GLN:HE21	2.32	0.42
2:I:51:ILE:O	2:I:54:LEU:HB3	2.19	0.42
2:I:61:PHE:O	2:I:62:ASP:HB3	2.19	0.42
2:J:54:LEU:HD12	2:J:55:PRO:HD2	2.00	0.42
2:K:169:SER:HA	2:K:176:LEU:HD23	2.00	0.42
2:K:249:PHE:CE2	2:K:251:PRO:HG3	2.53	0.42
2:L:227:PRO:HD3	2:L:277:PHE:CG	2.53	0.42
2:M:227:PRO:HD3	2:M:277:PHE:CG	2.53	0.42
2:M:89:VAL:C	2:M:91:PHE:N	2.72	0.42
2:O:113:SER:O	2:O:117:ARG:HG3	2.18	0.42
1:A:265:LEU:HB3	1:A:296:ALA:HB1	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:ILE:O	1:A:374:ALA:CB	2.68	0.42
1:A:510:LEU:HA	1:A:513:LEU:HD12	2.01	0.42
1:A:391:THR:O	1:A:573:THR:HA	2.19	0.42
1:A:775:ILE:C	1:A:777:LYS:N	2.71	0.42
1:A:864:GLU:CD	1:A:865:PRO:HD2	2.40	0.42
1:A:548:ARG:NH1	1:A:877:MET:CA	2.78	0.42
1:B:380:LYS:O	1:B:381:THR:C	2.58	0.42
1:B:636:LYS:O	1:B:637:LYS:CB	2.66	0.42
2:C:111:PRO:HB3	2:C:116:LEU:HD23	2.01	0.42
2:C:26:ASN:N	2:C:26:ASN:OD1	2.52	0.42
2:D:27:VAL:CG2	2:D:31:ILE:HD11	2.49	0.42
2:D:35:ASN:O	2:D:37:MET:N	2.53	0.42
2:E:63:PHE:N	2:E:63:PHE:CD1	2.87	0.42
2:F:69:THR:O	2:F:70:LEU:C	2.56	0.42
2:H:38:ILE:HG13	2:H:38:ILE:H	1.57	0.42
2:I:36:GLN:NE2	2:I:126:ARG:HD3	2.34	0.42
2:I:17:LYS:HG2	2:K:130:ASP:HA	2.01	0.42
2:L:106:ARG:H	2:L:106:ARG:CD	2.20	0.42
2:L:140:ASN:O	2:L:143:ASN:N	2.50	0.42
2:N:116:LEU:O	2:N:119:LEU:N	2.48	0.42
2:N:273:TYR:C	2:N:274:GLN:HE21	2.21	0.42
1:A:321:ILE:O	1:A:322:THR:C	2.58	0.42
1:A:383:ILE:HD11	1:A:550:LEU:CD2	2.49	0.42
1:A:660:ASP:CA	1:B:539:ARG:NH1	2.83	0.42
1:A:666:ARG:HA	1:A:669:LEU:HD12	2.00	0.42
1:A:714:ARG:CG	1:A:720:TYR:HD2	2.32	0.42
1:A:548:ARG:HH11	1:A:877:MET:N	2.17	0.42
1:B:192:ASN:O	1:B:193:SER:HB3	2.19	0.42
1:B:300:ARG:HA	1:B:301:PRO:HD3	1.76	0.42
1:B:443:GLN:C	1:B:445:MET:H	2.21	0.42
1:B:482:GLN:CA	1:B:493:LEU:HD22	2.49	0.42
1:B:557:LEU:O	1:B:558:MET:C	2.58	0.42
1:B:789:LEU:O	1:B:790:ARG:O	2.37	0.42
1:B:239:VAL:CG2	1:B:844:SER:O	2.61	0.42
1:B:853:ASP:O	1:B:854:LEU:CB	2.67	0.42
1:B:879:GLU:O	1:B:880:LEU:OXT	2.37	0.42
2:C:46:PHE:CE2	2:C:119:LEU:HD21	2.54	0.42
2:C:227:PRO:O	2:C:228:ASP:HB2	2.20	0.42
2:E:227:PRO:O	2:E:228:ASP:HB2	2.19	0.42
2:E:4:LEU:O	2:E:5:TYR:C	2.57	0.42
2:F:123:LYS:HG3	2:F:124:PHE:CD1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:136:ILE:HG23	2:F:137:GLU:N	2.34	0.42
2:F:168:ARG:HD2	2:F:175:ASN:O	2.20	0.42
2:J:131:ASN:ND2	2:J:131:ASN:N	2.67	0.42
2:J:163:SER:HB3	2:J:181:TRP:CZ2	2.54	0.42
2:K:139:TRP:HE1	2:K:143:ASN:HD22	1.66	0.42
2:L:163:SER:HB3	2:L:181:TRP:CZ2	2.54	0.42
2:L:24:TYR:O	2:L:26:ASN:N	2.52	0.42
2:L:62:ASP:H	2:L:63:PHE:HD1	1.66	0.42
2:N:163:SER:HB3	2:N:181:TRP:CZ2	2.54	0.42
2:N:168:ARG:HD2	2:N:175:ASN:O	2.20	0.42
1:A:319:ASP:OD2	1:A:570:THR:HG22	2.19	0.42
1:A:400:ASN:O	1:A:403:SER:HB2	2.20	0.42
1:A:570:THR:CG2	1:A:571:LEU:N	2.74	0.42
1:B:146:TRP:O	1:B:833:PHE:HB3	2.20	0.42
1:B:113:PRO:CG	1:B:609:ASN:HB3	2.49	0.42
2:C:128:ASN:O	2:C:129:PHE:HB2	2.20	0.42
2:E:24:TYR:CE1	2:E:31:ILE:HG13	2.54	0.42
2:F:153:HIS:NE2	2:G:153:HIS:NE2	2.67	0.42
2:G:136:ILE:HG23	2:G:137:GLU:N	2.33	0.42
2:G:163:SER:HB3	2:G:181:TRP:CZ2	2.54	0.42
2:G:89:VAL:C	2:G:91:PHE:N	2.73	0.42
2:I:168:ARG:HD2	2:I:175:ASN:O	2.20	0.42
2:K:23:LEU:H	2:K:26:ASN:ND2	2.17	0.42
2:L:227:PRO:O	2:L:228:ASP:HB2	2.20	0.42
2:L:66:LEU:HB3	2:L:67:GLY:H	1.66	0.42
2:M:145:ARG:CB	2:M:145:ARG:HH11	2.32	0.42
2:M:14:ALA:O	2:M:16:ASP:N	2.52	0.42
2:M:78:VAL:O	2:M:81:ALA:HB3	2.19	0.42
2:N:21:GLY:O	2:N:22:THR:O	2.36	0.42
2:N:34:PHE:O	2:N:37:MET:HB3	2.20	0.42
2:O:227:PRO:O	2:O:228:ASP:HB2	2.20	0.42
1:A:200:VAL:CG2	1:A:241:TYR:HD2	2.32	0.42
1:A:259:HIS:O	1:A:260:GLN:C	2.56	0.42
1:A:271:PHE:HA	1:A:274:ILE:CD1	2.47	0.42
1:A:351:GLN:O	1:A:353:LEU:N	2.53	0.42
1:A:443:GLN:HE22	1:A:522:PRO:HG3	1.84	0.42
1:A:546:LEU:HD21	1:A:588:ILE:HD12	1.99	0.42
1:A:594:ILE:HG23	1:A:595:PRO:HD2	2.01	0.42
1:A:593:VAL:HG12	1:A:594:ILE:N	2.35	0.42
1:A:876:ILE:O	1:A:877:MET:CB	2.68	0.42
1:B:195:ASP:O	1:B:196:ALA:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:VAL:HG13	1:B:242:PRO:O	2.20	0.42
1:B:465:ASN:O	1:B:466:PHE:C	2.58	0.42
1:B:555:GLU:OE2	1:B:871:PHE:CE2	2.69	0.42
2:C:9:LYS:HE3	2:C:13:ASP:OD1	2.19	0.42
2:E:163:SER:HB3	2:E:181:TRP:CZ2	2.54	0.42
2:E:59:TRP:N	2:E:59:TRP:CD1	2.87	0.42
2:G:168:ARG:HD2	2:G:175:ASN:O	2.20	0.42
2:I:78:VAL:O	2:I:81:ALA:HB3	2.20	0.42
2:J:227:PRO:O	2:J:228:ASP:HB2	2.20	0.42
2:J:74:ASP:O	2:J:75:ALA:C	2.57	0.42
2:J:6:SER:C	2:J:8:SER:N	2.73	0.42
2:M:3:VAL:O	2:M:4:LEU:C	2.57	0.42
2:N:101:VAL:HG12	2:N:350:ARG:HG2	2.01	0.42
2:O:6:SER:C	2:O:8:SER:N	2.73	0.42
1:A:125:ILE:H	1:A:125:ILE:HD12	1.77	0.42
1:A:211:ILE:C	1:A:213:GLN:H	2.23	0.42
1:A:409:TRP:CH2	1:A:547:THR:OG1	2.71	0.42
1:A:709:ASP:OD2	1:A:820:THR:HG21	2.20	0.42
1:A:775:ILE:HG13	1:A:775:ILE:H	1.35	0.42
1:A:839:MET:CG	1:A:840:HIS:N	2.83	0.42
1:A:853:ASP:O	1:A:854:LEU:HB2	2.18	0.42
1:B:390:ARG:HG3	1:B:391:THR:N	2.34	0.42
1:B:409:TRP:CZ3	1:B:413:VAL:CG2	3.02	0.42
1:B:496:ASN:HD22	1:B:498:ARG:CB	2.32	0.42
1:A:571:LEU:CD2	1:B:531:ARG:CZ	2.97	0.42
1:B:243:SER:HB3	1:B:842:LEU:HD12	2.01	0.42
2:E:168:ARG:HD2	2:E:175:ASN:O	2.20	0.42
2:F:227:PRO:O	2:F:228:ASP:HB2	2.20	0.42
2:G:9:LYS:HE3	2:G:13:ASP:OD1	2.19	0.42
2:H:136:ILE:HG23	2:H:137:GLU:N	2.34	0.42
2:K:78:VAL:O	2:K:81:ALA:HB3	2.19	0.42
2:L:168:ARG:HD2	2:L:175:ASN:O	2.20	0.42
2:N:227:PRO:O	2:N:228:ASP:HB2	2.19	0.42
1:A:440:PHE:O	1:A:441:GLY:C	2.58	0.42
1:A:517:GLN:HG3	1:A:517:GLN:O	2.20	0.42
1:A:707:TYR:N	1:A:707:TYR:CD1	2.88	0.42
1:A:850:VAL:C	1:A:851:TYR:CD1	2.93	0.42
1:B:482:GLN:O	1:B:483:VAL:CG2	2.68	0.42
1:B:546:LEU:HD23	1:B:546:LEU:HA	1.81	0.42
2:C:155:PRO:HA	2:C:337:ASP:HB2	2.02	0.42
2:E:9:LYS:HE3	2:E:13:ASP:OD1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:145:ARG:C	2:F:146:GLN:HG2	2.40	0.42
2:G:253:ILE:HG13	2:H:234:PHE:CE1	2.55	0.42
2:L:125:LYS:C	2:L:127:ILE:H	2.22	0.42
2:L:42:ASN:HB3	2:L:62:ASP:N	2.35	0.42
2:L:61:PHE:N	2:L:61:PHE:CD1	2.88	0.42
2:M:163:SER:HB3	2:M:181:TRP:CZ2	2.55	0.42
2:M:355:ILE:HA	2:M:356:PRO:HD3	1.96	0.42
2:O:124:PHE:O	2:O:127:ILE:HG13	2.19	0.42
2:O:23:LEU:HG	2:O:24:TYR:H	1.85	0.42
1:A:141:GLU:O	1:A:142:LEU:HD12	2.20	0.42
1:A:216:GLU:N	1:A:216:GLU:OE1	2.50	0.42
1:A:487:GLY:O	1:A:488:VAL:CB	2.68	0.42
1:B:183:LEU:O	1:B:184:LYS:C	2.57	0.42
1:B:253:ASN:O	1:B:256:PHE:HB2	2.20	0.42
1:B:310:LEU:H	1:B:310:LEU:HG	1.44	0.42
1:B:454:THR:CG2	1:B:476:ASN:ND2	2.61	0.42
1:B:570:THR:HG22	1:B:571:LEU:N	2.34	0.42
1:B:646:LEU:H	1:B:646:LEU:HG	1.51	0.42
1:B:856:ALA:C	1:B:858:VAL:N	2.72	0.42
2:D:163:SER:HB3	2:D:181:TRP:CZ2	2.54	0.42
2:E:129:PHE:CE1	2:E:130:ASP:HB3	2.54	0.42
2:E:3:VAL:O	2:E:4:LEU:C	2.57	0.42
2:E:61:PHE:CD1	2:E:61:PHE:N	2.87	0.42
2:I:104:SER:HB3	2:I:108:GLY:HA2	2.02	0.42
2:J:73:LEU:HD22	2:J:77:TYR:CD2	2.54	0.42
2:K:9:LYS:HE3	2:K:13:ASP:OD1	2.20	0.42
2:I:397:LYS:NZ	2:K:150:PHE:HA	2.34	0.42
2:K:227:PRO:O	2:K:228:ASP:HB2	2.20	0.42
2:J:253:ILE:HG13	2:K:234:PHE:CE1	2.55	0.42
2:M:14:ALA:C	2:M:18:ILE:HD12	2.40	0.42
2:M:7:LEU:HG	2:M:7:LEU:H	1.53	0.42
2:N:14:ALA:O	2:N:16:ASP:N	2.53	0.42
2:N:4:LEU:O	2:N:5:TYR:C	2.58	0.42
2:O:153:HIS:C	2:O:155:PRO:N	2.71	0.42
1:A:134:TYR:CE1	1:A:803:ASN:CG	2.93	0.42
1:A:201:ASP:O	1:A:204:THR:N	2.52	0.42
1:A:492:VAL:CG1	1:A:493:LEU:N	2.82	0.42
1:A:695:ALA:O	1:A:696:SER:HB3	2.20	0.42
1:A:810:TYR:O	1:A:813:ALA:N	2.53	0.42
1:B:287:ASN:HD22	1:B:287:ASN:HA	1.60	0.42
1:B:544:VAL:HG12	1:B:548:ARG:HE	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:746:GLN:HE22	2:D:64:GLY:HA2	1.85	0.42
1:B:148:TRP:NE1	1:B:833:PHE:HD1	2.18	0.42
2:C:168:ARG:HD2	2:C:175:ASN:O	2.20	0.42
2:D:51:ILE:O	2:D:52:GLY:C	2.58	0.42
2:E:14:ALA:O	2:E:16:ASP:N	2.52	0.42
2:G:23:LEU:HD23	2:G:25:SER:H	1.85	0.42
2:H:163:SER:HB3	2:H:181:TRP:CZ2	2.54	0.42
2:H:152:PHE:O	2:H:328:SER:HA	2.19	0.42
2:H:3:VAL:O	2:H:4:LEU:C	2.58	0.42
2:I:35:ASN:O	2:I:37:MET:N	2.52	0.42
2:I:74:ASP:O	2:I:75:ALA:C	2.57	0.42
2:K:35:ASN:O	2:K:37:MET:N	2.53	0.42
2:K:4:LEU:O	2:K:5:TYR:C	2.58	0.42
2:K:51:ILE:O	2:K:51:ILE:HG23	2.20	0.42
2:K:61:PHE:CD1	2:K:61:PHE:N	2.88	0.42
2:M:227:PRO:O	2:M:228:ASP:HB2	2.20	0.42
