



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:50 AM UTC

PDB ID : 4EIW / pdb_00004eiw
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.

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

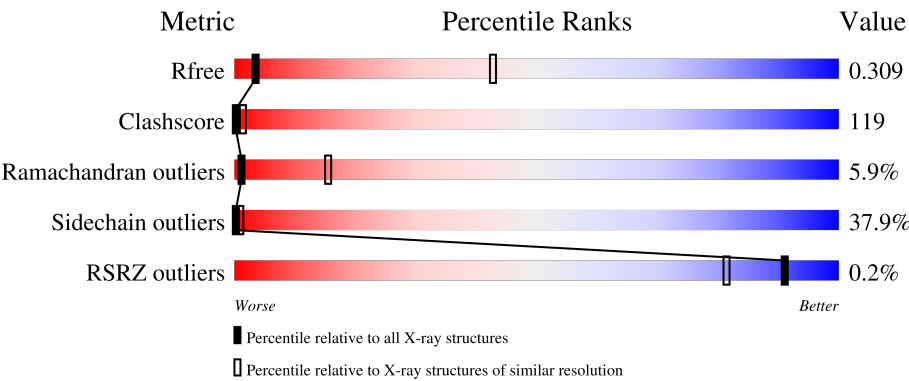
1 Overall quality at a glance i

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}	180053	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	508	14%48%26%•10%
1	B	508	8%48%26%5%12%
1	C	508	14%48%25%•10%
1	D	508	8%50%25%5%12%
1	E	508	15%47%26%•10%

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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

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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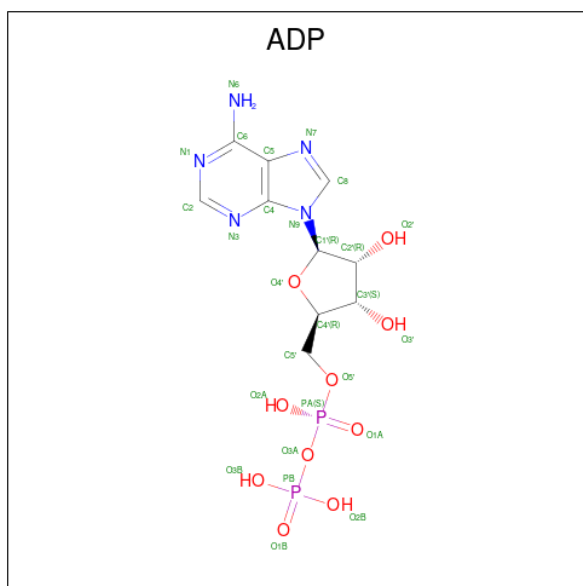
Chain	Residue	Modelled	Actual	Comment	Reference
B	124	GLY	-	expression tag	UNP Q5SI82
B	125	ALA	-	expression tag	UNP Q5SI82
B	399	LEU	GLY	engineered mutation	UNP Q5SI82
C	117	GLY	-	expression tag	UNP Q5SI82
C	118	PRO	-	expression tag	UNP Q5SI82
C	119	LEU	-	expression tag	UNP Q5SI82
C	120	GLY	-	expression 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 (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

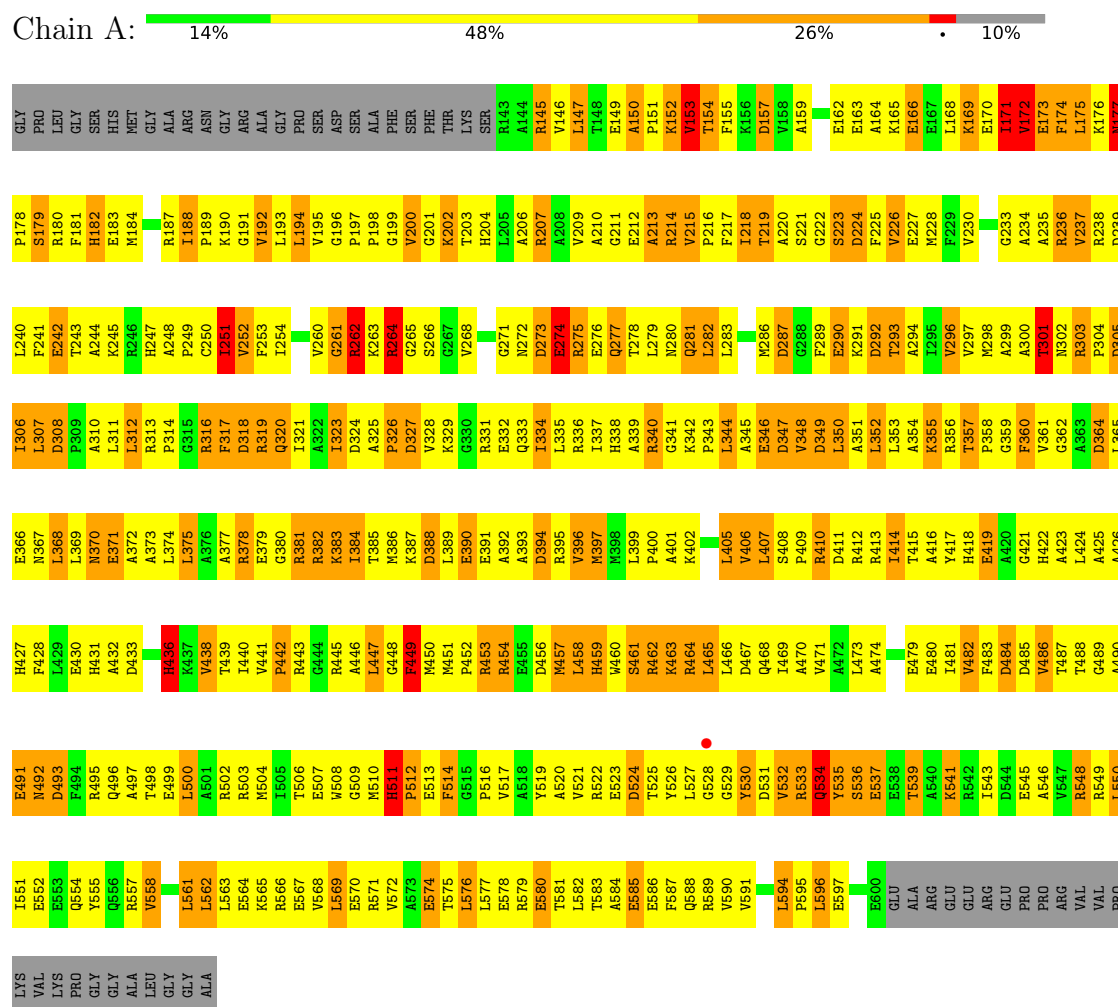


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	D	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	E	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	F	1	Total 27	C 10	N 5	O 10	P 2	0	0

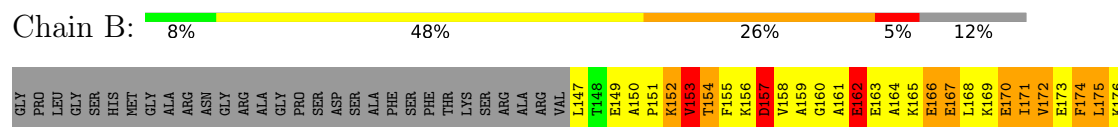
3 Residue-property plots

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

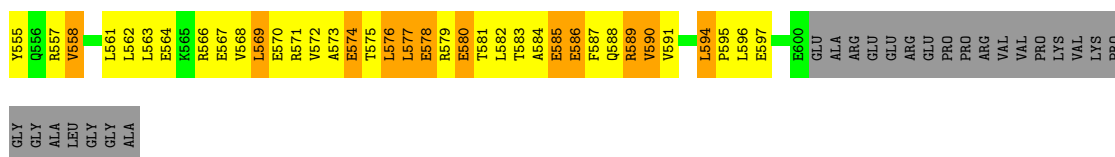
• Molecule 1: ATP-dependent zinc metalloprotease FtsH



• Molecule 1: ATP-dependent zinc metalloprotease FtsH

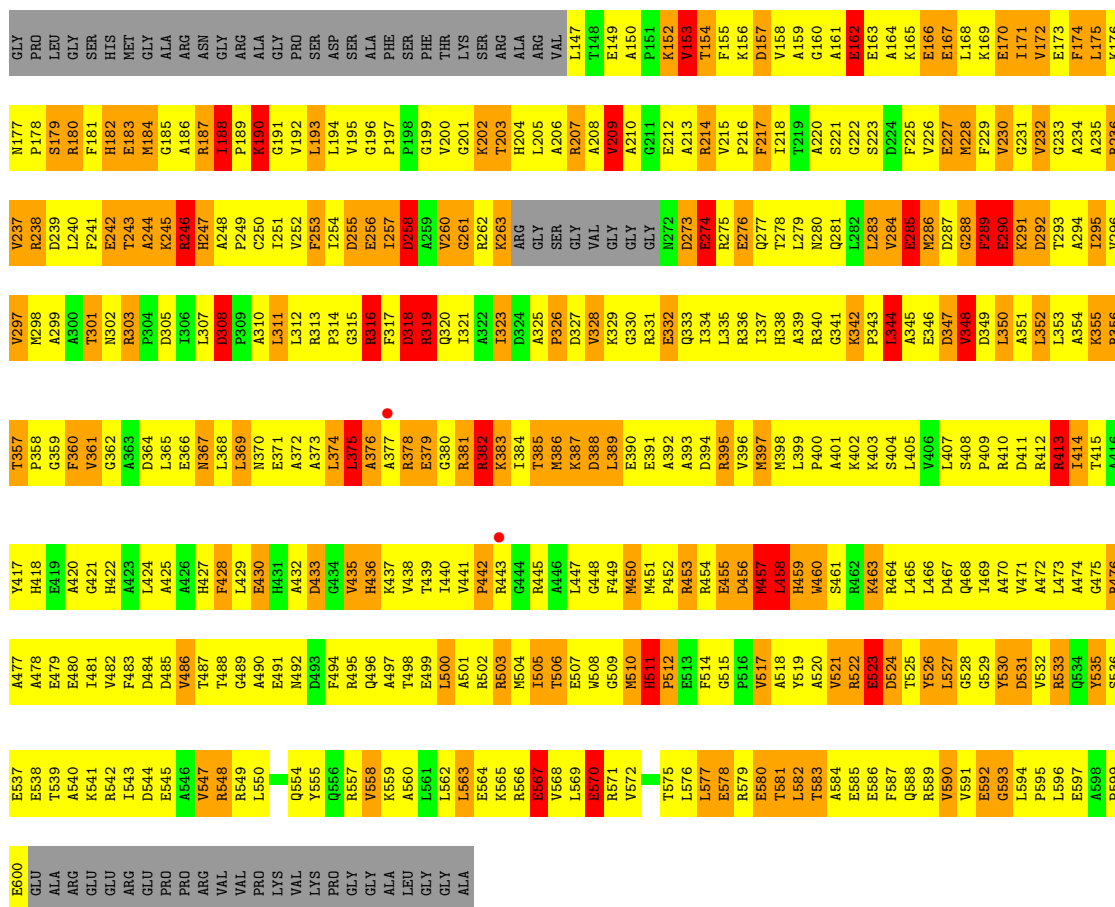






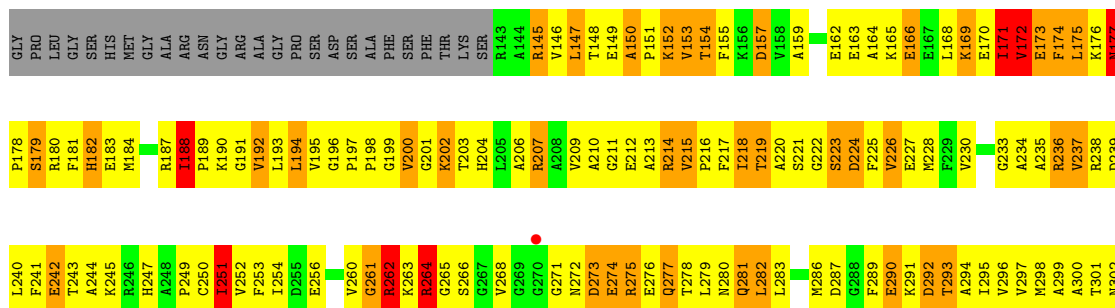
• Molecule 1: ATP-dependent zinc metalloprotease FtsH

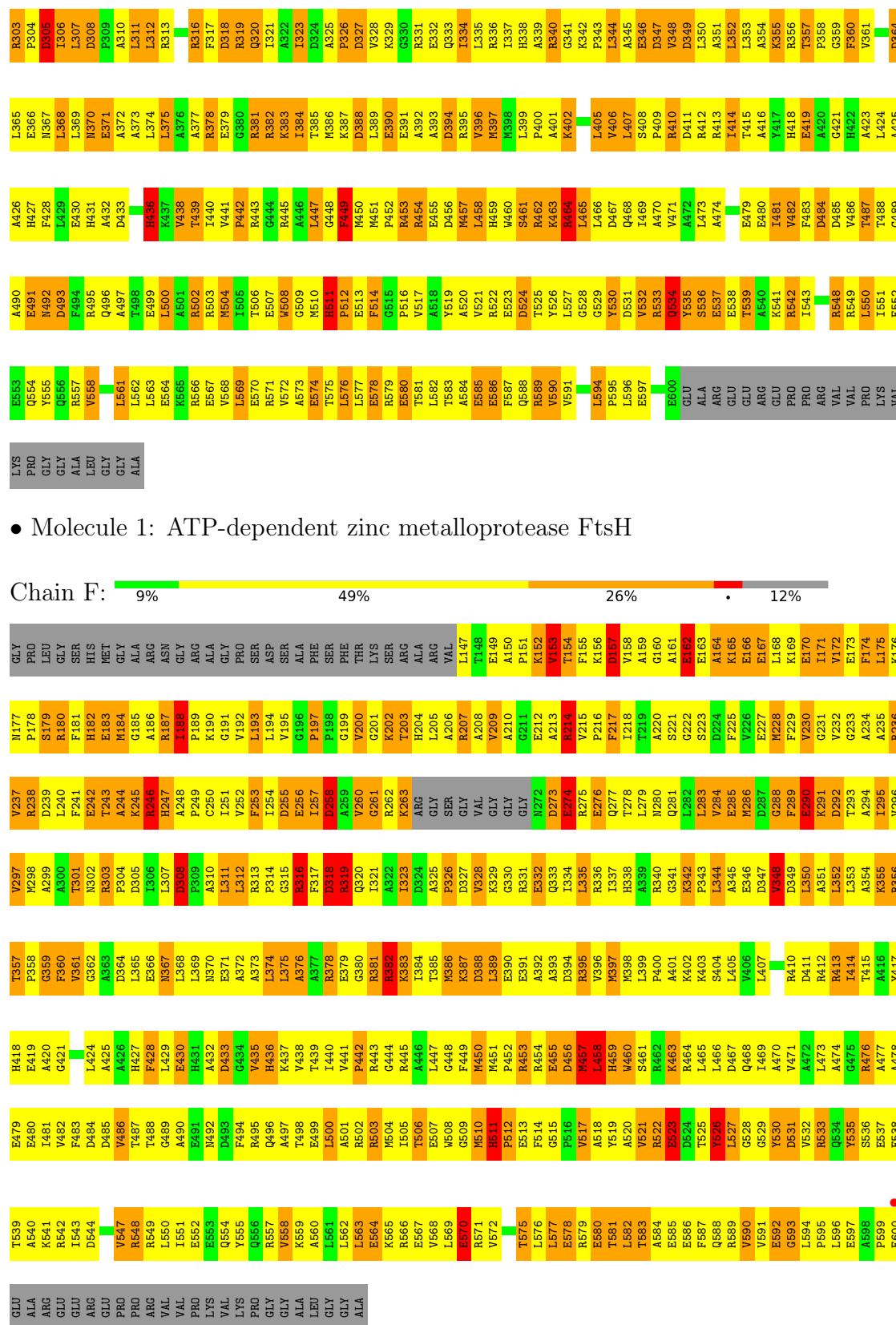
Chain D: 8% 50% 25% 5% 12%



• Molecule 1: ATP-dependent zinc metalloprotease FtsH

Chain E: 15% 47% 26% 10%





• 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 (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	99.1	Xtriage
Anisotropy	0.272	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 568.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.27$, $\langle L^2 \rangle = 0.11$	Xtriage
Estimated twinning fraction	0.237 for -h,-k,l	Xtriage
F_o, F_c correlation	0.81	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.80	3/3636 (0.1%)	1.17	22/4906 (0.4%)
1	B	0.82	2/3568 (0.1%)	1.26	40/4815 (0.8%)
1	C	0.82	3/3636 (0.1%)	1.22	34/4906 (0.7%)
1	D	0.81	2/3568 (0.1%)	1.24	35/4815 (0.7%)
1	E	0.81	8/3636 (0.2%)	1.19	25/4906 (0.5%)
1	F	0.78	0/3568	1.23	32/4815 (0.7%)
All	All	0.80	18/21612 (0.1%)	1.22	188/29163 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	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	E	214	ARG	CZ-NH2	-8.43	1.22	1.33
1	C	214	ARG	CZ-NH2	7.85	1.43	1.33
1	B	586	GLU	CD-OE1	-6.81	1.12	1.25
1	A	214	ARG	CZ-NH2	-6.71	1.24	1.33
1	E	319	ARG	CZ-NH1	-6.65	1.23	1.32
1	D	382	ARG	N-CA	-6.57	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	214	ARG	CD-NE	-6.44	1.37	1.46
1	E	214	ARG	CD-NE	-6.20	1.37	1.46
1	A	301	THR	CB-CG2	-5.82	1.33	1.52
1	E	214	ARG	CZ-NH1	-5.72	1.24	1.32
1	B	316	ARG	CZ-NH2	-5.66	1.26	1.33
1	C	214	ARG	CZ-NH1	-5.63	1.24	1.32
1	E	508	TRP	CA-C	-5.60	1.45	1.52
1	D	526	TYR	CA-C	-5.36	1.48	1.52
1	E	214	ARG	CA-C	-5.33	1.45	1.52
1	E	214	ARG	CA-CB	-5.26	1.44	1.53
1	E	214	ARG	CG-CD	-5.18	1.36	1.52
1	C	214	ARG	CA-CB	-5.06	1.45	1.53

All (188) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	511	HIS	CA-C-N	-12.31	104.45	119.84
1	D	511	HIS	C-N-CA	-12.31	104.45	119.84
1	F	511	HIS	CA-C-N	-11.79	105.11	119.84
1	F	511	HIS	C-N-CA	-11.79	105.11	119.84
1	A	177	ASN	CB-CA-C	-11.37	98.74	110.33
1	B	511	HIS	CA-C-N	-11.36	105.64	119.84
1	B	511	HIS	C-N-CA	-11.36	105.64	119.84
1	E	319	ARG	NE-CZ-NH2	11.29	129.36	119.20
1	C	214	ARG	N-CA-C	9.82	131.72	110.80
1	C	207	ARG	NE-CZ-NH2	8.96	127.26	119.20
1	B	236	ARG	NE-CZ-NH2	8.89	127.20	119.20
1	C	207	ARG	NE-CZ-NH1	-8.88	112.61	121.50
1	F	381	ARG	N-CA-C	8.88	124.06	109.95
1	C	275	ARG	CB-CA-C	-8.81	96.21	110.84
1	A	316	ARG	NE-CZ-NH1	-8.77	112.73	121.50
1	D	382	ARG	N-CA-CB	-8.65	99.39	110.90
1	B	381	ARG	N-CA-C	8.57	123.57	109.95
1	B	236	ARG	NE-CZ-NH1	-8.52	112.98	121.50
1	C	316	ARG	NE-CZ-NH2	8.47	126.82	119.20
1	E	511	HIS	CA-C-N	-8.41	109.33	119.84
1	E	511	HIS	C-N-CA	-8.41	109.33	119.84
1	B	458	LEU	N-CA-C	-8.36	96.52	107.73
1	E	214	ARG	N-CA-C	8.26	128.39	110.80
1	F	188	ILE	N-CA-C	7.98	115.74	109.19
1	C	496	GLN	CB-CA-C	-7.94	98.64	110.95
1	D	382	ARG	N-CA-C	-7.93	104.08	114.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	531	ASP	N-CA-C	7.84	122.02	109.24
1	F	531	ASP	N-CA-C	7.73	121.51	109.07
1	A	316	ARG	NE-CZ-NH2	7.66	126.09	119.20
1	B	348	VAL	N-CA-C	7.61	123.49	113.07
1	A	274	GLU	CB-CG-CD	-7.60	99.68	112.60
1	C	214	ARG	CA-CB-CG	-7.56	98.98	114.10
1	A	171	ILE	N-CA-CB	7.55	118.85	110.62
1	D	285	GLU	CB-CA-C	-7.51	98.98	110.92
1	C	481	ILE	CG1-CB-CG2	-7.49	88.25	110.70
1	C	177	ASN	CB-CA-C	-7.27	102.92	110.33
1	B	531	ASP	N-CA-C	7.25	120.74	109.07
1	E	316	ARG	NE-CZ-NH1	-7.17	114.33	121.50
1	D	289	PHE	N-CA-CB	-7.15	99.28	111.21
1	C	316	ARG	NE-CZ-NH1	-7.12	114.38	121.50
1	C	340	ARG	N-CA-C	6.93	119.85	111.40
1	B	515	GLY	CA-C-N	6.90	128.47	119.84
1	B	515	GLY	C-N-CA	6.90	128.47	119.84
1	F	348	VAL	N-CA-C	6.88	123.40	113.16
1	D	348	VAL	N-CA-C	6.86	123.39	113.16
1	F	458	LEU	N-CA-C	-6.82	96.27	110.80
1	E	533	ARG	N-CA-C	6.78	119.48	108.76
1	F	246	ARG	N-CA-C	-6.76	104.04	113.37
1	C	207	ARG	CG-CD-NE	-6.67	97.33	112.00
1	A	340	ARG	CB-CA-C	-6.65	100.65	110.95
1	D	526	TYR	CB-CA-C	-6.57	102.27	112.31
1	C	171	ILE	N-CA-CB	6.55	117.76	110.62
1	C	207	ARG	CD-NE-CZ	6.54	133.56	124.40
1	E	436	HIS	N-CA-C	6.53	119.37	108.13
1	F	526	TYR	N-CA-C	6.53	120.87	112.12
1	B	246	ARG	N-CA-C	-6.52	104.38	113.37
1	E	171	ILE	N-CA-CB	6.48	117.69	110.62
1	D	458	LEU	N-CA-C	-6.46	97.04	110.80
1	E	340	ARG	CB-CA-C	-6.44	100.96	110.95
1	F	515	GLY	CA-C-N	6.41	127.85	119.84
1	F	515	GLY	C-N-CA	6.41	127.85	119.84
1	D	381	ARG	N-CA-C	6.39	120.47	110.17
1	A	511	HIS	CA-C-N	-6.39	111.85	119.84
1	A	511	HIS	C-N-CA	-6.39	111.85	119.84
1	C	533	ARG	N-CA-C	6.35	118.80	108.76
1	C	436	HIS	N-CA-C	6.35	119.91	108.48
1	A	533	ARG	N-CA-C	6.34	118.78	108.76
1	B	236	ARG	CD-NE-CZ	6.28	133.20	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	511	HIS	CA-C-N	-6.25	112.03	119.84
1	C	511	HIS	C-N-CA	-6.25	112.03	119.84
1	F	214	ARG	CA-CB-CG	6.24	126.59	114.10
1	B	457	MET	N-CA-C	6.23	118.64	108.55
1	F	316	ARG	NE-CZ-NH2	6.18	124.76	119.20
1	F	289	PHE	N-CA-CB	-6.17	101.62	111.62
1	D	285	GLU	CA-CB-CG	6.17	126.44	114.10
1	D	382	ARG	CB-CG-CD	-6.17	97.11	111.30
1	B	154	THR	N-CA-C	-6.17	97.66	110.80
1	B	188	ILE	CA-C-N	6.16	127.54	119.84
1	B	188	ILE	C-N-CA	6.16	127.54	119.84
1	B	289	PHE	N-CA-CB	-6.16	101.64	111.62
1	F	318	ASP	N-CA-C	-6.15	97.11	108.24
1	D	286	MET	N-CA-C	-6.11	103.93	111.33
1	E	542	ARG	N-CA-C	-6.10	103.94	111.75
1	E	319	ARG	NH1-CZ-NH2	-6.10	111.37	119.30
1	B	318	ASP	N-CA-C	-6.04	97.31	108.24
1	A	436	HIS	N-CA-C	6.04	119.34	108.48
1	D	515	GLY	CA-C-N	6.03	127.38	119.84
1	D	515	GLY	C-N-CA	6.03	127.38	119.84
1	F	285	GLU	CB-CA-C	-6.01	101.36	110.92
1	E	316	ARG	NE-CZ-NH2	6.01	124.61	119.20
1	D	188	ILE	CA-C-N	5.98	127.31	119.84
1	D	188	ILE	C-N-CA	5.98	127.31	119.84
1	A	301	THR	OG1-CB-CG2	-5.92	97.46	109.30
1	B	316	ARG	NE-CZ-NH2	5.91	124.52	119.20
1	F	316	ARG	NE-CZ-NH1	-5.88	115.62	121.50
1	F	188	ILE	CA-C-N	5.87	127.17	119.84
1	F	188	ILE	C-N-CA	5.87	127.17	119.84
1	E	534	GLN	N-CA-C	5.86	119.17	107.62
1	B	381	ARG	NE-CZ-NH1	-5.86	115.64	121.50
1	E	251	ILE	CB-CA-C	-5.84	101.98	110.63
1	B	580	GLU	N-CA-C	5.83	123.22	110.80
1	B	483	PHE	N-CA-C	5.82	118.88	109.86
1	E	502	ARG	N-CA-C	-5.78	104.33	111.33
1	B	157	ASP	N-CA-CB	5.77	116.81	110.35
1	C	214	ARG	NE-CZ-NH1	-5.75	115.75	121.50
1	D	457	MET	N-CA-C	5.74	117.85	108.55
1	E	319	ARG	N-CA-C	5.72	116.95	108.60
1	C	481	ILE	CB-CG1-CD1	5.71	125.80	113.80
1	F	413	ARG	CB-CG-CD	5.69	124.39	111.30
1	B	285	GLU	CB-CA-C	-5.66	101.92	110.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	319	ARG	N-CA-C	5.66	116.86	108.60
1	C	534	GLN	N-CA-C	5.64	118.73	107.62
1	D	524	ASP	N-CA-C	5.64	115.47	108.19
1	E	187	ARG	N-CA-C	5.64	115.28	107.73
1	F	457	MET	N-CA-C	5.63	117.67	108.55
1	E	214	ARG	CA-CB-CG	-5.63	102.84	114.10
1	D	318	ASP	N-CA-C	-5.63	98.05	108.24
1	F	286	MET	N-CA-C	-5.62	105.15	111.28
1	C	251	ILE	CB-CA-C	-5.60	102.34	110.63
1	B	378	ARG	CG-CD-NE	5.60	124.32	112.00
1	A	251	ILE	CB-CA-C	-5.59	102.16	110.33
1	D	154	THR	N-CA-C	-5.59	98.90	110.80
1	B	308	ASP	CA-C-N	5.58	125.29	119.82
1	B	308	ASP	C-N-CA	5.58	125.29	119.82
1	A	534	GLN	N-CA-C	5.58	118.61	107.62
1	D	316	ARG	NE-CZ-NH2	5.58	124.22	119.20
1	D	342	LYS	CA-C-N	5.54	126.76	119.84
1	D	342	LYS	C-N-CA	5.54	126.76	119.84
1	C	275	ARG	CA-CB-CG	5.53	125.16	114.10
1	C	319	ARG	N-CA-C	5.50	116.62	108.60
1	A	187	ARG	N-CA-C	5.48	115.08	107.73
1	F	154	THR	N-CA-C	-5.48	99.12	110.80
1	B	526	TYR	CB-CA-C	-5.48	102.16	111.26
1	B	524	ASP	N-CA-C	5.47	115.25	108.19
1	A	274	GLU	N-CA-C	5.46	117.23	111.28
1	F	526	TYR	CB-CA-C	-5.45	102.22	111.26
1	E	464	ARG	CB-CA-C	-5.43	99.61	110.42
1	E	177	ASN	CB-CA-C	-5.41	104.81	110.33
1	B	232	VAL	N-CA-C	-5.40	105.11	111.00
1	C	497	ALA	N-CA-C	-5.40	105.29	111.07
1	C	187	ARG	N-CA-C	5.39	114.95	107.73
1	D	232	VAL	N-CA-C	-5.37	105.14	111.00
1	F	308	ASP	CA-C-N	5.36	125.03	119.56
1	F	308	ASP	C-N-CA	5.36	125.03	119.56
1	C	510	MET	N-CA-C	-5.35	99.60	108.75
1	D	308	ASP	CA-C-N	5.34	125.01	119.56
1	D	308	ASP	C-N-CA	5.34	125.01	119.56
1	D	567	GLU	CA-CB-CG	5.33	124.76	114.10
1	B	286	MET	N-CA-C	-5.31	104.91	111.33
1	D	344	LEU	N-CA-C	5.28	116.46	108.07
1	B	342	LYS	CA-C-N	5.26	126.42	119.84
1	B	342	LYS	C-N-CA	5.26	126.42	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	157	ASP	CB-CA-C	-5.26	104.29	112.07
1	D	246	ARG	CB-CG-CD	5.25	123.38	111.30
1	D	375	LEU	CA-CB-CG	5.24	134.64	116.30
1	F	342	LYS	CA-C-N	5.22	126.36	119.84
1	F	342	LYS	C-N-CA	5.22	126.36	119.84
1	C	502	ARG	N-CA-C	-5.21	105.03	111.33
1	B	196	GLY	CA-C-N	5.21	125.74	120.38
1	B	196	GLY	C-N-CA	5.21	125.74	120.38
1	F	382	ARG	CB-CG-CD	-5.20	99.34	111.30
1	E	305	ASP	N-CA-C	5.19	116.62	111.07
1	C	188	ILE	CB-CA-C	-5.18	101.93	111.36
1	D	190	LYS	CG-CD-CE	-5.17	99.42	111.30
1	A	214	ARG	N-CA-C	5.17	121.80	110.80
1	B	290	GLU	N-CA-C	5.16	116.91	109.07
1	C	274	GLU	CB-CA-C	-5.16	100.16	110.42
1	E	188	ILE	CB-CA-C	-5.15	101.99	111.36
1	B	203	THR	CB-CA-C	-5.14	102.58	110.81
1	F	290	GLU	N-CA-C	5.14	116.89	109.07
1	E	464	ARG	CB-CG-CD	5.12	123.08	111.30
1	C	531	ASP	N-CA-C	5.10	116.73	108.41
1	D	375	LEU	N-CA-C	-5.10	105.22	111.75
1	F	413	ARG	CB-CA-C	-5.10	100.27	110.42
1	A	171	ILE	CB-CG1-CD1	5.09	124.49	113.80
1	A	264	ARG	N-CA-C	5.09	121.64	110.80
1	E	481	ILE	CB-CA-C	-5.08	105.20	111.70
1	B	382	ARG	CB-CG-CD	-5.07	99.65	111.30
1	B	526	TYR	N-CA-C	5.07	118.91	112.12
1	C	214	ARG	CG-CD-NE	-5.06	100.87	112.00
1	A	274	GLU	CA-CB-CG	5.05	124.21	114.10
1	B	355	LYS	CB-CG-CD	-5.05	99.67	111.30
1	A	486	VAL	N-CA-C	-5.05	101.14	108.97
1	A	534	GLN	CB-CA-C	-5.04	102.56	111.22
1	C	264	ARG	N-CA-C	5.03	121.52	110.80
1	C	305	ASP	N-CA-C	5.03	116.45	111.07
1	D	290	GLU	N-CA-C	5.02	116.71	109.07
1	E	214	ARG	CD-NE-CZ	-5.00	117.40	124.40

