



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:22 PM GMT

PDB ID : 4EIW
Title : Whole cytosolic region of atp-dependent metalloprotease FtsH (G399L)
Authors : Suno, R.; Niwa, H.; Tsuchiya, D.; Yoshida, M.; Morikawa, K.
Deposited on : 2012-04-06
Resolution : 3.90 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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

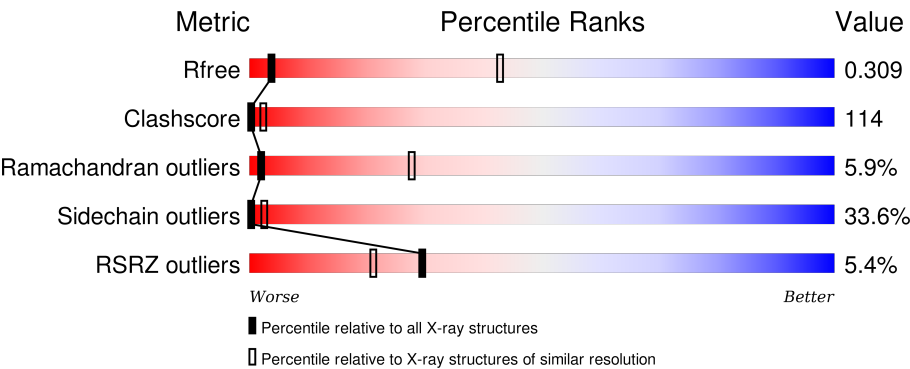
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	91344	1014 (4.28-3.52)
Clashscore	102246	1031 (4.24-3.56)
Ramachandran outliers	100387	1012 (4.26-3.54)
Sidechain outliers	100360	1004 (4.26-3.54)
RSRZ outliers	91569	1018 (4.28-3.52)

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	508	<div><div>4%</div><div>16%</div><div>49%</div><div>23%</div><div>10%</div></div>
1	B	508	<div><div>5%</div><div>9%</div><div>53%</div><div>22%</div><div>12%</div></div>
1	C	508	<div><div>6%</div><div>16%</div><div>49%</div><div>21%</div><div>10%</div></div>
1	D	508	<div><div>4%</div><div>9%</div><div>52%</div><div>23%</div><div>12%</div></div>
1	E	508	<div><div>6%</div><div>17%</div><div>49%</div><div>22%</div><div>10%</div></div>

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Mol	Chain	Length	Quality of chain
1	F	508	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ADP	B	2001	-	-	X	-
2	ADP	C	1001	-	-	X	-
2	ADP	D	2001	-	-	X	-
2	ADP	E	1001	-	-	X	-
2	ADP	F	2001	-	-	X	-

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 21429 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 ATP-dependent zinc metalloprotease FtsH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	458	Total	C	N	O	S	0	0	0
			3578	2245	658	662	13			
1	B	446	Total	C	N	O	S	0	0	0
			3511	2206	641	651	13			
1	C	458	Total	C	N	O	S	0	0	0
			3578	2245	658	662	13			
1	D	446	Total	C	N	O	S	0	0	0
			3511	2206	641	651	13			
1	E	458	Total	C	N	O	S	0	0	0
			3578	2245	658	662	13			
1	F	446	Total	C	N	O	S	0	0	0
			3511	2206	641	651	13			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	117	GLY	-	EXPRESSION TAG	UNP Q5SI82
A	118	PRO	-	EXPRESSION TAG	UNP Q5SI82
A	119	LEU	-	EXPRESSION TAG	UNP Q5SI82
A	120	GLY	-	EXPRESSION TAG	UNP Q5SI82
A	121	SER	-	EXPRESSION TAG	UNP Q5SI82
A	122	HIS	-	EXPRESSION TAG	UNP Q5SI82
A	123	MET	-	EXPRESSION TAG	UNP Q5SI82
A	124	GLY	-	EXPRESSION TAG	UNP Q5SI82
A	125	ALA	-	EXPRESSION TAG	UNP Q5SI82
A	399	LEU	GLY	ENGINEERED MUTATION	UNP Q5SI82
B	117	GLY	-	EXPRESSION TAG	UNP Q5SI82
B	118	PRO	-	EXPRESSION TAG	UNP Q5SI82
B	119	LEU	-	EXPRESSION TAG	UNP Q5SI82
B	120	GLY	-	EXPRESSION TAG	UNP Q5SI82
B	121	SER	-	EXPRESSION TAG	UNP Q5SI82
B	122	HIS	-	EXPRESSION TAG	UNP Q5SI82
B	123	MET	-	EXPRESSION TAG	UNP Q5SI82

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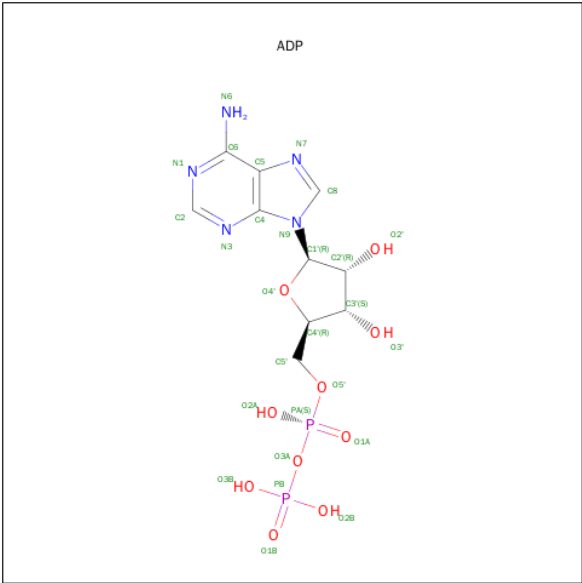
Chain	Residue	Modelled	Actual	Comment	Reference
B	124	GLY	-	EXPRESSION TAG	UNP Q5SI82
B	125	ALA	-	EXPRESSION TAG	UNP Q5SI82
B	399	LEU	GLY	ENGINEERED MUTATION	UNP Q5SI82
C	117	GLY	-	EXPRESSION TAG	UNP Q5SI82
C	118	PRO	-	EXPRESSION TAG	UNP Q5SI82
C	119	LEU	-	EXPRESSION TAG	UNP Q5SI82
C	120	GLY	-	EXPRESSION TAG	UNP Q5SI82
C	121	SER	-	EXPRESSION TAG	UNP Q5SI82
C	122	HIS	-	EXPRESSION TAG	UNP Q5SI82
C	123	MET	-	EXPRESSION TAG	UNP Q5SI82
C	124	GLY	-	EXPRESSION TAG	UNP Q5SI82
C	125	ALA	-	EXPRESSION TAG	UNP Q5SI82
C	399	LEU	GLY	ENGINEERED MUTATION	UNP Q5SI82
D	117	GLY	-	EXPRESSION TAG	UNP Q5SI82
D	118	PRO	-	EXPRESSION TAG	UNP Q5SI82
D	119	LEU	-	EXPRESSION TAG	UNP Q5SI82
D	120	GLY	-	EXPRESSION TAG	UNP Q5SI82
D	121	SER	-	EXPRESSION TAG	UNP Q5SI82
D	122	HIS	-	EXPRESSION TAG	UNP Q5SI82
D	123	MET	-	EXPRESSION TAG	UNP Q5SI82
D	124	GLY	-	EXPRESSION TAG	UNP Q5SI82
D	125	ALA	-	EXPRESSION TAG	UNP Q5SI82
D	399	LEU	GLY	ENGINEERED MUTATION	UNP Q5SI82
E	117	GLY	-	EXPRESSION TAG	UNP Q5SI82
E	118	PRO	-	EXPRESSION TAG	UNP Q5SI82
E	119	LEU	-	EXPRESSION TAG	UNP Q5SI82
E	120	GLY	-	EXPRESSION TAG	UNP Q5SI82
E	121	SER	-	EXPRESSION TAG	UNP Q5SI82
E	122	HIS	-	EXPRESSION TAG	UNP Q5SI82
E	123	MET	-	EXPRESSION TAG	UNP Q5SI82
E	124	GLY	-	EXPRESSION TAG	UNP Q5SI82
E	125	ALA	-	EXPRESSION TAG	UNP Q5SI82
E	399	LEU	GLY	ENGINEERED MUTATION	UNP Q5SI82
F	117	GLY	-	EXPRESSION TAG	UNP Q5SI82
F	118	PRO	-	EXPRESSION TAG	UNP Q5SI82
F	119	LEU	-	EXPRESSION TAG	UNP Q5SI82
F	120	GLY	-	EXPRESSION TAG	UNP Q5SI82
F	121	SER	-	EXPRESSION TAG	UNP Q5SI82
F	122	HIS	-	EXPRESSION TAG	UNP Q5SI82
F	123	MET	-	EXPRESSION TAG	UNP Q5SI82
F	124	GLY	-	EXPRESSION TAG	UNP Q5SI82
F	125	ALA	-	EXPRESSION TAG	UNP Q5SI82

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Chain	Residue	Modelled	Actual	Comment	Reference
F	399	LEU	GLY	ENGINEERED MUTATION	UNP Q5SI82

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

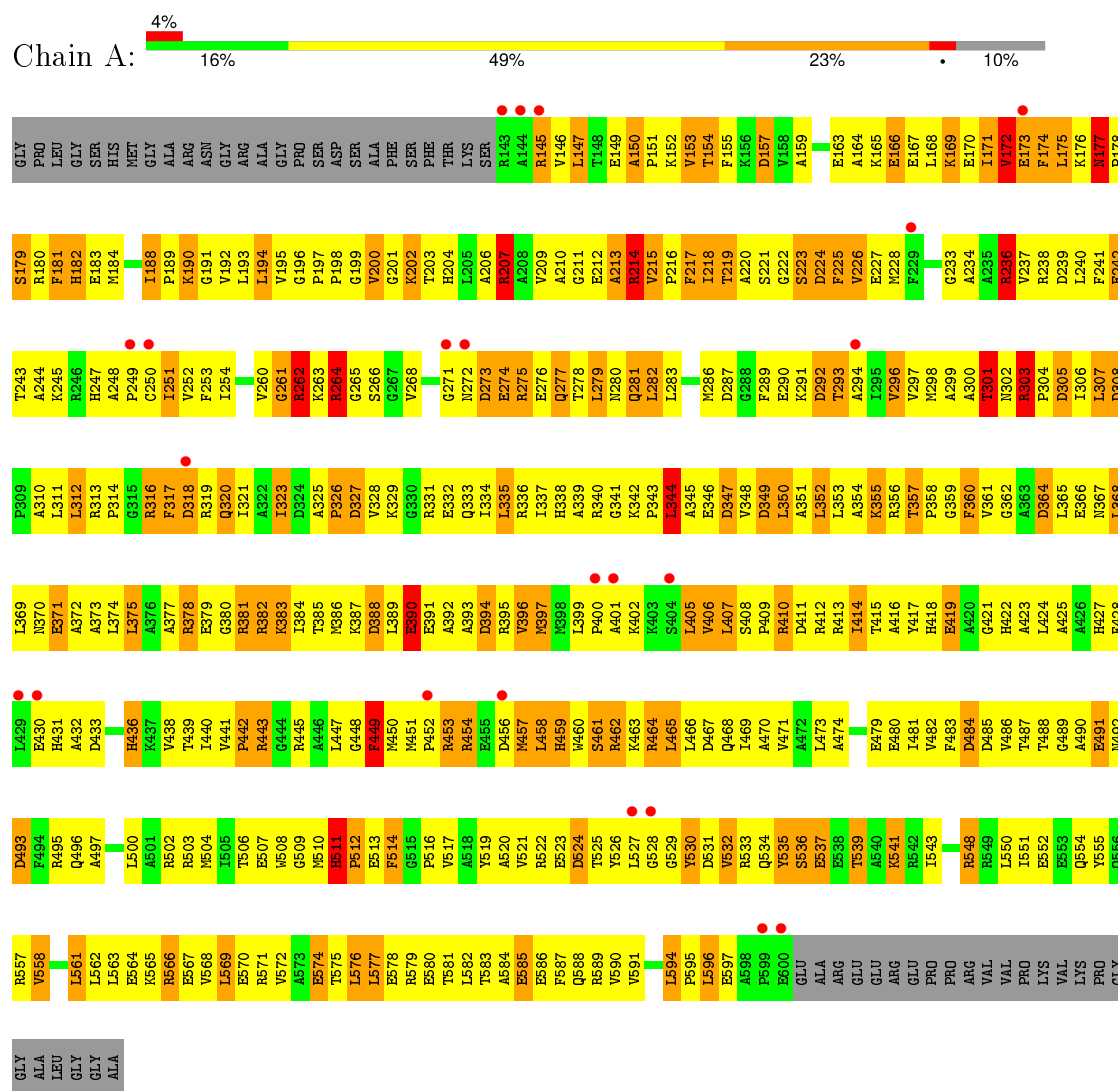


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

3 Residue-property plots

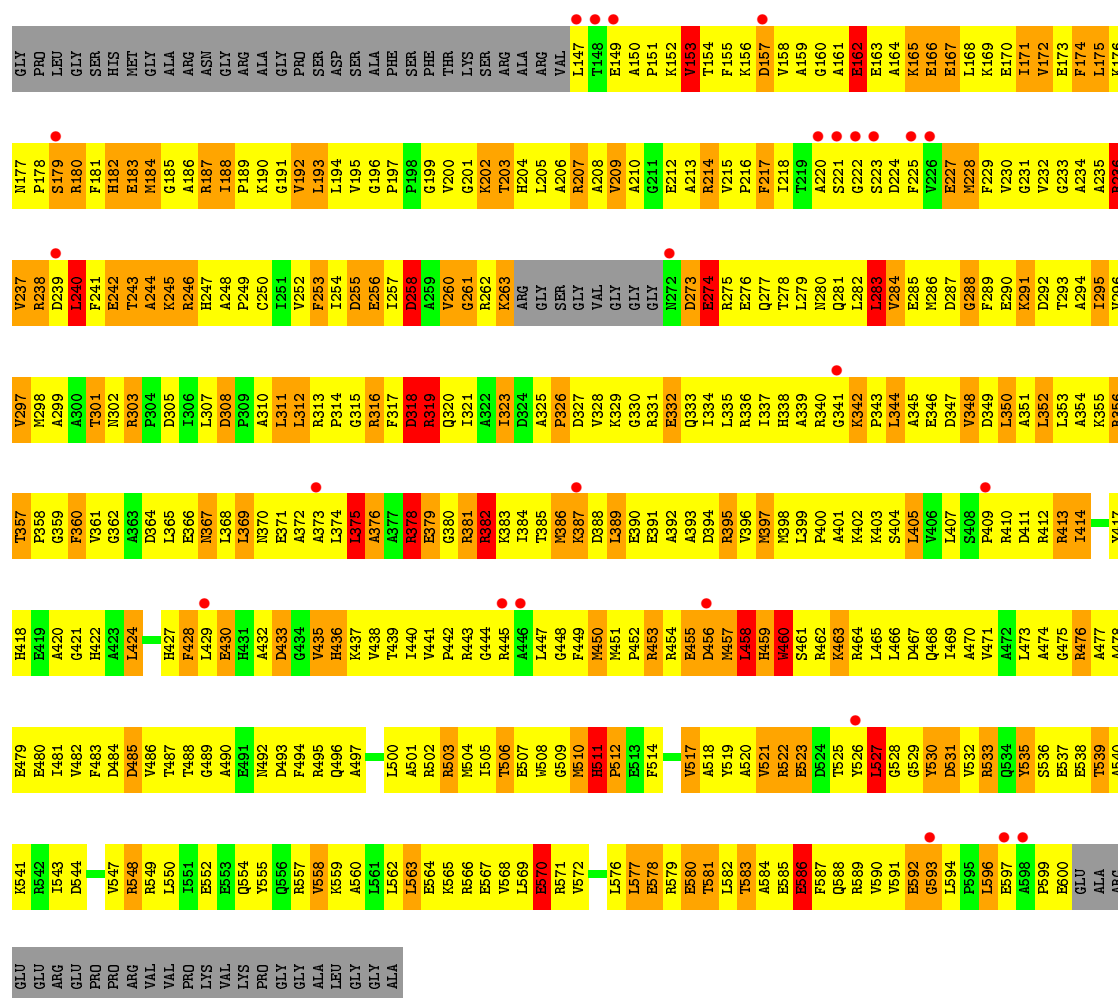
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

- Molecule 1: ATP-dependent zinc metalloprotease FtsH

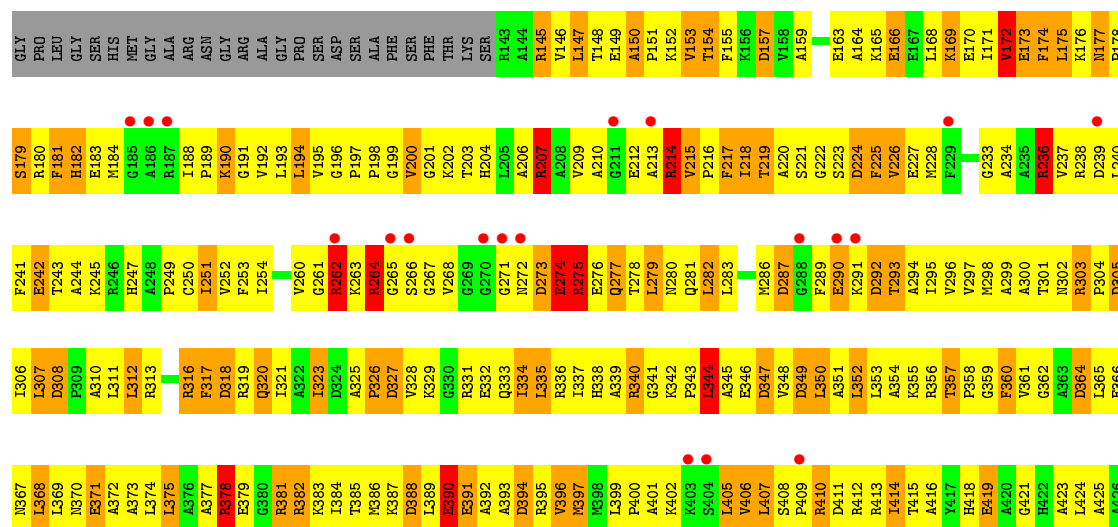
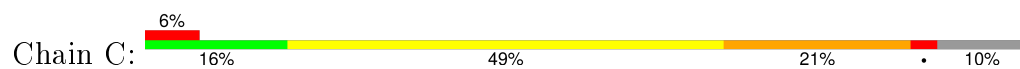


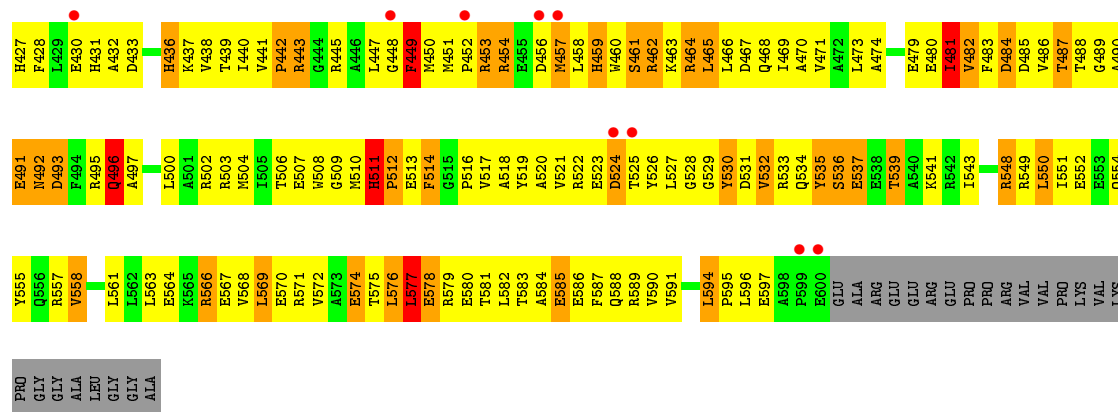
- Molecule 1: ATP-dependent zinc metalloprotease FtsH



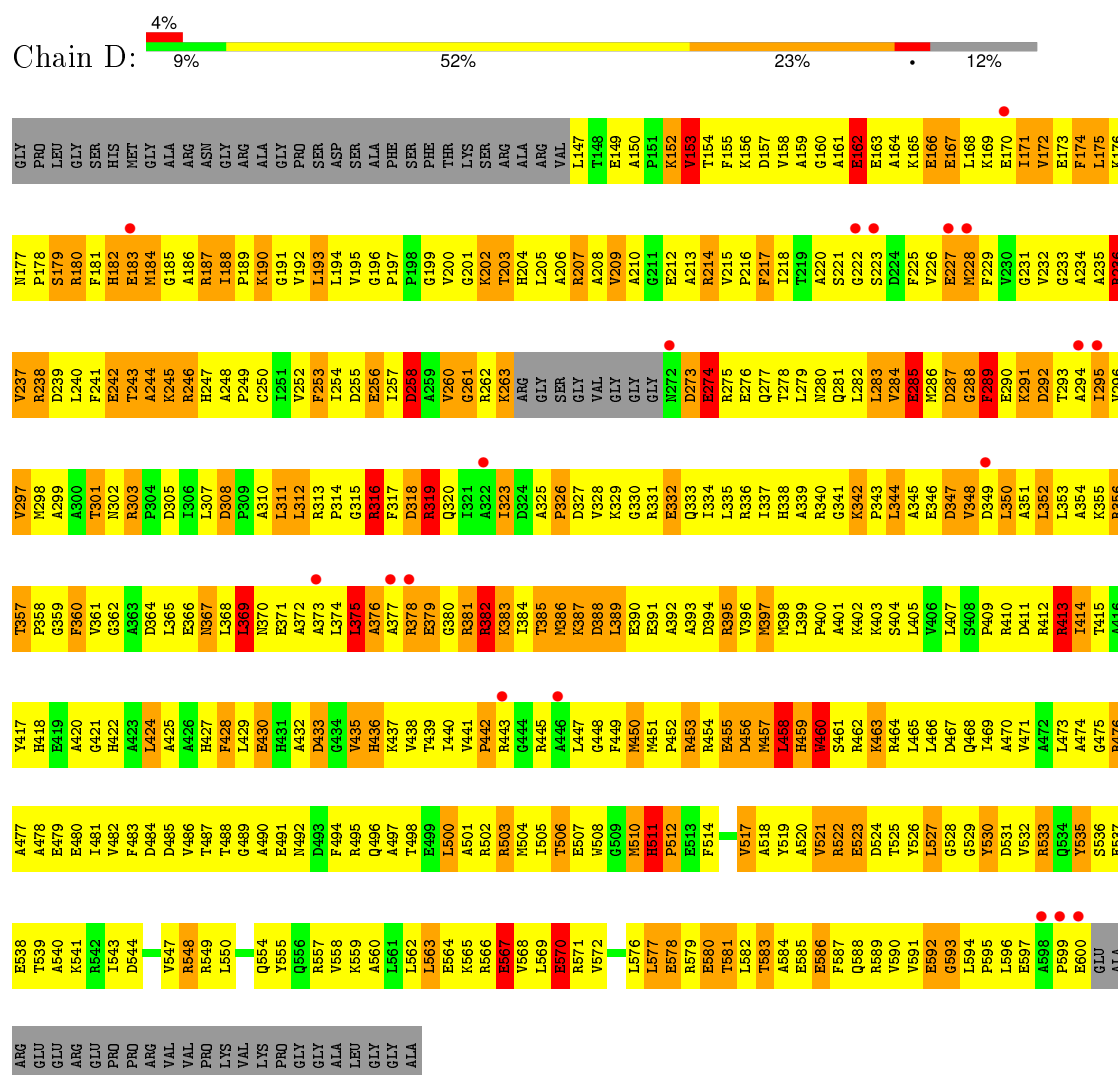


• Molecule 1: ATP-dependent zinc metalloprotease FtsH

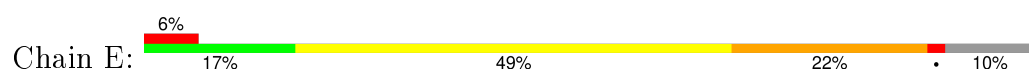


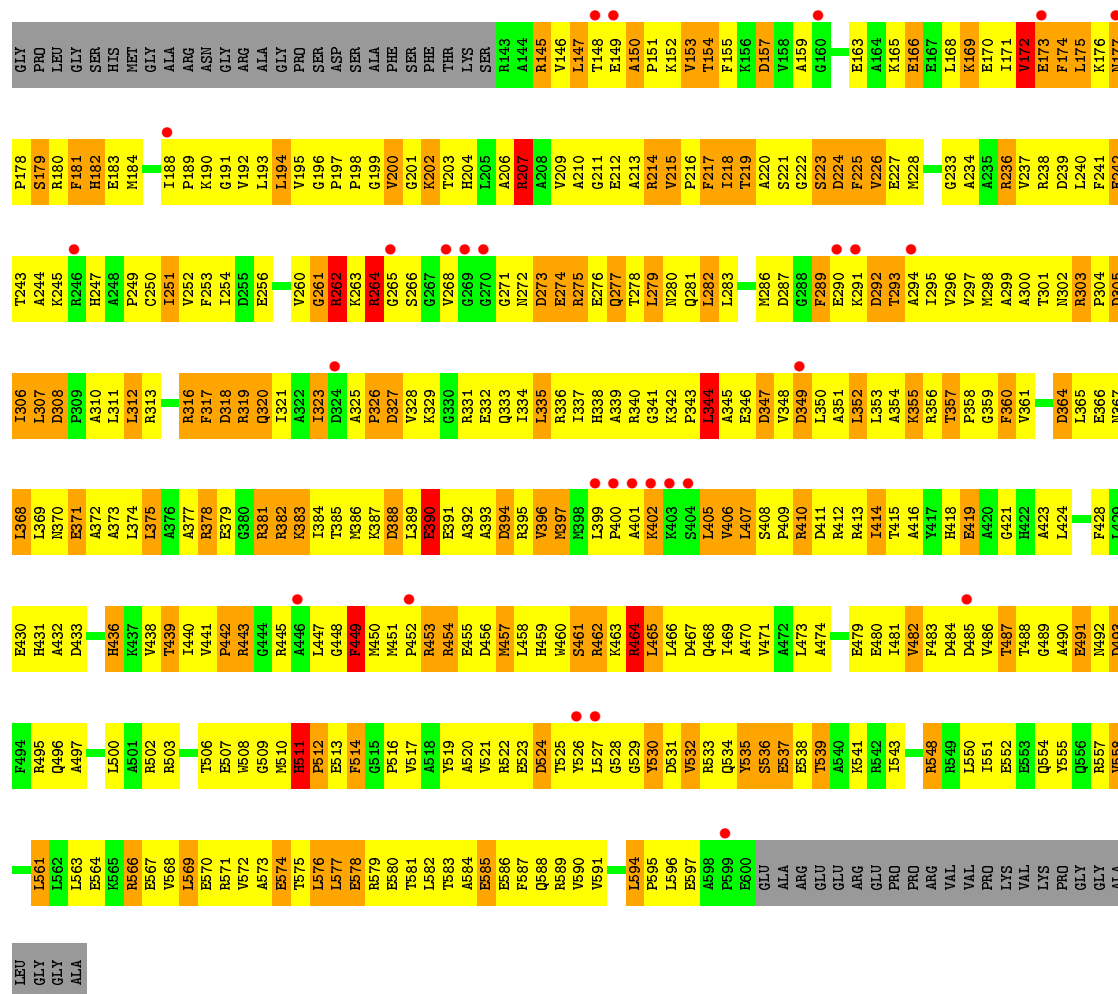


• Molecule 1: ATP-dependent zinc metalloprotease FtsH

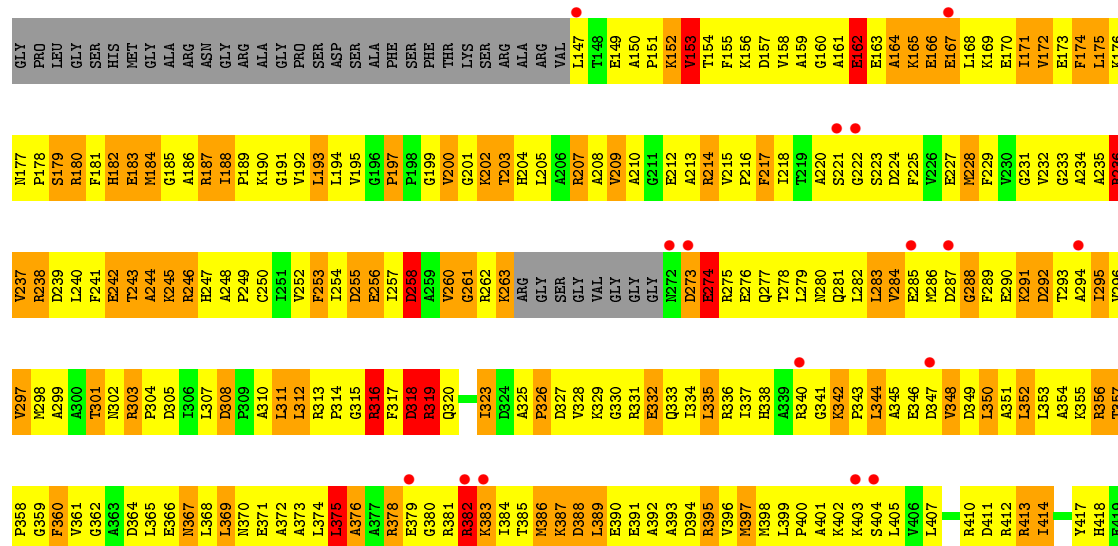
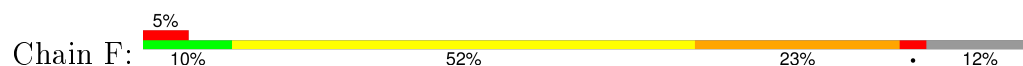


• Molecule 1: ATP-dependent zinc metalloprotease FtsH





• Molecule 1: ATP-dependent zinc metalloprotease FtsH





4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	146.15Å 146.15Å 349.06Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	71.53 – 3.90 71.53 – 3.90	Depositor EDS
% Data completeness (in resolution range)	97.1 (71.53-3.90) 97.1 (71.53-3.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.46 (at 3.89Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.299 , 0.312 0.298 , 0.309	Depositor DCC
R_{free} test set	1967 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	99.1	Xtriage
Anisotropy	0.272	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.17 , 17.8	EDS
Estimated twinning fraction	0.237 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.27$, $\langle L^2 \rangle = 0.11$	Xtriage
Outliers	0 of 39234 reflections	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	21429	wwPDB-VP
Average B, all atoms (Å ²)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.77% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ADP

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	0.60	3/3636 (0.1%)	0.95	16/4906 (0.3%)
1	B	0.63	3/3568 (0.1%)	1.01	18/4815 (0.4%)
1	C	0.59	2/3636 (0.1%)	1.03	24/4906 (0.5%)
1	D	0.60	2/3568 (0.1%)	0.98	17/4815 (0.4%)
1	E	0.61	6/3636 (0.2%)	0.96	13/4906 (0.3%)
1	F	0.58	2/3568 (0.1%)	0.96	12/4815 (0.2%)
All	All	0.60	18/21612 (0.1%)	0.98	100/29163 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	5
1	C	0	1
1	D	0	6
1	E	0	1
1	F	0	5
All	All	0	20

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	586	GLU	CD-OE1	-12.04	1.12	1.25
1	C	214	ARG	CZ-NH2	8.16	1.43	1.33
1	E	214	ARG	CZ-NH2	-8.12	1.22	1.33
1	E	319	ARG	CZ-NH1	-7.39	1.23	1.33
1	D	586	GLU	CD-OE1	-6.72	1.18	1.25
1	A	214	ARG	CZ-NH2	-6.40	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	214	ARG	CZ-NH1	-6.39	1.24	1.33
1	F	586	GLU	CD-OE1	-6.36	1.18	1.25
1	C	214	ARG	CZ-NH1	-6.30	1.24	1.33
1	E	214	ARG	CG-CD	-6.02	1.36	1.51
1	A	301	THR	CB-CG2	-5.76	1.33	1.52
1	B	460	TRP	CD2-CE2	5.54	1.48	1.41
1	A	214	ARG	CD-NE	-5.42	1.37	1.46
1	B	316	ARG	CZ-NH2	-5.36	1.26	1.33
1	E	316	ARG	CZ-NH1	-5.34	1.26	1.33
1	F	460	TRP	CD2-CE2	5.30	1.47	1.41
1	E	214	ARG	CD-NE	-5.23	1.37	1.46
1	D	460	TRP	CD2-CE2	5.20	1.47	1.41

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	319	ARG	NE-CZ-NH2	18.11	129.36	120.30
1	C	207	ARG	NE-CZ-NH1	-15.37	112.61	120.30
1	A	316	ARG	NE-CZ-NH1	-15.14	112.73	120.30
1	B	236	ARG	NE-CZ-NH1	-14.64	112.98	120.30
1	C	207	ARG	NE-CZ-NH2	13.93	127.26	120.30
1	B	236	ARG	NE-CZ-NH2	13.80	127.20	120.30
1	C	316	ARG	NE-CZ-NH2	13.04	126.82	120.30
1	E	316	ARG	NE-CZ-NH1	-11.95	114.33	120.30
1	C	316	ARG	NE-CZ-NH1	-11.85	114.38	120.30
1	A	316	ARG	NE-CZ-NH2	11.58	126.09	120.30
1	C	481	ILE	CG1-CB-CG2	-10.53	88.25	111.40
1	A	214	ARG	NE-CZ-NH1	9.92	125.26	120.30
1	F	316	ARG	NE-CZ-NH1	-9.37	115.62	120.30
1	B	381	ARG	NE-CZ-NH1	-9.32	115.64	120.30
1	C	214	ARG	NE-CZ-NH1	-9.09	115.75	120.30
1	F	316	ARG	NE-CZ-NH2	8.93	124.76	120.30
1	E	316	ARG	NE-CZ-NH2	8.61	124.61	120.30
1	B	316	ARG	NE-CZ-NH2	8.43	124.52	120.30
1	D	375	LEU	CA-CB-CG	8.41	134.64	115.30
1	F	236	ARG	NE-CZ-NH2	-8.32	116.14	120.30
1	D	289	PHE	CB-CG-CD1	-8.21	115.06	120.80
1	D	236	ARG	NE-CZ-NH2	-8.16	116.22	120.30
1	B	375	LEU	CA-CB-CG	7.99	133.66	115.30
1	D	316	ARG	NE-CZ-NH2	7.84	124.22	120.30
1	C	214	ARG	N-CA-C	7.67	131.72	111.00
1	B	283	LEU	CB-CG-CD1	-7.66	97.98	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	236	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	A	207	ARG	NE-CZ-NH1	7.41	124.00	120.30
1	A	214	ARG	NE-CZ-NH2	-7.37	116.61	120.30
1	D	236	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	E	319	ARG	NH1-CZ-NH2	-7.30	111.37	119.40
1	E	335	LEU	CA-CB-CG	7.21	131.88	115.30
1	C	207	ARG	CD-NE-CZ	7.12	133.56	123.60
1	E	207	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	A	335	LEU	CA-CB-CG	7.09	131.62	115.30
1	C	275	ARG	CB-CA-C	-7.09	96.21	110.40
1	F	375	LEU	CA-CB-CG	7.01	131.43	115.30
1	E	207	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	C	207	ARG	CG-CD-NE	-6.89	97.33	111.80
1	B	236	ARG	CD-NE-CZ	6.86	133.20	123.60
1	C	335	LEU	CA-CB-CG	6.70	130.72	115.30
1	A	207	ARG	NE-CZ-NH2	-6.59	117.01	120.30
1	D	381	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	C	214	ARG	CA-CB-CG	-6.55	98.98	113.40
1	E	214	ARG	N-CA-C	6.44	128.39	111.00
1	B	240	LEU	CA-CB-CG	6.42	130.06	115.30
1	D	289	PHE	N-CA-CB	-6.29	99.28	110.60
1	D	382	ARG	N-CA-CB	-6.22	99.39	110.60
1	C	214	ARG	NE-CZ-NH2	6.13	123.36	120.30
1	D	511	HIS	C-N-CD	6.12	141.25	128.40
1	E	214	ARG	NE-CZ-NH2	6.02	123.31	120.30
1	F	214	ARG	CA-CB-CG	5.99	126.59	113.40
1	B	378	ARG	CG-CD-NE	5.96	124.32	111.80
1	D	285	GLU	CA-CB-CG	5.93	126.44	113.40
1	F	511	HIS	C-N-CD	5.91	140.81	128.40
1	C	496	GLN	CB-CA-C	-5.88	98.64	110.40
1	C	577	LEU	CB-CG-CD1	-5.87	101.02	111.00
1	D	289	PHE	CB-CG-CD2	5.87	124.91	120.80
1	A	177	ASN	CB-CA-C	-5.83	98.74	110.40
1	E	577	LEU	CA-CB-CG	5.82	128.68	115.30
1	C	287	ASP	CB-CG-OD1	5.75	123.47	118.30
1	C	344	LEU	CA-CB-CG	5.72	128.45	115.30
1	D	285	GLU	CB-CA-C	-5.71	98.98	110.40
1	A	344	LEU	CA-CB-CG	5.61	128.20	115.30
1	D	382	ARG	CB-CG-CD	-5.58	97.11	111.60
1	D	282	LEU	CA-CB-CG	5.53	128.03	115.30
1	B	369	LEU	CA-CB-CG	5.52	127.99	115.30
1	A	303	ARG	NE-CZ-NH1	5.49	123.05	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	458	LEU	N-CA-C	-5.46	96.27	111.00
1	A	301	THR	OG1-CB-CG2	-5.45	97.46	110.00
1	B	511	HIS	C-N-CD	5.42	139.77	128.40
1	E	344	LEU	CA-CB-CG	5.40	127.72	115.30
1	E	464	ARG	CB-CA-C	-5.40	99.61	110.40
1	A	577	LEU	CA-CB-CG	5.39	127.70	115.30
1	A	274	GLU	CB-CG-CD	-5.38	99.68	114.20
1	B	282	LEU	CA-CB-CG	5.37	127.64	115.30
1	B	458	LEU	N-CA-C	-5.36	96.52	111.00
1	C	275	ARG	CA-CB-CG	5.35	125.16	113.40
1	F	282	LEU	CA-CB-CG	5.33	127.55	115.30
1	B	586	GLU	CG-CD-OE2	5.30	128.90	118.30
1	C	378	ARG	CG-CD-NE	5.28	122.89	111.80
1	B	527	LEU	CA-CB-CG	-5.27	103.17	115.30
1	C	378	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	B	165	LYS	CD-CE-NZ	-5.26	99.61	111.70
1	C	378	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	C	214	ARG	CG-CD-NE	-5.21	100.87	111.80
1	B	586	GLU	OE1-CD-OE2	-5.20	117.06	123.30
1	A	335	LEU	CB-CG-CD1	-5.19	102.18	111.00
1	D	458	LEU	N-CA-C	-5.17	97.04	111.00
1	A	236	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	D	567	GLU	CA-CB-CG	5.16	124.76	113.40
1	F	318	ASP	N-CA-C	-5.14	97.11	111.00
1	F	369	LEU	CA-CB-CG	5.12	127.08	115.30
1	D	369	LEU	CA-CB-CG	5.12	127.08	115.30
1	C	274	GLU	CB-CA-C	-5.12	100.16	110.40
1	B	318	ASP	N-CA-C	-5.07	97.31	111.00
1	C	236	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	F	413	ARG	CB-CA-C	-5.06	100.27	110.40
1	A	577	LEU	CB-CG-CD1	-5.06	102.40	111.00
1	E	287	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	213	ALA	Peptide
1	A	532	VAL	Peptide
1	B	244	ALA	Peptide
1	B	288	GLY	Peptide
1	B	382	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	B	510	MET	Peptide
1	B	523	GLU	Peptide
1	C	532	VAL	Peptide
1	D	244	ALA	Peptide
1	D	288	GLY	Peptide
1	D	347	ASP	Peptide
1	D	382	ARG	Peptide
1	D	510	MET	Peptide
1	D	523	GLU	Peptide
1	E	532	VAL	Peptide
1	F	244	ALA	Peptide
1	F	288	GLY	Peptide
1	F	382	ARG	Peptide
1	F	510	MET	Peptide
1	F	523	GLU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3578	0	3623	862	5
1	B	3511	0	3556	851	3
1	C	3578	0	3623	815	0
1	D	3511	0	3556	851	3
1	E	3578	0	3623	805	3
1	F	3511	0	3556	857	2
2	A	27	0	12	8	0
2	B	27	0	12	9	0
2	C	27	0	12	10	0
2	D	27	0	12	9	0
2	E	27	0	12	11	0
2	F	27	0	12	10	0
All	All	21429	0	21609	4895	8

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 114.