2:N:59:TRP:CD1	2:N:59:TRP:N	2.88	0.42
2:O:239:ASN:ND2	2:O:246:THR:HG22	2.29	0.42
2:O:1:MET:HG3	2:O:2:ASP:N	2.34	0.42
1:A:129:ARG:HG2	1:A:130:GLN:H	1.84	0.41
1:A:162:VAL:O	1:A:165:TYR:HB3	2.20	0.41
1:A:174:LEU:HA	1:A:177:MET:HB2	2.01	0.41
1:A:842:LEU:HD23	1:A:842:LEU:HA	1.76	0.41
1:A:853:ASP:OD1	1:A:854:LEU:N	2.53	0.41
1:B:224:PHE:CE1	2:O:71:LEU:N	2.87	0.41
1:B:501:HIS:O	1:B:503:ILE:N	2.53	0.41
1:B:526:LYS:O	1:B:530:GLN:HG2	2.20	0.41
2:C:235:PRO:HA	2:C:249:PHE:O	2.20	0.41
2:E:106:ARG:HB3	2:E:107:ASN:H	1.54	0.41
2:E:239:ASN:ND2	2:E:246:THR:HG22	2.30	0.41
2:E:89:VAL:C	2:E:91:PHE:N	2.73	0.41
2:H:227:PRO:O	2:H:228:ASP:HB2	2.20	0.41
2:I:27:VAL:O	2:I:31:ILE:HG12	2.19	0.41
2:L:124:PHE:O	2:L:126:ARG:N	2.53	0.41
2:L:235:PRO:HA	2:L:249:PHE:O	2.20	0.41
2:N:76:ASN:HA	2:O:75:ALA:HB3	2.01	0.41
2:N:89:VAL:C	2:N:91:PHE:N	2.71	0.41
2:O:125:LYS:O	2:O:127:ILE:N	2.51	0.41
1:A:124:ARG:HD2	1:A:203:GLU:OE1	2.20	0.41
1:A:275:PRO:C	1:A:277:ARG:H	2.23	0.41
1:A:275:PRO:CG	1:A:278:ILE:HD11	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:LEU:HD22	1:A:435:ILE:HD11	2.02	0.41
1:A:493:LEU:HD11	1:A:566:GLN:O	2.20	0.41
1:A:656:ARG:O	1:A:657:VAL:HG23	2.20	0.41
1:A:314:PHE:HZ	1:A:664:ARG:HG2	1.84	0.41
1:A:848:PHE:C	1:A:849:THR:OG1	2.58	0.41
1:B:371:ASN:O	1:B:372:SER:C	2.58	0.41
1:B:383:ILE:O	1:B:384:ALA:C	2.57	0.41
1:B:406:SER:O	1:B:409:TRP:N	2.51	0.41
1:B:466:PHE:CE1	2:H:80:THR:HG22	2.55	0.41
2:C:142:GLN:OE1	2:N:145:ARG:NH1	2.48	0.41
2:C:234:PHE:CE1	2:E:253:ILE:HG13	2.55	0.41
2:D:116:LEU:O	2:D:119:LEU:N	2.50	0.41
2:D:133:SER:O	2:D:134:GLU:C	2.59	0.41
2:D:1:MET:O	2:D:2:ASP:C	2.56	0.41
2:D:4:LEU:O	2:D:5:TYR:C	2.58	0.41
2:D:70:LEU:CD1	2:D:71:LEU:N	2.82	0.41
2:E:74:ASP:O	2:E:75:ALA:C	2.58	0.41
2:F:234:PHE:CE1	2:H:253:ILE:HG13	2.55	0.41
2:F:27:VAL:O	2:F:31:ILE:HG12	2.20	0.41
2:G:125:LYS:C	2:G:127:ILE:H	2.24	0.41
2:H:168:ARG:HD2	2:H:175:ASN:O	2.20	0.41
2:K:168:ARG:HD2	2:K:175:ASN:O	2.20	0.41
2:M:155:PRO:O	2:M:186:SER:HB3	2.20	0.41
2:O:38:ILE:HG22	2:O:42:ASN:ND2	2.33	0.41
1:A:170:TYR:CZ	1:A:682:PHE:HB2	2.55	0.41
1:A:236:ARG:HB2	1:A:238:VAL:CG2	2.47	0.41
1:A:382:LEU:O	1:A:385:ALA:HB3	2.20	0.41
1:A:647:LYS:HG2	1:A:654:VAL:HG21	1.99	0.41
1:B:456:PHE:O	1:B:457:GLN:O	2.38	0.41
1:B:646:LEU:O	1:B:649:LEU:HB2	2.20	0.41
1:B:721:VAL:CG1	1:B:722:ASN:H	2.30	0.41
2:D:168:ARG:HD2	2:D:175:ASN:O	2.20	0.41
2:E:128:ASN:O	2:E:129:PHE:CB	2.68	0.41
2:E:35:ASN:O	2:E:37:MET:N	2.53	0.41
2:G:144:ARG:O	2:G:145:ARG:CB	2.67	0.41
2:G:235:PRO:HA	2:G:249:PHE:O	2.21	0.41
2:I:14:ALA:O	2:I:16:ASP:N	2.53	0.41
2:J:239:ASN:ND2	2:J:246:THR:HG22	2.29	0.41
2:K:34:PHE:O	2:K:37:MET:HB3	2.20	0.41
2:L:151:THR:C	2:L:152:PHE:CD1	2.94	0.41
2:L:48:THR:O	2:L:56:ILE:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:6:SER:C	2:L:8:SER:N	2.73	0.41
2:M:153:HIS:NE2	2:N:153:HIS:CD2	2.88	0.41
2:M:253:ILE:HG13	2:N:234:PHE:CE1	2.55	0.41
2:M:6:SER:C	2:M:8:SER:N	2.73	0.41
2:N:239:ASN:ND2	2:N:246:THR:HG22	2.29	0.41
2:N:148:THR:OG1	2:N:332:GLU:HG2	2.20	0.41
2:O:4:LEU:O	2:O:5:TYR:C	2.58	0.41
1:A:414:VAL:C	1:A:416:ASN:H	2.22	0.41
1:A:163:ARG:NE	1:A:631:LEU:O	2.54	0.41
1:A:807:ASN:C	1:A:809:PHE:N	2.73	0.41
1:B:275:PRO:HB2	1:B:278:ILE:HD13	2.03	0.41
1:B:322:THR:HG22	1:B:390:ARG:HD3	2.02	0.41
1:B:449:ASN:ND2	1:B:455:PRO:HB3	2.36	0.41
1:B:743:ASP:OD2	1:B:745:ALA:CA	2.68	0.41
1:B:776:ALA:O	1:B:777:LYS:C	2.58	0.41
2:C:153:HIS:CD2	2:E:153:HIS:CE1	3.08	0.41
2:C:253:ILE:HG13	2:D:234:PHE:CE1	2.55	0.41
2:D:14:ALA:C	2:D:18:ILE:HD12	2.41	0.41
2:D:34:PHE:O	2:D:37:MET:HB3	2.20	0.41
2:F:6:SER:C	2:F:8:SER:N	2.73	0.41
2:G:35:ASN:O	2:G:37:MET:N	2.54	0.41
2:J:149:GLY:C	2:J:150:PHE:CD1	2.94	0.41
2:M:35:ASN:O	2:M:37:MET:N	2.53	0.41
2:M:66:LEU:O	2:M:67:GLY:C	2.58	0.41
2:N:78:VAL:O	2:N:81:ALA:N	2.39	0.41
2:O:61:PHE:N	2:O:61:PHE:CD1	2.87	0.41
2:O:74:ASP:O	2:O:75:ALA:C	2.58	0.41
1:A:542:GLN:N	1:A:542:GLN:OE1	2.53	0.41
1:B:191:LYS:HD3	1:B:191:LYS:HA	1.90	0.41
1:B:735:LEU:CG	1:B:760:VAL:O	2.59	0.41
1:B:807:ASN:C	1:B:809:PHE:H	2.23	0.41
1:B:812:VAL:C	1:B:814:ASN:H	2.23	0.41
2:D:227:PRO:O	2:D:228:ASP:HB2	2.20	0.41
2:D:253:ILE:HG13	2:E:234:PHE:CE1	2.55	0.41
2:D:74:ASP:O	2:D:75:ALA:C	2.59	0.41
2:D:6:SER:C	2:D:8:SER:N	2.73	0.41
2:G:11:LEU:HA	2:G:14:ALA:HB3	2.02	0.41
2:G:34:PHE:O	2:G:37:MET:HB3	2.20	0.41
2:H:34:PHE:O	2:H:37:MET:HB3	2.20	0.41
2:H:9:LYS:HE3	2:H:13:ASP:OD1	2.20	0.41
2:L:9:LYS:HE3	2:L:13:ASP:OD1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:74:ASP:O	2:N:75:ALA:C	2.58	0.41
2:O:53:ASN:HD22	2:O:354:ALA:HB3	1.86	0.41
1:A:855:LEU:O	1:A:856:ALA:C	2.56	0.41
1:B:190:ASN:HB2	1:B:199:VAL:CG2	2.50	0.41
1:B:270:ILE:HG23	1:B:854:LEU:HD21	2.03	0.41
1:B:493:LEU:CD1	1:B:567:HIS:HB2	2.50	0.41
1:B:712:LEU:HG	1:B:721:VAL:O	2.19	0.41
1:B:786:ILE:O	1:B:787:VAL:C	2.59	0.41
2:D:239:ASN:ND2	2:D:246:THR:HG22	2.29	0.41
2:I:239:ASN:ND2	2:I:246:THR:HG22	2.30	0.41
2:I:235:PRO:HA	2:I:249:PHE:O	2.21	0.41
2:I:3:VAL:O	2:I:4:LEU:C	2.57	0.41
2:I:253:ILE:HG13	2:J:234:PHE:CE1	2.55	0.41
2:J:59:TRP:N	2:J:59:TRP:CD1	2.86	0.41
2:I:234:PHE:CE1	2:K:253:ILE:HG13	2.55	0.41
2:O:14:ALA:O	2:O:16:ASP:N	2.52	0.41
1:A:178:PRO:CD	1:A:256:PHE:HE2	2.32	0.41
1:A:345:GLN:HG3	1:A:349:MET:CE	2.51	0.41
1:A:396:PHE:CD2	1:A:578:LEU:HD11	2.56	0.41
1:A:405:ILE:O	1:A:408:MET:HB2	2.21	0.41
1:A:304:LEU:H	1:A:615:ASN:ND2	2.19	0.41
1:A:679:LEU:O	1:A:681:ILE:N	2.54	0.41
1:B:136:ALA:O	1:B:137:ASN:HB3	2.21	0.41
1:B:166:PHE:CE2	1:B:689:MET:CA	2.99	0.41
1:B:178:PRO:CD	1:B:256:PHE:CE2	3.04	0.41
1:B:515:ARG:O	1:B:515:ARG:HG3	2.21	0.41
1:B:521:MET:SD	1:B:521:MET:N	2.94	0.41
1:B:552:TYR:O	1:B:553:ASN:C	2.58	0.41
2:C:61:PHE:CD1	2:C:61:PHE:N	2.89	0.41
2:C:6:SER:C	2:C:8:SER:N	2.74	0.41
2:D:124:PHE:CD1	2:D:124:PHE:N	2.89	0.41
2:G:227:PRO:O	2:G:228:ASP:HB2	2.20	0.41
2:F:253:ILE:HG13	2:G:234:PHE:CE1	2.55	0.41
2:J:11:LEU:HA	2:J:14:ALA:HB3	2.03	0.41
2:J:14:ALA:O	2:J:18:ILE:HD12	2.21	0.41
2:K:110:ALA:HB1	2:K:111:PRO:CD	2.50	0.41
2:L:21:GLY:O	2:L:22:THR:O	2.38	0.41
2:M:235:PRO:HA	2:M:249:PHE:O	2.21	0.41
2:O:35:ASN:O	2:O:37:MET:N	2.53	0.41
1:A:120:THR:HB	1:A:121:LYS:H	1.66	0.41
1:A:310:LEU:HD11	1:A:614:TYR:OH	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:ILE:HG13	1:A:503:ILE:H	1.72	0.41
1:A:701:GLN:CB	1:A:826:TYR:HD2	2.33	0.41
1:B:252:PHE:O	1:B:253:ASN:C	2.59	0.41
1:B:286:LEU:O	1:B:287:ASN:ND2	2.54	0.41
1:B:721:VAL:HG12	1:B:799:LEU:HD21	1.98	0.41
2:C:100:MET:HG3	2:C:388:VAL:HG11	2.01	0.41
2:C:145:ARG:CB	2:C:145:ARG:NH1	2.79	0.41
2:D:9:LYS:HE3	2:D:13:ASP:OD1	2.21	0.41
2:G:14:ALA:O	2:G:16:ASP:N	2.54	0.41
2:H:235:PRO:HA	2:H:249:PHE:O	2.21	0.41
2:H:6:SER:C	2:H:8:SER:N	2.74	0.41
2:I:153:HIS:CD2	2:K:153:HIS:CE1	3.08	0.41
2:J:136:ILE:HD12	2:J:139:TRP:HB3	2.03	0.41
2:L:23:LEU:HD22	2:L:72:ASN:OD1	2.21	0.41
2:L:150:PHE:O	2:L:330:VAL:HG13	2.20	0.41
2:L:35:ASN:OD1	2:L:65:LEU:HD22	2.21	0.41
2:M:124:PHE:CD1	2:M:124:PHE:N	2.89	0.41
2:M:168:ARG:HD2	2:M:175:ASN:O	2.20	0.41
2:L:253:ILE:HG13	2:M:234:PHE:CE1	2.55	0.41
2:N:7:LEU:H	2:N:7:LEU:HG	1.54	0.41
2:O:168:ARG:HD2	2:O:175:ASN:O	2.20	0.41
1:A:374:ALA:HB1	1:A:580:SER:HA	2.02	0.41
1:A:472:LEU:N	1:A:472:LEU:HD23	2.36	0.41
1:A:368:THR:HG23	1:A:579:THR:O	2.21	0.41
1:A:782:VAL:CG2	1:A:798:ILE:HD11	2.51	0.41
1:A:862:THR:HG22	1:A:863:VAL:N	2.36	0.41
1:B:349:MET:HB2	1:B:349:MET:HE2	1.88	0.41
1:B:489:LEU:C	1:B:489:LEU:HD23	2.41	0.41
2:D:235:PRO:HA	2:D:249:PHE:O	2.21	0.41
2:F:135:TYR:CZ	2:F:342:MET:HE3	2.56	0.41
2:F:9:LYS:HE3	2:F:13:ASP:OD1	2.21	0.41
2:I:106:ARG:HG2	2:I:107:ASN:H	1.84	0.41
2:J:9:LYS:HE3	2:J:13:ASP:OD1	2.21	0.41
2:J:27:VAL:O	2:J:28:SER:C	2.57	0.41
2:I:72:ASN:CG	2:K:126:ARG:NH1	2.74	0.41
2:L:1:MET:O	2:L:2:ASP:C	2.59	0.41
2:L:4:LEU:O	2:L:5:TYR:C	2.59	0.41
2:O:147:ARG:O	2:O:148:THR:CB	2.66	0.41
2:O:152:PHE:CD1	2:O:152:PHE:N	2.89	0.41
2:O:34:PHE:O	2:O:35:ASN:C	2.59	0.41
1:A:202:SER:O	1:A:205:ALA:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:ASN:HD21	1:A:869:VAL:H	1.69	0.41
1:A:382:LEU:HD12	1:A:382:LEU:HA	1.60	0.41