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	213	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	A	532	VAL	Peptide
1	B	244	ALA	Peptide
1	B	288	GLY	Peptide
1	B	382	ARG	Peptide
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	901	5
1	B	3511	0	3556	894	3
1	C	3578	0	3623	843	0
1	D	3511	0	3556	892	3
1	E	3578	0	3623	844	3
1	F	3511	0	3556	896	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	5119	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 119.

All (5119) 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:A:586:GLU:HB2	1:A:589:ARG:NH2	1.18	1.46
1:D:313:ARG:CD	1:D:314:PRO:HD2	1.40	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:CE2	1.90	1.39
1:A:316:ARG:NH1	1:A:317:PHE:CD2	1.91	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:HB2	1:E:303:ARG:NH1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:PHE:CZ	1:A:496:GLN:HG2	1.73	1.22
1:D:382:ARG:HH11	1:D:382:ARG:CG	1.50	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
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:A:263:LYS:NZ	1:A:276:GLU:OE2	1.75	1.20
1:A:303:ARG:HH11	1:A:303:ARG:CB	1.55	1.20
1:E:449:PHE:CZ	1:E:496:GLN:HG2	1.76	1.20
1:F:283:LEU:HD12	1:F:316:ARG:NH2	1.57	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:168:LEU:HB2	1:C:171:ILE:HD11	1.22	1.18
1:C:303:ARG:HH11	1:C:303:ARG:CB	1.57	1.18
1:E:303:ARG:HH11	1:E:303:ARG:CB	1.57	1.18
1:C:263:LYS:NZ	1:C:276:GLU:OE2	1.76	1.18
1:B:395:ARG:HG2	1:B:395:ARG:HH11	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:B:286:MET:HE1	1:B:316:ARG:HA	1.28	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: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:F:165:LYS:O	1:F:168:LEU:N	1.79	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:A:524:ASP:HA	1:A:529:GLY:HA2	1.15	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:PHE:CZ	1:C:278:THR:HB	1.83	1.14
1:F:283:LEU:CD1	1:F:316:ARG:NH2	2.10	1.14
1:B:589:ARG:HE	1:B:594:LEU:HD21	1.07	1.13
1:E:416:ALA:HB3	1:E:577:LEU:HD21	1.26	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
1:C:416:ALA:CB	1:C:577:LEU:HD23	1.78	1.13
1:C:524:ASP:HA	1:C:529:GLY:HA2	1.14	1.13
1:D:286:MET:HE1	1:D:316:ARG:HA	1.26	1.12
1:F:395:ARG:HG2	1:F:395:ARG:HH11	1.08	1.12
1:A:416:ALA:HB3	1:A:577:LEU:HD21	1.21	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:F:286:MET:HE1	1:F:316:ARG:HA	1.22	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:B:413:ARG:HG2	1:B:413:ARG:HH11	1.11	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: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:171:ILE:HD11	1:D:296:VAL:HG11	1.15	1.10
1:D:290:GLU:HG2	1:D:293:THR:HG23	1.28	1.10
1:E:236:ARG:HG3	1:E:237:VAL:N	1.50	1.10
1:A:416:ALA:HB2	1:A:577:LEU:HD23	1.15	1.10
1:C:172:VAL:HG23	1:C:213:ALA:HB2	1.28	1.10
1:C:263:LYS:HD2	1:C:276:GLU:CD	1.75	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: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:C:264:ARG:HG3	1:C:266:SER:H	1.08	1.10
1:E:182:HIS:HB2	1:E:291:LYS:HD2	1.31	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:376:ALA:C	1:B:381:ARG:HD2	1.76	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:A:428:PHE:CE1	1:A:432:ALA:HA	1.86	1.09
1:D:376:ALA:HA	1:D:381:ARG:HG3	1.33	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:A:263:LYS:NZ	1:A:276:GLU:CD	2.11	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: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:E:416:ALA:HB2	1:E:577:LEU:HD23	1.21	1.09
1:F:171:ILE:HD11	1:F:296:VAL:HG11	1.13	1.09
1:A:174:PHE:CE1	1:A:188:ILE:HD11	1.87	1.08
1:A:263:LYS:HD2	1:A:276:GLU:CD	1.77	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:C:174:PHE:CE1	1:C:188:ILE:HD11	1.87	1.08
1:C:262:ARG:HB3	1:C:275:ARG:HH12	1.10	1.08
1:C:263:LYS:NZ	1:C:276:GLU:CD	2.10	1.08
1:D:413:ARG:HG2	1:D:413:ARG:HH11	1.08	1.08
1:F:318:ASP:O	1:F:319:ARG:HB2	1.50	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:HG3	1:B:382:ARG:HH11	1.10	1.08
1:E:263:LYS:HD2	1:E:276:GLU:CD	1.79	1.08
1:F:238:ARG:NH1	1:F:239:ASP:N	2.02	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:238:ARG:NH1	1:F:239:ASP:H	1.50	1.08
1:A:182:HIS:HB2	1:A:291:LYS:HD2	1.27	1.07
1:C:170:GLU:O	1:C:174:PHE:HB3	1.50	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:E:413:ARG:HA	1:E:577:LEU:HD22	1.32	1.07
1:A:311:LEU:CD2	1:A:316:ARG:NH2	2.17	1.07
1:B:474:ALA:HA	1:B:558:VAL:HG11	1.33	1.07
1:C:453:ARG:NH2	1:C:460:TRP:HE1	1.51	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
1:C:147:LEU:HD21	1:C:151:PRO:HB3	1.13	1.07
1:C:264:ARG:HG3	1:C:266:SER:N	1.69	1.07
1:D:190:LYS:HE3	1:D:289:PHE:CE2	1.90	1.07
1:E:263:LYS:NZ	1:E:276:GLU:CD	2.12	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:D:459:HIS:ND1	1:D:459:HIS:O	1.88	1.06
1:F:400:PRO:O	1:F:404:SER:N	1.87	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:A:449:PHE:CE2	1:A:496:GLN:HG2	1.90	1.05
1:C:449:PHE:CE2	1:C:496:GLN:HG3	1.90	1.05
1:D:313:ARG:CD	1:D:314:PRO:CD	2.34	1.05
1:B:356:ARG:HH11	1:B:356:ARG:HG3	1.16	1.05
1:D:400:PRO:O	1:D:404:SER:N	1.87	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:D:356:ARG:HG3	1:D:356:ARG:HH11	1.14	1.05
1:D:395:ARG:HG2	1:D:395:ARG:HH11	1.16	1.05
1:D:412:ARG:NH1	1:D:440:ILE:HG21	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:E:342:LYS:HD2	1:E:343:PRO:HD2	1.39	1.05
1:F:412:ARG:NH1	1:F:440:ILE:HG21	1.70	1.05
1:A:262:ARG:HG2	1:A:275:ARG:HH22	1.22	1.04
1:C:225:PHE:HE1	1:C:233:GLY:CA	1.69	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:F:276:GLU:HA	1:F:279:LEU:HD13	1.35	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:238:ARG:NH1	1:B:239:ASP:N	2.04	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:C:342:LYS:HD2	1:C:343:PRO:HD2	1.37	1.04
1:A:147:LEU:HD21	1:A:151:PRO:CB	1.87	1.04
1:E:212:GLU:C	1:E:214:ARG:HG3	1.82	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
1:D:381:ARG:HH22	1:D:388:ASP:CG	1.66	1.04
1:E:533:ARG:NH2	1:E:534:GLN:O	1.91	1.04
1:F:313:ARG:HD2	1:F:314:PRO:HD2	1.05	1.04
1:D:238:ARG:NH1	1:D:239:ASP:N	2.05	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:E:152:LYS:HG3	1:E:153:VAL:HG23	1.39	1.03
1:F:482:VAL:HG13	1:F:483:PHE:HD2	1.24	1.03
1:B:376:ALA:CA	1:B:381:ARG:CD	2.10	1.03
1:B:482:VAL:HG13	1:B:483:PHE:HD2	1.21	1.03
1:A:342:LYS:HD3	1:F:184:MET:O	1.58	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:B:237:VAL:O	1:B:240:LEU:HB3	1.57	1.03
1:C:166:GLU:HB2	1:C:169:LYS:HZ2	1.22	1.03
1:D:382:ARG:HH11	1:D:382:ARG:HG3	0.87	1.02
1:A:264:ARG:CG	1:A:266:SER:H	1.71	1.02
1:F:290:GLU:HG2	1:F:293:THR:HG23	1.40	1.02
1:B:412:ARG:HH12	1:B:440:ILE:HG21	1.23	1.02
1:E:225:PHE:HE1	1:E:233:GLY:CA	1.72	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:C:218:ILE:HD11	1:C:250:CYS:SG	2.00	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:E:448:GLY:O	1:E:452:PRO:HD2	1.60	1.01
1:C:147:LEU:HD21	1:C:151:PRO:CB	1.88	1.01
1:A:533:ARG:NH2	1:A:534:GLN:O	1.94	1.01
1:B:165:LYS:HE2	1:B:205:LEU:HD23	1.38	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:459:HIS:ND1	1:B:459:HIS:O	1.92	1.01
1:C:152:LYS:HG3	1:C:153:VAL:HG23	1.42	1.01
1:D:348:VAL:CG2	1:D:352:LEU:HD22	1.91	1.01
1:E:263:LYS:HE3	1:E:276:GLU:OE1	1.58	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
1:B:326:PRO:HB3	1:B:360:PHE:O	1.60	1.01
1:C:589:ARG:NH1	1:C:589:ARG:HB3	1.76	1.01
1:D:453:ARG:CZ	1:D:495:ARG:HH21	1.73	1.01
1:E:286:MET:CB	1:E:316:ARG:CD	2.39	1.01
1:B:311:LEU:HA	1:B:316:ARG:NH1	1.75	1.00
1:C:286:MET:HG3	1:C:316:ARG:CD	1.90	1.00
1:D:313:ARG:HD2	1:D:314:PRO:HD2	1.01	1.00
1:D:348:VAL:HG21	1:D:352:LEU:HD22	1.43	1.00
1:D:382:ARG:HG3	1:D:382:ARG:NH1	1.69	1.00
1:A:152:LYS:HG3	1:A:153:VAL:HG23	1.44	1.00
1:C:416:ALA:HB3	1:C:577:LEU:HD23	1.01	1.00
1:D:238:ARG:NH1	1:D:239:ASP:H	1.56	1.00
1:B:439:THR:HG23	1:B:445:ARG:HH22	1.25	1.00
1:E:286:MET:HG3	1:E:316:ARG:HD2	1.40	1.00
1:E:589:ARG:HH21	1:E:596:LEU:HB3	0.98	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: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:A:263:LYS:HZ2	1:A:276:GLU:CD	1.68	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:236:ARG:HH12	1:B:278:THR:HG22	1.26	0.99
1:B:262:ARG:HG3	1:B:263:LYS:N	1.77	0.99
1:B:310:ALA:C	1:B:316:ARG:NH1	2.21	0.99
1:C:263:LYS:CD	1:C:276:GLU:OE1	2.11	0.99
1:F:313:ARG:CD	1:F:314:PRO:CD	2.40	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:A:264:ARG:HG3	1:A:266:SER:N	1.77	0.98
1:C:313:ARG:NH2	1:C:526:TYR:HA	1.77	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:589:ARG:HB3	1:E:589:ARG:NH1	1.78	0.98
1:F:453:ARG:NH1	1:F:495:ARG:HH21	1.59	0.98
1:A:586:GLU:HA	1:A:589:ARG:NE	1.77	0.98
1:F:459:HIS:ND1	1:F:459:HIS:O	1.94	0.98
1:A:311:LEU:CA	1:A:316:ARG:HH22	1.75	0.98
1:A:378:ARG:NH2	1:F:170:GLU:HB3	1.78	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
1:E:174:PHE:CZ	1:E:188:ILE:CD1	2.47	0.98
1:D:376:ALA:CA	1:D:381:ARG:HG3	1.92	0.98
1:E:413:ARG:HA	1:E:577:LEU:CD2	1.93	0.98
1:C:190:LYS:HD2	1:C:289:PHE:CE1	1.98	0.98
1:C:286:MET:CG	1:C:316:ARG:CD	2.41	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:166:GLU:HA	1:C:169:LYS:HG2	1.46	0.98
1:E:218:ILE:HD11	1:E:250:CYS:SG	2.04	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: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:D:262:ARG:HG3	1:D:263:LYS:N	1.77	0.97
1:A:166:GLU:HB2	1:A:169:LYS:HZ2	1.29	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:A:448:GLY:O	1:A:452:PRO:HD2	1.62	0.97
1:C:262:ARG:HG2	1:C:275:ARG:HH22	1.25	0.97
1:E:524:ASP:HA	1:E:529:GLY:CA	1.94	0.97
1:A:378:ARG:HA	1:F:173:GLU:OE1	1.63	0.97
1:A:571:ARG:HD2	1:A:590:VAL:O	1.64	0.97
1:E:286:MET:HB3	1:E:316:ARG:HG2	0.99	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: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:F:275:ARG:O	1:F:278:THR:OG1	1.82	0.97
1:A:145:ARG:NH2	1:A:219:THR:OG1	1.96	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:187:ARG:O	1:C:374:LEU:HD21	1.63	0.96
1:B:233:GLY:CA	1:B:236:ARG:HH22	1.78	0.96
1:B:453:ARG:CZ	1:B:495:ARG:HH21	1.77	0.96
1:C:215:VAL:HG21	1:C:250:CYS:HA	1.48	0.96
1:E:283:LEU:HG	1:E:316:ARG:HH12	1.29	0.96
1:B:453:ARG:NH1	1:B:495:ARG:HH21	1.62	0.96
1:A:292:ASP:HB2	1:B:227:GLU:OE2	1.63	0.96
1:B:171:ILE:CD1	1:B:296:VAL:HG11	1.96	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:A:374:LEU:CD2	1:F:187:ARG:O	2.14	0.96
1:B:190:LYS:NZ	1:B:289:PHE:CE2	2.26	0.96
1:C:263:LYS:NZ	1:C:276:GLU:OE1	1.99	0.96
1:D:275:ARG:O	1:D:278:THR:OG1	1.82	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:A:227:GLU:HG3	1:F:263:LYS:NZ	1.81	0.95
1:C:174:PHE:CZ	1:C:188:ILE:CD1	2.48	0.95
1:E:215:VAL:HG21	1:E:250:CYS:HA	1.47	0.95
1:E:326:PRO:HB3	1:E:360:PHE:O	1.64	0.95
1:F:337:ILE:HD12	1:F:340:ARG:HH12	1.30	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: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:F:313:ARG:CG	1:F:314:PRO:HD2	1.96	0.95
1:A:263:LYS:CD	1:A:276:GLU:OE1	2.14	0.94
1:A:313:ARG:HH22	1:A:526:TYR:C	1.75	0.94
1:A:524:ASP:HA	1:A:529:GLY:CA	1.97	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:190:LYS:HD2	1:A:289:PHE:CE1	2.02	0.94
1:B:313:ARG:HD2	1:B:314:PRO:CD	1.93	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:511:HIS:NE2	1:E:516:PRO:HD3	1.81	0.94
1:F:319:ARG:HG2	1:F:319:ARG:HH11	1.32	0.94
1:A:215:VAL:HG21	1:A:250:CYS:HA	1.49	0.94
1:A:520:ALA:HA	1:A:533:ARG:HD3	1.48	0.94
1:C:263:LYS:CD	1:C:276:GLU:CD	2.40	0.94
1:C:275:ARG:HG2	1:C:275:ARG:HH11	1.26	0.94
1:F:311:LEU:CA	1:F:316:ARG:NH1	2.10	0.94
1:F:412:ARG:HH12	1:F:440:ILE:CG2	1.81	0.94
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:A:511:HIS:NE2	1:A:516:PRO:HD3	1.83	0.94
1:A:582:LEU:HD23	1:A:587:PHE:HA	1.49	0.94
1:B:319:ARG:HG2	1:B:319:ARG:HH11	1.32	0.94
1:C:533:ARG:NH2	1:C:534:GLN:O	2.01	0.94
1:C:582:LEU:HD23	1:C:587:PHE:HA	1.49	0.94
1:D:263:LYS:NZ	1:E:227:GLU:HG3	1.82	0.94
1:E:166:GLU:HA	1:E:169:LYS:HG2	1.46	0.94
1:E:520:ALA:HA	1:E:533:ARG:HD3	1.50	0.94
1:F:376:ALA:CA	1:F:381:ARG:CD	2.28	0.94
1:F:578:GLU:HG2	1:F:579:ARG:N	1.81	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:C:286:MET:CB	1:C:316:ARG:HD3	1.90	0.93
1:D:233:GLY:CA	1:D:236:ARG:HH22	1.80	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:C:201:GLY:N	2:C:1001:ADP:O1A	1.99	0.93
1:D:190:LYS:CE	1:D:289:PHE:CE2	2.52	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: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:376:ALA:CB	1:F:381:ARG:HD2	1.98	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:453:ARG:CZ	1:F:495:ARG:HH21	1.80	0.93
1:A:263:LYS:NZ	1:A:276:GLU:OE1	2.00	0.93
1:B:283:LEU:HD12	1:B:316:ARG:HH21	1.32	0.93
1:C:533:ARG:HD2	1:C:534:GLN:H	1.34	0.93
1:C:215:VAL:HG23	1:C:216:PRO:HD2	1.51	0.93
1:D:385:THR:OG1	1:D:388:ASP:OD1	1.86	0.93
1:A:147:LEU:CD2	1:A:151:PRO:HB3	1.96	0.93
1:B:291:LYS:HG3	1:B:292:ASP:H	1.34	0.93
1:D:291:LYS:HG3	1:D:292:ASP:N	1.81	0.93
1:E:236:ARG:HG2	1:E:236:ARG:HH11	1.32	0.93
1:E:589:ARG:HH22	1:E:596:LEU:CB	1.70	0.93
1:B:310:ALA:O	1:B:316:ARG:NH1	2.02	0.93
1:B:352:LEU:HD23	1:B:353:LEU:N	1.82	0.93
1:C:236:ARG:HG2	1:C:236:ARG:HH11	1.32	0.93
1:E:582:LEU:HD23	1:E:587:PHE:HA	1.48	0.93
1:F:237:VAL:O	1:F:240:LEU:HB3	1.69	0.93
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:E:263:LYS:CD	1:E:276:GLU:OE1	2.15	0.92
1:F:215:VAL:CG2	1:F:216:PRO:HD2	1.99	0.92
1:A:262:ARG:CB	1:A:275:ARG:HH12	1.82	0.92
1:C:313:ARG:HH22	1:C:526:TYR:C	1.77	0.92
1:C:586:GLU:HA	1:C:589:ARG:HG3	1.51	0.92
1:F:165:LYS:NZ	1:F:205:LEU:HB3	1.84	0.92
1:B:381:ARG:NH1	1:B:388:ASP:OD2	2.02	0.92
1:D:352:LEU:HD23	1:D:353:LEU:N	1.84	0.92
1:E:166:GLU:HB2	1:E:169:LYS:HZ2	1.31	0.92
1:B:439:THR:HG23	1:B:445:ARG:NH2	1.83	0.92
1:C:173:GLU:HA	1:C:176:LYS:CG	1.98	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:A:453:ARG:NH1	1:A:460:TRP:CZ2	2.36	0.92
1:D:215:VAL:CG2	1:D:216:PRO:HD2	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:LYS:CD	1:A:276:GLU:CD	2.42	0.91
1:A:453:ARG:NH1	1:A:460:TRP:HZ2	1.67	0.91
1:A:453:ARG:HH11	1:A:453:ARG:HG3	1.34	0.91
1:B:460:TRP:HE3	1:B:460:TRP:H	1.18	0.91
1:F:233:GLY:CA	1:F:236:ARG:HH22	1.81	0.91
1:A:319:ARG:HH21	1:B:402:LYS:HZ1	1.17	0.91
1:A:481:ILE:HD12	1:A:563:LEU:HB3	1.51	0.91
1:B:454:ARG:NH2	1:B:526:TYR:O	2.02	0.91
1:C:511:HIS:NE2	1:C:516:PRO:HD3	1.84	0.91
1:F:439:THR:HG23	1:F:445:ARG:HH22	1.34	0.91
1:C:174:PHE:CZ	1:C:188:ILE:HD11	2.06	0.91
1:C:382:ARG:HG3	1:C:383:LYS:N	1.85	0.91
1:D:316:ARG:HG3	1:D:316:ARG:NH1	1.83	0.91
1:F:233:GLY:CA	1:F:236:ARG:NH2	2.32	0.91
1:D:257:ILE:O	1:D:260:VAL:N	2.03	0.91
1:E:313:ARG:HH22	1:E:526:TYR:C	1.77	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:313:ARG:NH1	1:C:526:TYR:O	2.04	0.91
1:C:589:ARG:HH22	1:C:596:LEU:CB	1.75	0.91
1:E:263:LYS:CD	1:E:276:GLU:CD	2.44	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:155:PHE:HD2	1:C:212:GLU:OE1	1.54	0.90
1:C:262:ARG:CB	1:C:275:ARG:HH12	1.84	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:B:238:ARG:HH12	1:B:239:ASP:HB3	1.35	0.90
1:C:166:GLU:HB2	1:C:169:LYS:NZ	1.85	0.90
1:D:263:LYS:HE2	1:E:228:MET:HE2	1.51	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:B:412:ARG:HH12	1:B:440:ILE:CG2	1.85	0.90
1:E:286:MET:HB2	1:E:316:ARG:HD3	1.54	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:F:526:TYR:O	1:F:527:LEU:C	2.15	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:LEU:HB2	1:A:171:ILE:CD1	2.01	0.90
1:A:201:GLY:N	2:A:1001:ADP:O1A	2.03	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:B:215:VAL:CG2	1:B:216:PRO:HD2	2.01	0.89
1:E:449:PHE:CB	1:E:468:GLN:NE2	2.35	0.89
1:B:395:ARG:HG2	1:B:395:ARG:NH1	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
1:B:413:ARG:HG2	1:B:413:ARG:NH1	1.78	0.89
1:C:509:GLY:C	1:D:476:ARG:HH22	1.80	0.89
1:C:519:TYR:O	1:C:533:ARG:NE	2.05	0.89
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: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:A:533:ARG:HD2	1:A:534:GLN:H	1.35	0.89
1:B:171:ILE:HD11	1:B:296:VAL:CG1	2.03	0.89
1:D:165:LYS:HE2	1:D:205:LEU:CD2	2.02	0.89
1:D:460:TRP:H	1:D:460:TRP:HE3	1.20	0.89
1:E:588:GLN:O	1:E:591:VAL:HB	1.72	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:A:286:MET:HG3	1:A:316:ARG:HD3	0.99	0.89
1:E:412:ARG:NH1	1:E:577:LEU:O	2.06	0.89
1:F:233:GLY:HA2	1:F:236:ARG:HH22	1.17	0.89
1:E:533:ARG:HD2	1:E:534:GLN:H	1.36	0.89
1:F:257:ILE:O	1:F:260:VAL:N	2.05	0.89
1:A:263:LYS:CE	1:A:276:GLU:CD	2.46	0.88
1:A:456:ASP:OD1	1:A:457:MET:N	2.06	0.88
1:B:238:ARG:HG2	1:B:281:GLN:NE2	1.88	0.88
1:C:155:PHE:CZ	1:C:168:LEU:HD11	2.08	0.88
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:327:ASP:OD1	1:D:328:VAL:N	2.06	0.88
1:F:286:MET:CE	1:F:316:ARG:HA	2.04	0.88
1:A:166:GLU:HB2	1:A:169:LYS:NZ	1.89	0.88
1:C:147:LEU:CD2	1:C:151:PRO:HB3	2.02	0.88
1:C:589:ARG:HH21	1:C:596:LEU:CB	1.64	0.88
1:E:313:ARG:HH22	1:E:526:TYR:HA	1.39	0.88
1:C:286:MET:HB3	1:C:316:ARG:CD	1.94	0.88
1:F:453:ARG:NH1	1:F:495:ARG:NH2	2.20	0.88
1:A:378:ARG:NH2	1:F:170:GLU:CB	2.34	0.88
1:B:356:ARG:HH11	1:B:356:ARG:CG	1.86	0.88
1:D:471:VAL:O	1:D:474:ALA:HB3	1.74	0.88
1:B:184:MET:SD	1:C:342:LYS:NZ	2.46	0.88
1:B:355:LYS:HE2	1:B:578:GLU:O	1.72	0.88
1:C:412:ARG:NH1	1:C:577:LEU:O	2.06	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:A:326:PRO:HB3	1:A:360:PHE:O	1.73	0.88
1:A:384:ILE:HG23	1:A:388:ASP:HB2	1.56	0.88
1:A:509:GLY:C	1:B:476:ARG:HH22	1.81	0.88
1:B:382:ARG:HG3	1:B:382:ARG:NH1	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:B:526:TYR:O	1:B:527:LEU:C	2.17	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:E:223:SER:C	1:E:225:PHE:H	1.81	0.87
1:F:302:ASN:HD21	1:F:443:ARG:NH2	1.71	0.87
1:C:384:ILE:HG23	1:C:388:ASP:HB2	1.56	0.87