All (4895) 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:E:416:ALA:CB	1:E:577:LEU:HD23	1.18	1.63
1:A:416:ALA:HB3	1:A:577:LEU:CD2	1.33	1.58
1:A:416:ALA:CB	1:A:577:LEU:HD23	1.15	1.55
1:F:376:ALA:CA	1:F:381:ARG:HD2	1.31	1.55
1:E:416:ALA:HB3	1:E:577:LEU:CD2	1.35	1.55
1:B:376:ALA:CA	1:B:381:ARG:HD2	1.18	1.54
1:B:376:ALA:HA	1:B:381:ARG:CD	1.38	1.54
1:A:286:MET:HG3	1:A:316:ARG:CD	1.39	1.49
1:B:313:ARG:CD	1:B:314:PRO:HD2	1.42	1.49
1:B:283:LEU:CD1	1:B:316:ARG:NH2	1.77	1.46
1:D:313:ARG:CD	1:D:314:PRO:HD2	1.40	1.46
1:A:586:GLU:HB2	1:A:589:ARG:NH2	1.18	1.46
1:F:311:LEU:HA	1:F:316:ARG:NH1	1.17	1.46
1:A:286:MET:CG	1:A:316:ARG:HD3	1.43	1.45
1:B:283:LEU:CD1	1:B:316:ARG:HH21	1.28	1.45
1:F:313:ARG:CD	1:F:314:PRO:HD2	1.45	1.44
1:E:589:ARG:NH2	1:E:596:LEU:CB	1.82	1.42
1:A:316:ARG:NH1	1:A:317:PHE:CD2	1.91	1.39
1:A:316:ARG:NH1	1:A:317:PHE:CE2	1.90	1.39
1:C:589:ARG:NH2	1:C:596:LEU:CB	1.82	1.39
1:A:286:MET:SD	1:A:316:ARG:HG3	1.65	1.36
1:B:283:LEU:HD11	1:B:316:ARG:NH2	1.06	1.36
1:F:376:ALA:HA	1:F:381:ARG:CD	1.55	1.34
1:A:263:LYS:CE	1:A:276:GLU:OE1	1.77	1.33
1:A:168:LEU:O	1:A:171:ILE:HD13	1.22	1.32
1:A:586:GLU:CB	1:A:589:ARG:HH21	1.43	1.31
1:C:263:LYS:CE	1:C:276:GLU:OE1	1.77	1.31
1:F:311:LEU:CA	1:F:316:ARG:HH12	1.41	1.30
1:E:263:LYS:CE	1:E:276:GLU:OE1	1.80	1.29
1:E:286:MET:HB3	1:E:316:ARG:CG	1.61	1.29
1:A:374:LEU:HD21	1:F:187:ARG:O	1.32	1.28
1:C:303:ARG:HB2	1:C:303:ARG:NH1	1.50	1.26
1:A:311:LEU:HA	1:A:316:ARG:NH2	1.49	1.25
1:C:286:MET:HB3	1:C:316:ARG:CG	1.64	1.25
1:E:303:ARG:NH1	1:E:303:ARG:HB2	1.50	1.25
1:A:303:ARG:HB2	1:A:303:ARG:NH1	1.48	1.25
1:A:416:ALA:CB	1:A:577:LEU:CD2	1.98	1.22
1:D:382:ARG:HH11	1:D:382:ARG:CG	1.50	1.22
1:A:449:PHE:CZ	1:A:496:GLN:HG2	1.73	1.22
1:F:233:GLY:HA2	1:F:236:ARG:NH2	1.54	1.21
1:D:233:GLY:HA2	1:D:236:ARG:NH2	1.53	1.21
1:E:416:ALA:CB	1:E:577:LEU:CD2	2.02	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:381:ARG:NH2	1:D:388:ASP:OD2	1.72	1.21
1:E:589:ARG:NH2	1:E:596:LEU:HB3	1.40	1.20
1:A:286:MET:CG	1:A:316:ARG:CD	2.05	1.20
1:C:449:PHE:CZ	1:C:496:GLN:HG3	1.75	1.20
1:F:283:LEU:HD12	1:F:316:ARG:NH2	1.57	1.20
1:A:263:LYS:NZ	1:A:276:GLU:OE2	1.75	1.20
1:E:449:PHE:CZ	1:E:496:GLN:HG2	1.76	1.20
1:A:303:ARG:CB	1:A:303:ARG:HH11	1.55	1.20
1:C:286:MET:CG	1:C:316:ARG:HD2	1.70	1.19
1:A:585:GLU:O	1:A:588:GLN:HG2	1.41	1.19
1:C:303:ARG:HH11	1:C:303:ARG:CB	1.57	1.18
1:C:168:LEU:HB2	1:C:171:ILE:HD11	1.22	1.18
1:E:303:ARG:CB	1:E:303:ARG:HH11	1.57	1.18
1:C:263:LYS:NZ	1:C:276:GLU:OE2	1.76	1.18
1:B:395:ARG:HH11	1:B:395:ARG:HG2	1.09	1.17
1:C:413:ARG:HA	1:C:577:LEU:HD22	1.25	1.17
1:C:286:MET:CB	1:C:316:ARG:CD	2.21	1.17
1:C:589:ARG:NH2	1:C:596:LEU:HB3	1.49	1.17
1:A:587:PHE:O	1:A:590:VAL:HG22	1.42	1.16
1:B:318:ASP:O	1:B:319:ARG:HB2	1.46	1.16
1:E:168:LEU:HB2	1:E:171:ILE:HD11	1.18	1.16
1:E:262:ARG:HB3	1:E:275:ARG:HH12	1.10	1.15
1:D:165:LYS:O	1:D:168:LEU:N	1.80	1.15
1:D:311:LEU:O	1:D:316:ARG:HG2	1.44	1.15
1:C:589:ARG:NH2	1:C:596:LEU:HB2	1.45	1.15
1:A:172:VAL:HG23	1:A:213:ALA:HB2	1.29	1.15
1:B:165:LYS:O	1:B:168:LEU:N	1.77	1.14
1:F:165:LYS:O	1:F:168:LEU:N	1.79	1.14
1:B:233:GLY:HA2	1:B:236:ARG:HH22	1.01	1.14
1:C:428:PHE:CE1	1:C:432:ALA:HA	1.82	1.14
1:E:589:ARG:NH2	1:E:596:LEU:HB2	1.53	1.14
1:F:283:LEU:CD1	1:F:316:ARG:HH21	1.60	1.14
1:E:263:LYS:NZ	1:E:276:GLU:OE2	1.79	1.14
1:F:589:ARG:HE	1:F:594:LEU:HD21	1.08	1.14
1:F:283:LEU:CD1	1:F:316:ARG:NH2	2.10	1.14
1:C:225:PHE:CZ	1:C:278:THR:HB	1.83	1.14
1:A:524:ASP:HA	1:A:529:GLY:HA2	1.15	1.14
1:E:416:ALA:HB3	1:E:577:LEU:HD21	1.26	1.13
1:B:589:ARG:HE	1:B:594:LEU:HD21	1.07	1.13
1:A:236:ARG:HG3	1:A:237:VAL:N	1.48	1.13
1:B:165:LYS:HD3	1:B:168:LEU:HD22	1.14	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:416:ALA:CB	1:C:577:LEU:HD23	1.78	1.13
1:F:395:ARG:HG2	1:F:395:ARG:HH11	1.08	1.12
1:C:524:ASP:HA	1:C:529:GLY:HA2	1.14	1.13
1:A:416:ALA:HB3	1:A:577:LEU:HD21	1.21	1.12
1:E:236:ARG:HG3	1:E:237:VAL:N	1.50	1.12
1:E:524:ASP:HA	1:E:529:GLY:HA2	1.13	1.12
1:A:413:ARG:HA	1:A:577:LEU:HD22	1.31	1.12
1:F:165:LYS:HD3	1:F:168:LEU:HD22	1.20	1.12
1:A:170:GLU:O	1:A:174:PHE:HB3	1.49	1.12
1:A:342:LYS:NZ	1:F:184:MET:SD	2.23	1.12
1:B:171:ILE:HD11	1:B:296:VAL:HG11	1.16	1.11
1:C:182:HIS:HB2	1:C:291:LYS:HD2	1.31	1.11
1:C:236:ARG:HG3	1:C:237:VAL:N	1.48	1.11
1:D:165:LYS:HD3	1:D:168:LEU:HD22	1.17	1.11
1:D:412:ARG:HH12	1:D:440:ILE:HG21	1.15	1.11
1:D:291:LYS:HG3	1:D:292:ASP:H	1.13	1.11
1:A:286:MET:HG3	1:A:316:ARG:HD2	1.27	1.11
1:E:170:GLU:O	1:E:174:PHE:HB3	1.50	1.11
1:E:283:LEU:HG	1:E:316:ARG:NH1	1.64	1.11
1:F:286:MET:HE1	1:F:316:ARG:HA	1.11	1.11
1:B:413:ARG:HH11	1:B:413:ARG:HG2	1.11	1.11
1:D:190:LYS:HE3	1:D:289:PHE:CZ	1.85	1.10
1:E:172:VAL:HG23	1:E:213:ALA:HB2	1.24	1.10
1:D:290:GLU:HG2	1:D:293:THR:HG23	1.28	1.10
1:D:171:ILE:HD11	1:D:296:VAL:HG11	1.15	1.10
1:A:416:ALA:HB2	1:A:577:LEU:HD23	1.15	1.10
1:B:286:MET:HE1	1:B:316:ARG:HA	1.17	1.10
1:F:190:LYS:NZ	1:F:289:PHE:HE2	1.49	1.10
1:F:382:ARG:HH11	1:F:382:ARG:HG3	1.11	1.10
1:C:172:VAL:HG23	1:C:213:ALA:HB2	1.28	1.10
1:A:286:MET:SD	1:A:316:ARG:CG	2.39	1.10
1:B:290:GLU:HG2	1:B:293:THR:HG23	1.33	1.10
1:E:182:HIS:HB2	1:E:291:LYS:HD2	1.31	1.10
1:C:264:ARG:HG3	1:C:266:SER:H	1.08	1.10
1:F:356:ARG:HH11	1:F:356:ARG:HG3	1.15	1.10
1:A:262:ARG:HB3	1:A:275:ARG:HH12	1.09	1.10
1:E:147:LEU:HD21	1:E:151:PRO:HB3	1.14	1.10
1:E:264:ARG:HG3	1:E:266:SER:N	1.65	1.10
1:E:428:PHE:CE1	1:E:432:ALA:HA	1.86	1.09
1:F:474:ALA:HA	1:F:558:VAL:HG11	1.34	1.09
1:E:174:PHE:CE1	1:E:188:ILE:HD11	1.86	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:165:LYS:HE2	1:F:205:LEU:HD23	1.24	1.09
1:F:412:ARG:HH12	1:F:440:ILE:HG21	1.16	1.09
1:B:190:LYS:NZ	1:B:289:PHE:HE2	1.49	1.09
1:D:280:ASN:O	1:D:284:VAL:HG12	1.51	1.09
1:A:311:LEU:HD23	1:A:316:ARG:NH2	1.68	1.09
1:E:145:ARG:NH2	1:E:219:THR:OG1	1.84	1.09
1:F:280:ASN:O	1:F:284:VAL:HG12	1.51	1.09
1:D:376:ALA:HA	1:D:381:ARG:HG3	1.33	1.09
1:A:428:PHE:CE1	1:A:432:ALA:HA	1.86	1.09
1:E:416:ALA:HB2	1:E:577:LEU:HD23	1.21	1.09
1:A:286:MET:CB	1:A:316:ARG:HD3	1.81	1.09
1:A:378:ARG:HH22	1:F:170:GLU:HB3	1.06	1.09
1:F:171:ILE:HD11	1:F:296:VAL:HG11	1.13	1.09
1:C:264:ARG:CG	1:C:266:SER:H	1.66	1.09
1:D:589:ARG:HE	1:D:594:LEU:HD21	1.09	1.09
1:A:174:PHE:CE1	1:A:188:ILE:HD11	1.87	1.08
1:A:263:LYS:HE3	1:A:276:GLU:OE1	1.51	1.08
1:D:165:LYS:HE2	1:D:205:LEU:HD23	1.34	1.08
1:D:286:MET:HE1	1:D:316:ARG:HA	1.23	1.08
1:F:318:ASP:O	1:F:319:ARG:HB2	1.50	1.08
1:D:413:ARG:HG2	1:D:413:ARG:HH11	1.08	1.08
1:C:262:ARG:HB3	1:C:275:ARG:HH12	1.10	1.08
1:C:174:PHE:CE1	1:C:188:ILE:HD11	1.87	1.08
1:A:225:PHE:CZ	1:A:278:THR:HB	1.88	1.08
1:E:225:PHE:CZ	1:E:278:THR:HB	1.88	1.08
1:F:283:LEU:HD12	1:F:316:ARG:HH21	0.92	1.08
1:D:276:GLU:HA	1:D:279:LEU:HD13	1.33	1.08
1:E:453:ARG:NH2	1:E:460:TRP:HE1	1.52	1.08
1:B:382:ARG:HH11	1:B:382:ARG:HG3	1.10	1.08
1:F:238:ARG:NH1	1:F:239:ASP:N	2.02	1.08
1:F:238:ARG:NH1	1:F:239:ASP:H	1.50	1.08
1:E:413:ARG:HA	1:E:577:LEU:HD22	1.32	1.07
1:A:182:HIS:HB2	1:A:291:LYS:HD2	1.27	1.07
1:D:316:ARG:HH11	1:D:316:ARG:HG3	0.99	1.07
1:D:318:ASP:O	1:D:319:ARG:HB2	1.48	1.07
1:C:170:GLU:O	1:C:174:PHE:HB3	1.50	1.07
1:A:311:LEU:CD2	1:A:316:ARG:NH2	2.17	1.07
1:C:453:ARG:NH2	1:C:460:TRP:HE1	1.51	1.07
1:B:474:ALA:HA	1:B:558:VAL:HG11	1.33	1.07
1:B:276:GLU:HA	1:B:279:LEU:HD13	1.32	1.07
1:B:280:ASN:O	1:B:284:VAL:HG12	1.52	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:LEU:HD21	1:C:151:PRO:HB3	1.13	1.07
1:D:190:LYS:HE3	1:D:289:PHE:CE2	1.90	1.07
1:C:264:ARG:HG3	1:C:266:SER:N	1.69	1.07
1:A:342:LYS:HD2	1:A:343:PRO:HD2	1.35	1.06
1:A:453:ARG:NH2	1:A:460:TRP:HE1	1.52	1.06
1:F:400:PRO:O	1:F:404:SER:N	1.87	1.06
1:D:459:HIS:ND1	1:D:459:HIS:O	1.88	1.06
1:A:313:ARG:NH2	1:A:526:TYR:HA	1.70	1.06
1:A:264:ARG:HG3	1:A:266:SER:H	1.12	1.05
1:C:263:LYS:HD2	1:C:276:GLU:CD	1.75	1.05
1:A:449:PHE:CE2	1:A:496:GLN:HG2	1.90	1.05
1:D:313:ARG:CD	1:D:314:PRO:CD	2.34	1.05
1:C:449:PHE:CE2	1:C:496:GLN:HG3	1.90	1.05
1:D:400:PRO:O	1:D:404:SER:N	1.87	1.05
1:B:356:ARG:HG3	1:B:356:ARG:HH11	1.16	1.05
1:B:238:ARG:NH1	1:B:239:ASP:H	1.55	1.05
1:B:412:ARG:NH1	1:B:440:ILE:HG21	1.72	1.05
1:E:313:ARG:NH2	1:E:526:TYR:HA	1.69	1.05
1:E:237:VAL:HG11	1:E:281:GLN:HB3	1.38	1.05
1:E:286:MET:CB	1:E:316:ARG:HG2	1.87	1.05
1:D:356:ARG:HH11	1:D:356:ARG:HG3	1.14	1.05
1:D:395:ARG:HH11	1:D:395:ARG:HG2	1.16	1.05
1:D:412:ARG:NH1	1:D:440:ILE:HG21	1.69	1.05
1:F:412:ARG:NH1	1:F:440:ILE:HG21	1.70	1.05
1:E:342:LYS:HD2	1:E:343:PRO:HD2	1.39	1.05
1:A:262:ARG:HG2	1:A:275:ARG:HH22	1.22	1.04
1:B:376:ALA:C	1:B:381:ARG:HD2	1.76	1.04
1:F:276:GLU:HA	1:F:279:LEU:HD13	1.35	1.04
1:D:474:ALA:HA	1:D:558:VAL:HG11	1.37	1.04
1:E:264:ARG:HG3	1:E:266:SER:H	0.88	1.04
1:C:225:PHE:HE1	1:C:233:GLY:CA	1.69	1.04
1:A:168:LEU:HB2	1:A:171:ILE:HD11	1.38	1.04
1:A:237:VAL:HG11	1:A:281:GLN:HB3	1.35	1.04
1:C:342:LYS:HD2	1:C:343:PRO:HD2	1.37	1.04
1:C:263:LYS:HE3	1:C:276:GLU:OE1	1.55	1.04
1:C:286:MET:HB2	1:C:316:ARG:HD3	1.39	1.04
1:B:238:ARG:NH1	1:B:239:ASP:N	2.04	1.04
1:A:147:LEU:HD21	1:A:151:PRO:CB	1.87	1.04
1:B:400:PRO:O	1:B:404:SER:N	1.89	1.04
1:F:326:PRO:HB3	1:F:360:PHE:O	1.56	1.04
1:B:313:ARG:CD	1:B:314:PRO:CD	2.36	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:313:ARG:HD2	1:F:314:PRO:HD2	1.05	1.04
1:A:263:LYS:HD2	1:A:276:GLU:CD	1.77	1.04
1:C:263:LYS:NZ	1:C:276:GLU:CD	2.10	1.04
1:E:533:ARG:NH2	1:E:534:GLN:O	1.91	1.04
1:D:238:ARG:NH1	1:D:239:ASP:N	2.05	1.03
1:A:263:LYS:NZ	1:A:276:GLU:CD	2.11	1.03
1:A:147:LEU:HD21	1:A:151:PRO:HB3	1.04	1.03
1:A:225:PHE:HE1	1:A:233:GLY:CA	1.71	1.03
1:F:482:VAL:HG13	1:F:483:PHE:HD2	1.24	1.03
1:E:152:LYS:HG3	1:E:153:VAL:HG23	1.39	1.03
1:B:376:ALA:CA	1:B:381:ARG:CD	2.10	1.03
1:E:263:LYS:HD2	1:E:276:GLU:CD	1.79	1.03
1:B:482:VAL:HG13	1:B:483:PHE:HD2	1.21	1.03
1:B:337:ILE:HD12	1:B:340:ARG:HH12	1.19	1.03
1:E:147:LEU:HD21	1:E:151:PRO:CB	1.88	1.03
1:A:342:LYS:HD3	1:F:184:MET:O	1.58	1.03
1:C:166:GLU:HB2	1:C:169:LYS:HZ2	1.22	1.03
1:B:237:VAL:O	1:B:240:LEU:HB3	1.57	1.03
1:D:382:ARG:HH11	1:D:382:ARG:HG3	0.87	1.02
1:F:290:GLU:HG2	1:F:293:THR:HG23	1.40	1.02
1:A:264:ARG:CG	1:A:266:SER:H	1.71	1.02
1:E:225:PHE:HE1	1:E:233:GLY:CA	1.72	1.02
1:B:412:ARG:HH12	1:B:440:ILE:HG21	1.23	1.02
1:E:263:LYS:NZ	1:E:276:GLU:CD	2.12	1.02
1:E:449:PHE:CE2	1:E:496:GLN:HG2	1.93	1.02
1:A:374:LEU:HD11	1:F:187:ARG:H	1.24	1.02
1:E:448:GLY:O	1:E:452:PRO:HD2	1.60	1.01
1:C:237:VAL:HG11	1:C:281:GLN:HB3	1.37	1.01
1:C:286:MET:HB3	1:C:316:ARG:HG2	1.04	1.01
1:D:326:PRO:HB3	1:D:360:PHE:O	1.58	1.01
1:C:218:ILE:HD11	1:C:250:CYS:SG	2.00	1.01
1:C:147:LEU:HD21	1:C:151:PRO:CB	1.88	1.01
1:B:165:LYS:HE2	1:B:205:LEU:HD23	1.38	1.01
1:E:263:LYS:HE3	1:E:276:GLU:OE1	1.58	1.01
1:A:533:ARG:NH2	1:A:534:GLN:O	1.94	1.01
1:D:348:VAL:CG2	1:D:352:LEU:HD22	1.91	1.01
1:B:459:HIS:O	1:B:459:HIS:ND1	1.92	1.01
1:C:152:LYS:HG3	1:C:153:VAL:HG23	1.42	1.01
1:A:218:ILE:HD11	1:A:250:CYS:SG	2.01	1.01
1:D:316:ARG:HH11	1:D:316:ARG:CG	1.71	1.01
1:F:302:ASN:HD21	1:F:443:ARG:HH22	1.05	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:PRO:HB3	1:B:360:PHE:O	1.60	1.01
1:E:286:MET:CB	1:E:316:ARG:CD	2.39	1.01
1:C:589:ARG:HB3	1:C:589:ARG:NH1	1.76	1.01
1:D:453:ARG:CZ	1:D:495:ARG:HH21	1.73	1.01
1:B:311:LEU:HA	1:B:316:ARG:NH1	1.75	1.00
1:D:313:ARG:HD2	1:D:314:PRO:HD2	1.01	1.00
1:C:286:MET:HG3	1:C:316:ARG:CD	1.90	1.00
1:D:382:ARG:NH1	1:D:382:ARG:HG3	1.69	1.00
1:D:348:VAL:HG21	1:D:352:LEU:HD22	1.43	1.00
1:D:238:ARG:NH1	1:D:239:ASP:H	1.56	1.00
1:C:416:ALA:HB3	1:C:577:LEU:HD23	1.01	1.00
1:A:152:LYS:HG3	1:A:153:VAL:HG23	1.44	1.00
1:E:589:ARG:HH21	1:E:596:LEU:HB3	0.98	1.00
1:E:286:MET:HG3	1:E:316:ARG:HD2	1.40	1.00
1:B:439:THR:HG23	1:B:445:ARG:HH22	1.25	1.00
1:C:589:ARG:HH21	1:C:596:LEU:HB3	0.95	1.00
1:B:263:LYS:NZ	1:C:227:GLU:HG3	1.77	1.00
1:E:212:GLU:C	1:E:214:ARG:HG3	1.82	0.99
1:A:378:ARG:HH22	1:F:170:GLU:CB	1.75	0.99
1:B:348:VAL:CG2	1:B:352:LEU:HD22	1.92	0.99
1:D:439:THR:HG23	1:D:445:ARG:HH22	1.23	0.99
1:A:166:GLU:HA	1:A:169:LYS:HG2	1.42	0.99
1:E:173:GLU:HA	1:E:176:LYS:CG	1.92	0.99
1:B:262:ARG:HG3	1:B:263:LYS:N	1.77	0.99
1:B:236:ARG:HH12	1:B:278:THR:HG22	1.26	0.99
1:D:381:ARG:HH22	1:D:388:ASP:CG	1.66	0.99
1:F:313:ARG:CD	1:F:314:PRO:CD	2.40	0.99
1:C:263:LYS:CD	1:C:276:GLU:OE1	2.11	0.99
1:F:190:LYS:NZ	1:F:289:PHE:CE2	2.28	0.99
1:B:313:ARG:HD2	1:B:314:PRO:HD2	1.02	0.98
1:D:313:ARG:CG	1:D:314:PRO:HD2	1.93	0.98
1:F:165:LYS:HE2	1:F:205:LEU:CD2	1.93	0.98
1:E:589:ARG:HB3	1:E:589:ARG:NH1	1.78	0.98
1:A:264:ARG:HG3	1:A:266:SER:N	1.77	0.98
1:F:453:ARG:NH1	1:F:495:ARG:HH21	1.59	0.98
1:C:313:ARG:NH2	1:C:526:TYR:HA	1.77	0.98
1:A:586:GLU:HA	1:A:589:ARG:NE	1.77	0.98
1:F:459:HIS:O	1:F:459:HIS:ND1	1.94	0.98
1:A:311:LEU:CA	1:A:316:ARG:HH22	1.75	0.98
1:D:233:GLY:HA2	1:D:236:ARG:HH22	1.15	0.98
1:D:319:ARG:HG2	1:D:319:ARG:HH11	1.26	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:174:PHE:CZ	1:E:188:ILE:CD1	2.47	0.98
1:A:378:ARG:NH2	1:F:170:GLU:HB3	1.78	0.98
1:E:413:ARG:HA	1:E:577:LEU:CD2	1.93	0.98
1:D:376:ALA:CA	1:D:381:ARG:HG3	1.92	0.98
1:E:262:ARG:HG2	1:E:275:ARG:HH22	1.24	0.98
1:F:262:ARG:HG3	1:F:263:LYS:N	1.78	0.98
1:C:286:MET:CG	1:C:316:ARG:CD	2.41	0.98
1:C:190:LYS:HD2	1:C:289:PHE:CE1	1.98	0.98
1:E:218:ILE:HD11	1:E:250:CYS:SG	2.04	0.98
1:C:166:GLU:HA	1:C:169:LYS:HG2	1.46	0.98
1:A:174:PHE:CZ	1:A:188:ILE:CD1	2.47	0.98
1:A:311:LEU:CA	1:A:316:ARG:NH2	2.26	0.98
1:B:522:ARG:HD2	1:B:530:TYR:HA	1.46	0.98
1:D:262:ARG:HG3	1:D:263:LYS:N	1.77	0.97
1:C:286:MET:HG3	1:C:316:ARG:HD2	0.99	0.97
1:D:188:ILE:HG23	1:D:189:PRO:HD2	1.45	0.97
1:B:348:VAL:HG21	1:B:352:LEU:HD22	1.46	0.97
1:C:416:ALA:HB3	1:C:577:LEU:CD2	1.94	0.97
1:B:313:ARG:CG	1:B:314:PRO:HD2	1.94	0.97
1:C:326:PRO:HB3	1:C:360:PHE:O	1.63	0.97
1:C:145:ARG:NH2	1:C:219:THR:OG1	1.97	0.97
1:C:262:ARG:HG2	1:C:275:ARG:HH22	1.25	0.97
1:A:448:GLY:O	1:A:452:PRO:HD2	1.62	0.97
1:E:524:ASP:HA	1:E:529:GLY:CA	1.94	0.97
1:E:286:MET:HB3	1:E:316:ARG:HG2	0.99	0.97
1:A:571:ARG:HD2	1:A:590:VAL:O	1.64	0.97
1:A:378:ARG:HA	1:F:173:GLU:OE1	1.63	0.97
1:F:171:ILE:CD1	1:F:296:VAL:HG11	1.93	0.97
1:D:337:ILE:HD12	1:D:340:ARG:HH12	1.29	0.97
1:F:275:ARG:O	1:F:278:THR:OG1	1.82	0.97
1:C:448:GLY:O	1:C:452:PRO:HD2	1.64	0.97
1:D:482:VAL:HG13	1:D:483:PHE:HD2	1.25	0.97
1:A:145:ARG:NH2	1:A:219:THR:OG1	1.96	0.97
1:A:316:ARG:NH1	1:A:317:PHE:HD2	1.50	0.97
1:A:286:MET:SD	1:A:316:ARG:CD	2.53	0.96
1:B:453:ARG:CZ	1:B:495:ARG:HH21	1.77	0.96
1:B:233:GLY:CA	1:B:236:ARG:HH22	1.78	0.96
1:B:187:ARG:O	1:C:374:LEU:HD21	1.63	0.96
1:E:283:LEU:HG	1:E:316:ARG:HH12	1.29	0.96
1:C:215:VAL:HG21	1:C:250:CYS:HA	1.48	0.96
1:B:453:ARG:NH1	1:B:495:ARG:HH21	1.62	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:ILE:CD1	1:B:296:VAL:HG11	1.96	0.96
1:A:292:ASP:HB2	1:B:227:GLU:OE2	1.63	0.96
1:D:171:ILE:CD1	1:D:296:VAL:HG11	1.94	0.96
1:B:188:ILE:HG23	1:B:189:PRO:HD2	1.44	0.96
1:F:291:LYS:HG3	1:F:292:ASP:H	1.31	0.96
1:A:586:GLU:CB	1:A:589:ARG:NH2	2.14	0.96
1:D:184:MET:SD	1:E:342:LYS:NZ	2.39	0.96
1:B:190:LYS:NZ	1:B:289:PHE:CE2	2.26	0.96
1:D:275:ARG:O	1:D:278:THR:OG1	1.82	0.96
1:A:374:LEU:CD2	1:F:187:ARG:O	2.14	0.96
1:C:263:LYS:NZ	1:C:276:GLU:OE1	1.99	0.96
1:D:313:ARG:HD2	1:D:314:PRO:CD	1.93	0.96
1:B:260:VAL:O	1:B:279:LEU:HD11	1.66	0.95
1:F:260:VAL:O	1:F:279:LEU:HD11	1.64	0.95
1:B:165:LYS:HD3	1:B:168:LEU:CD2	1.96	0.95
1:E:215:VAL:HG21	1:E:250:CYS:HA	1.47	0.95
1:A:227:GLU:HG3	1:F:263:LYS:NZ	1.81	0.95
1:F:337:ILE:HD12	1:F:340:ARG:HH12	1.30	0.95
1:C:174:PHE:CZ	1:C:188:ILE:CD1	2.48	0.95
1:E:326:PRO:HB3	1:E:360:PHE:O	1.64	0.95
1:A:166:GLU:HB2	1:A:169:LYS:HZ2	1.31	0.95
1:D:439:THR:HG23	1:D:445:ARG:NH2	1.80	0.95
1:B:578:GLU:HG2	1:B:579:ARG:N	1.81	0.95
1:E:263:LYS:NZ	1:E:276:GLU:OE1	1.99	0.95
1:F:313:ARG:CG	1:F:314:PRO:HD2	1.96	0.95
1:B:275:ARG:O	1:B:278:THR:OG1	1.83	0.95
1:D:302:ASN:HD21	1:D:443:ARG:HH22	1.06	0.95
1:A:263:LYS:CD	1:A:276:GLU:OE1	2.14	0.94
1:C:520:ALA:HA	1:C:533:ARG:HD3	1.48	0.94
1:D:487:THR:HG22	1:D:488:THR:H	1.30	0.94
1:A:524:ASP:HA	1:A:529:GLY:CA	1.97	0.94
1:A:190:LYS:HD2	1:A:289:PHE:CE1	2.02	0.94
1:B:310:ALA:C	1:B:316:ARG:NH1	2.21	0.94
1:B:313:ARG:HD2	1:B:314:PRO:CD	1.93	0.94
1:F:319:ARG:HH11	1:F:319:ARG:HG2	1.32	0.94
1:E:511:HIS:NE2	1:E:516:PRO:HD3	1.81	0.94
1:A:215:VAL:HG21	1:A:250:CYS:HA	1.49	0.94
1:F:311:LEU:CA	1:F:316:ARG:NH1	2.10	0.94
1:C:275:ARG:HG2	1:C:275:ARG:HH11	1.26	0.94
1:A:520:ALA:HA	1:A:533:ARG:HD3	1.48	0.94
1:F:412:ARG:HH12	1:F:440:ILE:CG2	1.81	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:VAL:O	1:D:279:LEU:HD11	1.68	0.94
1:B:203:THR:OG1	2:B:2001:ADP:O2A	1.84	0.94
1:D:190:LYS:NZ	1:D:289:PHE:HE2	1.65	0.94
1:D:453:ARG:NH1	1:D:495:ARG:HH21	1.65	0.94
1:A:413:ARG:HA	1:A:577:LEU:CD2	1.98	0.94
1:F:376:ALA:CA	1:F:381:ARG:CD	2.28	0.94
1:B:319:ARG:HG2	1:B:319:ARG:HH11	1.32	0.94
1:E:166:GLU:HA	1:E:169:LYS:HG2	1.46	0.94
1:D:263:LYS:NZ	1:E:227:GLU:HG3	1.82	0.94
1:A:582:LEU:HD23	1:A:587:PHE:HA	1.49	0.94
1:F:578:GLU:HG2	1:F:579:ARG:N	1.81	0.94
1:C:582:LEU:HD23	1:C:587:PHE:HA	1.49	0.94
1:C:533:ARG:NH2	1:C:534:GLN:O	2.01	0.94
1:E:520:ALA:HA	1:E:533:ARG:HD3	1.50	0.94
1:A:511:HIS:NE2	1:A:516:PRO:HD3	1.83	0.94
1:F:188:ILE:HG23	1:F:189:PRO:HD2	1.47	0.94
1:A:586:GLU:HB2	1:A:589:ARG:CZ	1.96	0.94
1:C:524:ASP:HA	1:C:529:GLY:CA	1.97	0.94
1:E:201:GLY:N	2:E:1001:ADP:O1A	2.01	0.94
1:B:579:ARG:O	1:B:579:ARG:HG2	1.65	0.93
1:D:233:GLY:CA	1:D:236:ARG:HH22	1.80	0.93
1:C:286:MET:CB	1:C:316:ARG:HD3	1.90	0.93
1:B:302:ASN:HD21	1:B:443:ARG:HH22	1.06	0.93
1:B:487:THR:HG22	1:B:488:THR:H	1.31	0.93
1:A:173:GLU:HA	1:A:176:LYS:CG	1.98	0.93
1:A:215:VAL:HG23	1:A:216:PRO:HD2	1.48	0.93
1:D:190:LYS:CE	1:D:289:PHE:CE2	2.52	0.93
1:C:201:GLY:N	2:C:1001:ADP:O1A	1.99	0.93
1:D:412:ARG:HH12	1:D:440:ILE:CG2	1.80	0.93
1:B:233:GLY:HA2	1:B:236:ARG:NH2	1.82	0.93
1:F:376:ALA:CB	1:F:381:ARG:HD2	1.98	0.93
1:D:233:GLY:CA	1:D:236:ARG:NH2	2.32	0.93
1:D:522:ARG:HD2	1:D:530:TYR:HA	1.50	0.93
1:F:453:ARG:CZ	1:F:495:ARG:HH21	1.80	0.93
1:B:283:LEU:HD12	1:B:316:ARG:HH21	1.32	0.93
1:A:263:LYS:NZ	1:A:276:GLU:OE1	2.00	0.93
1:C:533:ARG:HD2	1:C:534:GLN:H	1.34	0.93
1:D:385:THR:OG1	1:D:388:ASP:OD1	1.86	0.93
1:C:215:VAL:HG23	1:C:216:PRO:HD2	1.51	0.93
1:E:589:ARG:HH22	1:E:596:LEU:CB	1.70	0.93
1:A:147:LEU:CD2	1:A:151:PRO:HB3	1.96	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:291:LYS:HG3	1:D:292:ASP:N	1.81	0.93
1:E:236:ARG:HH11	1:E:236:ARG:HG2	1.32	0.93
1:B:291:LYS:HG3	1:B:292:ASP:H	1.34	0.93
1:E:582:LEU:HD23	1:E:587:PHE:HA	1.48	0.93
1:B:352:LEU:HD23	1:B:353:LEU:N	1.82	0.93
1:B:310:ALA:O	1:B:316:ARG:NH1	2.02	0.93
1:F:237:VAL:O	1:F:240:LEU:HB3	1.69	0.93
1:C:236:ARG:HG2	1:C:236:ARG:HH11	1.32	0.93
1:E:286:MET:HE1	1:E:297:VAL:HG11	1.50	0.92
1:F:215:VAL:CG2	1:F:216:PRO:HD2	1.99	0.92
1:E:263:LYS:CD	1:E:276:GLU:OE1	2.15	0.92
1:A:460:TRP:O	1:B:488:THR:HA	1.68	0.92
1:D:165:LYS:HD3	1:D:168:LEU:CD2	1.98	0.92
1:A:262:ARG:CB	1:A:275:ARG:HH12	1.82	0.92
1:F:165:LYS:NZ	1:F:205:LEU:HB3	1.84	0.92
1:C:586:GLU:HA	1:C:589:ARG:HG3	1.51	0.92
1:B:381:ARG:NH1	1:B:388:ASP:OD2	2.02	0.92
1:E:166:GLU:HB2	1:E:169:LYS:HZ2	1.31	0.92
1:D:352:LEU:HD23	1:D:353:LEU:N	1.84	0.92
1:C:173:GLU:HA	1:C:176:LYS:CG	1.98	0.92
1:B:439:THR:HG23	1:B:445:ARG:NH2	1.83	0.92
1:A:311:LEU:CB	1:A:316:ARG:HH22	1.82	0.92
1:D:190:LYS:NZ	1:D:289:PHE:CE2	2.37	0.92
1:D:190:LYS:CE	1:D:289:PHE:CZ	2.51	0.92
1:F:165:LYS:HD3	1:F:168:LEU:CD2	1.99	0.92
1:F:522:ARG:HD2	1:F:530:TYR:HA	1.49	0.92
1:D:215:VAL:CG2	1:D:216:PRO:HD2	2.00	0.92
1:A:453:ARG:NH1	1:A:460:TRP:CZ2	2.36	0.92
1:D:578:GLU:HG2	1:D:579:ARG:N	1.80	0.92
1:B:153:VAL:HG13	1:B:154:THR:N	1.85	0.92
1:A:316:ARG:NH1	1:A:317:PHE:HE2	1.51	0.91
1:D:454:ARG:NH2	1:D:526:TYR:O	2.02	0.91
1:E:190:LYS:HD2	1:E:289:PHE:CE1	2.05	0.91
1:F:233:GLY:CA	1:F:236:ARG:HH22	1.81	0.91
1:C:286:MET:HE1	1:C:297:VAL:HG11	1.51	0.91
1:A:453:ARG:HH11	1:A:453:ARG:HG3	1.34	0.91
1:A:453:ARG:NH1	1:A:460:TRP:HZ2	1.67	0.91
1:B:460:TRP:HE3	1:B:460:TRP:H	1.18	0.91
1:B:454:ARG:NH2	1:B:526:TYR:O	2.02	0.91
1:A:481:ILE:HD12	1:A:563:LEU:HB3	1.51	0.91
1:C:511:HIS:NE2	1:C:516:PRO:HD3	1.84	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:439:THR:HG23	1:F:445:ARG:HH22	1.34	0.91
1:C:382:ARG:HG3	1:C:383:LYS:N	1.85	0.91
1:D:316:ARG:NH1	1:D:316:ARG:HG3	1.83	0.91
1:F:233:GLY:CA	1:F:236:ARG:NH2	2.32	0.91
1:C:174:PHE:CZ	1:C:188:ILE:HD11	2.06	0.91
1:D:257:ILE:O	1:D:260:VAL:N	2.03	0.91
1:F:313:ARG:HD2	1:F:314:PRO:CD	1.97	0.91
1:C:274:GLU:O	1:C:277:GLN:HB3	1.70	0.91
1:A:174:PHE:CZ	1:A:188:ILE:HD11	2.05	0.91
1:C:589:ARG:HH22	1:C:596:LEU:CB	1.75	0.91
1:C:313:ARG:NH1	1:C:526:TYR:O	2.04	0.91
1:D:346:GLU:HG2	1:D:348:VAL:H	1.36	0.90
1:E:166:GLU:HB2	1:E:169:LYS:NZ	1.86	0.90
1:A:168:LEU:O	1:A:171:ILE:CD1	2.17	0.90
1:B:165:LYS:CD	1:B:168:LEU:HD22	2.01	0.90
1:C:262:ARG:CB	1:C:275:ARG:HH12	1.84	0.90
1:C:155:PHE:HD2	1:C:212:GLU:OE1	1.54	0.90
1:B:283:LEU:HD11	1:B:316:ARG:HH22	1.09	0.90
1:E:274:GLU:O	1:E:277:GLN:HB3	1.70	0.90
1:E:174:PHE:CZ	1:E:188:ILE:HD11	2.05	0.90
1:E:215:VAL:HG23	1:E:216:PRO:HD2	1.51	0.90
1:F:238:ARG:HH12	1:F:239:ASP:HB3	1.36	0.90
1:C:166:GLU:HB2	1:C:169:LYS:NZ	1.85	0.90
1:B:238:ARG:HH12	1:B:239:ASP:HB3	1.35	0.90
1:E:286:MET:HB2	1:E:316:ARG:HD3	1.54	0.90
1:A:313:ARG:HH22	1:A:526:TYR:C	1.75	0.90
1:B:412:ARG:HH12	1:B:440:ILE:CG2	1.85	0.90
1:A:236:ARG:HH11	1:A:236:ARG:HG2	1.33	0.90
1:D:453:ARG:NH1	1:D:495:ARG:NH2	2.20	0.90
1:A:201:GLY:N	2:A:1001:ADP:O1A	2.03	0.90
1:A:168:LEU:HB2	1:A:171:ILE:CD1	2.01	0.90
1:B:376:ALA:CB	1:B:381:ARG:HD2	2.01	0.90
1:B:376:ALA:HA	1:B:381:ARG:NE	1.87	0.89
1:E:262:ARG:CB	1:E:275:ARG:HH12	1.83	0.89
1:F:487:THR:HG22	1:F:488:THR:H	1.36	0.89
1:C:286:MET:CB	1:C:316:ARG:CG	2.47	0.89
1:E:449:PHE:CB	1:E:468:GLN:NE2	2.35	0.89
1:B:215:VAL:CG2	1:B:216:PRO:HD2	2.01	0.89
1:B:395:ARG:NH1	1:B:395:ARG:HG2	1.83	0.89
1:C:292:ASP:HB2	1:D:227:GLU:OE2	1.72	0.89
1:A:236:ARG:CG	1:A:237:VAL:N	2.35	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:VAL:O	1:D:240:LEU:HB3	1.71	0.89
1:F:238:ARG:HG2	1:F:281:GLN:NE2	1.88	0.89
1:C:519:TYR:O	1:C:533:ARG:NE	2.05	0.89
1:D:352:LEU:HD21	1:D:386:MET:HE1	1.55	0.89
1:B:413:ARG:NH1	1:B:413:ARG:HG2	1.78	0.89
1:F:439:THR:HG23	1:F:445:ARG:NH2	1.88	0.89
1:F:454:ARG:NH2	1:F:526:TYR:O	2.05	0.89
1:E:588:GLN:O	1:E:591:VAL:HB	1.72	0.89
1:B:171:ILE:HD11	1:B:296:VAL:CG1	2.03	0.89
1:D:460:TRP:HE3	1:D:460:TRP:H	1.20	0.89
1:A:533:ARG:HD2	1:A:534:GLN:H	1.35	0.89
1:D:165:LYS:HE2	1:D:205:LEU:CD2	2.02	0.89
1:A:412:ARG:NH1	1:A:577:LEU:O	2.05	0.89
1:E:236:ARG:CG	1:E:237:VAL:N	2.36	0.89
1:E:286:MET:CB	1:E:316:ARG:HD3	2.03	0.89
1:E:412:ARG:NH1	1:E:577:LEU:O	2.06	0.89
1:A:286:MET:HG3	1:A:316:ARG:HD3	0.99	0.89
1:F:233:GLY:HA2	1:F:236:ARG:HH22	1.17	0.89
1:F:257:ILE:O	1:F:260:VAL:N	2.05	0.89
1:C:263:LYS:CD	1:C:276:GLU:CD	2.40	0.89
1:E:533:ARG:HD2	1:E:534:GLN:H	1.36	0.89
1:F:171:ILE:HD11	1:F:296:VAL:CG1	2.01	0.88
1:F:190:LYS:HE3	1:F:289:PHE:CE2	2.08	0.88
1:C:155:PHE:CZ	1:C:168:LEU:HD11	2.08	0.88
1:B:238:ARG:HG2	1:B:281:GLN:NE2	1.88	0.88
1:A:456:ASP:OD1	1:A:457:MET:N	2.06	0.88
1:A:311:LEU:HA	1:A:316:ARG:HH21	1.30	0.88
1:A:588:GLN:O	1:A:591:VAL:HB	1.73	0.88
1:C:286:MET:CB	1:C:316:ARG:HG2	1.98	0.88
1:D:327:ASP:OD1	1:D:328:VAL:N	2.06	0.88
1:A:166:GLU:HB2	1:A:169:LYS:NZ	1.89	0.88
1:C:589:ARG:HH21	1:C:596:LEU:CB	1.64	0.88
1:C:147:LEU:CD2	1:C:151:PRO:HB3	2.02	0.88
1:E:313:ARG:HH22	1:E:526:TYR:HA	1.39	0.88
1:F:453:ARG:NH1	1:F:495:ARG:NH2	2.20	0.88
1:C:286:MET:HB3	1:C:316:ARG:CD	1.94	0.88
1:C:313:ARG:HH22	1:C:526:TYR:C	1.77	0.88
1:A:378:ARG:NH2	1:F:170:GLU:CB	2.34	0.88
1:D:471:VAL:O	1:D:474:ALA:HB3	1.74	0.88
1:B:356:ARG:CG	1:B:356:ARG:HH11	1.86	0.88
1:B:184:MET:SD	1:C:342:LYS:NZ	2.46	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:LYS:HE2	1:B:578:GLU:O	1.72	0.88
1:E:176:LYS:HD3	1:E:213:ALA:HA	1.54	0.88
1:E:211:GLY:O	1:E:214:ARG:HD2	1.72	0.88
1:C:412:ARG:NH1	1:C:577:LEU:O	2.06	0.88
1:A:326:PRO:HB3	1:A:360:PHE:O	1.73	0.88
1:B:382:ARG:NH1	1:B:382:ARG:HG3	1.74	0.88
1:D:165:LYS:CD	1:D:168:LEU:HD22	2.03	0.88
1:D:168:LEU:O	1:D:171:ILE:HG22	1.73	0.88
1:D:173:GLU:O	1:D:176:LYS:HG2	1.74	0.88
1:A:384:ILE:HG23	1:A:388:ASP:HB2	1.56	0.88
1:A:311:LEU:CD2	1:A:316:ARG:HH22	1.88	0.87
1:A:453:ARG:HH22	1:A:464:ARG:HH12	1.23	0.87
1:B:482:VAL:HG13	1:B:483:PHE:CD2	2.09	0.87
1:F:302:ASN:HD21	1:F:443:ARG:NH2	1.71	0.87
1:E:173:GLU:HA	1:E:176:LYS:HG3	1.52	0.87
1:E:313:ARG:NH1	1:E:526:TYR:O	2.07	0.87
1:C:384:ILE:HG23	1:C:388:ASP:HB2	1.56	0.87
1:B:503:ARG:HH22	1:B:522:ARG:NH2	1.73	0.87
1:E:456:ASP:OD1	1:E:457:MET:N	2.07	0.87
1:B:173:GLU:O	1:B:176:LYS:HG2	1.74	0.87
1:B:257:ILE:O	1:B:260:VAL:N	2.07	0.87
1:D:238:ARG:HH12	1:D:239:ASP:HB3	1.36	0.87
1:E:147:LEU:CD2	1:E:151:PRO:HB3	2.02	0.87
1:F:159:ALA:HB3	1:F:334:ILE:HG13	1.57	0.87
1:F:165:LYS:CD	1:F:168:LEU:HD22	2.04	0.87
1:A:263:LYS:CD	1:A:276:GLU:CD	2.42	0.87
1:B:453:ARG:NH1	1:B:495:ARG:NH2	2.23	0.87
1:C:430:GLU:O	1:C:431:HIS:HB3	1.75	0.87
1:F:345:ALA:HB2	1:F:383:LYS:HE3	1.56	0.87
1:F:395:ARG:HG2	1:F:395:ARG:NH1	1.81	0.87
1:E:453:ARG:HH22	1:E:460:TRP:HE1	1.21	0.87
1:A:449:PHE:CB	1:A:468:GLN:NE2	2.38	0.87
1:E:313:ARG:HH22	1:E:526:TYR:CA	1.87	0.87
1:A:155:PHE:HD2	1:A:212:GLU:OE1	1.58	0.87
1:F:460:TRP:H	1:F:460:TRP:HE3	1.19	0.87
1:F:470:ALA:O	1:F:558:VAL:HG21	1.74	0.87
1:D:301:THR:HG21	1:D:307:LEU:HD11	1.56	0.87
1:C:410:ARG:O	1:C:413:ARG:N	2.07	0.87
1:E:313:ARG:HH22	1:E:526:TYR:C	1.77	0.87
1:D:238:ARG:HG2	1:D:281:GLN:NE2	1.90	0.87
1:F:286:MET:HE1	1:F:316:ARG:CA	2.03	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:ILE:HD11	1:D:296:VAL:CG1	2.02	0.87
1:D:338:HIS:ND1	1:D:366:GLU:HG3	1.90	0.87
1:D:175:LEU:HD12	1:D:215:VAL:HG11	1.57	0.86
1:E:172:VAL:CG2	1:E:213:ALA:HB2	2.05	0.86
1:F:190:LYS:CE	1:F:289:PHE:CE2	2.57	0.86
1:B:175:LEU:HD12	1:B:215:VAL:HG11	1.57	0.86
1:B:291:LYS:HG3	1:B:292:ASP:N	1.89	0.86
1:D:153:VAL:HG13	1:D:154:THR:N	1.90	0.86
1:D:253:PHE:HE2	1:D:255:ASP:HB2	1.38	0.86
1:C:176:LYS:HD3	1:C:213:ALA:HA	1.55	0.86
1:B:283:LEU:HD12	1:B:316:ARG:NH2	1.86	0.86
1:B:301:THR:HG21	1:B:307:LEU:HD11	1.57	0.86
1:F:370:ASN:OD1	1:F:371:GLU:N	2.08	0.86
1:C:536:SER:OG	1:D:544:ASP:OD2	1.94	0.86
1:D:164:ALA:O	1:D:168:LEU:HD13	1.73	0.86
1:D:370:ASN:OD1	1:D:371:GLU:N	2.08	0.86
1:A:342:LYS:CD	1:A:343:PRO:HD2	2.04	0.86
1:F:173:GLU:O	1:F:176:LYS:HG2	1.75	0.86
1:E:263:LYS:CD	1:E:276:GLU:CD	2.44	0.86
1:C:308:ASP:OD1	1:C:310:ALA:N	2.09	0.86
1:A:313:ARG:CZ	1:A:526:TYR:HA	2.05	0.86
1:C:588:GLN:O	1:C:591:VAL:HB	1.75	0.86
1:C:467:ASP:OD1	1:C:557:ARG:NH2	2.08	0.86
1:D:345:ALA:HB2	1:D:383:LYS:HE3	1.55	0.86
1:E:428:PHE:CD1	1:E:432:ALA:HA	2.11	0.86
1:E:481:ILE:HD12	1:E:563:LEU:HB3	1.55	0.86
1:B:346:GLU:HG2	1:B:348:VAL:H	1.41	0.86
1:E:155:PHE:CZ	1:E:168:LEU:HD11	2.11	0.86
1:F:153:VAL:HG13	1:F:154:THR:N	1.91	0.86
1:E:264:ARG:CG	1:E:266:SER:H	1.83	0.86
1:D:356:ARG:HG3	1:D:356:ARG:NH1	1.83	0.86
1:C:428:PHE:CD1	1:C:432:ALA:HA	2.10	0.86
1:D:174:PHE:HB2	1:D:181:PHE:CE2	2.11	0.86
1:F:301:THR:HG21	1:F:307:LEU:HD11	1.56	0.86
1:C:456:ASP:OD1	1:C:457:MET:N	2.07	0.86
1:A:430:GLU:O	1:A:431:HIS:HB3	1.75	0.86
1:A:176:LYS:HD3	1:A:213:ALA:HA	1.58	0.85
1:B:164:ALA:O	1:B:168:LEU:HD13	1.76	0.85
1:C:233:GLY:HA2	1:C:236:ARG:NH1	1.91	0.85
1:D:209:VAL:HG13	1:D:210:ALA:H	1.40	0.85
1:D:253:PHE:CE2	1:D:255:ASP:HB2	2.11	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:346:GLU:HG2	1:F:348:VAL:H	1.41	0.85
1:F:382:ARG:NH1	1:F:382:ARG:HG3	1.73	0.85
1:A:155:PHE:CZ	1:A:168:LEU:HD11	2.11	0.85
1:D:313:ARG:CG	1:D:314:PRO:CD	2.54	0.85
1:E:155:PHE:HD2	1:E:212:GLU:OE1	1.57	0.85
1:A:449:PHE:HB3	1:A:468:GLN:NE2	1.91	0.85
1:A:174:PHE:CZ	1:A:188:ILE:HD13	2.12	0.85
1:B:382:ARG:HH11	1:B:382:ARG:CG	1.89	0.85
1:F:164:ALA:O	1:F:168:LEU:HD13	1.77	0.85
1:F:238:ARG:HH12	1:F:239:ASP:CB	1.89	0.85
1:C:449:PHE:CB	1:C:468:GLN:NE2	2.38	0.85
1:A:509:GLY:O	1:B:476:ARG:NH2	2.09	0.85
1:F:215:VAL:HG22	1:F:216:PRO:HD2	1.57	0.85
1:E:449:PHE:HB3	1:E:468:GLN:NE2	1.91	0.85
1:C:173:GLU:HA	1:C:176:LYS:HG3	1.59	0.85
1:F:526:TYR:O	1:F:527:LEU:C	2.15	0.85
1:E:384:ILE:HG23	1:E:388:ASP:HB2	1.58	0.85
1:B:327:ASP:OD1	1:B:328:VAL:N	2.08	0.85
1:D:579:ARG:HG2	1:D:579:ARG:O	1.76	0.85
1:D:311:LEU:O	1:D:316:ARG:CG	2.25	0.85
1:E:173:GLU:HA	1:E:176:LYS:HG2	1.59	0.85
1:F:168:LEU:O	1:F:171:ILE:HG22	1.74	0.85
1:A:374:LEU:HD11	1:F:187:ARG:N	1.91	0.85
1:C:202:LYS:HD2	1:C:300:ALA:HB1	1.59	0.85
1:C:453:ARG:HG3	1:C:453:ARG:HH11	1.42	0.85
1:A:453:ARG:HH22	1:A:460:TRP:HE1	1.20	0.85
1:D:159:ALA:HB3	1:D:334:ILE:HG13	1.56	0.85
1:A:410:ARG:O	1:A:413:ARG:N	2.10	0.85
1:A:316:ARG:HG2	1:A:317:PHE:H	1.41	0.85
1:A:352:LEU:CD1	1:A:356:ARG:HH21	1.90	0.85
1:B:168:LEU:O	1:B:171:ILE:HG22	1.76	0.85
1:C:589:ARG:CZ	1:C:589:ARG:HB3	2.07	0.85
1:D:356:ARG:HH11	1:D:356:ARG:CG	1.89	0.85
1:E:571:ARG:HD2	1:E:590:VAL:O	1.76	0.84
1:E:145:ARG:CZ	1:E:219:THR:OG1	2.25	0.84
1:E:308:ASP:OD1	1:E:310:ALA:N	2.10	0.84
1:B:238:ARG:HH12	1:B:239:ASP:CB	1.90	0.84
1:F:209:VAL:HG13	1:F:210:ALA:H	1.42	0.84
1:F:382:ARG:HH11	1:F:382:ARG:CG	1.89	0.84
1:E:473:LEU:HD22	1:E:555:TYR:HB2	1.57	0.84
1:E:342:LYS:CD	1:E:343:PRO:HD2	2.06	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:473:LEU:HD22	1:C:555:TYR:HB2	1.59	0.84
1:C:342:LYS:CD	1:C:343:PRO:HD2	2.06	0.84
1:C:382:ARG:CG	1:C:383:LYS:N	2.41	0.84
1:B:190:LYS:CE	1:B:289:PHE:CE2	2.60	0.84
1:B:356:ARG:NH1	1:B:356:ARG:HG3	1.82	0.84
1:A:172:VAL:CG2	1:A:213:ALA:HB2	2.07	0.84
1:B:352:LEU:HD21	1:B:386:MET:HE1	1.59	0.84
1:C:509:GLY:C	1:D:476:ARG:HH22	1.80	0.84
1:D:470:ALA:O	1:D:558:VAL:HG21	1.77	0.84
1:B:460:TRP:HE3	1:B:460:TRP:N	1.74	0.84
1:A:384:ILE:CG2	1:A:388:ASP:HB2	2.08	0.84
1:B:345:ALA:HB2	1:B:383:LYS:HE3	1.57	0.84
1:E:163:GLU:OE1	1:E:163:GLU:N	2.11	0.84
1:A:202:LYS:HD2	1:A:300:ALA:HB1	1.59	0.84
1:D:215:VAL:HG22	1:D:216:PRO:HD2	1.59	0.84
1:F:253:PHE:CE2	1:F:255:ASP:HB2	2.13	0.84
1:C:174:PHE:CZ	1:C:188:ILE:HD13	2.13	0.84
1:D:395:ARG:NH1	1:D:395:ARG:HG2	1.89	0.84
1:B:470:ALA:O	1:B:558:VAL:HG21	1.76	0.84
1:E:430:GLU:O	1:E:431:HIS:HB3	1.74	0.84
1:A:263:LYS:HZ2	1:A:276:GLU:CD	1.79	0.84
1:C:453:ARG:HH22	1:C:464:ARG:HH12	1.26	0.84
1:A:313:ARG:NH1	1:A:526:TYR:O	2.10	0.84
1:A:163:GLU:OE1	1:A:163:GLU:N	2.11	0.84
1:A:151:PRO:HD2	1:A:211:GLY:HA2	1.59	0.84
1:F:214:ARG:HH11	1:F:214:ARG:HG3	1.38	0.84
1:A:263:LYS:CE	1:A:276:GLU:CD	2.46	0.84
1:F:356:ARG:CG	1:F:356:ARG:HH11	1.88	0.84
1:A:428:PHE:CD1	1:A:432:ALA:HA	2.13	0.84
1:A:173:GLU:HA	1:A:176:LYS:HG2	1.60	0.84
1:B:190:LYS:HE3	1:B:289:PHE:CE2	2.12	0.84
1:B:311:LEU:CA	1:B:316:ARG:NH1	2.41	0.84
1:F:355:LYS:HE3	1:F:578:GLU:O	1.76	0.84
1:C:236:ARG:CG	1:C:237:VAL:N	2.34	0.84
1:A:308:ASP:OD1	1:A:310:ALA:N	2.11	0.84
1:A:283:LEU:HD11	1:A:311:LEU:HD21	1.59	0.83
1:B:370:ASN:OD1	1:B:371:GLU:N	2.10	0.83
1:B:262:ARG:HG3	1:B:263:LYS:H	1.43	0.83
1:C:571:ARG:HD2	1:C:590:VAL:O	1.78	0.83
1:C:453:ARG:HH22	1:C:460:TRP:HE1	1.22	0.83
1:E:202:LYS:HD2	1:E:300:ALA:HB1	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:313:ARG:HG3	1:D:314:PRO:CD	2.07	0.83
1:B:302:ASN:HD21	1:B:443:ARG:NH2	1.75	0.83
1:F:291:LYS:HG3	1:F:292:ASP:N	1.87	0.83
1:A:382:ARG:HG3	1:A:383:LYS:N	1.91	0.83
1:B:159:ALA:HB3	1:B:334:ILE:HG13	1.60	0.83
1:D:589:ARG:NE	1:D:596:LEU:HD11	1.92	0.83
1:B:174:PHE:HB2	1:B:181:PHE:CE2	2.13	0.83
1:B:253:PHE:HE2	1:B:255:ASP:HB2	1.42	0.83
1:F:356:ARG:NH1	1:F:356:ARG:HG3	1.83	0.83
1:A:313:ARG:HH22	1:A:526:TYR:CA	1.90	0.83
1:F:207:ARG:HB3	1:F:217:PHE:CZ	2.13	0.83
1:E:453:ARG:HH22	1:E:464:ARG:HH12	1.27	0.83
1:B:235:ALA:O	1:B:238:ARG:CZ	2.26	0.83
1:A:210:ALA:O	1:A:214:ARG:HA	1.79	0.83
1:B:165:LYS:HE2	1:B:205:LEU:CD2	2.08	0.83
1:B:257:ILE:H	1:B:257:ILE:HD12	1.43	0.83
1:C:470:ALA:HB1	1:C:558:VAL:HG23	1.59	0.83
1:A:509:GLY:C	1:B:476:ARG:HH22	1.81	0.83
1:B:526:TYR:O	1:B:527:LEU:C	2.17	0.83
1:E:589:ARG:HB3	1:E:589:ARG:CZ	2.08	0.83
1:F:175:LEU:HD12	1:F:215:VAL:HG11	1.59	0.83
1:E:470:ALA:HB1	1:E:558:VAL:HG23	1.59	0.83
1:D:302:ASN:HD21	1:D:443:ARG:NH2	1.75	0.83
1:C:384:ILE:CG2	1:C:388:ASP:HB2	2.09	0.83
1:B:207:ARG:HB3	1:B:217:PHE:CZ	2.14	0.83
1:B:313:ARG:CG	1:B:314:PRO:CD	2.57	0.83
1:D:257:ILE:HD12	1:D:257:ILE:H	1.43	0.83
1:E:215:VAL:CG2	1:E:250:CYS:HA	2.09	0.83
1:F:253:PHE:HE2	1:F:255:ASP:HB2	1.42	0.83
1:C:332:GLU:OE2	1:C:351:ALA:HA	1.79	0.83
1:C:352:LEU:CD1	1:C:356:ARG:HH21	1.92	0.83
1:C:371:GLU:HG3	1:C:392:ALA:HB1	1.58	0.83
1:A:262:ARG:HB3	1:A:275:ARG:NH1	1.92	0.82
1:B:253:PHE:CE2	1:B:255:ASP:HB2	2.13	0.82
1:D:526:TYR:O	1:D:527:LEU:C	2.16	0.82
1:E:223:SER:O	1:E:225:PHE:N	2.11	0.82
1:F:345:ALA:HB2	1:F:383:LYS:CE	2.08	0.82
1:D:325:ALA:HB3	1:D:326:PRO:HD3	1.58	0.82
1:F:482:VAL:HG13	1:F:483:PHE:CD2	2.12	0.82
1:F:430:GLU:OE1	1:F:430:GLU:HA	1.78	0.82
1:A:416:ALA:HB1	1:A:577:LEU:HD23	1.56	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:233:GLY:HA2	1:E:236:ARG:NH1	1.94	0.82
1:A:342:LYS:CD	1:F:184:MET:O	2.28	0.82
1:D:165:LYS:HA	1:D:168:LEU:HD22	1.62	0.82
1:B:215:VAL:HG22	1:B:216:PRO:HD2	1.61	0.82
1:A:233:GLY:O	1:A:236:ARG:HG2	1.79	0.82
1:C:449:PHE:HB3	1:C:468:GLN:NE2	1.94	0.82
1:D:345:ALA:HB2	1:D:383:LYS:CE	2.08	0.82
1:E:332:GLU:OE2	1:E:351:ALA:HA	1.79	0.82
1:C:163:GLU:OE1	1:C:163:GLU:N	2.11	0.82
1:B:345:ALA:HB2	1:B:383:LYS:CE	2.08	0.82
1:E:286:MET:HB3	1:E:316:ARG:CD	2.04	0.82
1:F:174:PHE:HB2	1:F:181:PHE:CE2	2.13	0.82
1:F:214:ARG:HG3	1:F:214:ARG:NH1	1.91	0.82
1:F:257:ILE:H	1:F:257:ILE:HD12	1.44	0.82
1:A:449:PHE:CE2	1:A:496:GLN:CG	2.62	0.82
1:D:376:ALA:C	1:D:381:ARG:HG3	1.99	0.82
1:E:197:PRO:HD2	1:E:200:VAL:HG21	1.61	0.82
1:A:332:GLU:OE2	1:A:351:ALA:HA	1.80	0.82
1:E:174:PHE:CZ	1:E:188:ILE:HD13	2.12	0.82
1:E:207:ARG:HB2	1:E:207:ARG:CZ	2.10	0.82
1:C:263:LYS:HD2	1:C:276:GLU:OE1	1.75	0.82
1:D:529:GLY:O	1:D:530:TYR:HB3	1.78	0.82
1:D:238:ARG:HH12	1:D:239:ASP:CB	1.92	0.82
1:C:197:PRO:HD2	1:C:200:VAL:HG21	1.59	0.82
1:C:263:LYS:CE	1:C:276:GLU:CD	2.47	0.82
1:B:529:GLY:O	1:B:530:TYR:HB3	1.79	0.82
1:A:313:ARG:HH22	1:A:526:TYR:HA	1.44	0.82
1:E:223:SER:C	1:E:225:PHE:H	1.81	0.82
1:A:377:ALA:HB1	1:F:181:PHE:CE1	2.15	0.82
1:F:262:ARG:HG3	1:F:263:LYS:H	1.45	0.82
1:C:460:TRP:O	1:D:488:THR:HA	1.80	0.82
1:F:571:ARG:HD2	1:F:590:VAL:O	1.80	0.82
1:B:343:PRO:HG2	1:B:383:LYS:HA	1.62	0.82
1:E:263:LYS:HD2	1:E:276:GLU:OE1	1.78	0.82
1:C:225:PHE:CE1	1:C:233:GLY:CA	2.60	0.82
1:A:470:ALA:HB1	1:A:558:VAL:HG23	1.62	0.82
1:F:327:ASP:OD1	1:F:328:VAL:N	2.12	0.81
1:E:313:ARG:CZ	1:E:526:TYR:HA	2.08	0.81
1:F:589:ARG:NE	1:F:596:LEU:HD11	1.95	0.81
1:B:471:VAL:O	1:B:474:ALA:HB3	1.80	0.81
1:A:197:PRO:HD2	1:A:200:VAL:HG21	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:ALA:O	1:A:357:THR:HG23	1.80	0.81
1:B:337:ILE:HD12	1:B:340:ARG:NH1	1.96	0.81
1:B:313:ARG:HG3	1:B:314:PRO:CD	2.10	0.81
1:F:286:MET:CE	1:F:316:ARG:HA	2.04	0.81
1:F:579:ARG:O	1:F:579:ARG:HG2	1.78	0.81
1:A:519:TYR:O	1:A:533:ARG:NE	2.12	0.81
1:E:416:ALA:HB1	1:E:577:LEU:HD23	1.57	0.81
1:A:207:ARG:CZ	1:A:207:ARG:HB2	2.10	0.81
1:A:352:LEU:HD12	1:A:356:ARG:HH21	1.45	0.81
1:B:209:VAL:HG13	1:B:210:ALA:H	1.44	0.81
1:F:337:ILE:O	1:F:340:ARG:NH1	2.13	0.81
1:D:482:VAL:HG13	1:D:483:PHE:CD2	2.13	0.81
1:D:378:ARG:C	1:D:380:GLY:H	1.84	0.81
1:B:523:GLU:HG2	1:B:530:TYR:O	1.81	0.81
1:C:225:PHE:HE1	1:C:233:GLY:HA2	1.43	0.81
1:C:155:PHE:CD2	1:C:212:GLU:OE1	2.33	0.81
1:C:172:VAL:CG2	1:C:213:ALA:HB2	2.07	0.81
1:B:568:VAL:O	1:B:572:VAL:HG23	1.79	0.81
1:D:243:THR:HA	1:D:246:ARG:HH21	1.45	0.81
1:F:338:HIS:ND1	1:F:366:GLU:HG3	1.94	0.81
1:C:173:GLU:HA	1:C:176:LYS:HG2	1.63	0.81
1:B:241:PHE:O	1:B:244:ALA:N	2.13	0.81
1:F:474:ALA:CA	1:F:558:VAL:HG11	2.11	0.81
1:E:352:LEU:HD21	1:E:386:MET:SD	2.21	0.81
1:E:371:GLU:HG3	1:E:392:ALA:HB1	1.62	0.81
1:E:410:ARG:O	1:E:413:ARG:N	2.14	0.81
1:F:375:LEU:HD11	1:F:388:ASP:HB3	1.61	0.81
1:F:155:PHE:CD2	1:F:212:GLU:OE2	2.34	0.81
1:F:238:ARG:HH12	1:F:239:ASP:N	1.78	0.81
1:C:262:ARG:HB3	1:C:275:ARG:NH1	1.93	0.81
1:C:352:LEU:HD12	1:C:356:ARG:HH21	1.46	0.81
1:D:523:GLU:HG2	1:D:530:TYR:O	1.81	0.81
1:E:155:PHE:CD2	1:E:212:GLU:OE1	2.33	0.81
1:F:460:TRP:N	1:F:460:TRP:HE3	1.77	0.81
1:A:178:PRO:HB3	1:A:294:ALA:HB2	1.62	0.80
1:C:215:VAL:CG2	1:C:250:CYS:HA	2.10	0.80
1:B:430:GLU:HA	1:B:430:GLU:OE1	1.81	0.80
1:E:225:PHE:CE1	1:E:233:GLY:CA	2.63	0.80
1:D:533:ARG:HH11	1:D:533:ARG:HG3	1.45	0.80
1:E:467:ASP:OD1	1:E:557:ARG:NH2	2.14	0.80
1:D:155:PHE:CD2	1:D:212:GLU:OE2	2.34	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:568:VAL:O	1:F:572:VAL:HG23	1.81	0.80
1:D:582:LEU:HD21	1:D:590:VAL:HG21	1.62	0.80
1:A:173:GLU:HA	1:A:176:LYS:HG3	1.61	0.80
1:B:328:VAL:CG2	1:B:355:LYS:HE3	2.11	0.80
1:B:579:ARG:O	1:B:581:THR:N	2.13	0.80
1:E:236:ARG:CG	1:E:236:ARG:HH11	1.93	0.80
1:C:223:SER:C	1:C:225:PHE:H	1.84	0.80
1:D:331:ARG:NH2	1:D:580:GLU:OE1	2.14	0.80
1:C:313:ARG:CZ	1:C:526:TYR:HA	2.10	0.80
1:F:521:VAL:HG23	1:F:532:VAL:HG13	1.62	0.80
1:D:262:ARG:HG3	1:D:263:LYS:H	1.45	0.80
1:D:355:LYS:HE3	1:D:578:GLU:O	1.81	0.80
1:E:586:GLU:HA	1:E:589:ARG:HG3	1.61	0.80
1:A:168:LEU:C	1:A:171:ILE:HD13	2.02	0.80
1:C:533:ARG:HD2	1:C:534:GLN:N	1.96	0.80
1:D:413:ARG:HG2	1:D:413:ARG:NH1	1.77	0.80
1:B:474:ALA:CA	1:B:558:VAL:HG11	2.11	0.80
1:A:371:GLU:HG3	1:A:392:ALA:HB1	1.62	0.80
1:B:325:ALA:HB3	1:B:326:PRO:HD3	1.62	0.80
1:E:168:LEU:CB	1:E:171:ILE:HD11	2.06	0.80
1:E:225:PHE:HE1	1:E:233:GLY:HA2	1.45	0.80
1:F:471:VAL:O	1:F:474:ALA:HB3	1.80	0.80
1:B:521:VAL:HG23	1:B:532:VAL:HG13	1.62	0.80
1:A:155:PHE:CD2	1:A:212:GLU:OE1	2.34	0.80
1:D:286:MET:CE	1:D:316:ARG:HA	2.09	0.80
1:E:215:VAL:HG11	1:E:250:CYS:HA	1.64	0.80
1:E:352:LEU:CD1	1:E:356:ARG:HH21	1.95	0.80
1:A:225:PHE:HE1	1:A:233:GLY:HA2	1.44	0.80
1:A:233:GLY:HA2	1:A:236:ARG:NH1	1.96	0.80
1:A:339:ALA:HA	1:A:369:LEU:HD21	1.63	0.80
1:E:172:VAL:HG23	1:E:213:ALA:CB	2.08	0.80
1:D:153:VAL:HG13	1:D:154:THR:H	1.46	0.80
1:A:223:SER:C	1:A:225:PHE:H	1.85	0.80
1:F:450:MET:HA	1:F:453:ARG:HD2	1.63	0.80
1:E:210:ALA:HB2	1:E:251:ILE:HD12	1.63	0.79
1:F:468:GLN:O	1:F:471:VAL:HG22	1.82	0.79
1:F:449:PHE:CE2	1:F:453:ARG:NH2	2.50	0.79
1:F:313:ARG:CG	1:F:314:PRO:CD	2.60	0.79
1:C:357:THR:HG1	1:C:360:PHE:HD1	1.29	0.79
1:E:382:ARG:HG3	1:E:383:LYS:N	1.98	0.79
1:D:236:ARG:HG2	1:D:237:VAL:N	1.97	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:219:THR:HB	1:E:253:PHE:HD2	1.47	0.79
1:D:348:VAL:HG21	1:D:352:LEU:CD2	2.12	0.79
1:F:582:LEU:HD21	1:F:590:VAL:HG21	1.63	0.79
1:E:354:ALA:O	1:E:357:THR:HG23	1.82	0.79
1:E:396:VAL:O	1:E:400:PRO:HD3	1.82	0.79
1:A:225:PHE:CE1	1:A:233:GLY:CA	2.61	0.79
1:F:274:GLU:O	1:F:277:GLN:HG2	1.81	0.79
1:C:313:ARG:HH22	1:C:526:TYR:CA	1.96	0.79
1:E:331:ARG:NH1	1:E:354:ALA:O	2.14	0.79
1:A:223:SER:O	1:A:225:PHE:N	2.15	0.79
1:D:235:ALA:O	1:D:238:ARG:HG3	1.83	0.79
1:B:589:ARG:NE	1:B:594:LEU:HD21	1.93	0.79
1:D:241:PHE:O	1:D:244:ALA:N	2.15	0.79
1:C:503:ARG:HG2	1:C:508:TRP:CZ3	2.18	0.79
1:D:460:TRP:HE3	1:D:460:TRP:N	1.80	0.79
1:C:223:SER:O	1:C:225:PHE:N	2.14	0.79
1:A:274:GLU:O	1:A:277:GLN:HB3	1.81	0.79
1:D:286:MET:HE1	1:D:316:ARG:CA	2.08	0.79
1:F:325:ALA:HB3	1:F:326:PRO:HD3	1.65	0.79
1:C:236:ARG:HH11	1:C:236:ARG:CG	1.96	0.79
1:C:178:PRO:HB3	1:C:294:ALA:HB2	1.65	0.79
1:B:165:LYS:HA	1:B:168:LEU:HD22	1.64	0.79
1:E:509:GLY:C	1:F:476:ARG:HH22	1.85	0.79
1:C:168:LEU:CB	1:C:171:ILE:HD11	2.09	0.79
1:E:339:ALA:HA	1:E:369:LEU:HD21	1.63	0.79
1:F:376:ALA:C	1:F:381:ARG:HD2	2.03	0.79
1:C:354:ALA:O	1:C:357:THR:HG23	1.83	0.79
1:A:461:SER:HA	1:B:487:THR:O	1.82	0.79
1:F:523:GLU:HG2	1:F:530:TYR:O	1.83	0.79
1:A:172:VAL:HG23	1:A:213:ALA:CB	2.11	0.78
1:F:241:PHE:O	1:F:244:ALA:N	2.16	0.78
1:E:263:LYS:CE	1:E:276:GLU:CD	2.50	0.78
1:A:236:ARG:CG	1:A:236:ARG:HH11	1.95	0.78
1:B:338:HIS:ND1	1:B:366:GLU:HG3	1.97	0.78
1:D:241:PHE:CE2	1:D:285:GLU:OE2	2.36	0.78
1:A:449:PHE:CZ	1:A:496:GLN:CG	2.63	0.78
1:B:241:PHE:CE2	1:B:285:GLU:OE2	2.36	0.78
1:E:536:SER:OG	1:F:544:ASP:OD2	2.02	0.78
1:F:378:ARG:C	1:F:380:GLY:H	1.86	0.78
1:E:286:MET:CB	1:E:316:ARG:CG	2.45	0.78
1:D:376:ALA:O	1:D:381:ARG:CG	2.31	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:GLU:O	1:B:277:GLN:HG2	1.83	0.78
1:C:396:VAL:O	1:C:400:PRO:HD3	1.83	0.78
1:D:199:GLY:N	2:D:2001:ADP:O2B	2.15	0.78
1:A:215:VAL:CG2	1:A:250:CYS:HA	2.14	0.78
1:D:238:ARG:HH12	1:D:239:ASP:N	1.82	0.78
1:E:262:ARG:HB3	1:E:275:ARG:NH1	1.93	0.78
1:A:382:ARG:CG	1:A:383:LYS:N	2.46	0.78
1:F:313:ARG:HG3	1:F:314:PRO:CD	2.12	0.78
1:F:238:ARG:HH11	1:F:239:ASP:N	1.77	0.78
1:A:264:ARG:CD	1:A:266:SER:HB2	2.13	0.78
1:D:474:ALA:CA	1:D:558:VAL:HG11	2.13	0.78
1:B:235:ALA:O	1:B:238:ARG:HG3	1.84	0.78
1:B:193:LEU:O	1:B:320:GLN:HB2	1.83	0.78
1:D:313:ARG:NE	1:D:314:PRO:HD2	1.97	0.78
1:D:319:ARG:CG	1:D:319:ARG:HH11	1.96	0.78
1:F:236:ARG:HG2	1:F:237:VAL:N	1.97	0.78
1:D:382:ARG:NH1	1:D:382:ARG:CG	2.17	0.78
1:C:346:GLU:OE1	1:C:346:GLU:N	2.17	0.78
1:E:233:GLY:O	1:E:236:ARG:HG2	1.82	0.78
1:E:533:ARG:HD2	1:E:534:GLN:N	1.99	0.78
1:B:313:ARG:NE	1:B:314:PRO:HD2	1.99	0.78
1:F:207:ARG:HB3	1:F:217:PHE:CE1	2.19	0.78
1:F:343:PRO:HG2	1:F:383:LYS:HA	1.66	0.78
1:F:331:ARG:NH2	1:F:580:GLU:OE1	2.15	0.78
1:E:465:LEU:HD22	1:E:508:TRP:HZ3	1.50	0.78
1:C:225:PHE:CE2	1:C:278:THR:HB	2.19	0.78
1:A:396:VAL:O	1:A:400:PRO:HD3	1.84	0.77
1:E:178:PRO:HB3	1:E:294:ALA:HB2	1.66	0.77
1:F:155:PHE:HA	1:F:158:VAL:HG23	1.67	0.77
1:F:235:ALA:O	1:F:238:ARG:HG3	1.84	0.77
1:A:263:LYS:HD2	1:A:276:GLU:OE1	1.79	0.77
1:B:207:ARG:HB3	1:B:217:PHE:CE1	2.20	0.77
1:A:585:GLU:O	1:A:588:GLN:CG	2.27	0.77
1:C:586:GLU:HA	1:C:589:ARG:CG	2.15	0.77
1:C:352:LEU:HD21	1:C:386:MET:SD	2.24	0.77
1:D:283:LEU:HD12	1:D:316:ARG:HH21	1.49	0.77
1:F:153:VAL:HG13	1:F:154:THR:H	1.48	0.77
1:F:352:LEU:HD11	1:F:386:MET:HE1	1.65	0.77
1:D:337:ILE:O	1:D:340:ARG:NH1	2.18	0.77
1:B:155:PHE:CD2	1:B:212:GLU:OE2	2.36	0.77
1:A:346:GLU:N	1:A:346:GLU:OE1	2.17	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:582:LEU:HD21	1:B:590:VAL:HG21	1.65	0.77
1:E:346:GLU:OE1	1:E:346:GLU:N	2.18	0.77
1:E:357:THR:HG1	1:E:360:PHE:HD1	1.33	0.77
1:F:165:LYS:HA	1:F:168:LEU:HD22	1.66	0.77
1:F:215:VAL:HG21	1:F:249:PRO:O	1.84	0.77
1:E:249:PRO:HA	1:E:294:ALA:O	1.85	0.77
1:E:519:TYR:O	1:E:533:ARG:NE	2.17	0.77
1:A:418:HIS:O	1:A:421:GLY:N	2.18	0.77
1:A:319:ARG:HH21	1:B:402:LYS:NZ	1.82	0.77
1:D:458:LEU:HD12	1:D:459:HIS:H	1.48	0.77
1:C:219:THR:HB	1:C:253:PHE:HD2	1.49	0.77
1:C:249:PRO:HA	1:C:294:ALA:O	1.84	0.77
1:B:450:MET:HA	1:B:453:ARG:HD2	1.65	0.77
1:B:414:ILE:HG23	1:B:483:PHE:CE1	2.20	0.77
1:A:225:PHE:CE2	1:A:278:THR:HB	2.19	0.77
1:B:337:ILE:O	1:B:340:ARG:NH1	2.18	0.77
1:E:286:MET:HG3	1:E:316:ARG:CD	2.15	0.77
1:B:413:ARG:CG	1:B:413:ARG:HH11	1.95	0.77
1:A:352:LEU:HD21	1:A:386:MET:SD	2.25	0.77
1:F:243:THR:HA	1:F:246:ARG:HH21	1.49	0.77
1:B:243:THR:HA	1:B:246:ARG:HH21	1.48	0.77
1:E:352:LEU:HD12	1:E:356:ARG:HH21	1.49	0.77
1:B:286:MET:O	1:B:289:PHE:HB2	1.85	0.76
1:A:536:SER:OG	1:B:544:ASP:OD2	2.02	0.76
1:E:449:PHE:CE2	1:E:496:GLN:CG	2.67	0.76
1:E:453:ARG:HG3	1:E:453:ARG:HH11	1.50	0.76
1:A:533:ARG:HD2	1:A:534:GLN:N	2.00	0.76
1:D:331:ARG:NH1	1:D:357:THR:O	2.17	0.76
1:B:276:GLU:HA	1:B:279:LEU:CD1	2.15	0.76
1:D:238:ARG:HH11	1:D:239:ASP:N	1.82	0.76
1:C:503:ARG:HD2	1:C:508:TRP:CE2	2.20	0.76
1:C:313:ARG:HH22	1:C:526:TYR:HA	1.50	0.76
1:A:174:PHE:CE2	1:A:188:ILE:HD13	2.20	0.76
1:B:331:ARG:NH2	1:B:580:GLU:OE1	2.18	0.76
1:B:348:VAL:HG21	1:B:352:LEU:CD2	2.15	0.76
1:D:274:GLU:O	1:D:277:GLN:HG2	1.85	0.76
1:C:461:SER:O	1:C:464:ARG:HB3	1.85	0.76
1:E:453:ARG:NH1	1:E:460:TRP:HZ2	1.83	0.76
1:A:311:LEU:HD22	1:A:316:ARG:NH2	2.00	0.76
1:B:331:ARG:NH1	1:B:357:THR:O	2.18	0.76
1:E:149:GLU:O	1:E:150:ALA:HB3	1.83	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:225:PHE:CE2	1:E:278:THR:HB	2.20	0.76
1:F:529:GLY:O	1:F:530:TYR:HB3	1.83	0.76
1:C:313:ARG:NH2	1:C:526:TYR:O	2.17	0.76
1:B:502:ARG:O	1:B:506:THR:HG23	1.86	0.76
1:B:376:ALA:CB	1:B:381:ARG:CD	2.60	0.76
1:C:233:GLY:O	1:C:236:ARG:HG2	1.85	0.76
1:B:238:ARG:HH11	1:B:239:ASP:N	1.82	0.76
1:B:215:VAL:HG21	1:B:249:PRO:O	1.85	0.76
1:F:588:GLN:O	1:F:591:VAL:HB	1.86	0.76
1:B:328:VAL:HG22	1:B:355:LYS:HE3	1.67	0.76
1:C:453:ARG:NH1	1:C:460:TRP:CZ2	2.54	0.76
1:D:207:ARG:HB2	1:D:217:PHE:CZ	2.20	0.76
1:C:210:ALA:HB2	1:C:251:ILE:HD12	1.67	0.76
1:F:412:ARG:HH22	1:F:440:ILE:HB	1.50	0.76
1:B:238:ARG:HH12	1:B:239:ASP:N	1.82	0.76
1:F:241:PHE:CE2	1:F:285:GLU:OE2	2.39	0.76
1:B:243:THR:HA	1:B:246:ARG:NH2	2.00	0.76
1:E:384:ILE:CG2	1:E:388:ASP:HB2	2.16	0.76
1:A:453:ARG:CZ	1:A:460:TRP:HE1	1.99	0.76
1:A:510:MET:O	1:A:512:PRO:HD2	1.86	0.76
1:B:412:ARG:HH22	1:B:440:ILE:HB	1.51	0.76
1:F:424:LEU:HD11	1:F:569:LEU:HA	1.67	0.76
1:A:211:GLY:HA2	1:A:214:ARG:HE	1.51	0.76
1:A:215:VAL:HG11	1:A:250:CYS:HA	1.67	0.76
1:B:158:VAL:HG22	1:B:204:HIS:CE1	2.21	0.76
1:F:235:ALA:O	1:F:238:ARG:CZ	2.33	0.76
1:F:238:ARG:HH12	1:F:239:ASP:CA	1.99	0.76
1:C:453:ARG:NH1	1:C:460:TRP:HZ2	1.82	0.76
1:D:450:MET:HA	1:D:453:ARG:HD2	1.67	0.76
1:F:449:PHE:HE2	1:F:492:ASN:HB3	1.51	0.76
1:C:166:GLU:CA	1:C:169:LYS:HG2	2.15	0.76
1:F:243:THR:HA	1:F:246:ARG:NH2	2.00	0.75
1:A:453:ARG:NH1	1:A:453:ARG:HG3	2.00	0.75
1:B:460:TRP:CE3	1:B:460:TRP:N	2.52	0.75
1:D:588:GLN:O	1:D:591:VAL:HB	1.86	0.75
1:E:339:ALA:CA	1:E:369:LEU:HD21	2.15	0.75
1:A:342:LYS:HD2	1:A:343:PRO:CD	2.13	0.75
1:D:521:VAL:HG23	1:D:532:VAL:HG13	1.67	0.75
1:B:238:ARG:HH12	1:B:239:ASP:CA	2.00	0.75
1:F:451:MET:HB3	1:F:452:PRO:HD3	1.69	0.75
1:A:219:THR:HB	1:A:253:PHE:HD2	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:PRO:HD2	1:B:200:VAL:HG11	1.69	0.75
1:D:276:GLU:HA	1:D:279:LEU:CD1	2.16	0.75
1:E:174:PHE:CE2	1:E:188:ILE:HD13	2.20	0.75
1:F:233:GLY:O	1:F:278:THR:HG22	1.85	0.75
1:C:584:ALA:O	1:C:587:PHE:HB3	1.85	0.75
1:C:390:GLU:O	1:C:393:ALA:HB3	1.86	0.75
1:B:247:HIS:HB3	1:B:250:CYS:SG	2.27	0.75
1:F:474:ALA:HA	1:F:558:VAL:CG1	2.16	0.75
1:C:339:ALA:CA	1:C:369:LEU:HD21	2.17	0.75
1:C:339:ALA:HA	1:C:369:LEU:HD21	1.66	0.75
1:C:393:ALA:O	1:C:396:VAL:HG12	1.86	0.75
1:A:503:ARG:HG2	1:A:508:TRP:CZ3	2.22	0.75
1:B:238:ARG:HB3	1:B:281:GLN:NE2	2.01	0.75
1:F:502:ARG:O	1:F:506:THR:HG23	1.86	0.75
1:A:339:ALA:CA	1:A:369:LEU:HD21	2.15	0.75
1:E:286:MET:CG	1:E:316:ARG:HD2	2.15	0.75
1:C:589:ARG:HH22	1:C:596:LEU:HB2	1.33	0.75
1:C:181:PHE:O	1:C:184:MET:HG2	1.87	0.75
1:A:388:ASP:OD1	1:A:388:ASP:N	2.20	0.75
1:C:449:PHE:CZ	1:C:496:GLN:CG	2.65	0.75
1:D:451:MET:HB3	1:D:452:PRO:HD3	1.69	0.75
1:A:210:ALA:O	1:A:214:ARG:HD3	1.87	0.75
1:C:174:PHE:CE2	1:C:188:ILE:HD13	2.22	0.75
1:C:172:VAL:HG23	1:C:213:ALA:CB	2.12	0.75
1:F:319:ARG:HH11	1:F:319:ARG:CG	2.00	0.74
1:B:451:MET:HB3	1:B:452:PRO:HD3	1.69	0.74
1:D:412:ARG:HH22	1:D:440:ILE:HB	1.49	0.74
1:F:410:ARG:O	1:F:413:ARG:N	2.20	0.74
1:E:393:ALA:O	1:E:396:VAL:HG12	1.87	0.74
1:A:331:ARG:NH1	1:A:354:ALA:O	2.20	0.74
1:C:381:ARG:HG3	1:C:381:ARG:HH11	1.52	0.74
1:D:233:GLY:O	1:D:278:THR:HG22	1.86	0.74
1:E:286:MET:CG	1:E:316:ARG:CD	2.65	0.74
1:F:337:ILE:HD12	1:F:340:ARG:NH1	2.01	0.74
1:C:313:ARG:CZ	1:C:526:TYR:O	2.34	0.74
1:E:335:LEU:CD2	1:E:353:LEU:HD23	2.17	0.74
1:E:584:ALA:O	1:E:587:PHE:HB3	1.86	0.74
1:A:166:GLU:CA	1:A:169:LYS:HG2	2.14	0.74
1:B:310:ALA:C	1:B:316:ARG:HH12	1.86	0.74
1:A:586:GLU:HA	1:A:589:ARG:HE	1.50	0.74
1:B:503:ARG:HH12	1:B:522:ARG:HH21	1.35	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:510:MET:O	1:E:512:PRO:HD2	1.87	0.74
1:F:503:ARG:HH22	1:F:522:ARG:NH2	1.85	0.74
1:B:233:GLY:O	1:B:278:THR:HG22	1.86	0.74
1:B:424:LEU:HD11	1:B:569:LEU:HA	1.69	0.74
1:F:171:ILE:HG13	1:F:296:VAL:HG21	1.69	0.74
1:C:196:GLY:N	1:C:202:LYS:NZ	2.35	0.74
1:D:153:VAL:CG1	1:D:154:THR:N	2.51	0.74
1:F:313:ARG:NE	1:F:314:PRO:HD2	2.00	0.74
1:B:449:PHE:HE2	1:B:492:ASN:HB3	1.52	0.74
1:D:365:LEU:O	1:D:368:LEU:HB3	1.88	0.74
1:E:342:LYS:HD2	1:E:343:PRO:CD	2.16	0.74
1:A:236:ARG:O	1:A:237:VAL:C	2.26	0.74
1:A:249:PRO:HA	1:A:294:ALA:O	1.87	0.74
1:F:331:ARG:NH1	1:F:357:THR:O	2.19	0.74
1:A:264:ARG:HG3	1:A:265:GLY:N	2.02	0.74
1:C:342:LYS:HD2	1:C:343:PRO:CD	2.16	0.74
1:E:465:LEU:HD22	1:E:508:TRP:CZ3	2.22	0.74
1:B:378:ARG:C	1:B:380:GLY:H	1.89	0.74
1:A:165:LYS:O	1:A:168:LEU:HG	1.87	0.74
1:C:449:PHE:CE2	1:C:496:GLN:CG	2.68	0.74
1:F:458:LEU:HD12	1:F:459:HIS:H	1.53	0.74
1:A:390:GLU:O	1:A:393:ALA:HB3	1.88	0.74
1:D:243:THR:HA	1:D:246:ARG:NH2	2.02	0.74
1:F:155:PHE:HD2	1:F:212:GLU:OE2	1.71	0.74
1:D:458:LEU:HD12	1:D:459:HIS:N	2.02	0.74
1:B:588:GLN:O	1:B:591:VAL:HB	1.88	0.74
1:A:313:ARG:NH2	1:A:526:TYR:O	2.20	0.74
1:E:418:HIS:O	1:E:421:GLY:N	2.21	0.74
1:F:199:GLY:N	2:F:2001:ADP:O2B	2.17	0.74
1:D:468:GLN:O	1:D:471:VAL:HG22	1.88	0.74
1:C:236:ARG:HG3	1:C:237:VAL:H	1.52	0.74
1:A:461:SER:OG	1:B:486:VAL:HG11	1.87	0.74
1:F:589:ARG:NE	1:F:594:LEU:HD21	1.94	0.74
1:E:413:ARG:CA	1:E:577:LEU:HD22	2.16	0.73
1:E:236:ARG:HG3	1:E:237:VAL:H	1.52	0.73
1:A:181:PHE:O	1:A:184:MET:HG2	1.87	0.73
1:D:235:ALA:O	1:D:238:ARG:CZ	2.36	0.73
1:E:166:GLU:CA	1:E:169:LYS:HG2	2.16	0.73
1:A:381:ARG:HG3	1:A:381:ARG:HH11	1.53	0.73
1:E:453:ARG:NH1	1:E:460:TRP:CZ2	2.55	0.73
1:D:346:GLU:HG3	1:D:386:MET:HG2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:571:ARG:HD2	1:D:590:VAL:O	1.88	0.73
1:E:390:GLU:O	1:E:393:ALA:HB3	1.87	0.73
1:A:410:ARG:HG3	1:A:411:ASP:N	2.04	0.73
1:F:376:ALA:HA	1:F:381:ARG:NE	2.04	0.73
1:F:376:ALA:HA	1:F:381:ARG:HD2	0.74	0.73
1:B:376:ALA:C	1:B:381:ARG:HB2	2.08	0.73
1:E:215:VAL:HG21	1:E:250:CYS:CA	2.17	0.73
1:D:155:PHE:HD2	1:D:212:GLU:OE2	1.71	0.73
1:B:236:ARG:NH1	1:B:278:THR:HG22	2.00	0.73
1:B:468:GLN:O	1:B:471:VAL:HG22	1.87	0.73
1:D:589:ARG:NE	1:D:594:LEU:HD21	1.95	0.73
1:A:313:ARG:NH2	1:A:526:TYR:CA	2.46	0.73
1:B:348:VAL:HG22	1:B:352:LEU:HD22	1.70	0.73
1:C:358:PRO:HA	1:C:359:GLY:C	2.08	0.73
1:C:474:ALA:HA	1:C:558:VAL:HG11	1.70	0.73
1:A:441:VAL:O	1:A:441:VAL:HG12	1.88	0.73
1:F:316:ARG:NH1	1:F:316:ARG:HG2	2.03	0.73
1:D:586:GLU:O	1:D:590:VAL:HG23	1.88	0.73
1:F:436:HIS:O	1:F:437:LYS:HG2	1.89	0.73
1:D:191:GLY:HA2	1:D:297:VAL:HG12	1.71	0.73
1:F:233:GLY:HA2	1:F:236:ARG:HH21	1.52	0.73
1:D:158:VAL:HG22	1:D:204:HIS:CE1	2.23	0.73
1:B:589:ARG:HB3	1:B:594:LEU:HD22	1.70	0.73
1:D:439:THR:CG2	1:D:445:ARG:HH22	2.00	0.73
1:D:430:GLU:HA	1:D:430:GLU:OE1	1.88	0.73
1:A:408:SER:HB2	1:A:409:PRO:HD2	1.71	0.73
1:A:236:ARG:HG3	1:A:237:VAL:H	1.49	0.73
1:F:247:HIS:HB3	1:F:250:CYS:SG	2.28	0.73
1:C:196:GLY:H	1:C:202:LYS:NZ	1.86	0.73
1:D:238:ARG:HH12	1:D:239:ASP:CA	2.01	0.73
1:D:413:ARG:HH11	1:D:413:ARG:CG	1.96	0.73
1:B:238:ARG:CB	1:B:281:GLN:NE2	2.52	0.73
1:F:460:TRP:N	1:F:460:TRP:CE3	2.54	0.73
1:A:236:ARG:O	1:A:239:ASP:OD1	2.07	0.73
1:F:193:LEU:O	1:F:320:GLN:HB2	1.88	0.73
1:B:501:ALA:HB1	1:B:550:LEU:HD23	1.70	0.73
1:D:155:PHE:HA	1:D:158:VAL:HG23	1.71	0.73
1:D:153:VAL:HB	1:D:207:ARG:HH11	1.54	0.73
1:E:382:ARG:HG3	1:E:383:LYS:H	1.51	0.73
1:C:215:VAL:HG21	1:C:250:CYS:CA	2.19	0.73
1:A:589:ARG:NH1	1:A:596:LEU:HB3	2.02	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:235:ALA:HA	1:F:238:ARG:CD	2.18	0.73
1:F:316:ARG:HH11	1:F:316:ARG:HG2	1.54	0.73
1:A:460:TRP:CD1	1:A:464:ARG:NH1	2.57	0.73
1:F:503:ARG:HH12	1:F:522:ARG:HH21	1.36	0.73
1:A:393:ALA:O	1:A:396:VAL:HG12	1.88	0.72
1:B:155:PHE:HD2	1:B:212:GLU:OE2	1.72	0.72
1:B:171:ILE:HG13	1:B:296:VAL:HG21	1.71	0.72
1:A:503:ARG:HD2	1:A:508:TRP:CE2	2.23	0.72
1:F:567:GLU:O	1:F:570:GLU:N	2.22	0.72
1:A:587:PHE:O	1:A:590:VAL:CG2	2.32	0.72
1:F:276:GLU:CA	1:F:279:LEU:HD13	2.18	0.72
1:E:453:ARG:HH21	1:E:464:ARG:NH2	1.86	0.72
1:D:412:ARG:NH2	1:D:440:ILE:HD13	2.03	0.72
1:D:313:ARG:HG3	1:D:314:PRO:N	2.04	0.72
1:E:224:ASP:HA	1:E:227:GLU:OE2	1.88	0.72
1:A:586:GLU:CA	1:A:589:ARG:NE	2.52	0.72
1:D:449:PHE:HE2	1:D:492:ASN:HB3	1.53	0.72
1:E:460:TRP:CD1	1:E:464:ARG:NH1	2.56	0.72
1:D:337:ILE:HD12	1:D:340:ARG:NH1	2.02	0.72
1:C:166:GLU:CB	1:C:169:LYS:HZ2	2.02	0.72
1:E:388:ASP:OD1	1:E:388:ASP:N	2.22	0.72
1:B:153:VAL:CG1	1:B:154:THR:N	2.50	0.72
1:B:163:GLU:N	1:B:163:GLU:OE1	2.22	0.72
1:E:196:GLY:N	1:E:202:LYS:NZ	2.36	0.72
1:D:378:ARG:O	1:D:380:GLY:N	2.21	0.72
1:A:196:GLY:N	1:A:202:LYS:NZ	2.38	0.72
1:B:153:VAL:HG13	1:B:154:THR:H	1.54	0.72
1:D:215:VAL:HG21	1:D:249:PRO:O	1.89	0.72
1:D:283:LEU:CD1	1:D:316:ARG:HH21	2.01	0.72
1:D:454:ARG:HH21	1:D:526:TYR:C	1.93	0.72
1:C:331:ARG:NH1	1:C:354:ALA:O	2.22	0.72
1:D:173:GLU:HA	1:D:176:LYS:HE3	1.71	0.72
1:D:171:ILE:HG13	1:D:296:VAL:HG21	1.70	0.72
1:F:392:ALA:O	1:F:396:VAL:HG12	1.88	0.72
1:C:441:VAL:O	1:C:441:VAL:HG12	1.87	0.72
1:E:461:SER:O	1:E:464:ARG:HB2	1.88	0.72
1:C:165:LYS:O	1:C:168:LEU:HG	1.89	0.72
1:C:215:VAL:HG11	1:C:250:CYS:HA	1.70	0.72
1:C:418:HIS:O	1:C:421:GLY:N	2.22	0.72
1:E:441:VAL:HG12	1:E:441:VAL:O	1.89	0.72
1:A:149:GLU:O	1:A:150:ALA:HB3	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ALA:HB2	1:A:251:ILE:HD12	1.70	0.72
1:C:224:ASP:HA	1:C:227:GLU:OE2	1.89	0.72
1:E:236:ARG:O	1:E:237:VAL:C	2.27	0.72
1:F:346:GLU:HG3	1:F:386:MET:CG	2.19	0.72
1:F:579:ARG:O	1:F:581:THR:N	2.22	0.72
1:A:461:SER:O	1:A:464:ARG:HB3	1.89	0.72
1:A:439:THR:OG1	1:A:440:ILE:N	2.23	0.72
1:B:474:ALA:HA	1:B:558:VAL:CG1	2.16	0.72
1:B:392:ALA:O	1:B:396:VAL:HG12	1.89	0.72
1:D:247:HIS:HB3	1:D:250:CYS:SG	2.29	0.72
1:E:181:PHE:O	1:E:184:MET:HG2	1.90	0.72
1:C:439:THR:OG1	1:C:440:ILE:N	2.23	0.72
1:C:335:LEU:CD2	1:C:353:LEU:HD23	2.19	0.72
1:A:465:LEU:HD22	1:A:508:TRP:HZ3	1.55	0.72
1:E:524:ASP:CA	1:E:529:GLY:HA2	2.08	0.72
1:F:466:LEU:HD11	1:F:504:MET:HE1	1.72	0.72
1:D:589:ARG:HB3	1:D:594:LEU:HD22	1.71	0.72
1:B:454:ARG:HH21	1:B:526:TYR:C	1.91	0.72