1:A:552:TYR:O	1:A:553:ASN:C	2.59	0.41
1:A:601:PHE:CD1	1:A:601:PHE:N	2.80	0.41
1:A:622:VAL:O	1:A:623:ALA:C	2.59	0.41
1:A:756:PRO:C	1:A:757:VAL:CG2	2.89	0.41
1:A:287:ASN:O	1:A:858:VAL:HA	2.20	0.41
1:B:159:ASP:OD2	1:B:761:GLY:CA	2.69	0.41
1:B:492:VAL:O	1:B:493:LEU:O	2.38	0.41
1:B:763:LEU:HD23	1:B:763:LEU:HA	1.80	0.41
1:B:771:VAL:O	1:B:775:ILE:HD13	2.21	0.41
1:B:791:LYS:O	1:B:792:VAL:CG1	2.66	0.41
2:C:33:GLN:O	2:C:36:GLN:HB3	2.21	0.41
2:D:128:ASN:HD22	2:E:19:VAL:CG2	2.34	0.41
2:D:31:ILE:O	2:D:32:GLN:C	2.59	0.41
2:E:23:LEU:HD22	2:E:25:SER:OG	2.21	0.41
2:F:24:TYR:C	2:F:26:ASN:H	2.24	0.41
2:H:91:PHE:O	2:H:95:VAL:HG23	2.21	0.41
2:I:9:LYS:HE3	2:I:13:ASP:OD1	2.20	0.41
2:I:227:PRO:O	2:I:228:ASP:HB2	2.20	0.41
2:I:397:LYS:HZ1	2:K:150:PHE:HA	1.86	0.41
2:J:168:ARG:HD2	2:J:175:ASN:O	2.20	0.41
2:L:14:ALA:O	2:L:16:ASP:N	2.54	0.41
2:L:26:ASN:OD1	2:N:33:GLN:HB2	2.21	0.41
2:N:124:PHE:C	2:N:126:ARG:H	2.24	0.41
2:O:23:LEU:CG	2:O:24:TYR:N	2.83	0.41
2:O:5:TYR:CE2	2:O:131:ASN:HA	2.55	0.41
1:A:609:ASN:O	1:A:610:PHE:C	2.59	0.41
1:A:726:ASN:HD22	1:A:726:ASN:HA	1.60	0.41
1:A:763:LEU:HA	1:A:764:PRO:HD3	1.68	0.41
1:A:771:VAL:HG12	1:A:809:PHE:CB	2.51	0.41
1:B:207:ILE:HG13	1:B:207:ILE:H	1.62	0.41
1:B:229:ARG:HD2	1:B:230:GLN:NE2	2.31	0.41
1:B:288:MET:HE1	1:B:288:MET:HA	2.02	0.41
1:B:379:PHE:O	1:B:380:LYS:C	2.59	0.41
1:B:411:LEU:HA	1:B:411:LEU:HD23	1.83	0.41
1:B:451:ASP:N	1:B:452:PRO:CD	2.82	0.41
1:B:415:PRO:HB3	1:B:480:PHE:HB2	2.01	0.41
1:B:672:LEU:O	1:B:673:PRO:O	2.38	0.41
2:C:5:TYR:HE2	2:C:130:ASP:O	2.04	0.41
2:C:204:ASN:HB3	2:C:296:ARG:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:67:GLY:C	2:C:69:THR:N	2.72	0.41
2:D:204:ASN:HB3	2:D:296:ARG:HB3	2.03	0.41
2:D:34:PHE:O	2:D:35:ASN:C	2.59	0.41
2:F:74:ASP:O	2:F:75:ALA:C	2.59	0.41
2:H:123:LYS:HG3	2:H:124:PHE:CD1	2.56	0.41
2:H:14:ALA:O	2:H:16:ASP:N	2.54	0.41
2:J:27:VAL:O	2:J:31:ILE:HG12	2.20	0.41
2:I:16:ASP:HB3	2:K:131:ASN:C	2.42	0.41
2:K:235:PRO:HA	2:K:249:PHE:O	2.21	0.41
2:L:42:ASN:CB	2:L:62:ASP:HA	2.51	0.41
2:N:235:PRO:HA	2:N:249:PHE:O	2.21	0.41
2:N:34:PHE:O	2:N:35:ASN:C	2.59	0.41
1:A:594:ILE:HA	1:A:595:PRO:HD3	1.86	0.40
1:B:401:TYR:N	1:B:401:TYR:CD1	2.74	0.40
1:B:743:ASP:OD1	1:B:744:TYR:N	2.53	0.40
1:B:747:ILE:H	1:B:747:ILE:HG22	1.51	0.40
1:B:854:LEU:HD22	1:B:855:LEU:N	2.36	0.40
1:B:869:VAL:HG13	1:B:873:ASN:CA	2.51	0.40
2:D:144:ARG:O	2:D:145:ARG:CB	2.65	0.40
2:D:38:ILE:HG13	2:D:38:ILE:H	1.57	0.40
2:E:235:PRO:HA	2:E:249:PHE:O	2.21	0.40
2:H:34:PHE:O	2:H:35:ASN:C	2.60	0.40
2:I:116:LEU:O	2:I:119:LEU:N	2.50	0.40
2:I:11:LEU:HA	2:I:14:ALA:HB3	2.02	0.40
2:J:110:ALA:CB	2:J:111:PRO:CD	2.96	0.40
2:J:126:ARG:NH1	2:K:72:ASN:ND2	2.69	0.40
2:J:133:SER:O	2:J:134:GLU:C	2.59	0.40
2:J:355:ILE:HA	2:J:356:PRO:HD3	1.96	0.40
2:I:144:ARG:HD2	2:J:82:ARG:CZ	2.51	0.40
2:K:38:ILE:H	2:K:38:ILE:HG13	1.58	0.40
2:L:131:ASN:HD22	2:L:131:ASN:N	2.19	0.40
2:L:234:PHE:CE1	2:N:253:ILE:HG13	2.55	0.40
1:A:200:VAL:O	1:A:201:ASP:HB3	2.21	0.40
1:A:249:ASP:O	1:A:250:TYR:C	2.60	0.40
1:A:264:PRO:O	1:A:265:LEU:HB2	2.22	0.40
1:A:283:ASN:ND2	1:A:869:VAL:H	2.18	0.40
1:A:594:ILE:HG23	1:A:595:PRO:N	2.36	0.40
1:A:714:ARG:O	1:A:715:ASP:C	2.59	0.40
1:A:785:GLN:HB2	1:A:786:ILE:H	1.60	0.40
1:A:793:ASP:OD1	1:A:793:ASP:N	2.54	0.40
1:B:224:PHE:HE1	2:O:70:LEU:C	2.24	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:543:LEU:O	1:B:544:VAL:C	2.58	0.40
1:B:558:MET:O	1:B:559:ALA:C	2.60	0.40
1:B:150:LEU:CD1	1:B:696:SER:HA	2.50	0.40
1:B:847:THR:HG22	1:B:847:THR:O	2.20	0.40
2:D:214:LEU:N	2:D:214:LEU:HD23	2.36	0.40
2:E:65:LEU:C	2:E:66:LEU:HG	2.42	0.40
2:E:91:PHE:O	2:E:95:VAL:HG23	2.22	0.40
2:F:65:LEU:HB3	2:F:66:LEU:H	1.69	0.40
2:G:104:SER:O	2:G:108:GLY:HA2	2.21	0.40
2:H:152:PHE:HB3	2:H:337:ASP:CB	2.51	0.40
2:H:65:LEU:O	2:H:66:LEU:HD23	2.22	0.40
2:I:204:ASN:HB3	2:I:296:ARG:HB3	2.03	0.40
2:L:153:HIS:CE1	2:M:153:HIS:CD2	3.09	0.40
1:A:338:GLU:O	1:A:339:LEU:HG	2.22	0.40
1:A:362:SER:HA	1:A:365:GLN:HE21	1.87	0.40
1:A:451:ASP:O	1:A:452:PRO:O	2.39	0.40
1:A:506:LEU:HD21	1:A:544:VAL:N	2.36	0.40
1:A:542:GLN:HA	1:A:545:ASP:OD2	2.20	0.40
1:A:707:TYR:H	1:A:707:TYR:HD1	1.69	0.40
1:A:715:ASP:O	1:A:718:TYR:O	2.39	0.40
1:B:497:ILE:HG23	2:I:68:THR:CG2	2.52	0.40
1:B:622:VAL:O	1:B:623:ALA:C	2.59	0.40
1:B:743:ASP:OD2	1:B:745:ALA:N	2.54	0.40
2:C:214:LEU:HD23	2:C:214:LEU:N	2.37	0.40
2:E:136:ILE:HD12	2:E:139:TRP:HB3	2.04	0.40
2:F:155:PRO:O	2:F:186:SER:HB3	2.21	0.40
2:F:14:ALA:O	2:F:16:ASP:N	2.54	0.40
2:F:204:ASN:HB3	2:F:296:ARG:HB3	2.03	0.40
2:G:4:LEU:O	2:G:5:TYR:C	2.59	0.40
2:H:23:LEU:H	2:H:26:ASN:HD21	1.67	0.40
2:I:145:ARG:NH1	2:I:145:ARG:CB	2.65	0.40
2:J:124:PHE:O	2:J:126:ARG:N	2.54	0.40
2:K:48:THR:O	2:K:56:ILE:HA	2.20	0.40
2:K:88:PHE:O	2:K:91:PHE:HB3	2.22	0.40
2:M:131:ASN:ND2	2:M:131:ASN:N	2.70	0.40
2:M:11:LEU:HA	2:M:14:ALA:HB3	2.04	0.40
2:M:204:ASN:HB3	2:M:296:ARG:HB3	2.04	0.40
2:O:204:ASN:HB3	2:O:296:ARG:HB3	2.03	0.40
2:O:9:LYS:HE3	2:O:13:ASP:OD1	2.21	0.40
1:A:154:THR:O	1:A:155:LEU:C	2.59	0.40
1:A:304:LEU:N	1:A:615:ASN:ND2	2.67	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:LEU:HD22	1:A:536:LEU:N	2.36	0.40
1:A:657:VAL:HA	1:A:658:PRO:HD3	1.64	0.40
1:A:163:ARG:NH2	1:A:736:GLU:OE1	2.52	0.40
1:A:854:LEU:HD22	1:A:855:LEU:H	1.86	0.40
1:B:190:ASN:HB3	1:B:197:GLY:O	2.21	0.40
1:B:239:VAL:HG21	1:B:845:ASN:O	2.21	0.40
1:B:244:ILE:O	1:B:244:ILE:HG23	2.22	0.40
1:B:639:LYS:O	1:B:641:ILE:N	2.55	0.40
1:B:804:SER:O	1:B:805:ASP:HB2	2.22	0.40
1:B:870:ALA:C	1:B:872:ASP:H	2.21	0.40
2:D:11:LEU:HA	2:D:14:ALA:HB3	2.03	0.40
2:D:124:PHE:O	2:D:126:ARG:N	2.54	0.40
2:F:11:LEU:HB2	2:F:395:LEU:HD21	2.04	0.40
2:H:108:GLY:C	2:H:110:ALA:N	2.75	0.40
2:I:31:ILE:O	2:I:32:GLN:C	2.59	0.40
2:K:11:LEU:HA	2:K:14:ALA:HB3	2.03	0.40
2:K:133:SER:O	2:K:134:GLU:C	2.60	0.40
2:L:59:TRP:CD1	2:L:59:TRP:N	2.88	0.40
2:M:31:ILE:O	2:M:32:GLN:C	2.60	0.40
2:N:91:PHE:O	2:N:95:VAL:HG23	2.21	0.40
2:O:100:MET:HG3	2:O:388:VAL:CG1	2.51	0.40
2:O:144:ARG:O	2:O:145:ARG:CG	2.69	0.40
2:O:34:PHE:O	2:O:37:MET:HB3	2.21	0.40
1:A:131:LEU:HA	1:A:132:PRO:HD3	1.90	0.40
1:A:303:LEU:HA	1:A:615:ASN:HD21	1.82	0.40
1:A:359:THR:HG22	1:A:359:THR:O	2.22	0.40
1:A:421:ARG:C	1:A:423:SER:H	2.25	0.40
1:A:510:LEU:HA	1:A:513:LEU:CD1	2.51	0.40
1:A:536:LEU:CD2	1:A:536:LEU:N	2.85	0.40
1:A:815:TYR:CD1	1:A:815:TYR:N	2.85	0.40
1:B:373:GLN:O	1:B:374:ALA:C	2.59	0.40
1:B:477:ASN:C	1:B:479:GLN:N	2.75	0.40
1:B:556:THR:HG22	1:B:557:LEU:N	2.36	0.40
1:B:746:GLN:O	1:B:750:MET:HG3	2.21	0.40
1:B:87:GLN:C	1:B:89:GLU:H	2.25	0.40
2:C:14:ALA:O	2:C:18:ILE:HD12	2.21	0.40
2:D:128:ASN:O	2:D:129:PHE:HB3	2.21	0.40
2:D:378:ARG:O	2:D:382:LEU:HB2	2.22	0.40
2:E:100:MET:HG3	2:E:388:VAL:HG11	2.04	0.40
2:F:235:PRO:HA	2:F:249:PHE:O	2.21	0.40
2:G:131:ASN:N	2:G:131:ASN:HD22	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:34:PHE:O	2:G:35:ASN:C	2.60	0.40
2:K:116:LEU:O	2:K:119:LEU:N	2.50	0.40
2:K:204:ASN:HB3	2:K:296:ARG:HB3	2.04	0.40
2:L:355:ILE:HA	2:L:356:PRO:HD3	1.96	0.40
2:L:74:ASP:O	2:L:75:ALA:C	2.59	0.40
2:M:4:LEU:O	2:M:5:TYR:C	2.58	0.40
2:O:101:VAL:HG23	2:O:102:ARG:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	779/880 (88%)	431 (55%)	199 (26%)	149 (19%)	0	2
1	B	808/880 (92%)	458 (57%)	204 (25%)	146 (18%)	0	3
2	C	395/397 (100%)	318 (80%)	54 (14%)	23 (6%)	2	27
2	D	395/397 (100%)	315 (80%)	50 (13%)	30 (8%)	1	19
2	E	395/397 (100%)	323 (82%)	49 (12%)	23 (6%)	2	27
2	F	395/397 (100%)	324 (82%)	47 (12%)	24 (6%)	2	25
2	G	395/397 (100%)	323 (82%)	49 (12%)	23 (6%)	2	27
2	H	395/397 (100%)	323 (82%)	50 (13%)	22 (6%)	2	27
2	I	395/397 (100%)	320 (81%)	51 (13%)	24 (6%)	2	25
2	J	395/397 (100%)	320 (81%)	53 (13%)	22 (6%)	2	27
2	K	395/397 (100%)	318 (80%)	52 (13%)	25 (6%)	1	25
2	L	395/397 (100%)	322 (82%)	47 (12%)	26 (7%)	1	24
2	M	395/397 (100%)	322 (82%)	52 (13%)	21 (5%)	2	29
2	N	395/397 (100%)	317 (80%)	50 (13%)	28 (7%)	1	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	O	395/397 (100%)	317 (80%)	47 (12%)	31 (8%)	1	19
All	All	6722/6921 (97%)	5051 (75%)	1054 (16%)	617 (9%)	1	15