1:D:526:TYR:O	1:D:527:LEU:C	2.16	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:449:PHE:CB	1:A:468:GLN:NE2	2.38	0.87
1:E:453:ARG:HH22	1:E:460:TRP:HE1	1.21	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:D:376:ALA:C	1:D:381:ARG:HG3	1.99	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:D:301:THR:HG21	1:D:307:LEU:HD11	1.56	0.87
1:F:460:TRP:HE3	1:F:460:TRP:H	1.19	0.87
1:F:470:ALA:O	1:F:558:VAL:HG21	1.74	0.87
1:C:410:ARG:O	1:C:413:ARG:N	2.07	0.87
1:C:263:LYS:CE	1:C:276:GLU:CD	2.47	0.87
1:D:171:ILE:HD11	1:D:296:VAL:CG1	2.02	0.87
1:D:238:ARG:HG2	1:D:281:GLN:NE2	1.90	0.87
1:D:338:HIS:ND1	1:D:366:GLU:HG3	1.90	0.87
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: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: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: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:F:370:ASN:OD1	1:F:371:GLU:N	2.08	0.86
1:A:313:ARG:CZ	1:A:526:TYR:HA	2.05	0.86
1:A:342:LYS:CD	1:A:343:PRO:HD2	2.04	0.86
1:C:308:ASP:OD1	1:C:310:ALA:N	2.09	0.86
1:C:536:SER:OG	1:D:544:ASP:OD2	1.94	0.86
1:D:378:ARG:C	1:D:380:GLY:H	1.84	0.86
1:F:173:GLU:O	1:F:176:LYS:HG2	1.75	0.86
1:C:467:ASP:OD1	1:C:557:ARG:NH2	2.08	0.86
1:C:588:GLN:O	1:C:591:VAL:HB	1.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:GLU:O	1:A:431:HIS:HB3	1.75	0.86
1:B:346:GLU:HG2	1:B:348:VAL:H	1.41	0.86
1:C:181:PHE:HA	1:C:184:MET:HE3	1.56	0.86
1:C:428:PHE:CD1	1:C:432:ALA:HA	2.10	0.86
1:C:456:ASP:OD1	1:C:457:MET:N	2.07	0.86
1:D:174:PHE:HB2	1:D:181:PHE:CE2	2.11	0.86
1:D:356:ARG:HG3	1:D:356:ARG:NH1	1.83	0.86
1:E:155:PHE:CZ	1:E:168:LEU:HD11	2.11	0.86
1:E:264:ARG:CG	1:E:266:SER:H	1.83	0.86
1:F:153:VAL:HG13	1:F:154:THR:N	1.91	0.86
1:F:301:THR:HG21	1:F:307:LEU:HD11	1.56	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
1:F:346:GLU:HG2	1:F:348:VAL:H	1.41	0.85
1:F:382:ARG:HG3	1:F:382:ARG:NH1	1.73	0.85
1:A:155:PHE:CZ	1:A:168:LEU:HD11	2.11	0.85
1:A:449:PHE:HB3	1:A:468:GLN:NE2	1.91	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: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:C:223:SER:C	1:C:225:PHE:H	1.84	0.85
1:F:164:ALA:O	1:F:168:LEU:HD13	1.77	0.85
1:A:509:GLY:O	1:B:476:ARG:NH2	2.09	0.85
1:C:449:PHE:CB	1:C:468:GLN:NE2	2.38	0.85
1:F:238:ARG:HH12	1:F:239:ASP:CB	1.89	0.85
1:C:173:GLU:HA	1:C:176:LYS:HG3	1.59	0.85
1:E:384:ILE:HG23	1:E:388:ASP:HB2	1.58	0.85
1:E:449:PHE:HB3	1:E:468:GLN:NE2	1.91	0.85
1:F:215:VAL:HG22	1:F:216:PRO:HD2	1.57	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:A:374:LEU:HD11	1:F:187:ARG:N	1.91	0.85
1:A:453:ARG:HH22	1:A:460:TRP:HE1	1.20	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:D:159:ALA:HB3	1:D:334:ILE:HG13	1.56	0.85
1:D:311:LEU:O	1:D:316:ARG:CG	2.25	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:410:ARG:O	1:A:413:ARG:N	2.10	0.85
1:B:168:LEU:O	1:B:171:ILE:HG22	1.76	0.85
1:C:589:ARG:HB3	1:C:589:ARG:CZ	2.07	0.85
1:D:356:ARG:HH11	1:D:356:ARG:CG	1.89	0.85
1:A:168:LEU:C	1:A:171:ILE:HD13	2.02	0.85
1:B:238:ARG:HH12	1:B:239:ASP:CB	1.90	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:E:571:ARG:HD2	1:E:590:VAL:O	1.76	0.84
1:C:473:LEU:HD22	1:C:555:TYR:HB2	1.59	0.84
1:E:342:LYS:CD	1:E:343:PRO:HD2	2.06	0.84
1:E:473:LEU:HD22	1:E:555:TYR:HB2	1.57	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:B:190:LYS:CE	1:B:289:PHE:CE2	2.60	0.84
1:B:356:ARG:HG3	1:B:356:ARG:NH1	1.82	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:A:172:VAL:CG2	1:A:213:ALA:HB2	2.07	0.84
1:A:223:SER:C	1:A:225:PHE:H	1.85	0.84
1:A:384:ILE:CG2	1:A:388:ASP:HB2	2.08	0.84
1:B:460:TRP:HE3	1:B:460:TRP:N	1.74	0.84
1:D:470:ALA:O	1:D:558:VAL:HG21	1.77	0.84
1:A:181:PHE:HA	1:A:184:MET:HE3	1.59	0.84
1:B:345:ALA:HB2	1:B:383:LYS:HE3	1.57	0.84
1:E:163:GLU:N	1:E:163:GLU:OE1	2.11	0.84
1:A:202:LYS:HD2	1:A:300:ALA:HB1	1.59	0.84
1:B:470:ALA:O	1:B:558:VAL:HG21	1.76	0.84
1:C:174:PHE:CZ	1:C:188:ILE:HD13	2.13	0.84
1:D:215:VAL:HG22	1:D:216:PRO:HD2	1.59	0.84
1:D:395:ARG:HG2	1:D:395:ARG:NH1	1.89	0.84
1:E:430:GLU:O	1:E:431:HIS:HB3	1.74	0.84
1:F:253:PHE:CE2	1:F:255:ASP:HB2	2.13	0.84
1:A:163:GLU:OE1	1:A:163:GLU:N	2.11	0.84
1:A:313:ARG:NH1	1:A:526:TYR:O	2.10	0.84
1:C:453:ARG:HH22	1:C:464:ARG:HH12	1.26	0.84
1:D:263:LYS:CE	1:E:228:MET:HE2	2.07	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:428:PHE:CD1	1:A:432:ALA:HA	2.13	0.84
1:F:356:ARG:HH11	1:F:356:ARG:CG	1.88	0.84
1:A:173:GLU:HA	1:A:176:LYS:HG2	1.60	0.84
1:A:308:ASP:OD1	1:A:310:ALA:N	2.11	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:C:236:ARG:CG	1:C:237:VAL:N	2.34	0.84
1:E:181:PHE:HA	1:E:184:MET:HE3	1.58	0.84
1:F:355:LYS:HE3	1:F:578:GLU:O	1.76	0.84
1:A:283:LEU:HD11	1:A:311:LEU:HD21	1.59	0.83
1:B:262:ARG:HG3	1:B:263:LYS:H	1.43	0.83
1:B:370:ASN:OD1	1:B:371:GLU:N	2.10	0.83
1:C:453:ARG:HH22	1:C:460:TRP:HE1	1.22	0.83
1:C:571:ARG:HD2	1:C:590:VAL:O	1.78	0.83
1:E:202:LYS:HD2	1:E:300:ALA:HB1	1.60	0.83
1:B:302:ASN:HD21	1:B:443:ARG:NH2	1.75	0.83
1:D:313:ARG:HG3	1:D:314:PRO:CD	2.07	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:E:509:GLY:C	1:F:476:ARG:HH22	1.85	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:E:263:LYS:CE	1:E:276:GLU:CD	2.50	0.83
1:F:376:ALA:C	1:F:381:ARG:HD2	2.03	0.83
1:A:313:ARG:HH22	1:A:526:TYR:CA	1.90	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:HG3	1:F:356:ARG:NH1	1.83	0.83
1:F:378:ARG:C	1:F:380:GLY:H	1.86	0.83
1:B:235:ALA:O	1:B:238:ARG:CZ	2.26	0.83
1:E:453:ARG:HH22	1:E:464:ARG:HH12	1.27	0.83
1:F:207:ARG:HB3	1:F:217:PHE:CZ	2.13	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:C:384:ILE:CG2	1:C:388:ASP:HB2	2.09	0.83
1:D:302:ASN:HD21	1:D:443:ARG:NH2	1.75	0.83
1:E:470:ALA:HB1	1:E:558:VAL:HG23	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:D:257:ILE:H	1:D:257:ILE:HD12	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: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:325:ALA:HB3	1:D:326:PRO:HD3	1.58	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:F:430:GLU:OE1	1:F:430:GLU:HA	1.78	0.82
1:F:482:VAL:HG13	1:F:483:PHE:CD2	2.12	0.82
1:A:342:LYS:CD	1:F:184:MET:O	2.28	0.82
1:A:416:ALA:HB1	1:A:577:LEU:HD23	1.56	0.82
1:B:215:VAL:HG22	1:B:216:PRO:HD2	1.61	0.82
1:C:286:MET:HE1	1:C:297:VAL:HG11	1.61	0.82
1:D:165:LYS:HA	1:D:168:LEU:HD22	1.62	0.82
1:E:233:GLY:HA2	1:E:236:ARG:NH1	1.94	0.82
1:A:233:GLY:O	1:A:236:ARG:HG2	1.79	0.82
1:C:163:GLU:OE1	1:C:163:GLU:N	2.11	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: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:A:449:PHE:CE2	1:A:496:GLN:CG	2.62	0.82
1:E:197:PRO:HD2	1:E:200:VAL:HG21	1.61	0.82
1:E:286:MET:HE1	1:E:297:VAL:HG11	1.61	0.82
1:F:257:ILE:H	1:F:257:ILE:HD12	1.44	0.82
1:A:332:GLU:OE2	1:A:351:ALA:HA	1.80	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:E:174:PHE:CZ	1:E:188:ILE:HD13	2.12	0.82
1:E:207:ARG:CZ	1:E:207:ARG:HB2	2.10	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:PRO:HD2	1:C:200:VAL:HG21	1.59	0.82
1:D:238:ARG:HH12	1:D:239:ASP:CB	1.92	0.82
1:A:313:ARG:HH22	1:A:526:TYR:HA	1.44	0.82
1:B:529:GLY:O	1:B:530:TYR:HB3	1.79	0.82
1:A:377:ALA:HB1	1:F:181:PHE:CE1	2.15	0.82
1:C:460:TRP:O	1:D:488:THR:HA	1.80	0.82
1:F:262:ARG:HG3	1:F:263:LYS:H	1.45	0.82
1:F:571:ARG:HD2	1:F:590:VAL:O	1.80	0.82
1:A:470:ALA:HB1	1:A:558:VAL:HG23	1.62	0.82
1:B:343:PRO:HG2	1:B:383:LYS:HA	1.62	0.82
1:C:225:PHE:CE1	1:C:233:GLY:CA	2.60	0.82
1:E:263:LYS:HD2	1:E:276:GLU:OE1	1.78	0.82
1:E:313:ARG:CZ	1:E:526:TYR:HA	2.08	0.81
1:F:327:ASP:OD1	1:F:328:VAL:N	2.12	0.81
1:B:471:VAL:O	1:B:474:ALA:HB3	1.80	0.81
1:F:589:ARG:NE	1:F:596:LEU:HD11	1.95	0.81
1:A:197:PRO:HD2	1:A:200:VAL:HG21	1.61	0.81
1:A:354:ALA:O	1:A:357:THR:HG23	1.80	0.81
1:A:519:TYR:O	1:A:533:ARG:NE	2.12	0.81
1:B:313:ARG:HG3	1:B:314:PRO:CD	2.10	0.81
1:B:337:ILE:HD12	1:B:340:ARG:NH1	1.96	0.81
1:E:263:LYS:HZ2	1:E:276:GLU:CD	1.80	0.81
1:F:579:ARG:O	1:F:579:ARG:HG2	1.78	0.81
1:A:207:ARG:HB2	1:A:207:ARG:CZ	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:D:482:VAL:HG13	1:D:483:PHE:CD2	2.13	0.81
1:E:416:ALA:HB1	1:E:577:LEU:HD23	1.57	0.81
1:F:337:ILE:O	1:F:340:ARG:NH1	2.13	0.81
1:B:286:MET:CE	1:B:316:ARG:HA	2.09	0.81
1:B:523:GLU:HG2	1:B:530:TYR:O	1.81	0.81
1:B:568:VAL:O	1:B:572:VAL:HG23	1.79	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:C:225:PHE:HE1	1:C:233:GLY:HA2	1.43	0.81
1:B:241:PHE:O	1:B:244:ALA:N	2.13	0.81
1:C:173:GLU:HA	1:C:176:LYS:HG2	1.63	0.81
1:D:243:THR:HA	1:D:246:ARG:HH21	1.45	0.81
1:D:286:MET:CE	1:D:316:ARG:HA	2.09	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:338:HIS:ND1	1:F:366:GLU:HG3	1.94	0.81
1:F:474:ALA:CA	1:F:558:VAL:HG11	2.11	0.81
1:C:262:ARG:HB3	1:C:275:ARG:NH1	1.93	0.81
1:E:410:ARG:O	1:E:413:ARG:N	2.14	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:F:375:LEU:HD11	1:F:388:ASP:HB3	1.61	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:HE3	1:F:460:TRP:N	1.77	0.81
1:A:178:PRO:HB3	1:A:294:ALA:HB2	1.62	0.80
1:B:430:GLU:HA	1:B:430:GLU:OE1	1.81	0.80
1:C:215:VAL:CG2	1:C:250:CYS:HA	2.10	0.80
1:D:155:PHE:CD2	1:D:212:GLU:OE2	2.34	0.80
1:D:533:ARG:HH11	1:D:533:ARG:HG3	1.45	0.80
1:D:582:LEU:HD21	1:D:590:VAL:HG21	1.62	0.80
1:E:225:PHE:CE1	1:E:233:GLY:CA	2.63	0.80
1:E:467:ASP:OD1	1:E:557:ARG:NH2	2.14	0.80
1:F:568:VAL:O	1:F:572:VAL:HG23	1.81	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:C:313:ARG:CZ	1:C:526:TYR:HA	2.10	0.80
1:D:331:ARG:NH2	1:D:580:GLU:OE1	2.14	0.80
1:E:236:ARG:HH11	1:E:236:ARG:CG	1.93	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:371:GLU:HG3	1:A:392:ALA:HB1	1.62	0.80
1:B:474:ALA:CA	1:B:558:VAL:HG11	2.11	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:325:ALA:HB3	1:B:326:PRO:HD3	1.62	0.80
1:B:521:VAL:HG23	1:B:532:VAL:HG13	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:A:155:PHE:CD2	1:A:212:GLU:OE1	2.34	0.80
1:E:215:VAL:HG11	1:E:250:CYS:HA	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:153:VAL:HG13	1:D:154:THR:H	1.46	0.80
1:E:172:VAL:HG23	1:E:213:ALA:CB	2.08	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: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:E:460:TRP:CD1	1:E:464:ARG:HH12	2.00	0.79
1:F:313:ARG:CG	1:F:314:PRO:CD	2.60	0.79
1:D:236:ARG:HG2	1:D:237:VAL:N	1.97	0.79
1:D:348:VAL:HG21	1:D:352:LEU:CD2	2.12	0.79
1:E:219:THR:HB	1:E:253:PHE:HD2	1.47	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:F:582:LEU:HD21	1:F:590:VAL:HG21	1.63	0.79
1:A:225:PHE:CE1	1:A:233:GLY:CA	2.61	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:F:274:GLU:O	1:F:277:GLN:HG2	1.81	0.79
1:A:223:SER:O	1:A:225:PHE:N	2.15	0.79
1:B:589:ARG:NE	1:B:594:LEU:HD21	1.93	0.79
1:D:235:ALA:O	1:D:238:ARG:HG3	1.83	0.79
1:C:223:SER:O	1:C:225:PHE:N	2.14	0.79
1:C:503:ARG:HG2	1:C:508:TRP:CZ3	2.18	0.79
1:D:241:PHE:O	1:D:244:ALA:N	2.15	0.79
1:D:460:TRP:HE3	1:D:460:TRP:N	1.80	0.79
1:A:236:ARG:O	1:A:237:VAL:C	2.26	0.79
1:A:274:GLU:O	1:A:277:GLN:HB3	1.81	0.79
1:C:178:PRO:HB3	1:C:294:ALA:HB2	1.65	0.79
1:C:236:ARG:HH11	1:C:236:ARG:CG	1.96	0.79
1:F:325:ALA:HB3	1:F:326:PRO:HD3	1.65	0.79
1:B:165:LYS:HA	1:B:168:LEU:HD22	1.64	0.79
1:B:378:ARG:C	1:B:380:GLY:H	1.89	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:A:461:SER:HA	1:B:487:THR:O	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:354:ALA:O	1:C:357:THR:HG23	1.83	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:F:394:ASP:HA	1:F:397:MET:HE3	1.63	0.78
1:A:236:ARG:HH11	1:A:236:ARG:CG	1.95	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: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:E:536:SER:OG	1:F:544:ASP:OD2	2.02	0.78
1:B:274:GLU:O	1:B:277:GLN:HG2	1.83	0.78
1:D:376:ALA:O	1:D:381:ARG:CG	2.31	0.78
1:E:286:MET:CB	1:E:316:ARG:CG	2.45	0.78
1:B:310:ALA:C	1:B:316:ARG:HH12	1.86	0.78
1:C:396:VAL:O	1:C:400:PRO:HD3	1.83	0.78
1:B:376:ALA:C	1:B:381:ARG:HB2	2.08	0.78
1:C:263:LYS:HZ1	1:C:276:GLU:CD	1.91	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:A:382:ARG:CG	1:A:383:LYS:N	2.46	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:F:313:ARG:HG3	1:F:314:PRO:CD	2.12	0.78
1:A:264:ARG:CD	1:A:266:SER:HB2	2.13	0.78
1:B:235:ALA:O	1:B:238:ARG:HG3	1.84	0.78
1:C:358:PRO:HA	1:C:359:GLY:C	2.08	0.78
1:D:474:ALA:CA	1:D:558:VAL:HG11	2.13	0.78
1:F:238:ARG:HH11	1:F:239:ASP:N	1.77	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:HH11	1:D:319:ARG:CG	1.96	0.78
1:D:382:ARG:CG	1:D:382:ARG:NH1	2.17	0.78
1:F:236:ARG:HG2	1:F:237:VAL:N	1.97	0.78
1:C:346:GLU:N	1:C:346:GLU:OE1	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:C:225:PHE:CE2	1:C:278:THR:HB	2.19	0.78
1:E:465:LEU:HD22	1:E:508:TRP:HZ3	1.50	0.78
1:F:207:ARG:HB3	1:F:217:PHE:CE1	2.19	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:331:ARG:NH2	1:F:580:GLU:OE1	2.15	0.78
1:F:343:PRO:HG2	1:F:383:LYS:HA	1.66	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:585:GLU:O	1:A:588:GLN:CG	2.27	0.77
1:B:207:ARG:HB3	1:B:217:PHE:CE1	2.20	0.77
1:C:352:LEU:HD21	1:C:386:MET:SD	2.24	0.77
1:C:586:GLU:HA	1:C:589:ARG:CG	2.15	0.77
1:D:283:LEU:HD12	1:D:316:ARG:HH21	1.49	0.77
1:D:337:ILE:O	1:D:340:ARG:NH1	2.18	0.77
1:F:153:VAL:HG13	1:F:154:THR:H	1.48	0.77
1:A:346:GLU:OE1	1:A:346:GLU:N	2.17	0.77
1:B:155:PHE:CD2	1:B:212:GLU:OE2	2.36	0.77
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:A:418:HIS:O	1:A:421:GLY:N	2.18	0.77
1:D:394:ASP:HA	1:D:397:MET:HE3	1.66	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:319:ARG:HH21	1:B:402:LYS:NZ	1.82	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:D:454:ARG:HH21	1:D:526:TYR:C	1.93	0.77
1:D:458:LEU:HD12	1:D:459:HIS:H	1.48	0.77
1:B:414:ILE:HG23	1:B:483:PHE:CE1	2.20	0.77
1:B:450:MET:HA	1:B:453:ARG:HD2	1.65	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:B:413:ARG:HH11	1:B:413:ARG:CG	1.95	0.77
1:E:236:ARG:O	1:E:237:VAL:C	2.27	0.77
1:E:286:MET:HG3	1:E:316:ARG:CD	2.15	0.77
1:A:352:LEU:HD21	1:A:386:MET:SD	2.25	0.77
1:B:243:THR:HA	1:B:246:ARG:HH21	1.48	0.77
1:B:454:ARG:HH21	1:B:526:TYR:C	1.91	0.77
1:E:352:LEU:HD12	1:E:356:ARG:HH21	1.49	0.77
1:F:243:THR:HA	1:F:246:ARG:HH21	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:ARG:HD2	1:A:534:GLN:N	2.00	0.76
1:A:536:SER:OG	1:B:544:ASP:OD2	2.02	0.76
1:B:286:MET:O	1:B:289:PHE:HB2	1.85	0.76
1:D:331:ARG:NH1	1:D:357:THR:O	2.17	0.76
1:E:449:PHE:CE2	1:E:496:GLN:CG	2.67	0.76
1:E:453:ARG:HH11	1:E:453:ARG:HG3	1.50	0.76
1:F:376:ALA:C	1:F:381:ARG:HB2	2.10	0.76
1:B:276:GLU:HA	1:B:279:LEU:CD1	2.15	0.76
1:C:313:ARG:HH22	1:C:526:TYR:HA	1.50	0.76
1:C:503:ARG:HD2	1:C:508:TRP:CE2	2.20	0.76
1:D:238:ARG:HH11	1:D:239:ASP:N	1.82	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:C:461:SER:O	1:C:464:ARG:HB3	1.85	0.76
1:D:274:GLU:O	1:D:277:GLN:HG2	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:B:502:ARG:O	1:B:506:THR:HG23	1.86	0.76
1:C:313:ARG:NH2	1:C:526:TYR:O	2.17	0.76
1:E:149:GLU:O	1:E:150:ALA:HB3	1.83	0.76
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:B:215:VAL:HG21	1:B:249:PRO:O	1.85	0.76
1:B:238:ARG:HH11	1:B:239:ASP:N	1.82	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: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:210:ALA:HB2	1:C:251:ILE:HD12	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: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:A:358:PRO:HA	1:A:359:GLY:C	2.11	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:F:241:PHE:CE2	1:F:285:GLU:OE2	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:166:GLU:CA	1:C:169:LYS:HG2	2.15	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: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:F:449:PHE:HE2	1:F:492:ASN:HB3	1.51	0.76
1:A:453:ARG:NH1	1:A:453:ARG:HG3	2.00	0.75
1:B:460:TRP:N	1:B:460:TRP:CE3	2.52	0.75
1:D:286:MET:HE1	1:D:316:ARG:CA	2.12	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:F:243:THR:HA	1:F:246:ARG:NH2	2.00	0.75
1:A:342:LYS:HD2	1:A:343:PRO:CD	2.13	0.75
1:B:238:ARG:HH12	1:B:239:ASP:CA	2.00	0.75
1:D:521:VAL:HG23	1:D:532:VAL:HG13	1.67	0.75
1:A:340:ARG:C	1:A:342:LYS:H	1.92	0.75
1:C:236:ARG:O	1:C:237:VAL:C	2.29	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
1:B:197:PRO:HD2	1:B:200:VAL:HG11	1.69	0.75
1:B:247:HIS:HB3	1:B:250:CYS:SG	2.27	0.75
1:C:390:GLU:O	1:C:393:ALA:HB3	1.86	0.75
1:C:584:ALA:O	1:C:587:PHE:HB3	1.85	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:F:474:ALA:HA	1:F:558:VAL:CG1	2.16	0.75
1:A:503:ARG:HG2	1:A:508:TRP:CZ3	2.22	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: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:A:388:ASP:OD1	1:A:388:ASP:N	2.20	0.75
1:C:181:PHE:O	1:C:184:MET:HG2	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:589:ARG:HH22	1:C:596:LEU:HB2	1.33	0.75
1:E:286:MET:CG	1:E:316:ARG:HD2	2.15	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:F:348:VAL:HG21	1:F:386:MET:HE2	1.68	0.75
1:A:210:ALA:O	1:A:214:ARG:HD3	1.87	0.75
1:C:172:VAL:HG23	1:C:213:ALA:CB	2.12	0.75
1:C:174:PHE:CE2	1:C:188:ILE:HD13	2.22	0.75
1:D:376:ALA:C	1:D:381:ARG:CG	2.60	0.75
1:B:451:MET:HB3	1:B:452:PRO:HD3	1.69	0.74
1:C:340:ARG:C	1:C:342:LYS:H	1.95	0.74
1:D:412:ARG:HH22	1:D:440:ILE:HB	1.49	0.74
1:E:393:ALA:O	1:E:396:VAL:HG12	1.87	0.74
1:F:319:ARG:HH11	1:F:319:ARG:CG	2.00	0.74
1:F:410:ARG:O	1:F:413:ARG:N	2.20	0.74
1:A:331:ARG:NH1	1:A:354:ALA:O	2.20	0.74
1:C:313:ARG:CZ	1:C:526:TYR:O	2.34	0.74
1:C:381:ARG:HH11	1:C:381:ARG:HG3	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:E:335:LEU:CD2	1:E:353:LEU:HD23	2.17	0.74
1:F:337:ILE:HD12	1:F:340:ARG:NH1	2.01	0.74
1:A:166:GLU:CA	1:A:169:LYS:HG2	2.14	0.74
1:A:586:GLU:HA	1:A:589:ARG:HE	1.50	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:B:503:ARG:HH12	1:B:522:ARG:HH21	1.35	0.74
1:E:510:MET:O	1:E:512:PRO:HD2	1.87	0.74