1:F:376:ALA:C	1:F:381:ARG:HB2	2.10	0.72
1:B:286:MET:HE1	1:B:316:ARG:CA	2.09	0.72
1:B:286:MET:O	1:B:289:PHE:CB	2.37	0.72
1:A:382:ARG:HG3	1:A:383:LYS:CB	2.20	0.72
1:D:214:ARG:HB3	1:D:214:ARG:HH11	1.54	0.72
1:A:286:MET:CG	1:A:316:ARG:HD2	1.99	0.71
1:B:170:GLU:HB3	1:C:378:ARG:HH22	1.55	0.71
1:F:153:VAL:CG1	1:F:154:THR:N	2.52	0.71
1:F:190:LYS:CE	1:F:289:PHE:CZ	2.73	0.71
1:D:414:ILE:HG23	1:D:483:PHE:CE1	2.24	0.71
1:D:579:ARG:O	1:D:581:THR:N	2.22	0.71
1:F:589:ARG:HB3	1:F:594:LEU:HD22	1.72	0.71
1:D:567:GLU:O	1:D:570:GLU:N	2.23	0.71
1:F:346:GLU:HG3	1:F:386:MET:HG2	1.70	0.71
1:E:263:LYS:HG2	1:E:264:ARG:H	1.56	0.71
1:E:474:ALA:HA	1:E:558:VAL:HG11	1.71	0.71
1:B:571:ARG:HD2	1:B:590:VAL:O	1.88	0.71
1:F:458:LEU:HD12	1:F:459:HIS:N	2.04	0.71
1:B:184:MET:O	1:C:342:LYS:HD3	1.89	0.71
1:D:242:GLU:HA	1:D:245:LYS:HB3	1.72	0.71
1:F:286:MET:O	1:F:289:PHE:HB2	1.90	0.71
1:C:453:ARG:NH2	1:C:460:TRP:NE1	2.33	0.71
1:C:233:GLY:HA2	1:C:236:ARG:HH12	1.53	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:ARG:O	1:C:239:ASP:OD1	2.07	0.71
1:B:238:ARG:HB3	1:B:281:GLN:HE22	1.55	0.71
1:B:284:VAL:O	1:B:288:GLY:N	2.24	0.71
1:B:376:ALA:HA	1:B:381:ARG:HD2	0.72	0.71
1:E:313:ARG:CZ	1:E:526:TYR:O	2.39	0.71
1:A:239:ASP:OD1	1:A:240:LEU:N	2.22	0.71
1:B:199:GLY:N	2:B:2001:ADP:O2B	2.20	0.71
1:E:381:ARG:HG3	1:E:381:ARG:HH11	1.53	0.71
1:F:586:GLU:O	1:F:590:VAL:HG23	1.91	0.71
1:F:414:ILE:HG23	1:F:483:PHE:CE1	2.26	0.71
1:C:149:GLU:O	1:C:150:ALA:HB3	1.88	0.71
1:E:410:ARG:HG3	1:E:411:ASP:N	2.04	0.71
1:A:358:PRO:HA	1:A:359:GLY:C	2.11	0.71
1:B:352:LEU:O	1:B:355:LYS:HB2	1.90	0.71
1:F:163:GLU:N	1:F:163:GLU:OE1	2.24	0.71
1:C:586:GLU:O	1:C:589:ARG:HB2	1.90	0.71
1:C:202:LYS:HB2	2:C:1001:ADP:O1B	1.90	0.71
1:C:520:ALA:HA	1:C:533:ARG:CD	2.20	0.71
1:D:424:LEU:HD11	1:D:569:LEU:HA	1.72	0.71
1:D:465:LEU:O	1:D:469:ILE:HG13	1.89	0.71
1:C:155:PHE:HZ	1:C:168:LEU:HD11	1.55	0.71
1:B:233:GLY:O	1:B:236:ARG:NH1	2.23	0.71
1:A:467:ASP:OD1	1:A:557:ARG:NH2	2.24	0.71
1:A:474:ALA:HA	1:A:558:VAL:HG11	1.70	0.71
1:A:488:THR:O	1:A:490:ALA:N	2.21	0.71
1:D:163:GLU:OE1	1:D:163:GLU:N	2.23	0.71
1:F:165:LYS:HZ1	1:F:205:LEU:HB3	1.54	0.71
1:A:263:LYS:HG2	1:A:264:ARG:H	1.56	0.71
1:A:533:ARG:CD	1:A:534:GLN:H	2.04	0.71
1:D:348:VAL:HG22	1:D:352:LEU:HD22	1.72	0.71
1:B:155:PHE:HA	1:B:158:VAL:HG23	1.71	0.71
1:B:332:GLU:OE1	1:B:351:ALA:HA	1.91	0.71
1:C:521:VAL:HG12	1:D:495:ARG:HD2	1.71	0.71
1:B:242:GLU:HA	1:B:245:LYS:HB3	1.72	0.71
1:D:502:ARG:O	1:D:506:THR:HG23	1.91	0.71
1:B:533:ARG:HG3	1:B:533:ARG:HH11	1.56	0.71
1:D:193:LEU:O	1:D:320:GLN:HB2	1.90	0.71
1:C:453:ARG:HH21	1:C:464:ARG:NH2	1.89	0.71
1:C:493:ASP:O	1:C:496:GLN:HB2	1.91	0.71
1:B:190:LYS:CE	1:B:289:PHE:CZ	2.74	0.70
1:F:284:VAL:O	1:F:288:GLY:N	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:ARG:O	1:C:237:VAL:C	2.29	0.70
1:D:428:PHE:CE1	1:D:432:ALA:HB1	2.26	0.70
1:A:178:PRO:HB3	1:A:294:ALA:CB	2.21	0.70
1:B:346:GLU:HG3	1:B:386:MET:CG	2.20	0.70
1:D:191:GLY:CA	1:D:297:VAL:HG12	2.21	0.70
1:E:165:LYS:O	1:E:168:LEU:HG	1.90	0.70
1:F:153:VAL:HB	1:F:207:ARG:HH11	1.56	0.70
1:F:286:MET:O	1:F:289:PHE:CB	2.39	0.70
1:D:346:GLU:HG3	1:D:386:MET:CG	2.21	0.70
1:E:196:GLY:H	1:E:202:LYS:NZ	1.87	0.70
1:A:384:ILE:HG23	1:A:388:ASP:CB	2.21	0.70
1:D:449:PHE:CE2	1:D:453:ARG:NH2	2.59	0.70
1:B:449:PHE:CE2	1:B:453:ARG:NH2	2.59	0.70
1:B:458:LEU:HD12	1:B:459:HIS:H	1.55	0.70
1:E:313:ARG:NH2	1:E:526:TYR:O	2.25	0.70
1:A:481:ILE:CD1	1:A:563:LEU:HB3	2.21	0.70
1:E:419:GLU:HA	1:E:419:GLU:OE1	1.92	0.70
1:F:381:ARG:NH1	1:F:388:ASP:OD2	2.25	0.70
1:B:311:LEU:N	1:B:316:ARG:NH1	2.38	0.70
1:A:340:ARG:C	1:A:342:LYS:H	1.92	0.70
1:E:503:ARG:HG2	1:E:508:TRP:CZ3	2.27	0.70
1:A:313:ARG:CZ	1:A:526:TYR:O	2.40	0.70
1:E:439:THR:OG1	1:E:440:ILE:N	2.22	0.70
1:A:311:LEU:HD22	1:A:316:ARG:CZ	2.22	0.70
1:A:586:GLU:CA	1:A:589:ARG:HE	2.05	0.70
1:B:365:LEU:O	1:B:368:LEU:HB3	1.92	0.70
1:F:238:ARG:HB3	1:F:281:GLN:NE2	2.06	0.70
1:C:408:SER:HB2	1:C:409:PRO:HD2	1.73	0.70
1:C:239:ASP:OD1	1:C:240:LEU:N	2.25	0.70
1:A:520:ALA:HA	1:A:533:ARG:CD	2.22	0.70
1:D:214:ARG:HH11	1:D:214:ARG:CB	2.05	0.70
1:A:335:LEU:CD2	1:A:353:LEU:HD23	2.21	0.70
1:D:284:VAL:O	1:D:288:GLY:N	2.24	0.70
1:A:588:GLN:O	1:A:591:VAL:CB	2.39	0.70
1:F:182:HIS:ND1	1:F:182:HIS:N	2.40	0.70
1:B:503:ARG:HH22	1:B:522:ARG:CZ	2.05	0.70
1:A:465:LEU:HD22	1:A:508:TRP:CZ3	2.26	0.70
1:F:501:ALA:O	1:F:505:ILE:HD12	1.92	0.70
1:D:376:ALA:C	1:D:381:ARG:CG	2.60	0.70
1:D:389:LEU:O	1:D:392:ALA:N	2.25	0.70
1:C:384:ILE:HG23	1:C:388:ASP:CB	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:GLY:HA2	1:A:443:ARG:HH21	1.55	0.70
1:C:340:ARG:C	1:C:342:LYS:H	1.95	0.70
1:A:227:GLU:HG3	1:F:263:LYS:HZ3	1.57	0.70
1:A:224:ASP:HA	1:A:227:GLU:OE2	1.91	0.70
1:C:333:GLN:HG3	1:C:336:ARG:NH1	2.06	0.70
1:D:165:LYS:O	1:D:168:LEU:HB2	1.91	0.70
1:D:220:ALA:O	1:D:254:ILE:HA	1.91	0.70
1:F:376:ALA:HB2	1:F:381:ARG:HH11	1.57	0.70
1:B:319:ARG:HH11	1:B:319:ARG:CG	2.02	0.70
1:E:215:VAL:CG1	1:E:250:CYS:HA	2.22	0.70
1:E:286:MET:O	1:E:289:PHE:CZ	2.45	0.70
1:A:381:ARG:N	1:F:180:ARG:NH2	2.40	0.70
1:A:453:ARG:HH21	1:A:464:ARG:NH2	1.89	0.70
1:D:215:VAL:HG23	1:D:216:PRO:HD2	1.73	0.70
1:D:460:TRP:N	1:D:460:TRP:CE3	2.58	0.70
1:D:568:VAL:O	1:D:572:VAL:HG23	1.92	0.70
1:F:525:THR:HG22	1:F:526:TYR:HD2	1.55	0.70
1:D:428:PHE:CE1	1:D:432:ALA:CB	2.74	0.70
1:A:413:ARG:CA	1:A:577:LEU:HD22	2.16	0.69
1:A:196:GLY:H	1:A:202:LYS:NZ	1.89	0.69
1:D:262:ARG:CG	1:D:263:LYS:N	2.54	0.69
1:E:236:ARG:NH1	1:E:236:ARG:HB3	2.06	0.69
1:F:355:LYS:CE	1:F:578:GLU:O	2.40	0.69
1:F:394:ASP:HA	1:F:397:MET:CE	2.22	0.69
1:E:453:ARG:NH2	1:E:460:TRP:NE1	2.35	0.69
1:C:275:ARG:HG2	1:C:275:ARG:NH1	2.01	0.69
1:E:340:ARG:C	1:E:342:LYS:H	1.93	0.69
1:F:454:ARG:HH21	1:F:526:TYR:C	1.94	0.69
1:D:216:PRO:HG3	1:D:247:HIS:ND1	2.07	0.69
1:F:216:PRO:HG3	1:F:247:HIS:ND1	2.06	0.69
1:C:460:TRP:CD1	1:C:464:ARG:NH1	2.59	0.69
1:D:201:GLY:O	1:D:205:LEU:HD13	1.92	0.69
1:B:215:VAL:HG23	1:B:216:PRO:HD2	1.72	0.69
1:E:449:PHE:CD2	1:E:449:PHE:N	2.60	0.69
1:E:503:ARG:HD2	1:E:508:TRP:CE2	2.27	0.69
1:C:207:ARG:HB2	1:C:207:ARG:CZ	2.21	0.69
1:A:215:VAL:HG21	1:A:250:CYS:CA	2.21	0.69
1:A:286:MET:HE1	1:A:297:VAL:HG11	1.74	0.69
1:F:158:VAL:HG22	1:F:204:HIS:CE1	2.26	0.69
1:F:173:GLU:HA	1:F:176:LYS:HE3	1.74	0.69
1:D:564:GLU:C	1:D:566:ARG:H	1.95	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:202:LYS:HG2	2:D:2001:ADP:O1A	1.92	0.69
1:B:187:ARG:H	1:C:374:LEU:HD11	1.58	0.69
1:A:283:LEU:HD11	1:A:311:LEU:CD2	2.21	0.69
1:F:253:PHE:HA	1:F:298:MET:HB3	1.74	0.69
1:C:533:ARG:CD	1:C:534:GLN:H	2.05	0.69
1:C:303:ARG:HB2	1:C:303:ARG:HH11	0.64	0.69
1:E:382:ARG:HD3	1:E:383:LYS:HB3	1.74	0.69
1:F:303:ARG:O	1:F:307:LEU:HD13	1.93	0.69
1:E:358:PRO:HA	1:E:359:GLY:C	2.11	0.69
1:A:234:ALA:O	1:A:237:VAL:HG12	1.92	0.69
1:B:286:MET:CE	1:B:316:ARG:HA	2.09	0.69
1:D:225:PHE:CD2	1:D:236:ARG:HD2	2.28	0.69
1:C:453:ARG:HG3	1:C:453:ARG:NH1	2.02	0.69
1:C:177:ASN:HD22	1:C:180:ARG:HD3	1.58	0.69
1:B:238:ARG:CG	1:B:281:GLN:NE2	2.55	0.69
1:B:439:THR:CG2	1:B:445:ARG:HH22	2.01	0.69
1:C:313:ARG:NH2	1:C:526:TYR:CA	2.52	0.69
1:F:424:LEU:O	1:F:427:HIS:N	2.23	0.69
1:A:387:LYS:HA	1:A:390:GLU:HB2	1.73	0.69
1:D:233:GLY:HA2	1:D:236:ARG:HH21	1.51	0.69
1:F:238:ARG:CB	1:F:281:GLN:NE2	2.56	0.69
1:F:332:GLU:OE1	1:F:351:ALA:HA	1.91	0.69
1:D:424:LEU:O	1:D:427:HIS:N	2.23	0.69
1:E:453:ARG:CZ	1:E:460:TRP:HE1	2.05	0.69
1:E:533:ARG:CZ	1:E:534:GLN:O	2.40	0.69
1:C:234:ALA:HB1	1:C:281:GLN:NE2	2.07	0.69
1:E:303:ARG:HH11	1:E:303:ARG:HB2	0.65	0.69
1:D:155:PHE:O	1:D:158:VAL:N	2.26	0.69
1:D:337:ILE:HG23	1:D:338:HIS:CD2	2.28	0.69
1:D:355:LYS:CE	1:D:578:GLU:O	2.41	0.69
1:B:424:LEU:O	1:B:427:HIS:N	2.24	0.69
1:C:469:ILE:HG23	1:C:497:ALA:HB1	1.73	0.69
1:D:228:MET:SD	1:D:232:VAL:HG12	2.33	0.69
1:D:235:ALA:HA	1:D:238:ARG:CD	2.22	0.69
1:E:234:ALA:HB1	1:E:281:GLN:NE2	2.08	0.69
1:E:236:ARG:O	1:E:239:ASP:OD1	2.10	0.69
1:E:239:ASP:OD1	1:E:240:LEU:N	2.26	0.69
1:A:584:ALA:O	1:A:587:PHE:HB3	1.92	0.69
1:F:242:GLU:HA	1:F:245:LYS:HB3	1.73	0.69
1:F:365:LEU:O	1:F:368:LEU:HB3	1.93	0.69
1:C:413:ARG:HA	1:C:577:LEU:CD2	2.15	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:453:ARG:CZ	1:C:460:TRP:HE1	2.05	0.69
1:A:453:ARG:HH22	1:A:464:ARG:NH1	1.90	0.69
1:A:469:ILE:HG23	1:A:497:ALA:HB1	1.75	0.69
1:D:197:PRO:HD2	1:D:200:VAL:HG11	1.75	0.69
1:B:567:GLU:O	1:B:570:GLU:N	2.26	0.69
1:A:486:VAL:HG21	1:F:463:LYS:HE3	1.73	0.69
1:E:340:ARG:O	1:E:342:LYS:N	2.25	0.69
1:B:436:HIS:O	1:B:437:LYS:HG2	1.93	0.69
1:F:215:VAL:HG23	1:F:216:PRO:HD2	1.73	0.69
1:C:357:THR:OG1	1:C:360:PHE:CD1	2.46	0.69
1:D:503:ARG:HH22	1:D:522:ARG:NH2	1.91	0.69
1:A:357:THR:HG1	1:A:360:PHE:HD1	1.37	0.69
1:B:193:LEU:HA	1:B:299:ALA:O	1.92	0.69
1:C:178:PRO:HB3	1:C:294:ALA:CB	2.23	0.69
1:C:286:MET:O	1:C:289:PHE:CZ	2.46	0.69
1:B:215:VAL:CG2	1:B:249:PRO:O	2.41	0.69
1:E:196:GLY:O	1:E:302:ASN:HA	1.92	0.69
1:C:388:ASP:OD1	1:C:388:ASP:N	2.22	0.69
1:D:341:GLY:O	1:D:342:LYS:HB2	1.93	0.69
1:A:197:PRO:HD2	1:A:200:VAL:CG2	2.22	0.68
1:B:313:ARG:HG3	1:B:314:PRO:N	2.08	0.68
1:A:196:GLY:O	1:A:302:ASN:HA	1.94	0.68
1:E:166:GLU:HA	1:E:169:LYS:CG	2.23	0.68
1:C:519:TYR:O	1:C:533:ARG:CD	2.41	0.68
1:E:453:ARG:HG3	1:E:453:ARG:NH1	2.06	0.68
1:A:473:LEU:HD22	1:A:555:TYR:HB2	1.76	0.68
1:C:166:GLU:HA	1:C:169:LYS:CG	2.23	0.68
1:F:238:ARG:CG	1:F:281:GLN:NE2	2.56	0.68
1:C:481:ILE:HG22	1:C:482:VAL:N	2.07	0.68
1:E:408:SER:HB2	1:E:409:PRO:HD2	1.76	0.68
1:D:263:LYS:HZ3	1:E:227:GLU:HG3	1.57	0.68
1:F:177:ASN:OD1	1:F:180:ARG:HB2	1.94	0.68
1:F:191:GLY:HA2	1:F:297:VAL:HG12	1.73	0.68
1:F:236:ARG:HH12	1:F:278:THR:HG22	1.57	0.68
1:E:500:LEU:O	1:E:503:ARG:HB3	1.93	0.68
1:B:235:ALA:HA	1:B:238:ARG:CD	2.23	0.68
1:F:428:PHE:CE1	1:F:432:ALA:CB	2.76	0.68
1:B:220:ALA:O	1:B:254:ILE:HA	1.94	0.68
1:F:376:ALA:O	1:F:381:ARG:HG3	1.94	0.68
1:E:520:ALA:HA	1:E:533:ARG:CD	2.22	0.68
1:C:234:ALA:O	1:C:237:VAL:HG12	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:412:ARG:NH2	1:F:440:ILE:HD13	2.09	0.68
1:D:177:ASN:OD1	1:D:180:ARG:HB2	1.92	0.68
1:F:220:ALA:O	1:F:254:ILE:HA	1.93	0.68
1:A:166:GLU:HA	1:A:169:LYS:CG	2.21	0.68
1:D:238:ARG:HB3	1:D:281:GLN:NE2	2.09	0.68
1:D:289:PHE:CD2	1:D:290:GLU:N	2.61	0.68
1:C:410:ARG:HG3	1:C:411:ASP:N	2.06	0.68
1:A:319:ARG:HH21	1:B:402:LYS:HZ1	1.39	0.68
1:E:178:PRO:HB3	1:E:294:ALA:CB	2.23	0.68
1:A:588:GLN:HA	1:A:591:VAL:CG2	2.23	0.68
1:F:215:VAL:CG2	1:F:249:PRO:O	2.42	0.68
1:C:357:THR:OG1	1:C:360:PHE:HD1	1.75	0.68
1:D:392:ALA:O	1:D:396:VAL:HG12	1.94	0.68
1:B:216:PRO:HG3	1:B:247:HIS:ND1	2.07	0.68
1:E:400:PRO:HG2	1:E:405:LEU:HD12	1.76	0.68
1:D:221:SER:HB2	1:D:256:GLU:OE1	1.93	0.68
1:F:564:GLU:C	1:F:566:ARG:H	1.95	0.68
1:B:201:GLY:O	1:B:205:LEU:HD13	1.94	0.68
1:B:328:VAL:HG23	1:B:580:GLU:HG3	1.76	0.68
1:E:283:LEU:CG	1:E:316:ARG:HH12	2.04	0.68
1:C:581:THR:O	1:C:582:LEU:HD12	1.94	0.68
1:C:195:VAL:HG11	1:C:304:PRO:HD3	1.74	0.68
1:B:487:THR:HG22	1:B:488:THR:N	2.06	0.68
1:D:165:LYS:NZ	1:D:205:LEU:HB3	2.08	0.68
1:B:238:ARG:HG2	1:B:281:GLN:HE22	1.57	0.68
1:E:197:PRO:HD2	1:E:200:VAL:CG2	2.23	0.68
1:E:586:GLU:HA	1:E:589:ARG:CG	2.24	0.68
1:B:386:MET:O	1:B:389:LEU:HD12	1.93	0.68
1:B:191:GLY:HA2	1:B:297:VAL:HG12	1.74	0.68
1:D:276:GLU:CA	1:D:279:LEU:HD13	2.17	0.68
1:F:193:LEU:HA	1:F:299:ALA:O	1.93	0.68
1:F:283:LEU:HD13	1:F:316:ARG:NH2	2.06	0.68
1:F:386:MET:O	1:F:389:LEU:HD12	1.94	0.68
1:F:389:LEU:O	1:F:392:ALA:N	2.27	0.68
1:C:197:PRO:HD2	1:C:200:VAL:CG2	2.23	0.68
1:E:449:PHE:CZ	1:E:496:GLN:CG	2.67	0.68
1:B:245:LYS:C	1:B:247:HIS:H	1.97	0.68
1:B:154:THR:HG23	1:B:156:LYS:HB3	1.76	0.68
1:B:253:PHE:HA	1:B:298:MET:HB3	1.76	0.68
1:E:275:ARG:O	1:E:279:LEU:HB2	1.94	0.68
1:F:245:LYS:C	1:F:247:HIS:H	1.97	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:449:PHE:HB2	1:E:468:GLN:NE2	2.07	0.68
1:A:453:ARG:NH2	1:A:460:TRP:NE1	2.35	0.68
1:B:586:GLU:O	1:B:590:VAL:HG23	1.92	0.68
1:A:236:ARG:NH1	1:A:236:ARG:HB3	2.09	0.67
1:B:177:ASN:OD1	1:B:180:ARG:HB2	1.94	0.67
1:B:202:LYS:HG2	2:B:2001:ADP:O1A	1.93	0.67
1:F:191:GLY:CA	1:F:297:VAL:HG12	2.24	0.67
1:B:458:LEU:HD12	1:B:459:HIS:N	2.08	0.67
1:D:174:PHE:CZ	1:D:294:ALA:HB1	2.29	0.67
1:B:165:LYS:O	1:B:168:LEU:HB2	1.94	0.67
1:F:225:PHE:HB3	1:F:278:THR:HG21	1.74	0.67
1:B:466:LEU:HD11	1:B:504:MET:HE1	1.75	0.67
1:C:313:ARG:HH12	1:C:526:TYR:C	1.97	0.67
1:A:400:PRO:HG2	1:A:405:LEU:HD12	1.76	0.67
1:B:395:ARG:CG	1:B:395:ARG:HH11	1.98	0.67
1:B:276:GLU:CA	1:B:279:LEU:HD13	2.16	0.67
1:A:585:GLU:OE2	1:A:589:ARG:NE	2.27	0.67
1:A:340:ARG:O	1:A:342:LYS:N	2.26	0.67
1:F:174:PHE:CZ	1:F:294:ALA:HB1	2.28	0.67
1:C:263:LYS:HZ1	1:C:276:GLU:CD	1.98	0.67
1:D:376:ALA:C	1:D:381:ARG:HB2	2.15	0.67
1:C:168:LEU:O	1:C:171:ILE:HD12	1.95	0.67
1:B:182:HIS:ND1	1:B:182:HIS:N	2.40	0.67
1:A:524:ASP:CA	1:A:529:GLY:HA2	2.10	0.67
1:D:188:ILE:HG23	1:D:189:PRO:CD	2.24	0.67
1:B:341:GLY:O	1:B:342:LYS:HB2	1.94	0.67
1:D:236:ARG:HH12	1:D:278:THR:HG22	1.59	0.67
1:E:234:ALA:O	1:E:237:VAL:HG12	1.95	0.67
1:C:519:TYR:HA	1:C:533:ARG:NH2	2.09	0.67
1:E:449:PHE:CB	1:E:468:GLN:HE22	2.05	0.67
1:D:376:ALA:O	1:D:381:ARG:HG3	1.93	0.67
1:B:564:GLU:C	1:B:566:ARG:H	1.95	0.67
1:D:253:PHE:HA	1:D:298:MET:HB3	1.76	0.67
1:B:362:GLY:HA2	1:B:365:LEU:HD12	1.76	0.67
1:B:191:GLY:CA	1:B:297:VAL:HG12	2.24	0.67
1:F:276:GLU:HA	1:F:279:LEU:CD1	2.16	0.67
1:C:264:ARG:HG2	1:C:266:SER:H	1.59	0.67
1:C:449:PHE:HB2	1:C:468:GLN:NE2	2.09	0.67
1:C:447:LEU:HA	1:C:496:GLN:HE21	1.57	0.67
1:B:277:GLN:HA	1:B:280:ASN:ND2	2.09	0.67
1:E:334:ILE:HD13	2:E:1001:ADP:C6	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:331:ARG:HD2	1:E:357:THR:HG23	1.77	0.67
1:D:237:VAL:CG2	1:D:281:GLN:HG3	2.24	0.67
1:A:586:GLU:CB	1:A:589:ARG:HE	2.07	0.67
1:F:201:GLY:O	1:F:205:LEU:HD13	1.95	0.67
1:E:263:LYS:HZ2	1:E:276:GLU:CD	1.80	0.67
1:D:332:GLU:OE1	1:D:351:ALA:HA	1.94	0.67
1:E:387:LYS:HA	1:E:390:GLU:HB2	1.76	0.67
1:F:190:LYS:HE3	1:F:289:PHE:CZ	2.30	0.67
1:D:452:PRO:HG3	1:E:402:LYS:HE3	1.77	0.67
1:C:168:LEU:O	1:C:171:ILE:CD1	2.43	0.67
1:E:357:THR:OG1	1:E:360:PHE:CD1	2.48	0.67
1:A:378:ARG:HA	1:F:173:GLU:CD	2.14	0.67
1:F:237:VAL:CG2	1:F:281:GLN:HG3	2.25	0.67
1:C:449:PHE:CB	1:C:468:GLN:HE22	2.08	0.67
1:D:154:THR:HG23	1:D:156:LYS:HB3	1.77	0.67
1:A:523:GLU:N	1:A:523:GLU:OE1	2.27	0.67
1:F:525:THR:HG22	1:F:526:TYR:CD2	2.29	0.67
1:C:517:VAL:HG23	1:D:498:THR:OG1	1.95	0.67
1:B:173:GLU:HA	1:B:176:LYS:HE3	1.76	0.67
1:C:196:GLY:O	1:C:302:ASN:HA	1.95	0.67
1:E:491:GLU:O	1:E:493:ASP:N	2.28	0.67
1:C:273:ASP:OD1	1:C:274:GLU:N	2.28	0.67
1:D:376:ALA:CB	1:D:381:ARG:HH11	2.07	0.67
1:E:335:LEU:HD21	1:E:353:LEU:HD23	1.76	0.67
1:A:174:PHE:CE1	1:A:188:ILE:CD1	2.69	0.67
1:A:234:ALA:HB1	1:A:281:GLN:NE2	2.10	0.67
1:B:155:PHE:O	1:B:158:VAL:N	2.27	0.67
1:B:352:LEU:HD23	1:B:353:LEU:H	1.60	0.67
1:D:238:ARG:CB	1:D:281:GLN:NE2	2.58	0.67
1:E:168:LEU:O	1:E:171:ILE:CD1	2.43	0.67
1:D:503:ARG:HH12	1:D:522:ARG:HH21	1.40	0.67
1:F:503:ARG:HH22	1:F:522:ARG:CZ	2.08	0.67
1:B:303:ARG:O	1:B:307:LEU:HD13	1.95	0.67
1:E:333:GLN:HG3	1:E:336:ARG:NH1	2.10	0.67
1:A:333:GLN:HG3	1:A:336:ARG:NH1	2.10	0.66
1:D:193:LEU:HA	1:D:299:ALA:O	1.93	0.66
1:D:238:ARG:HG2	1:D:281:GLN:HE22	1.59	0.66
1:F:311:LEU:C	1:F:311:LEU:HD12	2.14	0.66
1:F:335:LEU:CD1	1:F:365:LEU:HB3	2.24	0.66
1:E:453:ARG:HH22	1:E:464:ARG:NH1	1.93	0.66
1:D:153:VAL:HB	1:D:207:ARG:NH1	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:378:ARG:O	1:F:380:GLY:N	2.28	0.66
1:F:228:MET:SD	1:F:232:VAL:HG12	2.35	0.66
1:B:200:VAL:HG22	1:B:202:LYS:HD2	1.77	0.66
1:D:245:LYS:C	1:D:247:HIS:H	1.98	0.66
1:F:159:ALA:HB3	1:F:334:ILE:CG1	2.24	0.66
1:F:352:LEU:O	1:F:355:LYS:N	2.27	0.66
1:C:264:ARG:CD	1:C:266:SER:HB2	2.25	0.66
1:D:436:HIS:O	1:D:437:LYS:HG2	1.94	0.66
1:A:215:VAL:HG23	1:A:216:PRO:CD	2.24	0.66
1:F:277:GLN:HA	1:F:280:ASN:ND2	2.11	0.66
1:F:333:GLN:O	1:F:336:ARG:HB3	1.96	0.66
1:F:343:PRO:O	1:F:344:LEU:HB3	1.96	0.66
1:F:395:ARG:HH11	1:F:395:ARG:CG	1.96	0.66
1:D:394:ASP:HA	1:D:397:MET:HE3	1.77	0.66
1:B:228:MET:SD	1:B:232:VAL:HG12	2.35	0.66
1:E:357:THR:OG1	1:E:360:PHE:HD1	1.77	0.66
1:A:580:GLU:HG2	1:A:580:GLU:O	1.94	0.66
1:B:346:GLU:HG3	1:B:386:MET:HG2	1.77	0.66
1:F:238:ARG:HG2	1:F:281:GLN:HE22	1.59	0.66
1:F:237:VAL:HG22	1:F:281:GLN:HG3	1.77	0.66
1:F:362:GLY:HA2	1:F:365:LEU:HD12	1.77	0.66
1:C:387:LYS:HA	1:C:390:GLU:HB2	1.77	0.66
1:E:469:ILE:HG23	1:E:497:ALA:HB1	1.77	0.66
1:E:196:GLY:HA2	1:E:443:ARG:HH21	1.61	0.66
1:E:585:GLU:O	1:E:588:GLN:HG2	1.94	0.66
1:D:241:PHE:CD2	1:D:285:GLU:HG3	2.31	0.66
1:D:225:PHE:HB3	1:D:278:THR:HG21	1.77	0.66
1:E:215:VAL:HG11	1:E:250:CYS:CA	2.25	0.66
1:F:155:PHE:O	1:F:158:VAL:N	2.27	0.66
1:D:523:GLU:OE2	1:E:264:ARG:NH2	2.29	0.66
1:A:453:ARG:NH2	1:A:464:ARG:HH22	1.93	0.66
1:C:207:ARG:NH2	1:C:217:PHE:HD2	1.93	0.66
1:C:207:ARG:HH21	1:C:217:PHE:HD2	1.42	0.66
1:A:225:PHE:CE1	1:A:233:GLY:HA2	2.29	0.66
1:C:340:ARG:O	1:C:342:LYS:N	2.29	0.66
1:D:237:VAL:HG22	1:D:281:GLN:HG3	1.77	0.66
1:F:209:VAL:HG13	1:F:210:ALA:N	2.11	0.66
1:C:514:PHE:HB3	1:C:519:TYR:CE1	2.31	0.66
1:E:533:ARG:CD	1:E:534:GLN:H	2.06	0.66
1:C:523:GLU:OE1	1:C:523:GLU:N	2.28	0.66
1:D:428:PHE:CZ	1:D:432:ALA:HB1	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:277:GLN:HA	1:D:280:ASN:ND2	2.11	0.66
1:E:460:TRP:O	1:F:488:THR:HA	1.95	0.66
1:D:373:ALA:O	1:D:376:ALA:HB3	1.96	0.66
1:C:572:VAL:O	1:C:576:LEU:HB2	1.96	0.66
1:C:382:ARG:HG3	1:C:383:LYS:CB	2.25	0.66
1:D:241:PHE:CE2	1:D:285:GLU:HG3	2.31	0.66
1:A:381:ARG:O	1:F:180:ARG:NH2	2.29	0.66
1:C:462:ARG:HB2	1:C:510:MET:SD	2.35	0.66
1:A:449:PHE:CB	1:A:468:GLN:HE22	2.08	0.66
1:A:533:ARG:CZ	1:A:534:GLN:O	2.43	0.66
1:C:290:GLU:OE2	1:D:226:VAL:HG11	1.96	0.66
1:A:155:PHE:HZ	1:A:168:LEU:HD11	1.59	0.66
1:C:585:GLU:O	1:C:588:GLN:HG2	1.94	0.66
1:D:200:VAL:HG22	1:D:202:LYS:HD2	1.78	0.66
1:F:428:PHE:CE1	1:F:432:ALA:HB1	2.30	0.66
1:E:586:GLU:O	1:E:589:ARG:HB2	1.96	0.66
1:B:352:LEU:O	1:B:355:LYS:N	2.29	0.66
1:E:177:ASN:HD22	1:E:180:ARG:HD3	1.61	0.66
1:E:312:LEU:O	1:E:318:ASP:HA	1.95	0.66
1:C:263:LYS:HG2	1:C:264:ARG:H	1.60	0.66
1:C:467:ASP:O	1:C:470:ALA:HB3	1.96	0.66
1:C:225:PHE:CZ	1:C:278:THR:CB	2.72	0.66
1:D:159:ALA:HB3	1:D:334:ILE:CG1	2.25	0.66
1:B:410:ARG:O	1:B:413:ARG:N	2.29	0.66
1:E:313:ARG:NH2	1:E:526:TYR:CA	2.46	0.66
1:B:378:ARG:O	1:B:380:GLY:N	2.29	0.66
1:A:225:PHE:HE1	1:A:233:GLY:C	1.98	0.65
1:E:168:LEU:O	1:E:171:ILE:HD12	1.95	0.65
1:F:225:PHE:CD2	1:F:236:ARG:HD2	2.31	0.65
1:F:283:LEU:HD12	1:F:316:ARG:CZ	2.26	0.65
1:F:313:ARG:HG3	1:F:314:PRO:N	2.11	0.65
1:C:334:ILE:HD13	2:C:1001:ADP:C6	2.31	0.65
1:C:335:LEU:HD21	1:C:353:LEU:HD23	1.78	0.65
1:F:449:PHE:CZ	1:F:453:ARG:CZ	2.79	0.65
1:D:362:GLY:HA2	1:D:365:LEU:HD12	1.78	0.65
1:B:178:PRO:HG3	1:B:249:PRO:HG3	1.78	0.65
1:B:589:ARG:HB3	1:B:594:LEU:CD2	2.26	0.65
1:A:211:GLY:CA	1:A:214:ARG:HE	2.08	0.65
1:B:337:ILE:HG23	1:B:338:HIS:CD2	2.31	0.65
1:E:155:PHE:HZ	1:E:168:LEU:HD11	1.58	0.65
1:C:500:LEU:O	1:C:503:ARG:HB3	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:465:LEU:HD22	1:C:508:TRP:HZ3	1.61	0.65
1:D:466:LEU:HD11	1:D:504:MET:HE1	1.77	0.65
1:D:508:TRP:HD1	1:E:491:GLU:HG2	1.61	0.65
1:D:343:PRO:HG2	1:D:383:LYS:HA	1.79	0.65
1:B:225:PHE:HB3	1:B:278:THR:HG21	1.78	0.65
1:A:169:LYS:O	1:A:172:VAL:HG13	1.96	0.65
1:A:202:LYS:HB2	2:A:1001:ADP:O1B	1.96	0.65
1:A:316:ARG:HG2	1:A:317:PHE:N	2.11	0.65
1:A:357:THR:OG1	1:A:360:PHE:CD1	2.49	0.65
1:A:196:GLY:CA	1:A:443:ARG:NH2	2.60	0.65
1:B:263:LYS:HZ3	1:C:227:GLU:HG3	1.59	0.65
1:D:178:PRO:HG3	1:D:249:PRO:HG3	1.78	0.65
1:F:311:LEU:O	1:F:316:ARG:HG2	1.95	0.65
1:C:400:PRO:HG2	1:C:405:LEU:HD12	1.78	0.65
1:D:487:THR:HG22	1:D:488:THR:N	2.07	0.65
1:C:428:PHE:O	1:C:432:ALA:HB2	1.96	0.65
1:C:419:GLU:OE1	1:C:419:GLU:HA	1.95	0.65
1:A:215:VAL:CG1	1:A:250:CYS:HA	2.27	0.65
1:F:221:SER:HB2	1:F:256:GLU:OE1	1.97	0.65
1:A:264:ARG:HD2	1:A:266:SER:CB	2.26	0.65
1:C:333:GLN:HA	1:C:336:ARG:CZ	2.26	0.65
1:C:273:ASP:CG	1:C:274:GLU:N	2.49	0.65
1:E:428:PHE:O	1:E:432:ALA:HB2	1.96	0.65
1:B:318:ASP:O	1:B:319:ARG:CB	2.32	0.65
1:D:238:ARG:CG	1:D:281:GLN:NE2	2.58	0.65
1:E:225:PHE:HE1	1:E:233:GLY:C	2.00	0.65
1:F:153:VAL:HB	1:F:207:ARG:NH1	2.12	0.65
1:C:215:VAL:CG1	1:C:250:CYS:HA	2.27	0.65
1:E:313:ARG:HH12	1:E:526:TYR:C	1.99	0.65
1:F:202:LYS:HG2	2:F:2001:ADP:O1A	1.97	0.65
1:F:160:GLY:H	1:F:333:GLN:NE2	1.95	0.65
1:C:533:ARG:CD	1:C:534:GLN:N	2.60	0.65
1:A:512:PRO:HB2	1:A:514:PHE:HD2	1.61	0.65
1:A:519:TYR:O	1:A:533:ARG:CD	2.45	0.65
1:A:275:ARG:O	1:A:279:LEU:HB2	1.96	0.65
1:B:311:LEU:HD12	1:B:311:LEU:C	2.16	0.65
1:D:286:MET:CE	1:D:315:GLY:O	2.45	0.65
1:F:174:PHE:HB2	1:F:181:PHE:HE2	1.60	0.65
1:F:348:VAL:HG21	1:F:352:LEU:HD11	1.77	0.65
1:D:352:LEU:O	1:D:355:LYS:N	2.29	0.65
1:C:215:VAL:HG23	1:C:216:PRO:CD	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:ILE:HG23	1:B:189:PRO:CD	2.24	0.65
1:A:419:GLU:HA	1:A:419:GLU:OE1	1.97	0.65
1:B:221:SER:HB2	1:B:256:GLU:OE1	1.97	0.65
1:C:414:ILE:HG22	1:C:415:THR:N	2.12	0.65
1:D:463:LYS:O	1:D:466:LEU:N	2.29	0.65
1:C:312:LEU:O	1:C:318:ASP:HA	1.95	0.65
1:A:305:ASP:OD1	1:A:305:ASP:N	2.27	0.65
1:F:463:LYS:O	1:F:466:LEU:N	2.30	0.65
1:B:514:PHE:HB3	1:B:519:TYR:HE1	1.62	0.65
1:D:263:LYS:HZ2	1:E:227:GLU:HG3	1.60	0.65
1:E:233:GLY:HA2	1:E:236:ARG:HH12	1.61	0.65
1:E:510:MET:O	1:E:512:PRO:CD	2.44	0.65
1:A:449:PHE:CD2	1:A:449:PHE:N	2.64	0.65
1:D:394:ASP:HA	1:D:397:MET:CE	2.26	0.65
1:E:195:VAL:HG11	1:E:304:PRO:HD3	1.78	0.65
1:E:580:GLU:HG2	1:E:580:GLU:O	1.97	0.64
1:A:357:THR:OG1	1:A:360:PHE:HD1	1.77	0.64
1:B:389:LEU:O	1:B:392:ALA:N	2.30	0.64
1:C:264:ARG:HG3	1:C:265:GLY:N	2.11	0.64
1:C:225:PHE:CE1	1:C:233:GLY:HA2	2.29	0.64
1:D:328:VAL:HG23	1:D:580:GLU:HG3	1.79	0.64
1:D:344:LEU:HD22	1:D:346:GLU:OE1	1.97	0.64
1:B:463:LYS:O	1:B:466:LEU:N	2.30	0.64
1:B:412:ARG:NH2	1:B:440:ILE:HD13	2.12	0.64
1:D:174:PHE:HB2	1:D:181:PHE:HE2	1.58	0.64
1:C:488:THR:O	1:C:490:ALA:N	2.28	0.64
1:E:179:SER:O	1:E:182:HIS:HD2	1.80	0.64
1:E:283:LEU:CG	1:E:316:ARG:NH1	2.54	0.64
1:F:181:PHE:O	1:F:184:MET:N	2.30	0.64
1:B:510:MET:O	1:B:512:PRO:HD2	1.98	0.64
1:E:263:LYS:HZ1	1:E:276:GLU:CD	1.99	0.64
1:D:352:LEU:HD23	1:D:353:LEU:H	1.62	0.64
1:F:188:ILE:HG23	1:F:189:PRO:CD	2.25	0.64
1:E:567:GLU:HA	1:E:570:GLU:OE1	1.96	0.64
1:A:335:LEU:HD21	1:A:353:LEU:HD23	1.78	0.64
1:B:154:THR:CG2	1:B:156:LYS:HB3	2.27	0.64
1:B:394:ASP:HA	1:B:397:MET:CE	2.27	0.64
1:A:264:ARG:NE	1:A:266:SER:HB2	2.12	0.64
1:C:447:LEU:HA	1:C:496:GLN:NE2	2.12	0.64
1:D:386:MET:O	1:D:389:LEU:HD12	1.97	0.64
1:C:152:LYS:HG3	1:C:153:VAL:CG2	2.22	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:VAL:HA	1:C:157:ASP:OD2	1.98	0.64
1:C:580:GLU:HG2	1:C:580:GLU:O	1.97	0.64
1:B:190:LYS:HE3	1:B:289:PHE:CZ	2.33	0.64
1:D:474:ALA:HA	1:D:558:VAL:CG1	2.21	0.64
1:E:470:ALA:O	1:E:558:VAL:HG21	1.98	0.64
1:E:533:ARG:CD	1:E:534:GLN:N	2.60	0.64
1:B:587:PHE:O	1:B:591:VAL:HG23	1.97	0.64
1:D:273:ASP:N	1:D:273:ASP:OD1	2.29	0.64
1:F:376:ALA:CA	1:F:381:ARG:HH11	2.11	0.64
1:B:257:ILE:N	1:B:257:ILE:HD12	2.13	0.64
1:C:533:ARG:CZ	1:C:534:GLN:O	2.46	0.64
1:C:236:ARG:NH1	1:C:236:ARG:HB3	2.13	0.64
1:D:154:THR:CG2	1:D:156:LYS:HB3	2.28	0.64
1:B:237:VAL:HG22	1:B:281:GLN:HG3	1.79	0.64
1:F:586:GLU:O	1:F:589:ARG:HB2	1.98	0.64
1:F:439:THR:CG2	1:F:445:ARG:HH22	2.08	0.64
1:D:303:ARG:O	1:D:307:LEU:HD13	1.97	0.64
1:F:341:GLY:O	1:F:342:LYS:HB2	1.98	0.64
1:D:286:MET:O	1:D:289:PHE:CB	2.45	0.64
1:E:169:LYS:O	1:E:172:VAL:HG13	1.98	0.64
1:D:414:ILE:O	1:D:417:TYR:N	2.31	0.64
1:E:520:ALA:CA	1:E:533:ARG:HD3	2.26	0.64
1:A:453:ARG:NH2	1:A:464:ARG:NH2	2.46	0.64
1:D:207:ARG:HB2	1:D:217:PHE:CE1	2.31	0.64
1:D:209:VAL:HG13	1:D:210:ALA:N	2.10	0.64
1:A:262:ARG:CG	1:A:275:ARG:HH22	2.07	0.64
1:D:313:ARG:NE	1:D:314:PRO:CG	2.61	0.64
1:C:453:ARG:HH22	1:C:464:ARG:NH1	1.95	0.64
1:D:369:LEU:O	1:D:372:ALA:N	2.28	0.64
1:B:175:LEU:CD1	1:B:215:VAL:HG11	2.27	0.64
1:A:313:ARG:HH12	1:A:526:TYR:C	2.01	0.64
1:F:273:ASP:OD1	1:F:273:ASP:N	2.31	0.64
1:F:465:LEU:O	1:F:469:ILE:HG13	1.98	0.64
1:F:385:THR:HB	1:F:388:ASP:OD1	1.98	0.64
1:A:286:MET:O	1:A:289:PHE:CZ	2.50	0.64
1:B:379:GLU:OE1	1:B:381:ARG:NE	2.31	0.64
1:D:258:ASP:N	1:D:258:ASP:OD1	2.28	0.64
1:C:449:PHE:N	1:C:449:PHE:CD2	2.63	0.64
1:C:453:ARG:CG	1:C:453:ARG:HH11	2.10	0.64
1:C:518:ALA:CB	1:D:495:ARG:HA	2.27	0.64
1:C:190:LYS:HD2	1:C:289:PHE:HE1	1.59	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:MET:CE	1:B:236:ARG:HD3	2.27	0.64
1:B:237:VAL:CG2	1:B:281:GLN:HG3	2.27	0.64
1:B:465:LEU:O	1:B:469:ILE:HG13	1.98	0.64
1:E:481:ILE:CD1	1:E:563:LEU:HB3	2.27	0.64
1:A:467:ASP:O	1:A:470:ALA:HB3	1.98	0.64
1:A:252:VAL:O	1:A:298:MET:N	2.30	0.64
1:B:577:LEU:HG	1:B:578:GLU:N	2.13	0.64
1:B:286:MET:CE	1:B:315:GLY:O	2.46	0.64
1:D:241:PHE:CD1	1:D:242:GLU:N	2.66	0.64
1:F:165:LYS:O	1:F:168:LEU:HB2	1.98	0.64
1:F:175:LEU:CD1	1:F:215:VAL:HG11	2.28	0.64
1:F:253:PHE:HE2	1:F:255:ASP:CB	2.11	0.64
1:D:523:GLU:OE1	1:E:264:ARG:NH2	2.31	0.64
1:A:520:ALA:CA	1:A:533:ARG:HD3	2.27	0.64
1:D:160:GLY:H	1:D:333:GLN:NE2	1.96	0.64
1:A:177:ASN:HD22	1:A:180:ARG:HD3	1.63	0.63
1:B:174:PHE:CZ	1:B:294:ALA:HB1	2.33	0.63
1:D:225:PHE:CE2	1:D:236:ARG:HD2	2.32	0.63
1:B:428:PHE:CE1	1:B:432:ALA:CB	2.81	0.63
1:E:581:THR:O	1:E:582:LEU:HD12	1.98	0.63
1:F:376:ALA:CB	1:F:381:ARG:HH11	2.09	0.63
1:B:400:PRO:HA	1:B:403:LYS:HB2	1.81	0.63
1:E:212:GLU:N	1:E:214:ARG:HG3	2.13	0.63
1:E:225:PHE:CE1	1:E:233:GLY:HA2	2.31	0.63
1:A:567:GLU:HA	1:A:570:GLU:OE1	1.99	0.63
1:F:178:PRO:HG3	1:F:249:PRO:HG3	1.80	0.63
1:F:257:ILE:N	1:F:257:ILE:HD12	2.13	0.63
1:A:264:ARG:HD2	1:A:266:SER:HB2	1.78	0.63
1:C:465:LEU:HD22	1:C:508:TRP:CZ3	2.33	0.63
1:D:420:ALA:O	1:D:424:LEU:HD12	1.99	0.63
1:B:273:ASP:OD1	1:B:273:ASP:N	2.31	0.63
1:B:262:ARG:CG	1:B:263:LYS:N	2.54	0.63
1:E:212:GLU:O	1:E:214:ARG:HG3	1.98	0.63
1:F:214:ARG:HH11	1:F:214:ARG:CG	2.11	0.63
1:F:396:VAL:O	1:F:400:PRO:HD2	1.98	0.63
1:C:196:GLY:HA2	1:C:443:ARG:HH21	1.63	0.63
1:E:523:GLU:N	1:E:523:GLU:OE1	2.31	0.63
1:E:292:ASP:OD1	1:E:292:ASP:C	2.36	0.63
1:B:174:PHE:HB2	1:B:181:PHE:HE2	1.61	0.63
1:D:175:LEU:CD1	1:D:215:VAL:HG11	2.28	0.63
1:D:260:VAL:HG23	1:D:279:LEU:HD12	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:275:ARG:O	1:E:279:LEU:CB	2.47	0.63
1:A:588:GLN:O	1:A:591:VAL:N	2.31	0.63
1:C:503:ARG:HG2	1:C:508:TRP:CH2	2.33	0.63
1:A:461:SER:O	1:A:465:LEU:HD12	1.97	0.63
1:E:152:LYS:HG3	1:E:153:VAL:CG2	2.20	0.63
1:B:328:VAL:CG2	1:B:355:LYS:CE	2.76	0.63
1:D:526:TYR:HE2	1:E:256:GLU:OE2	1.81	0.63
1:E:252:VAL:O	1:E:298:MET:N	2.30	0.63
1:F:165:LYS:HZ3	1:F:205:LEU:HB3	1.60	0.63
1:F:238:ARG:HB3	1:F:281:GLN:HE22	1.60	0.63
1:E:467:ASP:O	1:E:470:ALA:HB3	1.98	0.63
1:D:577:LEU:HG	1:D:578:GLU:N	2.11	0.63
1:E:384:ILE:HG23	1:E:388:ASP:CB	2.26	0.63
1:D:215:VAL:CG2	1:D:249:PRO:O	2.45	0.63
1:A:596:LEU:HG	1:A:597:GLU:N	2.13	0.63
1:F:202:LYS:HD3	2:F:2001:ADP:O2B	1.99	0.63
1:F:260:VAL:HG23	1:F:279:LEU:HD12	1.79	0.63
1:C:252:VAL:O	1:C:298:MET:N	2.29	0.63
1:F:430:GLU:OE1	1:F:430:GLU:CA	2.46	0.63
1:E:589:ARG:CZ	1:E:589:ARG:CB	2.77	0.63
1:B:343:PRO:O	1:B:344:LEU:HB3	1.98	0.63
1:C:510:MET:O	1:C:512:PRO:HD2	1.98	0.63
1:D:410:ARG:O	1:D:413:ARG:HB2	1.98	0.63
1:E:461:SER:O	1:E:465:LEU:HD12	1.98	0.63
1:C:292:ASP:OD1	1:C:292:ASP:C	2.37	0.63
1:A:449:PHE:HB2	1:A:468:GLN:NE2	2.12	0.63
1:A:572:VAL:O	1:A:576:LEU:HB2	1.99	0.63
1:F:376:ALA:CB	1:F:381:ARG:CD	2.70	0.63
1:A:168:LEU:CB	1:A:171:ILE:CD1	2.77	0.63
1:E:215:VAL:HG23	1:E:216:PRO:CD	2.26	0.63
1:E:273:ASP:CG	1:E:274:GLU:N	2.51	0.63
1:C:169:LYS:O	1:C:172:VAL:HG13	1.99	0.63
1:A:152:LYS:HG3	1:A:153:VAL:CG2	2.25	0.63
1:A:414:ILE:HG22	1:A:415:THR:N	2.13	0.63
1:B:159:ALA:HB3	1:B:334:ILE:CG1	2.29	0.63
1:B:209:VAL:HG13	1:B:210:ALA:N	2.14	0.63
1:F:155:PHE:HA	1:F:158:VAL:CG2	2.29	0.63
1:E:514:PHE:HB3	1:E:519:TYR:CE1	2.34	0.63
1:A:539:THR:O	1:A:543:ILE:HG13	1.99	0.63
1:F:519:TYR:HB3	1:F:535:TYR:HD2	1.64	0.63
1:D:396:VAL:O	1:D:400:PRO:HD2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:597:GLU:O	1:D:599:PRO:HD3	1.98	0.63
1:A:155:PHE:HZ	1:A:209:VAL:HG22	1.64	0.62
1:B:318:ASP:N	1:B:318:ASP:OD1	2.24	0.62
1:D:317:PHE:HD1	1:D:317:PHE:N	1.97	0.62
1:E:453:ARG:HH21	1:E:464:ARG:HH22	1.47	0.62
1:E:447:LEU:HA	1:E:496:GLN:NE2	2.12	0.62
1:F:428:PHE:CZ	1:F:432:ALA:HB1	2.34	0.62
1:B:181:PHE:O	1:B:184:MET:N	2.32	0.62
1:E:149:GLU:O	1:E:150:ALA:CB	2.46	0.62
1:E:212:GLU:CA	1:E:214:ARG:HG3	2.29	0.62
1:E:273:ASP:OD1	1:E:274:GLU:N	2.31	0.62
1:B:152:LYS:HB2	1:B:207:ARG:NH1	2.14	0.62
1:B:396:VAL:O	1:B:400:PRO:HD2	2.00	0.62
1:D:318:ASP:O	1:D:319:ARG:CB	2.35	0.62
1:A:586:GLU:CB	1:A:589:ARG:NE	2.63	0.62
1:F:210:ALA:O	1:F:214:ARG:HA	2.00	0.62
1:F:327:ASP:O	1:F:331:ARG:CZ	2.47	0.62
1:C:264:ARG:CG	1:C:266:SER:N	2.41	0.62
1:D:400:PRO:HA	1:D:403:LYS:HB2	1.82	0.62
1:B:414:ILE:O	1:B:417:TYR:N	2.32	0.62
1:F:420:ALA:O	1:F:424:LEU:HD12	1.99	0.62
1:A:179:SER:O	1:A:182:HIS:HD2	1.82	0.62
1:B:165:LYS:NZ	1:B:205:LEU:HB3	2.15	0.62
1:B:253:PHE:HE2	1:B:255:ASP:CB	2.12	0.62
1:B:313:ARG:NE	1:B:314:PRO:CG	2.63	0.62
1:C:414:ILE:CG2	1:C:415:THR:N	2.63	0.62
1:D:510:MET:O	1:D:512:PRO:HD2	1.98	0.62
1:C:225:PHE:HZ	1:C:278:THR:HB	1.60	0.62
1:A:533:ARG:CD	1:A:534:GLN:N	2.61	0.62
1:B:586:GLU:O	1:B:589:ARG:HB2	1.99	0.62
1:D:589:ARG:HB3	1:D:594:LEU:CD2	2.29	0.62
1:F:258:ASP:N	1:F:258:ASP:OD1	2.31	0.62
1:E:166:GLU:CB	1:E:169:LYS:HZ2	2.09	0.62
1:F:400:PRO:HA	1:F:403:LYS:HB2	1.81	0.62
1:C:333:GLN:HG3	1:C:336:ARG:HH12	1.63	0.62
1:B:165:LYS:O	1:B:168:LEU:CA	2.48	0.62
1:B:328:VAL:HG21	1:B:355:LYS:CE	2.30	0.62
1:F:533:ARG:HG3	1:F:533:ARG:HH11	1.65	0.62
1:C:214:ARG:HG2	1:C:214:ARG:O	1.98	0.62
1:D:586:GLU:O	1:D:589:ARG:HB2	2.00	0.62
1:A:233:GLY:HA2	1:A:236:ARG:HH12	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:286:MET:O	1:E:289:PHE:CE1	2.52	0.62
1:E:191:GLY:HA2	1:E:297:VAL:HG22	1.81	0.62
1:E:453:ARG:NH2	1:E:464:ARG:HH22	1.97	0.62
1:C:524:ASP:CA	1:C:529:GLY:HA2	2.09	0.62
1:E:153:VAL:HA	1:E:157:ASP:OD2	1.99	0.62
1:B:258:ASP:N	1:B:258:ASP:OD1	2.31	0.62
1:E:414:ILE:HG22	1:E:415:THR:N	2.14	0.62
1:E:397:MET:HG3	1:E:406:VAL:HG13	1.82	0.62
1:A:195:VAL:HG22	1:A:301:THR:O	1.99	0.62
1:A:334:ILE:HD13	2:A:1001:ADP:C6	2.35	0.62
1:B:373:ALA:O	1:B:376:ALA:HB3	1.99	0.62
1:B:311:LEU:O	1:B:316:ARG:HD3	1.99	0.62
1:E:174:PHE:CE1	1:E:188:ILE:CD1	2.69	0.62
1:F:165:LYS:HE2	1:F:205:LEU:CG	2.30	0.62
1:C:331:ARG:HD2	1:C:357:THR:HG23	1.82	0.62
1:C:179:SER:O	1:C:182:HIS:HD2	1.82	0.62
1:D:181:PHE:O	1:D:184:MET:N	2.33	0.62
1:F:373:ALA:HA	1:F:384:ILE:HD11	1.82	0.62
1:A:236:ARG:NH1	1:A:236:ARG:CG	2.59	0.62
1:B:355:LYS:NZ	1:B:578:GLU:HG3	2.15	0.62
1:C:191:GLY:HA2	1:C:297:VAL:HG22	1.82	0.62
1:D:165:LYS:O	1:D:168:LEU:CA	2.47	0.62
1:B:225:PHE:HB3	1:B:236:ARG:NH1	2.14	0.62
1:A:428:PHE:O	1:A:432:ALA:HB2	2.00	0.62
1:D:255:ASP:O	1:D:256:GLU:HG2	2.00	0.62
1:E:572:VAL:O	1:E:576:LEU:HB2	1.99	0.61
1:B:382:ARG:HB3	1:B:383:LYS:HB2	1.82	0.61
1:D:238:ARG:HB3	1:D:281:GLN:HE22	1.63	0.61
1:E:225:PHE:CZ	1:E:278:THR:CB	2.76	0.61
1:F:190:LYS:HZ1	1:F:289:PHE:HE2	0.70	0.61
1:C:276:GLU:OE2	1:C:527:LEU:HD11	2.00	0.61
1:D:517:VAL:HG11	1:D:519:TYR:OH	1.99	0.61
1:E:519:TYR:O	1:E:533:ARG:CD	2.47	0.61
1:C:177:ASN:ND2	1:C:180:ARG:HD3	2.16	0.61
1:F:378:ARG:C	1:F:380:GLY:N	2.52	0.61
1:B:260:VAL:HG23	1:B:279:LEU:HD12	1.82	0.61
1:F:255:ASP:O	1:F:256:GLU:HG2	1.99	0.61
1:A:449:PHE:HE2	1:A:496:GLN:NE2	1.97	0.61
1:A:153:VAL:HA	1:A:157:ASP:OD2	2.01	0.61
1:E:390:GLU:O	1:E:393:ALA:N	2.33	0.61
1:A:430:GLU:O	1:A:431:HIS:CB	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:LEU:HD12	1:A:299:ALA:O	1.99	0.61
1:A:292:ASP:OD1	1:A:292:ASP:C	2.37	0.61
1:B:313:ARG:NE	1:B:314:PRO:CD	2.62	0.61
1:F:215:VAL:HG22	1:F:216:PRO:CD	2.29	0.61
1:C:453:ARG:NH2	1:C:464:ARG:HH22	1.97	0.61
1:D:511:HIS:C	1:D:512:PRO:O	2.38	0.61
1:A:510:MET:O	1:A:512:PRO:CD	2.47	0.61
1:D:253:PHE:HE2	1:D:255:ASP:CB	2.11	0.61
1:F:507:GLU:HG3	1:F:520:ALA:O	2.00	0.61
1:A:166:GLU:CB	1:A:169:LYS:HZ2	2.08	0.61
1:A:440:ILE:HG22	1:A:441:VAL:HG23	1.83	0.61
1:F:241:PHE:CD1	1:F:242:GLU:N	2.68	0.61
1:F:159:ALA:HB1	1:F:333:GLN:CG	2.31	0.61
1:D:382:ARG:HG2	1:D:382:ARG:NH1	2.11	0.61
1:D:344:LEU:HA	1:D:383:LYS:HG3	1.83	0.61
1:B:241:PHE:CD1	1:B:242:GLU:N	2.68	0.61
1:E:338:HIS:CE1	1:E:366:GLU:HG3	2.36	0.61
1:A:333:GLN:HA	1:A:336:ARG:CZ	2.30	0.61
1:D:314:PRO:C	1:D:316:ARG:H	2.02	0.61
1:A:581:THR:O	1:A:582:LEU:HD12	2.00	0.61
1:F:225:PHE:CE2	1:F:236:ARG:HD2	2.35	0.61
1:F:382:ARG:HB3	1:F:383:LYS:HB2	1.82	0.61
1:F:394:ASP:HA	1:F:397:MET:HE3	1.81	0.61
1:E:469:ILE:O	1:E:473:LEU:HD12	2.01	0.61
1:B:428:PHE:CE1	1:B:432:ALA:HB1	2.34	0.61
1:F:376:ALA:HA	1:F:381:ARG:NH1	2.16	0.61
1:A:215:VAL:HG11	1:A:250:CYS:CA	2.29	0.61
1:A:312:LEU:O	1:A:318:ASP:HA	2.00	0.61
1:F:235:ALA:HA	1:F:238:ARG:CG	2.29	0.61
1:B:367:ASN:C	1:B:367:ASN:OD1	2.39	0.61
1:B:391:GLU:O	1:B:395:ARG:HB3	2.01	0.61
1:A:319:ARG:NH2	1:B:402:LYS:NZ	2.48	0.61
1:E:150:ALA:HB2	1:E:214:ARG:HH21	1.66	0.61
1:A:381:ARG:CG	1:A:382:ARG:H	2.13	0.61
1:F:317:PHE:N	1:F:317:PHE:HD1	1.99	0.61
1:B:501:ALA:O	1:B:505:ILE:HD12	2.00	0.61
1:C:225:PHE:HE1	1:C:233:GLY:C	2.03	0.61
1:B:154:THR:HG23	1:B:156:LYS:H	1.66	0.61
1:C:347:ASP:OD1	1:C:347:ASP:N	2.33	0.61
1:E:212:GLU:O	1:E:214:ARG:CG	2.49	0.61
1:E:449:PHE:HB2	1:E:468:GLN:HE22	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:428:PHE:HE1	1:C:432:ALA:HA	1.61	0.61
1:D:587:PHE:O	1:D:591:VAL:HG23	2.00	0.61
1:B:597:GLU:O	1:B:599:PRO:HD3	2.01	0.61
1:B:190:LYS:HZ1	1:B:289:PHE:HE2	0.69	0.61
1:D:215:VAL:HG22	1:D:216:PRO:CD	2.31	0.61
1:D:235:ALA:HA	1:D:238:ARG:CG	2.30	0.61
1:D:318:ASP:OD1	1:D:318:ASP:N	2.24	0.61
1:E:223:SER:C	1:E:225:PHE:N	2.48	0.61
1:F:348:VAL:HG21	1:F:352:LEU:CD1	2.31	0.61
1:F:352:LEU:CD1	1:F:353:LEU:N	2.64	0.61
1:C:520:ALA:CA	1:C:533:ARG:HD3	2.25	0.61
1:A:447:LEU:HA	1:A:496:GLN:NE2	2.15	0.61
1:B:589:ARG:CB	1:B:594:LEU:HD22	2.30	0.61
1:A:313:ARG:NH2	1:A:526:TYR:C	2.51	0.61
1:B:378:ARG:C	1:B:380:GLY:N	2.54	0.61
1:A:195:VAL:HG11	1:A:304:PRO:HD3	1.81	0.61
1:A:275:ARG:O	1:A:279:LEU:CB	2.48	0.61
1:A:311:LEU:CD2	1:A:316:ARG:CZ	2.79	0.61
1:C:381:ARG:CG	1:C:382:ARG:H	2.14	0.61
1:D:285:GLU:O	1:D:289:PHE:HB2	2.01	0.61
1:B:430:GLU:CA	1:B:430:GLU:OE1	2.48	0.61
1:A:410:ARG:HG3	1:A:411:ASP:H	1.65	0.60
1:A:191:GLY:HA2	1:A:297:VAL:HG22	1.83	0.60
1:F:369:LEU:O	1:F:372:ALA:N	2.33	0.60
1:F:394:ASP:O	1:F:397:MET:HG2	2.01	0.60
1:F:328:VAL:HG23	1:F:580:GLU:HG3	1.83	0.60
1:C:337:ILE:HD12	1:C:338:HIS:CD2	2.36	0.60
1:D:171:ILE:CG1	1:D:296:VAL:HG21	2.30	0.60
1:A:338:HIS:CE1	1:A:366:GLU:HG3	2.36	0.60
1:B:311:LEU:CA	1:B:316:ARG:HH11	2.11	0.60
1:A:263:LYS:HZ1	1:A:276:GLU:CD	2.02	0.60
1:C:390:GLU:O	1:C:393:ALA:N	2.34	0.60
1:D:327:ASP:O	1:D:331:ARG:CZ	2.49	0.60
1:A:347:ASP:N	1:A:347:ASP:OD1	2.34	0.60
1:F:367:ASN:OD1	1:F:367:ASN:C	2.39	0.60
1:F:577:LEU:HG	1:F:578:GLU:N	2.15	0.60
1:D:367:ASN:C	1:D:367:ASN:OD1	2.40	0.60
1:C:166:GLU:O	1:C:169:LYS:CG	2.49	0.60
1:B:238:ARG:CG	1:B:281:GLN:HE22	2.13	0.60
1:B:589:ARG:NE	1:B:596:LEU:HD21	2.15	0.60
1:E:196:GLY:CA	1:E:443:ARG:NH2	2.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:371:GLU:OE1	1:E:395:ARG:NH1	2.34	0.60
1:E:488:THR:O	1:E:490:ALA:N	2.29	0.60
1:A:150:ALA:HB2	1:A:214:ARG:NH1	2.17	0.60
1:A:225:PHE:CE1	1:A:233:GLY:C	2.74	0.60
1:B:317:PHE:N	1:B:317:PHE:HD1	1.99	0.60
1:B:317:PHE:N	1:B:317:PHE:CD1	2.69	0.60
1:D:290:GLU:CG	1:D:293:THR:HG23	2.18	0.60
1:B:503:ARG:NH2	1:B:522:ARG:CZ	2.64	0.60
1:C:357:THR:N	1:C:358:PRO:HD2	2.16	0.60
1:B:369:LEU:O	1:B:372:ALA:N	2.33	0.60
1:E:166:GLU:O	1:E:169:LYS:HG2	2.01	0.60
1:F:294:ALA:C	1:F:295:ILE:HG12	2.21	0.60
1:C:567:GLU:HA	1:C:570:GLU:OE1	2.00	0.60
1:C:589:ARG:CZ	1:C:589:ARG:CB	2.78	0.60
1:C:491:GLU:O	1:C:493:ASP:N	2.34	0.60
1:D:165:LYS:HE2	1:D:205:LEU:CG	2.31	0.60
1:A:196:GLY:HA2	1:A:443:ARG:NH2	2.16	0.60
1:D:257:ILE:N	1:D:257:ILE:HD12	2.13	0.60
1:D:289:PHE:HD2	1:D:290:GLU:N	2.00	0.60
1:D:319:ARG:C	1:D:320:GLN:OE1	2.40	0.60
1:C:266:SER:C	1:C:268:VAL:H	2.05	0.60
1:C:387:LYS:O	1:C:390:GLU:HB2	2.02	0.60
1:D:501:ALA:HB1	1:D:550:LEU:HD23	1.83	0.60
1:D:343:PRO:O	1:D:344:LEU:HB3	2.00	0.60
1:B:410:ARG:O	1:B:413:ARG:HB2	2.01	0.60
1:B:467:ASP:O	1:B:470:ALA:HB3	2.01	0.60
1:E:440:ILE:HG22	1:E:441:VAL:HG23	1.84	0.60
1:E:586:GLU:O	1:E:590:VAL:HG13	2.01	0.60
1:A:211:GLY:C	1:A:214:ARG:HE	2.05	0.60
1:A:331:ARG:HD2	1:A:357:THR:HG23	1.83	0.60
1:B:159:ALA:HB1	1:B:333:GLN:CG	2.31	0.60
1:F:171:ILE:CG1	1:F:296:VAL:HG21	2.31	0.60
1:C:394:ASP:N	1:C:394:ASP:OD1	2.35	0.60
1:B:237:VAL:HG22	1:B:281:GLN:CG	2.31	0.60
1:A:275:ARG:HG3	1:A:275:ARG:NH1	2.17	0.60
1:D:239:ASP:HA	1:D:242:GLU:OE1	2.02	0.60
1:E:310:ALA:O	1:E:316:ARG:NH2	2.34	0.60
1:F:276:GLU:HA	1:F:279:LEU:HB2	1.84	0.60
1:E:453:ARG:NH2	1:E:464:ARG:NH2	2.50	0.60
1:A:514:PHE:HB3	1:A:519:TYR:CE1	2.36	0.60
1:E:333:GLN:HA	1:E:336:ARG:CZ	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:335:LEU:HD22	1:E:353:LEU:HD23	1.83	0.60
1:C:430:GLU:O	1:C:431:HIS:CB	2.47	0.60
1:B:355:LYS:CE	1:B:578:GLU:O	2.46	0.60
1:B:394:ASP:HA	1:B:397:MET:HE2	1.84	0.60
1:D:311:LEU:C	1:D:311:LEU:HD12	2.22	0.60
1:E:166:GLU:O	1:E:169:LYS:CG	2.50	0.60
1:F:337:ILE:HG23	1:F:338:HIS:CD2	2.36	0.60
1:C:519:TYR:HA	1:C:533:ARG:CZ	2.31	0.60
1:A:453:ARG:NH2	1:A:464:ARG:NH1	2.50	0.60
1:F:461:SER:O	1:F:464:ARG:HB3	2.02	0.60
1:E:346:GLU:CD	1:E:347:ASP:H	2.04	0.60
1:D:410:ARG:O	1:D:413:ARG:N	2.34	0.60
1:E:264:ARG:HE	1:E:266:SER:HB2	1.65	0.60
1:A:303:ARG:HB2	1:A:303:ARG:HH11	0.62	0.60
1:A:191:GLY:HA2	1:A:297:VAL:CG2	2.32	0.59
1:A:286:MET:HB3	1:A:316:ARG:HD3	1.80	0.59
1:E:318:ASP:OD1	1:E:318:ASP:N	2.34	0.59
1:F:517:VAL:HG11	1:F:519:TYR:OH	2.02	0.59
1:D:394:ASP:O	1:D:397:MET:HG2	2.02	0.59
1:C:210:ALA:O	1:C:214:ARG:HG3	2.02	0.59
1:A:337:ILE:HD12	1:A:338:HIS:CD2	2.36	0.59
1:B:165:LYS:HZ2	1:B:168:LEU:HD23	1.67	0.59
1:B:385:THR:HB	1:B:388:ASP:OD1	2.02	0.59
1:B:390:GLU:O	1:B:393:ALA:HB3	2.02	0.59
1:B:286:MET:HA	1:B:289:PHE:HD1	1.67	0.59
1:A:346:GLU:CD	1:A:347:ASP:H	2.05	0.59
1:F:237:VAL:HG22	1:F:281:GLN:CG	2.32	0.59
1:F:216:PRO:HG2	1:F:250:CYS:HB3	1.83	0.59
1:C:215:VAL:HG11	1:C:250:CYS:CA	2.31	0.59
1:F:583:THR:N	1:F:586:GLU:OE2	2.35	0.59
1:D:294:ALA:C	1:D:295:ILE:HG12	2.23	0.59
1:E:357:THR:N	1:E:358:PRO:HD2	2.17	0.59
1:C:149:GLU:O	1:C:150:ALA:CB	2.50	0.59
1:A:274:GLU:HA	1:A:277:GLN:HB3	1.84	0.59
1:B:180:ARG:O	1:B:184:MET:HB3	2.02	0.59
1:B:333:GLN:O	1:B:336:ARG:HB3	2.01	0.59
1:D:237:VAL:HG22	1:D:281:GLN:CG	2.31	0.59
1:F:239:ASP:HA	1:F:242:GLU:OE1	2.02	0.59
1:C:514:PHE:HB3	1:C:519:TYR:HE1	1.68	0.59
1:E:453:ARG:CG	1:E:453:ARG:HH11	2.15	0.59
1:D:159:ALA:HB1	1:D:333:GLN:CG	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:376:ALA:HB2	1:D:381:ARG:NH1	2.17	0.59
1:D:395:ARG:CG	1:D:395:ARG:HH11	2.02	0.59
1:C:155:PHE:HZ	1:C:209:VAL:HG22	1.67	0.59
1:B:238:ARG:CB	1:B:281:GLN:HE22	2.13	0.59
1:A:390:GLU:O	1:A:393:ALA:N	2.35	0.59
1:B:294:ALA:C	1:B:295:ILE:HG12	2.21	0.59
1:B:319:ARG:C	1:B:320:GLN:OE1	2.41	0.59
1:F:152:LYS:HB2	1:F:207:ARG:NH1	2.18	0.59
1:A:263:LYS:HG2	1:A:264:ARG:N	2.17	0.59
1:A:264:ARG:HE	1:A:266:SER:HB2	1.66	0.59
1:D:390:GLU:O	1:D:393:ALA:HB3	2.01	0.59
1:B:301:THR:CG2	1:B:303:ARG:H	2.14	0.59
1:A:308:ASP:C	1:A:308:ASP:OD1	2.39	0.59
1:D:286:MET:HA	1:D:289:PHE:HD1	1.67	0.59
1:F:279:LEU:O	1:F:283:LEU:HB2	2.02	0.59
1:A:453:ARG:HH11	1:A:453:ARG:CG	2.12	0.59
1:C:313:ARG:NH2	1:C:526:TYR:C	2.52	0.59
1:B:428:PHE:CZ	1:B:432:ALA:HB1	2.38	0.59
1:B:160:GLY:H	1:B:333:GLN:NE2	1.99	0.59
1:B:157:ASP:HB3	1:B:337:ILE:HG12	1.83	0.59
1:A:589:ARG:HH12	1:A:596:LEU:HB3	1.67	0.59
1:F:327:ASP:O	1:F:331:ARG:NE	2.35	0.59
1:E:453:ARG:NH2	1:E:464:ARG:HH12	1.99	0.59
1:C:318:ASP:N	1:C:318:ASP:OD1	2.33	0.59
1:A:511:HIS:HE1	1:B:552:GLU:OE2	1.85	0.59
1:C:166:GLU:O	1:C:169:LYS:HG2	2.02	0.59
1:B:420:ALA:O	1:B:424:LEU:HD12	2.03	0.59
1:A:190:LYS:HD2	1:A:289:PHE:HE1	1.66	0.59
1:D:317:PHE:CD1	1:D:317:PHE:N	2.68	0.59
1:A:266:SER:C	1:A:268:VAL:H	2.05	0.59
1:E:264:ARG:CD	1:E:266:SER:HB2	2.32	0.59
1:D:331:ARG:O	1:D:335:LEU:HG	2.03	0.59
1:A:166:GLU:O	1:A:169:LYS:CG	2.51	0.59
1:D:313:ARG:NE	1:D:314:PRO:CD	2.59	0.59
1:F:180:ARG:HH12	1:F:184:MET:HE1	1.68	0.59
1:F:286:MET:CE	1:F:315:GLY:O	2.50	0.59
1:B:501:ALA:CB	1:B:550:LEU:HD23	2.33	0.59
1:F:418:HIS:NE2	1:F:479:GLU:OE1	2.36	0.59
1:B:237:VAL:O	1:B:240:LEU:CB	2.44	0.59
1:B:216:PRO:HG2	1:B:250:CYS:HB3	1.84	0.59
1:B:507:GLU:HG3	1:B:520:ALA:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:597:GLU:O	1:F:599:PRO:HD3	2.03	0.59
1:B:157:ASP:OD1	1:B:157:ASP:N	2.34	0.59
1:B:171:ILE:CG1	1:B:296:VAL:HG21	2.33	0.59
1:D:216:PRO:HG2	1:D:250:CYS:HB3	1.84	0.59
1:F:257:ILE:CD1	1:F:257:ILE:H	2.14	0.59
1:E:266:SER:C	1:E:268:VAL:H	2.05	0.59
1:D:583:THR:N	1:D:586:GLU:OE2	2.35	0.59
1:C:371:GLU:OE1	1:C:395:ARG:NH1	2.36	0.59
1:A:414:ILE:CG2	1:A:415:THR:N	2.65	0.59
1:F:376:ALA:HA	1:F:381:ARG:CZ	2.32	0.59
1:A:400:PRO:O	1:A:405:LEU:HD11	2.03	0.59
1:E:191:GLY:HA2	1:E:297:VAL:CG2	2.33	0.59
1:C:440:ILE:HG22	1:C:441:VAL:HG23	1.84	0.59
1:A:264:ARG:HG2	1:A:266:SER:H	1.65	0.59
1:B:449:PHE:CZ	1:B:453:ARG:CZ	2.86	0.59
1:B:235:ALA:HA	1:B:238:ARG:CG	2.33	0.59
1:E:479:GLU:OE2	1:E:488:THR:HG23	2.03	0.59
1:F:338:HIS:HB3	1:F:369:LEU:CD1	2.33	0.58
1:D:449:PHE:CZ	1:D:453:ARG:CZ	2.86	0.58
1:D:517:VAL:CG1	1:D:519:TYR:CZ	2.86	0.58
1:E:465:LEU:CD2	1:E:508:TRP:CZ3	2.86	0.58
1:D:155:PHE:HA	1:D:158:VAL:CG2	2.33	0.58
1:D:438:VAL:HG22	1:D:439:THR:N	2.17	0.58
1:E:589:ARG:CZ	1:E:596:LEU:HB2	2.27	0.58
1:B:257:ILE:H	1:B:257:ILE:CD1	2.14	0.58
1:D:182:HIS:N	1:D:182:HIS:ND1	2.40	0.58
1:A:438:VAL:HG23	1:A:439:THR:N	2.18	0.58
1:F:262:ARG:CG	1:F:263:LYS:N	2.55	0.58
1:C:196:GLY:CA	1:C:443:ARG:NH2	2.66	0.58
1:C:264:ARG:NE	1:C:266:SER:HB2	2.18	0.58
1:C:390:GLU:O	1:C:393:ALA:CB	2.51	0.58
1:C:453:ARG:NH2	1:C:464:ARG:HH12	1.98	0.58
1:D:589:ARG:CB	1:D:594:LEU:HD22	2.32	0.58
1:D:301:THR:CG2	1:D:303:ARG:H	2.16	0.58
1:A:225:PHE:CZ	1:A:278:THR:CB	2.77	0.58
1:B:153:VAL:HB	1:B:207:ARG:HH11	1.68	0.58
1:E:145:ARG:NH2	1:E:219:THR:HG1	1.98	0.58
1:F:192:VAL:O	1:F:317:PHE:CE2	2.56	0.58
1:F:286:MET:HA	1:F:289:PHE:HD1	1.67	0.58
1:F:317:PHE:N	1:F:317:PHE:CD1	2.70	0.58
1:F:366:GLU:O	1:F:369:LEU:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:390:GLU:O	1:F:393:ALA:HB3	2.04	0.58
1:B:511:HIS:C	1:B:512:PRO:O	2.41	0.58
1:C:449:PHE:HB2	1:C:468:GLN:HE22	1.66	0.58
1:C:371:GLU:HG3	1:C:392:ALA:CB	2.32	0.58
1:A:286:MET:O	1:A:289:PHE:CE1	2.56	0.58
1:B:376:ALA:CB	1:B:381:ARG:HD3	2.33	0.58
1:C:586:GLU:CA	1:C:589:ARG:HG3	2.30	0.58
1:C:397:MET:HG3	1:C:406:VAL:HG13	1.84	0.58
1:A:513:GLU:O	1:B:548:ARG:NH2	2.37	0.58
1:A:275:ARG:HG3	1:A:275:ARG:HH11	1.69	0.58
1:A:357:THR:N	1:A:358:PRO:HD2	2.17	0.58
1:B:153:VAL:HB	1:B:207:ARG:NH1	2.18	0.58
1:C:346:GLU:CD	1:C:347:ASP:H	2.06	0.58
1:D:257:ILE:CD1	1:D:257:ILE:H	2.14	0.58
1:C:264:ARG:HE	1:C:266:SER:HB2	1.68	0.58
1:E:507:GLU:CD	1:E:522:ARG:HE	2.07	0.58
1:F:517:VAL:HG13	1:F:519:TYR:CZ	2.39	0.58
1:B:244:ALA:O	1:B:250:CYS:SG	2.61	0.58
1:B:585:GLU:HA	1:B:588:GLN:OE1	2.04	0.58
1:F:301:THR:CG2	1:F:303:ARG:H	2.15	0.58
1:E:337:ILE:HD12	1:E:338:HIS:CD2	2.39	0.58
1:A:479:GLU:OE2	1:A:488:THR:HG23	2.03	0.58
1:A:336:ARG:O	1:A:339:ALA:N	2.37	0.58
1:F:201:GLY:N	2:F:2001:ADP:O1A	2.33	0.58
1:C:438:VAL:HG23	1:C:439:THR:N	2.19	0.58
1:D:463:LYS:O	1:D:464:ARG:C	2.41	0.58
1:E:264:ARG:NE	1:E:266:SER:HB2	2.19	0.58
1:A:509:GLY:C	1:B:476:ARG:NH2	2.56	0.58
1:B:239:ASP:HA	1:B:242:GLU:OE1	2.03	0.58
1:E:336:ARG:O	1:E:339:ALA:N	2.36	0.58
1:E:155:PHE:HZ	1:E:209:VAL:HG22	1.69	0.58
1:E:238:ARG:CZ	1:E:238:ARG:HB2	2.34	0.58
1:A:276:GLU:OE2	1:A:527:LEU:HD11	2.03	0.58
1:E:503:ARG:HG2	1:E:508:TRP:CH2	2.38	0.58
1:F:438:VAL:HG22	1:F:439:THR:N	2.19	0.58
1:E:400:PRO:O	1:E:405:LEU:HD11	2.03	0.58
1:A:340:ARG:C	1:A:342:LYS:N	2.57	0.58
1:F:245:LYS:CG	1:F:246:ARG:N	2.66	0.58
1:A:264:ARG:CG	1:A:266:SER:N	2.47	0.58
1:C:338:HIS:CE1	1:C:366:GLU:HG3	2.39	0.58
1:C:319:ARG:O	1:C:320:GLN:NE2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:ARG:NH2	1:A:552:GLU:OE1	2.35	0.58
1:D:333:GLN:O	1:D:336:ARG:HB3	2.04	0.58
1:D:233:GLY:C	1:D:236:ARG:HH22	2.07	0.58
1:D:526:TYR:O	1:D:528:GLY:N	2.37	0.58
1:E:236:ARG:NH1	1:E:236:ARG:CB	2.67	0.58
1:C:400:PRO:O	1:C:405:LEU:HD11	2.03	0.58
1:A:503:ARG:HG2	1:A:508:TRP:CH2	2.39	0.58
1:B:237:VAL:HA	1:B:240:LEU:HD12	1.86	0.58
1:F:463:LYS:O	1:F:464:ARG:C	2.41	0.58
1:C:349:ASP:O	1:C:349:ASP:OD1	2.22	0.58
1:E:189:PRO:O	1:E:190:LYS:HG2	2.04	0.58
1:E:225:PHE:CE1	1:E:233:GLY:C	2.76	0.58
1:D:526:TYR:CE2	1:E:256:GLU:OE2	2.57	0.58
1:F:159:ALA:CB	1:F:334:ILE:HG13	2.32	0.58
1:D:418:HIS:NE2	1:D:479:GLU:OE1	2.37	0.58
1:E:381:ARG:CG	1:E:382:ARG:H	2.16	0.58
1:B:236:ARG:HG2	1:B:237:VAL:N	2.17	0.58
1:F:480:GLU:OE1	1:F:555:TYR:OH	2.21	0.58
1:B:331:ARG:O	1:B:335:LEU:HG	2.04	0.57
1:B:373:ALA:HA	1:B:384:ILE:HD11	1.86	0.57
1:E:212:GLU:O	1:E:214:ARG:CD	2.52	0.57
1:B:512:PRO:HB2	1:B:514:PHE:HD2	1.69	0.57
1:C:514:PHE:N	1:C:514:PHE:CD2	2.72	0.57
1:E:453:ARG:NH2	1:E:464:ARG:NH1	2.51	0.57
1:F:589:ARG:HB3	1:F:594:LEU:CD2	2.33	0.57
1:F:373:ALA:O	1:F:376:ALA:HB3	2.05	0.57
1:A:168:LEU:CA	1:A:171:ILE:CD1	2.82	0.57
1:A:286:MET:SD	1:A:316:ARG:HD2	2.36	0.57
1:D:276:GLU:HA	1:D:279:LEU:HB2	1.86	0.57
1:E:210:ALA:O	1:E:214:ARG:HA	2.04	0.57
1:C:585:GLU:OE1	1:C:586:GLU:N	2.37	0.57
1:B:215:VAL:HG22	1:B:216:PRO:CD	2.33	0.57
1:B:245:LYS:CG	1:B:246:ARG:N	2.65	0.57
1:A:318:ASP:OD1	1:A:318:ASP:N	2.38	0.57
1:B:337:ILE:CD1	1:B:340:ARG:HH12	2.07	0.57
1:F:286:MET:HA	1:F:289:PHE:CD1	2.40	0.57
1:C:335:LEU:HD22	1:C:353:LEU:HD23	1.85	0.57
1:C:453:ARG:NH2	1:C:464:ARG:NH1	2.52	0.57
1:D:501:ALA:O	1:D:505:ILE:HD12	2.05	0.57
1:F:503:ARG:HH12	1:F:522:ARG:NH2	2.00	0.57
1:D:159:ALA:CB	1:D:334:ILE:HG13	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:348:VAL:HG13	1:D:350:LEU:H	1.69	0.57
1:F:414:ILE:O	1:F:417:TYR:N	2.38	0.57
1:E:347:ASP:N	1:E:347:ASP:OD1	2.37	0.57
1:E:430:GLU:O	1:E:431:HIS:CB	2.48	0.57
1:C:479:GLU:OE2	1:C:488:THR:HG23	2.03	0.57
1:A:394:ASP:OD1	1:A:394:ASP:N	2.36	0.57
1:A:169:LYS:HA	1:A:172:VAL:CG1	2.35	0.57
1:A:188:ILE:O	1:A:190:LYS:NZ	2.35	0.57
1:B:290:GLU:CG	1:B:293:THR:HG23	2.23	0.57
1:E:247:HIS:O	1:E:250:CYS:HB2	2.04	0.57
1:F:165:LYS:O	1:F:168:LEU:CA	2.51	0.57
1:F:233:GLY:C	1:F:236:ARG:HH22	2.07	0.57
1:F:238:ARG:CG	1:F:281:GLN:HE22	2.15	0.57
1:F:244:ALA:O	1:F:250:CYS:SG	2.62	0.57
1:B:549:ARG:O	1:B:550:LEU:C	2.42	0.57
1:D:549:ARG:O	1:D:550:LEU:C	2.42	0.57
1:C:191:GLY:HA2	1:C:297:VAL:CG2	2.35	0.57
1:A:491:GLU:HG2	1:F:508:TRP:HD1	1.68	0.57
1:F:517:VAL:CG1	1:F:519:TYR:CZ	2.87	0.57
1:B:285:GLU:O	1:B:288:GLY:N	2.37	0.57
1:F:413:ARG:HG3	1:F:413:ARG:NH1	2.17	0.57
1:A:200:VAL:CG1	1:A:323:ILE:HG13	2.35	0.57
1:B:308:ASP:OD1	1:B:308:ASP:C	2.42	0.57
1:E:211:GLY:C	1:E:214:ARG:CG	2.72	0.57
1:A:378:ARG:CA	1:F:173:GLU:OE1	2.45	0.57
1:D:523:GLU:CD	1:E:264:ARG:NH2	2.58	0.57
1:C:225:PHE:CE1	1:C:233:GLY:C	2.78	0.57
1:A:460:TRP:HB3	1:A:465:LEU:HD11	1.85	0.57
1:F:512:PRO:HB2	1:F:514:PHE:HD2	1.69	0.57
1:F:589:ARG:CB	1:F:594:LEU:HD22	2.34	0.57
1:B:463:LYS:O	1:B:464:ARG:C	2.41	0.57
1:E:313:ARG:NH2	1:E:526:TYR:C	2.52	0.57
1:E:334:ILE:CD1	2:E:1001:ADP:C6	2.86	0.57
1:E:394:ASP:O	1:E:397:MET:N	2.37	0.57
1:F:526:TYR:O	1:F:528:GLY:N	2.38	0.57
1:A:397:MET:HG3	1:A:406:VAL:HG13	1.86	0.57
1:A:237:VAL:HG11	1:A:281:GLN:CB	2.24	0.57
1:B:394:ASP:O	1:B:397:MET:HG2	2.05	0.57
1:C:345:ALA:HB3	1:C:385:THR:HA	1.87	0.57
1:E:519:TYR:HA	1:E:533:ARG:CZ	2.35	0.57
1:C:275:ARG:O	1:C:279:LEU:HB2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:154:THR:HG23	1:D:156:LYS:H	1.70	0.57
1:E:371:GLU:HG3	1:E:392:ALA:CB	2.34	0.57
1:A:371:GLU:HG3	1:A:392:ALA:CB	2.34	0.57
1:A:371:GLU:OE1	1:A:395:ARG:NH1	2.38	0.57
1:D:163:GLU:O	1:D:167:GLU:HB3	2.04	0.57
1:A:212:GLU:O	1:A:214:ARG:HB2	2.04	0.57
1:E:275:ARG:NH1	1:E:275:ARG:HG3	2.19	0.57
1:B:519:TYR:HB3	1:B:535:TYR:HD2	1.69	0.57
1:E:519:TYR:HA	1:E:533:ARG:NH2	2.20	0.57
1:C:223:SER:C	1:C:225:PHE:N	2.51	0.57
1:E:382:ARG:HD3	1:E:383:LYS:CB	2.34	0.57
1:B:238:ARG:NH1	1:B:239:ASP:HB3	2.14	0.57
1:E:414:ILE:CG2	1:E:415:THR:N	2.67	0.57
1:A:177:ASN:ND2	1:A:180:ARG:HD3	2.19	0.57
1:A:333:GLN:HG3	1:A:336:ARG:HH12	1.70	0.57
1:A:196:GLY:C	1:A:443:ARG:NH2	2.58	0.57
1:B:335:LEU:CD2	1:B:365:LEU:HB3	2.35	0.57
1:B:289:PHE:CD2	1:B:290:GLU:N	2.73	0.57
1:D:235:ALA:C	1:D:238:ARG:HG3	2.25	0.57
1:F:180:ARG:O	1:F:184:MET:HB3	2.05	0.57
1:B:512:PRO:HB2	1:B:514:PHE:CD2	2.39	0.57
1:D:381:ARG:CZ	1:D:388:ASP:OD2	2.48	0.57
1:D:595:PRO:O	1:D:596:LEU:HD12	2.05	0.57
1:A:585:GLU:OE2	1:A:589:ARG:HD3	2.04	0.57
1:F:391:GLU:O	1:F:394:ASP:OD1	2.22	0.57
1:C:519:TYR:O	1:C:533:ARG:CG	2.53	0.57
1:D:519:TYR:HB3	1:D:535:TYR:HD2	1.69	0.57
1:D:433:ASP:OD1	1:D:433:ASP:N	2.38	0.57
1:B:255:ASP:O	1:B:256:GLU:HG2	2.03	0.57
1:D:244:ALA:O	1:D:250:CYS:SG	2.63	0.57
1:D:286:MET:O	1:D:289:PHE:HB3	2.04	0.57
1:E:236:ARG:CG	1:E:236:ARG:NH1	2.58	0.57
1:E:236:ARG:O	1:E:238:ARG:N	2.37	0.57
1:C:470:ALA:O	1:C:558:VAL:HG21	2.05	0.57
1:D:177:ASN:O	1:D:180:ARG:HB3	2.05	0.57
1:E:202:LYS:HB2	2:E:1001:ADP:O1B	2.04	0.57
1:A:394:ASP:O	1:A:397:MET:N	2.38	0.57
1:F:421:GLY:HA2	1:F:562:LEU:HD11	1.86	0.57
1:E:410:ARG:HG3	1:E:411:ASP:H	1.68	0.56
1:D:308:ASP:OD1	1:D:308:ASP:C	2.42	0.56
1:A:583:THR:HG22	1:A:586:GLU:CD	2.26	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:586:GLU:O	1:C:590:VAL:HG13	2.05	0.56
1:C:263:LYS:HD2	1:C:276:GLU:CG	2.35	0.56
1:C:461:SER:O	1:C:465:LEU:HD12	2.04	0.56
1:C:310:ALA:O	1:C:316:ARG:NH2	2.38	0.56
1:A:507:GLU:CD	1:A:522:ARG:HE	2.09	0.56
1:F:512:PRO:HB2	1:F:514:PHE:CD2	2.40	0.56
1:F:587:PHE:O	1:F:591:VAL:HG23	2.06	0.56
1:D:238:ARG:CG	1:D:281:GLN:HE22	2.17	0.56
1:D:313:ARG:HG3	1:D:314:PRO:CG	2.36	0.56
1:E:150:ALA:HB2	1:E:214:ARG:NH2	2.19	0.56
1:F:245:LYS:C	1:F:247:HIS:N	2.58	0.56
1:C:283:LEU:O	1:C:286:MET:HB2	2.05	0.56
1:A:469:ILE:O	1:A:473:LEU:HD12	2.05	0.56
1:F:467:ASP:O	1:F:470:ALA:HB3	2.06	0.56
1:B:187:ARG:O	1:C:374:LEU:CD2	2.48	0.56
1:E:331:ARG:HD2	1:E:357:THR:CG2	2.35	0.56
1:E:390:GLU:O	1:E:393:ALA:CB	2.52	0.56
1:B:421:GLY:HA2	1:B:562:LEU:HD11	1.87	0.56
1:E:585:GLU:OE1	1:E:586:GLU:N	2.37	0.56
1:A:407:LEU:O	1:A:407:LEU:HD12	2.05	0.56
1:A:247:HIS:O	1:A:250:CYS:HB2	2.05	0.56
1:B:170:GLU:HB3	1:C:378:ARG:NH2	2.20	0.56
1:B:279:LEU:O	1:B:283:LEU:HB2	2.05	0.56
1:D:245:LYS:CG	1:D:246:ARG:N	2.68	0.56
1:D:261:GLY:O	1:D:308:ASP:N	2.34	0.56
1:D:286:MET:HA	1:D:289:PHE:CD1	2.40	0.56
1:D:286:MET:HE2	1:D:315:GLY:O	2.05	0.56
1:F:210:ALA:O	1:F:214:ARG:N	2.38	0.56
1:C:516:PRO:HB2	1:D:494:PHE:CD1	2.40	0.56
1:B:503:ARG:NH2	1:B:522:ARG:NH2	2.49	0.56
1:C:334:ILE:CD1	2:C:1001:ADP:C6	2.88	0.56
1:C:394:ASP:O	1:C:397:MET:N	2.37	0.56
1:E:460:TRP:HB3	1:E:465:LEU:HD11	1.86	0.56
1:C:219:THR:HA	1:C:253:PHE:O	2.06	0.56
1:A:305:ASP:O	1:A:307:LEU:N	2.39	0.56
1:A:453:ARG:NH1	1:A:460:TRP:CE2	2.74	0.56
1:B:245:LYS:C	1:B:247:HIS:N	2.58	0.56
1:B:245:LYS:HG3	1:B:246:ARG:N	2.20	0.56
1:D:589:ARG:CZ	1:D:596:LEU:HD11	2.35	0.56
1:E:196:GLY:O	1:E:202:LYS:NZ	2.30	0.56
1:E:368:LEU:HD13	1:E:393:ALA:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:525:THR:HG22	1:F:526:TYR:H	1.71	0.56
1:B:165:LYS:HE2	1:B:205:LEU:CG	2.36	0.56
1:B:391:GLU:O	1:B:394:ASP:OD1	2.23	0.56
1:C:263:LYS:HZ2	1:C:276:GLU:CD	1.80	0.56
1:F:447:LEU:O	1:F:450:MET:HG3	2.06	0.56
1:B:477:ALA:O	1:B:481:ILE:HG13	2.06	0.56
1:B:449:PHE:CE2	1:B:492:ASN:HB3	2.37	0.56
1:A:238:ARG:CZ	1:A:238:ARG:HB2	2.35	0.56
1:D:245:LYS:C	1:D:247:HIS:N	2.59	0.56
1:F:180:ARG:NH1	1:F:184:MET:HE1	2.20	0.56
1:F:235:ALA:C	1:F:238:ARG:HG3	2.26	0.56
1:C:407:LEU:HD12	1:C:407:LEU:O	2.05	0.56
1:F:503:ARG:NH2	1:F:522:ARG:CZ	2.68	0.56
1:F:592:GLU:O	1:F:594:LEU:N	2.39	0.56
1:B:338:HIS:HB3	1:B:369:LEU:CD1	2.35	0.56
1:A:588:GLN:HG3	1:A:589:ARG:N	2.21	0.56
1:F:192:VAL:C	1:F:317:PHE:CE2	2.79	0.56
1:C:196:GLY:O	1:C:202:LYS:NZ	2.31	0.56
1:E:449:PHE:HE2	1:E:496:GLN:NE2	2.03	0.56
1:C:275:ARG:O	1:C:279:LEU:CB	2.53	0.56
1:A:500:LEU:O	1:A:504:MET:HG2	2.05	0.56
1:A:459:HIS:HB2	1:B:488:THR:HB	1.87	0.56
1:D:327:ASP:O	1:D:331:ARG:NE	2.38	0.56
1:C:166:GLU:C	1:C:169:LYS:HG2	2.26	0.56
1:B:236:ARG:HH12	1:B:278:THR:CG2	2.11	0.56
1:E:345:ALA:HB3	1:E:385:THR:HA	1.88	0.56
1:A:525:THR:O	1:A:528:GLY:N	2.39	0.56
1:E:407:LEU:O	1:E:407:LEU:HD12	2.06	0.56
1:B:331:ARG:HD2	1:B:354:ALA:O	2.05	0.56
1:E:147:LEU:HD23	1:E:217:PHE:HB3	1.88	0.56
1:E:308:ASP:OD1	1:E:308:ASP:C	2.43	0.56
1:F:397:MET:O	1:F:400:PRO:HG2	2.06	0.56
1:C:199:GLY:O	1:C:361:VAL:HG22	2.06	0.56
1:E:263:LYS:HG2	1:E:264:ARG:N	2.20	0.56
1:F:487:THR:HG22	1:F:488:THR:N	2.14	0.56
1:A:449:PHE:HB3	1:A:468:GLN:HE22	1.68	0.56
1:D:376:ALA:CB	1:D:381:ARG:NH1	2.69	0.56
1:A:316:ARG:HH11	1:A:317:PHE:HE2	1.22	0.56
1:A:390:GLU:O	1:A:393:ALA:CB	2.53	0.56
1:B:276:GLU:HA	1:B:279:LEU:HB2	1.87	0.56
1:E:262:ARG:CG	1:E:275:ARG:HH22	2.08	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:585:GLU:CD	1:C:586:GLU:N	2.59	0.56
1:C:589:ARG:CZ	1:C:596:LEU:HB2	2.28	0.56
1:C:305:ASP:OD1	1:C:305:ASP:N	2.28	0.56
1:C:512:PRO:HB2	1:C:514:PHE:HD2	1.71	0.56
1:C:519:TYR:C	1:C:533:ARG:NE	2.59	0.56
1:E:514:PHE:HB3	1:E:519:TYR:HE1	1.71	0.56
1:C:145:ARG:CZ	1:C:219:THR:OG1	2.53	0.56
1:A:449:PHE:HB2	1:A:468:GLN:HE22	1.71	0.56
1:A:438:VAL:HG11	1:A:587:PHE:CD1	2.41	0.56
1:A:536:SER:O	1:A:537:GLU:C	2.44	0.56
1:E:554:GLN:O	1:E:557:ARG:HB3	2.06	0.56