All (617) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	LYS
1	A	130	GLN
1	A	193	SER
1	A	198	LYS
1	A	220	ALA
1	A	234	ALA
1	A	246	HIS
1	A	252	PHE
1	A	260	GLN
1	A	275	PRO
1	A	283	ASN
1	A	287	ASN
1	A	306	ASP
1	A	315	GLU
1	A	338	GLU
1	A	340	VAL
1	A	356	GLU
1	A	358	LEU
1	A	370	ILE
1	A	413	VAL
1	A	443	GLN
1	A	446	HIS
1	A	451	ASP
1	A	452	PRO
1	A	453	GLN
1	A	484	VAL
1	A	485	ILE
1	A	488	VAL
1	A	489	LEU
1	A	501	HIS
1	A	523	VAL
1	A	558	MET
1	A	564	ASN
1	A	570	THR
1	A	573	THR
1	A	585	CYS

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Mol	Chain	Res	Type
1	A	650	HIS
1	A	651	ILE
1	A	660	ASP
1	A	661	GLN
1	A	689	MET
1	A	701	GLN
1	A	715	ASP
1	A	743	ASP
1	A	745	ALA
1	A	770	SER
1	A	771	VAL
1	A	772	ILE
1	A	781	THR
1	A	782	VAL
1	A	785	GLN
1	A	786	ILE
1	A	808	ASP
1	A	811	LEU
1	A	814	ASN
1	A	828	GLN
1	A	854	LEU
1	A	855	LEU
1	A	856	ALA
1	A	857	PHE
1	B	191	LYS
1	B	194	ARG
1	B	195	ASP
1	B	196	ALA
1	B	200	VAL
1	B	215	GLU
1	B	218	GLU
1	B	226	ALA
1	B	227	GLU
1	B	252	PHE
1	B	306	ASP
1	B	355	LEU
1	B	361	GLN
1	B	369	GLY
1	B	400	ASN
1	B	417	ASP
1	B	446	HIS
1	B	447	TYR