1:E:584:ALA:O	1:E:587:PHE:HB3	1.86	0.74
1:F:503:ARG:HH22	1:F:522:ARG:NH2	1.85	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:171:ILE:HG13	1:F:296:VAL:HG21	1.69	0.74
1:F:454:ARG:HH21	1:F:526:TYR:C	1.94	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:F:313:ARG:NE	1:F:314:PRO:HD2	2.00	0.74
1:A:249:PRO:HA	1:A:294:ALA:O	1.87	0.74
1:A:453:ARG:HH22	1:A:460:TRP:NE1	1.84	0.74
1:F:331:ARG:NH1	1:F:357:THR:O	2.19	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:E:340:ARG:C	1:E:342:LYS:H	1.93	0.74
1:F:458:LEU:HD12	1:F:459:HIS:H	1.53	0.74
1:A:313:ARG:NH2	1:A:526:TYR:O	2.20	0.74
1:A:390:GLU:O	1:A:393:ALA:HB3	1.88	0.74
1:A:460:TRP:CD1	1:A:464:ARG:HH12	2.05	0.74
1:B:588:GLN:O	1:B:591:VAL:HB	1.88	0.74
1:D:243:THR:HA	1:D:246:ARG:NH2	2.02	0.74
1:D:458:LEU:HD12	1:D:459:HIS:N	2.02	0.74
1:D:564:GLU:C	1:D:566:ARG:H	1.95	0.74
1:E:418:HIS:O	1:E:421:GLY:N	2.21	0.74
1:F:155:PHE:HD2	1:F:212:GLU:OE2	1.71	0.74
1:A:461:SER:OG	1:B:486:VAL:HG11	1.87	0.74
1:C:236:ARG:HG3	1:C:237:VAL:H	1.52	0.74
1:D:468:GLN:O	1:D:471:VAL:HG22	1.88	0.74
1:E:358:PRO:HA	1:E:359:GLY:C	2.11	0.74
1:F:199:GLY:N	2:F:2001:ADP:O2B	2.17	0.74
1:F:589:ARG:NE	1:F:594:LEU:HD21	1.94	0.74
1:E:236:ARG:HG3	1:E:237:VAL:H	1.52	0.73
1:E:413:ARG:CA	1:E:577:LEU:HD22	2.16	0.73
1:A:181:PHE:O	1:A:184:MET:HG2	1.87	0.73
1:A:263:LYS:HD2	1:A:276:GLU:OE1	1.79	0.73
1:A:381:ARG:HH11	1:A:381:ARG:HG3	1.53	0.73
1:C:453:ARG:HH22	1:C:460:TRP:NE1	1.85	0.73
1:D:235:ALA:O	1:D:238:ARG:CZ	2.36	0.73
1:D:346:GLU:HG3	1:D:386:MET:HG2	1.70	0.73
1:D:571:ARG:HD2	1:D:590:VAL:O	1.88	0.73
1:E:166:GLU:CA	1:E:169:LYS:HG2	2.16	0.73
1:E:390:GLU:O	1:E:393:ALA:HB3	1.87	0.73
1:E:453:ARG:NH1	1:E:460:TRP:CZ2	2.55	0.73
1:A:313:ARG:NH2	1:A:526:TYR:CA	2.46	0.73
1:A:410:ARG:HG3	1:A:411:ASP:N	2.04	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:155:PHE:HD2	1:D:212:GLU:OE2	1.71	0.73
1:D:589:ARG:NE	1:D:594:LEU:HD21	1.95	0.73
1:E:215:VAL:HG21	1:E:250:CYS:CA	2.17	0.73
1:F:376:ALA:HA	1:F:381:ARG:NE	2.04	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:376:ALA:HA	1:F:381:ARG:HD2	0.74	0.73
1:B:348:VAL:HG22	1:B:352:LEU:HD22	1.70	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:D:586:GLU:O	1:D:590:VAL:HG23	1.88	0.73
1:F:316:ARG:NH1	1:F:316:ARG:HG2	2.03	0.73
1:F:436:HIS:O	1:F:437:LYS:HG2	1.89	0.73
1:B:589:ARG:HB3	1:B:594:LEU:HD22	1.70	0.73
1:D:158:VAL:HG22	1:D:204:HIS:CE1	2.23	0.73
1:D:191:GLY:HA2	1:D:297:VAL:HG12	1.71	0.73
1:D:430:GLU:OE1	1:D:430:GLU:HA	1.88	0.73
1:D:439:THR:CG2	1:D:445:ARG:HH22	2.00	0.73
1:E:453:ARG:HH22	1:E:460:TRP:NE1	1.86	0.73
1:F:233:GLY:HA2	1:F:236:ARG:HH21	1.52	0.73
1:A:236:ARG:HG3	1:A:237:VAL:H	1.49	0.73
1:A:408:SER:HB2	1:A:409:PRO:HD2	1.71	0.73
1:C:196:GLY:H	1:C:202:LYS:NZ	1.86	0.73
1:F:247:HIS:HB3	1:F:250:CYS:SG	2.28	0.73
1:B:238:ARG:CB	1:B:281:GLN:NE2	2.52	0.73
1:B:394:ASP:HA	1:B:397:MET:HE3	1.68	0.73
1:C:460:TRP:CD1	1:C:464:ARG:HH12	2.07	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: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:A:264:ARG:HG3	1:A:265:GLY:N	2.02	0.73
1:B:348:VAL:HG21	1:B:386:MET:HE2	1.69	0.73
1:B:501:ALA:HB1	1:B:550:LEU:HD23	1.70	0.73
1:C:215:VAL:HG21	1:C:250:CYS:CA	2.19	0.73
1:D:153:VAL:HB	1:D:207:ARG:HH11	1.54	0.73
1:D:155:PHE:HA	1:D:158:VAL:HG23	1.71	0.73
1:E:382:ARG:HG3	1:E:383:LYS:H	1.51	0.73
1:F:193:LEU:O	1:F:320:GLN:HB2	1.88	0.73
1:A:460:TRP:CD1	1:A:464:ARG:NH1	2.57	0.73
1:A:589:ARG:NH1	1:A:596:LEU:HB3	2.02	0.73
1:F:235:ALA:HA	1:F:238:ARG:CD	2.18	0.73
1:F:316:ARG:HG2	1:F:316:ARG:HH11	1.54	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:A:503:ARG:HD2	1:A:508:TRP:CE2	2.23	0.72
1:B:155:PHE:HD2	1:B:212:GLU:OE2	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:ILE:HG13	1:B:296:VAL:HG21	1.71	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:D:412:ARG:NH2	1:D:440:ILE:HD13	2.03	0.72
1:E:453:ARG:HH21	1:E:464:ARG:NH2	1.86	0.72
1:F:276:GLU:CA	1:F:279:LEU:HD13	2.18	0.72
1:A:586:GLU:CA	1:A:589:ARG:NE	2.52	0.72
1:C:166:GLU:CB	1:C:169:LYS:HZ2	2.02	0.72
1:D:313:ARG:HG3	1:D:314:PRO:N	2.04	0.72
1:D:337:ILE:HD12	1:D:340:ARG:NH1	2.02	0.72
1:D:449:PHE:HE2	1:D:492:ASN:HB3	1.53	0.72
1:E:224:ASP:HA	1:E:227:GLU:OE2	1.88	0.72
1:E:388:ASP:OD1	1:E:388:ASP:N	2.22	0.72
1:E:460:TRP:CD1	1:E:464:ARG:NH1	2.56	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:B:245:LYS:C	1:B:247:HIS:H	1.97	0.72
1:D:378:ARG:O	1:D:380:GLY:N	2.21	0.72
1:E:196:GLY:N	1:E:202:LYS:NZ	2.36	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:C:313:ARG:HH12	1:C:526:TYR:C	1.97	0.72
1:C:331:ARG:NH1	1:C:354:ALA:O	2.22	0.72
1:D:171:ILE:HG13	1:D:296:VAL:HG21	1.70	0.72
1:D:173:GLU:HA	1:D:176:LYS:HE3	1.71	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: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: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:F:245:LYS:C	1:F:247:HIS:H	1.97	0.72
1:F:392:ALA:O	1:F:396:VAL:HG12	1.88	0.72
1:F:564:GLU:C	1:F:566:ARG:H	1.95	0.72
1:A:149:GLU:O	1:A:150:ALA:HB3	1.90	0.72
1:A:210:ALA:HB2	1:A:251:ILE:HD12	1.70	0.72
1:A:461:SER:O	1:A:464:ARG:HB3	1.89	0.72
1:B:564:GLU:C	1:B:566:ARG:H	1.95	0.72
1:C:224:ASP:HA	1:C:227:GLU:OE2	1.89	0.72
1:D:376:ALA:C	1:D:381:ARG:HB2	2.15	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:441:VAL:O	1:E:441:VAL:HG12	1.89	0.72
1:F:311:LEU:C	1:F:311:LEU:HD12	2.14	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: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:A:465:LEU:HD22	1:A:508:TRP:HZ3	1.55	0.72
1:B:392:ALA:O	1:B:396:VAL:HG12	1.89	0.72
1:C:335:LEU:CD2	1:C:353:LEU:HD23	2.19	0.72
1:C:439:THR:OG1	1:C:440:ILE:N	2.23	0.72
1:D:247:HIS:HB3	1:D:250:CYS:SG	2.29	0.72
1:D:589:ARG:HB3	1:D:594:LEU:HD22	1.71	0.72
1:E:181:PHE:O	1:E:184:MET:HG2	1.90	0.72
1:E:524:ASP:CA	1:E:529:GLY:HA2	2.08	0.72
1:A:286:MET:HE1	1:A:297:VAL:HG11	1.70	0.72
1:A:382:ARG:HG3	1:A:383:LYS:CB	2.20	0.72
1:B:286:MET:O	1:B:289:PHE:CB	2.37	0.72
1:D:214:ARG:HH11	1:D:214:ARG:HB3	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:D:414:ILE:HG23	1:D:483:PHE:CE1	2.24	0.71
1:D:567:GLU:O	1:D:570:GLU:N	2.23	0.71
1:D:579:ARG:O	1:D:581:THR:N	2.22	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:F:589:ARG:HB3	1:F:594:LEU:HD22	1.72	0.71
1:A:378:ARG:HA	1:F:173:GLU:CD	2.14	0.71
1:B:571:ARG:HD2	1:B:590:VAL:O	1.88	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:F:346:GLU:HG3	1:F:386:MET:HG2	1.70	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: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:C:233:GLY:HA2	1:C:236:ARG:HH12	1.53	0.71
1:C:236:ARG:O	1:C:239:ASP:OD1	2.07	0.71
1:C:453:ARG:NH2	1:C:460:TRP:NE1	2.33	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:B:376:ALA:HA	1:B:381:ARG:HD2	0.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:149:GLU:O	1:C:150:ALA:HB3	1.88	0.71
1:E:381:ARG:HH11	1:E:381:ARG:HG3	1.53	0.71
1:F:414:ILE:HG23	1:F:483:PHE:CE1	2.26	0.71
1:F:586:GLU:O	1:F:590:VAL:HG23	1.91	0.71
1:B:352:LEU:O	1:B:355:LYS:HB2	1.90	0.71
1:C:586:GLU:O	1:C:589:ARG:HB2	1.90	0.71
1:E:410:ARG:HG3	1:E:411:ASP:N	2.04	0.71
1:F:163:GLU:OE1	1:F:163:GLU:N	2.24	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:B:233:GLY:O	1:B:236:ARG:NH1	2.23	0.71
1:C:155:PHE:HZ	1:C:168:LEU:HD11	1.55	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:163:GLU:OE1	1:D:163:GLU:N	2.23	0.71
1:D:245:LYS:C	1:D:247:HIS:H	1.98	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: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:F:165:LYS:HZ1	1:F:205:LEU:HB3	1.54	0.71
1:B:155:PHE:HA	1:B:158:VAL:HG23	1.71	0.71
1:B:242:GLU:HA	1:B:245:LYS:HB3	1.72	0.71
1:B:332:GLU:OE1	1:B:351:ALA:HA	1.91	0.71
1:B:533:ARG:HH11	1:B:533:ARG:HG3	1.56	0.71
1:C:521:VAL:HG12	1:D:495:ARG:HD2	1.71	0.71
1:D:502:ARG:O	1:D:506:THR:HG23	1.91	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:D:193:LEU:O	1:D:320:GLN:HB2	1.90	0.71
1:B:190:LYS:CE	1:B:289:PHE:CZ	2.74	0.70
1:D:428:PHE:CE1	1:D:432:ALA:HB1	2.26	0.70
1:F:284:VAL:O	1:F:288:GLY:N	2.24	0.70
1:A:178:PRO:HB3	1:A:294:ALA:CB	2.21	0.70
1:A:384:ILE:HG23	1:A:388:ASP:CB	2.21	0.70
1:B:346:GLU:HG3	1:B:386:MET:CG	2.20	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:191:GLY:CA	1:D:297:VAL:HG12	2.21	0.70
1:D:346:GLU:HG3	1:D:386:MET:CG	2.21	0.70
1:E:165:LYS:O	1:E:168:LEU:HG	1.90	0.70
1:E:196:GLY:H	1:E:202:LYS:NZ	1.87	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:A:481:ILE:CD1	1:A:563:LEU:HB3	2.21	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:D:449:PHE:CE2	1:D:453:ARG:NH2	2.59	0.70
1:E:313:ARG:NH2	1:E:526:TYR:O	2.25	0.70
1:E:419:GLU:OE1	1:E:419:GLU:HA	1.92	0.70
1:A:227:GLU:HG3	1:F:263:LYS:HZ3	1.56	0.70
1:A:313:ARG:CZ	1:A:526:TYR:O	2.40	0.70
1:B:311:LEU:N	1:B:316:ARG:NH1	2.38	0.70
1:E:503:ARG:HG2	1:E:508:TRP:CZ3	2.27	0.70
1:F:381:ARG:NH1	1:F:388:ASP:OD2	2.25	0.70
1:A:225:PHE:HE1	1:A:233:GLY:C	1.98	0.70
1:A:286:MET:HE1	1:A:297:VAL:HG21	1.73	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:E:439:THR:OG1	1:E:440:ILE:N	2.22	0.70
1:A:520:ALA:HA	1:A:533:ARG:CD	2.22	0.70
1:B:365:LEU:O	1:B:368:LEU:HB3	1.92	0.70
1:C:239:ASP:OD1	1:C:240:LEU:N	2.25	0.70
1:C:408:SER:HB2	1:C:409:PRO:HD2	1.73	0.70
1:D:214:ARG:HH11	1:D:214:ARG:CB	2.05	0.70
1:F:238:ARG:HB3	1:F:281:GLN:NE2	2.06	0.70
1:A:335:LEU:CD2	1:A:353:LEU:HD23	2.21	0.70
1:A:465:LEU:HD22	1:A:508:TRP:CZ3	2.26	0.70
1:A:588:GLN:O	1:A:591:VAL:CB	2.39	0.70
1:B:503:ARG:HH22	1:B:522:ARG:CZ	2.05	0.70
1:C:384:ILE:HG23	1:C:388:ASP:CB	2.21	0.70
1:D:284:VAL:O	1:D:288:GLY:N	2.24	0.70
1:D:389:LEU:O	1:D:392:ALA:N	2.25	0.70
1:F:182:HIS:ND1	1:F:182:HIS:N	2.40	0.70
1:F:501:ALA:O	1:F:505:ILE:HD12	1.92	0.70
1:A:196:GLY:HA2	1:A:443:ARG:HH21	1.55	0.70
1:A:224:ASP:HA	1:A:227:GLU:OE2	1.91	0.70
1:B:311:LEU:C	1:B:311:LEU:HD12	2.16	0.70
1:C:333:GLN:HG3	1:C:336:ARG:NH1	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:319:ARG:HH11	1:B:319:ARG:CG	2.02	0.70
1:C:273:ASP:CG	1:C:274:GLU:N	2.49	0.70
1:E:215:VAL:CG1	1:E:250:CYS:HA	2.22	0.70
1:E:225:PHE:HE1	1:E:233:GLY:C	2.00	0.70
1:E:286:MET:O	1:E:289:PHE:CZ	2.45	0.70
1:E:313:ARG:HH12	1:E:526:TYR:C	1.99	0.70
1:F:376:ALA:HB2	1:F:381:ARG:HH11	1.57	0.70
1:D:215:VAL:HG23	1:D:216:PRO:HD2	1.73	0.70
1:D:428:PHE:CE1	1:D:432:ALA:CB	2.74	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:A:196:GLY:H	1:A:202:LYS:NZ	1.89	0.69
1:A:413:ARG:CA	1:A:577:LEU:HD22	2.16	0.69
1:C:275:ARG:HG2	1:C:275:ARG:NH1	2.01	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:E:453:ARG:NH2	1:E:460:TRP:NE1	2.35	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:B:215:VAL:HG23	1:B:216:PRO:HD2	1.72	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: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:207:ARG:HB2	1:C:207:ARG:CZ	2.21	0.69
1:E:449:PHE:N	1:E:449:PHE:CD2	2.60	0.69
1:E:503:ARG:HD2	1:E:508:TRP:CE2	2.27	0.69
1:A:215:VAL:HG21	1:A:250:CYS:CA	2.21	0.69
1:B:187:ARG:H	1:C:374:LEU:HD11	1.58	0.69
1:D:202:LYS:HG2	2:D:2001:ADP:O1A	1.92	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:A:283:LEU:HD11	1:A:311:LEU:CD2	2.21	0.69
1:C:303:ARG:HB2	1:C:303:ARG:HH11	0.64	0.69
1:C:533:ARG:CD	1:C:534:GLN:H	2.05	0.69
1:E:382:ARG:HD3	1:E:383:LYS:HB3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:253:PHE:HA	1:F:298:MET:HB3	1.74	0.69
1:F:303:ARG:O	1:F:307:LEU:HD13	1.93	0.69
1:A:234:ALA:O	1:A:237:VAL:HG12	1.92	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:177:ASN:HD22	1:C:180:ARG:HD3	1.58	0.69
1:C:313:ARG:NH2	1:C:526:TYR:CA	2.52	0.69
1:C:453:ARG:HG3	1:C:453:ARG:NH1	2.02	0.69
1:D:225:PHE:CD2	1:D:236:ARG:HD2	2.28	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:B:424:LEU:O	1:B:427:HIS:N	2.24	0.69
1:C:234:ALA:HB1	1:C:281:GLN:NE2	2.07	0.69
1:C:469:ILE:HG23	1:C:497:ALA:HB1	1.73	0.69
1:D:155:PHE:O	1:D:158:VAL:N	2.26	0.69
1:D:228:MET:SD	1:D:232:VAL:HG12	2.33	0.69
1:D:233:GLY:HA2	1:D:236:ARG:HH21	1.51	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:D:424:LEU:O	1:D:427:HIS:N	2.23	0.69
1:E:303:ARG:HB2	1:E:303:ARG:HH11	0.65	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: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: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:A:486:VAL:HG21	1:F:463:LYS:HE3	1.73	0.69
1:A:584:ALA:O	1:A:587:PHE:HB3	1.92	0.69
1:B:436:HIS:O	1:B:437:LYS:HG2	1.93	0.69
1:B:567:GLU:O	1:B:570:GLU:N	2.26	0.69
1:C:413:ARG:HA	1:C:577:LEU:CD2	2.15	0.69
1:C:453:ARG:CZ	1:C:460:TRP:HE1	2.05	0.69
1:D:197:PRO:HD2	1:D:200:VAL:HG11	1.75	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:E:263:LYS:HZ1	1:E:276:GLU:CD	1.99	0.69
1:E:340:ARG:O	1:E:342:LYS:N	2.25	0.69
1:F:242:GLU:HA	1:F:245:LYS:HB3	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:365:LEU:O	1:F:368:LEU:HB3	1.93	0.69
1:A:313:ARG:HH12	1:A:526:TYR:C	2.01	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:F:215:VAL:HG23	1:F:216:PRO:HD2	1.73	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:B:215:VAL:CG2	1:B:249:PRO:O	2.41	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: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:E:196:GLY:O	1:E:302:ASN:HA	1.92	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: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:C:519:TYR:O	1:C:533:ARG:CD	2.41	0.68
1:E:166:GLU:HA	1:E:169:LYS:CG	2.23	0.68
1:E:453:ARG:HG3	1:E:453:ARG:NH1	2.06	0.68
1:C:481:ILE:HG22	1:C:482:VAL:N	2.07	0.68
1:F:238:ARG:CG	1:F:281:GLN:NE2	2.56	0.68
1:B:220:ALA:O	1:B:254:ILE:HA	1.94	0.68
1:B:235:ALA:HA	1:B:238:ARG:CD	2.23	0.68
1:E:408:SER:HB2	1:E:409:PRO:HD2	1.76	0.68
1:E:500:LEU:O	1:E:503:ARG:HB3	1.93	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:F:428:PHE:CE1	1:F:432:ALA:CB	2.76	0.68
1:C:234:ALA:O	1:C:237:VAL:HG12	1.94	0.68
1:D:177:ASN:OD1	1:D:180:ARG:HB2	1.92	0.68
1:E:520:ALA:HA	1:E:533:ARG:CD	2.22	0.68
1:F:220:ALA:O	1:F:254:ILE:HA	1.93	0.68
1:F:376:ALA:O	1:F:381:ARG:HG3	1.94	0.68
1:F:412:ARG:NH2	1:F:440:ILE:HD13	2.09	0.68
1:A:166:GLU:HA	1:A:169:LYS:CG	2.21	0.68
1:C:410:ARG:HG3	1:C:411:ASP:N	2.06	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:348:VAL:HG21	1:D:386:MET:HE2	1.75	0.68
1:E:292:ASP:C	1:E:292:ASP:OD1	2.36	0.68
1:A:588:GLN:HA	1:A:591:VAL:CG2	2.23	0.68
1:B:216:PRO:HG3	1:B:247:HIS:ND1	2.07	0.68
1:C:357:THR:OG1	1:C:360:PHE:HD1	1.75	0.68
1:D:221:SER:HB2	1:D:256:GLU:OE1	1.93	0.68
1:D:392:ALA:O	1:D:396:VAL:HG12	1.94	0.68
1:E:178:PRO:HB3	1:E:294:ALA:CB	2.23	0.68
1:E:400:PRO:HG2	1:E:405:LEU:HD12	1.76	0.68
1:F:215:VAL:CG2	1:F:249:PRO:O	2.42	0.68
1:B:201:GLY:O	1:B:205:LEU:HD13	1.94	0.68
1:B:238:ARG:HG2	1:B:281:GLN:HE22	1.57	0.68
1:B:328:VAL:HG23	1:B:580:GLU:HG3	1.76	0.68
1:B:487:THR:HG22	1:B:488:THR:N	2.06	0.68
1:C:195:VAL:HG11	1:C:304:PRO:HD3	1.74	0.68
1:C:581:THR:O	1:C:582:LEU:HD12	1.94	0.68
1:D:165:LYS:NZ	1:D:205:LEU:HB3	2.08	0.68
1:E:197:PRO:HD2	1:E:200:VAL:CG2	2.23	0.68
1:E:283:LEU:CG	1:E:316:ARG:HH12	2.04	0.68
1:B:191:GLY:HA2	1:B:297:VAL:HG12	1.74	0.68
1:B:386:MET:O	1:B:389:LEU:HD12	1.93	0.68
1:C:197:PRO:HD2	1:C:200:VAL:CG2	2.23	0.68
1:D:276:GLU:CA	1:D:279:LEU:HD13	2.17	0.68
1:E:449:PHE:CZ	1:E:496:GLN:CG	2.67	0.68
1:E:586:GLU:HA	1:E:589:ARG:CG	2.24	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:A:223:SER:C	1:A:225:PHE:N	2.51	0.68
1:A:453:ARG:NH2	1:A:460:TRP:NE1	2.35	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:B:586:GLU:O	1:B:590:VAL:HG23	1.92	0.68
1:C:292:ASP:C	1:C:292:ASP:OD1	2.37	0.68
1:E:275:ARG:O	1:E:279:LEU:HB2	1.94	0.68
1:E:449:PHE:HB2	1:E:468:GLN:NE2	2.07	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:B:458:LEU:HD12	1:B:459:HIS:N	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:PHE:CZ	1:D:294:ALA:HB1	2.29	0.67
1:E:273:ASP:CG	1:E:274:GLU:N	2.51	0.67
1:F:191:GLY:CA	1:F:297:VAL:HG12	2.24	0.67
1:B:165:LYS:O	1:B:168:LEU:HB2	1.94	0.67
1:D:263:LYS:HZ3	1:E:227:GLU:HG3	1.59	0.67
1:F:225:PHE:HB3	1:F:278:THR:HG21	1.74	0.67
1:A:340:ARG:O	1:A:342:LYS:N	2.26	0.67
1:A:400:PRO:HG2	1:A:405:LEU:HD12	1.76	0.67
1:A:524:ASP:CA	1:A:529:GLY:HA2	2.10	0.67
1:A:585:GLU:OE2	1:A:589:ARG:NE	2.27	0.67
1:B:182:HIS:ND1	1:B:182:HIS:N	2.40	0.67
1:B:276:GLU:CA	1:B:279:LEU:HD13	2.16	0.67
1:B:341:GLY:O	1:B:342:LYS:HB2	1.94	0.67
1:B:395:ARG:HH11	1:B:395:ARG:CG	1.98	0.67
1:C:168:LEU:O	1:C:171:ILE:HD12	1.95	0.67
1:D:188:ILE:HG23	1:D:189:PRO:CD	2.24	0.67
1:F:174:PHE:CZ	1:F:294:ALA:HB1	2.28	0.67
1:C:519:TYR:HA	1:C:533:ARG:NH2	2.09	0.67
1:D:236:ARG:HH12	1:D:278:THR:HG22	1.59	0.67
1:D:253:PHE:HA	1:D:298:MET:HB3	1.76	0.67
1:D:376:ALA:O	1:D:381:ARG:HG3	1.93	0.67
1:E:234:ALA:O	1:E:237:VAL:HG12	1.95	0.67
1:E:449:PHE:CB	1:E:468:GLN:HE22	2.05	0.67
1:B:191:GLY:CA	1:B:297:VAL:HG12	2.24	0.67
1:B:277:GLN:HA	1:B:280:ASN:ND2	2.09	0.67
1:B:362:GLY:HA2	1:B:365:LEU:HD12	1.76	0.67
1:C:264:ARG:HG2	1:C:266:SER:H	1.59	0.67
1:C:447:LEU:HA	1:C:496:GLN:HE21	1.57	0.67
1:C:449:PHE:HB2	1:C:468:GLN:NE2	2.09	0.67
1:E:331:ARG:HD2	1:E:357:THR:HG23	1.77	0.67
1:E:334:ILE:HD13	2:E:1001:ADP:C6	2.30	0.67
1:F:276:GLU:HA	1:F:279:LEU:CD1	2.16	0.67
1:A:586:GLU:CB	1:A:589:ARG:HE	2.07	0.67
1:D:237:VAL:CG2	1:D:281:GLN:HG3	2.24	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:201:GLY:O	1:F:205:LEU:HD13	1.95	0.67
1:C:168:LEU:O	1:C:171:ILE:CD1	2.43	0.67
1:D:452:PRO:HG3	1:E:402:LYS:HE3	1.77	0.67
1:E:357:THR:OG1	1:E:360:PHE:CD1	2.48	0.67
1:F:190:LYS:HE3	1:F:289:PHE:CZ	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:GLU:OE1	1:A:523:GLU:N	2.27	0.67
1:C:449:PHE:CB	1:C:468:GLN:HE22	2.08	0.67
1:C:517:VAL:HG23	1:D:498:THR:OG1	1.95	0.67
1:D:154:THR:HG23	1:D:156:LYS:HB3	1.77	0.67
1:F:237:VAL:CG2	1:F:281:GLN:HG3	2.25	0.67