1:C:177:ASN:HD22	1:C:180:ARG:CD	2.17	0.56
1:C:234:ALA:HB1	1:C:281:GLN:CD	2.26	0.56
1:C:238:ARG:HB2	1:C:238:ARG:CZ	2.35	0.56
1:D:335:LEU:CD2	1:D:365:LEU:HB3	2.36	0.56
1:C:247:HIS:O	1:C:250:CYS:HB2	2.05	0.56
1:E:196:GLY:HA2	1:E:443:ARG:NH2	2.21	0.56
1:A:283:LEU:O	1:A:286:MET:HB2	2.05	0.56
1:B:311:LEU:HA	1:B:316:ARG:HH11	1.61	0.56
1:E:166:GLU:C	1:E:169:LYS:HG2	2.26	0.56
1:F:344:LEU:HA	1:F:383:LYS:HG3	1.88	0.56
1:B:537:GLU:O	1:B:540:ALA:HB3	2.05	0.56
1:C:401:ALA:HB3	1:C:405:LEU:HD21	1.88	0.56
1:B:438:VAL:HG22	1:B:439:THR:N	2.20	0.56
1:B:210:ALA:O	1:B:214:ARG:HA	2.07	0.55
1:F:216:PRO:HG2	1:F:250:CYS:CB	2.37	0.55
1:F:308:ASP:OD1	1:F:308:ASP:C	2.45	0.55
1:C:438:VAL:HG11	1:C:587:PHE:CD1	2.41	0.55
1:C:174:PHE:CZ	1:C:294:ALA:HB1	2.41	0.55
1:C:308:ASP:OD1	1:C:308:ASP:C	2.43	0.55
1:E:387:LYS:O	1:E:390:GLU:HB2	2.06	0.55
1:F:521:VAL:HG23	1:F:532:VAL:CG1	2.34	0.55
1:A:196:GLY:O	1:A:202:LYS:NZ	2.31	0.55
1:A:368:LEU:HG	1:A:369:LEU:N	2.20	0.55
1:B:344:LEU:HA	1:B:383:LYS:HG3	1.88	0.55
1:E:275:ARG:HH11	1:E:275:ARG:HG3	1.70	0.55
1:A:370:ASN:OD1	1:A:374:LEU:HD13	2.06	0.55
1:E:394:ASP:N	1:E:394:ASP:OD1	2.38	0.55
1:A:568:VAL:O	1:A:572:VAL:HG23	2.06	0.55
1:B:376:ALA:HB1	1:B:381:ARG:CD	2.36	0.55
1:B:286:MET:HA	1:B:289:PHE:CD1	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:MET:O	1:B:289:PHE:CD1	2.59	0.55
1:D:316:ARG:NH1	1:D:316:ARG:CG	2.42	0.55
1:F:319:ARG:C	1:F:320:GLN:OE1	2.44	0.55
1:D:461:SER:O	1:D:464:ARG:HB3	2.06	0.55
1:A:223:SER:C	1:A:225:PHE:N	2.51	0.55
1:B:263:LYS:HZ2	1:C:227:GLU:HG3	1.69	0.55
1:C:453:ARG:NH2	1:C:464:ARG:NH2	2.52	0.55
1:E:451:MET:HB2	1:E:452:PRO:HD3	1.88	0.55
1:A:514:PHE:CD2	1:A:514:PHE:N	2.75	0.55
1:D:165:LYS:O	1:D:168:LEU:CB	2.54	0.55
1:F:585:GLU:HA	1:F:588:GLN:OE1	2.06	0.55
1:F:589:ARG:HE	1:F:594:LEU:CD2	2.00	0.55
1:A:194:LEU:HA	1:A:321:ILE:O	2.06	0.55
1:E:438:VAL:HG11	1:E:587:PHE:CD1	2.41	0.55
1:A:168:LEU:O	1:A:169:LYS:C	2.45	0.55
1:A:262:ARG:HG2	1:A:275:ARG:NH2	2.06	0.55
1:B:165:LYS:NZ	1:B:168:LEU:CD2	2.70	0.55
1:B:327:ASP:O	1:B:331:ARG:NE	2.39	0.55
1:A:345:ALA:HB3	1:A:385:THR:HA	1.88	0.55
1:F:352:LEU:HD13	1:F:353:LEU:N	2.21	0.55
1:B:503:ARG:HH12	1:B:522:ARG:NH2	2.03	0.55
1:C:196:GLY:H	1:C:202:LYS:HZ1	1.55	0.55
1:A:145:ARG:CZ	1:A:219:THR:OG1	2.54	0.55
1:A:319:ARG:NH2	1:B:402:LYS:HZ3	2.04	0.55
1:B:194:LEU:HD23	1:B:323:ILE:HD11	1.89	0.55
1:D:237:VAL:C	1:D:240:LEU:HB3	2.27	0.55
1:F:233:GLY:C	1:F:236:ARG:NH2	2.60	0.55
1:D:449:PHE:CE2	1:D:492:ASN:HB3	2.40	0.55
1:D:511:HIS:O	1:D:512:PRO:O	2.24	0.55
1:C:174:PHE:CD2	1:C:175:LEU:N	2.74	0.55
1:B:239:ASP:O	1:B:242:GLU:OE2	2.24	0.55
1:E:340:ARG:C	1:E:342:LYS:N	2.58	0.55
1:A:495:ARG:HD2	1:F:521:VAL:HG12	1.88	0.55
1:D:524:ASP:H	1:E:306:ILE:HD11	1.70	0.55
1:A:531:ASP:C	1:A:531:ASP:OD1	2.45	0.55
1:A:166:GLU:O	1:A:169:LYS:HG2	2.07	0.55
1:A:174:PHE:CD2	1:A:175:LEU:N	2.75	0.55
1:C:382:ARG:CG	1:C:383:LYS:H	2.19	0.55
1:F:245:LYS:HG3	1:F:246:ARG:N	2.21	0.55
1:C:436:HIS:HB3	1:C:584:ALA:HB1	1.88	0.55
1:D:477:ALA:O	1:D:481:ILE:HG13	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:557:ARG:O	1:D:560:ALA:HB3	2.05	0.55
1:F:449:PHE:CE2	1:F:492:ASN:HB3	2.37	0.55
1:B:494:PHE:O	1:B:495:ARG:C	2.45	0.55
1:C:552:GLU:O	1:C:555:TYR:HB3	2.07	0.55
1:A:236:ARG:O	1:A:238:ARG:N	2.39	0.55
1:A:589:ARG:NH1	1:A:596:LEU:CB	2.69	0.55
1:F:181:PHE:HA	1:F:184:MET:HG2	1.88	0.55
1:F:355:LYS:NZ	1:F:578:GLU:HG3	2.22	0.55
1:C:339:ALA:N	1:C:369:LEU:HD21	2.22	0.55
1:D:467:ASP:OD1	1:D:557:ARG:NH2	2.40	0.55
1:E:276:GLU:OE2	1:E:527:LEU:HD11	2.06	0.55
1:E:197:PRO:C	1:E:302:ASN:OD1	2.45	0.55
1:A:338:HIS:ND1	1:A:366:GLU:HG3	2.22	0.55
1:B:155:PHE:HA	1:B:158:VAL:CG2	2.37	0.55
1:B:257:ILE:O	1:B:260:VAL:HG13	2.07	0.55
1:D:216:PRO:HB2	1:D:218:ILE:HD11	1.88	0.55
1:D:233:GLY:C	1:D:236:ARG:NH2	2.60	0.55
1:D:234:ALA:O	1:D:237:VAL:HG13	2.07	0.55
1:D:236:ARG:O	1:D:239:ASP:OD1	2.25	0.55
1:E:219:THR:HA	1:E:253:PHE:O	2.07	0.55
1:F:241:PHE:CE2	1:F:285:GLU:CG	2.90	0.55
1:F:344:LEU:HG	1:F:346:GLU:OE1	2.06	0.55
1:F:348:VAL:HG21	1:F:386:MET:HE2	1.89	0.55
1:C:414:ILE:HG22	1:C:415:THR:H	1.71	0.55
1:A:491:GLU:O	1:A:493:ASP:N	2.40	0.55
1:F:459:HIS:O	1:F:459:HIS:CG	2.60	0.55
1:B:327:ASP:O	1:B:331:ARG:CZ	2.54	0.55
1:E:174:PHE:CD2	1:E:175:LEU:N	2.74	0.55
1:F:154:THR:HG23	1:F:156:LYS:H	1.71	0.55
1:C:453:ARG:HH21	1:C:464:ARG:HH22	1.49	0.55
1:C:286:MET:O	1:C:289:PHE:CE1	2.59	0.55
1:A:500:LEU:O	1:A:503:ARG:HB3	2.06	0.55
1:D:155:PHE:CE2	1:D:212:GLU:OE2	2.59	0.55
1:D:373:ALA:HA	1:D:384:ILE:HD11	1.88	0.55
1:E:334:ILE:HD13	2:E:1001:ADP:N1	2.22	0.55
1:C:481:ILE:HD11	1:C:563:LEU:HB3	1.89	0.55
1:A:154:THR:OG1	1:A:155:PHE:N	2.38	0.54
1:A:335:LEU:HD22	1:A:353:LEU:HD23	1.88	0.54
1:A:387:LYS:O	1:A:390:GLU:HB2	2.06	0.54
1:A:585:GLU:OE1	1:A:586:GLU:N	2.39	0.54
1:F:236:ARG:O	1:F:239:ASP:OD1	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:263:LYS:HG2	1:C:264:ARG:N	2.21	0.54
1:C:463:LYS:HD2	1:D:486:VAL:CG2	2.37	0.54
1:C:179:SER:HA	1:C:182:HIS:NE2	2.23	0.54
1:A:462:ARG:HB2	1:A:510:MET:SD	2.47	0.54
1:F:501:ALA:HB1	1:F:550:LEU:HD23	1.89	0.54
1:B:234:ALA:O	1:B:237:VAL:HG13	2.07	0.54
1:B:235:ALA:C	1:B:238:ARG:HG3	2.28	0.54
1:E:199:GLY:O	1:E:361:VAL:HG22	2.06	0.54
1:B:525:THR:HG22	1:B:526:TYR:H	1.73	0.54
1:D:253:PHE:C	1:D:253:PHE:CD2	2.80	0.54
1:C:367:ASN:O	1:C:371:GLU:HB3	2.07	0.54
1:A:234:ALA:HB1	1:A:281:GLN:CD	2.27	0.54
1:F:313:ARG:NE	1:F:314:PRO:CG	2.70	0.54
1:F:313:ARG:NE	1:F:314:PRO:CD	2.66	0.54
1:F:394:ASP:HA	1:F:397:MET:HE2	1.88	0.54
1:C:197:PRO:C	1:C:302:ASN:OD1	2.46	0.54
1:C:336:ARG:CG	1:C:337:ILE:N	2.69	0.54
1:C:336:ARG:O	1:C:339:ALA:N	2.38	0.54
1:D:430:GLU:CA	1:D:430:GLU:OE1	2.54	0.54
1:F:433:ASP:OD1	1:F:433:ASP:N	2.39	0.54
1:A:199:GLY:O	1:A:361:VAL:HG22	2.07	0.54
1:A:197:PRO:C	1:A:302:ASN:OD1	2.45	0.54
1:A:283:LEU:CD1	1:A:311:LEU:HD21	2.36	0.54
1:A:339:ALA:N	1:A:369:LEU:HD21	2.22	0.54
1:B:348:VAL:HG13	1:B:350:LEU:H	1.72	0.54
1:C:381:ARG:HH11	1:C:381:ARG:CG	2.20	0.54
1:D:193:LEU:C	1:D:194:LEU:HD12	2.28	0.54
1:A:381:ARG:CG	1:A:381:ARG:HH11	2.21	0.54
1:F:257:ILE:O	1:F:260:VAL:HG13	2.07	0.54
1:C:334:ILE:HD13	2:C:1001:ADP:N1	2.23	0.54
1:C:516:PRO:HB2	1:D:494:PHE:CE1	2.42	0.54
1:C:506:THR:HA	1:C:519:TYR:HD1	1.72	0.54
1:C:236:ARG:O	1:C:238:ARG:N	2.39	0.54
1:D:391:GLU:O	1:D:394:ASP:OD1	2.26	0.54
1:C:147:LEU:HD23	1:C:217:PHE:HB3	1.88	0.54
1:D:203:THR:HG23	1:D:253:PHE:CZ	2.41	0.54
1:D:222:GLY:N	1:D:255:ASP:O	2.37	0.54
1:E:194:LEU:HA	1:E:321:ILE:O	2.08	0.54
1:A:189:PRO:O	1:A:190:LYS:HG2	2.07	0.54
1:A:215:VAL:CG2	1:A:216:PRO:N	2.70	0.54
1:B:190:LYS:NZ	1:B:289:PHE:CZ	2.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:234:ALA:HB1	1:E:281:GLN:CD	2.27	0.54
1:E:283:LEU:O	1:E:286:MET:HB2	2.07	0.54
1:E:174:PHE:CZ	1:E:294:ALA:HB1	2.41	0.54
1:E:189:PRO:HD3	1:E:319:ARG:NH1	2.23	0.54
1:F:311:LEU:O	1:F:311:LEU:HD12	2.07	0.54
1:A:263:LYS:HD2	1:A:276:GLU:CG	2.36	0.54
1:C:236:ARG:NH1	1:C:236:ARG:CG	2.60	0.54
1:A:519:TYR:O	1:A:533:ARG:CG	2.56	0.54
1:D:207:ARG:HB2	1:D:217:PHE:CE2	2.41	0.54
1:D:391:GLU:O	1:D:395:ARG:HB3	2.06	0.54
1:D:180:ARG:O	1:D:184:MET:HB3	2.06	0.54
1:C:194:LEU:HA	1:C:321:ILE:O	2.08	0.54
1:A:174:PHE:CZ	1:A:294:ALA:HB1	2.42	0.54
1:A:353:LEU:O	1:A:357:THR:HG22	2.06	0.54
1:B:192:VAL:C	1:B:317:PHE:CE2	2.80	0.54
1:D:238:ARG:CB	1:D:281:GLN:HE22	2.20	0.54
1:D:283:LEU:HD12	1:D:316:ARG:NH2	2.20	0.54
1:C:353:LEU:O	1:C:357:THR:HG22	2.08	0.54
1:E:519:TYR:O	1:E:533:ARG:CG	2.56	0.54
1:D:165:LYS:CD	1:D:168:LEU:CD2	2.77	0.54
1:E:333:GLN:HG3	1:E:336:ARG:HH12	1.71	0.54
1:B:433:ASP:OD1	1:B:433:ASP:N	2.41	0.54
1:A:149:GLU:O	1:A:150:ALA:CB	2.53	0.54
1:A:179:SER:C	1:A:181:PHE:H	2.10	0.54
1:B:311:LEU:N	1:B:316:ARG:HH12	2.04	0.54
1:D:190:LYS:NZ	1:D:289:PHE:CZ	2.73	0.54
1:A:583:THR:HG22	1:A:586:GLU:OE1	2.07	0.54
1:F:190:LYS:HD2	1:F:289:PHE:HZ	1.71	0.54
1:F:237:VAL:C	1:F:240:LEU:HB3	2.28	0.54
1:C:196:GLY:C	1:C:443:ARG:NH2	2.61	0.54
1:D:512:PRO:HB2	1:D:514:PHE:CD2	2.43	0.54
1:D:166:GLU:O	1:D:169:LYS:HG2	2.07	0.54
1:C:218:ILE:HG12	1:C:251:ILE:O	2.08	0.54
1:D:180:ARG:NH1	1:D:184:MET:HE1	2.22	0.54
1:E:339:ALA:N	1:E:369:LEU:HD21	2.23	0.54
1:E:401:ALA:HB3	1:E:405:LEU:HD21	1.89	0.54
1:A:236:ARG:NH1	1:A:236:ARG:CB	2.70	0.54
1:B:163:GLU:O	1:B:167:GLU:HB3	2.07	0.54
1:B:192:VAL:O	1:B:317:PHE:CE2	2.60	0.54
1:E:211:GLY:O	1:E:214:ARG:CD	2.53	0.54
1:A:588:GLN:HA	1:A:591:VAL:HG23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:165:LYS:CE	1:F:205:LEU:CG	2.86	0.54
1:F:203:THR:HG23	1:F:253:PHE:CZ	2.42	0.54
1:F:234:ALA:O	1:F:237:VAL:HG13	2.07	0.54
1:E:263:LYS:HD2	1:E:276:GLU:CG	2.38	0.54
1:E:449:PHE:N	1:E:449:PHE:HD2	2.04	0.54
1:D:199:GLY:H	2:D:2001:ADP:PB	2.29	0.54
1:B:277:GLN:HA	1:B:280:ASN:HD21	1.72	0.54
1:E:338:HIS:ND1	1:E:366:GLU:HG3	2.22	0.54
1:E:305:ASP:O	1:E:307:LEU:N	2.41	0.54
1:E:438:VAL:HG23	1:E:439:THR:N	2.23	0.54
1:A:325:ALA:N	1:A:326:PRO:CD	2.71	0.54
1:B:210:ALA:O	1:B:214:ARG:N	2.41	0.54
1:B:319:ARG:NH1	1:B:319:ARG:CG	2.67	0.54
1:E:179:SER:O	1:E:182:HIS:CD2	2.60	0.54
1:A:374:LEU:CD1	1:F:186:ALA:HB1	2.38	0.54
1:A:342:LYS:CE	1:F:184:MET:SD	2.95	0.54
1:F:216:PRO:HB2	1:F:218:ILE:HD11	1.90	0.54
1:E:512:PRO:HB2	1:E:514:PHE:HD2	1.72	0.54
1:B:418:HIS:NE2	1:B:479:GLU:OE1	2.40	0.54
1:D:201:GLY:N	2:D:2001:ADP:O1A	2.34	0.54
1:D:207:ARG:CB	1:D:217:PHE:CZ	2.91	0.54
1:A:541:LYS:HA	1:F:536:SER:OG	2.07	0.54
1:E:589:ARG:HH22	1:E:596:LEU:HB2	1.38	0.54
1:B:344:LEU:HG	1:B:346:GLU:OE1	2.08	0.54
1:B:313:ARG:HG3	1:B:314:PRO:CG	2.38	0.54
1:D:237:VAL:CG2	1:D:281:GLN:CG	2.86	0.54
1:D:313:ARG:CG	1:D:314:PRO:N	2.70	0.54
1:A:585:GLU:OE2	1:A:589:ARG:CD	2.56	0.54
1:F:238:ARG:CB	1:F:281:GLN:HE22	2.18	0.54
1:D:503:ARG:HH12	1:D:522:ARG:NH2	2.05	0.54
1:C:319:ARG:C	1:C:320:GLN:NE2	2.61	0.54
1:B:241:PHE:CE2	1:B:285:GLU:CG	2.91	0.54
1:F:417:TYR:CE1	1:F:482:VAL:HG21	2.42	0.54
1:E:202:LYS:CD	1:E:300:ALA:HB1	2.36	0.54
1:E:334:ILE:O	1:E:335:LEU:C	2.47	0.54
1:A:563:LEU:HD12	1:A:564:GLU:N	2.22	0.54
1:E:305:ASP:OD1	1:E:305:ASP:N	2.26	0.54
1:F:375:LEU:CD1	1:F:388:ASP:HB3	2.36	0.54
1:A:219:THR:HA	1:A:253:PHE:O	2.08	0.54
1:B:170:GLU:CB	1:C:378:ARG:HH22	2.20	0.54
1:D:285:GLU:O	1:D:288:GLY:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:238:ARG:NH1	1:F:239:ASP:HB3	2.15	0.54
1:F:511:HIS:C	1:F:512:PRO:O	2.45	0.54
1:B:236:ARG:O	1:B:239:ASP:OD1	2.26	0.54
1:E:368:LEU:HD13	1:E:393:ALA:CA	2.37	0.54
1:F:454:ARG:NH2	1:F:528:GLY:C	2.61	0.54
1:A:196:GLY:O	1:A:302:ASN:OD1	2.25	0.53
1:B:334:ILE:O	1:B:337:ILE:HG22	2.09	0.53
1:D:319:ARG:CG	1:D:319:ARG:NH1	2.62	0.53
1:F:177:ASN:O	1:F:180:ARG:HB3	2.07	0.53
1:F:261:GLY:O	1:F:308:ASP:N	2.35	0.53
1:F:285:GLU:O	1:F:288:GLY:N	2.41	0.53
1:F:289:PHE:CD2	1:F:290:GLU:N	2.75	0.53
1:F:327:ASP:O	1:F:331:ARG:NH2	2.41	0.53
1:D:522:ARG:HD2	1:D:530:TYR:CA	2.32	0.53
1:D:334:ILE:O	1:D:337:ILE:HG22	2.08	0.53
1:C:551:ILE:O	1:C:552:GLU:C	2.46	0.53
1:A:367:ASN:O	1:A:371:GLU:HB3	2.07	0.53
1:A:166:GLU:C	1:A:169:LYS:HG2	2.28	0.53
1:A:218:ILE:HG12	1:A:251:ILE:O	2.08	0.53
1:A:311:LEU:HB3	1:A:316:ARG:HH22	1.73	0.53
1:A:336:ARG:CG	1:A:337:ILE:N	2.72	0.53
1:B:165:LYS:CD	1:B:168:LEU:CD2	2.76	0.53
1:B:328:VAL:HG21	1:B:355:LYS:HE3	1.88	0.53
1:D:257:ILE:O	1:D:260:VAL:HG13	2.08	0.53
1:E:179:SER:HA	1:E:182:HIS:NE2	2.24	0.53
1:F:166:GLU:O	1:F:169:LYS:HG2	2.08	0.53
1:D:517:VAL:HG11	1:D:519:TYR:CZ	2.43	0.53
1:D:152:LYS:HB2	1:D:207:ARG:NH1	2.23	0.53
1:E:367:ASN:O	1:E:371:GLU:HB3	2.09	0.53
1:D:480:GLU:OE1	1:D:555:TYR:OH	2.26	0.53
1:F:376:ALA:CA	1:F:381:ARG:NH1	2.71	0.53
1:A:240:LEU:O	1:A:243:THR:OG1	2.20	0.53
1:A:292:ASP:OD1	1:A:293:THR:N	2.41	0.53
1:A:334:ILE:CD1	2:A:1001:ADP:C6	2.91	0.53
1:B:253:PHE:CD2	1:B:253:PHE:C	2.82	0.53
1:E:177:ASN:ND2	1:E:180:ARG:HD3	2.22	0.53
1:B:522:ARG:HD2	1:B:530:TYR:CA	2.31	0.53
1:C:305:ASP:O	1:C:307:LEU:N	2.41	0.53
1:C:368:LEU:HD13	1:C:393:ALA:HA	1.89	0.53
1:C:461:SER:HA	1:D:487:THR:O	2.08	0.53
1:D:467:ASP:O	1:D:470:ALA:HB3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:467:ASP:O	1:E:471:VAL:HG23	2.08	0.53
1:E:379:GLU:HG3	1:E:381:ARG:HB2	1.91	0.53
1:B:216:PRO:HG2	1:B:250:CYS:CB	2.39	0.53
1:F:417:TYR:CD2	1:F:483:PHE:HE2	2.26	0.53
1:C:410:ARG:HG3	1:C:411:ASP:H	1.73	0.53
1:C:202:LYS:CD	1:C:300:ALA:HB1	2.36	0.53
1:A:448:GLY:O	1:A:449:PHE:C	2.46	0.53
1:A:493:ASP:OD1	1:A:493:ASP:N	2.41	0.53
1:A:465:LEU:CD2	1:A:508:TRP:CZ3	2.92	0.53
1:D:202:LYS:HD3	2:D:2001:ADP:O2B	2.08	0.53
1:D:165:LYS:HZ1	1:D:205:LEU:HB3	1.73	0.53
1:B:592:GLU:O	1:B:594:LEU:N	2.41	0.53
1:A:313:ARG:NH1	1:A:526:TYR:HA	2.24	0.53
1:E:196:GLY:C	1:E:443:ARG:NH2	2.61	0.53
1:A:525:THR:OG1	1:A:528:GLY:HA3	2.08	0.53
1:B:177:ASN:O	1:B:180:ARG:HB3	2.08	0.53
1:A:587:PHE:CD2	1:A:588:GLN:N	2.76	0.53
1:A:586:GLU:CB	1:A:589:ARG:CZ	2.72	0.53
1:F:163:GLU:O	1:F:167:GLU:HB3	2.08	0.53
1:F:212:GLU:O	1:F:214:ARG:HG2	2.09	0.53
1:C:507:GLU:CD	1:C:522:ARG:HE	2.12	0.53
1:A:552:GLU:O	1:A:555:TYR:HB3	2.09	0.53
1:E:334:ILE:CD1	2:E:1001:ADP:N6	2.71	0.53
1:C:563:LEU:HD12	1:C:564:GLU:N	2.23	0.53
1:C:594:LEU:O	1:C:594:LEU:HG	2.09	0.53
1:A:319:ARG:O	1:A:320:GLN:NE2	2.42	0.53
1:B:201:GLY:N	2:B:2001:ADP:O1A	2.39	0.53
1:E:169:LYS:HA	1:E:172:VAL:CG1	2.38	0.53
1:A:585:GLU:CD	1:A:586:GLU:N	2.62	0.53
1:F:194:LEU:HD23	1:F:323:ILE:HD11	1.90	0.53
1:C:368:LEU:HD13	1:C:393:ALA:CA	2.39	0.53
1:F:467:ASP:OD1	1:F:557:ARG:NH2	2.42	0.53
1:D:441:VAL:O	1:D:443:ARG:N	2.42	0.53
1:F:477:ALA:O	1:F:481:ILE:HG13	2.09	0.53
1:A:349:ASP:OD1	1:A:349:ASP:O	2.26	0.53
1:E:585:GLU:CD	1:E:586:GLU:N	2.62	0.53
1:A:334:ILE:O	1:A:335:LEU:C	2.46	0.53
1:A:368:LEU:HD13	1:A:393:ALA:HA	1.91	0.53
1:B:366:GLU:O	1:B:369:LEU:HB2	2.08	0.53
1:B:397:MET:O	1:B:400:PRO:HG2	2.09	0.53
1:F:155:PHE:CE2	1:F:212:GLU:OE2	2.61	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:318:ASP:OD1	1:F:318:ASP:N	2.21	0.53
1:A:537:GLU:N	1:B:537:GLU:OE2	2.41	0.53
1:D:517:VAL:HG13	1:D:519:TYR:CZ	2.44	0.53
1:E:525:THR:O	1:E:528:GLY:N	2.42	0.53
1:E:539:THR:O	1:E:543:ILE:HG13	2.08	0.53
1:F:451:MET:HB3	1:F:452:PRO:CD	2.38	0.53
1:B:447:LEU:O	1:B:449:PHE:N	2.41	0.53
1:D:171:ILE:HG23	1:D:172:VAL:N	2.23	0.53
1:A:401:ALA:HB3	1:A:405:LEU:HD21	1.91	0.53
1:B:181:PHE:O	1:B:185:GLY:N	2.42	0.53
1:F:210:ALA:O	1:F:214:ARG:CA	2.57	0.53
1:F:253:PHE:C	1:F:253:PHE:CD2	2.82	0.53
1:F:331:ARG:HD2	1:F:354:ALA:O	2.09	0.53
1:D:417:TYR:CE1	1:D:482:VAL:HG21	2.44	0.53
1:D:463:LYS:HE3	1:E:486:VAL:HG21	1.91	0.53
1:F:494:PHE:O	1:F:495:ARG:C	2.45	0.53
1:B:216:PRO:HB2	1:B:218:ILE:HD11	1.89	0.53
1:E:200:VAL:CG1	1:E:323:ILE:HG13	2.39	0.53
1:E:336:ARG:CG	1:E:337:ILE:N	2.71	0.53
1:C:193:LEU:HD12	1:C:299:ALA:O	2.09	0.53
1:A:155:PHE:CZ	1:A:209:VAL:HG22	2.44	0.53
1:B:158:VAL:CG1	1:B:205:LEU:HD11	2.38	0.53
1:B:262:ARG:CG	1:B:263:LYS:H	2.18	0.53
1:D:277:GLN:HA	1:D:280:ASN:HD21	1.74	0.53
1:E:319:ARG:O	1:E:320:GLN:NE2	2.41	0.53
1:A:382:ARG:HG3	1:A:383:LYS:HB2	1.91	0.53
1:F:391:GLU:O	1:F:395:ARG:HB3	2.08	0.53
1:A:264:ARG:HD2	1:A:266:SER:OG	2.09	0.53
1:E:514:PHE:CD2	1:E:514:PHE:N	2.77	0.53
1:F:514:PHE:HB3	1:F:519:TYR:HE1	1.74	0.53
1:D:592:GLU:O	1:D:594:LEU:N	2.42	0.53
1:E:343:PRO:C	1:E:344:LEU:HD13	2.28	0.53
1:A:424:LEU:HD22	1:A:569:LEU:HA	1.90	0.53
1:E:349:ASP:O	1:E:349:ASP:OD1	2.26	0.53
1:A:214:ARG:NH1	1:A:214:ARG:HG2	2.23	0.53
1:B:165:LYS:O	1:B:168:LEU:CB	2.57	0.53
1:C:345:ALA:O	1:C:348:VAL:HB	2.09	0.53
1:E:168:LEU:O	1:E:169:LYS:C	2.47	0.53
1:A:227:GLU:HG3	1:F:263:LYS:HZ1	1.68	0.53
1:F:186:ALA:O	1:F:187:ARG:HB3	2.08	0.53
1:C:196:GLY:HA2	1:C:443:ARG:NH2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:461:SER:HA	1:F:487:THR:O	2.09	0.53
1:C:262:ARG:CG	1:C:275:ARG:HH22	2.12	0.53
1:C:318:ASP:O	1:C:319:ARG:HG3	2.09	0.53
1:A:521:VAL:HG12	1:B:495:ARG:HD2	1.90	0.53
1:D:387:LYS:HG3	1:D:388:ASP:N	2.21	0.53
1:C:169:LYS:HA	1:C:172:VAL:CG1	2.38	0.53
1:D:585:GLU:HA	1:D:588:GLN:OE1	2.09	0.53
1:D:181:PHE:O	1:D:185:GLY:N	2.42	0.53
1:D:181:PHE:HA	1:D:184:MET:HG2	1.89	0.53
1:B:181:PHE:HA	1:B:184:MET:HG2	1.90	0.52
1:C:343:PRO:C	1:C:344:LEU:HD13	2.30	0.52
1:B:319:ARG:O	1:B:320:GLN:HB3	2.09	0.52
1:E:179:SER:C	1:E:181:PHE:H	2.13	0.52
1:F:165:LYS:HZ1	1:F:205:LEU:CB	2.21	0.52
1:D:459:HIS:CG	1:D:459:HIS:O	2.56	0.52
1:F:479:GLU:OE2	1:F:488:THR:HG23	2.09	0.52
1:C:189:PRO:O	1:C:190:LYS:HG2	2.08	0.52
1:B:479:GLU:OE2	1:B:488:THR:HG23	2.10	0.52
1:F:526:TYR:N	1:F:526:TYR:CD2	2.76	0.52
1:D:421:GLY:HA2	1:D:562:LEU:HD11	1.90	0.52
1:F:376:ALA:O	1:F:381:ARG:CG	2.57	0.52
1:A:172:VAL:CB	1:A:213:ALA:HB2	2.39	0.52
1:B:158:VAL:HG11	1:B:205:LEU:HD11	1.91	0.52
1:D:263:LYS:HE2	1:E:228:MET:HE1	1.91	0.52
1:E:240:LEU:O	1:E:243:THR:OG1	2.22	0.52
1:C:460:TRP:HB3	1:C:465:LEU:HD11	1.91	0.52
1:E:521:VAL:HG12	1:F:495:ARG:HD2	1.92	0.52
1:D:335:LEU:HD21	1:D:365:LEU:HB3	1.90	0.52
1:E:568:VAL:O	1:E:572:VAL:HG23	2.10	0.52
1:A:179:SER:HA	1:A:182:HIS:NE2	2.24	0.52
1:E:177:ASN:HD22	1:E:180:ARG:CD	2.22	0.52
1:E:178:PRO:O	1:E:182:HIS:CD2	2.62	0.52
1:E:190:LYS:HD2	1:E:289:PHE:HE1	1.70	0.52
1:E:212:GLU:O	1:E:214:ARG:HD3	2.10	0.52
1:F:277:GLN:HA	1:F:280:ASN:HD21	1.74	0.52
1:C:354:ALA:O	1:C:357:THR:CG2	2.57	0.52
1:C:510:MET:O	1:C:512:PRO:CD	2.57	0.52
1:C:525:THR:O	1:C:528:GLY:N	2.42	0.52
1:F:356:ARG:O	1:F:358:PRO:HD3	2.10	0.52
1:D:187:ARG:O	1:E:374:LEU:HD21	2.08	0.52
1:B:521:VAL:HG23	1:B:532:VAL:CG1	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:LEU:HD13	1:A:393:ALA:CA	2.39	0.52
1:D:243:THR:HG22	1:D:244:ALA:N	2.25	0.52
1:A:436:HIS:HB3	1:A:584:ALA:HB1	1.90	0.52
1:F:165:LYS:CD	1:F:168:LEU:CD2	2.79	0.52
1:F:235:ALA:HA	1:F:238:ARG:HD3	1.91	0.52
1:C:451:MET:HB2	1:C:452:PRO:HD3	1.92	0.52
1:D:554:GLN:O	1:D:557:ARG:HB3	2.09	0.52
1:A:503:ARG:NH2	1:A:522:ARG:NH1	2.57	0.52
1:D:348:VAL:HG11	1:D:386:MET:SD	2.49	0.52
1:B:463:LYS:HE3	1:C:486:VAL:HG21	1.90	0.52
1:E:442:PRO:HG2	1:E:443:ARG:H	1.74	0.52
1:A:273:ASP:CG	1:A:274:GLU:N	2.63	0.52
1:B:171:ILE:HG23	1:B:172:VAL:N	2.23	0.52
1:B:180:ARG:NH1	1:B:184:MET:HE1	2.24	0.52
1:D:216:PRO:HG2	1:D:250:CYS:CB	2.39	0.52
1:E:241:PHE:O	1:E:244:ALA:N	2.42	0.52
1:A:374:LEU:CD1	1:F:187:ARG:H	2.11	0.52
1:D:417:TYR:CD2	1:D:483:PHE:HE2	2.28	0.52
1:C:463:LYS:HD2	1:D:486:VAL:HG22	1.90	0.52
1:D:331:ARG:HH22	1:D:580:GLU:CD	2.10	0.52
1:D:376:ALA:C	1:D:381:ARG:CB	2.77	0.52
1:B:571:ARG:HH12	1:B:593:GLY:H	1.57	0.52
1:E:354:ALA:HA	1:E:357:THR:CG2	2.39	0.52
1:D:507:GLU:HG3	1:D:520:ALA:O	2.10	0.52
1:A:574:GLU:C	1:A:574:GLU:OE1	2.48	0.52
1:A:583:THR:N	1:A:586:GLU:OE2	2.36	0.52
1:A:343:PRO:C	1:A:344:LEU:HD13	2.29	0.52
1:F:174:PHE:HZ	1:F:294:ALA:CA	2.22	0.52
1:F:348:VAL:HG13	1:F:350:LEU:H	1.73	0.52
1:C:470:ALA:HB1	1:C:558:VAL:CG2	2.36	0.52
1:A:451:MET:HB2	1:A:452:PRO:HD3	1.92	0.52
1:D:350:LEU:HA	1:D:353:LEU:HB3	1.91	0.52
1:C:568:VAL:O	1:C:572:VAL:HG23	2.09	0.52
1:F:381:ARG:CZ	1:F:388:ASP:OD2	2.57	0.52
1:C:379:GLU:HG3	1:C:381:ARG:HB2	1.92	0.52
1:D:194:LEU:HD23	1:D:323:ILE:HD11	1.92	0.52
1:E:236:ARG:HG3	1:E:237:VAL:CA	2.37	0.52
1:A:374:LEU:HA	1:A:377:ALA:HB3	1.92	0.52
1:F:350:LEU:HA	1:F:353:LEU:HB3	1.91	0.52
1:C:207:ARG:NH2	1:C:217:PHE:CD2	2.76	0.52
1:B:281:GLN:O	1:B:285:GLU:OE1	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:PHE:HZ	1:D:294:ALA:CA	2.23	0.52
1:A:241:PHE:O	1:A:244:ALA:N	2.43	0.52
1:A:286:MET:HE3	1:A:297:VAL:HG21	1.90	0.52
1:B:190:LYS:HD2	1:B:289:PHE:HZ	1.73	0.52
1:B:297:VAL:HG13	1:B:317:PHE:HZ	1.75	0.52
1:F:165:LYS:CE	1:F:205:LEU:HG	2.39	0.52
1:B:505:ILE:HD13	1:B:547:VAL:HG23	1.90	0.52
1:C:325:ALA:N	1:C:326:PRO:CD	2.72	0.52
1:D:503:ARG:HG2	1:D:508:TRP:CZ2	2.44	0.52
1:E:462:ARG:HB2	1:E:510:MET:SD	2.50	0.52
1:C:179:SER:C	1:C:181:PHE:H	2.13	0.52
1:D:338:HIS:HB3	1:D:369:LEU:CD1	2.40	0.52
1:C:218:ILE:CG1	1:C:251:ILE:O	2.57	0.52
1:D:378:ARG:C	1:D:380:GLY:N	2.51	0.52
1:B:398:MET:O	1:B:401:ALA:HB3	2.09	0.52
1:C:574:GLU:OE1	1:C:575:THR:N	2.43	0.52
1:D:398:MET:O	1:D:401:ALA:HB3	2.10	0.52
1:E:436:HIS:HB3	1:E:584:ALA:HB1	1.92	0.52
1:B:180:ARG:HH12	1:B:184:MET:HE1	1.75	0.52
1:D:245:LYS:HG3	1:D:246:ARG:N	2.24	0.52
1:D:281:GLN:O	1:D:285:GLU:OE1	2.28	0.52
1:D:319:ARG:O	1:D:320:GLN:HB3	2.10	0.52
1:C:334:ILE:CD1	2:C:1001:ADP:N6	2.73	0.52
1:C:449:PHE:N	1:C:449:PHE:HD2	2.08	0.52
1:E:447:LEU:CB	1:E:496:GLN:HE22	2.23	0.52
1:C:219:THR:HB	1:C:253:PHE:CD2	2.38	0.52
1:C:225:PHE:CE1	1:C:233:GLY:HA3	2.43	0.52
1:D:355:LYS:NZ	1:D:578:GLU:O	2.43	0.52
1:E:378:ARG:HG2	1:E:379:GLU:N	2.23	0.52
1:F:557:ARG:O	1:F:560:ALA:HB3	2.10	0.52
1:E:331:ARG:CZ	1:E:358:PRO:HD3	2.39	0.52
1:E:353:LEU:O	1:E:357:THR:HG22	2.09	0.52
1:A:331:ARG:HD2	1:A:357:THR:CG2	2.40	0.52
1:B:202:LYS:HD3	2:B:2001:ADP:O2B	2.10	0.52
1:B:350:LEU:HA	1:B:353:LEU:HB3	1.91	0.52
1:D:190:LYS:CE	1:D:289:PHE:HZ	2.13	0.52
1:D:260:VAL:HG23	1:D:279:LEU:CD1	2.40	0.52
1:F:237:VAL:CG2	1:F:281:GLN:CG	2.88	0.52
1:D:455:GLU:O	1:D:457:MET:N	2.43	0.52
1:D:470:ALA:O	1:D:474:ALA:HB2	2.10	0.52
1:C:539:THR:OG1	1:D:544:ASP:OD2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:453:ARG:HA	1:F:456:ASP:OD2	2.10	0.52
1:C:241:PHE:O	1:C:244:ALA:N	2.43	0.52
1:D:180:ARG:HH12	1:D:184:MET:HE1	1.73	0.52
1:A:334:ILE:HD13	2:A:1001:ADP:N1	2.26	0.51
1:A:206:ALA:HB1	1:A:217:PHE:HZ	1.75	0.51
1:A:238:ARG:O	1:A:241:PHE:N	2.43	0.51
1:B:173:GLU:OE1	1:C:378:ARG:HA	2.10	0.51
1:B:174:PHE:HZ	1:B:294:ALA:HA	1.76	0.51
1:B:376:ALA:C	1:B:381:ARG:CD	2.61	0.51
1:A:346:GLU:OE1	1:A:347:ASP:OD1	2.28	0.51
1:F:180:ARG:NH1	1:F:184:MET:CE	2.73	0.51
1:C:200:VAL:CG1	1:C:323:ILE:HG13	2.39	0.51
1:C:175:LEU:O	1:C:249:PRO:HG3	2.10	0.51
1:D:366:GLU:O	1:D:369:LEU:HB2	2.09	0.51
1:B:417:TYR:CD2	1:B:483:PHE:HE2	2.26	0.51
1:E:345:ALA:O	1:E:348:VAL:HB	2.10	0.51
1:B:526:TYR:O	1:B:528:GLY:N	2.42	0.51
1:F:376:ALA:HA	1:F:381:ARG:HH11	1.74	0.51
1:A:172:VAL:O	1:A:213:ALA:HB1	2.10	0.51
1:B:159:ALA:H	2:B:2001:ADP:HN62	1.57	0.51
1:B:166:GLU:O	1:B:169:LYS:HG2	2.10	0.51
1:D:192:VAL:O	1:D:317:PHE:CE2	2.64	0.51
1:F:158:VAL:CG1	1:F:205:LEU:HD11	2.40	0.51
1:C:368:LEU:HG	1:C:369:LEU:N	2.25	0.51
1:C:174:PHE:HB2	1:C:181:PHE:CE2	2.46	0.51
1:D:352:LEU:O	1:D:353:LEU:C	2.48	0.51
1:D:338:HIS:CE1	1:D:366:GLU:HG3	2.44	0.51
1:D:376:ALA:O	1:D:381:ARG:HG2	2.10	0.51
1:B:467:ASP:OD1	1:B:557:ARG:NH2	2.43	0.51
1:A:594:LEU:O	1:A:594:LEU:HG	2.11	0.51
1:B:583:THR:O	1:B:584:ALA:C	2.48	0.51
1:E:193:LEU:HD12	1:E:299:ALA:O	2.09	0.51
1:A:379:GLU:HG3	1:A:381:ARG:HB2	1.92	0.51
1:B:523:GLU:OE1	1:C:264:ARG:NH2	2.43	0.51
1:C:334:ILE:O	1:C:335:LEU:C	2.48	0.51
1:C:397:MET:SD	1:C:406:VAL:CG1	2.98	0.51
1:C:525:THR:OG1	1:C:528:GLY:HA3	2.11	0.51
1:C:179:SER:O	1:C:182:HIS:CD2	2.61	0.51
1:C:240:LEU:O	1:C:243:THR:OG1	2.25	0.51
1:C:241:PHE:O	1:C:242:GLU:C	2.49	0.51
1:B:455:GLU:O	1:B:457:MET:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:331:ARG:HD2	1:D:354:ALA:O	2.11	0.51
1:C:154:THR:OG1	1:C:155:PHE:N	2.43	0.51
1:B:175:LEU:HB3	1:B:213:ALA:HB1	1.93	0.51
1:B:215:VAL:HG22	1:B:250:CYS:HB3	1.92	0.51
1:B:356:ARG:O	1:B:358:PRO:HD3	2.11	0.51
1:E:594:LEU:HG	1:E:594:LEU:O	2.10	0.51
1:A:354:ALA:HA	1:A:357:THR:CG2	2.40	0.51
1:D:175:LEU:O	1:D:249:PRO:CB	2.58	0.51
1:E:206:ALA:HB1	1:E:217:PHE:HZ	1.75	0.51
1:F:174:PHE:HZ	1:F:294:ALA:HA	1.75	0.51
1:C:338:HIS:ND1	1:C:366:GLU:HG3	2.25	0.51
1:A:313:ARG:NH1	1:A:526:TYR:CA	2.73	0.51
1:E:196:GLY:H	1:E:202:LYS:HZ1	1.55	0.51
1:A:169:LYS:O	1:A:172:VAL:CG1	2.58	0.51
1:A:236:ARG:HG3	1:A:237:VAL:CA	2.36	0.51
1:B:355:LYS:HZ3	1:B:578:GLU:HG3	1.74	0.51
1:E:218:ILE:CG1	1:E:251:ILE:O	2.59	0.51
1:F:171:ILE:HG23	1:F:172:VAL:N	2.25	0.51
1:F:222:GLY:N	1:F:255:ASP:O	2.40	0.51
1:F:281:GLN:O	1:F:285:GLU:OE1	2.29	0.51
1:F:318:ASP:O	1:F:319:ARG:CB	2.35	0.51
1:D:447:LEU:O	1:D:449:PHE:N	2.43	0.51
1:D:452:PRO:O	1:D:456:ASP:N	2.43	0.51
1:C:236:ARG:NH1	1:C:236:ARG:CB	2.73	0.51
1:A:464:ARG:CG	1:A:464:ARG:HH11	2.23	0.51
1:B:452:PRO:O	1:B:456:ASP:N	2.43	0.51
1:D:210:ALA:O	1:D:214:ARG:N	2.41	0.51
1:B:175:LEU:O	1:B:249:PRO:CB	2.58	0.51
1:B:557:ARG:O	1:B:560:ALA:HB3	2.11	0.51
1:E:313:ARG:HH12	1:E:526:TYR:CA	2.23	0.51
1:F:428:PHE:CE1	1:F:432:ALA:C	2.84	0.51
1:F:193:LEU:HB3	1:F:317:PHE:HD2	1.76	0.51
1:D:514:PHE:HB3	1:D:519:TYR:HE1	1.74	0.51
1:C:236:ARG:HG3	1:C:237:VAL:CA	2.36	0.51
1:C:292:ASP:OD1	1:C:293:THR:N	2.43	0.51
1:D:327:ASP:O	1:D:331:ARG:NH2	2.43	0.51
1:F:567:GLU:O	1:F:570:GLU:CB	2.58	0.51
1:B:461:SER:O	1:B:464:ARG:HB3	2.10	0.51
1:E:563:LEU:HD12	1:E:564:GLU:N	2.25	0.51
1:A:334:ILE:O	1:A:337:ILE:HG13	2.10	0.51
1:B:180:ARG:NH1	1:B:184:MET:CE	2.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:175:LEU:O	1:E:249:PRO:HG3	2.10	0.51
1:F:286:MET:O	1:F:289:PHE:CD1	2.64	0.51
1:C:554:GLN:O	1:C:557:ARG:HB3	2.11	0.51
1:D:563:LEU:O	1:D:566:ARG:HB3	2.11	0.51
1:C:174:PHE:CE1	1:C:188:ILE:CD1	2.70	0.51
1:C:181:PHE:HA	1:C:184:MET:HE2	1.91	0.51
1:E:313:ARG:NH1	1:E:526:TYR:CA	2.74	0.51
1:B:186:ALA:O	1:B:187:ARG:HB3	2.09	0.51
1:B:454:ARG:HH21	1:B:526:TYR:CA	2.24	0.51
1:E:583:THR:HG22	1:E:586:GLU:CD	2.31	0.51
1:F:375:LEU:HD11	1:F:388:ASP:CB	2.38	0.51
1:A:169:LYS:O	1:A:172:VAL:N	2.44	0.51
1:A:218:ILE:CG1	1:A:251:ILE:O	2.58	0.51
1:D:191:GLY:HA3	1:D:297:VAL:HG12	1.92	0.51
1:D:319:ARG:HG2	1:D:319:ARG:NH1	2.06	0.51
1:E:166:GLU:HB2	1:E:169:LYS:HZ1	1.75	0.51
1:F:215:VAL:HG22	1:F:250:CYS:HB3	1.93	0.51
1:C:459:HIS:HE1	1:D:411:ASP:HB3	1.76	0.51
1:D:521:VAL:HG12	1:E:495:ARG:HD2	1.93	0.51
1:B:592:GLU:O	1:B:594:LEU:CB	2.59	0.51
1:B:459:HIS:O	1:B:459:HIS:CG	2.60	0.51
1:C:313:ARG:NH1	1:C:526:TYR:HA	2.26	0.51
1:E:513:GLU:O	1:F:548:ARG:NH2	2.44	0.51
1:E:566:ARG:O	1:E:569:LEU:N	2.44	0.51
1:E:589:ARG:HH21	1:E:596:LEU:CB	1.74	0.51
1:A:416:ALA:HB2	1:A:577:LEU:CD2	2.06	0.51
1:B:286:MET:SD	1:B:316:ARG:HG2	2.51	0.51
1:D:225:PHE:HA	1:D:236:ARG:CZ	2.41	0.51
1:D:290:GLU:HG3	1:D:292:ASP:HB3	1.93	0.51
1:F:190:LYS:NZ	1:F:289:PHE:CZ	2.77	0.51
1:F:243:THR:HG22	1:F:244:ALA:N	2.25	0.51
1:C:450:MET:HG3	1:C:451:MET:H	1.76	0.51
1:F:505:ILE:HD13	1:F:547:VAL:HG23	1.91	0.51
1:F:572:VAL:O	1:F:576:LEU:HB2	2.11	0.51
1:E:524:ASP:OD1	1:E:524:ASP:N	2.43	0.51
1:F:410:ARG:HA	1:F:413:ARG:HG2	1.93	0.51
1:E:346:GLU:OE1	1:E:347:ASP:OD1	2.28	0.51
1:A:470:ALA:O	1:A:558:VAL:HG21	2.10	0.51
1:E:292:ASP:OD1	1:E:293:THR:N	2.43	0.51
1:A:397:MET:SD	1:A:406:VAL:CG1	2.99	0.51
1:B:480:GLU:OE1	1:B:555:TYR:OH	2.27	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:381:ARG:HH22	1:F:388:ASP:CG	2.15	0.51
1:A:241:PHE:O	1:A:242:GLU:C	2.48	0.51
1:A:316:ARG:O	1:A:317:PHE:C	2.50	0.51
1:A:331:ARG:CZ	1:A:358:PRO:HD3	2.40	0.51
1:E:191:GLY:CA	1:E:297:VAL:HG22	2.41	0.51
1:A:586:GLU:HG2	1:A:587:PHE:N	2.26	0.51
1:F:175:LEU:HB3	1:F:213:ALA:HB1	1.93	0.51
1:F:241:PHE:CD2	1:F:285:GLU:HG2	2.46	0.51
1:F:331:ARG:HH22	1:F:580:GLU:CD	2.13	0.51
1:F:332:GLU:HB2	1:F:354:ALA:HB2	1.93	0.51
1:B:536:SER:OG	1:C:541:LYS:HA	2.11	0.51
1:C:331:ARG:HD2	1:C:357:THR:CG2	2.40	0.51
1:C:503:ARG:NH2	1:C:522:ARG:NH1	2.58	0.51
1:D:503:ARG:HH22	1:D:522:ARG:CZ	2.23	0.51
1:F:522:ARG:HD2	1:F:530:TYR:CA	2.33	0.51
1:B:585:GLU:O	1:B:587:PHE:N	2.44	0.51
1:D:572:VAL:O	1:D:576:LEU:HB2	2.11	0.51
1:C:374:LEU:HA	1:C:377:ALA:HB3	1.93	0.51
1:E:354:ALA:O	1:E:357:THR:CG2	2.56	0.51
1:E:371:GLU:OE2	1:E:395:ARG:HD2	2.10	0.51
1:F:469:ILE:HG22	1:F:473:LEU:HD12	1.92	0.51
1:A:414:ILE:HG22	1:A:415:THR:H	1.75	0.50
1:B:286:MET:O	1:B:289:PHE:CG	2.63	0.50
1:A:512:PRO:HB2	1:A:514:PHE:CD2	2.46	0.50
1:D:397:MET:O	1:D:400:PRO:HG2	2.11	0.50
1:B:417:TYR:CE1	1:B:482:VAL:HG21	2.45	0.50
1:D:538:GLU:O	1:D:541:LYS:N	2.44	0.50
1:D:428:PHE:CE1	1:D:432:ALA:C	2.85	0.50
1:B:155:PHE:CE2	1:B:212:GLU:OE2	2.64	0.50
1:B:297:VAL:HG13	1:B:317:PHE:CZ	2.47	0.50
1:D:454:ARG:HH21	1:D:526:TYR:CA	2.23	0.50
1:A:345:ALA:HB1	1:A:347:ASP:OD1	2.12	0.50
1:F:335:LEU:HB3	1:F:350:LEU:HD13	1.92	0.50
1:F:345:ALA:CB	1:F:383:LYS:HE3	2.37	0.50
1:C:178:PRO:O	1:C:182:HIS:CD2	2.65	0.50
1:C:188:ILE:O	1:C:190:LYS:NZ	2.38	0.50
1:A:519:TYR:HA	1:A:533:ARG:NH2	2.27	0.50
1:D:355:LYS:NZ	1:D:578:GLU:HG3	2.26	0.50
1:C:215:VAL:CG2	1:C:216:PRO:N	2.75	0.50
1:B:237:VAL:CG2	1:B:281:GLN:CG	2.87	0.50
1:F:592:GLU:O	1:F:594:LEU:CB	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:329:LYS:O	1:E:332:GLU:HB3	2.11	0.50
1:B:335:LEU:HD21	1:B:365:LEU:HB3	1.92	0.50
1:C:346:GLU:OE1	1:C:347:ASP:OD1	2.29	0.50
1:C:378:ARG:HG3	1:C:379:GLU:N	2.21	0.50
1:D:236:ARG:NH1	1:D:237:VAL:HG12	2.27	0.50
1:D:262:ARG:CG	1:D:263:LYS:H	2.19	0.50
1:F:260:VAL:HG23	1:F:279:LEU:CD1	2.41	0.50
1:F:352:LEU:O	1:F:355:LYS:HB2	2.10	0.50
1:C:198:PRO:HD3	1:C:302:ASN:ND2	2.27	0.50
1:C:331:ARG:CZ	1:C:358:PRO:HD3	2.41	0.50
1:D:508:TRP:CD1	1:E:491:GLU:HG2	2.45	0.50
1:B:451:MET:HB3	1:B:452:PRO:CD	2.37	0.50
1:D:325:ALA:CB	1:D:326:PRO:HD3	2.37	0.50
1:B:243:THR:HG22	1:B:244:ALA:N	2.26	0.50
1:F:595:PRO:O	1:F:596:LEU:HD12	2.11	0.50
1:F:441:VAL:O	1:F:443:ARG:N	2.44	0.50
1:E:300:ALA:O	1:E:301:THR:HG22	2.11	0.50
1:F:454:ARG:NH2	1:F:526:TYR:HA	2.26	0.50
1:A:357:THR:OG1	1:A:360:PHE:HB2	2.12	0.50
1:B:174:PHE:HZ	1:B:294:ALA:CA	2.24	0.50
1:C:382:ARG:HG2	1:C:383:LYS:H	1.75	0.50
1:C:447:LEU:HB2	1:C:496:GLN:HE22	1.77	0.50
1:B:538:GLU:HB2	1:C:541:LYS:NZ	2.26	0.50
1:D:451:MET:HB3	1:D:452:PRO:CD	2.38	0.50
1:D:479:GLU:OE2	1:D:488:THR:HG23	2.11	0.50
1:E:381:ARG:CG	1:E:381:ARG:HH11	2.21	0.50
1:C:168:LEU:O	1:C:169:LYS:C	2.47	0.50
1:A:313:ARG:HH12	1:A:526:TYR:CA	2.25	0.50
1:E:368:LEU:HG	1:E:369:LEU:N	2.25	0.50
1:C:469:ILE:O	1:C:473:LEU:HD12	2.11	0.50
1:E:389:LEU:O	1:E:392:ALA:HB3	2.11	0.50
1:F:564:GLU:C	1:F:566:ARG:N	2.65	0.50
1:A:479:GLU:OE2	1:A:488:THR:N	2.45	0.50
1:E:479:GLU:OE2	1:E:488:THR:N	2.45	0.50
1:B:193:LEU:HB3	1:B:317:PHE:HD2	1.77	0.50
1:D:278:THR:O	1:D:281:GLN:HB3	2.12	0.50
1:D:285:GLU:C	1:D:288:GLY:H	2.14	0.50
1:F:207:ARG:O	1:F:210:ALA:N	2.45	0.50
1:F:225:PHE:HA	1:F:236:ARG:CZ	2.42	0.50
1:C:357:THR:OG1	1:C:360:PHE:HB2	2.11	0.50
1:E:507:GLU:HB2	1:E:520:ALA:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:LEU:O	1:C:286:MET:HG2	2.11	0.50
1:F:549:ARG:O	1:F:550:LEU:C	2.49	0.50
1:D:329:LYS:O	1:D:332:GLU:HB3	2.12	0.50
1:B:175:LEU:HD12	1:B:215:VAL:CG1	2.36	0.50
1:E:325:ALA:N	1:E:326:PRO:CD	2.74	0.50
1:E:334:ILE:O	1:E:337:ILE:HG13	2.10	0.50
1:E:397:MET:SD	1:E:406:VAL:CG1	2.99	0.50
1:E:302:ASN:HB3	1:E:443:ARG:HH12	1.76	0.50
1:E:536:SER:O	1:E:537:GLU:C	2.49	0.50
1:C:574:GLU:C	1:C:574:GLU:OE1	2.49	0.50
1:A:279:LEU:O	1:A:282:LEU:N	2.45	0.50
1:A:325:ALA:N	1:A:326:PRO:HD2	2.27	0.50
1:B:158:VAL:HG22	1:B:204:HIS:ND1	2.26	0.50
1:B:260:VAL:HG23	1:B:279:LEU:CD1	2.42	0.50
1:E:218:ILE:HG12	1:E:251:ILE:O	2.11	0.50
1:E:319:ARG:C	1:E:320:GLN:NE2	2.65	0.50
1:F:297:VAL:HG13	1:F:317:PHE:HZ	1.77	0.50
1:C:408:SER:C	1:C:410:ARG:H	2.14	0.50
1:C:325:ALA:N	1:C:326:PRO:HD2	2.27	0.50
1:C:450:MET:O	1:C:454:ARG:HB3	2.12	0.50
1:F:449:PHE:CZ	1:F:496:GLN:OE1	2.64	0.50
1:C:279:LEU:O	1:C:282:LEU:N	2.44	0.50
1:A:580:GLU:CG	1:A:580:GLU:O	2.59	0.50
1:F:398:MET:O	1:F:401:ALA:HB3	2.11	0.50
1:E:583:THR:HG22	1:E:586:GLU:OE1	2.10	0.50
1:F:387:LYS:HG3	1:F:388:ASP:N	2.25	0.50
1:A:196:GLY:H	1:A:202:LYS:HZ1	1.58	0.50
1:B:345:ALA:CB	1:B:383:LYS:HE3	2.37	0.50
1:D:239:ASP:O	1:D:242:GLU:OE2	2.30	0.50
1:E:241:PHE:O	1:E:242:GLU:C	2.49	0.50
1:F:334:ILE:O	1:F:337:ILE:HG22	2.12	0.50
1:C:449:PHE:HE2	1:C:496:GLN:NE2	2.10	0.50
1:C:493:ASP:N	1:C:493:ASP:OD1	2.44	0.50
1:A:445:ARG:O	1:A:447:LEU:N	2.45	0.50
1:D:158:VAL:HG22	1:D:204:HIS:ND1	2.26	0.50
1:B:238:ARG:HA	1:B:241:PHE:CE2	2.47	0.50
1:B:285:GLU:C	1:B:288:GLY:H	2.15	0.50
1:C:524:ASP:OD1	1:C:524:ASP:N	2.44	0.50
1:F:554:GLN:O	1:F:557:ARG:HB3	2.11	0.50
1:E:313:ARG:NH1	1:E:526:TYR:HA	2.27	0.50
1:C:313:ARG:NH1	1:C:526:TYR:CA	2.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:567:GLU:O	1:D:570:GLU:CB	2.59	0.50
1:A:286:MET:HB3	1:A:316:ARG:HB2	1.94	0.50
1:C:382:ARG:HG3	1:C:383:LYS:HB2	1.93	0.50
1:E:210:ALA:HA	1:E:251:ILE:HD11	1.94	0.50
1:A:345:ALA:O	1:A:348:VAL:HB	2.12	0.50
1:C:566:ARG:O	1:C:569:LEU:N	2.45	0.50
1:C:365:LEU:O	1:C:368:LEU:HB3	2.11	0.50
1:D:447:LEU:O	1:D:450:MET:HG3	2.11	0.50
1:E:448:GLY:O	1:E:449:PHE:C	2.51	0.50
1:D:389:LEU:O	1:D:390:GLU:C	2.50	0.50
1:B:585:GLU:O	1:B:586:GLU:C	2.50	0.50
1:B:301:THR:HG22	1:B:303:ARG:H	1.77	0.50
1:A:211:GLY:HA2	1:A:214:ARG:NE	2.25	0.50
1:A:319:ARG:C	1:A:320:GLN:NE2	2.65	0.50
1:D:238:ARG:NH1	1:D:239:ASP:HB3	2.16	0.50
1:D:313:ARG:HG3	1:D:314:PRO:HG2	1.94	0.50
1:D:313:ARG:O	1:D:316:ARG:HB3	2.12	0.50
1:E:282:LEU:O	1:E:286:MET:HG2	2.12	0.50
1:C:334:ILE:O	1:C:337:ILE:HG13	2.11	0.50
1:C:463:LYS:HB2	1:D:486:VAL:HG11	1.94	0.50
1:E:503:ARG:NH2	1:E:522:ARG:NH1	2.60	0.50
1:E:525:THR:OG1	1:E:528:GLY:HA3	2.11	0.50
1:A:450:MET:HG3	1:A:451:MET:H	1.77	0.50
1:F:510:MET:O	1:F:512:PRO:HD2	2.12	0.50
1:B:441:VAL:O	1:B:443:ARG:N	2.45	0.50
1:A:179:SER:O	1:A:182:HIS:CD2	2.62	0.49
1:A:588:GLN:HA	1:A:591:VAL:HG21	1.92	0.49
1:F:181:PHE:O	1:F:185:GLY:N	2.44	0.49
1:C:354:ALA:HA	1:C:357:THR:CG2	2.42	0.49
1:D:512:PRO:HB2	1:D:514:PHE:HD2	1.76	0.49
1:E:447:LEU:HA	1:E:496:GLN:HE21	1.76	0.49
1:B:449:PHE:CZ	1:B:496:GLN:OE1	2.65	0.49
1:A:428:PHE:HE1	1:A:432:ALA:HA	1.66	0.49
1:A:175:LEU:O	1:A:249:PRO:HG3	2.12	0.49
1:A:178:PRO:O	1:A:182:HIS:CD2	2.64	0.49
1:A:365:LEU:O	1:A:368:LEU:HB3	2.12	0.49
1:B:376:ALA:O	1:B:381:ARG:CG	2.60	0.49
1:E:174:PHE:HB2	1:E:181:PHE:CE2	2.47	0.49
1:E:215:VAL:CG2	1:E:216:PRO:N	2.74	0.49
1:F:197:PRO:HD2	1:F:200:VAL:HG11	1.94	0.49
1:F:225:PHE:CD2	1:F:225:PHE:N	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:236:ARG:NH1	1:F:237:VAL:HG12	2.26	0.49
1:C:436:HIS:HB3	1:C:584:ALA:CB	2.42	0.49
1:B:529:GLY:O	1:B:530:TYR:CB	2.55	0.49
1:D:563:LEU:O	1:D:566:ARG:CB	2.61	0.49
1:A:514:PHE:HB3	1:A:519:TYR:HE1	1.73	0.49
1:D:336:ARG:O	1:D:339:ALA:N	2.27	0.49
1:C:171:ILE:HD12	1:C:172:VAL:H	1.76	0.49
1:B:554:GLN:O	1:B:557:ARG:HB3	2.11	0.49
1:D:174:PHE:HZ	1:D:294:ALA:HA	1.76	0.49
1:C:531:ASP:C	1:C:531:ASP:OD1	2.51	0.49
1:A:150:ALA:CB	1:A:214:ARG:NH1	2.75	0.49
1:A:225:PHE:CE1	1:A:233:GLY:HA3	2.47	0.49
1:B:311:LEU:HA	1:B:316:ARG:CZ	2.39	0.49
1:D:241:PHE:HE2	1:D:285:GLU:OE2	1.91	0.49
1:F:193:LEU:C	1:F:194:LEU:HD12	2.33	0.49
1:F:338:HIS:CE1	1:F:366:GLU:HG3	2.47	0.49
1:A:264:ARG:CD	1:A:266:SER:CB	2.87	0.49
1:C:302:ASN:HB3	1:C:443:ARG:HH12	1.76	0.49
1:C:357:THR:N	1:C:358:PRO:CD	2.74	0.49
1:C:448:GLY:O	1:C:449:PHE:C	2.50	0.49
1:C:539:THR:O	1:C:543:ILE:HG13	2.13	0.49
1:E:460:TRP:HD1	1:E:464:ARG:NH1	2.08	0.49
1:C:206:ALA:HB1	1:C:217:PHE:HZ	1.77	0.49
1:B:242:GLU:CA	1:B:245:LYS:HB3	2.41	0.49
1:D:186:ALA:O	1:D:187:ARG:HB3	2.12	0.49
1:F:443:ARG:O	1:F:445:ARG:N	2.45	0.49
1:F:454:ARG:HH21	1:F:526:TYR:CA	2.25	0.49
1:E:537:GLU:N	1:F:537:GLU:OE2	2.41	0.49
1:C:594:LEU:HD12	1:C:595:PRO:O	2.12	0.49
1:A:147:LEU:HD23	1:A:217:PHE:HB3	1.93	0.49
1:B:336:ARG:C	1:B:338:HIS:N	2.62	0.49
1:D:454:ARG:NH2	1:D:528:GLY:C	2.66	0.49
1:F:313:ARG:HG3	1:F:314:PRO:CG	2.41	0.49
1:C:519:TYR:HB3	1:C:535:TYR:HD2	1.76	0.49
1:D:564:GLU:C	1:D:566:ARG:N	2.64	0.49
1:A:453:ARG:HH21	1:A:464:ARG:HH22	1.55	0.49
1:A:449:PHE:CE2	1:A:496:GLN:NE2	2.79	0.49
1:C:313:ARG:HH12	1:C:526:TYR:CA	2.25	0.49
1:E:195:VAL:HG22	1:E:301:THR:O	2.12	0.49
1:A:354:ALA:O	1:A:357:THR:CG2	2.55	0.49
1:B:308:ASP:OD1	1:B:310:ALA:N	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:154:THR:OG1	1:E:155:PHE:N	2.44	0.49
1:F:241:PHE:HE2	1:F:285:GLU:OE2	1.90	0.49
1:F:334:ILE:HG21	1:F:365:LEU:HD12	1.93	0.49
1:E:470:ALA:C	1:E:558:VAL:HG21	2.32	0.49
1:C:191:GLY:CA	1:C:297:VAL:HG22	2.43	0.49
1:D:209:VAL:CG1	1:D:210:ALA:H	2.20	0.49
1:C:370:ASN:OD1	1:C:374:LEU:HD13	2.12	0.49
1:B:454:ARG:NH2	1:B:528:GLY:C	2.66	0.49
1:A:389:LEU:O	1:A:392:ALA:HB3	2.11	0.49
1:E:580:GLU:O	1:E:580:GLU:CG	2.60	0.49
1:A:273:ASP:OD1	1:A:274:GLU:N	2.46	0.49
1:F:239:ASP:O	1:F:242:GLU:OE2	2.30	0.49
1:D:566:ARG:O	1:D:569:LEU:HB3	2.13	0.49
1:C:237:VAL:HG11	1:C:281:GLN:CB	2.26	0.49
2:A:1001:ADP:N3	2:A:1001:ADP:H2'	2.27	0.49
1:A:219:THR:HB	1:A:253:PHE:CD2	2.40	0.49
1:B:174:PHE:C	1:B:174:PHE:CD2	2.86	0.49
1:B:376:ALA:O	1:B:381:ARG:HG3	2.12	0.49
1:B:261:GLY:O	1:B:308:ASP:N	2.38	0.49
1:E:279:LEU:O	1:E:282:LEU:N	2.45	0.49
1:F:165:LYS:O	1:F:168:LEU:CB	2.60	0.49
1:F:191:GLY:HA3	1:F:297:VAL:HG12	1.94	0.49
1:D:453:ARG:HA	1:D:456:ASP:OD2	2.13	0.49
1:C:172:VAL:CB	1:C:213:ALA:HB2	2.41	0.49
1:D:183:GLU:OE1	1:D:184:MET:HB3	2.13	0.49
1:B:334:ILE:HG21	1:B:365:LEU:HD12	1.94	0.49
1:E:169:LYS:O	1:E:172:VAL:CG1	2.60	0.49
1:A:378:ARG:NH1	1:F:170:GLU:HB2	2.28	0.49
1:F:175:LEU:O	1:F:249:PRO:CB	2.61	0.49
1:F:319:ARG:O	1:F:320:GLN:HB3	2.11	0.49
1:F:336:ARG:C	1:F:338:HIS:N	2.64	0.49
1:F:352:LEU:O	1:F:353:LEU:C	2.49	0.49
1:F:360:PHE:HE1	1:F:364:ASP:HB3	1.77	0.49
1:F:335:LEU:HD13	1:F:365:LEU:HB3	1.93	0.49
1:C:583:THR:HG22	1:C:586:GLU:CD	2.32	0.49
2:C:1001:ADP:N3	2:C:1001:ADP:H2'	2.28	0.49
1:D:409:PRO:O	1:D:413:ARG:HD3	2.13	0.49
1:C:155:PHE:CZ	1:C:209:VAL:HG22	2.47	0.49
1:B:567:GLU:O	1:B:570:GLU:CB	2.61	0.49
1:D:525:THR:HG22	1:D:526:TYR:H	1.77	0.49
1:E:236:ARG:NH1	1:E:236:ARG:HG2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:260:VAL:HG23	1:E:261:GLY:H	1.78	0.49
1:C:329:LYS:O	1:C:332:GLU:HB3	2.12	0.49
1:C:442:PRO:HG2	1:C:443:ARG:H	1.78	0.49
1:C:503:ARG:CG	1:C:508:TRP:CE3	2.95	0.49
1:B:278:THR:O	1:B:281:GLN:HB3	2.13	0.49
1:D:174:PHE:CD2	1:D:174:PHE:C	2.85	0.49
1:E:374:LEU:HA	1:E:377:ALA:HB3	1.93	0.49
1:E:357:THR:OG1	1:E:360:PHE:HB2	2.11	0.49
1:F:564:GLU:O	1:F:566:ARG:N	2.45	0.49
1:E:220:ALA:O	1:E:254:ILE:HA	2.13	0.49
1:A:408:SER:C	1:A:410:ARG:H	2.15	0.49
1:A:203:THR:OG1	2:A:1001:ADP:O2A	2.20	0.49
1:A:260:VAL:HG23	1:A:261:GLY:H	1.76	0.49
1:B:191:GLY:HA3	1:B:297:VAL:HG12	1.94	0.49
1:D:238:ARG:CB	1:D:238:ARG:HH11	2.26	0.49
1:F:159:ALA:H	2:F:2001:ADP:HN62	1.61	0.49
1:F:174:PHE:CZ	1:F:294:ALA:CB	2.95	0.49
1:F:286:MET:O	1:F:289:PHE:CG	2.65	0.49
1:C:447:LEU:CA	1:C:496:GLN:NE2	2.75	0.49
1:C:507:GLU:HB2	1:C:520:ALA:HB3	1.94	0.49
1:D:469:ILE:HG22	1:D:473:LEU:HD12	1.95	0.49
1:A:447:LEU:CB	1:A:496:GLN:HE22	2.25	0.49
1:D:360:PHE:HE1	1:D:364:ASP:HB3	1.77	0.49
1:B:589:ARG:NE	1:B:596:LEU:CD2	2.76	0.49
1:E:198:PRO:HD3	1:E:302:ASN:ND2	2.27	0.49
1:E:373:ALA:HA	1:E:384:ILE:CD1	2.42	0.49
1:E:574:GLU:C	1:E:574:GLU:OE1	2.52	0.48
1:B:369:LEU:O	1:B:370:ASN:C	2.51	0.48
1:D:215:VAL:HG22	1:D:250:CYS:HB3	1.94	0.48
1:F:199:GLY:H	2:F:2001:ADP:PB	2.34	0.48
1:F:238:ARG:HH11	1:F:238:ARG:CB	2.26	0.48
1:C:359:GLY:HA3	1:C:360:PHE:CG	2.48	0.48
1:F:503:ARG:NH2	1:F:522:ARG:NH2	2.59	0.48
1:D:334:ILE:HG21	1:D:365:LEU:HD12	1.94	0.48
1:C:389:LEU:O	1:C:392:ALA:HB3	2.12	0.48
1:C:220:ALA:O	1:C:254:ILE:HA	2.13	0.48
1:A:198:PRO:HD3	1:A:302:ASN:ND2	2.28	0.48
1:A:210:ALA:HB2	1:A:251:ILE:CD1	2.42	0.48
1:B:360:PHE:HE1	1:B:364:ASP:HB3	1.79	0.48
1:D:225:PHE:N	1:D:225:PHE:CD2	2.80	0.48
1:D:175:LEU:O	1:D:249:PRO:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:181:PHE:HA	1:E:184:MET:HE2	1.95	0.48
1:E:262:ARG:HG2	1:E:275:ARG:NH2	2.08	0.48
1:F:190:LYS:HG3	1:F:190:LYS:O	2.12	0.48
1:F:348:VAL:HG11	1:F:386:MET:SD	2.53	0.48
1:C:408:SER:HB2	1:C:409:PRO:CD	2.43	0.48
1:C:416:ALA:HB2	1:C:440:ILE:HD11	1.94	0.48
1:C:447:LEU:CB	1:C:496:GLN:NE2	2.77	0.48
1:D:159:ALA:H	2:D:2001:ADP:HN62	1.61	0.48
1:D:336:ARG:C	1:D:338:HIS:N	2.61	0.48
1:B:241:PHE:CD2	1:B:285:GLU:HG2	2.48	0.48
1:E:196:GLY:O	1:E:302:ASN:OD1	2.30	0.48
1:B:454:ARG:NH2	1:B:526:TYR:HA	2.29	0.48
1:C:580:GLU:O	1:C:580:GLU:CG	2.61	0.48
1:E:594:LEU:HD12	1:E:595:PRO:O	2.13	0.48
1:D:548:ARG:NH1	1:D:548:ARG:HG2	2.28	0.48
1:D:312:LEU:HD23	1:D:312:LEU:O	2.13	0.48
1:E:483:PHE:C	1:E:485:ASP:H	2.17	0.48
1:B:212:GLU:O	1:B:214:ARG:HG3	2.13	0.48
1:E:236:ARG:HH11	1:E:236:ARG:CB	2.26	0.48
1:E:520:ALA:HA	1:E:533:ARG:CG	2.43	0.48
1:C:260:VAL:HG23	1:C:261:GLY:H	1.78	0.48
1:C:273:ASP:CG	1:C:274:GLU:H	2.17	0.48
1:A:519:TYR:HA	1:A:533:ARG:CZ	2.43	0.48
1:B:447:LEU:O	1:B:450:MET:HG3	2.12	0.48
1:E:357:THR:N	1:E:358:PRO:CD	2.76	0.48
1:F:566:ARG:O	1:F:569:LEU:HB3	2.13	0.48
1:F:548:ARG:NH1	1:F:548:ARG:HG2	2.28	0.48
1:A:233:GLY:O	1:A:236:ARG:CG	2.58	0.48
1:B:207:ARG:O	1:B:210:ALA:N	2.47	0.48
1:B:193:LEU:C	1:B:194:LEU:HD12	2.34	0.48
1:B:313:ARG:HG3	1:B:314:PRO:HG2	1.96	0.48
1:D:175:LEU:HD12	1:D:215:VAL:CG1	2.37	0.48
1:E:212:GLU:N	1:E:214:ARG:CG	2.76	0.48
1:E:147:LEU:HD23	1:E:217:PHE:CB	2.43	0.48
1:F:311:LEU:C	1:F:316:ARG:NH1	2.66	0.48
1:B:511:HIS:O	1:B:512:PRO:O	2.31	0.48
1:C:196:GLY:O	1:C:302:ASN:OD1	2.31	0.48
1:C:328:VAL:HG12	1:C:329:LYS:N	2.27	0.48
1:C:249:PRO:HB3	1:C:294:ALA:HB3	1.95	0.48
1:A:453:ARG:NH2	1:A:464:ARG:CZ	2.76	0.48
1:F:517:VAL:CG1	1:F:519:TYR:OH	2.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:ASP:O	1:D:204:HIS:HE1	1.96	0.48
1:D:344:LEU:HB2	1:D:384:ILE:O	2.13	0.48
1:B:238:ARG:HA	1:B:241:PHE:HE2	1.78	0.48
1:B:274:GLU:HA	1:B:277:GLN:HE21	1.78	0.48
1:E:397:MET:HG3	1:E:406:VAL:CG1	2.43	0.48
1:E:443:ARG:HG2	1:E:443:ARG:O	2.14	0.48
1:A:576:LEU:O	1:A:580:GLU:N	2.32	0.48
1:F:376:ALA:HB1	1:F:381:ARG:CD	2.42	0.48
1:B:394:ASP:HA	1:B:397:MET:HE3	1.94	0.48
1:B:313:ARG:CG	1:B:314:PRO:N	2.74	0.48
1:D:242:GLU:CA	1:D:245:LYS:HB3	2.42	0.48
1:A:380:GLY:C	1:F:180:ARG:NH2	2.66	0.48
1:F:183:GLU:OE1	1:F:184:MET:HB3	2.14	0.48
1:C:520:ALA:HA	1:C:533:ARG:CG	2.43	0.48
1:E:462:ARG:CG	1:E:463:LYS:N	2.76	0.48
1:D:165:LYS:CE	1:D:205:LEU:HG	2.43	0.48
1:B:225:PHE:CD2	1:B:236:ARG:NE	2.81	0.48
1:D:180:ARG:NH1	1:D:184:MET:CE	2.76	0.48
1:F:454:ARG:HH21	1:F:526:TYR:HA	1.78	0.48
1:A:554:GLN:O	1:A:557:ARG:HB3	2.14	0.48
1:A:200:VAL:HG11	1:A:323:ILE:HG13	1.96	0.48
1:A:302:ASN:HB3	1:A:443:ARG:HH12	1.78	0.48
1:B:157:ASP:HB3	1:B:337:ILE:CD1	2.44	0.48
1:B:190:LYS:O	1:B:190:LYS:HG3	2.14	0.48
1:E:147:LEU:HB3	1:E:217:PHE:O	2.12	0.48
1:F:397:MET:HA	1:F:400:PRO:HG2	1.95	0.48
1:C:445:ARG:O	1:C:447:LEU:N	2.47	0.48
1:C:228:MET:CG	1:C:236:ARG:HH22	2.27	0.48
1:A:447:LEU:HA	1:A:496:GLN:HE21	1.77	0.48
1:D:174:PHE:CZ	1:D:294:ALA:CB	2.96	0.48
1:C:373:ALA:HA	1:C:384:ILE:CD1	2.43	0.48
1:F:563:LEU:O	1:F:566:ARG:CB	2.61	0.48
1:E:414:ILE:HG22	1:E:415:THR:H	1.78	0.48
1:F:388:ASP:OD1	1:F:388:ASP:N	2.46	0.48
1:A:174:PHE:HB2	1:A:181:PHE:CE2	2.48	0.48
1:A:179:SER:C	1:A:181:PHE:N	2.65	0.48
1:A:311:LEU:CG	1:A:316:ARG:HH22	2.25	0.48
1:D:286:MET:O	1:D:289:PHE:CD1	2.67	0.48
1:E:238:ARG:O	1:E:239:ASP:C	2.51	0.48
1:F:285:GLU:C	1:F:288:GLY:H	2.16	0.48
1:F:336:ARG:HD3	1:F:336:ARG:HA	1.50	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:400:PRO:HB2	1:F:404:SER:OG	2.14	0.48
1:C:467:ASP:O	1:C:471:VAL:HG23	2.13	0.48
1:E:519:TYR:C	1:E:533:ARG:NE	2.67	0.48
1:F:476:ARG:NH1	1:F:487:THR:HG21	2.29	0.48
1:C:280:ASN:O	1:C:281:GLN:C	2.52	0.48
1:F:505:ILE:HG23	1:F:514:PHE:CD2	2.48	0.48
1:D:369:LEU:O	1:D:370:ASN:C	2.51	0.48
1:B:564:GLU:O	1:B:566:ARG:N	2.47	0.48
1:E:300:ALA:O	1:E:301:THR:CG2	2.62	0.48
1:D:228:MET:SD	1:D:232:VAL:CG1	3.01	0.48
1:A:177:ASN:HD22	1:A:180:ARG:CD	2.25	0.48
1:A:280:ASN:O	1:A:281:GLN:C	2.50	0.48
1:B:222:GLY:N	1:B:255:ASP:O	2.43	0.48
1:B:311:LEU:HD12	1:B:311:LEU:O	2.13	0.48
1:E:215:VAL:HG21	1:E:250:CYS:CB	2.43	0.48
1:F:175:LEU:O	1:F:249:PRO:HG2	2.14	0.48
1:F:159:ALA:HB1	1:F:333:GLN:HG3	1.96	0.48
1:D:410:ARG:O	1:D:413:ARG:CB	2.61	0.48
1:C:179:SER:C	1:C:181:PHE:N	2.67	0.48
1:C:274:GLU:HB3	1:C:275:ARG:H	1.43	0.48
1:D:397:MET:HA	1:D:400:PRO:HG2	1.95	0.48
1:B:468:GLN:O	1:B:471:VAL:N	2.45	0.48
1:F:470:ALA:O	1:F:474:ALA:HB2	2.14	0.48
1:D:592:GLU:O	1:D:594:LEU:CB	2.61	0.48
1:D:302:ASN:ND2	1:D:443:ARG:NH2	2.55	0.48
1:E:328:VAL:HG12	1:E:329:LYS:N	2.29	0.48
1:E:531:ASP:OD1	1:E:531:ASP:C	2.52	0.48
1:B:336:ARG:HA	1:B:336:ARG:HD3	1.47	0.48
1:E:179:SER:C	1:E:181:PHE:N	2.67	0.48
1:F:237:VAL:HG21	1:F:281:GLN:HG3	1.96	0.48
1:F:159:ALA:HA	1:F:333:GLN:HE21	1.79	0.48
1:C:410:ARG:HA	1:C:413:ARG:HB3	1.96	0.48
1:C:449:PHE:HB3	1:C:468:GLN:HE22	1.72	0.48
1:C:528:GLY:HA2	1:C:530:TYR:CE2	2.49	0.48
1:E:506:THR:CG2	1:E:543:ILE:HD13	2.44	0.48
1:A:460:TRP:HD1	1:A:464:ARG:NH1	2.10	0.48
1:B:453:ARG:HA	1:B:456:ASP:OD2	2.14	0.48
1:D:356:ARG:O	1:D:358:PRO:HD3	2.13	0.48
1:D:374:LEU:C	1:D:374:LEU:HD23	2.34	0.48
1:F:302:ASN:ND2	1:F:443:ARG:HH22	1.89	0.48
1:E:325:ALA:N	1:E:326:PRO:HD2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:ALA:HB1	1:A:558:VAL:CG2	2.40	0.48
1:C:479:GLU:OE2	1:C:488:THR:N	2.47	0.48
1:B:428:PHE:CE1	1:B:432:ALA:C	2.87	0.48
1:C:575:THR:HA	1:C:578:GLU:OE1	2.13	0.48
1:A:562:LEU:O	1:A:565:LYS:N	2.47	0.48
1:B:199:GLY:H	2:B:2001:ADP:PB	2.34	0.48
1:B:387:LYS:HG3	1:B:388:ASP:N	2.26	0.48
1:B:286:MET:HE2	1:B:315:GLY:O	2.14	0.48
1:B:314:PRO:C	1:B:316:ARG:H	2.16	0.48
1:E:169:LYS:O	1:E:172:VAL:N	2.46	0.48
1:F:238:ARG:HA	1:F:241:PHE:CE2	2.49	0.48
1:F:242:GLU:CA	1:F:245:LYS:HB3	2.43	0.48
1:F:338:HIS:CB	1:F:369:LEU:HD11	2.43	0.48
1:B:488:THR:O	1:B:490:ALA:N	2.47	0.48
1:D:154:THR:OG1	1:D:212:GLU:OE2	2.32	0.48
1:D:158:VAL:CG1	1:D:205:LEU:HD11	2.44	0.48
1:D:159:ALA:HB1	1:D:333:GLN:HG3	1.96	0.48
1:C:169:LYS:O	1:C:172:VAL:N	2.47	0.48
1:B:233:GLY:CA	1:B:236:ARG:NH2	2.59	0.48
1:B:564:GLU:C	1:B:566:ARG:N	2.64	0.48
1:C:576:LEU:O	1:C:580:GLU:N	2.35	0.48
1:A:400:PRO:HG2	1:A:405:LEU:CD1	2.44	0.47
1:B:338:HIS:CB	1:B:369:LEU:HD11	2.44	0.47
1:C:345:ALA:HB1	1:C:347:ASP:OD1	2.13	0.47
1:B:170:GLU:CB	1:C:378:ARG:NH2	2.77	0.47
1:F:154:THR:CG2	1:F:156:LYS:HB3	2.44	0.47
1:F:157:ASP:O	1:F:204:HIS:CE1	2.67	0.47
1:F:297:VAL:HG13	1:F:317:PHE:CZ	2.48	0.47
1:F:261:GLY:O	1:F:308:ASP:HB3	2.14	0.47
1:C:470:ALA:C	1:C:558:VAL:HG21	2.35	0.47
1:D:564:GLU:O	1:D:566:ARG:N	2.46	0.47
1:F:449:PHE:CE2	1:F:453:ARG:CZ	2.97	0.47
1:B:571:ARG:HH12	1:B:593:GLY:N	2.11	0.47
1:B:196:GLY:O	1:B:302:ASN:HA	2.14	0.47
1:A:594:LEU:HD12	1:A:595:PRO:O	2.13	0.47
1:A:182:HIS:CD2	1:A:182:HIS:H	2.30	0.47
1:A:207:ARG:HH21	1:A:217:PHE:HD2	1.62	0.47
1:A:357:THR:HG1	1:A:360:PHE:CB	2.27	0.47
1:A:387:LYS:CA	1:A:390:GLU:HB2	2.42	0.47
1:E:182:HIS:CD2	1:E:182:HIS:H	2.30	0.47
1:F:203:THR:OG1	2:F:2001:ADP:O1B	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:157:ASP:O	1:F:204:HIS:HE1	1.96	0.47
1:F:393:ALA:O	1:F:397:MET:HB3	2.15	0.47
1:B:517:VAL:CG2	1:B:518:ALA:N	2.76	0.47
1:C:357:THR:C	1:C:360:PHE:HD1	2.17	0.47
1:C:536:SER:O	1:C:537:GLU:C	2.51	0.47
1:D:517:VAL:CG1	1:D:519:TYR:OH	2.63	0.47
1:F:452:PRO:O	1:F:456:ASP:CG	2.53	0.47
1:A:520:ALA:HA	1:A:533:ARG:CG	2.44	0.47
1:D:199:GLY:O	1:D:361:VAL:HG22	2.13	0.47
1:D:344:LEU:CD2	1:D:346:GLU:OE1	2.61	0.47
1:B:225:PHE:HA	1:B:236:ARG:CZ	2.44	0.47
1:B:460:TRP:CD1	1:B:464:ARG:HG2	2.49	0.47
1:F:563:LEU:O	1:F:566:ARG:HB3	2.14	0.47
1:A:191:GLY:CA	1:A:297:VAL:HG22	2.44	0.47
1:D:263:LYS:HE2	1:E:228:MET:CE	2.43	0.47
1:E:210:ALA:HB2	1:E:251:ILE:CD1	2.38	0.47
1:A:462:ARG:HH12	1:A:511:HIS:H	1.62	0.47
1:A:506:THR:HA	1:A:519:TYR:HD1	1.79	0.47
1:D:388:ASP:OD1	1:D:388:ASP:N	2.42	0.47
1:B:241:PHE:HE2	1:B:285:GLU:OE2	1.90	0.47
1:D:438:VAL:CG2	1:D:439:THR:N	2.76	0.47
1:F:436:HIS:O	1:F:437:LYS:CG	2.61	0.47
1:B:162:GLU:HA	1:B:162:GLU:OE1	2.15	0.47
1:A:357:THR:N	1:A:358:PRO:CD	2.77	0.47
1:B:201:GLY:O	1:B:204:HIS:HB3	2.13	0.47
1:D:225:PHE:CD2	1:D:236:ARG:CD	2.95	0.47
1:F:290:GLU:CG	1:F:293:THR:HG23	2.29	0.47
1:C:195:VAL:HG22	1:C:301:THR:O	2.13	0.47
1:C:331:ARG:O	1:C:335:LEU:HG	2.14	0.47
1:E:519:TYR:HB3	1:E:535:TYR:HD2	1.78	0.47
1:D:157:ASP:O	1:D:204:HIS:CE1	2.67	0.47
1:F:589:ARG:CD	1:F:596:LEU:HD11	2.44	0.47
1:B:409:PRO:O	1:B:413:ARG:HD3	2.14	0.47
1:C:479:GLU:OE2	1:C:487:THR:HA	2.15	0.47
1:A:238:ARG:O	1:A:239:ASP:C	2.51	0.47
1:B:376:ALA:HB1	1:B:381:ARG:HD3	1.95	0.47
1:B:384:ILE:HG22	1:B:385:THR:N	2.30	0.47
1:D:247:HIS:O	1:D:249:PRO:O	2.33	0.47
1:E:172:VAL:CB	1:E:213:ALA:HB2	2.44	0.47
1:F:168:LEU:O	1:F:171:ILE:N	2.48	0.47
1:F:175:LEU:HD12	1:F:215:VAL:CG1	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:589:ARG:HH11	1:C:589:ARG:HB3	1.73	0.47
1:E:449:PHE:HE2	1:E:496:GLN:HE21	1.63	0.47
1:E:462:ARG:HH12	1:E:511:HIS:H	1.62	0.47
1:D:169:LYS:O	1:D:172:VAL:HG22	2.14	0.47
1:F:571:ARG:HH12	1:F:593:GLY:H	1.63	0.47
1:E:523:GLU:O	1:E:529:GLY:HA2	2.14	0.47
1:D:571:ARG:HH12	1:D:593:GLY:H	1.61	0.47
1:F:302:ASN:ND2	1:F:443:ARG:NH2	2.52	0.47
1:B:186:ALA:HB1	1:C:374:LEU:CD1	2.44	0.47
1:E:159:ALA:HB1	1:E:333:GLN:HB3	1.96	0.47
1:C:548:ARG:NH2	1:C:552:GLU:OE1	2.43	0.47
1:A:311:LEU:HD22	1:A:316:ARG:NH1	2.28	0.47
1:B:165:LYS:HZ2	1:B:168:LEU:CD2	2.27	0.47
1:D:274:GLU:HA	1:D:277:GLN:HE21	1.80	0.47
1:A:436:HIS:HB3	1:A:584:ALA:CB	2.45	0.47
1:F:169:LYS:O	1:F:172:VAL:HG22	2.15	0.47
1:F:235:ALA:O	1:F:238:ARG:NH1	2.48	0.47
1:F:262:ARG:CG	1:F:263:LYS:H	2.20	0.47
1:C:357:THR:HG1	1:C:360:PHE:CB	2.28	0.47
1:D:165:LYS:CE	1:D:205:LEU:CG	2.93	0.47
1:E:589:ARG:HH22	1:E:596:LEU:N	2.13	0.47
1:A:331:ARG:O	1:A:335:LEU:HG	2.14	0.47
1:A:329:LYS:O	1:A:332:GLU:HB3	2.15	0.47
1:B:159:ALA:CB	1:B:334:ILE:HG13	2.36	0.47
1:B:332:GLU:HB2	1:B:354:ALA:HB2	1.95	0.47
1:B:397:MET:HA	1:B:400:PRO:HG2	1.95	0.47
1:E:207:ARG:HH21	1:E:217:PHE:HD2	1.61	0.47
1:D:454:ARG:NH2	1:D:526:TYR:HA	2.29	0.47
1:E:188:ILE:CG2	1:E:189:PRO:HD2	2.45	0.47
1:E:191:GLY:CA	1:E:297:VAL:CG2	2.93	0.47
1:E:192:VAL:O	1:E:298:MET:HA	2.14	0.47
1:F:158:VAL:HG22	1:F:204:HIS:ND1	2.29	0.47
1:D:510:MET:O	1:D:512:PRO:CD	2.61	0.47
1:F:494:PHE:O	1:F:496:GLN:N	2.47	0.47
1:D:505:ILE:HD13	1:D:547:VAL:HG23	1.95	0.47
1:F:449:PHE:CZ	1:F:453:ARG:NH2	2.81	0.47
1:C:192:VAL:N	1:C:297:VAL:O	2.39	0.47
1:B:455:GLU:O	1:B:456:ASP:C	2.53	0.47
1:D:336:ARG:O	1:D:338:HIS:N	2.47	0.47
1:D:381:ARG:NH2	1:D:388:ASP:CG	2.47	0.47
1:E:382:ARG:CG	1:E:383:LYS:N	2.75	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:LYS:O	1:C:172:VAL:CG1	2.61	0.47
1:C:210:ALA:HA	1:C:251:ILE:HD11	1.96	0.47
1:F:301:THR:HG22	1:F:303:ARG:H	1.79	0.47
1:E:331:ARG:O	1:E:335:LEU:HG	2.15	0.47
1:E:408:SER:C	1:E:410:ARG:H	2.17	0.47
1:E:576:LEU:O	1:E:580:GLU:N	2.39	0.47
1:A:316:ARG:HG2	1:A:317:PHE:CD2	2.49	0.47
1:B:331:ARG:HH22	1:B:580:GLU:CD	2.14	0.47
1:B:159:ALA:HA	1:B:333:GLN:HE21	1.79	0.47
1:B:338:HIS:CE1	1:B:366:GLU:HG3	2.50	0.47
1:E:206:ALA:CB	1:E:217:PHE:HZ	2.28	0.47
1:A:348:VAL:HG12	1:A:348:VAL:O	2.14	0.47
1:F:314:PRO:C	1:F:316:ARG:H	2.18	0.47
1:C:277:GLN:HG3	1:C:278:THR:N	2.28	0.47
1:A:449:PHE:HZ	1:A:496:GLN:HG2	1.60	0.47
1:F:533:ARG:NH1	1:F:535:TYR:CD1	2.83	0.47
1:D:400:PRO:O	1:D:403:LYS:N	2.48	0.47
1:A:524:ASP:OD1	1:A:524:ASP:N	2.47	0.47
1:B:410:ARG:O	1:B:411:ASP:C	2.53	0.47
1:B:563:LEU:O	1:B:566:ARG:CB	2.62	0.47
1:E:345:ALA:HB1	1:E:347:ASP:OD1	2.14	0.47
1:D:536:SER:OG	1:E:541:LYS:HA	2.15	0.47
1:F:428:PHE:CZ	1:F:433:ASP:N	2.83	0.47
1:E:413:ARG:HA	1:E:577:LEU:HD21	1.91	0.47
1:A:225:PHE:CE1	1:A:236:ARG:HG2	2.50	0.47
1:D:175:LEU:HB3	1:D:213:ALA:HB1	1.97	0.47
1:D:237:VAL:HG21	1:D:281:GLN:HG3	1.95	0.47
1:D:238:ARG:HA	1:D:241:PHE:CE2	2.50	0.47
1:E:168:LEU:O	1:E:171:ILE:HG13	2.14	0.47
1:E:172:VAL:O	1:E:213:ALA:HB1	2.15	0.47
1:F:369:LEU:O	1:F:370:ASN:C	2.53	0.47
1:D:559:LYS:O	1:D:563:LEU:HB2	2.15	0.47
1:E:528:GLY:HA2	1:E:530:TYR:CE2	2.50	0.47
1:E:365:LEU:O	1:E:368:LEU:HB3	2.14	0.47
1:C:371:GLU:OE2	1:C:395:ARG:HD2	2.14	0.47
1:C:272:ASN:OD1	1:C:272:ASN:C	2.53	0.47
1:A:361:VAL:CG1	1:A:364:ASP:HB2	2.45	0.47
1:B:154:THR:OG1	1:B:212:GLU:OE2	2.33	0.47
1:B:194:LEU:HD23	1:B:323:ILE:CD1	2.45	0.47
1:D:308:ASP:OD1	1:D:310:ALA:N	2.46	0.47
1:F:319:ARG:NH1	1:F:319:ARG:CG	2.66	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:506:THR:CG2	1:C:543:ILE:HD13	2.45	0.47
1:C:514:PHE:HD2	1:C:514:PHE:H	1.62	0.47
1:C:189:PRO:HG3	1:C:319:ARG:NH1	2.31	0.47
1:C:228:MET:HG3	1:C:236:ARG:HH22	1.80	0.47
1:D:199:GLY:O	1:D:361:VAL:CG2	2.63	0.47
1:D:344:LEU:HA	1:D:383:LYS:CG	2.44	0.47
1:C:172:VAL:O	1:C:213:ALA:HB1	2.15	0.47
1:E:428:PHE:HE1	1:E:432:ALA:HA	1.67	0.47
1:E:410:ARG:HA	1:E:413:ARG:HB3	1.97	0.46
1:A:359:GLY:HA3	1:A:360:PHE:CG	2.50	0.46
1:E:147:LEU:C	1:E:147:LEU:HD12	2.35	0.46
1:A:596:LEU:HG	1:A:597:GLU:H	1.80	0.46
1:C:300:ALA:O	1:C:301:THR:HG22	2.15	0.46
1:C:387:LYS:C	1:C:390:GLU:HB2	2.35	0.46
1:C:387:LYS:CA	1:C:390:GLU:HB2	2.44	0.46
1:D:458:LEU:HD11	1:D:460:TRP:HB3	1.96	0.46
1:E:449:PHE:CE2	1:E:496:GLN:NE2	2.83	0.46
1:A:450:MET:O	1:A:454:ARG:HB3	2.15	0.46
1:C:147:LEU:C	1:C:147:LEU:HD12	2.36	0.46
1:B:225:PHE:CD2	1:B:225:PHE:N	2.81	0.46
1:A:292:ASP:OD2	1:B:227:GLU:OE1	2.33	0.46
1:B:336:ARG:O	1:B:339:ALA:N	2.23	0.46
1:B:157:ASP:HB3	1:B:337:ILE:CG1	2.45	0.46
1:B:263:LYS:HA	1:B:263:LYS:HD2	1.39	0.46
1:A:377:ALA:HB1	1:F:181:PHE:CD1	2.50	0.46
1:F:154:THR:HG23	1:F:156:LYS:HB3	1.96	0.46
1:C:583:THR:HG22	1:C:586:GLU:OE1	2.15	0.46
1:B:505:ILE:HG23	1:B:514:PHE:CD2	2.50	0.46
1:C:352:LEU:HD11	1:C:356:ARG:HH21	1.76	0.46
1:D:455:GLU:O	1:D:456:ASP:C	2.54	0.46
1:F:455:GLU:O	1:F:457:MET:N	2.48	0.46
1:C:182:HIS:CD2	1:C:182:HIS:H	2.32	0.46
1:C:238:ARG:O	1:C:239:ASP:C	2.52	0.46
1:C:316:ARG:O	1:C:317:PHE:C	2.54	0.46
1:D:379:GLU:OE1	1:D:381:ARG:NE	2.48	0.46
1:D:345:ALA:CB	1:D:383:LYS:HE3	2.36	0.46
1:C:210:ALA:O	1:C:214:ARG:HA	2.15	0.46
1:C:147:LEU:HD23	1:C:217:PHE:CB	2.44	0.46
1:B:469:ILE:HG23	1:B:497:ALA:HB1	1.98	0.46
1:F:410:ARG:O	1:F:411:ASP:C	2.53	0.46
1:E:348:VAL:HG12	1:E:348:VAL:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:357:THR:HG1	1:E:360:PHE:CB	2.28	0.46
1:B:506:THR:OG1	1:B:520:ALA:HB3	2.15	0.46
1:A:171:ILE:HG22	1:A:188:ILE:CG2	2.44	0.46
1:A:249:PRO:HB3	1:A:294:ALA:HB3	1.96	0.46
1:B:336:ARG:O	1:B:338:HIS:N	2.48	0.46
1:D:311:LEU:HA	1:D:316:ARG:CZ	2.45	0.46
1:E:312:LEU:HD21	1:E:320:GLN:OE1	2.16	0.46
1:C:570:GLU:O	1:C:571:ARG:C	2.54	0.46
1:C:361:VAL:O	1:C:365:LEU:HG	2.16	0.46
1:D:517:VAL:CG2	1:D:518:ALA:N	2.78	0.46