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Mol	Chain	Res	Type
1	B	451	ASP
1	B	457	GLN
1	B	458	ILE
1	B	479	GLN
1	B	481	ARG
1	B	503	ILE
1	B	504	ASN
1	B	574	GLU
1	B	585	CYS
1	B	634	TYR
1	B	640	ALA
1	B	651	ILE
1	B	655	ALA
1	B	673	PRO
1	B	699	ILE
1	B	702	GLY
1	B	724	ALA
1	B	764	PRO
1	B	765	PHE
1	B	777	LYS
1	B	782	VAL
1	B	785	GLN
1	B	786	ILE
1	B	790	ARG
1	B	792	VAL
1	B	805	ASP
1	B	806	SER
1	B	855	LEU
1	B	856	ALA
1	B	875	ARG
2	C	22	THR
2	C	70	LEU
2	C	134	GLU
2	D	25	SER
2	D	70	LEU
2	D	126	ARG
2	D	128	ASN
2	D	134	GLU
2	D	148	THR
2	E	22	THR
2	E	25	SER
2	E	106	ARG

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Mol	Chain	Res	Type
2	E	134	GLU
2	F	22	THR
2	F	62	ASP
2	F	70	LEU
2	F	105	GLN
2	F	134	GLU
2	F	145	ARG
2	F	148	THR
2	G	20	GLU
2	G	22	THR
2	G	134	GLU
2	G	148	THR
2	H	22	THR
2	H	107	ASN
2	H	134	GLU
2	I	25	SER
2	I	62	ASP
2	I	134	GLU
2	I	148	THR
2	J	20	GLU
2	J	70	LEU
2	J	106	ARG
2	J	134	GLU
2	K	22	THR
2	K	70	LEU
2	K	126	ARG
2	K	128	ASN
2	K	134	GLU
2	K	148	THR
2	L	22	THR
2	L	62	ASP
2	L	126	ARG
2	L	134	GLU
2	L	145	ARG
2	L	148	THR
2	M	22	THR
2	M	25	SER
2	M	128	ASN
2	M	134	GLU
2	N	22	THR
2	N	25	SER
2	N	70	LEU

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Mol	Chain	Res	Type
2	N	128	ASN
2	N	134	GLU
2	N	148	THR
2	O	65	LEU
2	O	68	THR
2	O	70	LEU
2	O	134	GLU
2	O	145	ARG
2	O	148	THR
1	A	143	ARG
1	A	202	SER
1	A	215	GLU
1	A	219	GLY
1	A	226	ALA
1	A	227	GLU
1	A	253	ASN
1	A	264	PRO
1	A	307	ARG
1	A	336	LEU
1	A	352	ASP
1	A	369	GLY
1	A	415	PRO
1	A	438	PRO
1	A	441	GLY
1	A	458	ILE
1	A	465	ASN
1	A	503	ILE
1	A	559	ALA
1	A	571	LEU
1	A	590	ASN
1	A	608	VAL
1	A	630	ARG
1	A	654	VAL
1	A	680	ASP
1	A	739	MET
1	A	804	SER
1	A	815	TYR
1	A	823	THR
1	A	847	THR
1	A	866	ILE
1	B	73	LEU
1	B	141	GLU

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Mol	Chain	Res	Type
1	B	142	LEU
1	B	212	PHE
1	B	230	GLN
1	B	253	ASN
1	B	261	LEU
1	B	264	PRO
1	B	265	LEU
1	B	278	ILE
1	B	282	VAL
1	B	283	ASN
1	B	307	ARG
1	B	313	ASN
1	B	338	GLU
1	B	388	SER
1	B	436	ILE
1	B	438	PRO
1	B	443	GLN
1	B	452	PRO
1	B	465	ASN
1	B	478	ASN
1	B	487	GLY
1	B	488	VAL
1	B	489	LEU
1	B	493	LEU
1	B	496	ASN
1	B	500	GLY
1	B	520	THR
1	B	524	ASP
1	B	608	VAL
1	B	631	LEU
1	B	637	LYS
1	B	638	MET
1	B	654	VAL
1	B	674	VAL
1	B	676	VAL
1	B	787	VAL
1	B	854	LEU
2	C	7	LEU
2	C	20	GLU
2	C	25	SER
2	C	62	ASP
2	C	106	ARG