1:F:525:THR:HG22	1:F:526:TYR:CD2	2.29	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: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:E:491:GLU:O	1:E:493:ASP:N	2.28	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:303:ARG:O	1:B:307:LEU:HD13	1.95	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:D:503:ARG:HH12	1:D:522:ARG:HH21	1.40	0.67
1:E:168:LEU:O	1:E:171:ILE:CD1	2.43	0.67
1:E:333:GLN:HG3	1:E:336:ARG:NH1	2.10	0.67
1:F:503:ARG:HH22	1:F:522:ARG:CZ	2.08	0.67
1:A:333:GLN:HG3	1:A:336:ARG:NH1	2.10	0.66
1:D:153:VAL:HB	1:D:207: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:E:453:ARG:HH22	1:E:464:ARG:NH1	1.93	0.66
1:F:228:MET:SD	1:F:232:VAL:HG12	2.35	0.66
1:F:335:LEU:CD1	1:F:365:LEU:HB3	2.24	0.66
1:F:378:ARG:O	1:F:380:GLY:N	2.28	0.66
1:B:200:VAL:HG22	1:B:202:LYS:HD2	1.77	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: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:A:215:VAL:HG23	1:A:216:PRO:CD	2.24	0.66
1:A:580:GLU:O	1:A:580:GLU:HG2	1.94	0.66
1:B:228:MET:SD	1:B:232:VAL:HG12	2.35	0.66
1:D:466:LEU:HD11	1:D:504:MET:HE1	1.76	0.66
1:E:357:THR:OG1	1:E:360:PHE:HD1	1.77	0.66
1:F:277:GLN:HA	1:F:280:ASN:ND2	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:346:GLU:HG3	1:B:386:MET:HG2	1.77	0.66
1:C:387:LYS:HA	1:C:390:GLU:HB2	1.77	0.66
1:D:378:ARG:C	1:D:380:GLY:N	2.51	0.66
1:E:196:GLY:HA2	1:E:443:ARG:HH21	1.61	0.66
1:E:469:ILE:HG23	1:E:497:ALA:HB1	1.77	0.66
1:F:237:VAL:HG22	1:F:281:GLN:HG3	1.77	0.66
1:F:238:ARG:HG2	1:F:281:GLN:HE22	1.59	0.66
1:F:362:GLY:HA2	1:F:365:LEU:HD12	1.77	0.66
1:F:378:ARG:C	1:F:380:GLY:N	2.52	0.66
1:A:292:ASP:C	1:A:292:ASP:OD1	2.37	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:D:225:PHE:HB3	1:D:278:THR:HG21	1.77	0.66
1:D:241:PHE:CD2	1:D:285:GLU:HG3	2.31	0.66
1:D:511:HIS:C	1:D:512:PRO:O	2.38	0.66
1:D:523:GLU:OE2	1:E:264:ARG:NH2	2.29	0.66
1:E:215:VAL:HG11	1:E:250:CYS:CA	2.25	0.66
1:E:585:GLU:O	1:E:588:GLN:HG2	1.94	0.66
1:F:155:PHE:O	1:F:158:VAL:N	2.27	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:C:514:PHE:HB3	1:C:519:TYR:CE1	2.31	0.66
1:C:523:GLU:N	1:C:523:GLU:OE1	2.28	0.66
1:D:237:VAL:HG22	1:D:281:GLN:HG3	1.77	0.66
1:D:428:PHE:CZ	1:D:432:ALA:HB1	2.31	0.66
1:E:533:ARG:CD	1:E:534:GLN:H	2.06	0.66
1:F:209:VAL:HG13	1:F:210:ALA:N	2.11	0.66
1:C:572:VAL:O	1:C:576:LEU:HB2	1.96	0.66
1:D:277:GLN:HA	1:D:280:ASN:ND2	2.11	0.66
1:D:373:ALA:O	1:D:376:ALA:HB3	1.96	0.66
1:E:460:TRP:O	1:F:488:THR:HA	1.95	0.66
1:A:381:ARG:O	1:F:180:ARG:NH2	2.29	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:C:382:ARG:HG3	1:C:383:LYS:CB	2.25	0.66
1:C:462:ARG:HB2	1:C:510:MET:SD	2.35	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:241:PHE:CE2	1:D:285:GLU:HG3	2.31	0.66
1:A:155:PHE:HZ	1:A:168:LEU:HD11	1.59	0.66
1:B:367:ASN:OD1	1:B:367:ASN:C	2.39	0.66
1:C:225:PHE:HE1	1:C:233:GLY:C	2.03	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:B:352:LEU:O	1:B:355:LYS:N	2.29	0.66
1:B:378:ARG:O	1:B:380:GLY:N	2.29	0.66
1:B:410:ARG:O	1:B:413:ARG:N	2.29	0.66
1:C:225:PHE:CZ	1:C:278:THR:CB	2.72	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:D:159:ALA:HB3	1:D:334:ILE:CG1	2.25	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:E:313:ARG:NH2	1:E:526:TYR:CA	2.46	0.66
1:E:586:GLU:O	1:E:589:ARG:HB2	1.96	0.66
1:B:178:PRO:HG3	1:B:249:PRO:HG3	1.78	0.65
1:B:466:LEU:HD11	1:B:504:MET:HE1	1.77	0.65
1:B:589:ARG:HB3	1:B:594:LEU:CD2	2.26	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:D:362:GLY:HA2	1:D:365:LEU:HD12	1.78	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:F:449:PHE:CZ	1:F:453:ARG:CZ	2.79	0.65
1:A:211:GLY:CA	1:A:214:ARG:HE	2.08	0.65
1:B:225:PHE:HB3	1:B:278:THR:HG21	1.78	0.65
1:B:337:ILE:HG23	1:B:338:HIS:CD2	2.31	0.65
1:C:465:LEU:HD22	1:C:508:TRP:HZ3	1.61	0.65
1:C:500:LEU:O	1:C:503:ARG:HB3	1.96	0.65
1:D:263:LYS:HZ2	1:E:227:GLU:HG3	1.58	0.65
1:D:343:PRO:HG2	1:D:383:LYS:HA	1.79	0.65
1:D:508:TRP:HD1	1:E:491:GLU:HG2	1.61	0.65
1:E:155:PHE:HZ	1:E:168:LEU:HD11	1.58	0.65
1:A:169:LYS:O	1:A:172:VAL:HG13	1.96	0.65
1:A:196:GLY:CA	1:A:443:ARG:NH2	2.60	0.65
1:A:202:LYS:HB2	2:A:1001:ADP:O1B	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:ARG:NH2	1:A:526:TYR:C	2.51	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:B:263:LYS:HZ3	1:C:227:GLU:HG3	1.59	0.65
1:C:400:PRO:HG2	1:C:405:LEU:HD12	1.78	0.65
1:C:419:GLU:OE1	1:C:419:GLU:HA	1.95	0.65
1:C:428:PHE:O	1:C:432:ALA:HB2	1.96	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:A:215:VAL:CG1	1:A:250:CYS:HA	2.27	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:D:487:THR:HG22	1:D:488:THR:N	2.07	0.65
1:E:428:PHE:O	1:E:432:ALA:HB2	1.96	0.65
1:F:221:SER:HB2	1:F:256:GLU:OE1	1.97	0.65
1:B:318:ASP:O	1:B:319:ARG:CB	2.32	0.65
1:C:215:VAL:CG1	1:C:250:CYS:HA	2.27	0.65
1:D:238:ARG:CG	1:D:281:GLN:NE2	2.58	0.65
1:D:367:ASN:C	1:D:367:ASN:OD1	2.40	0.65
1:F:153:VAL:HB	1:F:207:ARG:NH1	2.12	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:C:533:ARG:CD	1:C:534:GLN:N	2.60	0.65
1:F:160:GLY:H	1:F:333:GLN:NE2	1.95	0.65
1:F:202:LYS:HG2	2:F:2001:ADP:O1A	1.97	0.65
1:A:225:PHE:CE1	1:A:233:GLY:C	2.74	0.65
1:A:275:ARG:O	1:A:279:LEU:HB2	1.96	0.65
1:A:419:GLU:OE1	1:A:419:GLU:HA	1.97	0.65
1:B:188:ILE:HG23	1:B:189:PRO:CD	2.24	0.65
1:C:215:VAL:HG23	1:C:216:PRO:CD	2.27	0.65
1:D:286:MET:CE	1:D:315:GLY:O	2.45	0.65
1:D:319:ARG:C	1:D:320:GLN:OE1	2.40	0.65
1:D:352:LEU:O	1:D:355:LYS:N	2.29	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:A:305:ASP:OD1	1:A:305:ASP:N	2.27	0.65
1:B:221:SER:HB2	1:B:256:GLU:OE1	1.97	0.65
1:C:266:SER:C	1:C:268:VAL:H	2.05	0.65
1:C:312:LEU:O	1:C:318:ASP:HA	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:294:ALA:C	1:F:295:ILE:HG12	2.21	0.65
1:F:463:LYS:O	1:F:466:LEU:N	2.30	0.65
1:A:211:GLY:C	1:A:214:ARG:HE	2.05	0.65
1:B:514:PHE:HB3	1:B:519:TYR:HE1	1.62	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: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:F:466:LEU:HD11	1:F:504:MET:HE1	1.79	0.65
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:B:412:ARG:NH2	1:B:440:ILE:HD13	2.12	0.64
1:B:463:LYS:O	1:B:466:LEU:N	2.30	0.64
1:C:225:PHE:CE1	1:C:233:GLY:HA2	2.29	0.64
1:C:264:ARG:HG3	1:C:265:GLY:N	2.11	0.64
1:C:488:THR:O	1:C:490:ALA:N	2.28	0.64
1:D:174:PHE:HB2	1:D:181:PHE:HE2	1.58	0.64
1:D:311:LEU:HD12	1:D:311:LEU:C	2.22	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:E:266:SER:C	1:E:268:VAL:H	2.05	0.64
1:E:346:GLU:CD	1:E:347:ASP:H	2.04	0.64
1:E:580:GLU:O	1:E:580:GLU:HG2	1.97	0.64
1:F:367:ASN:C	1:F:367:ASN:OD1	2.39	0.64
1:B:510:MET:O	1:B:512:PRO:HD2	1.98	0.64
1:D:352:LEU:HD23	1:D:353:LEU:H	1.62	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:F:188:ILE:HG23	1:F:189:PRO:CD	2.25	0.64
1:A:264:ARG:NE	1:A:266:SER:HB2	2.12	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:378:ARG:C	1:B:380:GLY:N	2.54	0.64
1:C:152:LYS:HG3	1:C:153:VAL:CG2	2.22	0.64
1:C:153:VAL:HA	1:C:157:ASP:OD2	1.98	0.64
1:C:447:LEU:HA	1:C:496:GLN:NE2	2.12	0.64
1:C:580:GLU:O	1:C:580:GLU:HG2	1.97	0.64
1:D:386:MET:O	1:D:389:LEU:HD12	1.97	0.64
1:E:567:GLU:HA	1:E:570:GLU:OE1	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:GLU:CD	1:A:347:ASP:H	2.05	0.64
1:B:190:LYS:HE3	1:B:289:PHE:CZ	2.33	0.64
1:B:587:PHE:O	1:B:591:VAL:HG23	1.97	0.64
1:D:273:ASP:OD1	1:D:273:ASP:N	2.29	0.64
1:D:294:ALA:C	1:D:295:ILE:HG12	2.23	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:237:VAL:HG22	1:B:281:GLN:HG3	1.79	0.64
1:B:257:ILE:HD12	1:B:257:ILE:N	2.13	0.64
1:C:236:ARG:NH1	1:C:236:ARG:HB3	2.13	0.64
1:C:533:ARG:CZ	1:C:534:GLN:O	2.46	0.64
1:D:154:THR:CG2	1:D:156:LYS:HB3	2.28	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:F:376:ALA:CA	1:F:381:ARG:HH11	2.11	0.64
1:F:439:THR:CG2	1:F:445:ARG:HH22	2.08	0.64
1:F:586:GLU:O	1:F:589:ARG:HB2	1.98	0.64
1:A:308:ASP:OD1	1:A:308:ASP:C	2.39	0.64
1:A:453:ARG:NH2	1:A:464:ARG:NH2	2.46	0.64
1:B:319:ARG:C	1:B:320:GLN:OE1	2.41	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:D:286:MET:O	1:D:289:PHE:CB	2.45	0.64
1:D:414:ILE:O	1:D:417:TYR:N	2.31	0.64
1:E:169:LYS:O	1:E:172:VAL:HG13	1.98	0.64
1:E:520:ALA:CA	1:E:533:ARG:HD3	2.26	0.64
1:A:262:ARG:CG	1:A:275:ARG:HH22	2.07	0.64
1:B:175:LEU:CD1	1:B:215:VAL:HG11	2.27	0.64
1:C:453:ARG:HH22	1:C:464:ARG:NH1	1.95	0.64
1:D:313:ARG:NE	1:D:314:PRO:CG	2.61	0.64
1:D:369:LEU:O	1:D:372:ALA:N	2.28	0.64
1:F:273:ASP:N	1:F:273:ASP:OD1	2.31	0.64
1:F:465:LEU:O	1:F:469:ILE:HG13	1.98	0.64
1:A:286:MET:O	1:A:289:PHE:CZ	2.50	0.64
1:A:467:ASP:O	1:A:470:ALA:HB3	1.98	0.64
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:379:GLU:OE1	1:B:381:ARG:NE	2.31	0.64
1:B:465:LEU:O	1:B:469:ILE:HG13	1.98	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:C:449:PHE:CD2	1:C:449:PHE:N	2.63	0.64
1:C:453:ARG:HH11	1:C:453:ARG:CG	2.10	0.64
1:C:518:ALA:CB	1:D:495:ARG:HA	2.27	0.64
1:D:258:ASP:OD1	1:D:258:ASP:N	2.28	0.64
1:D:314:PRO:C	1:D:316:ARG:H	2.02	0.64
1:E:225:PHE:CE1	1:E:233:GLY:C	2.76	0.64
1:E:481:ILE:CD1	1:E:563:LEU:HB3	2.27	0.64
1:F:385:THR:HB	1:F:388:ASP:OD1	1.98	0.64
1:A:252:VAL:O	1:A:298:MET:N	2.30	0.64
1:A:266:SER:C	1:A:268:VAL:H	2.05	0.64
1:B:286:MET:CE	1:B:315:GLY:O	2.46	0.64
1:B:577:LEU:HG	1:B:578:GLU:N	2.13	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: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:D:523:GLU:OE1	1:E:264:ARG:NH2	2.31	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:B:294:ALA:C	1:B:295:ILE:HG12	2.21	0.63
1:B:428:PHE:CE1	1:B:432:ALA:CB	2.81	0.63
1:D:225:PHE:CE2	1:D:236:ARG:HD2	2.32	0.63
1:A:264:ARG:HD2	1:A:266:SER:HB2	1.78	0.63
1:A:567:GLU:HA	1:A:570:GLU:OE1	1.99	0.63
1:B:273:ASP:OD1	1:B:273:ASP:N	2.31	0.63
1:B:400:PRO:HA	1:B:403:LYS:HB2	1.81	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: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:E:581:THR:O	1:E:582:LEU:HD12	1.98	0.63
1:F:178:PRO:HG3	1:F:249:PRO:HG3	1.80	0.63
1:F:257:ILE:HD12	1:F:257:ILE:N	2.13	0.63
1:F:376:ALA:CB	1:F:381:ARG:HH11	2.09	0.63
1:B:262:ARG:CG	1:B:263:LYS:N	2.54	0.63
1:B:394:ASP:HA	1:B:397:MET:CE	2.27	0.63
1:C:196:GLY:HA2	1:C:443:ARG:HH21	1.63	0.63
1:E:212:GLU:O	1:E:214:ARG:HG3	1.98	0.63
1:E:523:GLU:OE1	1:E:523:GLU:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:461:SER:O	1:A:465:LEU:HD12	1.97	0.63
1:A:588:GLN:O	1:A:591:VAL:N	2.31	0.63
1:B:174:PHE:HB2	1:B:181:PHE:HE2	1.61	0.63
1:B:511:HIS:C	1:B:512:PRO:O	2.41	0.63
1:C:503:ARG:HG2	1:C:508:TRP:CH2	2.33	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
1:E:152:LYS:HG3	1:E:153:VAL:CG2	2.20	0.63
1:E:275:ARG:O	1:E:279:LEU:CB	2.47	0.63
1:A:166:GLU:CB	1:A:169:LYS:HZ2	2.07	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:D:577:LEU:HG	1:D:578:GLU:N	2.11	0.63
1:E:252:VAL:O	1:E:298:MET:N	2.30	0.63
1:E:384:ILE:HG23	1:E:388:ASP:CB	2.26	0.63
1:E:467:ASP:O	1:E:470:ALA:HB3	1.98	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:A:596:LEU:HG	1:A:597:GLU:N	2.13	0.63
1:C:252:VAL:O	1:C:298:MET:N	2.29	0.63
1:C:346:GLU:CD	1:C:347:ASP:H	2.06	0.63
1:D:215:VAL:CG2	1:D:249:PRO:O	2.45	0.63
1:F:190:LYS:HZ1	1:F:289:PHE:HE2	0.71	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:F:430:GLU:OE1	1:F:430:GLU:CA	2.46	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: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:E:507:GLU:CD	1:E:522:ARG:HE	2.07	0.63
1:E:589:ARG:CZ	1:E:589:ARG:CB	2.77	0.63
1:A:152:LYS:HG3	1:A:153:VAL:CG2	2.25	0.63
1:A:168:LEU:CB	1:A:171:ILE:CD1	2.77	0.63
1:C:169:LYS:O	1:C:172:VAL:HG13	1.99	0.63
1:D:463:LYS:O	1:D:464:ARG:C	2.41	0.63
1:E:215:VAL:HG23	1:E:216:PRO:CD	2.26	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:376:ALA:CB	1:F:381:ARG:CD	2.70	0.63
1:A:414:ILE:HG22	1:A:415:THR:N	2.13	0.63
1:A:509:GLY:C	1:B:476:ARG:NH2	2.56	0.63
1:A:539:THR:O	1:A:543:ILE:HG13	1.99	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:D:396:VAL:O	1:D:400:PRO:HD2	1.99	0.63
1:D:597:GLU:O	1:D:599:PRO:HD3	1.98	0.63
1:E:450:MET:HE1	1:E:499:GLU:OE2	1.99	0.63
1:E:514:PHE:HB3	1:E:519:TYR:CE1	2.34	0.63
1:F:155:PHE:HA	1:F:158:VAL:CG2	2.29	0.63
1:F:519:TYR:HB3	1:F:535:TYR:HD2	1.64	0.63
1:A:155:PHE:HZ	1:A:209:VAL:HG22	1.64	0.62
1:B:318:ASP:OD1	1:B:318:ASP:N	2.24	0.62
1:D:317:PHE:N	1:D:317:PHE:HD1	1.97	0.62
1:E:447:LEU:HA	1:E:496:GLN:NE2	2.12	0.62
1:E:453:ARG:HH21	1:E:464:ARG:HH22	1.47	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:D:233:GLY:C	1:D:236:ARG:HH22	2.07	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:F:463:LYS:O	1:F:464:ARG:C	2.41	0.62
1:A:586:GLU:CB	1:A:589:ARG:NE	2.63	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:B:414:ILE:O	1:B:417:TYR:N	2.32	0.62
1:C:264:ARG:CG	1:C:266:SER:N	2.41	0.62
1:D:318:ASP:O	1:D:319:ARG:CB	2.35	0.62
1:D:400:PRO:HA	1:D:403:LYS:HB2	1.82	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: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:A:533:ARG:CD	1:A:534:GLN:N	2.61	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:B:586:GLU:O	1:B:589:ARG:HB2	1.99	0.62
1:C:225:PHE:HZ	1:C:278:THR:HB	1.60	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:589:ARG:HB3	1:D:594:LEU:CD2	2.29	0.62
1:B:245:LYS:C	1:B:247:HIS:N	2.58	0.62
1:C:333:GLN:HG3	1:C:336:ARG:HH12	1.63	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: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:C:214:ARG:O	1:C:214:ARG:HG2	1.98	0.62
1:D:586:GLU:O	1:D:589:ARG:HB2	2.00	0.62
1:F:233:GLY:C	1:F:236:ARG:HH22	2.07	0.62
1:F:533:ARG:HG3	1:F:533:ARG:HH11	1.65	0.62
1:A:233:GLY:HA2	1:A:236:ARG:HH12	1.65	0.62
1:B:549:ARG:O	1:B:550:LEU:C	2.42	0.62
1:C:524:ASP:CA	1:C:529:GLY:HA2	2.09	0.62
1:D:549:ARG:O	1:D:550:LEU:C	2.42	0.62
1:E:153:VAL:HA	1:E:157:ASP:OD2	1.99	0.62
1:E:191:GLY:HA2	1:E:297:VAL:HG22	1.81	0.62
1:E:286:MET:O	1:E:289:PHE:CE1	2.52	0.62
1:E:453:ARG:NH2	1:E:464:ARG:HH22	1.97	0.62
1:A:195:VAL:HG22	1:A:301:THR:O	1.99	0.62
1:B:258:ASP:N	1:B:258:ASP:OD1	2.31	0.62
1:B:308:ASP:C	1:B:308:ASP:OD1	2.42	0.62
1:B:376:ALA:C	1:B:381:ARG:CD	2.61	0.62
1:B:463:LYS:O	1:B:464:ARG:C	2.41	0.62
1:C:225:PHE:CE1	1:C:233:GLY:C	2.78	0.62
1:D:523:GLU:CD	1:E:264:ARG:NH2	2.58	0.62
1:E:211:GLY:C	1:E:214:ARG:CG	2.72	0.62
1:E:397:MET:HG3	1:E:406:VAL:HG13	1.82	0.62
1:E:414:ILE:HG22	1:E:415:THR:N	2.14	0.62
1:A:334:ILE:HD13	2:A:1001:ADP:C6	2.35	0.62
1:B:311:LEU:O	1:B:316:ARG:HD3	1.99	0.62
1:B:373:ALA:O	1:B:376:ALA:HB3	1.99	0.62
1:C:179:SER:O	1:C:182:HIS:HD2	1.82	0.62
1:C:331:ARG:HD2	1:C:357:THR:HG23	1.82	0.62
1:D:181:PHE:O	1:D:184:MET:N	2.33	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:A:236:ARG:CG	1:A:236:ARG:NH1	2.59	0.62
1:A:428:PHE:O	1:A:432:ALA:HB2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:PHE:HB3	1:B:236:ARG:NH1	2.14	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:C:223:SER:C	1:C:225:PHE:N	2.51	0.62
1:D:165:LYS:O	1:D:168:LEU:CA	2.47	0.62
1:D:255:ASP:O	1:D:256:GLU:HG2	2.00	0.62
1:E:163:GLU:H	1:E:163:GLU:CD	2.08	0.62
1:F:373:ALA:HA	1:F:384:ILE:HD11	1.82	0.62
1:B:382:ARG:HB3	1:B:383:LYS:HB2	1.82	0.61
1:C:177:ASN:ND2	1:C:180:ARG:HD3	2.16	0.61
1:C:276:GLU:OE2	1:C:527:LEU:HD11	2.00	0.61
1:D:235:ALA:C	1:D:238:ARG:HG3	2.25	0.61
1:D:238:ARG:HB3	1:D:281:GLN:HE22	1.63	0.61
1:D:517:VAL:HG11	1:D:519:TYR:OH	1.99	0.61
1:E:225:PHE:CZ	1:E:278:THR:CB	2.76	0.61
1:E:519:TYR:O	1:E:533:ARG:CD	2.47	0.61
1:E:572:VAL:O	1:E:576:LEU:HB2	1.99	0.61
1:A:153:VAL:HA	1:A:157:ASP:OD2	2.01	0.61
1:A:193:LEU:HD12	1:A:299:ALA:O	1.99	0.61
1:A:430:GLU:O	1:A:431:HIS:CB	2.48	0.61
1:A:449:PHE:HE2	1:A:496:GLN:NE2	1.97	0.61
1:B:260:VAL:HG23	1:B:279:LEU:HD12	1.82	0.61
1:E:390:GLU:O	1:E:393:ALA:N	2.33	0.61
1:F:255:ASP:O	1:F:256:GLU:HG2	1.99	0.61
1:F:258:ASP:OD1	1:F:258:ASP:N	2.31	0.61
1:A:196:GLY:C	1:A:443:ARG:NH2	2.58	0.61
1:A:507:GLU:CD	1:A:522:ARG:HE	2.09	0.61
1:A:510:MET:O	1:A:512:PRO:CD	2.47	0.61
1:B:313:ARG:NE	1:B:314:PRO:CD	2.62	0.61
1:C:453:ARG:NH2	1:C:464:ARG:HH22	1.97	0.61
1:D:253:PHE:HE2	1:D:255:ASP:CB	2.11	0.61
1:E:313:ARG:NH2	1:E:526:TYR:C	2.52	0.61
1:F:215:VAL:HG22	1:F:216:PRO:CD	2.29	0.61
1:F:507:GLU:HG3	1:F:520:ALA:O	2.00	0.61
1:A:440:ILE:HG22	1:A:441:VAL:HG23	1.83	0.61
1:A:583:THR:HG22	1:A:586:GLU:CD	2.26	0.61
1:B:241:PHE:CD1	1:B:242:GLU:N	2.68	0.61
1:D:308:ASP:C	1:D:308:ASP:OD1	2.42	0.61
1:D:344:LEU:HA	1:D:383:LYS:HG3	1.83	0.61
1:D:382:ARG:NH1	1:D:382:ARG:HG2	2.11	0.61
1:E:338:HIS:CE1	1:E:366:GLU:HG3	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:159:ALA:HB1	1:F:333:GLN:CG	2.31	0.61
1:F:241:PHE:CD1	1:F:242:GLU:N	2.68	0.61
1:A:333:GLN:HA	1:A:336:ARG:CZ	2.30	0.61
1:A:581:THR:O	1:A:582:LEU:HD12	2.00	0.61
1:B:428:PHE:CE1	1:B:432:ALA:HB1	2.34	0.61
1:E:469:ILE:O	1:E:473:LEU:HD12	2.01	0.61
1:F:225:PHE:CE2	1:F:236:ARG:HD2	2.35	0.61
1:F:245:LYS:C	1:F:247:HIS:N	2.58	0.61
1:F:382:ARG:HB3	1:F:383:LYS:HB2	1.82	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:F:376:ALA:HA	1:F:381:ARG:NH1	2.16	0.61
1:A:319:ARG:NH2	1:B:402:LYS:NZ	2.48	0.61
1:A:381:ARG:CG	1:A:382:ARG:H	2.13	0.61
1:B:391:GLU:O	1:B:395:ARG:HB3	2.01	0.61
1:B:501:ALA:O	1:B:505:ILE:HD12	2.00	0.61
1:E:150:ALA:HB2	1:E:214:ARG:HH21	1.66	0.61
1:F:317:PHE:N	1:F:317:PHE:HD1	1.99	0.61
1:B:154:THR:HG23	1:B:156:LYS:H	1.66	0.61
1:B:597:GLU:O	1:B:599:PRO:HD3	2.01	0.61
1:C:347:ASP:OD1	1:C:347:ASP:N	2.33	0.61
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: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
1:A:195:VAL:HG11	1:A:304:PRO:HD3	1.81	0.61
1:A:447:LEU:HA	1:A:496:GLN:NE2	2.15	0.61
1:B:190:LYS:HZ1	1:B:289:PHE:HE2	0.69	0.61
1:B:589:ARG:CB	1:B:594:LEU:HD22	2.30	0.61
1:C:520:ALA:CA	1:C:533:ARG:HD3	2.25	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:F:235:ALA:C	1:F:238:ARG:HG3	2.26	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: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:B:430:GLU:OE1	1:B:430:GLU:CA	2.48	0.61