1:F:452:PRO:O	1:F:456:ASP:N	2.48	0.46
1:F:503:ARG:HG2	1:F:508:TRP:CZ2	2.49	0.46
1:D:200:VAL:HG12	1:D:325:ALA:HB2	1.98	0.46
1:D:352:LEU:O	1:D:355:LYS:HB2	2.16	0.46
1:C:168:LEU:O	1:C:171:ILE:HG13	2.15	0.46
1:C:210:ALA:HB2	1:C:251:ILE:CD1	2.43	0.46
1:F:572:VAL:HG11	1:F:587:PHE:HE1	1.80	0.46
1:B:563:LEU:O	1:B:566:ARG:HB3	2.15	0.46
1:D:572:VAL:HG11	1:D:587:PHE:HE1	1.81	0.46
1:E:436:HIS:HB3	1:E:584:ALA:CB	2.45	0.46
1:A:282:LEU:O	1:A:286:MET:HG2	2.15	0.46
1:B:297:VAL:CG1	1:B:317:PHE:CE1	2.98	0.46
1:E:249:PRO:HB3	1:E:294:ALA:HB3	1.98	0.46
1:A:378:ARG:HH12	1:F:170:GLU:HB2	1.80	0.46
1:D:411:ASP:O	1:D:414:ILE:HG13	2.16	0.46
1:C:282:LEU:HG	1:C:283:LEU:HD12	1.97	0.46
1:A:507:GLU:HB2	1:A:520:ALA:HB3	1.98	0.46
1:D:159:ALA:HA	1:D:333:GLN:HE21	1.80	0.46
1:B:469:ILE:HG22	1:B:473:LEU:HD12	1.96	0.46
1:F:467:ASP:O	1:F:471:VAL:HG13	2.16	0.46
1:D:571:ARG:HH12	1:D:593:GLY:N	2.13	0.46
1:A:212:GLU:C	1:A:214:ARG:HB2	2.34	0.46
1:A:253:PHE:HA	1:A:298:MET:O	2.16	0.46
1:B:384:ILE:CG2	1:B:385:THR:N	2.79	0.46
1:E:155:PHE:CZ	1:E:209:VAL:HG22	2.49	0.46
1:F:204:HIS:CD2	2:F:2001:ADP:H2'	2.50	0.46
1:F:256:GLU:CG	1:F:256:GLU:O	2.62	0.46
1:C:361:VAL:CG1	1:C:364:ASP:HB2	2.45	0.46
1:D:476:ARG:NH1	1:D:487:THR:HG21	2.30	0.46
1:C:190:LYS:CD	1:C:289:PHE:CE1	2.87	0.46
1:A:551:ILE:O	1:A:552:GLU:C	2.52	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:361:VAL:CG1	1:E:364:ASP:HB2	2.46	0.46
1:A:373:ALA:HA	1:A:384:ILE:CD1	2.46	0.46
1:D:399:LEU:O	1:D:402:LYS:HB3	2.16	0.46
1:A:191:GLY:CA	1:A:297:VAL:CG2	2.93	0.46
1:A:198:PRO:HD3	1:A:302:ASN:HD21	1.81	0.46
1:D:242:GLU:HA	1:D:245:LYS:CB	2.43	0.46
1:D:241:PHE:CZ	1:D:285:GLU:OE2	2.67	0.46
1:D:454:ARG:HH21	1:D:526:TYR:HA	1.80	0.46
1:E:225:PHE:CE1	1:E:236:ARG:HG2	2.51	0.46
1:F:174:PHE:CD2	1:F:174:PHE:C	2.89	0.46
1:F:242:GLU:HA	1:F:245:LYS:CB	2.45	0.46
1:C:407:LEU:HA	1:C:411:ASP:HB2	1.97	0.46
1:A:305:ASP:C	1:A:307:LEU:N	2.68	0.46
1:A:449:PHE:HE2	1:A:496:GLN:HE21	1.60	0.46
1:B:494:PHE:O	1:B:496:GLN:N	2.48	0.46
1:D:201:GLY:O	1:D:204:HIS:HB3	2.16	0.46
1:D:329:LYS:CG	1:D:330:GLY:N	2.78	0.46
1:C:218:ILE:H	1:C:218:ILE:HG12	1.64	0.46
1:B:228:MET:SD	1:B:232:VAL:CG1	3.04	0.46
1:F:438:VAL:CG2	1:F:439:THR:N	2.79	0.46
1:A:481:ILE:HG22	1:A:482:VAL:N	2.31	0.46
1:F:454:ARG:HA	1:F:454:ARG:HH11	1.80	0.46
1:F:374:LEU:HD23	1:F:374:LEU:C	2.36	0.46
1:A:408:SER:HB2	1:A:409:PRO:CD	2.41	0.46
1:A:215:VAL:HG22	1:A:216:PRO:N	2.30	0.46
1:B:328:VAL:HG22	1:B:355:LYS:CE	2.38	0.46
1:B:336:ARG:O	1:B:337:ILE:C	2.54	0.46
1:B:400:PRO:O	1:B:403:LYS:N	2.49	0.46
1:E:316:ARG:O	1:E:317:PHE:C	2.51	0.46
1:C:464:ARG:CG	1:C:464:ARG:HH11	2.29	0.46
1:C:520:ALA:HA	1:C:533:ARG:HG2	1.96	0.46
1:D:455:GLU:HG2	1:D:455:GLU:O	2.16	0.46
1:D:521:VAL:HG23	1:D:532:VAL:CG1	2.42	0.46
1:C:308:ASP:OD1	1:C:310:ALA:CB	2.64	0.46
1:A:503:ARG:CG	1:A:508:TRP:CE3	2.99	0.46
1:D:164:ALA:C	1:D:168:LEU:HD13	2.35	0.46
1:D:202:LYS:N	2:D:2001:ADP:O1A	2.49	0.46
1:E:311:LEU:HD23	1:E:311:LEU:HA	1.68	0.46
1:B:149:GLU:O	1:B:150:ALA:C	2.54	0.46
1:A:410:ARG:CG	1:A:411:ASP:N	2.77	0.46
1:A:312:LEU:HD21	1:A:320:GLN:OE1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:LYS:CG	1:B:330:GLY:N	2.78	0.46
1:C:340:ARG:C	1:C:342:LYS:N	2.59	0.46
1:B:314:PRO:HA	1:B:318:ASP:OD2	2.16	0.46
1:D:192:VAL:C	1:D:317:PHE:CE2	2.89	0.46
1:D:286:MET:HB2	1:D:286:MET:HE3	1.82	0.46
1:E:238:ARG:O	1:E:241:PHE:N	2.48	0.46
1:E:280:ASN:O	1:E:281:GLN:C	2.54	0.46
1:F:199:GLY:O	1:F:361:VAL:HG22	2.14	0.46
1:F:238:ARG:HH12	1:F:239:ASP:H	1.43	0.46
1:E:469:ILE:HD11	1:E:500:LEU:HB3	1.98	0.46
1:F:488:THR:O	1:F:490:ALA:N	2.48	0.46
1:F:517:VAL:HG11	1:F:519:TYR:CZ	2.51	0.46
1:D:207:ARG:O	1:D:210:ALA:N	2.49	0.46
1:F:571:ARG:O	1:F:575:THR:HG23	2.16	0.46
1:A:523:GLU:O	1:A:529:GLY:HA2	2.16	0.46
1:D:585:GLU:O	1:D:587:PHE:N	2.49	0.46
1:B:443:ARG:O	1:B:445:ARG:N	2.49	0.46
1:A:272:ASN:C	1:A:272:ASN:OD1	2.54	0.46
1:A:159:ALA:HB1	1:A:333:GLN:HB3	1.97	0.46
1:B:389:LEU:O	1:B:390:GLU:C	2.54	0.46
1:D:286:MET:O	1:D:289:PHE:CG	2.69	0.46
1:D:297:VAL:HG13	1:D:317:PHE:CZ	2.51	0.46
1:E:207:ARG:CB	1:E:207:ARG:CZ	2.91	0.46
1:C:462:ARG:HG3	1:C:466:LEU:HD11	1.97	0.46
1:D:469:ILE:HG23	1:D:497:ALA:HB1	1.98	0.46
1:D:501:ALA:CB	1:D:550:LEU:HD23	2.45	0.46
1:E:520:ALA:HA	1:E:533:ARG:HG2	1.96	0.46
1:C:262:ARG:HG2	1:C:275:ARG:NH2	2.09	0.46
1:C:192:VAL:O	1:C:298:MET:HA	2.16	0.46
1:A:503:ARG:HG2	1:A:508:TRP:CE3	2.51	0.46
1:D:165:LYS:NZ	1:D:168:LEU:CD2	2.79	0.46
1:B:242:GLU:HA	1:B:245:LYS:CB	2.42	0.46
1:E:370:ASN:C	1:E:370:ASN:OD1	2.55	0.46
1:B:454:ARG:HH11	1:B:454:ARG:HA	1.81	0.46
1:F:537:GLU:O	1:F:540:ALA:HB3	2.16	0.46
1:F:538:GLU:O	1:F:541:LYS:N	2.49	0.46
1:E:441:VAL:O	1:E:441:VAL:CG1	2.61	0.46
1:D:297:VAL:HG13	1:D:317:PHE:HZ	1.81	0.46
1:D:314:PRO:HA	1:D:318:ASP:OD2	2.16	0.46
1:E:173:GLU:CA	1:E:176:LYS:HG3	2.36	0.46
1:F:329:LYS:CG	1:F:330:GLY:N	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:ASP:C	1:C:307:LEU:N	2.69	0.46
1:C:356:ARG:C	1:C:358:PRO:HD2	2.37	0.46
1:F:447:LEU:O	1:F:449:PHE:N	2.49	0.46
1:B:228:MET:HE3	1:B:236:ARG:HD3	1.98	0.46
1:B:301:THR:HG23	1:B:303:ARG:H	1.81	0.46
1:A:410:ARG:O	1:A:411:ASP:C	2.54	0.45
1:A:155:PHE:HZ	1:A:209:VAL:CG2	2.29	0.45
1:A:174:PHE:O	1:A:177:ASN:C	2.55	0.45
1:A:206:ALA:CB	1:A:217:PHE:HZ	2.29	0.45
1:A:237:VAL:O	1:A:240:LEU:HB3	2.16	0.45
1:A:192:VAL:N	1:A:297:VAL:O	2.43	0.45
1:B:352:LEU:O	1:B:353:LEU:C	2.53	0.45
1:E:168:LEU:C	1:E:168:LEU:HD12	2.36	0.45
1:F:238:ARG:HA	1:F:241:PHE:HE2	1.81	0.45
1:C:450:MET:HE2	1:C:451:MET:SD	2.56	0.45
1:C:503:ARG:CD	1:C:508:TRP:CE2	2.95	0.45
1:C:459:HIS:CE1	1:D:411:ASP:HB3	2.51	0.45
1:D:476:ARG:CZ	1:D:487:THR:HG21	2.46	0.45
1:E:462:ARG:HG3	1:E:466:LEU:HD11	1.98	0.45
1:E:506:THR:HA	1:E:519:TYR:HD1	1.80	0.45
1:E:534:GLN:N	1:E:534:GLN:CD	2.70	0.45
1:C:228:MET:HG3	1:C:236:ARG:NH2	2.31	0.45
1:A:520:ALA:HA	1:A:533:ARG:HG2	1.98	0.45
1:D:428:PHE:HE1	1:D:432:ALA:C	2.19	0.45
1:D:537:GLU:O	1:D:540:ALA:HB3	2.16	0.45
1:F:384:ILE:HG22	1:F:385:THR:N	2.30	0.45
1:A:328:VAL:HG12	1:A:329:LYS:N	2.30	0.45
1:E:147:LEU:O	1:E:216:PRO:HB3	2.17	0.45
1:E:274:GLU:O	1:E:277:GLN:CB	2.54	0.45
1:F:313:ARG:CG	1:F:314:PRO:N	2.76	0.45
1:F:329:LYS:O	1:F:332:GLU:HB3	2.16	0.45
1:B:523:GLU:OE2	1:C:264:ARG:NH2	2.50	0.45
1:D:410:ARG:O	1:D:411:ASP:C	2.54	0.45
1:D:354:ALA:O	1:D:357:THR:HG23	2.15	0.45
1:B:175:LEU:O	1:B:249:PRO:HG2	2.15	0.45
1:F:571:ARG:HH12	1:F:593:GLY:N	2.14	0.45
1:F:428:PHE:CD1	1:F:432:ALA:HB3	2.50	0.45
1:E:408:SER:HB2	1:E:409:PRO:CD	2.44	0.45
1:E:410:ARG:CG	1:E:411:ASP:N	2.77	0.45
1:A:182:HIS:HD1	1:A:291:LYS:HB2	1.81	0.45
1:A:274:GLU:C	1:A:277:GLN:HB3	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:ARG:HG2	1:A:443:ARG:O	2.16	0.45
1:F:274:GLU:HA	1:F:277:GLN:HE21	1.80	0.45
1:F:357:THR:HB	1:F:360:PHE:CD2	2.52	0.45
1:C:300:ALA:O	1:C:301:THR:CG2	2.64	0.45
1:E:469:ILE:HG13	1:E:500:LEU:HD23	1.97	0.45
1:E:552:GLU:O	1:E:555:TYR:HB3	2.16	0.45
1:A:503:ARG:HG3	1:A:504:MET:N	2.28	0.45
1:A:506:THR:CG2	1:A:543:ILE:HD13	2.46	0.45
1:F:511:HIS:O	1:F:512:PRO:O	2.34	0.45
1:D:336:ARG:O	1:D:337:ILE:C	2.53	0.45
1:D:379:GLU:OE1	1:D:381:ARG:CD	2.65	0.45
1:B:470:ALA:O	1:B:474:ALA:HB2	2.16	0.45
1:E:359:GLY:HA3	1:E:360:PHE:CG	2.51	0.45
1:C:372:ALA:CB	1:C:389:LEU:HD23	2.47	0.45
1:E:517:VAL:HG23	1:F:498:THR:OG1	2.16	0.45
1:F:384:ILE:CG2	1:F:385:THR:N	2.79	0.45
1:A:277:GLN:HG3	1:A:278:THR:N	2.32	0.45
1:A:361:VAL:O	1:A:365:LEU:HG	2.17	0.45
1:D:261:GLY:O	1:D:308:ASP:HB3	2.16	0.45
1:D:527:LEU:HD11	1:E:226:VAL:HG12	1.97	0.45
1:E:308:ASP:OD1	1:E:310:ALA:CB	2.65	0.45
1:F:165:LYS:NZ	1:F:205:LEU:CB	2.68	0.45
1:F:165:LYS:O	1:F:167:GLU:N	2.50	0.45
1:C:438:VAL:HG22	1:C:582:LEU:HB2	1.99	0.45
1:C:198:PRO:HD3	1:C:302:ASN:HD21	1.81	0.45
1:D:449:PHE:CZ	1:D:496:GLN:OE1	2.69	0.45
1:C:222:GLY:O	1:C:225:PHE:HB2	2.17	0.45
1:B:589:ARG:CZ	1:B:596:LEU:HD22	2.46	0.45
1:E:487:THR:OG1	1:E:488:THR:N	2.49	0.45
1:F:162:GLU:OE1	1:F:162:GLU:HA	2.16	0.45
1:F:381:ARG:NH2	1:F:388:ASP:OD2	2.50	0.45
1:A:218:ILE:H	1:A:218:ILE:HG12	1.65	0.45
1:B:184:MET:O	1:C:342:LYS:CD	2.63	0.45
1:B:329:LYS:O	1:B:332:GLU:HB3	2.16	0.45
1:C:381:ARG:NH1	1:C:381:ARG:CG	2.79	0.45
1:E:189:PRO:HD3	1:E:319:ARG:HH11	1.82	0.45
1:B:503:ARG:HG2	1:B:508:TRP:CZ2	2.51	0.45
1:C:519:TYR:CA	1:C:533:ARG:CZ	2.95	0.45
1:C:459:HIS:HE1	1:D:411:ASP:CB	2.29	0.45
1:A:449:PHE:HD2	1:A:449:PHE:N	2.11	0.45
1:B:241:PHE:CZ	1:B:285:GLU:OE2	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:ARG:O	1:B:413:ARG:CB	2.65	0.45
1:A:528:GLY:HA2	1:A:530:TYR:CE2	2.52	0.45
1:A:286:MET:CE	1:A:297:VAL:HG21	2.46	0.45
1:C:345:ALA:HA	1:C:383:LYS:HD3	1.97	0.45
1:A:574:GLU:OE1	1:A:575:THR:N	2.49	0.45
1:F:247:HIS:O	1:F:249:PRO:O	2.34	0.45
1:F:278:THR:O	1:F:281:GLN:HB3	2.16	0.45
1:F:352:LEU:HD12	1:F:353:LEU:N	2.30	0.45
1:F:449:PHE:HZ	1:F:496:GLN:OE1	2.00	0.45
1:F:523:GLU:O	1:F:530:TYR:N	2.43	0.45
1:D:350:LEU:O	1:D:353:LEU:N	2.50	0.45
1:B:175:LEU:O	1:B:249:PRO:HB2	2.17	0.45
1:F:582:LEU:CD2	1:F:590:VAL:HG21	2.42	0.45
1:F:460:TRP:CD1	1:F:464:ARG:HG2	2.52	0.45
1:D:583:THR:O	1:D:584:ALA:C	2.55	0.45
1:E:200:VAL:N	2:E:1001:ADP:O1A	2.50	0.45
1:B:454:ARG:HH21	1:B:526:TYR:HA	1.81	0.45
1:F:162:GLU:OE1	1:F:162:GLU:CA	2.64	0.45
1:A:196:GLY:C	1:A:202:LYS:HZ1	2.18	0.45
1:A:212:GLU:O	1:A:214:ARG:CB	2.65	0.45
1:A:387:LYS:C	1:A:390:GLU:HB2	2.37	0.45
1:C:346:GLU:OE1	1:C:347:ASP:N	2.45	0.45
1:D:175:LEU:O	1:D:249:PRO:HB2	2.17	0.45
1:E:286:MET:CG	1:E:316:ARG:HG2	2.45	0.45
1:A:381:ARG:CG	1:A:381:ARG:NH1	2.80	0.45
1:F:352:LEU:HD11	1:F:386:MET:CE	2.40	0.45
1:B:510:MET:O	1:B:512:PRO:CD	2.63	0.45
1:C:361:VAL:HG12	1:C:364:ASP:HB2	1.99	0.45
1:D:503:ARG:NH2	1:D:522:ARG:CZ	2.80	0.45
1:E:453:ARG:NH2	1:E:464:ARG:CZ	2.79	0.45
1:E:470:ALA:HB1	1:E:558:VAL:CG2	2.38	0.45
1:C:236:ARG:HG2	1:C:236:ARG:NH1	2.12	0.45
1:C:274:GLU:C	1:C:277:GLN:HB3	2.34	0.45
1:A:464:ARG:NH1	1:A:464:ARG:HG2	2.32	0.45
1:A:519:TYR:C	1:A:533:ARG:NE	2.68	0.45
1:D:336:ARG:HA	1:D:336:ARG:HD3	1.51	0.45
1:D:393:ALA:O	1:D:397:MET:HB3	2.17	0.45
1:D:301:THR:HG23	1:D:303:ARG:H	1.80	0.45
1:D:302:ASN:ND2	1:D:443:ARG:HH22	1.91	0.45
1:D:443:ARG:O	1:D:445:ARG:N	2.50	0.45
1:B:342:LYS:HA	1:B:342:LYS:HD2	1.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:PHE:C	1:A:485:ASP:H	2.20	0.45
1:A:236:ARG:CB	1:A:236:ARG:HH11	2.29	0.45
1:A:361:VAL:HG12	1:A:364:ASP:HB2	1.99	0.45
1:F:202:LYS:CD	2:F:2001:ADP:O2B	2.65	0.45
1:F:255:ASP:OD1	1:F:256:GLU:N	2.49	0.45
1:C:462:ARG:HH12	1:C:511:HIS:H	1.64	0.45
1:E:447:LEU:HB2	1:E:496:GLN:HE22	1.82	0.45
1:A:519:TYR:HB3	1:A:535:TYR:HD2	1.82	0.45
1:E:334:ILE:HD11	2:E:1001:ADP:N6	2.32	0.45
1:F:428:PHE:CE1	1:F:433:ASP:N	2.84	0.45
1:E:424:LEU:HD22	1:E:569:LEU:HA	1.99	0.45
1:B:312:LEU:O	1:B:312:LEU:HD23	2.16	0.45
1:E:407:LEU:H	1:E:407:LEU:HG	1.57	0.45
1:A:168:LEU:C	1:A:168:LEU:HD12	2.38	0.45
1:A:352:LEU:HD11	1:A:356:ARG:HH21	1.74	0.45
1:B:286:MET:HE3	1:B:286:MET:HB2	1.87	0.45
1:C:159:ALA:HB1	1:C:333:GLN:HB3	1.99	0.45
1:B:536:SER:HB2	1:C:537:GLU:OE2	2.17	0.45
1:E:548:ARG:NH2	1:E:552:GLU:OE1	2.46	0.45
1:C:233:GLY:O	1:C:236:ARG:CG	2.62	0.45
1:C:236:ARG:CG	1:C:237:VAL:H	2.18	0.45
1:C:238:ARG:O	1:C:241:PHE:N	2.50	0.45
1:C:191:GLY:CA	1:C:297:VAL:CG2	2.94	0.45
1:D:157:ASP:O	1:D:158:VAL:HG23	2.16	0.45
1:B:438:VAL:CG2	1:B:439:THR:N	2.80	0.45
1:E:372:ALA:CB	1:E:389:LEU:HD23	2.47	0.45
1:E:305:ASP:C	1:E:307:LEU:N	2.70	0.45
1:A:204:HIS:CD2	2:A:1001:ADP:C2	3.04	0.45
1:A:442:PRO:HG2	1:A:443:ARG:H	1.81	0.45
1:B:153:VAL:O	1:B:154:THR:HB	2.17	0.45
1:B:344:LEU:HA	1:B:383:LYS:CG	2.46	0.45
1:E:286:MET:CG	1:E:316:ARG:CG	2.94	0.45
1:F:201:GLY:O	1:F:204:HIS:HB3	2.17	0.45
1:F:313:ARG:HG3	1:F:314:PRO:HG2	1.98	0.45
1:A:527:LEU:O	1:A:527:LEU:HD12	2.16	0.45
1:B:517:VAL:HG13	1:B:519:TYR:CZ	2.52	0.45
1:C:397:MET:HG3	1:C:406:VAL:CG1	2.46	0.45
1:C:451:MET:HB2	1:C:452:PRO:CD	2.47	0.45
1:D:505:ILE:HG23	1:D:514:PHE:CD2	2.52	0.45
1:C:271:GLY:O	1:C:275:ARG:NE	2.50	0.45
1:F:508:TRP:O	1:F:510:MET:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:PRO:HD2	1:D:200:VAL:CG1	2.45	0.45
1:F:468:GLN:O	1:F:471:VAL:N	2.49	0.45
1:E:586:GLU:HG2	1:E:587:PHE:N	2.30	0.44
1:E:589:ARG:HB3	1:E:589:ARG:HH11	1.74	0.44
1:B:207:ARG:CB	1:B:217:PHE:CZ	2.96	0.44
1:B:354:ALA:O	1:B:357:THR:HG23	2.17	0.44
1:D:175:LEU:O	1:D:249:PRO:CG	2.65	0.44
1:D:279:LEU:O	1:D:283:LEU:HB2	2.17	0.44
1:E:228:MET:HG3	1:E:236:ARG:NH2	2.31	0.44
1:E:237:VAL:HG11	1:E:281:GLN:CB	2.27	0.44
1:E:236:ARG:O	1:E:239:ASP:N	2.51	0.44
1:E:225:PHE:HZ	1:E:278:THR:HB	1.66	0.44
1:A:582:LEU:CD2	1:A:587:PHE:HA	2.34	0.44
1:F:200:VAL:HA	1:F:361:VAL:HG23	1.99	0.44
1:F:158:VAL:HG11	1:F:205:LEU:HD11	1.98	0.44
1:F:314:PRO:HA	1:F:318:ASP:OD2	2.16	0.44
1:F:338:HIS:HB3	1:F:369:LEU:HD12	1.99	0.44
1:F:344:LEU:HA	1:F:383:LYS:CG	2.47	0.44
1:C:337:ILE:CD1	1:C:338:HIS:CD2	3.00	0.44
1:E:263:LYS:CG	1:E:264:ARG:H	2.28	0.44
1:A:447:LEU:HB2	1:A:496:GLN:HE22	1.80	0.44
1:A:465:LEU:O	1:A:469:ILE:HG13	2.17	0.44
1:D:332:GLU:HB2	1:D:354:ALA:HB2	1.98	0.44
1:E:153:VAL:HG13	1:E:157:ASP:CB	2.47	0.44
1:D:307:LEU:CD1	1:D:307:LEU:H	2.31	0.44
1:B:150:ALA:HA	1:B:151:PRO:HD2	1.84	0.44
1:F:376:ALA:C	1:F:381:ARG:CB	2.84	0.44
1:A:280:ASN:HA	1:A:283:LEU:HB2	1.99	0.44
1:A:327:ASP:OD1	1:A:329:LYS:N	2.50	0.44
1:D:193:LEU:HB3	1:D:317:PHE:HD2	1.82	0.44
1:D:525:THR:HG22	1:D:526:TYR:CD2	2.52	0.44
1:E:211:GLY:C	1:E:214:ARG:HG2	2.37	0.44
1:E:233:GLY:O	1:E:236:ARG:CG	2.61	0.44
1:E:277:GLN:HG3	1:E:278:THR:N	2.31	0.44
1:E:192:VAL:N	1:E:297:VAL:O	2.38	0.44
1:A:438:VAL:HG22	1:A:582:LEU:HB2	2.00	0.44
1:A:382:ARG:CG	1:A:383:LYS:H	2.29	0.44
1:F:238:ARG:HH11	1:F:238:ARG:CG	2.30	0.44
1:E:454:ARG:HG3	1:E:455:GLU:N	2.32	0.44
1:C:312:LEU:HD21	1:C:320:GLN:OE1	2.16	0.44
1:D:338:HIS:CB	1:D:369:LEU:HD11	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:LEU:HB3	1:C:217:PHE:O	2.17	0.44
1:F:583:THR:O	1:F:584:ALA:C	2.56	0.44
1:B:566:ARG:O	1:B:569:LEU:HB3	2.17	0.44
1:C:370:ASN:C	1:C:370:ASN:OD1	2.55	0.44
1:E:387:LYS:CA	1:E:390:GLU:HB2	2.44	0.44
1:A:467:ASP:HA	1:A:557:ARG:NH2	2.32	0.44
1:F:149:GLU:O	1:F:150:ALA:C	2.56	0.44
1:A:220:ALA:O	1:A:254:ILE:HA	2.16	0.44
1:E:587:PHE:CD2	1:E:588:GLN:N	2.85	0.44
1:A:147:LEU:HD23	1:A:217:PHE:CB	2.47	0.44
1:B:343:PRO:HG2	1:B:383:LYS:CA	2.40	0.44
1:F:225:PHE:CD2	1:F:236:ARG:CD	2.99	0.44
1:F:308:ASP:OD1	1:F:310:ALA:N	2.45	0.44
1:A:263:LYS:CG	1:A:264:ARG:H	2.27	0.44
1:D:452:PRO:O	1:D:456:ASP:CA	2.65	0.44
1:E:266:SER:C	1:E:268:VAL:N	2.71	0.44
1:A:305:ASP:OD2	1:A:447:LEU:HD13	2.16	0.44
1:D:170:GLU:HG2	1:D:171:ILE:N	2.32	0.44
1:D:428:PHE:CD1	1:D:432:ALA:HB3	2.52	0.44
1:D:428:PHE:CZ	1:D:433:ASP:N	2.85	0.44
1:F:312:LEU:HD23	1:F:312:LEU:O	2.17	0.44
1:A:182:HIS:CB	1:A:291:LYS:HD2	2.20	0.44
1:A:291:LYS:O	1:A:292:ASP:C	2.56	0.44
1:B:353:LEU:O	1:B:357:THR:CG2	2.65	0.44
1:B:361:VAL:HG13	1:B:364:ASP:CG	2.38	0.44
1:D:454:ARG:HA	1:D:454:ARG:HH11	1.83	0.44
1:E:273:ASP:CG	1:E:274:GLU:H	2.20	0.44
1:F:382:ARG:HD2	1:F:382:ARG:HA	1.08	0.44
1:C:454:ARG:HB2	1:C:460:TRP:HH2	1.82	0.44
1:C:503:ARG:HG2	1:C:508:TRP:CE3	2.51	0.44
1:C:533:ARG:HA	1:C:533:ARG:HD2	1.91	0.44
1:D:533:ARG:NH1	1:D:533:ARG:HG3	2.21	0.44
1:E:471:VAL:O	1:E:474:ALA:HB3	2.17	0.44
1:E:519:TYR:O	1:E:533:ARG:HG2	2.17	0.44
1:A:451:MET:HB2	1:A:452:PRO:CD	2.47	0.44
1:F:503:ARG:CG	1:F:508:TRP:CZ2	3.00	0.44
1:D:168:LEU:O	1:D:171:ILE:N	2.51	0.44
1:B:231:GLY:H	1:B:277:GLN:HE22	1.65	0.44
1:E:198:PRO:HD3	1:E:302:ASN:HD21	1.82	0.44
1:E:387:LYS:C	1:E:390:GLU:HB2	2.38	0.44
1:F:525:THR:CG2	1:F:526:TYR:CD2	2.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:548:ARG:NH1	1:B:548:ARG:HG2	2.32	0.44
1:A:215:VAL:CG2	1:A:216:PRO:CD	2.93	0.44
1:A:318:ASP:O	1:A:319:ARG:HG3	2.18	0.44
1:D:215:VAL:O	1:D:216:PRO:C	2.56	0.44
1:E:225:PHE:CE1	1:E:233:GLY:HA3	2.48	0.44
1:F:154:THR:OG1	1:F:212:GLU:OE2	2.35	0.44
1:F:231:GLY:H	1:F:277:GLN:HE22	1.65	0.44
1:A:266:SER:C	1:A:268:VAL:N	2.70	0.44
1:B:538:GLU:O	1:B:541:LYS:N	2.50	0.44
1:C:327:ASP:OD1	1:C:327:ASP:C	2.56	0.44
1:C:509:GLY:O	1:D:476:ARG:NH2	2.36	0.44
1:C:519:TYR:C	1:C:533:ARG:CZ	2.86	0.44
1:E:464:ARG:O	1:E:465:LEU:C	2.56	0.44
1:F:476:ARG:CZ	1:F:487:THR:HG21	2.47	0.44
1:A:548:ARG:NH1	1:F:513:GLU:O	2.50	0.44
1:D:353:LEU:O	1:D:357:THR:CG2	2.65	0.44
1:C:168:LEU:C	1:C:168:LEU:HD12	2.38	0.44
1:B:238:ARG:NH1	1:B:239:ASP:CA	2.67	0.44
1:F:147:LEU:HD13	1:F:149:GLU:OE1	2.18	0.44
1:E:588:GLN:O	1:E:591:VAL:CB	2.55	0.44
1:F:373:ALA:CA	1:F:384:ILE:HD11	2.45	0.44
1:A:236:ARG:O	1:A:239:ASP:N	2.51	0.44
1:C:382:ARG:HH11	1:C:383:LYS:HB2	1.83	0.44
1:D:257:ILE:HG22	1:D:261:GLY:H	1.83	0.44
1:D:260:VAL:O	1:D:262:ARG:N	2.46	0.44
1:D:231:GLY:H	1:D:277:GLN:HE22	1.65	0.44
1:D:526:TYR:O	1:D:528:GLY:CA	2.65	0.44
1:E:171:ILE:HD12	1:E:172:VAL:H	1.81	0.44
1:A:370:ASN:OD1	1:A:370:ASN:C	2.55	0.44
1:C:586:GLU:HG2	1:C:587:PHE:N	2.32	0.44
1:C:465:LEU:CD2	1:C:508:TRP:CZ3	2.99	0.44
1:E:511:HIS:O	1:E:512:PRO:O	2.36	0.44
1:A:503:ARG:CD	1:A:508:TRP:CE2	2.98	0.44
1:C:206:ALA:CB	1:C:217:PHE:HZ	2.31	0.44
1:B:572:VAL:O	1:B:576:LEU:HB2	2.18	0.44
1:B:592:GLU:O	1:B:594:LEU:HB3	2.18	0.44
1:E:352:LEU:HD11	1:E:356:ARG:HH21	1.80	0.44
1:E:399:LEU:N	1:E:400:PRO:CD	2.81	0.44
1:F:526:TYR:O	1:F:528:GLY:CA	2.66	0.44
1:E:481:ILE:HG22	1:E:482:VAL:N	2.31	0.44
1:E:413:ARG:O	1:E:577:LEU:HD21	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:ARG:HA	1:A:413:ARG:HB3	2.00	0.44
1:A:237:VAL:HG13	1:A:238:ARG:N	2.32	0.44
1:A:378:ARG:HG2	1:A:379:GLU:N	2.22	0.44
1:F:153:VAL:O	1:F:154:THR:HB	2.17	0.44
1:F:209:VAL:CG1	1:F:210:ALA:H	2.21	0.44
1:C:203:THR:HG23	2:C:1001:ADP:O2A	2.18	0.44
1:C:400:PRO:HG2	1:C:405:LEU:CD1	2.46	0.44
1:E:551:ILE:O	1:E:552:GLU:C	2.56	0.44
1:D:374:LEU:HD23	1:D:375:LEU:N	2.33	0.44
1:B:175:LEU:O	1:B:249:PRO:CG	2.66	0.44
1:B:238:ARG:N	1:B:281:GLN:HE21	2.16	0.44
1:D:585:GLU:O	1:D:586:GLU:C	2.56	0.44
1:D:301:THR:HG22	1:D:303:ARG:H	1.82	0.44
1:F:525:THR:HG22	1:F:526:TYR:N	2.33	0.44
1:D:506:THR:OG1	1:D:520:ALA:HB3	2.17	0.44
1:B:161:ALA:O	1:B:164:ALA:HB3	2.18	0.44
1:B:355:LYS:HZ1	1:B:578:GLU:HG3	1.83	0.44
1:B:355:LYS:NZ	1:B:578:GLU:O	2.51	0.44
1:F:178:PRO:O	1:F:182:HIS:CE1	2.71	0.44
1:A:381:ARG:C	1:F:180:ARG:HH22	2.18	0.44
1:F:355:LYS:NZ	1:F:578:GLU:O	2.51	0.44
1:C:266:SER:C	1:C:268:VAL:N	2.70	0.44
1:B:476:ARG:O	1:B:479:GLU:N	2.51	0.44
1:C:147:LEU:HD21	1:C:151:PRO:CG	2.46	0.44
1:C:218:ILE:CD1	1:C:250:CYS:SG	2.91	0.44
1:F:589:ARG:CZ	1:F:596:LEU:HD11	2.45	0.44
1:B:585:GLU:C	1:B:587:PHE:N	2.71	0.44
1:C:290:GLU:CD	1:D:226:VAL:HG11	2.37	0.44
1:B:162:GLU:OE1	1:B:162:GLU:CA	2.66	0.44
1:E:272:ASN:OD1	1:E:272:ASN:C	2.55	0.44
1:A:192:VAL:O	1:A:298:MET:HA	2.18	0.44
1:D:286:MET:HG3	1:D:287:ASP:OD1	2.18	0.44
1:E:282:LEU:HG	1:E:283:LEU:HD12	2.00	0.44
1:A:378:ARG:NH2	1:F:170:GLU:HB2	2.28	0.44
1:F:159:ALA:CA	1:F:333:GLN:HE21	2.31	0.44
1:F:274:GLU:HB2	1:F:275:ARG:H	1.65	0.44
1:D:494:PHE:O	1:D:495:ARG:C	2.56	0.44
1:C:518:ALA:HB2	1:D:495:ARG:HA	2.00	0.44
1:C:518:ALA:HB3	1:D:495:ARG:HA	2.00	0.44
1:E:450:MET:HG3	1:E:451:MET:H	1.83	0.44
1:A:493:ASP:O	1:A:496:GLN:CB	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:LYS:HZ2	1:D:168:LEU:HD23	1.83	0.44
1:F:301:THR:HG23	1:F:303:ARG:H	1.81	0.44
1:B:307:LEU:HD12	1:B:307:LEU:N	2.33	0.44
1:B:187:ARG:N	1:C:374:LEU:HD11	2.27	0.44
1:A:467:ASP:O	1:A:471:VAL:HG23	2.18	0.44
1:A:397:MET:SD	1:A:406:VAL:HG11	2.58	0.44
1:A:228:MET:CG	1:A:236:ARG:HH22	2.31	0.43
1:A:282:LEU:HG	1:A:283:LEU:HD12	2.00	0.43
1:B:174:PHE:CZ	1:B:294:ALA:CB	3.00	0.43
1:B:357:THR:HB	1:B:360:PHE:CD2	2.53	0.43
1:B:367:ASN:O	1:B:371:GLU:HG2	2.17	0.43
1:B:297:VAL:CG1	1:B:317:PHE:CZ	3.01	0.43
1:F:343:PRO:HG2	1:F:383:LYS:CA	2.43	0.43
1:B:517:VAL:CG1	1:B:519:TYR:CZ	3.01	0.43
1:C:462:ARG:O	1:C:465:LEU:N	2.51	0.43
1:C:527:LEU:O	1:C:527:LEU:HD12	2.18	0.43
1:D:414:ILE:HG12	1:D:414:ILE:H	1.65	0.43
1:D:558:VAL:HG12	1:D:559:LYS:N	2.32	0.43
1:E:449:PHE:CB	1:E:468:GLN:HE21	2.28	0.43
1:C:252:VAL:O	1:C:297:VAL:HA	2.18	0.43
1:A:462:ARG:HG3	1:A:466:LEU:HD11	1.99	0.43
1:D:210:ALA:O	1:D:214:ARG:HA	2.18	0.43
1:B:582:LEU:CD2	1:B:590:VAL:HG21	2.43	0.43
1:F:411:ASP:O	1:F:414:ILE:HG13	2.18	0.43
1:E:370:ASN:OD1	1:E:374:LEU:HD13	2.18	0.43
1:F:428:PHE:HE1	1:F:432:ALA:C	2.20	0.43
1:A:566:ARG:O	1:A:569:LEU:N	2.51	0.43
1:C:311:LEU:HA	1:C:311:LEU:HD23	1.68	0.43
1:E:574:GLU:OE1	1:E:575:THR:N	2.51	0.43
1:A:180:ARG:O	1:A:184:MET:HE2	2.18	0.43
1:B:159:ALA:HB1	1:B:333:GLN:HG3	1.98	0.43
1:B:348:VAL:HG21	1:B:386:MET:HE2	2.00	0.43
1:D:297:VAL:CG1	1:D:317:PHE:CZ	3.01	0.43
1:F:361:VAL:HG13	1:F:364:ASP:CG	2.38	0.43
1:F:389:LEU:O	1:F:390:GLU:C	2.56	0.43
1:E:503:ARG:CD	1:E:508:TRP:CE2	3.00	0.43
1:F:453:ARG:HH12	1:F:495:ARG:NH2	2.08	0.43
1:D:158:VAL:HG11	1:D:205:LEU:HD11	2.00	0.43
1:B:563:LEU:CD1	1:B:563:LEU:C	2.87	0.43
1:C:153:VAL:HG13	1:C:157:ASP:CB	2.48	0.43
1:D:196:GLY:O	1:D:302:ASN:HA	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:357:THR:C	1:E:360:PHE:HD1	2.21	0.43
1:D:538:GLU:HB2	1:E:541:LYS:NZ	2.34	0.43
1:B:393:ALA:O	1:B:397:MET:HB3	2.18	0.43
1:B:261:GLY:O	1:B:308:ASP:HB3	2.18	0.43
1:D:194:LEU:HD23	1:D:323:ILE:CD1	2.49	0.43
1:A:587:PHE:HD2	1:A:588:GLN:N	2.15	0.43
1:F:194:LEU:HD23	1:F:323:ILE:CD1	2.48	0.43
1:F:360:PHE:CE1	1:F:364:ASP:HB3	2.54	0.43
1:C:408:SER:O	1:C:410:ARG:N	2.45	0.43
1:C:200:VAL:HG11	1:C:323:ILE:HG13	2.00	0.43
1:E:511:HIS:C	1:E:512:PRO:O	2.56	0.43
1:C:174:PHE:HB2	1:C:181:PHE:CZ	2.53	0.43
1:C:238:ARG:HG2	1:C:242:GLU:OE2	2.18	0.43
1:C:261:GLY:O	1:C:262:ARG:HB2	2.18	0.43
1:A:445:ARG:O	1:A:448:GLY:N	2.51	0.43
1:A:454:ARG:HB2	1:A:460:TRP:HH2	1.84	0.43
1:B:237:VAL:HG21	1:B:281:GLN:HG3	1.98	0.43
1:D:589:ARG:C	1:D:591:VAL:N	2.70	0.43
1:D:595:PRO:C	1:D:596:LEU:HD12	2.38	0.43
1:E:346:GLU:CD	1:E:347:ASP:N	2.71	0.43
1:D:307:LEU:HD12	1:D:307:LEU:N	2.32	0.43
1:A:541:LYS:HD3	1:F:538:GLU:CB	2.48	0.43
1:A:397:MET:HG3	1:A:406:VAL:CG1	2.47	0.43
1:E:408:SER:O	1:E:410:ARG:N	2.48	0.43
1:B:173:GLU:O	1:B:176:LYS:N	2.52	0.43
1:B:176:LYS:HE2	1:B:176:LYS:HB3	1.83	0.43
1:B:210:ALA:O	1:B:214:ARG:CA	2.67	0.43
1:F:179:SER:HA	1:F:182:HIS:NE2	2.33	0.43
1:F:175:LEU:O	1:F:249:PRO:CG	2.66	0.43
1:F:297:VAL:CG1	1:F:317:PHE:CE1	3.02	0.43
1:F:325:ALA:CB	1:F:326:PRO:HD3	2.42	0.43
1:F:397:MET:O	1:F:400:PRO:CD	2.66	0.43
1:C:411:ASP:O	1:C:415:THR:OG1	2.28	0.43
1:C:586:GLU:HA	1:C:589:ARG:CB	2.49	0.43
1:C:585:GLU:O	1:C:588:GLN:N	2.51	0.43
1:C:443:ARG:O	1:C:443:ARG:HG2	2.18	0.43
1:D:468:GLN:O	1:D:471:VAL:N	2.51	0.43
1:E:493:ASP:O	1:E:496:GLN:CB	2.65	0.43
1:E:516:PRO:HB2	1:F:494:PHE:CE1	2.53	0.43
1:A:453:ARG:NH1	1:A:460:TRP:NE1	2.66	0.43
1:B:452:PRO:O	1:B:456:ASP:CA	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:HIS:CD2	2:D:2001:ADP:H2'	2.53	0.43
1:B:235:ALA:HA	1:B:238:ARG:NE	2.33	0.43
1:D:589:ARG:CD	1:D:596:LEU:HD11	2.48	0.43
1:A:371:GLU:OE2	1:A:395:ARG:HD2	2.17	0.43
1:B:436:HIS:O	1:B:437:LYS:CG	2.64	0.43
1:B:428:PHE:C	1:B:428:PHE:HD1	2.21	0.43
1:A:425:ALA:C	1:A:427:HIS:N	2.72	0.43
1:A:147:LEU:O	1:A:216:PRO:HB3	2.19	0.43
1:B:183:GLU:OE1	1:B:184:MET:HB3	2.17	0.43
1:B:200:VAL:HA	1:B:361:VAL:HG23	2.00	0.43
1:B:248:ALA:HB1	1:B:294:ALA:HB3	1.99	0.43
1:B:375:LEU:HD21	1:B:388:ASP:O	2.18	0.43
1:C:382:ARG:HG3	1:C:383:LYS:CA	2.48	0.43
1:E:228:MET:CG	1:E:236:ARG:HH22	2.31	0.43
1:A:346:GLU:CD	1:A:347:ASP:N	2.71	0.43
1:C:327:ASP:OD1	1:C:329:LYS:N	2.51	0.43
1:C:358:PRO:CA	1:C:359:GLY:C	2.84	0.43
1:C:145:ARG:HH11	1:C:145:ARG:CB	2.30	0.43
1:B:455:GLU:O	1:B:455:GLU:HG2	2.19	0.43
1:F:568:VAL:HG13	1:F:591:VAL:HA	2.00	0.43
1:D:248:ALA:HB1	1:D:294:ALA:HB3	2.00	0.43
1:E:327:ASP:OD1	1:E:329:LYS:N	2.51	0.43
1:E:336:ARG:O	1:E:337:ILE:C	2.55	0.43
1:F:559:LYS:O	1:F:563:LEU:HB2	2.18	0.43
1:D:428:PHE:CE1	1:D:433:ASP:N	2.87	0.43
1:F:342:LYS:HA	1:F:342:LYS:HD2	1.66	0.43
1:B:428:PHE:CZ	1:B:433:ASP:N	2.87	0.43
1:D:149:GLU:O	1:D:150:ALA:C	2.57	0.43
1:E:570:GLU:O	1:E:571:ARG:C	2.57	0.43
1:B:170:GLU:HG2	1:B:171:ILE:N	2.33	0.43
1:B:391:GLU:O	1:B:395:ARG:CB	2.66	0.43
1:C:344:LEU:HB3	1:C:348:VAL:HG11	2.00	0.43
1:A:574:GLU:O	1:A:575:THR:C	2.57	0.43
1:A:346:GLU:OE1	1:A:347:ASP:N	2.44	0.43
1:A:227:GLU:CG	1:F:263:LYS:NZ	2.67	0.43
1:C:596:LEU:HG	1:C:597:GLU:N	2.34	0.43
1:C:357:THR:O	1:C:360:PHE:CD1	2.72	0.43
1:C:188:ILE:HG22	1:C:190:LYS:H	1.84	0.43
1:B:478:ALA:O	1:B:479:GLU:C	2.57	0.43
1:D:200:VAL:HA	1:D:361:VAL:HG23	2.01	0.43
1:B:247:HIS:O	1:B:249:PRO:O	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:559:LYS:O	1:B:563:LEU:HB2	2.18	0.43
1:D:177:ASN:OD1	1:D:180:ARG:CB	2.65	0.43
1:E:361:VAL:HG12	1:E:364:ASP:HB2	1.99	0.43
1:E:361:VAL:O	1:E:365:LEU:HG	2.18	0.43
1:D:428:PHE:C	1:D:428:PHE:HD1	2.22	0.43
1:A:145:ARG:HH11	1:A:145:ARG:CB	2.32	0.43
1:A:225:PHE:CE1	1:A:233:GLY:O	2.72	0.43
1:A:228:MET:SD	1:A:236:ARG:NH2	2.89	0.43
1:A:286:MET:HA	1:A:289:PHE:CE2	2.54	0.43
1:B:399:LEU:O	1:B:402:LYS:HB3	2.19	0.43
1:D:241:PHE:C	1:D:243:THR:N	2.71	0.43
1:E:261:GLY:O	1:E:262:ARG:HB2	2.19	0.43
1:F:202:LYS:N	2:F:2001:ADP:O1A	2.52	0.43
1:F:225:PHE:CG	1:F:236:ARG:NH1	2.86	0.43
1:F:297:VAL:CG1	1:F:317:PHE:CZ	3.01	0.43
1:F:355:LYS:HA	1:F:355:LYS:HD2	1.46	0.43
1:C:462:ARG:HH11	1:C:510:MET:HB3	1.84	0.43
1:E:451:MET:HB2	1:E:452:PRO:CD	2.47	0.43
1:E:454:ARG:HB2	1:E:460:TRP:HH2	1.84	0.43
1:E:512:PRO:HB2	1:E:514:PHE:CD2	2.54	0.43
1:D:428:PHE:CE1	1:D:432:ALA:HB3	2.52	0.43
1:F:228:MET:SD	1:F:232:VAL:CG1	3.04	0.43
1:B:374:LEU:HD23	1:B:374:LEU:C	2.38	0.43
1:A:408:SER:O	1:A:410:ARG:N	2.47	0.43
1:A:332:GLU:O	1:A:335:LEU:HB2	2.19	0.43
1:B:257:ILE:HG22	1:B:261:GLY:H	1.83	0.43
1:E:177:ASN:HA	1:E:178:PRO:HD2	1.91	0.43
1:A:587:PHE:C	1:A:587:PHE:CD2	2.92	0.43
1:C:503:ARG:HD2	1:C:508:TRP:CD2	2.52	0.43
1:D:417:TYR:CZ	1:D:482:VAL:HG21	2.54	0.43
1:E:503:ARG:CG	1:E:508:TRP:CE3	3.02	0.43
1:A:480:GLU:OE1	1:A:555:TYR:OH	2.30	0.43
1:A:449:PHE:CE2	1:A:496:GLN:CD	2.92	0.43
1:F:503:ARG:HA	1:F:503:ARG:HD3	1.58	0.43
1:D:394:ASP:HA	1:D:397:MET:HE2	1.98	0.43
1:D:583:THR:HG22	1:D:586:GLU:OE1	2.19	0.43
1:E:327:ASP:OD1	1:E:327:ASP:C	2.57	0.43
1:A:471:VAL:O	1:A:474:ALA:HB3	2.19	0.43
1:E:372:ALA:O	1:E:375:LEU:HB3	2.19	0.43
1:D:428:PHE:C	1:D:428:PHE:CD1	2.92	0.43
1:D:342:LYS:HD2	1:D:342:LYS:HA	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:597:GLU:O	1:B:599:PRO:CD	2.66	0.43
1:A:287:ASP:OD1	1:A:287:ASP:N	2.51	0.43
1:E:438:VAL:HG22	1:E:582:LEU:HB2	2.01	0.43
1:A:200:VAL:HG13	1:A:323:ILE:HG13	2.00	0.43
1:B:165:LYS:CE	1:B:205:LEU:HG	2.48	0.43
1:B:164:ALA:C	1:B:168:LEU:HD13	2.37	0.43
1:B:338:HIS:HB3	1:B:369:LEU:HD12	2.00	0.43
1:D:235:ALA:HA	1:D:238:ARG:HD3	2.00	0.43
1:E:234:ALA:HB1	1:E:281:GLN:HG2	2.01	0.43
1:E:252:VAL:O	1:E:297:VAL:HA	2.19	0.43
1:E:274:GLU:C	1:E:277:GLN:HB3	2.36	0.43
1:A:378:ARG:NH2	1:F:170:GLU:CA	2.80	0.43
1:B:523:GLU:O	1:B:530:TYR:N	2.43	0.43
1:C:203:THR:OG1	1:C:204:HIS:N	2.52	0.43
1:C:204:HIS:CD2	2:C:1001:ADP:C2	3.07	0.43
1:C:399:LEU:N	1:C:400:PRO:CD	2.81	0.43
1:C:448:GLY:O	1:C:452:PRO:CD	2.52	0.43
1:E:445:ARG:O	1:E:447:LEU:N	2.52	0.43
1:B:449:PHE:HZ	1:B:496:GLN:OE1	2.01	0.43
1:D:355:LYS:HD2	1:D:355:LYS:HA	1.44	0.43
1:B:178:PRO:O	1:B:182:HIS:CE1	2.72	0.43
1:B:225:PHE:CB	1:B:236:ARG:NH1	2.79	0.43
1:F:585:GLU:O	1:F:586:GLU:C	2.55	0.43
1:F:585:GLU:O	1:F:587:PHE:N	2.52	0.43
1:F:594:LEU:C	1:F:594:LEU:HD23	2.39	0.43
1:F:458:LEU:HD11	1:F:460:TRP:HB3	2.01	0.43
1:D:568:VAL:HG11	1:D:591:VAL:HG13	2.00	0.43
1:E:344:LEU:HB3	1:E:348:VAL:HG11	1.99	0.43
1:B:307:LEU:CD1	1:B:307:LEU:H	2.31	0.43
1:D:255:ASP:OD1	1:D:256:GLU:N	2.52	0.43
1:C:371:GLU:CG	1:C:392:ALA:HB1	2.40	0.43
1:C:483:PHE:C	1:C:485:ASP:H	2.23	0.43
1:A:411:ASP:O	1:A:415:THR:OG1	2.29	0.43
1:A:337:ILE:CD1	1:A:338:HIS:CD2	3.01	0.43
1:B:169:LYS:O	1:B:172:VAL:HG22	2.19	0.43
1:B:382:ARG:HA	1:B:382:ARG:HD2	1.08	0.43
1:C:348:VAL:O	1:C:348:VAL:HG12	2.18	0.43
1:F:160:GLY:N	1:F:333:GLN:NE2	2.66	0.43
1:F:367:ASN:O	1:F:371:GLU:HG2	2.19	0.43
1:C:460:TRP:HD1	1:C:464:ARG:NH1	2.13	0.43
1:C:500:LEU:O	1:C:504:MET:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:471:VAL:O	1:D:474:ALA:CB	2.58	0.43
1:D:533:ARG:NH1	1:D:535:TYR:CD1	2.86	0.43
1:A:453:ARG:NH1	1:A:460:TRP:HE1	2.16	0.43
1:B:215:VAL:CG2	1:B:216:PRO:CD	2.87	0.43
1:B:238:ARG:CB	1:B:238:ARG:HH11	2.32	0.43
1:E:400:PRO:HG2	1:E:405:LEU:CD1	2.44	0.43
1:D:203:THR:HG23	1:D:253:PHE:CE1	2.53	0.43
1:C:480:GLU:OE1	1:C:555:TYR:OH	2.31	0.43
1:A:372:ALA:CB	1:A:389:LEU:HD23	2.48	0.43
1:E:479:GLU:OE2	1:E:487:THR:HA	2.19	0.43
1:B:539:THR:O	1:B:543:ILE:HG13	2.18	0.43
1:D:422:HIS:CD2	1:D:475:GLY:CA	3.02	0.43
1:E:574:GLU:O	1:E:575:THR:C	2.57	0.42
1:A:399:LEU:N	1:A:400:PRO:CD	2.83	0.42
1:E:147:LEU:HD21	1:E:151:PRO:CG	2.45	0.42
1:E:188:ILE:O	1:E:190:LYS:NZ	2.42	0.42
1:F:190:LYS:CD	1:F:289:PHE:CZ	3.02	0.42
1:F:353:LEU:O	1:F:357:THR:CG2	2.66	0.42
1:C:263:LYS:CG	1:C:264:ARG:H	2.29	0.42
1:C:264:ARG:HD2	1:C:266:SER:CB	2.49	0.42
1:D:518:ALA:CB	1:E:495:ARG:HA	2.48	0.42
1:E:493:ASP:OD1	1:E:493:ASP:N	2.50	0.42
1:E:527:LEU:O	1:E:530:TYR:OH	2.30	0.42
1:C:297:VAL:HG23	1:C:317:PHE:CE1	2.54	0.42
1:A:453:ARG:HH11	1:A:460:TRP:HZ2	1.57	0.42
1:A:462:ARG:CG	1:A:463:LYS:N	2.81	0.42
1:B:449:PHE:CE2	1:B:453:ARG:CZ	3.01	0.42
1:D:173:GLU:O	1:D:176:LYS:N	2.51	0.42
1:B:411:ASP:O	1:B:414:ILE:HG13	2.18	0.42
1:B:554:GLN:HA	1:B:554:GLN:OE1	2.19	0.42
1:E:346:GLU:OE1	1:E:347:ASP:N	2.45	0.42
1:F:301:THR:HG23	1:F:302:ASN:N	2.34	0.42
1:B:188:ILE:HA	1:B:188:ILE:HD13	1.80	0.42
1:D:253:PHE:HA	1:D:298:MET:CB	2.46	0.42
1:A:308:ASP:OD1	1:A:310:ALA:CB	2.67	0.42
1:B:428:PHE:CE1	1:B:433:ASP:N	2.87	0.42
1:E:355:LYS:HD3	1:E:355:LYS:HA	1.88	0.42
1:C:350:LEU:HG	1:C:350:LEU:H	1.48	0.42
1:A:336:ARG:O	1:A:337:ILE:C	2.58	0.42
1:B:253:PHE:HA	1:B:298:MET:CB	2.47	0.42
1:F:175:LEU:O	1:F:249:PRO:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:257:ILE:HG22	1:F:261:GLY:H	1.84	0.42
1:C:410:ARG:CG	1:C:411:ASP:N	2.79	0.42
1:B:538:GLU:C	1:B:540:ALA:N	2.72	0.42
1:C:334:ILE:HD11	2:C:1001:ADP:N6	2.34	0.42
1:C:508:TRP:HD1	1:D:491:GLU:HG2	1.84	0.42
1:E:480:GLU:OE1	1:E:555:TYR:OH	2.29	0.42
1:F:455:GLU:O	1:F:455:GLU:HG2	2.19	0.42
1:C:236:ARG:O	1:C:239:ASP:N	2.52	0.42
1:D:159:ALA:CA	1:D:333:GLN:HE21	2.32	0.42
1:D:352:LEU:HD11	1:D:356:ARG:NH1	2.33	0.42
1:D:376:ALA:HA	1:D:381:ARG:NH1	2.34	0.42
1:C:172:VAL:HG22	1:C:173:GLU:N	2.34	0.42
1:B:216:PRO:HG3	1:B:247:HIS:CE1	2.53	0.42
1:D:187:ARG:H	1:E:374:LEU:HD11	1.82	0.42
1:A:153:VAL:HG13	1:A:157:ASP:CB	2.48	0.42
1:F:536:SER:O	1:F:538:GLU:N	2.51	0.42
1:B:147:LEU:HD13	1:B:149:GLU:OE1	2.19	0.42
1:B:321:ILE:HA	1:B:321:ILE:HD12	1.82	0.42
1:E:416:ALA:HB2	1:E:577:LEU:CD2	2.11	0.42
1:B:397:MET:O	1:B:400:PRO:CD	2.68	0.42
1:E:168:LEU:O	1:E:171:ILE:CG1	2.67	0.42
1:E:234:ALA:O	1:E:237:VAL:CG1	2.65	0.42
1:E:316:ARG:O	1:E:318:ASP:N	2.51	0.42
1:F:205:LEU:HA	1:F:208:ALA:HB3	2.02	0.42
1:F:238:ARG:O	1:F:239:ASP:C	2.56	0.42
1:F:286:MET:SD	1:F:316:ARG:HG3	2.59	0.42
1:F:193:LEU:HB3	1:F:317:PHE:CD2	2.54	0.42
1:D:488:THR:O	1:D:490:ALA:N	2.53	0.42
1:E:462:ARG:HG3	1:E:463:LYS:N	2.28	0.42
1:C:237:VAL:HG13	1:C:238:ARG:N	2.34	0.42
1:C:234:ALA:HB1	1:C:281:GLN:HG2	2.01	0.42
1:B:215:VAL:HG21	1:B:249:PRO:C	2.38	0.42
1:E:157:ASP:N	1:E:157:ASP:OD1	2.51	0.42
1:C:157:ASP:OD1	1:C:157:ASP:N	2.51	0.42
1:F:532:VAL:O	1:F:532:VAL:HG13	2.19	0.42
1:F:506:THR:OG1	1:F:520:ALA:HB3	2.19	0.42
1:E:424:LEU:HD12	1:E:424:LEU:HA	1.83	0.42
1:A:147:LEU:HB3	1:A:217:PHE:O	2.19	0.42
1:A:169:LYS:HA	1:A:172:VAL:HG13	2.01	0.42
1:A:215:VAL:HG21	1:A:250:CYS:CB	2.49	0.42
1:A:236:ARG:CG	1:A:237:VAL:H	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:ARG:C	1:A:238:ARG:N	2.71	0.42
1:B:256:GLU:CG	1:B:256:GLU:O	2.67	0.42
1:B:159:ALA:CA	1:B:333:GLN:HE21	2.32	0.42
1:D:225:PHE:CG	1:D:236:ARG:NH1	2.88	0.42
1:E:236:ARG:CG	1:E:237:VAL:H	2.19	0.42
1:E:237:VAL:HG13	1:E:238:ARG:N	2.35	0.42
1:F:215:VAL:O	1:F:216:PRO:C	2.56	0.42
1:F:319:ARG:HB3	1:F:319:ARG:NH1	2.35	0.42
1:F:348:VAL:CG2	1:F:352:LEU:CD1	2.98	0.42
1:C:471:VAL:O	1:C:474:ALA:HB3	2.20	0.42
1:D:328:VAL:HG21	1:D:579:ARG:HA	2.01	0.42
1:B:228:MET:O	1:B:229:PHE:HB2	2.20	0.42
1:B:417:TYR:CZ	1:B:482:VAL:HG21	2.55	0.42
1:E:200:VAL:HG11	1:E:323:ILE:HG13	2.01	0.42
1:A:372:ALA:O	1:A:375:LEU:HB3	2.20	0.42
1:F:563:LEU:C	1:F:563:LEU:CD1	2.88	0.42
1:A:458:LEU:HD12	1:A:458:LEU:C	2.39	0.42
1:E:582:LEU:HA	1:E:586:GLU:OE2	2.20	0.42
1:D:178:PRO:O	1:D:182:HIS:CE1	2.72	0.42
1:D:311:LEU:C	1:D:316:ARG:HG2	2.31	0.42
1:E:174:PHE:O	1:E:177:ASN:C	2.58	0.42
1:A:344:LEU:HB3	1:A:348:VAL:HG11	2.01	0.42
1:F:216:PRO:HG3	1:F:247:HIS:CE1	2.53	0.42
1:F:233:GLY:O	1:F:236:ARG:NH2	2.53	0.42
1:F:203:THR:HG23	1:F:253:PHE:CE1	2.54	0.42
1:F:328:VAL:HG22	1:F:355:LYS:CD	2.49	0.42
1:C:581:THR:O	1:C:582:LEU:CD1	2.66	0.42
1:C:587:PHE:CD2	1:C:588:GLN:N	2.88	0.42
1:C:336:ARG:O	1:C:337:ILE:C	2.57	0.42
1:C:527:LEU:O	1:C:530:TYR:OH	2.31	0.42
1:E:264:ARG:HB3	1:E:265:GLY:H	1.50	0.42
1:C:225:PHE:CE1	1:C:236:ARG:NH1	2.87	0.42
1:C:274:GLU:O	1:C:277:GLN:CB	2.54	0.42
1:A:445:ARG:C	1:A:447:LEU:N	2.73	0.42
1:A:454:ARG:HD3	1:A:454:ARG:C	2.39	0.42
1:A:463:LYS:HB2	1:B:486:VAL:HG11	2.00	0.42
1:D:373:ALA:CA	1:D:384:ILE:HD11	2.49	0.42
1:B:458:LEU:HG	1:B:460:TRP:CE3	2.55	0.42
1:B:464:ARG:O	1:B:467:ASP:N	2.51	0.42
1:B:558:VAL:HG12	1:B:559:LYS:N	2.33	0.42
2:E:1001:ADP:H2'	2:E:1001:ADP:N3	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:302:ASN:HB3	1:E:443:ARG:NH1	2.35	0.42
1:D:147:LEU:HD13	1:D:149:GLU:OE1	2.19	0.42
1:C:425:ALA:C	1:C:427:HIS:N	2.71	0.42
1:F:399:LEU:O	1:F:402:LYS:HB3	2.20	0.42
1:A:350:LEU:H	1:A:350:LEU:HG	1.47	0.42
1:E:586:GLU:CA	1:E:589:ARG:HG3	2.41	0.42
1:A:188:ILE:CG2	1:A:189:PRO:HD2	2.50	0.42
1:B:155:PHE:O	1:B:156:LYS:C	2.57	0.42
1:B:199:GLY:O	1:B:361:VAL:HG22	2.19	0.42
1:B:193:LEU:HB3	1:B:317:PHE:CD2	2.54	0.42
1:F:215:VAL:HG21	1:F:249:PRO:C	2.38	0.42
1:F:344:LEU:CG	1:F:346:GLU:OE1	2.67	0.42
1:F:357:THR:HG1	1:F:360:PHE:HD2	1.65	0.42
1:D:414:ILE:O	1:D:415:THR:C	2.57	0.42
1:F:455:GLU:O	1:F:456:ASP:C	2.58	0.42
1:C:273:ASP:C	1:C:273:ASP:OD1	2.58	0.42
1:B:477:ALA:O	1:B:478:ALA:C	2.55	0.42
1:B:476:ARG:HD3	1:B:494:PHE:HZ	1.85	0.42
1:F:517:VAL:CG2	1:F:518:ALA:N	2.81	0.42
1:B:215:VAL:O	1:B:216:PRO:C	2.55	0.42
1:F:464:ARG:O	1:F:467:ASP:N	2.53	0.42
1:A:408:SER:CB	1:A:409:PRO:HD2	2.45	0.42
1:A:251:ILE:HG23	1:A:296:VAL:HG23	2.01	0.42
1:A:271:GLY:O	1:A:275:ARG:NE	2.50	0.42
1:A:327:ASP:C	1:A:327:ASP:OD1	2.57	0.42
1:A:338:HIS:ND1	1:A:366:GLU:HB2	2.35	0.42
1:B:165:LYS:CE	1:B:205:LEU:CG	2.98	0.42
1:B:205:LEU:HA	1:B:208:ALA:HB3	2.02	0.42
1:E:449:PHE:CD1	1:E:468:GLN:NE2	2.87	0.42
1:A:462:ARG:O	1:A:466:LEU:HD12	2.19	0.42
1:F:529:GLY:O	1:F:530:TYR:CB	2.58	0.42
1:D:155:PHE:HB2	1:D:158:VAL:HB	2.01	0.42
1:D:361:VAL:HG13	1:D:364:ASP:CG	2.40	0.42
1:C:155:PHE:HZ	1:C:209:VAL:CG2	2.31	0.42
1:A:561:LEU:O	1:A:564:GLU:HB3	2.19	0.42
1:A:470:ALA:C	1:A:558:VAL:HG21	2.39	0.42
1:B:428:PHE:CD1	1:B:428:PHE:C	2.92	0.42
1:A:155:PHE:CZ	1:A:209:VAL:CG2	3.03	0.42
1:B:197:PRO:HD2	1:B:200:VAL:CG1	2.44	0.42
1:B:328:VAL:HG23	1:B:580:GLU:CG	2.47	0.42
1:B:373:ALA:CA	1:B:384:ILE:HD11	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:145:ARG:HH11	1:E:145:ARG:CB	2.32	0.42
1:E:147:LEU:HD12	1:E:148:THR:N	2.35	0.42
1:E:222:GLY:O	1:E:225:PHE:HB2	2.20	0.42
1:A:582:LEU:HA	1:A:586:GLU:OE2	2.19	0.42
1:A:381:ARG:CG	1:A:382:ARG:N	2.81	0.42
1:F:164:ALA:C	1:F:168:LEU:HD13	2.36	0.42
1:F:236:ARG:O	1:F:237:VAL:C	2.58	0.42
1:C:589:ARG:HH22	1:C:596:LEU:N	2.17	0.42
1:C:361:VAL:HG22	1:C:362:GLY:N	2.35	0.42
1:D:563:LEU:CD1	1:D:563:LEU:C	2.87	0.42
1:D:355:LYS:HZ3	1:D:578:GLU:HG3	1.85	0.42
1:F:417:TYR:CZ	1:F:482:VAL:HG21	2.55	0.42
1:D:307:LEU:HD12	1:D:307:LEU:H	1.85	0.42
1:C:194:LEU:H	1:C:194:LEU:HD12	1.85	0.42
1:A:407:LEU:HA	1:A:411:ASP:HB2	2.02	0.42
1:A:180:ARG:HG2	1:A:180:ARG:H	1.50	0.42
1:A:252:VAL:HB	1:A:297:VAL:HA	2.01	0.42
1:A:356:ARG:C	1:A:358:PRO:HD2	2.40	0.42
1:B:157:ASP:O	1:B:204:HIS:CE1	2.73	0.42
1:B:376:ALA:C	1:B:381:ARG:CB	2.84	0.42
1:D:238:ARG:HA	1:D:241:PHE:HE2	1.84	0.42
1:D:238:ARG:NH1	1:D:239:ASP:CA	2.69	0.42
1:E:175:LEU:O	1:E:175:LEU:HD12	2.20	0.42
1:E:253:PHE:HA	1:E:298:MET:O	2.20	0.42
1:F:173:GLU:O	1:F:176:LYS:N	2.50	0.42
1:F:172:VAL:O	1:F:175:LEU:HB2	2.20	0.42
1:F:253:PHE:HA	1:F:298:MET:CB	2.45	0.42
1:F:400:PRO:O	1:F:403:LYS:N	2.52	0.42
1:C:325:ALA:O	1:C:327:ASP:N	2.53	0.42
1:C:332:GLU:HA	1:C:335:LEU:HD12	2.02	0.42
1:C:453:ARG:NH2	1:C:464:ARG:CZ	2.82	0.42
1:D:449:PHE:CZ	1:D:453:ARG:NH2	2.88	0.42
1:D:478:ALA:O	1:D:482:VAL:HG12	2.20	0.42
1:D:200:VAL:HG12	1:D:325:ALA:CB	2.50	0.42
1:D:360:PHE:CE1	1:D:364:ASP:HB3	2.53	0.42
1:D:375:LEU:HD21	1:D:388:ASP:O	2.19	0.42
1:C:216:PRO:HG2	1:C:247:HIS:CD2	2.55	0.42
1:F:567:GLU:O	1:F:568:VAL:C	2.59	0.42
1:F:307:LEU:N	1:F:307:LEU:HD12	2.35	0.42
1:E:204:HIS:CD2	2:E:1001:ADP:C2	3.07	0.42
1:E:163:GLU:H	1:E:163:GLU:CD	2.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:533:ARG:HG3	1:B:533:ARG:NH1	2.31	0.42
1:D:162:GLU:OE1	1:D:162:GLU:CA	2.68	0.42
1:E:571:ARG:O	1:E:575:THR:HG23	2.20	0.42
1:A:277:GLN:CG	1:A:278:THR:N	2.83	0.42
1:A:311:LEU:HD23	1:A:316:ARG:HH21	1.75	0.42
1:B:168:LEU:O	1:B:171:ILE:N	2.52	0.42
1:B:157:ASP:O	1:B:204:HIS:HE1	2.03	0.42
1:B:388:ASP:N	1:B:388:ASP:OD1	2.48	0.42
1:D:233:GLY:O	1:D:236:ARG:NH2	2.52	0.42
1:E:180:ARG:H	1:E:180:ARG:HG2	1.51	0.42
1:E:180:ARG:O	1:E:184:MET:HE2	2.19	0.42
1:E:174:PHE:HZ	1:E:294:ALA:HB1	1.85	0.42
1:F:333:GLN:O	1:F:336:ARG:CB	2.65	0.42
1:C:264:ARG:HD2	1:C:266:SER:HB2	2.00	0.42
1:C:333:GLN:HA	1:C:336:ARG:NH2	2.35	0.42
1:D:452:PRO:O	1:D:456:ASP:CG	2.59	0.42
1:D:453:ARG:CZ	1:D:495:ARG:NH2	2.57	0.42
1:D:449:PHE:HZ	1:D:496:GLN:OE1	2.03	0.42
1:E:461:SER:OG	1:F:486:VAL:HG11	2.19	0.42
1:C:252:VAL:HB	1:C:297:VAL:HA	2.02	0.42
1:D:154:THR:HG23	1:D:156:LYS:N	2.35	0.42
1:D:214:ARG:CB	1:D:214:ARG:NH1	2.80	0.42
1:C:215:VAL:HG21	1:C:250:CYS:CB	2.49	0.42
1:C:250:CYS:HB3	1:C:295:ILE:HG13	2.01	0.42
1:B:589:ARG:CZ	1:B:596:LEU:CD2	2.97	0.42
1:A:172:VAL:HG22	1:A:173:GLU:N	2.35	0.41
1:A:174:PHE:CG	1:A:175:LEU:N	2.85	0.41
1:A:203:THR:OG1	1:A:204:HIS:N	2.52	0.41
1:A:222:GLY:O	1:A:225:PHE:HB2	2.19	0.41
1:A:361:VAL:HG22	1:A:362:GLY:N	2.35	0.41
1:B:255:ASP:OD1	1:B:256:GLU:N	2.53	0.41
1:B:355:LYS:HA	1:B:355:LYS:HD3	1.68	0.41
1:E:174:PHE:HB2	1:E:181:PHE:CZ	2.55	0.41
1:E:228:MET:HG3	1:E:236:ARG:HH22	1.85	0.41
1:A:382:ARG:HG2	1:A:383:LYS:H	1.84	0.41
1:F:241:PHE:CZ	1:F:285:GLU:OE2	2.73	0.41
1:F:350:LEU:O	1:F:353:LEU:N	2.53	0.41
1:C:586:GLU:HA	1:C:589:ARG:HB2	2.02	0.41
1:B:536:SER:O	1:B:538:GLU:N	2.53	0.41
1:C:332:GLU:O	1:C:335:LEU:HB2	2.20	0.41
1:C:442:PRO:HB3	1:C:445:ARG:NH2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:447:LEU:CB	1:C:496:GLN:HE22	2.33	0.41
1:D:477:ALA:O	1:D:478:ALA:C	2.58	0.41
1:E:468:GLN:O	1:E:471:VAL:HB	2.20	0.41
1:A:464:ARG:CG	1:A:464:ARG:NH1	2.80	0.41
1:D:206:ALA:O	1:D:209:VAL:CG1	2.67	0.41
1:E:356:ARG:C	1:E:358:PRO:HD2	2.39	0.41
1:E:589:ARG:HH22	1:E:596:LEU:CA	2.30	0.41
1:B:332:GLU:CD	1:B:351:ALA:HA	2.41	0.41
1:D:235:ALA:O	1:D:238:ARG:NH1	2.53	0.41
1:D:319:ARG:NH1	1:D:319:ARG:HB3	2.36	0.41
1:D:525:THR:HG22	1:D:526:TYR:HD2	1.84	0.41
1:F:158:VAL:HG13	1:F:205:LEU:HD11	2.02	0.41
1:F:344:LEU:CD1	1:F:346:GLU:OE1	2.68	0.41
1:C:566:ARG:O	1:C:567:GLU:C	2.56	0.41
1:B:500:LEU:O	1:B:503:ARG:CB	2.68	0.41
1:B:508:TRP:O	1:B:509:GLY:C	2.58	0.41
1:C:462:ARG:O	1:C:466:LEU:HD12	2.20	0.41
1:C:236:ARG:HH11	1:C:236:ARG:CB	2.32	0.41
1:F:500:LEU:O	1:F:503:ARG:CB	2.67	0.41
1:D:153:VAL:O	1:D:154:THR:HB	2.20	0.41
1:D:202:LYS:CD	2:D:2001:ADP:O2B	2.68	0.41
1:D:349:ASP:C	1:D:350:LEU:HG	2.40	0.41
1:F:412:ARG:O	1:F:413:ARG:C	2.59	0.41
1:F:307:LEU:CD1	1:F:307:LEU:H	2.32	0.41
1:B:301:THR:HG23	1:B:302:ASN:N	2.35	0.41
1:C:313:ARG:NH1	1:C:526:TYR:C	2.66	0.41
1:E:200:VAL:HG13	1:E:323:ILE:HG13	2.01	0.41
1:E:442:PRO:CG	1:E:443:ARG:H	2.33	0.41
1:E:407:LEU:HA	1:E:411:ASP:HB2	2.01	0.41
1:E:423:ALA:HB1	1:E:587:PHE:CE1	2.55	0.41
1:D:215:VAL:CG2	1:D:216:PRO:CD	2.86	0.41
1:D:238:ARG:HH11	1:D:238:ARG:CG	2.32	0.41
1:E:226:VAL:HG22	1:E:274:GLU:HG2	2.03	0.41
1:A:345:ALA:CB	1:A:347:ASP:OD1	2.69	0.41
1:F:336:ARG:O	1:F:338:HIS:N	2.53	0.41
1:A:517:VAL:HG21	1:B:547:VAL:HG12	2.02	0.41
1:C:512:PRO:HB2	1:C:514:PHE:CD2	2.52	0.41
1:C:234:ALA:O	1:C:237:VAL:CG1	2.65	0.41
1:D:205:LEU:HA	1:D:208:ALA:HB3	2.01	0.41
1:D:346:GLU:OE2	1:D:348:VAL:HG12	2.20	0.41
1:E:381:ARG:CG	1:E:381:ARG:NH1	2.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:ALA:CB	1:C:217:PHE:CD1	3.04	0.41
1:B:235:ALA:O	1:B:238:ARG:NH1	2.53	0.41
1:B:236:ARG:O	1:B:237:VAL:C	2.59	0.41
1:A:495:ARG:HD2	1:F:521:VAL:CG1	2.50	0.41
1:F:228:MET:O	1:F:229:PHE:HB2	2.20	0.41
1:C:391:GLU:HG3	1:C:391:GLU:O	2.21	0.41
1:A:174:PHE:HB2	1:A:181:PHE:CZ	2.56	0.41
1:A:203:THR:HG22	1:A:253:PHE:CZ	2.55	0.41
1:A:279:LEU:HD11	1:A:311:LEU:HD11	2.02	0.41
1:B:154:THR:HG23	1:B:156:LYS:N	2.33	0.41
1:B:353:LEU:O	1:B:357:THR:HG23	2.20	0.41
1:B:190:LYS:CD	1:B:289:PHE:CZ	3.04	0.41
1:D:249:PRO:O	1:D:250:CYS:HB3	2.20	0.41
1:E:188:ILE:HG22	1:E:189:PRO:CD	2.50	0.41
1:F:280:ASN:O	1:F:283:LEU:HB3	2.19	0.41
1:C:566:ARG:HG2	1:C:567:GLU:N	2.35	0.41
1:B:538:GLU:O	1:B:540:ALA:N	2.53	0.41
1:C:196:GLY:C	1:C:202:LYS:HZ1	2.19	0.41
1:C:305:ASP:OD2	1:C:447:LEU:HD13	2.20	0.41
1:C:445:ARG:O	1:C:448:GLY:N	2.51	0.41
1:C:462:ARG:CG	1:C:463:LYS:N	2.83	0.41
1:D:460:TRP:CD1	1:D:464:ARG:HG2	2.54	0.41
1:D:517:VAL:HG13	1:D:519:TYR:CE1	2.55	0.41
1:C:253:PHE:HA	1:C:298:MET:O	2.19	0.41
1:A:448:GLY:O	1:A:452:PRO:CD	2.51	0.41
1:D:155:PHE:O	1:D:156:LYS:C	2.59	0.41
1:D:172:VAL:CG2	1:D:173:GLU:N	2.82	0.41
1:B:405:LEU:HD12	1:B:405:LEU:O	2.20	0.41
1:E:575:THR:HA	1:E:578:GLU:OE1	2.20	0.41
1:A:357:THR:C	1:A:360:PHE:HD1	2.24	0.41
1:B:206:ALA:O	1:B:209:VAL:CG1	2.69	0.41
1:B:400:PRO:HB2	1:B:404:SER:OG	2.21	0.41
1:B:402:LYS:HE3	1:B:403:LYS:HG3	2.03	0.41
1:D:179:SER:HA	1:D:182:HIS:NE2	2.35	0.41
1:D:237:VAL:HG13	1:D:281:GLN:HG2	2.03	0.41
1:F:176:LYS:HB3	1:F:176:LYS:HE2	1.83	0.41
1:B:508:TRP:O	1:B:510:MET:HG3	2.20	0.41
1:C:491:GLU:O	1:C:492:ASN:C	2.58	0.41
1:C:519:TYR:O	1:C:533:ARG:HG2	2.19	0.41
1:D:529:GLY:O	1:D:530:TYR:CB	2.55	0.41
1:C:277:GLN:CG	1:C:278:THR:N	2.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:286:MET:HA	1:C:289:PHE:CE2	2.54	0.41
1:B:453:ARG:HH12	1:B:495:ARG:NH2	2.12	0.41
1:D:301:THR:HG23	1:D:302:ASN:N	2.36	0.41
1:C:549:ARG:O	1:C:550:LEU:C	2.58	0.41
1:E:596:LEU:HG	1:E:597:GLU:N	2.36	0.41
1:A:261:GLY:O	1:A:262:ARG:HB2	2.20	0.41
1:A:328:VAL:HG22	1:A:331:ARG:HH12	1.86	0.41
1:A:331:ARG:NH2	1:A:358:PRO:HG3	2.35	0.41
1:B:165:LYS:O	1:B:167:GLU:N	2.53	0.41
1:B:206:ALA:HB1	1:B:298:MET:HG2	2.02	0.41
1:B:345:ALA:HB2	1:B:383:LYS:NZ	2.35	0.41
1:D:283:LEU:HD13	1:D:316:ARG:HH21	1.82	0.41
1:F:243:THR:CA	1:F:246:ARG:HH21	2.26	0.41
1:F:286:MET:HE2	1:F:315:GLY:O	2.21	0.41
1:C:424:LEU:HD22	1:C:569:LEU:HA	2.02	0.41
1:C:264:ARG:HG2	1:C:267:GLY:H	1.85	0.41
1:C:396:VAL:CG1	1:C:397:MET:N	2.83	0.41
1:C:302:ASN:HB3	1:C:443:ARG:NH1	2.35	0.41
1:C:468:GLN:O	1:C:471:VAL:HB	2.20	0.41
1:D:500:LEU:O	1:D:503:ARG:CB	2.69	0.41
1:C:181:PHE:HA	1:C:184:MET:CE	2.51	0.41
1:C:236:ARG:C	1:C:238:ARG:N	2.71	0.41
1:A:519:TYR:O	1:A:533:ARG:HG2	2.20	0.41
1:C:523:GLU:O	1:C:529:GLY:HA2	2.21	0.41
1:F:301:THR:CG2	1:F:302:ASN:N	2.83	0.41
1:F:428:PHE:CE1	1:F:432:ALA:HB3	2.52	0.41
1:B:428:PHE:CD1	1:B:432:ALA:HB3	2.56	0.41
1:D:162:GLU:HA	1:D:162:GLU:OE1	2.19	0.41
1:E:570:GLU:O	1:E:573:ALA:HB3	2.21	0.41
1:A:147:LEU:C	1:A:147:LEU:HD12	2.40	0.41
1:A:168:LEU:HA	1:A:171:ILE:HD12	2.02	0.41
1:A:234:ALA:HB1	1:A:281:GLN:HG2	2.02	0.41
1:B:202:LYS:CD	2:B:2001:ADP:O2B	2.68	0.41
1:B:327:ASP:HB3	1:B:330:GLY:H	1.86	0.41
1:B:338:HIS:HB3	1:B:369:LEU:HD11	2.03	0.41
1:B:343:PRO:O	1:B:344:LEU:CB	2.68	0.41
1:B:335:LEU:HD23	1:B:365:LEU:HB3	2.00	0.41
1:E:172:VAL:HG22	1:E:173:GLU:N	2.34	0.41
1:E:271:GLY:O	1:E:275:ARG:NE	2.54	0.41
1:E:277:GLN:CG	1:E:278:THR:N	2.83	0.41
1:E:297:VAL:HG23	1:E:317:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:172:VAL:CG2	1:F:173:GLU:N	2.84	0.41
1:F:241:PHE:C	1:F:243:THR:N	2.72	0.41
1:F:249:PRO:O	1:F:250:CYS:HB3	2.21	0.41
1:F:248:ALA:HB1	1:F:294:ALA:HB3	2.02	0.41
1:B:508:TRP:HD1	1:C:491:GLU:HG2	1.85	0.41
1:E:503:ARG:CZ	1:E:522:ARG:CZ	2.99	0.41
1:E:538:GLU:O	1:E:539:THR:C	2.59	0.41
1:F:452:PRO:O	1:F:456:ASP:CA	2.68	0.41
1:C:191:GLY:O	1:C:317:PHE:HA	2.21	0.41
1:D:349:ASP:O	1:D:350:LEU:CG	2.68	0.41
1:D:376:ALA:HB2	1:D:381:ARG:HH11	1.79	0.41
1:C:168:LEU:O	1:C:171:ILE:CG1	2.68	0.41
1:B:241:PHE:C	1:B:243:THR:N	2.71	0.41
1:D:184:MET:SD	1:E:342:LYS:CE	3.08	0.41
1:C:372:ALA:O	1:C:375:LEU:HB3	2.20	0.41
1:F:428:PHE:C	1:F:428:PHE:HD1	2.24	0.41
1:D:597:GLU:O	1:D:599:PRO:CD	2.66	0.41
1:F:150:ALA:HA	1:F:151:PRO:HD2	1.85	0.41
1:F:551:ILE:HG22	1:F:552:GLU:N	2.35	0.41
1:A:214:ARG:CG	1:A:214:ARG:NH1	2.78	0.41
1:A:218:ILE:CD1	1:A:250:CYS:SG	2.92	0.41
1:B:172:VAL:CG2	1:B:173:GLU:N	2.84	0.41
1:B:202:LYS:N	2:B:2001:ADP:O1A	2.52	0.41
1:C:346:GLU:CD	1:C:347:ASP:N	2.72	0.41
1:E:274:GLU:HB3	1:E:275:ARG:H	1.56	0.41
1:A:570:GLU:O	1:A:571:ARG:C	2.58	0.41
1:F:161:ALA:O	1:F:164:ALA:HB3	2.21	0.41
1:F:352:LEU:HD12	1:F:353:LEU:H	1.86	0.41
1:C:423:ALA:HB1	1:C:436:HIS:HE1	1.85	0.41
1:C:200:VAL:HG13	1:C:323:ILE:HG13	2.03	0.41
1:E:447:LEU:CA	1:E:496:GLN:NE2	2.82	0.41
1:C:180:ARG:O	1:C:184:MET:HE2	2.21	0.41
1:D:387:LYS:O	1:D:390:GLU:HB3	2.20	0.41
1:C:212:GLU:C	1:C:214:ARG:HB2	2.41	0.41
1:D:589:ARG:O	1:D:590:VAL:C	2.58	0.41
1:E:328:VAL:HG22	1:E:331:ARG:HH12	1.86	0.41
1:E:331:ARG:NH2	1:E:358:PRO:HG3	2.36	0.41
1:D:422:HIS:CD2	1:D:475:GLY:HA3	2.56	0.41
1:B:422:HIS:CD2	1:B:475:GLY:CA	3.04	0.41
1:E:576:LEU:O	1:E:577:LEU:C	2.59	0.41
1:E:408:SER:CB	1:E:409:PRO:HD2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:GLU:HG2	1:A:167:GLU:N	2.34	0.41
1:B:327:ASP:O	1:B:331:ARG:NH2	2.54	0.41
1:E:210:ALA:HB2	1:E:217:PHE:CD1	2.56	0.41
1:D:527:LEU:HD11	1:E:226:VAL:CG1	2.51	0.41
1:E:236:ARG:C	1:E:238:ARG:N	2.70	0.41
1:D:280:ASN:HA	1:D:283:LEU:CD2	2.51	0.41
1:D:257:ILE:HD11	1:D:299:ALA:HB1	2.03	0.41
1:E:177:ASN:N	1:E:177:ASN:OD1	2.54	0.41
1:F:155:PHE:C	1:F:157:ASP:N	2.71	0.41
1:F:274:GLU:O	1:F:275:ARG:C	2.59	0.41
1:F:207:ARG:CB	1:F:217:PHE:CZ	2.95	0.41
1:F:286:MET:HB2	1:F:286:MET:HE3	1.91	0.41
1:F:311:LEU:C	1:F:311:LEU:CD1	2.87	0.41
1:F:353:LEU:O	1:F:357:THR:HG23	2.21	0.41
1:F:354:ALA:O	1:F:357:THR:HG23	2.20	0.41
1:F:391:GLU:O	1:F:395:ARG:CB	2.69	0.41
1:C:509:GLY:C	1:D:476:ARG:NH2	2.61	0.41
1:D:417:TYR:O	1:D:420:ALA:HB3	2.21	0.41
1:D:458:LEU:HG	1:D:460:TRP:CE3	2.56	0.41
1:C:463:LYS:H	1:D:486:VAL:CG1	2.34	0.41
1:E:451:MET:CB	1:E:452:PRO:HD3	2.51	0.41
1:C:180:ARG:HG2	1:C:180:ARG:H	1.53	0.41
1:C:291:LYS:O	1:C:292:ASP:C	2.59	0.41
1:C:286:MET:CE	1:C:297:VAL:HG21	2.50	0.41
1:F:509:GLY:O	1:F:510:MET:HG2	2.21	0.41
1:D:212:GLU:O	1:D:214:ARG:HG3	2.21	0.41
1:D:357:THR:HB	1:D:360:PHE:CD2	2.56	0.41
1:D:376:ALA:CA	1:D:381:ARG:CG	2.80	0.41
1:D:381:ARG:NH1	1:D:384:ILE:HA	2.35	0.41
1:C:215:VAL:CG2	1:C:216:PRO:CD	2.97	0.41
1:B:567:GLU:O	1:B:568:VAL:C	2.59	0.41
1:B:572:VAL:HG11	1:B:587:PHE:HE1	1.86	0.41
1:B:589:ARG:CD	1:B:596:LEU:HD21	2.50	0.41
1:B:468:GLN:O	1:B:469:ILE:C	2.59	0.41
1:D:594:LEU:C	1:D:594:LEU:HD23	2.41	0.41
1:E:153:VAL:CG1	1:E:157:ASP:HB2	2.51	0.41
1:F:441:VAL:O	1:F:442:PRO:C	2.58	0.41
1:A:157:ASP:OD1	1:A:157:ASP:N	2.53	0.41
1:B:307:LEU:HD12	1:B:307:LEU:H	1.86	0.41
1:E:196:GLY:CA	1:E:202:LYS:NZ	2.84	0.41
1:E:337:ILE:CD1	1:E:338:HIS:CD2	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:GLU:O	1:A:164:ALA:C	2.59	0.41
1:C:163:GLU:O	1:C:164:ALA:C	2.59	0.41
1:B:521:VAL:HG12	1:C:495:ARG:HD2	2.03	0.41
1:F:424:LEU:O	1:F:425:ALA:C	2.60	0.41
1:D:228:MET:O	1:D:229:PHE:HB2	2.20	0.41
1:C:513:GLU:O	1:D:548:ARG:CZ	2.69	0.41
1:A:182:HIS:N	1:A:182:HIS:CD2	2.89	0.41
1:A:225:PHE:HB3	1:A:226:VAL:H	1.77	0.41
1:A:352:LEU:CD1	1:A:356:ARG:NH2	2.72	0.41
1:D:215:VAL:HG21	1:D:249:PRO:C	2.41	0.41
1:E:203:THR:HG22	1:E:253:PHE:CZ	2.56	0.41
1:E:250:CYS:HB3	1:E:295:ILE:HG13	2.02	0.41
1:A:378:ARG:HA	1:F:173:GLU:OE2	2.20	0.41
1:F:199:GLY:O	1:F:361:VAL:CG2	2.69	0.41
1:F:336:ARG:O	1:F:337:ILE:C	2.58	0.41
1:D:468:GLN:O	1:D:469:ILE:C	2.58	0.41
1:C:226:VAL:HG22	1:C:274:GLU:HG2	2.02	0.41
1:B:492:ASN:O	1:B:493:ASP:C	2.59	0.41
1:D:376:ALA:HB1	1:D:381:ARG:CB	2.51	0.41
1:B:179:SER:HA	1:B:182:HIS:NE2	2.36	0.41
1:B:467:ASP:O	1:B:471:VAL:HG13	2.20	0.41
1:D:594:LEU:O	1:D:594:LEU:HD23	2.20	0.41
1:B:412:ARG:NH2	1:B:440:ILE:HB	2.28	0.41
1:D:180:ARG:NH2	1:E:377:ALA:HA	2.36	0.41
1:E:199:GLY:HA2	2:E:1001:ADP:PA	2.61	0.41
1:C:373:ALA:HA	1:C:384:ILE:HD11	2.02	0.41
1:C:372:ALA:HB3	1:C:389:LEU:HD23	2.03	0.41
1:B:428:PHE:HE1	1:B:432:ALA:C	2.23	0.41
1:A:513:GLU:O	1:B:548:ARG:CZ	2.68	0.41
1:A:248:ALA:HA	1:A:249:PRO:HA	1.92	0.40
1:A:252:VAL:O	1:A:297:VAL:HA	2.21	0.40
1:A:423:ALA:HB1	1:A:587:PHE:CE1	2.57	0.40
1:A:571:ARG:O	1:A:575:THR:HG23	2.20	0.40
1:F:160:GLY:H	1:F:333:GLN:HE22	1.68	0.40
1:F:260:VAL:O	1:F:262:ARG:N	2.48	0.40
1:C:410:ARG:O	1:C:411:ASP:C	2.58	0.40
1:C:445:ARG:C	1:C:447:LEU:N	2.74	0.40
1:C:514:PHE:HB3	1:C:519:TYR:OH	2.20	0.40
1:C:147:LEU:HD12	1:C:148:THR:N	2.36	0.40
1:C:171:ILE:O	1:C:172:VAL:C	2.59	0.40
1:C:210:ALA:HB2	1:C:217:PHE:CD1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:VAL:C	1:B:232:VAL:H	2.24	0.40
1:B:568:VAL:HG13	1:B:591:VAL:HA	2.02	0.40
1:B:459:HIS:C	1:B:459:HIS:HD1	2.15	0.40
1:B:483:PHE:C	1:B:485:ASP:H	2.24	0.40
1:E:561:LEU:O	1:E:564:GLU:HB3	2.21	0.40
1:E:411:ASP:O	1:E:415:THR:OG1	2.31	0.40
1:A:407:LEU:HG	1:A:407:LEU:H	1.57	0.40
1:A:413:ARG:O	1:A:577:LEU:HD21	2.21	0.40
1:B:360:PHE:CE1	1:B:364:ASP:HB3	2.55	0.40
1:C:381:ARG:CG	1:C:382:ARG:N	2.81	0.40
1:D:216:PRO:HG3	1:D:247:HIS:CE1	2.56	0.40
1:E:238:ARG:HG2	1:E:242:GLU:OE2	2.21	0.40
1:E:286:MET:HA	1:E:289:PHE:CE2	2.57	0.40
1:A:382:ARG:HG3	1:A:383:LYS:CA	2.51	0.40
1:F:155:PHE:HB2	1:F:158:VAL:HB	2.03	0.40
1:F:192:VAL:O	1:F:317:PHE:HE2	2.04	0.40
1:F:260:VAL:C	1:F:279:LEU:HD11	2.38	0.40
1:F:238:ARG:N	1:F:281:GLN:HE21	2.20	0.40
1:C:331:ARG:NH2	1:C:358:PRO:HG3	2.36	0.40
1:E:461:SER:O	1:E:462:ARG:C	2.60	0.40
1:C:316:ARG:O	1:C:318:ASP:N	2.54	0.40
1:F:303:ARG:HA	1:F:304:PRO:HD2	1.90	0.40
1:F:307:LEU:H	1:F:307:LEU:HD12	1.86	0.40
1:D:441:VAL:O	1:D:442:PRO:C	2.59	0.40
1:E:396:VAL:CG1	1:E:397:MET:N	2.84	0.40
1:D:256:GLU:CG	1:D:256:GLU:O	2.69	0.40
1:F:538:GLU:O	1:F:540:ALA:N	2.54	0.40
1:E:582:LEU:HD21	1:E:590:VAL:HG11	2.02	0.40
1:B:329:LYS:HG2	1:B:330:GLY:N	2.36	0.40
1:B:344:LEU:CD1	1:B:346:GLU:OE1	2.70	0.40
1:D:257:ILE:O	1:D:258:ASP:C	2.60	0.40
1:A:422:HIS:O	1:A:423:ALA:C	2.59	0.40
1:F:349:ASP:C	1:F:350:LEU:HG	2.41	0.40
1:C:464:ARG:O	1:C:465:LEU:C	2.57	0.40
1:D:508:TRP:O	1:D:510:MET:HG3	2.22	0.40
1:E:450:MET:O	1:E:454:ARG:HB3	2.21	0.40
1:B:452:PRO:O	1:B:456:ASP:CG	2.60	0.40
1:D:155:PHE:C	1:D:157:ASP:N	2.69	0.40
1:D:367:ASN:O	1:D:371:GLU:HG2	2.22	0.40
1:D:377:ALA:N	1:D:381:ARG:HB2	2.35	0.40
1:C:176:LYS:HG2	1:C:176:LYS:H	1.76	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:ALA:O	1:B:238:ARG:NE	2.51	0.40
1:B:567:GLU:O	1:B:570:GLU:HB3	2.21	0.40
1:B:460:TRP:HD1	1:B:464:ARG:HG2	1.86	0.40
1:C:484:ASP:C	1:C:486:VAL:H	2.23	0.40
1:C:153:VAL:CG1	1:C:157:ASP:HB2	2.51	0.40
1:B:188:ILE:HD12	1:B:189:PRO:HD3	2.03	0.40
1:D:536:SER:HB2	1:E:537:GLU:OE2	2.20	0.40
1:F:538:GLU:C	1:F:540:ALA:N	2.72	0.40
1:B:531:ASP:N	1:B:531:ASP:OD1	2.55	0.40
1:A:166:GLU:HB2	1:A:169:LYS:HZ1	1.82	0.40
1:A:173:GLU:CA	1:A:176:LYS:HG3	2.43	0.40
1:A:314:PRO:HA	1:A:318:ASP:HB3	2.04	0.40
1:B:346:GLU:OE2	1:B:348:VAL:HG12	2.22	0.40
1:B:313:ARG:O	1:B:316:ARG:HB2	2.21	0.40
1:D:193:LEU:HD12	1:D:194:LEU:H	1.86	0.40
1:E:173:GLU:HG2	1:E:174:PHE:N	2.37	0.40
1:E:182:HIS:CD2	1:E:182:HIS:N	2.90	0.40
1:E:226:VAL:CG2	1:E:274:GLU:HG2	2.51	0.40
1:F:180:ARG:HH12	1:F:184:MET:CE	2.31	0.40
1:F:241:PHE:O	1:F:243:THR:N	2.54	0.40
1:F:263:LYS:HD2	1:F:263:LYS:HA	1.38	0.40
1:A:263:LYS:CG	1:A:264:ARG:N	2.83	0.40
1:D:464:ARG:O	1:D:467:ASP:N	2.55	0.40
1:D:478:ALA:O	1:D:479:GLU:C	2.58	0.40
1:D:505:ILE:HG21	1:D:543:ILE:HG12	2.04	0.40
1:D:518:ALA:HB3	1:E:495:ARG:HA	2.03	0.40
1:B:417:TYR:O	1:B:420:ALA:HB3	2.21	0.40
1:F:478:ALA:O	1:F:482:VAL:HG12	2.21	0.40
1:D:568:VAL:HG13	1:D:591:VAL:HA	2.02	0.40
1:F:469:ILE:HG23	1:F:497:ALA:HB1	2.02	0.40
1:F:597:GLU:O	1:F:599:PRO:CD	2.68	0.40
1:B:422:HIS:CD2	1:B:475:GLY:HA3	2.57	0.40
1:A:355:LYS:HD3	1:A:355:LYS:HA	1.90	0.40
1:E:572:VAL:O	1:E:573:ALA:C	2.60	0.40
1:A:316:ARG:O	1:A:318:ASP:N	2.55	0.40
1:A:333:GLN:HA	1:A:336:ARG:NH2	2.36	0.40
1:B:349:ASP:C	1:B:350:LEU:HG	2.41	0.40
1:B:387:LYS:O	1:B:390:GLU:HB3	2.21	0.40
1:B:260:VAL:O	1:B:262:ARG:N	2.47	0.40
1:E:174:PHE:CG	1:E:175:LEU:N	2.85	0.40
1:E:252:VAL:HB	1:E:297:VAL:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:182:HIS:HD1	1:E:291:LYS:HB2	1.86	0.40
1:F:183:GLU:OE1	1:F:184:MET:N	2.55	0.40
1:F:216:PRO:O	1:F:250:CYS:HB2	2.22	0.40
1:F:345:ALA:HB2	1:F:383:LYS:NZ	2.37	0.40
1:D:424:LEU:O	1:D:425:ALA:C	2.60	0.40
1:D:467:ASP:O	1:D:471:VAL:HG13	2.21	0.40
1:D:514:PHE:HB3	1:D:519:TYR:CE1	2.56	0.40
1:C:225:PHE:HB3	1:C:226:VAL:H	1.73	0.40
1:D:161:ALA:O	1:D:164:ALA:HB3	2.21	0.40
1:D:332:GLU:CD	1:D:351:ALA:HA	2.42	0.40
1:D:173:GLU:OE1	1:E:378:ARG:HA	2.21	0.40
1:B:249:PRO:O	1:B:250:CYS:HB3	2.21	0.40
1:E:397:MET:SD	1:E:406:VAL:HG11	2.62	0.40
1:B:525:THR:HG22	1:B:526:TYR:N	2.34	0.40
1:A:194:LEU:HD12	1:A:194:LEU:H	1.87	0.40