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Mol	Chain	Res	Type
2	C	130	ASP
2	C	148	THR
2	D	7	LEU
2	D	20	GLU
2	D	42	ASN
2	D	65	LEU
2	D	67	GLY
2	D	69	THR
2	D	72	ASN
2	D	90	ASP
2	D	106	ARG
2	D	147	ARG
2	E	7	LEU
2	E	62	ASP
2	E	90	ASP
2	E	126	ARG
2	E	128	ASN
2	E	130	ASP
2	E	148	THR
2	F	7	LEU
2	F	25	SER
2	F	128	ASN
2	G	7	LEU
2	G	25	SER
2	G	125	LYS
2	G	126	ARG
2	H	7	LEU
2	H	25	SER
2	H	42	ASN
2	H	51	ILE
2	H	62	ASP
2	H	68	THR
2	H	109	ILE
2	H	128	ASN
2	I	7	LEU
2	I	90	ASP
2	I	125	LYS
2	I	147	ARG
2	J	7	LEU
2	J	51	ILE
2	J	62	ASP
2	J	90	ASP

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Mol	Chain	Res	Type
2	J	126	ARG
2	J	128	ASN
2	J	130	ASP
2	K	7	LEU
2	K	20	GLU
2	K	62	ASP
2	K	106	ARG
2	K	125	LYS
2	L	7	LEU
2	L	25	SER
2	L	69	THR
2	L	72	ASN
2	L	106	ARG
2	L	128	ASN
2	L	147	ARG
2	M	7	LEU
2	M	42	ASN
2	M	90	ASP
2	N	7	LEU
2	N	42	ASN
2	N	62	ASP
2	N	65	LEU
2	N	90	ASP
2	N	145	ARG
2	O	7	LEU
2	O	22	THR
2	O	25	SER
2	O	62	ASP
2	O	90	ASP
2	O	105	GLN
1	A	137	ASN
1	A	142	LEU
1	A	218	GLU
1	A	254	GLU
1	A	265	LEU
1	A	276	GLU
1	A	496	ASN
1	A	497	ILE
1	A	521	MET
1	A	525	TYR
1	A	579	THR
1	A	597	PRO

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Mol	Chain	Res	Type
1	A	648	ARG
1	A	658	PRO
1	A	676	VAL
1	A	687	MET
1	A	696	SER
1	A	773	SER
1	A	816	ASP
1	A	849	THR
1	B	237	ASN
1	B	254	GLU
1	B	273	TYR
1	B	359	THR
1	B	387	LEU
1	B	421	ARG
1	B	549	LEU
1	B	579	THR
1	B	581	VAL
1	B	590	ASN
1	B	635	GLN
1	B	656	ARG
1	B	670	ARG
1	B	675	GLU
1	B	794	THR
1	B	849	THR
2	C	13	ASP
2	C	42	ASN
2	C	69	THR
2	C	90	ASP
2	C	126	ARG
2	D	13	ASP
2	D	32	GLN
2	D	62	ASP
2	D	68	THR
2	D	125	LYS
2	E	13	ASP
2	E	32	GLN
2	E	70	LEU
2	F	13	ASP
2	F	32	GLN
2	F	90	ASP
2	F	126	ARG
2	F	130	ASP

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Mol	Chain	Res	Type
2	G	13	ASP
2	G	32	GLN
2	G	42	ASN
2	G	90	ASP
2	G	128	ASN
2	H	13	ASP
2	H	32	GLN
2	H	90	ASP
2	I	13	ASP
2	I	32	GLN
2	I	126	ARG
2	I	128	ASN
2	I	146	GLN
2	J	13	ASP
2	J	42	ASN
2	K	13	ASP
2	K	25	SER
2	K	32	GLN
2	K	90	ASP
2	K	111	PRO
2	L	13	ASP
2	L	20	GLU
2	L	41	MET
2	L	90	ASP
2	L	125	LYS
2	M	13	ASP
2	M	106	ARG
2	N	13	ASP
2	N	67	GLY
2	N	106	ARG
2	N	125	LYS
2	N	155	PRO
2	O	20	GLU
2	O	24	TYR
2	O	32	GLN
2	O	42	ASN
2	O	73	LEU
2	O	106	ARG
2	O	126	ARG
2	O	155	PRO
1	A	131	LEU
1	A	144	ASN

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Mol	Chain	Res	Type
1	A	155	LEU
1	A	187	ALA
1	A	195	ASP
1	A	206	SER
1	A	212	PHE
1	A	299	ILE
1	A	333	VAL
1	A	372	SER
1	A	387	LEU
1	A	457	GLN
1	A	518	PHE
1	A	524	ASP
1	A	549	LEU
1	A	552	TYR
1	A	557	LEU
1	A	581	VAL
1	A	700	ALA
1	A	730	PHE
1	A	853	ASP
1	A	877	MET
1	B	85	GLU
1	B	101	LYS
1	B	185	ASP
1	B	193	SER
1	B	206	SER
1	B	294	SER
1	B	302	ASN
1	B	372	SER
1	B	442	MET
1	B	466	PHE
1	B	483	VAL
1	B	552	TYR
1	B	564	ASN
1	B	597	PRO
1	B	639	LYS
1	B	680	ASP
1	B	731	GLN
2	C	32	GLN
2	C	38	ILE
2	C	89	VAL
2	D	38	ILE
2	D	41	MET

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Mol	Chain	Res	Type
2	D	89	VAL
2	D	123	LYS
2	D	145	ARG
2	E	38	ILE
2	F	20	GLU
2	F	38	ILE
2	F	42	ASN
2	G	38	ILE
2	G	130	ASP
2	G	145	ARG
2	H	36	GLN
2	H	38	ILE
2	H	89	VAL
2	H	106	ARG
2	I	36	GLN
2	I	38	ILE
2	I	42	ASN
2	I	89	VAL
2	I	145	ARG
2	J	32	GLN
2	J	36	GLN
2	J	38	ILE
2	J	89	VAL
2	K	9	LYS
2	K	36	GLN
2	K	38	ILE
2	K	89	VAL
2	L	32	GLN
2	L	36	GLN
2	L	38	ILE
2	M	20	GLU
2	M	32	GLN
2	M	38	ILE
2	M	55	PRO
2	M	89	VAL
2	M	126	ARG
2	N	20	GLU
2	N	32	GLN
2	N	36	GLN
2	N	38	ILE
2	N	89	VAL
2	N	126	ARG

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Mol	Chain	Res	Type
2	O	13	ASP
2	O	38	ILE
2	O	89	VAL
2	O	128	ASN
1	A	152	LYS
1	A	196	ALA
1	A	351	GLN
1	B	86	ILE
1	B	103	SER
1	B	207	ILE
1	B	277	ARG
1	B	399	THR
1	B	416	ASN
1	B	437	TYR
1	B	827	LYS
2	C	36	GLN
2	C	145	ARG
2	D	9	LYS
2	D	36	GLN
2	E	36	GLN
2	E	55	PRO
2	E	89	VAL
2	F	9	LYS
2	F	36	GLN
2	F	89	VAL
2	G	36	GLN
2	G	89	VAL
2	G	123	LYS
2	G	155	PRO
2	H	9	LYS
2	H	130	ASP
2	I	9	LYS
2	I	41	MET
2	J	125	LYS
2	K	42	ASN
2	K	130	ASP
2	L	9	LYS
2	L	65	LEU
2	L	89	VAL
2	M	36	GLN
2	M	41	MET
2	M	145	ARG

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Mol	Chain	Res	Type
2	N	9	LYS
2	N	69	THR
2	O	9	LYS
2	O	36	GLN
2	O	41	MET
1	A	207	ILE
1	A	422	GLU
1	A	622	VAL
1	A	733	ILE
1	A	819	PRO
1	B	521	MET
1	B	557	LEU
1	B	622	VAL
1	B	677	ARG
1	B	781	THR
1	B	857	PHE
2	C	3	VAL
2	E	9	LYS
2	E	20	GLU
2	E	42	ASN
2	F	55	PRO
2	G	3	VAL
2	G	9	LYS
2	I	123	LYS
2	J	3	VAL
2	J	9	LYS
2	J	69	THR
2	K	3	VAL
2	K	147	ARG
2	L	3	VAL
2	N	3	VAL
2	O	3	VAL
1	A	247	PRO
1	A	334	PRO
1	B	519	PRO
1	B	723	ILE
1	B	865	PRO
2	D	3	VAL
2	E	3	VAL
2	F	3	VAL
2	H	3	VAL
2	I	3	VAL

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Mol	Chain	Res	Type
2	M	3	VAL
1	A	502	VAL
1	A	606	VAL
1	B	415	PRO
2	E	78	VAL
2	I	78	VAL
2	I	101	VAL
2	L	78	VAL
2	N	78	VAL
1	A	405	ILE
1	A	699	ILE
1	B	128	PRO
1	B	370	ILE
1	B	405	ILE
1	B	413	VAL
2	C	78	VAL
2	F	78	VAL
2	H	78	VAL
2	J	78	VAL
2	K	78	VAL
2	M	78	VAL
2	M	101	VAL
2	N	101	VAL
2	O	51	ILE
2	O	78	VAL
2	O	101	VAL
1	A	500	GLY
1	B	435	ILE
1	B	606	VAL
2	C	67	GLY
2	D	78	VAL
2	G	78	VAL
1	A	787	VAL
1	B	246	HIS
1	B	544	VAL

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	715/809 (88%)	603 (84%)	112 (16%)	3	21
1	B	744/809 (92%)	635 (85%)	109 (15%)	3	24
2	C	350/350 (100%)	325 (93%)	25 (7%)	17	55
2	D	350/350 (100%)	322 (92%)	28 (8%)	14	50
2	E	350/350 (100%)	325 (93%)	25 (7%)	17	55
2	F	350/350 (100%)	327 (93%)	23 (7%)	19	57
2	G	350/350 (100%)	327 (93%)	23 (7%)	19	57
2	H	350/350 (100%)	329 (94%)	21 (6%)	22	60
2	I	350/350 (100%)	327 (93%)	23 (7%)	19	57
2	J	350/350 (100%)	327 (93%)	23 (7%)	19	57
2	K	350/350 (100%)	327 (93%)	23 (7%)	19	57
2	L	350/350 (100%)	321 (92%)	29 (8%)	13	49
2	M	350/350 (100%)	325 (93%)	25 (7%)	17	55
2	N	350/350 (100%)	324 (93%)	26 (7%)	16	53
2	O	350/350 (100%)	329 (94%)	21 (6%)	22	60
All	All	6009/6168 (97%)	5473 (91%)	536 (9%)	11	45

All (536) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	PRO
1	A	122	LEU
1	A	125	ILE
1	A	126	PHE
1	A	142	LEU
1	A	147	TYR
1	A	154	THR
1	A	157	ASP
1	A	169	LEU
1	A	180	TYR
1	A	193	SER
1	A	204	THR
1	A	215	GLU
1	A	216	GLU
1	A	229	ARG
1	A	230	GLN