1:C:166:GLU:C	1:C:169:LYS:HG2	2.26	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:192:VAL:C	1:F:317:PHE:CE2	2.79	0.61
1:A:191:GLY:HA2	1:A:297:VAL:HG22	1.83	0.60
1:A:410:ARG:HG3	1:A:411:ASP:H	1.65	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:E:308:ASP:OD1	1:E:308:ASP:C	2.43	0.60
1:F:328:VAL:HG23	1:F:580:GLU:HG3	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: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:C:390:GLU:O	1:C:393:ALA:N	2.34	0.60
1:C:519:TYR:C	1:C:533:ARG:NE	2.59	0.60
1:C:585:GLU:CD	1:C:586:GLU:N	2.59	0.60
1:D:327:ASP:O	1:D:331:ARG:CZ	2.49	0.60
1:A:347:ASP:OD1	1:A:347:ASP:N	2.34	0.60
1:A:536:SER:O	1:A:537:GLU:C	2.44	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:C:166:GLU:O	1:C:169:LYS:CG	2.49	0.60
1:C:234:ALA:HB1	1:C:281:GLN:CD	2.26	0.60
1:E:166:GLU:C	1:E:169:LYS:HG2	2.26	0.60
1:E:196:GLY:CA	1:E:443:ARG:NH2	2.65	0.60
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:F:577:LEU:HG	1:F:578:GLU:N	2.15	0.60
1:A:150:ALA:HB2	1:A:214:ARG:NH1	2.17	0.60
1:B:317:PHE:N	1:B:317:PHE:CD1	2.69	0.60
1:B:317:PHE:N	1:B:317:PHE:HD1	1.99	0.60
1:B:503:ARG:NH2	1:B:522:ARG:CZ	2.64	0.60
1:C:308:ASP:OD1	1:C:308:ASP:C	2.43	0.60
1:C:357:THR:N	1:C:358:PRO:HD2	2.16	0.60
1:D:290:GLU:CG	1:D:293:THR:HG23	2.18	0.60
1:F:319:ARG:C	1:F:320:GLN:OE1	2.44	0.60
1:B:369:LEU:O	1:B:372:ALA:N	2.33	0.60
1:C:491:GLU:O	1:C:493:ASP:N	2.34	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:D:165:LYS:HE2	1:D:205:LEU:CG	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:166:GLU:O	1:E:169:LYS:HG2	2.01	0.60
1:F:308:ASP:C	1:F:308:ASP:OD1	2.45	0.60
1:A:196:GLY:HA2	1:A:443:ARG:NH2	2.16	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:C:387:LYS:O	1:C:390:GLU:HB2	2.02	0.60
1:D:257:ILE:HD12	1:D:257:ILE:N	2.13	0.60
1:D:289:PHE:HD2	1:D:290:GLU:N	2.00	0.60
1:D:343:PRO:O	1:D:344:LEU:HB3	2.00	0.60
1:D:501:ALA:HB1	1:D:550:LEU:HD23	1.83	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:B:237:VAL:HG22	1:B:281:GLN:CG	2.31	0.60
1:C:394:ASP:N	1:C:394:ASP:OD1	2.35	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:F:171:ILE:CG1	1:F:296:VAL:HG21	2.31	0.60
1:A:275:ARG:NH1	1:A:275:ARG:HG3	2.17	0.60
1:A:514:PHE:HB3	1:A:519:TYR:CE1	2.36	0.60
1:C:430:GLU:O	1:C:431:HIS:CB	2.47	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:E:333:GLN:HA	1:E:336:ARG:CZ	2.32	0.60
1:E:335:LEU:HD22	1:E:353:LEU:HD23	1.83	0.60
1:E:453:ARG:NH2	1:E:464:ARG:NH2	2.50	0.60
1:F:276:GLU:HA	1:F:279:LEU:HB2	1.84	0.60
1:A:168:LEU:O	1:A:169:LYS:C	2.45	0.60
1:A:453:ARG:NH2	1:A:464:ARG:NH1	2.50	0.60
1:B:355:LYS:CE	1:B:578:GLU:O	2.46	0.60
1:C:519:TYR:HA	1:C:533:ARG:CZ	2.31	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:F:461:SER:O	1:F:464:ARG:HB3	2.02	0.60
1:A:303:ARG:HB2	1:A:303:ARG:HH11	0.62	0.60
1:A:531:ASP:C	1:A:531:ASP:OD1	2.45	0.60
1:D:237:VAL:C	1:D:240:LEU:HB3	2.27	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:F:233:GLY:C	1:F:236:ARG:NH2	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:494:PHE:O	1:B:495:ARG:C	2.45	0.59
1:C:210:ALA:O	1:C:214:ARG:HG3	2.02	0.59
1:D:394:ASP:O	1:D:397:MET:HG2	2.02	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:A:337:ILE:HD12	1:A:338:HIS:CD2	2.36	0.59
1:B:286:MET:HA	1:B:289:PHE:HD1	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:C:149:GLU:O	1:C:150:ALA:CB	2.50	0.59
1:C:215:VAL:HG11	1:C:250:CYS:CA	2.31	0.59
1:D:233:GLY:C	1:D:236:ARG:NH2	2.60	0.59
1:E:357:THR:N	1:E:358:PRO:HD2	2.17	0.59
1:F:216:PRO:HG2	1:F:250:CYS:HB3	1.83	0.59
1:F:237:VAL:HG22	1:F:281:GLN:CG	2.32	0.59
1:F:583:THR:N	1:F:586:GLU:OE2	2.35	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:238:ARG:CB	1:B:281:GLN:HE22	2.13	0.59
1:B:333:GLN:O	1:B:336:ARG:HB3	2.01	0.59
1:C:155:PHE:HZ	1:C:209:VAL:HG22	1.67	0.59
1:C:514:PHE:HB3	1:C:519:TYR:HE1	1.68	0.59
1:D:159:ALA:HB1	1:D:333:GLN:CG	2.32	0.59
1:D:237:VAL:HG22	1:D:281:GLN:CG	2.31	0.59
1:D:376:ALA:HB2	1:D:381:ARG:NH1	2.17	0.59
1:D:395:ARG:HH11	1:D:395:ARG:CG	2.02	0.59
1:E:197:PRO:C	1:E:302:ASN:OD1	2.45	0.59
1:E:234:ALA:HB1	1:E:281:GLN:CD	2.27	0.59
1:E:453:ARG:HH11	1:E:453:ARG:CG	2.15	0.59
1:F:239:ASP:HA	1:F:242:GLU:OE1	2.02	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:A:390:GLU:O	1:A:393:ALA:N	2.35	0.59
1:B:301:THR:CG2	1:B:303:ARG:H	2.14	0.59
1:D:390:GLU:O	1:D:393:ALA:HB3	2.01	0.59
1:F:152:LYS:HB2	1:F:207:ARG:NH1	2.18	0.59
1:A:453:ARG:HH11	1:A:453:ARG:CG	2.12	0.59
1:B:235:ALA:C	1:B:238:ARG:HG3	2.28	0.59
1:B:428:PHE:CZ	1:B:432:ALA:HB1	2.38	0.59
1:D:253:PHE:C	1:D:253:PHE:CD2	2.80	0.59
1:D:286:MET:HA	1:D:289:PHE:HD1	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:279:LEU:O	1:F:283:LEU:HB2	2.02	0.59
1:A:234:ALA:HB1	1:A:281:GLN:CD	2.27	0.59
1:A:511:HIS:HE1	1:B:552:GLU:OE2	1.85	0.59
1:A:589:ARG:HH12	1:A:596:LEU:HB3	1.67	0.59
1:B:157:ASP:HB3	1:B:337:ILE:HG12	1.83	0.59
1:B:160:GLY:H	1:B:333:GLN:NE2	1.99	0.59
1:B:192:VAL:C	1:B:317:PHE:CE2	2.80	0.59
1:B:420:ALA:O	1:B:424:LEU:HD12	2.03	0.59
1:C:166:GLU:O	1:C:169:LYS:HG2	2.02	0.59
1:C:197:PRO:C	1:C:302:ASN:OD1	2.46	0.59
1:C:318:ASP:OD1	1:C:318:ASP:N	2.33	0.59
1:E:453:ARG:NH2	1:E:464:ARG:HH12	1.99	0.59
1:F:327:ASP:O	1:F:331:ARG:NE	2.35	0.59
1:A:190:LYS:HD2	1:A:289:PHE:HE1	1.66	0.59
1:A:197:PRO:C	1:A:302:ASN:OD1	2.45	0.59
1:C:340:ARG:C	1:C:342:LYS:N	2.59	0.59
1:D:193:LEU:C	1:D:194:LEU:HD12	2.28	0.59
1:D:317:PHE:N	1:D:317:PHE:CD1	2.68	0.59
1:D:331:ARG:O	1:D:335:LEU:HG	2.03	0.59
1:E:264:ARG:CD	1:E:266:SER:HB2	2.32	0.59
1:A:166:GLU:O	1:A:169:LYS:CG	2.51	0.59
1:B:216:PRO:HG2	1:B:250:CYS:HB3	1.84	0.59
1:B:237:VAL:O	1:B:240:LEU:CB	2.44	0.59
1:B:501:ALA:CB	1:B:550:LEU:HD23	2.33	0.59
1:B:507:GLU:HG3	1:B:520:ALA:O	2.02	0.59
1:D:313:ARG:NE	1:D:314:PRO:CD	2.59	0.59
1:F:286:MET:CE	1:F:315:GLY:O	2.50	0.59
1:F:418:HIS:NE2	1:F:479:GLU:OE1	2.36	0.59
1:F:597:GLU:O	1:F:599:PRO:HD3	2.03	0.59
1:B:157:ASP:N	1:B:157:ASP:OD1	2.34	0.59
1:B:171:ILE:CG1	1:B:296:VAL:HG21	2.33	0.59
1:C:371:GLU:OE1	1:C:395:ARG:NH1	2.36	0.59
1:D:216:PRO:HG2	1:D:250:CYS:HB3	1.84	0.59
1:D:583:THR:N	1:D:586:GLU:OE2	2.35	0.59
1:E:196:GLY:C	1:E:443:ARG:NH2	2.61	0.59
1:F:257:ILE:H	1:F:257:ILE:CD1	2.14	0.59
1:A:264:ARG:HG2	1:A:266:SER:H	1.65	0.59
1:A:400:PRO:O	1:A:405:LEU:HD11	2.03	0.59
1:A:414:ILE:CG2	1:A:415:THR:N	2.65	0.59
1:B:235:ALA:HA	1:B:238:ARG:CG	2.33	0.59
1:B:449:PHE:CZ	1:B:453:ARG:CZ	2.86	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:440:ILE:HG22	1:C:441:VAL:HG23	1.84	0.59
1:E:191:GLY:HA2	1:E:297:VAL:CG2	2.33	0.59
1:E:479:GLU:OE2	1:E:488:THR:HG23	2.03	0.59
1:F:237:VAL:C	1:F:240:LEU:HB3	2.28	0.59
1:F:376:ALA:HA	1:F:381:ARG:CZ	2.32	0.59
1:A:179:SER:C	1:A:181:PHE:H	2.10	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: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:212:GLU:C	1:E:214:ARG:CG	2.69	0.58
1:E:465:LEU:CD2	1:E:508:TRP:CZ3	2.86	0.58
1:F:338:HIS:HB3	1:F:369:LEU:CD1	2.33	0.58
1:A:438:VAL:HG23	1:A:439:THR:N	2.18	0.58
1:B:257:ILE:H	1:B:257:ILE:CD1	2.14	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:182:HIS:ND1	1:D:182:HIS:N	2.40	0.58
1:D:301:THR:CG2	1:D:303:ARG:H	2.16	0.58
1:D:589:ARG:CB	1:D:594:LEU:HD22	2.32	0.58
1:E:589:ARG:CZ	1:E:596:LEU:HB2	2.27	0.58
1:F:262:ARG:CG	1:F:263:LYS:N	2.55	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:C:319:ARG:C	1:C:320:GLN:NE2	2.61	0.58
1:C:371:GLU:HG3	1:C:392:ALA:CB	2.32	0.58
1:C:449:PHE:HB2	1:C:468:GLN:HE22	1.66	0.58
1:D:245:LYS:C	1:D:247:HIS:N	2.59	0.58
1:E:145:ARG:NH2	1:E:219:THR:HG1	1.98	0.58
1:E:334:ILE:O	1:E:335:LEU:C	2.47	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
1:F:390:GLU:O	1:F:393:ALA:HB3	2.04	0.58
1:F:511:HIS:C	1:F:512:PRO:O	2.45	0.58
1:A:286:MET:O	1:A:289:PHE:CE1	2.56	0.58
1:A:513:GLU:O	1:B:548:ARG:NH2	2.37	0.58
1:B:165:LYS:HZ2	1:B:168:LEU:HD23	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:ALA:CB	1:B:381:ARG:HD3	2.33	0.58
1:C:397:MET:HG3	1:C:406:VAL:HG13	1.84	0.58
1:C:586:GLU:CA	1:C:589:ARG:HG3	2.30	0.58
1:D:352:LEU:HD21	1:D:386:MET:HE1	1.86	0.58
1:F:454:ARG:NH2	1:F:528:GLY:C	2.61	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:A:479:GLU:OE2	1:A:488:THR:HG23	2.03	0.58
1:B:153:VAL:HB	1:B:207:ARG:NH1	2.18	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:C:264:ARG:HE	1:C:266:SER:HB2	1.68	0.58
1:C:551:ILE:O	1:C:552:GLU:C	2.46	0.58
1:D:257:ILE:H	1:D:257:ILE:CD1	2.14	0.58
1:E:337:ILE:HD12	1:E:338:HIS:CD2	2.39	0.58
1:F:301:THR:CG2	1:F:303:ARG:H	2.15	0.58
1:F:517:VAL:HG13	1:F:519:TYR:CZ	2.39	0.58
1:A:166:GLU:C	1:A:169:LYS:HG2	2.28	0.58
1:A:336:ARG:O	1:A:339:ALA:N	2.37	0.58
1:B:239:ASP:HA	1:B:242:GLU:OE1	2.03	0.58
1:C:438:VAL:HG23	1:C:439:THR:N	2.19	0.58
1:E:264:ARG:NE	1:E:266:SER:HB2	2.19	0.58
1:E:336:ARG:O	1:E:339:ALA:N	2.36	0.58
1:F:201:GLY:N	2:F:2001:ADP:O1A	2.33	0.58
1:F:286:MET:HE1	1:F:316:ARG:CA	2.15	0.58
1:A:276:GLU:OE2	1:A:527:LEU:HD11	2.03	0.58
1:A:585:GLU:CD	1:A:586:GLU:N	2.62	0.58
1:B:253:PHE:C	1:B:253:PHE:CD2	2.82	0.58
1:E:155:PHE:HZ	1:E:209:VAL:HG22	1.69	0.58
1:E:238:ARG:HB2	1:E:238:ARG:CZ	2.34	0.58
1:E:400:PRO:O	1:E:405: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:A:264:ARG:CG	1:A:266:SER:N	2.47	0.58
1:A:448:GLY:O	1:A:449:PHE:C	2.46	0.58
1:A:548:ARG:NH2	1:A:552:GLU:OE1	2.35	0.58
1:C:319:ARG:O	1:C:320:GLN:NE2	2.37	0.58
1:C:338:HIS:CE1	1:C:366:GLU:HG3	2.39	0.58
1:D:333:GLN:O	1:D:336:ARG:HB3	2.04	0.58
1:E:240:LEU:O	1:E:243:THR:OG1	2.22	0.58
1:F:245:LYS:CG	1:F:246:ARG:N	2.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:196:GLY:C	1:C:443:ARG:NH2	2.61	0.58
1:C:349:ASP:OD1	1:C:349:ASP:O	2.22	0.58
1:C:400:PRO:O	1:C:405:LEU:HD11	2.03	0.58
1:D:286:MET:HE2	1:D:315:GLY:O	2.03	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:B:236:ARG:HG2	1:B:237:VAL:N	2.17	0.58
1:D:418:HIS:NE2	1:D:479:GLU:OE1	2.37	0.58
1:D:526:TYR:CE2	1:E:256:GLU:OE2	2.57	0.58
1:E:189:PRO:O	1:E:190:LYS:HG2	2.04	0.58
1:E:381:ARG:CG	1:E:382:ARG:H	2.16	0.58
1:F:159:ALA:CB	1:F:334:ILE:HG13	2.32	0.58
1:F:480:GLU:OE1	1:F:555:TYR:OH	2.21	0.58
1:A:334:ILE:O	1:A:335:LEU:C	2.46	0.57
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:B:512:PRO:HB2	1:B:514:PHE:HD2	1.69	0.57
1:C:514:PHE:CD2	1:C:514:PHE:N	2.72	0.57
1:E:212:GLU:O	1:E:214:ARG:CD	2.52	0.57
1:E:453:ARG:NH2	1:E:464:ARG:NH1	2.51	0.57
1:E:585:GLU:CD	1:E:586:GLU:N	2.62	0.57
1:F:589:ARG:HB3	1:F:594:LEU:CD2	2.33	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: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:C:585:GLU:OE1	1:C:586:GLU:N	2.37	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:F:253:PHE:C	1:F:253:PHE:CD2	2.82	0.57
1:F:373:ALA:O	1:F:376:ALA:HB3	2.05	0.57
1:F:494:PHE:O	1:F:495:ARG:C	2.45	0.57
1:A:318:ASP:N	1:A:318:ASP:OD1	2.38	0.57
1:A:394:ASP:OD1	1:A:394:ASP:N	2.36	0.57
1:B:337:ILE:CD1	1:B:340:ARG:HH12	2.07	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:C:479:GLU:OE2	1:C:488:THR:HG23	2.03	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:D:501:ALA:O	1:D:505:ILE:HD12	2.05	0.57
1:E:343:PRO:C	1:E:344:LEU:HD13	2.28	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:F:286:MET:HA	1:F:289:PHE:CD1	2.40	0.57
1:F:414:ILE:O	1:F:417:TYR:N	2.38	0.57
1:F:503:ARG:HH12	1:F:522:ARG:NH2	2.00	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:A:491:GLU:HG2	1:F:508:TRP:HD1	1.68	0.57
1:B:285:GLU:O	1:B:288:GLY:N	2.37	0.57
1:B:290:GLU:CG	1:B:293:THR:HG23	2.23	0.57
1:C:191:GLY:HA2	1:C:297:VAL:CG2	2.35	0.57
1:E:168:LEU:O	1:E:169:LYS:C	2.47	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: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:F:413:ARG:HG3	1:F:413:ARG:NH1	2.17	0.57
1:F:517:VAL:CG1	1:F:519:TYR:CZ	2.87	0.57
1:A:200:VAL:CG1	1:A:323:ILE:HG13	2.35	0.57
1:A:378:ARG:CA	1:F:173:GLU:OE1	2.45	0.57
1:A:397:MET:HG3	1:A:406:VAL:HG13	1.86	0.57
1:A:460:TRP:HB3	1:A:465:LEU:HD11	1.85	0.57
1:C:343:PRO:C	1:C:344:LEU:HD13	2.30	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:512:PRO:HB2	1:F:514:PHE:HD2	1.69	0.57
1:F:526:TYR:O	1:F:528:GLY:N	2.38	0.57
1:F:589:ARG:CB	1:F:594:LEU:HD22	2.34	0.57
1:A:237:VAL:HG11	1:A:281:GLN:CB	2.24	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:B:310:ALA:C	1:B:316:ARG:HH11	1.99	0.57
1:B:394:ASP:O	1:B:397:MET:HG2	2.05	0.57
1:C:275:ARG:O	1:C:279:LEU:HB2	2.03	0.57
1:C:345:ALA:HB3	1:C:385:THR:HA	1.87	0.57
1:D:154:THR:HG23	1:D:156:LYS:H	1.70	0.57
1:D:163:GLU:O	1:D:167:GLU:HB3	2.04	0.57
1:E:371:GLU:HG3	1:E:392:ALA:CB	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:519:TYR:HA	1:E:533:ARG:CZ	2.35	0.57
1:A:212:GLU:O	1:A:214:ARG:HB2	2.04	0.57
1:B:238:ARG:NH1	1:B:239:ASP:HB3	2.14	0.57
1:B:519:TYR:HB3	1:B:535:TYR:HD2	1.69	0.57
1:E:275:ARG:NH1	1:E:275:ARG:HG3	2.19	0.57
1:E:382:ARG:HD3	1:E:383:LYS:CB	2.34	0.57
1:E:460:TRP:NE1	1:E:464:ARG:HH12	2.01	0.57
1:E:519:TYR:HA	1:E:533:ARG:NH2	2.20	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:B:289:PHE:CD2	1:B:290:GLU:N	2.73	0.57
1:B:335:LEU:CD2	1:B:365:LEU:HB3	2.35	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:E:414:ILE:CG2	1:E:415:THR:N	2.67	0.57
1:F:180:ARG:O	1:F:184:MET:HB3	2.05	0.57
1:A:273:ASP:CG	1:A:274:GLU:N	2.63	0.57
1:A:585:GLU:OE2	1:A:589:ARG:HD3	2.04	0.57
1:C:519:TYR:O	1:C:533:ARG:CG	2.53	0.57
1:D:331:ARG:HH22	1:D:580:GLU:CD	2.10	0.57
1:D:433:ASP:N	1:D:433:ASP:OD1	2.38	0.57
1:D:519:TYR:HB3	1:D:535:TYR:HD2	1.69	0.57
1:F:391:GLU:O	1:F:394:ASP:OD1	2.22	0.57
1:A:394:ASP:O	1:A:397:MET:N	2.38	0.57
1:A:574:GLU:C	1:A:574:GLU:OE1	2.48	0.57
1:B:255:ASP:O	1:B:256:GLU:HG2	2.03	0.57
1:C:470:ALA:O	1:C:558:VAL:HG21	2.05	0.57
1:C:507:GLU:CD	1:C:522:ARG:HE	2.12	0.57
1:D:177:ASN:O	1:D:180:ARG:HB3	2.05	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:D:376:ALA:C	1:D:381:ARG:CB	2.77	0.57
1:E:202:LYS:HB2	2:E:1001:ADP:O1B	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:F:421:GLY:HA2	1:F:562:LEU:HD11	1.86	0.57
1:C:263:LYS:HD2	1:C:276:GLU:CG	2.35	0.56
1:C:310:ALA:O	1:C:316:ARG:NH2	2.38	0.56
1:C:461:SER:O	1:C:465:LEU:HD12	2.04	0.56
1:C:586:GLU:O	1:C:590:VAL:HG13	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:410:ARG:HG3	1:E:411:ASP:H	1.68	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:A:469:ILE:O	1:A:473:LEU:HD12	2.05	0.56
1:B:187:ARG:O	1:C:374:LEU:CD2	2.48	0.56
1:B:421:GLY:HA2	1:B:562:LEU:HD11	1.87	0.56
1:C:283:LEU:O	1:C:286:MET:HB2	2.05	0.56
1:C:286:MET:HE1	1:C:297:VAL:HG21	1.87	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: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:F:467:ASP:O	1:F:470:ALA:HB3	2.06	0.56
1:A:247:HIS:O	1:A:250:CYS:HB2	2.05	0.56
1:A:305:ASP:O	1:A:307:LEU:N	2.39	0.56
1:A:343:PRO:C	1:A:344:LEU:HD13	2.29	0.56
1:A:407:LEU:HD12	1:A:407:LEU:O	2.05	0.56
1:A:453:ARG:NH1	1:A:460:TRP:CE2	2.74	0.56
1:B:170:GLU:HB3	1:C:378:ARG:NH2	2.20	0.56
1:B:245:LYS:HG3	1:B:246:ARG:N	2.20	0.56
1:B:279:LEU:O	1:B:283:LEU:HB2	2.05	0.56
1:B:503:ARG:NH2	1:B:522:ARG:NH2	2.49	0.56
1:C:179:SER:C	1:C:181:PHE:H	2.13	0.56
1:C:219:THR:HA	1:C:253:PHE:O	2.06	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:C:516:PRO:HB2	1:D:494:PHE:CD1	2.40	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: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
1:E:460:TRP:HB3	1:E:465:LEU:HD11	1.86	0.56
1:E:585:GLU:OE1	1:E:586:GLU:N	2.37	0.56
1:F:210:ALA:O	1:F:214:ARG:N	2.38	0.56
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:B:449:PHE:CE2	1:B:492:ASN:HB3	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:477:ALA:O	1:B:481:ILE:HG13	2.06	0.56
1:F:447:LEU:O	1:F:450:MET:HG3	2.06	0.56
1:A:238:ARG:CZ	1:A:238:ARG:HB2	2.35	0.56
1:B:583:THR:O	1:B:584:ALA:C	2.48	0.56
1:C:241:PHE:O	1:C:242:GLU:C	2.49	0.56
1:C:407:LEU:O	1:C:407:LEU:HD12	2.05	0.56
1:D:352:LEU:O	1:D:353:LEU:C	2.48	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:A:459:HIS:HB2	1:B:488:THR:HB	1.87	0.56
1:A:500:LEU:O	1:A:504:MET:HG2	2.05	0.56
1:A:525:THR:O	1:A:528:GLY:N	2.39	0.56
1:A:588:GLN:HG3	1:A:589:ARG:N	2.21	0.56
1:B:236:ARG:HH12	1:B:278:THR:CG2	2.11	0.56
1:B:338:HIS:HB3	1:B:369:LEU:CD1	2.35	0.56
1:C:196:GLY:O	1:C:202:LYS:NZ	2.31	0.56
1:C:275:ARG:O	1:C:279:LEU:CB	2.53	0.56
1:C:334:ILE:O	1:C:335:LEU:C	2.48	0.56
1:D:327:ASP:O	1:D:331:ARG:NE	2.38	0.56
1:E:345:ALA:HB3	1:E:385:THR:HA	1.88	0.56
1:E:449:PHE:HE2	1:E:496:GLN:NE2	2.03	0.56
1:A:449:PHE:HB3	1:A:468:GLN:HE22	1.68	0.56
1:B:331:ARG:HD2	1:B:354:ALA:O	2.05	0.56
1:C:199:GLY:O	1:C:361:VAL:HG22	2.06	0.56
1:D:376:ALA:CB	1:D:381:ARG:NH1	2.69	0.56
1:E:147:LEU:HD23	1:E:217:PHE:HB3	1.88	0.56
1:E:263:LYS:HG2	1:E:264:ARG:N	2.20	0.56
1:E:407:LEU:HD12	1:E:407:LEU:O	2.06	0.56
1:F:397:MET:O	1:F:400:PRO:HG2	2.06	0.56
1:F:487:THR:HG22	1:F:488:THR:N	2.14	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:A:449:PHE:HB2	1:A:468:GLN:HE22	1.71	0.56
1:B:276:GLU:HA	1:B:279:LEU:HB2	1.87	0.56
1:C:145:ARG:CZ	1:C:219:THR:OG1	2.53	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:589:ARG:CZ	1:C:596:LEU:HB2	2.28	0.56
1:E:179:SER:C	1:E:181:PHE:H	2.13	0.56
1:E:262:ARG:CG	1:E:275:ARG:HH22	2.08	0.56
1:E:514:PHE:HB3	1:E:519:TYR:HE1	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:VAL:HG11	1:A:587:PHE:CD1	2.41	0.56
1:C:177:ASN:HD22	1:C:180:ARG:CD	2.17	0.56
1:C:238:ARG:HB2	1:C:238:ARG:CZ	2.35	0.56
1:C:247:HIS:O	1:C:250:CYS:HB2	2.05	0.56
1:D:335:LEU:CD2	1:D:365:LEU:HB3	2.36	0.56
1:E:196:GLY:HA2	1:E:443:ARG:NH2	2.21	0.56
1:E:554:GLN:O	1:E:557:ARG:HB3	2.06	0.56
1:E:583:THR:HG22	1:E:586:GLU:CD	2.31	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:B:438:VAL:HG22	1:B:439:THR:N	2.20	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:F:344:LEU:HA	1:F:383:LYS:HG3	1.88	0.56