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:570:GLU:CG	1:D:382:ARG:NH2[3_564]	1.61	0.59
1:A:417:TYR:OH	1:D:382:ARG:NE[3_564]	1.74	0.46
1:A:177:ASN:OD1	1:E:214:ARG:NH2[6_665]	1.85	0.35
1:B:238:ARG:NE	1:F:378:ARG:NH2[6_665]	1.91	0.29
1:A:570:GLU:CB	1:D:382:ARG:NH2[3_564]	2.08	0.12
1:A:176:LYS:O	1:E:214:ARG:NH1[6_665]	2.11	0.09
1:B:238:ARG:CZ	1:F:378:ARG:NH2[6_665]	2.17	0.03
1:B:224:ASP:OD2	1:E:180:ARG:NH2[6_665]	2.17	0.03

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	456/508 (90%)	323 (71%)	111 (24%)	22 (5%)	3	32
1	B	442/508 (87%)	289 (65%)	125 (28%)	28 (6%)	2	26
1	C	456/508 (90%)	323 (71%)	112 (25%)	21 (5%)	3	33
1	D	442/508 (87%)	288 (65%)	121 (27%)	33 (8%)	1	21
1	E	456/508 (90%)	324 (71%)	110 (24%)	22 (5%)	3	32
1	F	442/508 (87%)	288 (65%)	120 (27%)	34 (8%)	1	20
All	All	2694/3048 (88%)	1835 (68%)	699 (26%)	160 (6%)	2	28