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Mol	Chain	Res	Type
1	A	239	VAL
1	A	247	PRO
1	A	259	HIS
1	A	271	PHE
1	A	273	TYR
1	A	278	ILE
1	A	280	ASN
1	A	286	LEU
1	A	288	MET
1	A	295	THR
1	A	298	TYR
1	A	303	LEU
1	A	305	GLN
1	A	310	LEU
1	A	311	HIS
1	A	316	SER
1	A	318	TRP
1	A	342	THR
1	A	347	GLN
1	A	348	LYS
1	A	354	GLN
1	A	366	PHE
1	A	371	ASN
1	A	382	LEU
1	A	389	GLN
1	A	391	THR
1	A	392	MET
1	A	395	ASP
1	A	401	TYR
1	A	414	VAL
1	A	419	PHE
1	A	423	SER
1	A	424	LEU
1	A	428	GLN
1	A	436	ILE
1	A	443	GLN
1	A	445	MET
1	A	447	TYR
1	A	449	ASN
1	A	471	TRP
1	A	473	HIS
1	A	480	PHE

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Mol	Chain	Res	Type
1	A	495	ASP
1	A	505	GLN
1	A	515	ARG
1	A	516	GLN
1	A	520	THR
1	A	521	MET
1	A	525	TYR
1	A	534	LEU
1	A	540	LEU
1	A	563	MET
1	A	564	ASN
1	A	565	MET
1	A	571	LEU
1	A	587	LEU
1	A	594	ILE
1	A	600	LEU
1	A	601	PHE
1	A	616	GLU
1	A	634	TYR
1	A	638	MET
1	A	641	ILE
1	A	646	LEU
1	A	676	VAL
1	A	680	ASP
1	A	701	GLN
1	A	704	ILE
1	A	707	TYR
1	A	717	MET
1	A	718	TYR
1	A	720	TYR
1	A	723	ILE
1	A	726	ASN
1	A	730	PHE
1	A	743	ASP
1	A	744	TYR
1	A	747	ILE
1	A	753	ASN
1	A	759	LEU
1	A	765	PHE
1	A	771	VAL
1	A	775	ILE
1	A	782	VAL

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Mol	Chain	Res	Type
1	A	793	ASP
1	A	798	ILE
1	A	799	LEU
1	A	802	ILE
1	A	816	ASP
1	A	829	VAL
1	A	837	ASN
1	A	839	MET
1	A	848	PHE
1	A	849	THR
1	A	861	ASP
1	A	872	ASP
1	B	74	GLU
1	B	126	PHE
1	B	134	TYR
1	B	135	ARG
1	B	153	ASP
1	B	157	ASP
1	B	169	LEU
1	B	180	TYR
1	B	182	LEU
1	B	190	ASN
1	B	194	ARG
1	B	201	ASP
1	B	204	THR
1	B	215	GLU
1	B	217	THR
1	B	239	VAL
1	B	271	PHE
1	B	286	LEU
1	B	287	ASN
1	B	298	TYR
1	B	310	LEU
1	B	311	HIS
1	B	312	ASP
1	B	314	PHE
1	B	316	SER
1	B	318	TRP
1	B	336	LEU
1	B	347	GLN
1	B	348	LYS
1	B	352	ASP

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Mol	Chain	Res	Type
1	B	353	LEU
1	B	358	LEU
1	B	382	LEU
1	B	389	GLN
1	B	392	MET
1	B	396	PHE
1	B	397	VAL
1	B	401	TYR
1	B	424	LEU
1	B	428	GLN
1	B	436	ILE
1	B	451	ASP
1	B	453	GLN
1	B	457	GLN
1	B	471	TRP
1	B	476	ASN
1	B	494	ASN
1	B	495	ASP
1	B	497	ILE
1	B	498	ARG
1	B	499	ASN
1	B	505	GLN
1	B	518	PHE
1	B	521	MET
1	B	525	TYR
1	B	534	LEU
1	B	540	LEU
1	B	542	GLN
1	B	560	CYS
1	B	562	THR
1	B	590	ASN
1	B	600	LEU
1	B	601	PHE
1	B	616	GLU
1	B	634	TYR
1	B	638	MET
1	B	641	ILE
1	B	646	LEU
1	B	652	PHE
1	B	660	ASP
1	B	674	VAL
1	B	676	VAL

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Mol	Chain	Res	Type
1	B	680	ASP
1	B	697	ASP
1	B	707	TYR
1	B	709	ASP
1	B	710	MET
1	B	725	ARG
1	B	727	LEU
1	B	728	ASP
1	B	730	PHE
1	B	734	ASN
1	B	744	TYR
1	B	747	ILE
1	B	759	LEU
1	B	765	PHE
1	B	771	VAL
1	B	774	LEU
1	B	782	VAL
1	B	783	PHE
1	B	786	ILE
1	B	789	LEU
1	B	790	ARG
1	B	791	LYS
1	B	798	ILE
1	B	799	LEU
1	B	808	ASP
1	B	810	TYR
1	B	812	VAL
1	B	818	VAL
1	B	823	THR
1	B	832	GLN
1	B	836	ARG
1	B	839	MET
1	B	841	MET
1	B	857	PHE
1	B	871	PHE
1	B	872	ASP
1	B	876	ILE
2	C	1	MET
2	C	2	ASP
2	C	13	ASP
2	C	22	THR
2	C	26	ASN

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Mol	Chain	Res	Type
2	C	59	TRP
2	C	68	THR
2	C	106	ARG
2	C	128	ASN
2	C	129	PHE
2	C	142	GLN
2	C	147	ARG
2	C	150	PHE
2	C	152	PHE
2	C	170	GLN
2	C	214	LEU
2	C	225	LEU
2	C	255	ARG
2	C	274	GLN
2	C	284	ASN
2	C	370	LEU
2	C	374	TYR
2	C	378	ARG
2	C	382	LEU
2	C	385	VAL
2	D	1	MET
2	D	2	ASP
2	D	13	ASP
2	D	19	VAL
2	D	68	THR
2	D	70	LEU
2	D	73	LEU
2	D	103	GLU
2	D	106	ARG
2	D	109	ILE
2	D	117	ARG
2	D	129	PHE
2	D	142	GLN
2	D	143	ASN
2	D	147	ARG
2	D	150	PHE
2	D	152	PHE
2	D	170	GLN
2	D	214	LEU
2	D	225	LEU
2	D	255	ARG
2	D	274	GLN

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Mol	Chain	Res	Type
2	D	284	ASN
2	D	370	LEU
2	D	374	TYR
2	D	378	ARG
2	D	382	LEU
2	D	385	VAL
2	E	1	MET
2	E	2	ASP
2	E	13	ASP
2	E	26	ASN
2	E	59	TRP
2	E	69	THR
2	E	103	GLU
2	E	109	ILE
2	E	128	ASN
2	E	129	PHE
2	E	142	GLN
2	E	148	THR
2	E	150	PHE
2	E	152	PHE
2	E	170	GLN
2	E	214	LEU
2	E	225	LEU
2	E	255	ARG
2	E	274	GLN
2	E	284	ASN
2	E	370	LEU
2	E	374	TYR
2	E	378	ARG
2	E	382	LEU
2	E	385	VAL
2	F	2	ASP
2	F	13	ASP
2	F	60	ASN
2	F	61	PHE
2	F	105	GLN
2	F	109	ILE
2	F	128	ASN
2	F	129	PHE
2	F	142	GLN
2	F	148	THR
2	F	150	PHE

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Mol	Chain	Res	Type
2	F	152	PHE
2	F	170	GLN
2	F	214	LEU
2	F	225	LEU
2	F	255	ARG
2	F	274	GLN
2	F	284	ASN
2	F	370	LEU
2	F	374	TYR
2	F	378	ARG
2	F	382	LEU
2	F	385	VAL
2	G	2	ASP
2	G	13	ASP
2	G	26	ASN
2	G	63	PHE
2	G	106	ARG
2	G	109	ILE
2	G	117	ARG
2	G	129	PHE
2	G	142	GLN
2	G	143	ASN
2	G	145	ARG
2	G	152	PHE
2	G	170	GLN
2	G	214	LEU
2	G	225	LEU
2	G	255	ARG
2	G	274	GLN
2	G	284	ASN
2	G	370	LEU
2	G	374	TYR
2	G	378	ARG
2	G	382	LEU
2	G	385	VAL
2	H	1	MET
2	H	2	ASP
2	H	13	ASP
2	H	103	GLU
2	H	106	ARG
2	H	128	ASN
2	H	129	PHE

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Mol	Chain	Res	Type
2	H	142	GLN
2	H	150	PHE
2	H	152	PHE
2	H	170	GLN
2	H	214	LEU
2	H	225	LEU
2	H	255	ARG
2	H	274	GLN
2	H	284	ASN
2	H	370	LEU
2	H	374	TYR
2	H	378	ARG
2	H	382	LEU
2	H	385	VAL
2	I	1	MET
2	I	2	ASP
2	I	13	ASP
2	I	48	THR
2	I	61	PHE
2	I	106	ARG
2	I	109	ILE
2	I	117	ARG
2	I	129	PHE
2	I	142	GLN
2	I	150	PHE
2	I	152	PHE
2	I	170	GLN
2	I	214	LEU
2	I	225	LEU
2	I	255	ARG
2	I	274	GLN
2	I	284	ASN
2	I	370	LEU
2	I	374	TYR
2	I	378	ARG
2	I	382	LEU
2	I	385	VAL
2	J	1	MET
2	J	2	ASP
2	J	13	ASP
2	J	19	VAL
2	J	59	TRP

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Mol	Chain	Res	Type
2	J	106	ARG
2	J	109	ILE
2	J	128	ASN
2	J	129	PHE
2	J	142	GLN
2	J	150	PHE
2	J	152	PHE
2	J	170	GLN
2	J	214	LEU
2	J	225	LEU
2	J	255	ARG
2	J	274	GLN
2	J	284	ASN
2	J	370	LEU
2	J	374	TYR
2	J	378	ARG
2	J	382	LEU
2	J	385	VAL
2	K	1	MET
2	K	2	ASP
2	K	13	ASP
2	K	59	TRP
2	K	62	ASP
2	K	106	ARG
2	K	109	ILE
2	K	129	PHE
2	K	142	GLN
2	K	143	ASN
2	K	150	PHE
2	K	152	PHE
2	K	170	GLN
2	K	214	LEU
2	K	225	LEU
2	K	255	ARG
2	K	274	GLN
2	K	284	ASN
2	K	370	LEU
2	K	374	TYR
2	K	378	ARG
2	K	382	LEU
2	K	385	VAL
2	L	1	MET