1:B:210:ALA:O	1:B:214:ARG:HA	2.07	0.55
1:C:174:PHE:CZ	1:C:294:ALA:HB1	2.41	0.55
1:C:438:VAL:HG11	1:C:587:PHE:CD1	2.41	0.55
1:E:387:LYS:O	1:E:390:GLU:HB2	2.06	0.55
1:F:216:PRO:HG2	1:F:250:CYS:CB	2.37	0.55
1:F:428:PHE:CE1	1:F:432:ALA:C	2.84	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:A:370:ASN:OD1	1:A:374:LEU:HD13	2.06	0.55
1:A:568:VAL:O	1:A:572:VAL:HG23	2.06	0.55
1:B:344:LEU:HA	1:B:383:LYS:HG3	1.88	0.55
1:E:275:ARG:HG3	1:E:275:ARG:HH11	1.70	0.55
1:E:394:ASP:N	1:E:394:ASP:OD1	2.38	0.55
1:A:241:PHE:O	1:A:242:GLU:C	2.48	0.55
1:A:316:ARG:O	1:A:317:PHE:C	2.50	0.55
1:B:286:MET:O	1:B:289:PHE:CD1	2.59	0.55
1:B:286:MET:HA	1:B:289:PHE:CD1	2.41	0.55
1:B:376:ALA:HB1	1:B:381:ARG:CD	2.36	0.55
1:D:316:ARG:CG	1:D:316:ARG:NH1	2.42	0.55
1:D:461:SER:O	1:D:464:ARG:HB3	2.06	0.55
1:F:331:ARG:HH22	1:F:580:GLU:CD	2.13	0.55
1:F:381:ARG:HH22	1:F:388:ASP:CG	2.15	0.55
1:A:194:LEU:HA	1:A:321:ILE:O	2.06	0.55
1:A:514:PHE:CD2	1:A:514:PHE:N	2.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:LYS:O	1:D:168:LEU:CB	2.54	0.55
1:D:428:PHE:CE1	1:D:432:ALA:C	2.85	0.55
1:E:451:MET:HB2	1:E:452:PRO:HD3	1.88	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:262:ARG:HG2	1:A:275:ARG:NH2	2.06	0.55
1:A:345:ALA:HB3	1:A:385:THR:HA	1.88	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:B:503:ARG:HH12	1:B:522:ARG:NH2	2.03	0.55
1:E:438:VAL:HG11	1:E:587:PHE:CD1	2.41	0.55
1:F:352:LEU:HD13	1:F:353:LEU:N	2.21	0.55
1:A:145:ARG:CZ	1:A:219:THR:OG1	2.54	0.55
1:A:495:ARG:HD2	1:F:521:VAL:HG12	1.88	0.55
1:B:194:LEU:HD23	1:B:323:ILE:HD11	1.89	0.55
1:B:239:ASP:O	1:B:242:GLU:OE2	2.24	0.55
1:C:174:PHE:CD2	1:C:175:LEU:N	2.74	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:D:524:ASP:H	1:E:306:ILE:HD11	1.70	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:168:LEU:O	1:C:169:LYS:C	2.47	0.55
1:C:382:ARG:CG	1:C:383:LYS:H	2.19	0.55
1:C:436:HIS:HB3	1:C:584:ALA:HB1	1.88	0.55
1:C:552:GLU:O	1:C:555:TYR:HB3	2.07	0.55
1:D:285:GLU:C	1:D:288:GLY:H	2.14	0.55
1:D:477:ALA:O	1:D:481:ILE:HG13	2.07	0.55
1:D:557:ARG:O	1:D:560:ALA:HB3	2.05	0.55
1:F:180:ARG:NH1	1:F:184:MET:HE3	2.21	0.55
1:F:245:LYS:HG3	1:F:246:ARG:N	2.21	0.55
1:F:449:PHE:CE2	1:F:492:ASN:HB3	2.37	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: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:536:SER:O	1:E:537:GLU:C	2.49	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:F:549:ARG:O	1:F:550:LEU:C	2.49	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:564:GLU:C	1:F:566:ARG:N	2.65	0.55
1:A:319:ARG:C	1:A:320:GLN:NE2	2.65	0.55
1:A:338:HIS:ND1	1:A:366:GLU:HG3	2.22	0.55
1:A:491:GLU:O	1:A:493:ASP:N	2.40	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:C:408:SER:C	1:C:410:ARG:H	2.14	0.55
1:C:414:ILE:HG22	1:C:415:THR:H	1.71	0.55
1:C:574:GLU:C	1:C:574:GLU:OE1	2.49	0.55
1:D:216:PRO:HB2	1:D:218:ILE:HD11	1.88	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:459:HIS:O	1:F:459:HIS:CG	2.60	0.55
1:A:500:LEU:O	1:A:503:ARG:HB3	2.06	0.55
1:B:285:GLU:C	1:B:288:GLY:H	2.15	0.55
1:B:327:ASP:O	1:B:331:ARG:CZ	2.54	0.55
1:C:286:MET:O	1:C:289:PHE:CE1	2.59	0.55
1:C:453:ARG:HH21	1:C:464:ARG:HH22	1.49	0.55
1:C:481:ILE:HD11	1:C:563:LEU:HB3	1.89	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:174:PHE:CD2	1:E:175:LEU:N	2.74	0.55
1:E:241:PHE:O	1:E:242:GLU:C	2.49	0.55
1:E:319:ARG:C	1:E:320:GLN:NE2	2.65	0.55
1:E:334:ILE:HD13	2:E:1001:ADP:N1	2.22	0.55
1:F:154:THR:HG23	1:F:156:LYS:H	1.71	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:462:ARG:HB2	1:A:510:MET:SD	2.47	0.54
1:A:585:GLU:OE1	1:A:586:GLU:N	2.39	0.54
1:B:234:ALA:O	1:B:237:VAL:HG13	2.07	0.54
1:B:525:THR:HG22	1:B:526:TYR:H	1.73	0.54
1:B:585:GLU:O	1:B:586:GLU:C	2.50	0.54
1:C:179:SER:HA	1:C:182:HIS:NE2	2.23	0.54
1:C:263:LYS:HG2	1:C:264:ARG:N	2.21	0.54
1:C:367:ASN:O	1:C:371:GLU:HB3	2.07	0.54
1:C:463:LYS:HD2	1:D:486:VAL:CG2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:389:LEU:O	1:D:390:GLU:C	2.50	0.54
1:E:199:GLY:O	1:E:361:VAL:HG22	2.06	0.54
1:E:448:GLY:O	1:E:449:PHE:C	2.51	0.54
1:F:236:ARG:O	1:F:239:ASP:OD1	2.25	0.54
1:F:501:ALA:HB1	1:F:550:LEU:HD23	1.89	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:OE1	1:D:430:GLU:CA	2.54	0.54
1:F:313:ARG:NE	1:F:314:PRO:CD	2.66	0.54
1:F:313:ARG:NE	1:F:314:PRO:CG	2.70	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: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:A:381:ARG:HH11	1:A:381:ARG:CG	2.21	0.54
1:B:348:VAL:HG13	1:B:350:LEU:H	1.72	0.54
1:C:147:LEU:HD23	1:C:217:PHE:HB3	1.88	0.54
1:C:236:ARG:O	1:C:238:ARG:N	2.39	0.54
1:C:334:ILE:HD13	2:C:1001:ADP:N1	2.23	0.54
1:C:381:ARG:HH11	1:C:381:ARG:CG	2.20	0.54
1:C:506:THR:HA	1:C:519:TYR:HD1	1.72	0.54
1:C:516:PRO:HB2	1:D:494:PHE:CE1	2.42	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:D:391:GLU:O	1:D:394:ASP:OD1	2.26	0.54
1:E:194:LEU:HA	1:E:321:ILE:O	2.08	0.54
1:F:257:ILE:O	1:F:260:VAL:HG13	2.07	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:A:263:LYS:HD2	1:A:276:GLU:CG	2.36	0.54
1:A:519:TYR:O	1:A:533:ARG:CG	2.56	0.54
1:B:190:LYS:NZ	1:B:289:PHE:CZ	2.73	0.54
1:C:194:LEU:HA	1:C:321:ILE:O	2.08	0.54
1:C:236:ARG:NH1	1:C:236:ARG:CG	2.60	0.54
1:C:531:ASP:C	1:C:531:ASP:OD1	2.51	0.54
1:D:180:ARG:O	1:D:184:MET:HB3	2.06	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: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:E:283:LEU:O	1:E:286:MET:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:PHE:CZ	1:A:294:ALA:HB1	2.42	0.54
1:A:179:SER:C	1:A:181:PHE:N	2.65	0.54
1:A:353:LEU:O	1:A:357:THR:HG22	2.06	0.54
1:B:433:ASP:N	1:B:433:ASP:OD1	2.41	0.54
1:C:353:LEU:O	1:C:357:THR:HG22	2.08	0.54
1:C:448:GLY:O	1:C:449:PHE:C	2.50	0.54
1:D:165:LYS:CD	1:D:168:LEU:CD2	2.77	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:E:333:GLN:HG3	1:E:336:ARG:HH12	1.71	0.54
1:E:519:TYR:O	1:E:533:ARG:CG	2.56	0.54
1:F:193:LEU:C	1:F:194:LEU:HD12	2.33	0.54
1:A:149:GLU:O	1:A:150:ALA:CB	2.53	0.54
1:A:583:THR:HG22	1:A:586:GLU:OE1	2.07	0.54
1:B:311:LEU:N	1:B:316:ARG:HH12	2.04	0.54
1:B:336:ARG:C	1:B:338:HIS:N	2.62	0.54
1:C:218:ILE:HG12	1:C:251:ILE:O	2.08	0.54
1:D:166:GLU:O	1:D:169:LYS:HG2	2.07	0.54
1:D:190:LYS:NZ	1:D:289:PHE:CZ	2.73	0.54
1:D:336:ARG:C	1:D:338:HIS:N	2.61	0.54
1:D:454:ARG:NH2	1:D:528:GLY:C	2.66	0.54
1:D:512:PRO:HB2	1:D:514:PHE:CD2	2.43	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:F:190:LYS:HD2	1:F:289:PHE:HZ	1.71	0.54
1:A:236:ARG:NH1	1:A:236:ARG:CB	2.70	0.54
1:A:588:GLN:HA	1:A:591:VAL:HG23	1.89	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:B:277:GLN:HA	1:B:280:ASN:HD21	1.72	0.54
1:B:454:ARG:NH2	1:B:528:GLY:C	2.66	0.54
1:D:199:GLY:H	2:D:2001:ADP:PB	2.29	0.54
1:E:211:GLY:O	1:E:214:ARG:CD	2.53	0.54
1:E:263:LYS:HD2	1:E:276:GLU:CG	2.38	0.54
1:E:305:ASP:O	1:E:307:LEU:N	2.41	0.54
1:E:338:HIS:ND1	1:E:366:GLU:HG3	2.22	0.54
1:E:449:PHE:N	1:E:449:PHE:HD2	2.04	0.54
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:A:325:ALA:N	1:A:326:PRO:CD	2.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:LYS:CE	1:F:184:MET:SD	2.95	0.54
1:A:374:LEU:CD1	1:F:186:ALA:HB1	2.38	0.54
1:A:460:TRP:NE1	1:A:464:ARG:HH12	2.04	0.54
1:A:541:LYS:HA	1:F:536:SER:OG	2.07	0.54
1:B:210:ALA:O	1:B:214:ARG:N	2.41	0.54
1:B:319:ARG:CG	1:B:319:ARG:NH1	2.67	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:E:179:SER:O	1:E:182:HIS:CD2	2.60	0.54
1:E:512:PRO:HB2	1:E:514:PHE:HD2	1.72	0.54
1:F:216:PRO:HB2	1:F:218:ILE:HD11	1.90	0.54
1:A:563:LEU:HD12	1:A:564:GLU:N	2.22	0.54
1:A:585:GLU:OE2	1:A:589:ARG:CD	2.56	0.54
1:B:174:PHE:C	1:B:174:PHE:CD2	2.86	0.54
1:B:241:PHE:CE2	1:B:285:GLU:CG	2.91	0.54
1:B:313:ARG:HG3	1:B:314:PRO:CG	2.38	0.54
1:B:344:LEU:HG	1:B:346:GLU:OE1	2.08	0.54
1:C:196:GLY:H	1:C:202:LYS:HZ1	1.56	0.54
1:C:583:THR:HG22	1:C:586:GLU:CD	2.32	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:D:503:ARG:HH12	1:D:522:ARG:NH2	2.05	0.54
1:E:202:LYS:CD	1:E:300:ALA:HB1	2.36	0.54
1:E:305:ASP:OD1	1:E:305:ASP:N	2.26	0.54
1:E:589:ARG:HH22	1:E:596:LEU:HB2	1.38	0.54
1:F:238:ARG:CB	1:F:281:GLN:HE22	2.18	0.54
1:F:417:TYR:CE1	1:F:482:VAL:HG21	2.42	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:B:236:ARG:O	1:B:239:ASP:OD1	2.26	0.54
1:C:509:GLY:C	1:D:476:ARG:NH2	2.61	0.54
1:D:285:GLU:O	1:D:288:GLY:N	2.40	0.54
1:E:368:LEU:HD13	1:E:393:ALA:CA	2.37	0.54
1:F:238:ARG:NH1	1:F:239:ASP:HB3	2.15	0.54
1:F:336:ARG:C	1:F:338:HIS:N	2.64	0.54
1:F:352:LEU:O	1:F:353:LEU:C	2.49	0.54
1:F:375:LEU:CD1	1:F:388:ASP:HB3	2.36	0.54
1:A:196:GLY:O	1:A:302:ASN:OD1	2.25	0.53
1:A:367:ASN:O	1:A:371:GLU:HB3	2.07	0.53
1:A:408:SER:C	1:A:410:ARG:H	2.15	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:ILE:O	1:B:337:ILE:HG22	2.09	0.53
1:D:174:PHE:CD2	1:D:174:PHE:C	2.85	0.53
1:D:319:ARG:CG	1:D:319:ARG:NH1	2.62	0.53
1:D:334:ILE:O	1:D:337:ILE:HG22	2.08	0.53
1:D:522:ARG:HD2	1:D:530:TYR:CA	2.32	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: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:152:LYS:HB2	1:D:207:ARG:NH1	2.23	0.53
1:D:257:ILE:O	1:D:260:VAL:HG13	2.08	0.53
1:D:480:GLU:OE1	1:D:555:TYR:OH	2.26	0.53
1:D:517:VAL:HG11	1:D:519:TYR:CZ	2.43	0.53
1:E:179:SER:HA	1:E:182:HIS:NE2	2.24	0.53
1:E:367:ASN:O	1:E:371:GLU:HB3	2.09	0.53
1:E:470:ALA:C	1:E:558:VAL:HG21	2.32	0.53
1:F:166:GLU:O	1:F:169:LYS:HG2	2.08	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:216:PRO:HG2	1:B:250:CYS:CB	2.39	0.53
1:B:369:LEU:O	1:B:370:ASN:C	2.51	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
1:E:177:ASN:ND2	1:E:180:ARG:HD3	2.22	0.53
1:E:379:GLU:HG3	1:E:381:ARG:HB2	1.91	0.53
1:E:467:ASP:O	1:E:471:VAL:HG23	2.08	0.53
1:E:483:PHE:C	1:E:485:ASP:H	2.17	0.53
1:E:574:GLU:C	1:E:574:GLU:OE1	2.52	0.53
1:F:352:LEU:HD11	1:F:386:MET:HE1	1.90	0.53
1:F:376:ALA:CA	1:F:381:ARG:NH1	2.71	0.53
1:F:417:TYR:CD2	1:F:483:PHE:HE2	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:ARG:NH1	1:A:526:TYR:HA	2.24	0.53
1:A:465:LEU:CD2	1:A:508:TRP:CZ3	2.92	0.53
1:A:493:ASP:N	1:A:493:ASP:OD1	2.41	0.53
1:A:525:THR:OG1	1:A:528:GLY:HA3	2.08	0.53
1:B:592:GLU:O	1:B:594:LEU:N	2.41	0.53
1:C:202:LYS:CD	1:C:300:ALA:HB1	2.36	0.53
1:C:410:ARG:HG3	1:C:411:ASP:H	1.73	0.53
1:D:165:LYS:HZ1	1:D:205:LEU:HB3	1.73	0.53
1:D:202:LYS:HD3	2:D:2001:ADP:O2B	2.08	0.53
1:E:438:VAL:HG23	1:E:439:THR:N	2.23	0.53
1:F:311:LEU:HD12	1:F:311:LEU:O	2.07	0.53
1:A:552:GLU:O	1:A:555:TYR:HB3	2.09	0.53
1:A:586:GLU:CB	1:A:589:ARG:CZ	2.72	0.53
1:A:587:PHE:CD2	1:A:588:GLN:N	2.76	0.53
1:B:177:ASN:O	1:B:180:ARG:HB3	2.08	0.53
1:C:273:ASP:CG	1:C:274:GLU:H	2.17	0.53
1:C:460:TRP:NE1	1:C:464:ARG:HH12	2.06	0.53
1:C:563:LEU:HD12	1:C:564:GLU:N	2.23	0.53
1:C:594:LEU:HG	1:C:594:LEU:O	2.09	0.53
1:E:334:ILE:CD1	2:E:1001:ADP:N6	2.71	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:F:311:LEU:C	1:F:316:ARG:NH1	2.66	0.53
1:A:319:ARG:O	1:A:320:GLN:NE2	2.42	0.53
1:A:349:ASP:OD1	1:A:349:ASP:O	2.26	0.53
1:A:380:GLY:C	1:F:180:ARG:NH2	2.66	0.53
1:B:193:LEU:C	1:B:194:LEU:HD12	2.34	0.53
1:B:201:GLY:N	2:B:2001:ADP:O1A	2.39	0.53
1:B:286:MET:HE2	1:B:315:GLY:O	2.07	0.53
1:C:368:LEU:HD13	1:C:393:ALA:CA	2.39	0.53
1:D:441:VAL:O	1:D:443:ARG:N	2.42	0.53
1:E:169:LYS:HA	1:E:172:VAL:CG1	2.38	0.53
1:F:194:LEU:HD23	1:F:323:ILE:HD11	1.90	0.53
1:F:467:ASP:OD1	1:F:557:ARG:NH2	2.42	0.53
1:F:477:ALA:O	1:F:481:ILE:HG13	2.09	0.53
1:A:368:LEU:HD13	1:A:393:ALA:HA	1.91	0.53
1:A:537:GLU:N	1:B:537:GLU:OE2	2.41	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:374:LEU:C	1:D:374:LEU:HD23	2.34	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:155:PHE:CE2	1:F:212:GLU:OE2	2.61	0.53
1:F:318:ASP:OD1	1:F:318:ASP:N	2.21	0.53
1:F:451:MET:HB3	1:F:452:PRO:CD	2.38	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:B:216:PRO:HB2	1:B:218:ILE:HD11	1.89	0.53
1:C:193:LEU:HD12	1:C:299: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: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:F:210:ALA:O	1:F:214:ARG:CA	2.57	0.53
1:F:331:ARG:HD2	1:F:354:ALA:O	2.09	0.53
1:A:155:PHE:CZ	1:A:209:VAL:HG22	2.44	0.53
1:A:264:ARG:HD2	1:A:266:SER:OG	2.09	0.53
1:A:280:ASN:O	1:A:281:GLN:C	2.50	0.53
1:A:382:ARG:HG3	1:A:383:LYS:HB2	1.91	0.53
1:A:424:LEU:HD22	1:A:569:LEU:HA	1.90	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:C:280:ASN:O	1:C:281:GLN:C	2.52	0.53
1:D:277:GLN:HA	1:D:280:ASN:HD21	1.74	0.53
1:D:369:LEU:O	1:D:370:ASN:C	2.51	0.53
1:D:592:GLU:O	1:D:594:LEU:N	2.42	0.53
1:E:238:ARG:O	1:E:239:ASP:C	2.51	0.53
1:E:319:ARG:O	1:E:320:GLN:NE2	2.41	0.53
1:E:349:ASP:O	1:E:349:ASP:OD1	2.26	0.53
1:E:514:PHE:N	1:E:514:PHE:CD2	2.77	0.53
1:E:519:TYR:C	1:E:533:ARG:NE	2.67	0.53
1:F:285:GLU:C	1:F:288:GLY:H	2.16	0.53
1:F:391:GLU:O	1:F:395:ARG:HB3	2.08	0.53
1:F:514:PHE:HB3	1:F:519:TYR:HE1	1.74	0.53
1:A:214:ARG:NH1	1:A:214:ARG:HG2	2.23	0.53
1:A:521:VAL:HG12	1:B:495:ARG:HD2	1.90	0.53
1:B:165:LYS:O	1:B:168:LEU:CB	2.57	0.53
1:B:206:ALA:HA	1:B:298:MET:HE2	1.91	0.53
1:C:169:LYS:HA	1:C:172:VAL:CG1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:GLY:HA2	1:C:443:ARG:NH2	2.24	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:C:345:ALA:O	1:C:348:VAL:HB	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:D:387:LYS:HG3	1:D:388:ASP:N	2.21	0.53
1:D:585:GLU:HA	1:D:588:GLN:OE1	2.09	0.53
1:E:461:SER:HA	1:F:487:THR:O	2.09	0.53
1:E:531:ASP:OD1	1:E:531:ASP:C	2.52	0.53
1:F:186:ALA:O	1:F:187:ARG:HB3	2.08	0.53
1:B:181:PHE:HA	1:B:184:MET:HG2	1.90	0.52
1:B:319:ARG:O	1:B:320:GLN:HB3	2.09	0.52
1:B:479:GLU:OE2	1:B:488:THR:HG23	2.10	0.52
1:C:189:PRO:O	1:C:190:LYS:HG2	2.08	0.52
1:D:421:GLY:HA2	1:D:562:LEU:HD11	1.90	0.52
1:D:459:HIS:O	1:D:459:HIS:CG	2.56	0.52
1:E:286:MET:HE1	1:E:297:VAL:HG21	1.89	0.52
1:F:165:LYS:HZ1	1:F:205:LEU:CB	2.21	0.52
1:F:479:GLU:OE2	1:F:488:THR:HG23	2.09	0.52
1:F:526:TYR:CD2	1:F:526:TYR:N	2.76	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:C:357:THR:C	1:C:360:PHE:HD1	2.17	0.52
1:C:460:TRP:HB3	1:C:465:LEU:HD11	1.91	0.52
1:D:335:LEU:HD21	1:D:365:LEU:HB3	1.90	0.52
1:E:521:VAL:HG12	1:F:495:ARG:HD2	1.92	0.52
1:F:376:ALA:O	1:F:381:ARG:CG	2.57	0.52
1:A:179:SER:HA	1:A:182:HIS:NE2	2.24	0.52
1:B:314:PRO:C	1:B:316:ARG:H	2.16	0.52
1:B:521:VAL:HG23	1:B:532:VAL:CG1	2.37	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:D:187:ARG:O	1:E:374:LEU:HD21	2.08	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:E:568:VAL:O	1:E:572:VAL:HG23	2.10	0.52
1:F:277:GLN:HA	1:F:280:ASN:HD21	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:356:ARG:O	1:F:358:PRO:HD3	2.10	0.52
1:A:368:LEU:HD13	1:A:393:ALA:CA	2.39	0.52
1:A:436:HIS:HB3	1:A:584:ALA:HB1	1.90	0.52
1:A:503:ARG:NH2	1:A:522:ARG:NH1	2.57	0.52
1:B:352:LEU:HD21	1:B:386:MET:HE1	1.92	0.52
1:B:428:PHE:CE1	1:B:432:ALA:C	2.87	0.52
1:B:463:LYS:HE3	1:C:486:VAL:HG21	1.90	0.52
1:B:564:GLU:C	1:B:566:ARG:N	2.64	0.52
1:C:451:MET:HB2	1:C:452:PRO:HD3	1.92	0.52
1:D:243:THR:HG22	1:D:244:ALA:N	2.25	0.52
1:D:348:VAL:HG11	1:D:386:MET:SD	2.49	0.52
1:D:554:GLN:O	1:D:557:ARG:HB3	2.09	0.52
1:E:442:PRO:HG2	1:E:443:ARG:H	1.74	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:A:374:LEU:CD1	1:F:187:ARG:H	2.11	0.52
1:B:571:ARG:HH12	1:B:593:GLY:H	1.57	0.52
1:C:274:GLU:C	1:C:277:GLN:HB3	2.34	0.52
1:C:463:LYS:HD2	1:D:486:VAL:HG22	1.90	0.52
1:C:536:SER:O	1:C:537:GLU:C	2.51	0.52
1:D:216:PRO:HG2	1:D:250:CYS:CB	2.39	0.52
1:D:417:TYR:CD2	1:D:483:PHE:HE2	2.28	0.52
1:D:507:GLU:HG3	1:D:520:ALA:O	2.10	0.52
1:E:241:PHE:O	1:E:244:ALA:N	2.42	0.52
1:E:354:ALA:HA	1:E:357:THR:CG2	2.39	0.52
1:F:452:PRO:O	1:F:456:ASP:CG	2.53	0.52
1:A:451:MET:HB2	1:A:452:PRO:HD3	1.92	0.52
1:A:583:THR:N	1:A:586:GLU:OE2	2.36	0.52
1:B:171:ILE:HG23	1:B:172:VAL:N	2.23	0.52
1:C:470:ALA:HB1	1:C:558:VAL:CG2	2.36	0.52
1:C:568:VAL:O	1:C:572:VAL:HG23	2.09	0.52
1:D:350:LEU:HA	1:D:353:LEU:HB3	1.91	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:A:374:LEU:HA	1:A:377:ALA:HB3	1.92	0.52
1:B:281:GLN:O	1:B:285:GLU:OE1	2.28	0.52
1:B:331:ARG:HH22	1:B:580:GLU:CD	2.14	0.52
1:C:207:ARG:NH2	1:C:217:PHE:CD2	2.76	0.52
1:C:379:GLU:HG3	1:C:381:ARG:HB2	1.92	0.52
1:D:174:PHE:HZ	1:D:294:ALA:CA	2.23	0.52
1:D:194:LEU:HD23	1:D:323:ILE:HD11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:236:ARG:HG3	1:E:237:VAL:CA	2.37	0.52
1:F:350:LEU:HA	1:F:353:LEU:HB3	1.91	0.52
1:F:381:ARG:CZ	1:F:388:ASP:OD2	2.57	0.52
1:A:241:PHE:O	1:A:244:ALA:N	2.43	0.52
1:B:180:ARG:NH1	1:B:184:MET:HE3	2.24	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:B:398:MET:O	1:B:401:ALA:HB3	2.09	0.52
1:B:505:ILE:HD13	1:B:547:VAL:HG23	1.90	0.52
1:C:218:ILE:CG1	1:C:251:ILE:O	2.57	0.52
1:C:325:ALA:N	1:C:326:PRO:CD	2.72	0.52
1:C:574:GLU:OE1	1:C:575:THR:N	2.43	0.52
1:D:338:HIS:HB3	1:D:369:LEU:CD1	2.40	0.52
1:D:398:MET:O	1:D:401:ALA:HB3	2.10	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:F:165:LYS:CE	1:F:205:LEU:HG	2.39	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: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: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:D:355:LYS:NZ	1:D:578:GLU:O	2.43	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:E:378:ARG:HG2	1:E:379:GLU:N	2.23	0.52
1:E:436:HIS:HB3	1:E:584:ALA:HB1	1.92	0.52
1:E:447:LEU:CB	1:E:496:GLN:HE22	2.23	0.52
1:F:557:ARG:O	1:F:560:ALA:HB3	2.10	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:B:455:GLU:O	1:B:456:ASP:C	2.53	0.52
1:C:241:PHE:O	1:C:244:ALA:N	2.43	0.52
1:C:539:THR:OG1	1:D:544:ASP:OD2	2.25	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:237:VAL:CG2	1:F:281:GLN:CG	2.88	0.52
1:F:352:LEU:HD11	1:F:386:MET:CE	2.40	0.52
1:F:453:ARG:HA	1:F:456:ASP:OD2	2.10	0.52