All (160) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	153	VAL
1	A	511	HIS
1	B	153	VAL
1	B	274	GLU
1	B	379	GLU
1	B	511	HIS
1	B	580	GLU
1	C	153	VAL
1	D	153	VAL
1	D	274	GLU
1	D	319	ARG
1	D	379	GLU
1	D	511	HIS
1	D	580	GLU
1	E	153	VAL
1	E	511	HIS
1	F	153	VAL
1	F	274	GLU
1	F	379	GLU
1	F	511	HIS
1	F	580	GLU
1	A	169	LYS
1	A	224	ASP
1	A	390	GLU
1	A	449	PHE
1	A	457	MET
1	A	489	GLY
1	A	492	ASN
1	A	512	PRO
1	B	180	ARG

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Mol	Chain	Res	Type
1	B	319	ARG
1	B	376	ALA
1	B	435	VAL
1	B	456	ASP
1	B	489	GLY
1	B	512	PRO
1	B	530	TYR
1	B	593	GLY
1	C	224	ASP
1	C	341	GLY
1	C	390	GLU
1	C	457	MET
1	C	489	GLY
1	C	492	ASN
1	C	512	PRO
1	D	180	ARG
1	D	292	ASP
1	D	305	ASP
1	D	376	ALA
1	D	435	VAL
1	D	489	GLY
1	D	512	PRO
1	D	530	TYR
1	D	593	GLY
1	E	224	ASP
1	E	449	PHE
1	E	457	MET
1	E	489	GLY
1	E	492	ASN
1	E	512	PRO
1	F	180	ARG
1	F	319	ARG
1	F	376	ALA
1	F	435	VAL
1	F	489	GLY
1	F	512	PRO
1	F	530	TYR
1	F	593	GLY
1	A	172	VAL
1	A	262	ARG
1	A	264	ARG
1	A	341	GLY