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Mol	Chain	Res	Type
2	L	2	ASP
2	L	13	ASP
2	L	19	VAL
2	L	22	THR
2	L	25	SER
2	L	59	TRP
2	L	62	ASP
2	L	72	ASN
2	L	103	GLU
2	L	106	ARG
2	L	109	ILE
2	L	125	LYS
2	L	129	PHE
2	L	142	GLN
2	L	143	ASN
2	L	150	PHE
2	L	152	PHE
2	L	170	GLN
2	L	214	LEU
2	L	225	LEU
2	L	255	ARG
2	L	274	GLN
2	L	284	ASN
2	L	370	LEU
2	L	374	TYR
2	L	378	ARG
2	L	382	LEU
2	L	385	VAL
2	M	1	MET
2	M	2	ASP
2	M	13	ASP
2	M	22	THR
2	M	59	TRP
2	M	71	LEU
2	M	103	GLU
2	M	106	ARG
2	M	117	ARG
2	M	125	LYS
2	M	129	PHE
2	M	142	GLN
2	M	150	PHE
2	M	152	PHE

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Mol	Chain	Res	Type
2	M	170	GLN
2	M	214	LEU
2	M	225	LEU
2	M	255	ARG
2	M	274	GLN
2	M	284	ASN
2	M	370	LEU
2	M	374	TYR
2	M	378	ARG
2	M	382	LEU
2	M	385	VAL
2	N	1	MET
2	N	2	ASP
2	N	13	ASP
2	N	58	ASN
2	N	60	ASN
2	N	66	LEU
2	N	73	LEU
2	N	103	GLU
2	N	106	ARG
2	N	109	ILE
2	N	129	PHE
2	N	142	GLN
2	N	145	ARG
2	N	150	PHE
2	N	152	PHE
2	N	170	GLN
2	N	214	LEU
2	N	225	LEU
2	N	255	ARG
2	N	274	GLN
2	N	284	ASN
2	N	370	LEU
2	N	374	TYR
2	N	378	ARG
2	N	382	LEU
2	N	385	VAL
2	O	2	ASP
2	O	13	ASP
2	O	23	LEU
2	O	25	SER
2	O	106	ARG

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Mol	Chain	Res	Type
2	O	107	ASN
2	O	109	ILE
2	O	129	PHE
2	O	142	GLN
2	O	150	PHE
2	O	170	GLN
2	O	214	LEU
2	O	225	LEU
2	O	255	ARG
2	O	274	GLN
2	O	284	ASN
2	O	370	LEU
2	O	374	TYR
2	O	378	ARG
2	O	382	LEU
2	O	385	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (220) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	GLN
1	A	137	ASN
1	A	168	ASN
1	A	230	GLN
1	A	246	HIS
1	A	260	GLN
1	A	309	ASN
1	A	347	GLN
1	A	365	GLN
1	A	428	GLN
1	A	443	GLN
1	A	453	GLN
1	A	462	GLN
1	A	473	HIS
1	A	490	ASN
1	A	496	ASN
1	A	553	ASN
1	A	605	ASN
1	A	609	ASN
1	A	613	ASN
1	A	615	ASN
1	A	661	GLN

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Mol	Chain	Res	Type
1	A	683	ASN
1	A	701	GLN
1	A	722	ASN
1	A	726	ASN
1	A	803	ASN
1	A	807	ASN
1	A	840	HIS
1	A	873	ASN
1	B	119	GLN
1	B	168	ASN
1	B	190	ASN
1	B	230	GLN
1	B	237	ASN
1	B	240	ASN
1	B	246	HIS
1	B	287	ASN
1	B	302	ASN
1	B	305	GLN
1	B	311	HIS
1	B	347	GLN
1	B	371	ASN
1	B	449	ASN
1	B	465	ASN
1	B	473	HIS
1	B	476	ASN
1	B	477	ASN
1	B	491	GLN
1	B	517	GLN
1	B	553	ASN
1	B	564	ASN
1	B	590	ASN
1	B	602	HIS
1	B	605	ASN
1	B	609	ASN
1	B	611	HIS
1	B	615	ASN
1	B	629	ASN
1	B	635	GLN
1	B	683	ASN
1	B	746	GLN
1	B	807	ASN
1	B	814	ASN

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Mol	Chain	Res	Type
1	B	831	GLN
1	B	840	HIS
1	B	878	ASN
2	C	26	ASN
2	C	35	ASN
2	C	53	ASN
2	C	72	ASN
2	C	128	ASN
2	C	131	ASN
2	C	143	ASN
2	C	146	GLN
2	C	167	ASN
2	C	239	ASN
2	C	274	GLN
2	C	284	ASN
2	C	345	ASN
2	D	26	ASN
2	D	128	ASN
2	D	131	ASN
2	D	142	GLN
2	D	146	GLN
2	D	167	ASN
2	D	239	ASN
2	D	274	GLN
2	D	284	ASN
2	D	345	ASN
2	E	26	ASN
2	E	53	ASN
2	E	94	ASN
2	E	131	ASN
2	E	142	GLN
2	E	167	ASN
2	E	239	ASN
2	E	274	GLN
2	E	284	ASN
2	E	345	ASN
2	F	32	GLN
2	F	53	ASN
2	F	72	ASN
2	F	94	ASN
2	F	128	ASN
2	F	131	ASN

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Mol	Chain	Res	Type
2	F	142	GLN
2	F	167	ASN
2	F	239	ASN
2	F	274	GLN
2	F	284	ASN
2	F	345	ASN
2	G	26	ASN
2	G	35	ASN
2	G	53	ASN
2	G	128	ASN
2	G	131	ASN
2	G	142	GLN
2	G	167	ASN
2	G	239	ASN
2	G	274	GLN
2	G	284	ASN
2	G	345	ASN
2	H	26	ASN
2	H	53	ASN
2	H	83	ASN
2	H	94	ASN
2	H	107	ASN
2	H	128	ASN
2	H	131	ASN
2	H	142	GLN
2	H	167	ASN
2	H	239	ASN
2	H	274	GLN
2	H	284	ASN
2	H	345	ASN
2	I	32	GLN
2	I	53	ASN
2	I	76	ASN
2	I	94	ASN
2	I	128	ASN
2	I	131	ASN
2	I	143	ASN
2	I	146	GLN
2	I	167	ASN
2	I	239	ASN
2	I	274	GLN
2	I	284	ASN

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Mol	Chain	Res	Type
2	I	345	ASN
2	J	26	ASN
2	J	53	ASN
2	J	94	ASN
2	J	128	ASN
2	J	131	ASN
2	J	142	GLN
2	J	146	GLN
2	J	167	ASN
2	J	239	ASN
2	J	274	GLN
2	J	284	ASN
2	J	345	ASN
2	K	26	ASN
2	K	53	ASN
2	K	72	ASN
2	K	94	ASN
2	K	131	ASN
2	K	143	ASN
2	K	167	ASN
2	K	239	ASN
2	K	274	GLN
2	K	284	ASN
2	K	345	ASN
2	L	53	ASN
2	L	72	ASN
2	L	131	ASN
2	L	140	ASN
2	L	143	ASN
2	L	146	GLN
2	L	167	ASN
2	L	239	ASN
2	L	274	GLN
2	L	284	ASN
2	L	345	ASN
2	M	36	GLN
2	M	53	ASN
2	M	128	ASN
2	M	131	ASN
2	M	142	GLN
2	M	143	ASN
2	M	167	ASN

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Mol	Chain	Res	Type
2	M	239	ASN
2	M	274	GLN
2	M	284	ASN
2	M	345	ASN
2	N	26	ASN
2	N	32	GLN
2	N	53	ASN
2	N	94	ASN
2	N	128	ASN
2	N	131	ASN
2	N	140	ASN
2	N	142	GLN
2	N	146	GLN
2	N	167	ASN
2	N	239	ASN
2	N	274	GLN
2	N	284	ASN
2	N	345	ASN
2	O	35	ASN
2	O	53	ASN
2	O	131	ASN
2	O	140	ASN
2	O	142	GLN
2	O	143	ASN
2	O	153	HIS
2	O	167	ASN
2	O	239	ASN
2	O	274	GLN
2	O	284	ASN
2	O	345	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	781/880 (88%)	-0.21	0 100 100	62, 136, 196, 209	0
1	B	810/880 (92%)	-0.22	1 (0%) 95 94	53, 131, 186, 209	0
2	C	397/397 (100%)	-0.33	2 (0%) 90 86	81, 147, 203, 209	0
2	D	397/397 (100%)	-0.35	0 100 100	90, 154, 208, 209	0
2	E	397/397 (100%)	-0.34	0 100 100	72, 151, 201, 209	0
2	F	397/397 (100%)	-0.36	4 (1%) 82 75	100, 182, 209, 209	0
2	G	397/397 (100%)	-0.37	1 (0%) 93 91	82, 176, 209, 209	0
2	H	397/397 (100%)	-0.31	4 (1%) 82 75	96, 174, 209, 209	0
2	I	397/397 (100%)	-0.44	0 100 100	83, 157, 208, 209	0
2	J	397/397 (100%)	-0.44	0 100 100	77, 155, 203, 209	0
2	K	397/397 (100%)	-0.40	0 100 100	79, 156, 208, 209	0
2	L	397/397 (100%)	-0.25	6 (1%) 74 65	77, 150, 207, 209	0
2	M	397/397 (100%)	-0.29	1 (0%) 93 91	81, 150, 208, 209	0
2	N	397/397 (100%)	-0.29	3 (0%) 86 79	83, 150, 201, 209	0
2	O	397/397 (100%)	-0.27	2 (0%) 90 86	75, 150, 200, 209	0
All	All	6752/6921 (97%)	-0.31	24 (0%) 92 88	53, 153, 208, 209	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	397	LYS	4.2
2	L	324	LEU	3.4
2	G	397	LYS	3.1
2	H	397	LYS	3.0
2	F	20	GLU	2.9
2	N	397	LYS	2.8
1	B	351	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
2	C	335	LEU	2.5
2	H	20	GLU	2.5
2	L	15	ARG	2.4
2	H	294	LEU	2.4
2	F	1	MET	2.4
2	M	365	MET	2.4
2	N	335	LEU	2.4
2	H	318	ALA	2.3
2	L	397	LYS	2.3
2	L	290	LEU	2.2
2	O	157	ILE	2.1
2	O	15	ARG	2.1
2	L	225	LEU	2.1
2	L	288	ILE	2.1
2	N	125	LYS	2.1
2	F	318	ALA	2.1
2	F	397	LYS	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	ZN	F	398	1/1	0.99	0.16	-0.06	51,51,51,51	0
3	ZN	I	398	1/1	1.00	0.18	-0.12	51,51,51,51	0
3	ZN	C	398	1/1	1.00	0.16	-0.63	51,51,51,51	0
3	ZN	L	398	1/1	0.99	0.13	-0.82	51,51,51,51	0
3	ZN	O	398	1/1	1.00	0.20	-	51,51,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.