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Mol	Chain	Res	Type
1	A	442	PRO
1	B	305	ASP
1	B	565	LYS
1	C	169	LYS
1	C	172	VAL
1	C	262	ARG
1	C	264	ARG
1	C	442	PRO
1	C	449	PHE
1	C	458	LEU
1	C	511	HIS
1	D	162	GLU
1	D	383	LYS
1	D	413	ARG
1	D	442	PRO
1	D	456	ASP
1	D	565	LYS
1	E	262	ARG
1	E	264	ARG
1	E	341	GLY
1	E	390	GLU
1	E	442	PRO
1	E	464	ARG
1	F	162	GLU
1	F	305	ASP
1	F	456	ASP
1	F	565	LYS
1	A	458	LEU
1	B	162	GLU
1	B	448	GLY
1	B	570	GLU
1	C	150	ALA
1	D	570	GLU
1	E	150	ALA
1	E	169	LYS
1	E	172	VAL
1	E	458	LEU
1	F	283	LEU
1	F	442	PRO
1	F	570	GLU
1	A	150	ALA
1	A	410	ARG

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Mol	Chain	Res	Type
1	B	258	ASP
1	B	283	LEU
1	B	442	PRO
1	C	214	ARG
1	C	274	GLU
1	C	410	ARG
1	D	258	ASP
1	D	283	LEU
1	D	369	LEU
1	D	567	GLU
1	E	410	ARG
1	F	165	LYS
1	F	258	ASP
1	F	527	LEU
1	A	202	LYS
1	A	484	ASP
1	B	228	MET
1	B	359	GLY
1	D	228	MET
1	D	261	GLY
1	D	448	GLY
1	D	527	LEU
1	E	202	LYS
1	F	164	ALA
1	F	228	MET
1	F	292	ASP
1	F	383	LYS
1	F	444	GLY
1	F	448	GLY
1	B	261	GLY
1	D	326	PRO
1	F	359	GLY
1	D	359	GLY
1	F	261	GLY
1	F	326	PRO
1	B	209	VAL
1	B	326	PRO
1	B	444	GLY
1	D	209	VAL
1	F	209	VAL
1	A	261	GLY
1	F	197	PRO

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Mol	Chain	Res	Type
1	A	326	PRO
1	C	326	PRO
1	E	261	GLY
1	E	326	PRO

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	365/402 (91%)	240 (66%)	125 (34%)	0	2
1	B	361/402 (90%)	242 (67%)	119 (33%)	0	3
1	C	365/402 (91%)	240 (66%)	125 (34%)	0	2
1	D	361/402 (90%)	241 (67%)	120 (33%)	0	3
1	E	365/402 (91%)	244 (67%)	121 (33%)	0	3
1	F	361/402 (90%)	240 (66%)	121 (34%)	0	2
All	All	2178/2412 (90%)	1447 (66%)	731 (34%)	0	2

All (731) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	ARG
1	A	146	VAL
1	A	147	LEU
1	A	154	THR
1	A	157	ASP
1	A	166	GLU
1	A	171	ILE
1	A	172	VAL
1	A	173	GLU
1	A	174	PHE
1	A	175	LEU
1	A	177	ASN
1	A	179	SER
1	A	181	PHE

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Mol	Chain	Res	Type
1	A	182	HIS
1	A	183	GLU
1	A	188	ILE
1	A	190	LYS
1	A	194	LEU
1	A	200	VAL
1	A	207	ARG
1	A	214	ARG
1	A	215	VAL
1	A	217	PHE
1	A	218	ILE
1	A	219	THR
1	A	221	SER
1	A	223	SER
1	A	225	PHE
1	A	226	VAL
1	A	236	ARG
1	A	242	GLU
1	A	245	LYS
1	A	251	ILE
1	A	262	ARG
1	A	264	ARG
1	A	273	ASP
1	A	275	ARG
1	A	277	GLN
1	A	279	LEU
1	A	281	GLN
1	A	282	LEU
1	A	290	GLU
1	A	292	ASP
1	A	293	THR
1	A	296	VAL
1	A	301	THR
1	A	303	ARG
1	A	305	ASP
1	A	306	ILE
1	A	307	LEU
1	A	308	ASP
1	A	312	LEU
1	A	317	PHE
1	A	318	ASP
1	A	320	GLN

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Mol	Chain	Res	Type
1	A	323	ILE
1	A	327	ASP
1	A	344	LEU
1	A	347	ASP
1	A	349	ASP
1	A	350	LEU
1	A	352	LEU
1	A	355	LYS
1	A	357	THR
1	A	360	PHE
1	A	364	ASP
1	A	368	LEU
1	A	371	GLU
1	A	375	LEU
1	A	378	ARG
1	A	381	ARG
1	A	382	ARG
1	A	383	LYS
1	A	388	ASP
1	A	390	GLU
1	A	391	GLU
1	A	394	ASP
1	A	396	VAL
1	A	397	MET
1	A	402	LYS
1	A	405	LEU
1	A	406	VAL
1	A	407	LEU
1	A	414	ILE
1	A	419	GLU
1	A	433	ASP
1	A	436	HIS
1	A	443	ARG
1	A	449	PHE
1	A	453	ARG
1	A	454	ARG
1	A	459	HIS
1	A	461	SER
1	A	462	ARG
1	A	464	ARG
1	A	465	LEU
1	A	484	ASP

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Mol	Chain	Res	Type
1	A	487	THR
1	A	491	GLU
1	A	493	ASP
1	A	502	ARG
1	A	511	HIS
1	A	514	PHE
1	A	524	ASP
1	A	530	TYR
1	A	532	VAL
1	A	535	TYR
1	A	536	SER
1	A	537	GLU
1	A	539	THR
1	A	541	LYS
1	A	548	ARG
1	A	550	LEU
1	A	558	VAL
1	A	561	LEU
1	A	566	ARG
1	A	569	LEU
1	A	574	GLU
1	A	576	LEU
1	A	578	GLU
1	A	579	ARG
1	A	585	GLU
1	A	594	LEU
1	A	596	LEU
1	B	153	VAL
1	B	157	ASP
1	B	162	GLU
1	B	166	GLU
1	B	167	GLU
1	B	171	ILE
1	B	172	VAL
1	B	174	PHE
1	B	175	LEU
1	B	179	SER
1	B	182	HIS
1	B	183	GLU
1	B	184	MET
1	B	187	ARG
1	B	188	ILE

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Mol	Chain	Res	Type
1	B	192	VAL
1	B	193	LEU
1	B	195	VAL
1	B	202	LYS
1	B	203	THR
1	B	207	ARG
1	B	214	ARG
1	B	217	PHE
1	B	223	SER
1	B	227	GLU
1	B	236	ARG
1	B	237	VAL
1	B	238	ARG
1	B	240	LEU
1	B	242	GLU
1	B	243	THR
1	B	245	LYS
1	B	246	ARG
1	B	252	VAL
1	B	253	PHE
1	B	255	ASP
1	B	256	GLU
1	B	258	ASP
1	B	260	VAL
1	B	263	LYS
1	B	273	ASP
1	B	274	GLU
1	B	284	VAL
1	B	287	ASP
1	B	291	LYS
1	B	295	ILE
1	B	297	VAL
1	B	301	THR
1	B	303	ARG
1	B	308	ASP
1	B	311	LEU
1	B	312	LEU
1	B	318	ASP
1	B	319	ARG
1	B	323	ILE
1	B	332	GLU
1	B	342	LYS

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Mol	Chain	Res	Type
1	B	344	LEU
1	B	347	ASP
1	B	348	VAL
1	B	350	LEU
1	B	352	LEU
1	B	356	ARG
1	B	357	THR
1	B	360	PHE
1	B	367	ASN
1	B	375	LEU
1	B	378	ARG
1	B	382	ARG
1	B	386	MET
1	B	387	LYS
1	B	389	LEU
1	B	395	ARG
1	B	397	MET
1	B	405	LEU
1	B	407	LEU
1	B	413	ARG
1	B	414	ILE
1	B	424	LEU
1	B	428	PHE
1	B	429	LEU
1	B	430	GLU
1	B	433	ASP
1	B	435	VAL
1	B	436	HIS
1	B	450	MET
1	B	453	ARG
1	B	455	GLU
1	B	457	MET
1	B	458	LEU
1	B	459	HIS
1	B	460	TRP
1	B	462	ARG
1	B	463	LYS
1	B	476	ARG
1	B	484	ASP
1	B	485	ASP
1	B	503	ARG
1	B	506	THR

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Mol	Chain	Res	Type
1	B	517	VAL
1	B	521	VAL
1	B	522	ARG
1	B	527	LEU
1	B	531	ASP
1	B	533	ARG
1	B	535	TYR
1	B	539	THR
1	B	548	ARG
1	B	558	VAL
1	B	563	LEU
1	B	570	GLU
1	B	577	LEU
1	B	578	GLU
1	B	581	THR
1	B	583	THR
1	B	586	GLU
1	B	592	GLU
1	B	596	LEU
1	B	600	GLU
1	C	145	ARG
1	C	146	VAL
1	C	147	LEU
1	C	154	THR
1	C	157	ASP
1	C	166	GLU
1	C	172	VAL
1	C	173	GLU
1	C	174	PHE
1	C	175	LEU
1	C	177	ASN
1	C	179	SER
1	C	181	PHE
1	C	182	HIS
1	C	183	GLU
1	C	190	LYS
1	C	194	LEU
1	C	200	VAL
1	C	207	ARG
1	C	215	VAL
1	C	217	PHE
1	C	218	ILE

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Mol	Chain	Res	Type
1	C	219	THR
1	C	221	SER
1	C	225	PHE
1	C	226	VAL
1	C	236	ARG
1	C	242	GLU
1	C	245	LYS
1	C	251	ILE
1	C	262	ARG
1	C	264	ARG
1	C	273	ASP
1	C	274	GLU
1	C	275	ARG
1	C	277	GLN
1	C	279	LEU
1	C	282	LEU
1	C	287	ASP
1	C	290	GLU
1	C	292	ASP
1	C	293	THR
1	C	296	VAL
1	C	303	ARG
1	C	305	ASP
1	C	306	ILE
1	C	307	LEU
1	C	308	ASP
1	C	312	LEU
1	C	317	PHE
1	C	318	ASP
1	C	320	GLN
1	C	323	ILE
1	C	327	ASP
1	C	334	ILE
1	C	340	ARG
1	C	344	LEU
1	C	347	ASP
1	C	349	ASP
1	C	350	LEU
1	C	352	LEU
1	C	355	LYS
1	C	357	THR
1	C	360	PHE

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Mol	Chain	Res	Type
1	C	364	ASP
1	C	368	LEU
1	C	371	GLU
1	C	375	LEU
1	C	378	ARG
1	C	381	ARG
1	C	382	ARG
1	C	388	ASP
1	C	390	GLU
1	C	391	GLU
1	C	394	ASP
1	C	396	VAL
1	C	397	MET
1	C	402	LYS
1	C	405	LEU
1	C	406	VAL
1	C	407	LEU
1	C	414	ILE
1	C	419	GLU
1	C	433	ASP
1	C	436	HIS
1	C	437	LYS
1	C	443	ARG
1	C	449	PHE
1	C	453	ARG
1	C	454	ARG
1	C	459	HIS
1	C	461	SER
1	C	462	ARG
1	C	464	ARG
1	C	465	LEU
1	C	481	ILE
1	C	482	VAL
1	C	484	ASP
1	C	487	THR
1	C	491	GLU
1	C	493	ASP
1	C	496	GLN
1	C	502	ARG
1	C	511	HIS
1	C	514	PHE
1	C	524	ASP

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Mol	Chain	Res	Type
1	C	530	TYR
1	C	532	VAL
1	C	535	TYR
1	C	536	SER
1	C	537	GLU
1	C	539	THR
1	C	548	ARG
1	C	550	LEU
1	C	558	VAL
1	C	561	LEU
1	C	566	ARG
1	C	569	LEU
1	C	574	GLU
1	C	576	LEU
1	C	577	LEU
1	C	578	GLU
1	C	579	ARG
1	C	585	GLU
1	C	594	LEU
1	D	152	LYS
1	D	153	VAL
1	D	162	GLU
1	D	166	GLU
1	D	167	GLU
1	D	171	ILE
1	D	172	VAL
1	D	174	PHE
1	D	175	LEU
1	D	179	SER
1	D	182	HIS
1	D	183	GLU
1	D	184	MET
1	D	187	ARG
1	D	188	ILE
1	D	190	LYS
1	D	193	LEU
1	D	195	VAL
1	D	202	LYS
1	D	203	THR
1	D	207	ARG
1	D	214	ARG
1	D	217	PHE

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Mol	Chain	Res	Type
1	D	223	SER
1	D	227	GLU
1	D	236	ARG
1	D	237	VAL
1	D	238	ARG
1	D	242	GLU
1	D	243	THR
1	D	245	LYS
1	D	246	ARG
1	D	252	VAL
1	D	253	PHE
1	D	256	GLU
1	D	258	ASP
1	D	260	VAL
1	D	263	LYS
1	D	273	ASP
1	D	274	GLU
1	D	284	VAL
1	D	285	GLU
1	D	287	ASP
1	D	289	PHE
1	D	291	LYS
1	D	295	ILE
1	D	297	VAL
1	D	301	THR
1	D	303	ARG
1	D	308	ASP
1	D	311	LEU
1	D	312	LEU
1	D	316	ARG
1	D	318	ASP
1	D	319	ARG
1	D	323	ILE
1	D	332	GLU
1	D	342	LYS
1	D	344	LEU
1	D	347	ASP
1	D	348	VAL
1	D	350	LEU
1	D	352	LEU
1	D	356	ARG
1	D	357	THR

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Mol	Chain	Res	Type
1	D	360	PHE
1	D	367	ASN
1	D	375	LEU
1	D	378	ARG
1	D	382	ARG
1	D	385	THR
1	D	386	MET
1	D	387	LYS
1	D	388	ASP
1	D	389	LEU
1	D	395	ARG
1	D	397	MET
1	D	405	LEU
1	D	407	LEU
1	D	413	ARG
1	D	414	ILE
1	D	424	LEU
1	D	428	PHE
1	D	429	LEU
1	D	430	GLU
1	D	433	ASP
1	D	435	VAL
1	D	436	HIS
1	D	450	MET
1	D	453	ARG
1	D	455	GLU
1	D	457	MET
1	D	458	LEU
1	D	459	HIS
1	D	460	TRP
1	D	462	ARG
1	D	463	LYS
1	D	476	ARG
1	D	484	ASP
1	D	485	ASP
1	D	500	LEU
1	D	503	ARG
1	D	506	THR
1	D	517	VAL
1	D	521	VAL
1	D	522	ARG
1	D	531	ASP

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Mol	Chain	Res	Type
1	D	533	ARG
1	D	535	TYR
1	D	539	THR
1	D	548	ARG
1	D	563	LEU
1	D	567	GLU
1	D	570	GLU
1	D	577	LEU
1	D	578	GLU
1	D	581	THR
1	D	583	THR
1	D	592	GLU
1	D	600	GLU
1	E	145	ARG
1	E	146	VAL
1	E	147	LEU
1	E	154	THR
1	E	157	ASP
1	E	166	GLU
1	E	172	VAL
1	E	173	GLU
1	E	174	PHE
1	E	175	LEU
1	E	177	ASN
1	E	179	SER
1	E	181	PHE
1	E	182	HIS
1	E	183	GLU
1	E	194	LEU
1	E	200	VAL
1	E	207	ARG
1	E	215	VAL
1	E	217	PHE
1	E	218	ILE
1	E	219	THR
1	E	221	SER
1	E	223	SER
1	E	225	PHE
1	E	226	VAL
1	E	236	ARG
1	E	242	GLU
1	E	245	LYS

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Mol	Chain	Res	Type
1	E	251	ILE
1	E	262	ARG
1	E	264	ARG
1	E	273	ASP
1	E	274	GLU
1	E	275	ARG
1	E	277	GLN
1	E	279	LEU
1	E	282	LEU
1	E	289	PHE
1	E	290	GLU
1	E	292	ASP
1	E	293	THR
1	E	296	VAL
1	E	303	ARG
1	E	305	ASP
1	E	306	ILE
1	E	307	LEU
1	E	308	ASP
1	E	312	LEU
1	E	317	PHE
1	E	318	ASP
1	E	320	GLN
1	E	323	ILE
1	E	327	ASP
1	E	344	LEU
1	E	347	ASP
1	E	349	ASP
1	E	350	LEU
1	E	352	LEU
1	E	355	LYS
1	E	357	THR
1	E	360	PHE
1	E	364	ASP
1	E	368	LEU
1	E	371	GLU
1	E	375	LEU
1	E	378	ARG
1	E	381	ARG
1	E	382	ARG
1	E	383	LYS
1	E	388	ASP

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Mol	Chain	Res	Type
1	E	390	GLU
1	E	391	GLU
1	E	394	ASP
1	E	396	VAL
1	E	397	MET
1	E	402	LYS
1	E	405	LEU
1	E	406	VAL
1	E	407	LEU
1	E	414	ILE
1	E	419	GLU
1	E	433	ASP
1	E	436	HIS
1	E	439	THR
1	E	443	ARG
1	E	449	PHE
1	E	453	ARG
1	E	454	ARG
1	E	459	HIS
1	E	461	SER
1	E	462	ARG
1	E	464	ARG
1	E	465	LEU
1	E	482	VAL
1	E	484	ASP
1	E	487	THR
1	E	491	GLU
1	E	493	ASP
1	E	502	ARG
1	E	511	HIS
1	E	514	PHE
1	E	524	ASP
1	E	530	TYR
1	E	532	VAL
1	E	535	TYR
1	E	536	SER
1	E	537	GLU
1	E	539	THR
1	E	548	ARG
1	E	550	LEU
1	E	558	VAL
1	E	561	LEU

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Mol	Chain	Res	Type
1	E	566	ARG
1	E	569	LEU
1	E	574	GLU
1	E	576	LEU
1	E	578	GLU
1	E	579	ARG
1	E	585	GLU
1	E	594	LEU
1	F	152	LYS
1	F	153	VAL
1	F	162	GLU
1	F	166	GLU
1	F	167	GLU
1	F	171	ILE
1	F	172	VAL
1	F	174	PHE
1	F	175	LEU
1	F	179	SER
1	F	182	HIS
1	F	183	GLU
1	F	184	MET
1	F	187	ARG
1	F	188	ILE
1	F	193	LEU
1	F	195	VAL
1	F	200	VAL
1	F	202	LYS
1	F	203	THR
1	F	207	ARG
1	F	217	PHE
1	F	223	SER
1	F	224	ASP
1	F	227	GLU
1	F	236	ARG
1	F	237	VAL
1	F	238	ARG
1	F	242	GLU
1	F	243	THR
1	F	245	LYS
1	F	246	ARG
1	F	252	VAL
1	F	253	PHE

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Mol	Chain	Res	Type
1	F	255	ASP
1	F	256	GLU
1	F	258	ASP
1	F	260	VAL
1	F	263	LYS
1	F	273	ASP
1	F	274	GLU
1	F	284	VAL
1	F	287	ASP
1	F	291	LYS
1	F	295	ILE
1	F	297	VAL
1	F	301	THR
1	F	303	ARG
1	F	308	ASP
1	F	311	LEU
1	F	312	LEU
1	F	316	ARG
1	F	318	ASP
1	F	319	ARG
1	F	323	ILE
1	F	332	GLU
1	F	335	LEU
1	F	342	LYS
1	F	344	LEU
1	F	347	ASP
1	F	348	VAL
1	F	350	LEU
1	F	352	LEU
1	F	356	ARG
1	F	357	THR
1	F	360	PHE
1	F	367	ASN
1	F	375	LEU
1	F	378	ARG
1	F	382	ARG
1	F	386	MET
1	F	387	LYS
1	F	388	ASP
1	F	389	LEU
1	F	395	ARG
1	F	397	MET

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Mol	Chain	Res	Type
1	F	405	LEU
1	F	407	LEU
1	F	414	ILE
1	F	424	LEU
1	F	428	PHE
1	F	429	LEU
1	F	430	GLU
1	F	433	ASP
1	F	435	VAL
1	F	436	HIS
1	F	450	MET
1	F	453	ARG
1	F	455	GLU
1	F	457	MET
1	F	458	LEU
1	F	459	HIS
1	F	460	TRP
1	F	462	ARG
1	F	463	LYS
1	F	476	ARG
1	F	484	ASP
1	F	485	ASP
1	F	500	LEU
1	F	503	ARG
1	F	506	THR
1	F	517	VAL
1	F	521	VAL
1	F	522	ARG
1	F	526	TYR
1	F	527	LEU
1	F	531	ASP
1	F	533	ARG
1	F	535	TYR
1	F	539	THR
1	F	548	ARG
1	F	557	ARG
1	F	558	VAL
1	F	563	LEU
1	F	570	GLU
1	F	577	LEU
1	F	578	GLU
1	F	581	THR

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Mol	Chain	Res	Type
1	F	583	THR
1	F	592	GLU
1	F	600	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	182	HIS
1	A	204	HIS
1	A	320	GLN
1	A	468	GLN
1	A	496	GLN
1	A	511	HIS
1	B	204	HIS
1	B	277	GLN
1	B	281	GLN
1	B	302	ASN
1	B	333	GLN
1	B	338	HIS
1	B	431	HIS
1	C	177	ASN
1	C	182	HIS
1	C	204	HIS
1	C	468	GLN
1	C	496	GLN
1	D	204	HIS
1	D	277	GLN
1	D	281	GLN
1	D	302	ASN
1	D	333	GLN
1	D	338	HIS
1	D	431	HIS
1	E	182	HIS
1	E	204	HIS
1	E	320	GLN
1	E	468	GLN
1	E	496	GLN
1	F	204	HIS
1	F	277	GLN
1	F	281	GLN
1	F	302	ASN
1	F	333	GLN

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Mol	Chain	Res	Type
1	F	338	HIS
1	F	431	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	ADP	A	1001	-	22,29,29	1.11	1 (4%)	27,45,45	2.06	4 (14%)
2	ADP	B	2001	-	22,29,29	1.09	2 (9%)	27,45,45	2.06	4 (14%)
2	ADP	C	1001	-	22,29,29	1.13	2 (9%)	27,45,45	2.29	5 (18%)
2	ADP	D	2001	-	22,29,29	1.06	2 (9%)	27,45,45	1.97	5 (18%)
2	ADP	E	1001	-	22,29,29	1.10	2 (9%)	27,45,45	1.86	5 (18%)
2	ADP	F	2001	-	22,29,29	1.05	1 (4%)	27,45,45	2.15	4 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	1001	-	-	0/12/32/32	0/3/3/3
2	ADP	B	2001	-	-	0/12/32/32	0/3/3/3
2	ADP	C	1001	-	-	0/12/32/32	0/3/3/3
2	ADP	D	2001	-	-	0/12/32/32	0/3/3/3
2	ADP	E	1001	-	-	0/12/32/32	0/3/3/3
2	ADP	F	2001	-	-	0/12/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1001	ADP	O4'-C1'	2.01	1.43	1.41
2	B	2001	ADP	O4'-C1'	2.17	1.43	1.41
2	D	2001	ADP	O4'-C1'	2.19	1.44	1.41
2	C	1001	ADP	O4'-C1'	2.32	1.44	1.41
2	D	2001	ADP	C5-C4	3.03	1.47	1.40
2	B	2001	ADP	C5-C4	3.23	1.47	1.40
2	C	1001	ADP	C5-C4	3.26	1.47	1.40
2	E	1001	ADP	C5-C4	3.39	1.48	1.40
2	F	2001	ADP	C5-C4	3.43	1.48	1.40
2	A	1001	ADP	C5-C4	3.45	1.48	1.40

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1001	ADP	N3-C2-N1	-7.88	122.86	128.89
2	B	2001	ADP	N3-C2-N1	-6.68	123.78	128.89
2	D	2001	ADP	N3-C2-N1	-6.61	123.83	128.89
2	A	1001	ADP	N3-C2-N1	-6.53	123.89	128.89
2	F	2001	ADP	N3-C2-N1	-6.48	123.93	128.89
2	F	2001	ADP	C2'-C1'-N9	-6.07	105.02	114.29
2	E	1001	ADP	N3-C2-N1	-5.88	124.39	128.89
2	C	1001	ADP	C2'-C1'-N9	-5.21	106.33	114.29
2	A	1001	ADP	C2'-C1'-N9	-4.98	106.69	114.29
2	B	2001	ADP	C2'-C1'-N9	-4.82	106.93	114.29
2	A	1001	ADP	PA-O3A-PB	-4.31	118.21	132.67
2	C	1001	ADP	PA-O3A-PB	-4.26	118.40	132.67
2	D	2001	ADP	C4-C5-N7	-4.18	105.63	109.48
2	E	1001	ADP	PA-O3A-PB	-4.10	118.92	132.67
2	B	2001	ADP	PA-O3A-PB	-4.04	119.13	132.67
2	E	1001	ADP	C2'-C1'-N9	-3.79	108.51	114.29
2	D	2001	ADP	C2'-C1'-N9	-3.75	108.57	114.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2001	ADP	PA-O3A-PB	-3.73	120.17	132.67
2	C	1001	ADP	C4-C5-N7	-3.62	106.15	109.48
2	F	2001	ADP	C4-C5-N7	-3.49	106.27	109.48
2	A	1001	ADP	C4-C5-N7	-3.28	106.46	109.48
2	B	2001	ADP	C4-C5-N7	-3.20	106.54	109.48
2	E	1001	ADP	C4-C5-N7	-3.11	106.61	109.48
2	D	2001	ADP	PA-O3A-PB	-2.77	123.39	132.67
2	E	1001	ADP	O3B-PB-O2B	2.02	115.08	107.38
2	C	1001	ADP	O2B-PB-O1B	2.05	117.17	110.58
2	D	2001	ADP	O3B-PB-O2B	2.27	116.03	107.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	ADP	8	0
2	B	2001	ADP	9	0
2	C	1001	ADP	10	0
2	D	2001	ADP	9	0
2	E	1001	ADP	11	0
2	F	2001	ADP	10	0

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	458/508 (90%)	0.04	22 (4%) 34 25	21, 118, 174, 229	0
1	B	446/508 (87%)	0.02	25 (5%) 28 20	16, 125, 176, 241	0
1	C	458/508 (90%)	0.19	28 (6%) 25 16	21, 129, 184, 237	0
1	D	446/508 (87%)	-0.08	19 (4%) 39 28	23, 103, 173, 241	0
1	E	458/508 (90%)	0.08	28 (6%) 25 16	24, 130, 179, 223	0
1	F	446/508 (87%)	0.09	24 (5%) 29 21	21, 128, 173, 261	0
All	All	2712/3048 (88%)	0.06	146 (5%) 29 21	16, 124, 177, 261	0

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	525	THR	6.6
1	E	404	SER	6.5
1	B	148	THR	5.8
1	B	147	LEU	5.7
1	E	269	GLY	5.3
1	C	271	GLY	5.2
1	A	145	ARG	5.2
1	F	272	ASN	5.2
1	E	294	ALA	5.0
1	F	431	HIS	4.6
1	A	272	ASN	4.6
1	A	250	CYS	4.6
1	E	403	LYS	4.5
1	D	228	MET	4.4
1	D	183	GLU	4.3
1	C	270	GLY	4.1
1	B	446	ALA	4.1
1	F	598	ALA	3.8
1	C	404	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	429	LEU	3.7
1	A	144	ALA	3.7
1	E	446	ALA	3.6
1	C	409	PRO	3.5
1	D	227	GLU	3.4
1	D	378	ARG	3.4
1	A	527	LEU	3.4
1	F	451	MET	3.4
1	D	377	ALA	3.4
1	B	429	LEU	3.4
1	E	290	GLU	3.4
1	A	294	ALA	3.4
1	E	270	GLY	3.4
1	C	239	ASP	3.3
1	B	597	GLU	3.3
1	F	382	ARG	3.3
1	F	600	GLU	3.3
1	D	272	ASN	3.3
1	E	526	TYR	3.3
1	C	430	GLU	3.3
1	C	186	ALA	3.2
1	B	222	GLY	3.2
1	B	598	ALA	3.2
1	D	599	PRO	3.2
1	B	456	ASP	3.2
1	E	402	LYS	3.2
1	F	383	LYS	3.1
1	C	448	GLY	3.1
1	C	456	ASP	3.1
1	E	149	GLU	3.1
1	E	527	LEU	3.1
1	E	265	GLY	3.1
1	C	229	PHE	3.1
1	C	403	LYS	3.1
1	F	452	PRO	3.1
1	C	599	PRO	3.1
1	A	143	ARG	3.0
1	C	265	GLY	3.0
1	F	222	GLY	3.0
1	F	347	ASP	3.0
1	C	290	GLU	3.0
1	E	401	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	600	GLU	2.9
1	D	170	GLU	2.9
1	F	287	ASP	2.9
1	F	450	MET	2.9
1	E	148	THR	2.8
1	A	249	PRO	2.8
1	B	239	ASP	2.8
1	F	147	LEU	2.8
1	F	404	SER	2.8
1	B	149	GLU	2.7
1	D	373	ALA	2.7
1	D	443	ARG	2.7
1	B	373	ALA	2.7
1	F	403	LYS	2.7
1	B	220	ALA	2.7
1	E	324	ASP	2.7
1	C	187	ARG	2.6
1	E	246	ARG	2.6
1	C	452	PRO	2.6
1	E	291	LYS	2.6
1	E	160	GLY	2.6
1	F	167	GLU	2.6
1	F	294	ALA	2.6
1	B	387	LYS	2.6
1	C	291	LYS	2.6
1	D	322	ALA	2.6
1	B	526	TYR	2.5
1	E	268	VAL	2.5
1	B	341	GLY	2.5
1	D	222	GLY	2.5
1	A	600	GLU	2.5
1	B	221	SER	2.4
1	A	401	ALA	2.4
1	E	177	ASN	2.4
1	D	294	ALA	2.4
1	B	226	VAL	2.4
1	D	600	GLU	2.4
1	C	266	SER	2.4
1	A	318	ASP	2.4
1	D	598	ALA	2.4
1	C	288	GLY	2.3
1	B	179	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	213	ALA	2.3
1	C	211	GLY	2.3
1	F	285	GLU	2.3
1	C	262	ARG	2.3
1	A	400	PRO	2.3
1	C	272	ASN	2.3
1	A	229	PHE	2.3
1	F	340	ARG	2.3
1	B	223	SER	2.3
1	C	524	ASP	2.3
1	E	452	PRO	2.3
1	F	597	GLU	2.3
1	D	446	ALA	2.3
1	B	225	PHE	2.2
1	B	593	GLY	2.2
1	A	456	ASP	2.2
1	D	223	SER	2.2
1	C	525	THR	2.2
1	A	271	GLY	2.2
1	A	173	GLU	2.2
1	A	452	PRO	2.2
1	A	528	GLY	2.2
1	E	485	ASP	2.2
1	A	430	GLU	2.1
1	B	157	ASP	2.1
1	D	349	ASP	2.1
1	F	273	ASP	2.1
1	E	173	GLU	2.1
1	B	445	ARG	2.1
1	D	295	ILE	2.1
1	A	404	SER	2.1
1	B	409	PRO	2.1
1	B	272	ASN	2.1
1	E	188	ILE	2.0
1	E	599	PRO	2.0
1	C	185	GLY	2.0
1	C	457	MET	2.0
1	A	599	PRO	2.0
1	E	399	LEU	2.0
1	E	400	PRO	2.0
1	F	221	SER	2.0
1	F	379	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	349	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
2	ADP	C	1001	27/27	0.80	0.29	0.11	70,73,74,76	0
2	ADP	D	2001	27/27	0.90	0.20	0.06	58,64,74,74	0
2	ADP	F	2001	27/27	0.89	0.18	-0.39	64,69,74,74	0
2	ADP	A	1001	27/27	0.90	0.19	-0.44	63,66,70,71	0
2	ADP	E	1001	27/27	0.90	0.21	-0.95	66,70,72,73	0
2	ADP	B	2001	27/27	0.92	0.15	-1.13	65,72,75,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.