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:A:334:ILE:HD13	2:A:1001:ADP:N1	2.26	0.51
1:A:346:GLU:OE1	1:A:347:ASP:OD1	2.28	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:410:ARG:O	1:B:411:ASP:C	2.53	0.51
1:B:417:TYR:CD2	1:B:483:PHE:HE2	2.26	0.51
1:B:526:TYR:O	1:B:528:GLY:N	2.42	0.51
1:C:175:LEU:O	1:C:249:PRO:HG3	2.10	0.51
1:C:200:VAL:CG1	1:C:323:ILE:HG13	2.39	0.51
1:D:366:GLU:O	1:D:369:LEU:HB2	2.09	0.51
1:D:381:ARG:NH2	1:D:388:ASP:CG	2.47	0.51
1:E:179:SER:C	1:E:181:PHE:N	2.67	0.51
1:E:345:ALA:O	1:E:348:VAL:HB	2.10	0.51
1:E:408:SER:C	1:E:410:ARG:H	2.17	0.51
1:F:180:ARG:NH1	1:F:184:MET:CE	2.73	0.51
1:A:172:VAL:O	1:A:213:ALA:HB1	2.10	0.51
1:A:594:LEU:HG	1:A:594:LEU:O	2.11	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:B:467:ASP:OD1	1:B:557:ARG:NH2	2.43	0.51
1:C:174:PHE:HB2	1:C:181:PHE:CE2	2.46	0.51
1:C:272:ASN:C	1:C:272:ASN:OD1	2.53	0.51
1:C:368:LEU:HG	1:C:369:LEU:N	2.25	0.51
1:C:387:LYS:C	1:C:390:GLU:HB2	2.35	0.51
1:D:192:VAL:O	1:D:317:PHE:CE2	2.64	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:E:193:LEU:HD12	1:E:299:ALA:O	2.09	0.51
1:F:158:VAL:CG1	1:F:205:LEU:HD11	2.40	0.51
1:F:314:PRO:C	1:F:316:ARG:H	2.18	0.51
1:F:369:LEU:O	1:F:370:ASN:C	2.53	0.51
1:F:376:ALA:HA	1:F:381:ARG:HH11	1.74	0.51
1:A:212:GLU:C	1:A:214:ARG:HB2	2.34	0.51
1:A:379:GLU:HG3	1:A:381:ARG:HB2	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:ARG:O	1:B:358:PRO:HD3	2.11	0.51
1:B:455:GLU:O	1:B:457:MET:N	2.43	0.51
1:B:523:GLU:OE1	1:C:264:ARG:NH2	2.43	0.51
1:C:154:THR:OG1	1:C:155:PHE:N	2.43	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: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:D:331:ARG:HD2	1:D:354:ALA:O	2.11	0.51
1:E:594:LEU:HG	1:E:594:LEU:O	2.10	0.51
1:A:227:GLU:HG3	1:F:263:LYS:HZ1	1.69	0.51
1:A:313:ARG:NH1	1:A:526:TYR:CA	2.73	0.51
1:A:354:ALA:HA	1:A:357:THR:CG2	2.40	0.51
1:C:238:ARG:O	1:C:239:ASP:C	2.52	0.51
1:C:338:HIS:ND1	1:C:366:GLU:HG3	2.25	0.51
1:C:470:ALA:C	1:C:558:VAL:HG21	2.35	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: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:A:464:ARG:HH11	1:A:464:ARG:CG	2.23	0.51
1:B:175:LEU:O	1:B:249:PRO:CB	2.58	0.51
1:B:355:LYS:HZ2	1:B:578:GLU:HG3	1.74	0.51
1:B:452:PRO:O	1:B:456:ASP:N	2.43	0.51
1:B:557:ARG:O	1:B:560:ALA:HB3	2.11	0.51
1:C:236:ARG:NH1	1:C:236:ARG:CB	2.73	0.51
1:C:316:ARG:O	1:C:317:PHE:C	2.54	0.51
1:D:210:ALA:O	1:D:214:ARG:N	2.41	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:D:455:GLU:O	1:D:456:ASP:C	2.54	0.51
1:E:147:LEU:C	1:E:147:LEU:HD12	2.35	0.51
1:E:218:ILE:CG1	1:E:251:ILE:O	2.59	0.51
1:E:313:ARG:HH12	1:E:526:TYR:CA	2.23	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:B:461:SER:O	1:B:464:ARG:HB3	2.10	0.51
1:C:236:ARG:HG3	1:C:237:VAL:CA	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:292:ASP:OD1	1:C:293:THR:N	2.43	0.51
1:C:570:GLU:O	1:C:571:ARG:C	2.54	0.51
1:D:180:ARG:NH1	1:D:184:MET:HE3	2.26	0.51
1:D:327:ASP:O	1:D:331:ARG:NH2	2.43	0.51
1:D:514:PHE:HB3	1:D:519:TYR:HE1	1.74	0.51
1:E:196:GLY:C	1:E:202:LYS:HZ1	2.15	0.51
1:E:563:LEU:HD12	1:E:564:GLU:N	2.25	0.51
1:F:193:LEU:HB3	1:F:317:PHE:HD2	1.76	0.51
1:F:567:GLU:O	1:F:570:GLU:CB	2.58	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
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:C:174:PHE:CE1	1:C:188:ILE:CD1	2.70	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:E:175:LEU:O	1:E:249:PRO:HG3	2.10	0.51
1:E:313:ARG:NH1	1:E:526:TYR:CA	2.74	0.51
1:F:286:MET:O	1:F:289:PHE:CD1	2.64	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:A:238:ARG:O	1:A:239:ASP:C	2.51	0.51
1:A:551:ILE:O	1:A:552:GLU:C	2.52	0.51
1:B:459:HIS:O	1:B:459:HIS:CG	2.60	0.51
1:B:592:GLU:O	1:B:594:LEU:CB	2.59	0.51
1:C:313:ARG:NH1	1:C:526:TYR:HA	2.26	0.51
1:C:459:HIS:HE1	1:D:411:ASP:HB3	1.76	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:D:521:VAL:HG12	1:E:495:ARG:HD2	1.93	0.51
1:E:166:GLU:HB2	1:E:169:LYS:HZ1	1.75	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:F:215:VAL:HG22	1:F:250:CYS:HB3	1.93	0.51
1:F:375:LEU:HD11	1:F:388:ASP:CB	2.38	0.51
1:A:305:ASP:C	1:A:307:LEU:N	2.68	0.51
1:A:397:MET:SD	1:A:406:VAL:CG1	2.99	0.51
1:A:416:ALA:HB2	1:A:577:LEU:CD2	2.06	0.51
1:A:470:ALA:O	1:A:558:VAL:HG21	2.10	0.51
1:B:286:MET:SD	1:B:316:ARG:HG2	2.51	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:C:450:MET:HG3	1:C:451:MET:H	1.76	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:E:346:GLU:OE1	1:E:347:ASP:OD1	2.28	0.51
1:E:524:ASP:N	1:E:524:ASP:OD1	2.43	0.51
1:E:589:ARG:HH21	1:E:596:LEU:CB	1.74	0.51
1:F:174:PHE:C	1:F:174:PHE:CD2	2.89	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:F:374:LEU:HD23	1:F:374:LEU:C	2.36	0.51
1:F:410:ARG:O	1:F:411:ASP:C	2.53	0.51
1:F:410:ARG:HA	1:F:413:ARG:HG2	1.93	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:A:331:ARG:CZ	1:A:358:PRO:HD3	2.40	0.51
1:A:586:GLU:HG2	1:A:587:PHE:N	2.26	0.51
1:B:149:GLU:O	1:B:150:ALA:C	2.54	0.51
1:B:336:ARG:O	1:B:337:ILE:C	2.54	0.51
1:B:536:SER:OG	1:C:541:LYS:HA	2.11	0.51
1:B:585:GLU:O	1:B:587:PHE:N	2.44	0.51
1:C:331:ARG:HD2	1:C:357:THR:CG2	2.40	0.51
1:C:374:LEU:HA	1:C:377:ALA:HB3	1.93	0.51
1:C:503:ARG:NH2	1:C:522:ARG:NH1	2.58	0.51
1:D:164:ALA:C	1:D:168:LEU:HD13	2.35	0.51
1:D:503:ARG:HH22	1:D:522:ARG:CZ	2.23	0.51
1:D:572:VAL:O	1:D:576:LEU:HB2	2.11	0.51
1:E:191:GLY:CA	1:E:297:VAL:HG22	2.41	0.51
1:E:316:ARG:O	1:E:317:PHE:C	2.51	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: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:332:GLU:HB2	1:F:354:ALA:HB2	1.93	0.51
1:F:469:ILE:HG22	1:F:473:LEU:HD12	1.92	0.51
1:F:522:ARG:HD2	1:F:530:TYR:CA	2.33	0.51
1:A:414:ILE:HG22	1:A:415:THR:H	1.75	0.50
1:A:512:PRO:HB2	1:A:514:PHE:CD2	2.46	0.50
1:B:286:MET:O	1:B:289:PHE:CG	2.63	0.50
1:B:417:TYR:CE1	1:B:482:VAL:HG21	2.45	0.50
1:D:192:VAL:C	1:D:317:PHE:CE2	2.89	0.50
1:D:397:MET:O	1:D:400:PRO:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:538:GLU:O	1:D:541:LYS:N	2.44	0.50
1:E:280:ASN:O	1:E:281:GLN:C	2.54	0.50
1:A:345:ALA:HB1	1:A:347:ASP:OD1	2.12	0.50
1:A:519:TYR:HA	1:A:533:ARG:NH2	2.27	0.50
1:B:155:PHE:CE2	1:B:212:GLU:OE2	2.64	0.50
1:B:237:VAL:CG2	1:B:281:GLN:CG	2.87	0.50
1:B:297:VAL:HG13	1:B:317:PHE:CZ	2.47	0.50
1:B:389:LEU:O	1:B:390:GLU:C	2.54	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:C:215:VAL:CG2	1:C:216:PRO:N	2.75	0.50
1:D:355:LYS:NZ	1:D:578:GLU:HG3	2.26	0.50
1:D:454:ARG:HH21	1:D:526:TYR:CA	2.23	0.50
1:E:329:LYS:O	1:E:332:GLU:HB3	2.11	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:F:592:GLU:O	1:F:594:LEU:CB	2.60	0.50
1:B:243:THR:HG22	1:B:244:ALA:N	2.26	0.50
1:B:335:LEU:HD21	1:B:365:LEU:HB3	1.92	0.50
1:B:451:MET:HB3	1:B:452:PRO:CD	2.37	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:C:346:GLU:OE1	1:C:347:ASP:OD1	2.29	0.50
1:C:450:MET:HE1	1:C:499:GLU:OE2	2.12	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:D:325:ALA:CB	1:D:326:PRO:HD3	2.37	0.50
1:D:508:TRP:CD1	1:E:491:GLU:HG2	2.45	0.50
1:E:300:ALA:O	1:E:301:THR:HG22	2.11	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:F:441:VAL:O	1:F:443:ARG:N	2.44	0.50
1:F:454:ARG:NH2	1:F:526:TYR:HA	2.26	0.50
1:F:595:PRO:O	1:F:596:LEU:HD12	2.11	0.50
1:A:174:PHE:O	1:A:177:ASN:C	2.55	0.50
1:A:313:ARG:HH12	1:A:526:TYR:CA	2.25	0.50
1:A:357:THR:OG1	1:A:360:PHE:HB2	2.12	0.50
1:A:410:ARG:O	1:A:411:ASP:C	2.54	0.50
1:A:450:MET:HE1	1:A:499:GLU:OE2	2.12	0.50
1:A:479:GLU:OE2	1:A:488:THR:N	2.45	0.50
1:B:174:PHE:HZ	1:B:294:ALA:CA	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:LEU:O	1:B:353:LEU:C	2.53	0.50
1:B:538:GLU:HB2	1:C:541:LYS:NZ	2.26	0.50
1:C:147:LEU:C	1:C:147:LEU:HD12	2.36	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:C:469:ILE:O	1:C:473:LEU:HD12	2.11	0.50
1:D:428:PHE:HE1	1:D:432:ALA:C	2.19	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:368:LEU:HG	1:E:369:LEU:N	2.25	0.50
1:E:381:ARG:HH11	1:E:381:ARG:CG	2.21	0.50
1:E:389:LEU:O	1:E:392:ALA:HB3	2.11	0.50
1:E:479:GLU:OE2	1:E:488:THR:N	2.45	0.50
1:E:534:GLN:N	1:E:534:GLN:CD	2.70	0.50
1:A:263:LYS:HZ1	1:A:276:GLU:CD	2.13	0.50
1:B:175:LEU:HD12	1:B:215:VAL:CG1	2.36	0.50
1:B:193:LEU:HB3	1:B:317:PHE:HD2	1.77	0.50
1:C:282:LEU:O	1:C:286:MET:HG2	2.11	0.50
1:C:357:THR:OG1	1:C:360:PHE:HB2	2.11	0.50
1:D:278:THR:O	1:D:281:GLN:HB3	2.12	0.50
1:D:329:LYS:O	1:D:332:GLU:HB3	2.12	0.50
1:D:336:ARG:O	1:D:337:ILE:C	2.53	0.50
1:D:410:ARG:O	1:D:411:ASP:C	2.54	0.50
1:E:168:LEU:C	1:E:168:LEU:HD12	2.36	0.50
1:E:302:ASN:HB3	1:E:443:ARG:HH12	1.76	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:370:ASN:C	1:E:370:ASN:OD1	2.55	0.50
1:E:397:MET:SD	1:E:406:VAL:CG1	2.99	0.50
1:E:507:GLU:HB2	1:E:520:ALA:HB3	1.92	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:A:274:GLU:C	1:A:277:GLN:HB3	2.37	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:A:580:GLU:O	1:A:580:GLU:CG	2.59	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:C:179:SER:C	1:C:181:PHE:N	2.67	0.50
1:C:279:LEU:O	1:C:282:LEU:N	2.44	0.50
1:C:325:ALA:N	1:C:326:PRO:HD2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:450:MET:O	1:C:454:ARG:HB3	2.12	0.50
1:E:218:ILE:HG12	1:E:251:ILE:O	2.11	0.50
1:E:292:ASP:OD1	1:E:293:THR:N	2.43	0.50
1:F:297:VAL:HG13	1:F:317:PHE:HZ	1.77	0.50
1:F:398:MET:O	1:F:401:ALA:HB3	2.11	0.50
1:F:449:PHE:CZ	1:F:496:GLN:OE1	2.64	0.50
1:A:196:GLY:H	1:A:202:LYS:HZ1	1.58	0.50
1:A:445:ARG:O	1:A:447:LEU:N	2.45	0.50
1:B:238:ARG:HA	1:B:241:PHE:CE2	2.47	0.50
1:B:345:ALA:CB	1:B:383:LYS:HE3	2.37	0.50
1:C:313:ARG:NH1	1:C:526:TYR:CA	2.75	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:C:524:ASP:OD1	1:C:524:ASP:N	2.44	0.50
1:D:158:VAL:HG22	1:D:204:HIS:ND1	2.26	0.50
1:D:239:ASP:O	1:D:242:GLU:OE2	2.30	0.50
1:D:567:GLU:O	1:D:570:GLU:CB	2.59	0.50
1:E:273:ASP:CG	1:E:274:GLU:H	2.20	0.50
1:E:313:ARG:NH1	1:E:526:TYR:HA	2.27	0.50
1:E:583:THR:HG22	1:E:586:GLU:OE1	2.10	0.50
1:F:334:ILE:O	1:F:337:ILE:HG22	2.12	0.50
1:F:387:LYS:HG3	1:F:388:ASP:N	2.25	0.50
1:F:554:GLN:O	1:F:557:ARG:HB3	2.11	0.50
1:A:286:MET:HB3	1:A:316:ARG:HB2	1.94	0.50
1:A:345:ALA:O	1:A:348:VAL:HB	2.12	0.50
1:B:301:THR:HG22	1:B:303:ARG:H	1.77	0.50
1:C:356:ARG:C	1:C:358:PRO:HD2	2.37	0.50
1:C:365:LEU:O	1:C:368:LEU:HB3	2.11	0.50
1:C:382:ARG:HG3	1:C:383:LYS:HB2	1.93	0.50
1:C:566:ARG:O	1:C:569:LEU:N	2.45	0.50
1:D:447:LEU:O	1:D:450:MET:HG3	2.11	0.50
1:E:188:ILE:O	1:E:190:LYS:NZ	2.42	0.50
1:E:210:ALA:HA	1:E:251:ILE:HD11	1.94	0.50
1:A:211:GLY:HA2	1:A:214:ARG:NE	2.25	0.50
1:A:450:MET:HG3	1:A:451:MET:H	1.77	0.50
1:B:441:VAL:O	1:B:443:ARG:N	2.45	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:583:THR:O	1:D:584:ALA:C	2.55	0.50
1:E:282:LEU:O	1:E:286:MET:HG2	2.12	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:F:510:MET:O	1:F:512:PRO:HD2	2.12	0.50
1:A:179:SER:O	1:A:182:HIS:CD2	2.62	0.49
1:A:196:GLY:C	1:A:202:LYS:HZ1	2.18	0.49
1:A:387:LYS:C	1:A:390:GLU:HB2	2.37	0.49
1:A:428:PHE:HE1	1:A:432:ALA:HA	1.66	0.49
1:A:519:TYR:C	1:A:533:ARG:NE	2.68	0.49
1:A:588:GLN:HA	1:A:591:VAL:HG21	1.92	0.49
1:B:449:PHE:CZ	1:B:496:GLN:OE1	2.65	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:F:181:PHE:O	1:F:185:GLY:N	2.44	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:A:483:PHE:C	1:A:485:ASP:H	2.20	0.49
1:A:514:PHE:HB3	1:A:519:TYR:HE1	1.73	0.49
1:B:376:ALA:O	1:B:381:ARG:CG	2.60	0.49
1:B:529:GLY:O	1:B:530:TYR:CB	2.55	0.49
1:B:554:GLN:O	1:B:557:ARG:HB3	2.11	0.49
1:C:171:ILE:HD12	1:C:172:VAL:H	1.76	0.49
1:C:436:HIS:HB3	1:C:584:ALA:CB	2.42	0.49
1:D:174:PHE:HZ	1:D:294:ALA:HA	1.76	0.49
1:D:206:ALA:HA	1:D:298:MET:HE2	1.93	0.49
1:D:336:ARG:O	1:D:339:ALA:N	2.27	0.49
1:D:563:LEU:O	1:D:566:ARG:CB	2.61	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
1:F:236:ARG:NH1	1:F:237:VAL:HG12	2.26	0.49
1:A:150:ALA:CB	1:A:214:ARG:NH1	2.75	0.49
1:A:168:LEU:C	1:A:168:LEU:HD12	2.38	0.49
1:A:225:PHE:CE1	1:A:233:GLY:HA3	2.47	0.49
1:A:264:ARG:CD	1:A:266:SER:CB	2.87	0.49
1:A:272:ASN:C	1:A:272:ASN:OD1	2.54	0.49
1:A:346:GLU:CD	1:A:347:ASP:N	2.71	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:GLU:CA	1:B:245:LYS:HB3	2.41	0.49
1:B:311:LEU:HA	1:B:316:ARG:CZ	2.39	0.49
1:C:206:ALA:HB1	1:C:217:PHE:HZ	1.77	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:539:THR:O	1:C:543:ILE:HG13	2.13	0.49
1:C:594:LEU:HD12	1:C:595:PRO:O	2.12	0.49
1:D:241:PHE:HE2	1:D:285:GLU:OE2	1.91	0.49
1:E:460:TRP:HD1	1:E:464:ARG:NH1	2.08	0.49
1:E:537:GLU:N	1:F:537:GLU:OE2	2.41	0.49
1:F:338:HIS:CE1	1:F:366:GLU:HG3	2.47	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:A:147:LEU:HD23	1:A:217:PHE:HB3	1.93	0.49
1:A:449:PHE:CE2	1:A:496:GLN:NE2	2.79	0.49
1:A:453:ARG:HH21	1:A:464:ARG:HH22	1.55	0.49
1:C:313:ARG:HH12	1:C:526:TYR:CA	2.25	0.49
1:C:519:TYR:HB3	1:C:535:TYR:HD2	1.76	0.49
1:E:195:VAL:HG22	1:E:301:THR:O	2.12	0.49
1:E:305:ASP:C	1:E:307:LEU:N	2.70	0.49
1:F:313:ARG:HG3	1:F:314:PRO:CG	2.41	0.49
1:A:354:ALA:O	1:A:357:THR:CG2	2.55	0.49
1:A:389:LEU:O	1:A:392:ALA:HB3	2.11	0.49
1:B:308:ASP:OD1	1:B:310:ALA:N	2.43	0.49
1:C:191:GLY:CA	1:C:297:VAL:HG22	2.43	0.49
1:C:370:ASN:OD1	1:C:374:LEU:HD13	2.12	0.49
1:D:209:VAL:CG1	1:D:210:ALA:H	2.20	0.49
1:E:154:THR:OG1	1:E:155:PHE:N	2.44	0.49
1:F:149:GLU:O	1:F:150:ALA:C	2.56	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:A:273:ASP:OD1	1:A:274:GLU:N	2.46	0.49
1:C:237:VAL:HG11	1:C:281:GLN:CB	2.26	0.49
1:C:370:ASN:OD1	1:C:370:ASN:C	2.55	0.49
1:D:566:ARG:O	1:D:569:LEU:HB3	2.13	0.49
1:E:196:GLY:H	1:E:202:LYS:HZ1	1.56	0.49
1:E:580:GLU:O	1:E:580:GLU:CG	2.60	0.49
1:F:239:ASP:O	1:F:242:GLU:OE2	2.30	0.49
1:F:583:THR:O	1:F:584:ALA:C	2.56	0.49
1:A:219:THR:HB	1:A:253:PHE:CD2	2.40	0.49
2:A:1001:ADP:N3	2:A:1001:ADP:H2'	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:GLY:O	1:B:308:ASP:N	2.38	0.49
1:B:376:ALA:O	1:B:381:ARG:HG3	2.12	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:D:453:ARG:HA	1:D:456:ASP:OD2	2.13	0.49
1:E:211:GLY:C	1:E:214:ARG:HG2	2.37	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:F:376:ALA:C	1:F:381:ARG:CB	2.84	0.49
1:A:291:LYS:O	1:A:292:ASP:C	2.56	0.49
1:A:378:ARG:NH1	1:F:170:GLU:HB2	2.28	0.49
1:B:334:ILE:HG21	1:B:365:LEU:HD12	1.94	0.49
1:B:361:VAL:HG13	1:B:364:ASP:CG	2.38	0.49
1:B:567:GLU:O	1:B:570:GLU:CB	2.61	0.49
1:C:155:PHE:CZ	1:C:209:VAL:HG22	2.47	0.49
1:C:305:ASP:C	1:C:307:LEU:N	2.69	0.49
2:C:1001:ADP:H2'	2:C:1001:ADP:N3	2.28	0.49
1:D:409:PRO:O	1:D:413:ARG:HD3	2.13	0.49
1:E:169:LYS:O	1:E:172:VAL:CG1	2.60	0.49
1:E:387:LYS:C	1:E:390:GLU:HB2	2.38	0.49
1:E:464:ARG:O	1:E:465:LEU:C	2.56	0.49
1:F:164:ALA:C	1:F:168:LEU:HD13	2.36	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:335:LEU:HD13	1:F:365:LEU:HB3	1.93	0.49
1:F:360:PHE:HE1	1:F:364:ASP:HB3	1.77	0.49
1:B:278:THR:O	1:B:281:GLN:HB3	2.13	0.49
1:C:327:ASP:C	1:C:327:ASP:OD1	2.56	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:C:519:TYR:C	1:C:533:ARG:CZ	2.86	0.49
1:D:215:VAL:O	1:D:216:PRO:C	2.56	0.49
1:D:525:THR:HG22	1:D:526:TYR:H	1.77	0.49
1:E:220:ALA:O	1:E:254:ILE:HA	2.13	0.49
1:E:236:ARG:HG2	1:E:236:ARG:NH1	2.11	0.49
1:E:260:VAL:HG23	1:E:261:GLY:H	1.78	0.49
1:E:357:THR:OG1	1:E:360:PHE:HB2	2.11	0.49
1:E:374:LEU:HA	1:E:377:ALA:HB3	1.93	0.49
1:F:564:GLU:O	1:F:566:ARG:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:VAL:HG23	1:A:261:GLY:H	1.76	0.49
1:A:266:SER:C	1:A:268:VAL:N	2.70	0.49
1:A:370:ASN:OD1	1:A:370:ASN:C	2.55	0.49
1:A:447:LEU:CB	1:A:496:GLN:HE22	2.25	0.49
1:B:191:GLY:HA3	1:B:297:VAL:HG12	1.94	0.49
1:B:589:ARG:NE	1:B:596:LEU:CD2	2.76	0.49
1:C:196:GLY:C	1:C:202:LYS:HZ1	2.15	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:186:ALA:O	1:D:187:ARG:HB3	2.12	0.49
1:D:238:ARG:HH11	1:D:238:ARG:CB	2.26	0.49
1:D:360:PHE:HE1	1:D:364:ASP:HB3	1.77	0.49
1:D:469:ILE:HG22	1:D:473:LEU:HD12	1.95	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: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:B:376:ALA:C	1:B:381:ARG:CB	2.84	0.48
1:C:220:ALA:O	1:C:254:ILE:HA	2.13	0.48
1:C:359:GLY:HA3	1:C:360:PHE:CG	2.48	0.48
1:C:389:LEU:O	1:C:392:ALA:HB3	2.12	0.48
1:D:215:VAL:HG22	1:D:250:CYS:HB3	1.94	0.48
1:D:334:ILE:HG21	1:D:365:LEU:HD12	1.94	0.48
1:D:585:GLU:O	1:D:586:GLU:C	2.56	0.48
1:E:551:ILE:O	1:E:552:GLU:C	2.56	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:F:503:ARG:NH2	1:F:522:ARG:NH2	2.59	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:A:381:ARG:C	1:F:180:ARG:HH22	2.18	0.48
1:B:241:PHE:CD2	1:B:285:GLU:HG2	2.48	0.48
1:B:360:PHE:HE1	1:B:364:ASP:HB3	1.79	0.48
1:B:454:ARG:NH2	1:B:526:TYR:HA	2.29	0.48
1:C:290:GLU:CD	1:D:226:VAL:HG11	2.37	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:C:450:MET:HE2	1:C:451:MET:SD	2.53	0.48
1:C:580:GLU:O	1:C:580:GLU:CG	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:ALA:H	2:D:2001:ADP:HN62	1.61	0.48
1:D:175:LEU:O	1:D:249:PRO:HG2	2.13	0.48
1:D:225:PHE:CD2	1:D:225:PHE:N	2.80	0.48
1:D:312:LEU:HD23	1:D:312:LEU:O	2.13	0.48
1:D:548:ARG:NH1	1:D:548:ARG:HG2	2.28	0.48
1:E:196:GLY:O	1:E:302:ASN:OD1	2.30	0.48
1:E:262:ARG:HG2	1:E:275:ARG:NH2	2.08	0.48
1:E:272:ASN:C	1:E:272:ASN:OD1	2.55	0.48
1:E:594:LEU:HD12	1:E:595:PRO:O	2.13	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:F:428:PHE:HE1	1:F:432:ALA:C	2.20	0.48
1:A:519:TYR:HA	1:A:533:ARG:CZ	2.43	0.48
1:B:212:GLU:O	1:B:214:ARG:HG3	2.13	0.48
1:B:447:LEU:O	1:B:450:MET:HG3	2.12	0.48
1:C:168:LEU:C	1:C:168:LEU:HD12	2.38	0.48
1:C:260:VAL:HG23	1:C:261:GLY:H	1.78	0.48
1:C:266:SER:C	1:C:268:VAL:N	2.70	0.48
1:D:494:PHE:O	1:D:495:ARG:C	2.56	0.48
1:E:236:ARG:HH11	1:E:236:ARG:CB	2.26	0.48
1:E:266:SER:C	1:E:268:VAL:N	2.71	0.48
1:E:357:THR:N	1:E:358:PRO:CD	2.76	0.48
1:E:520:ALA:HA	1:E:533:ARG:CG	2.43	0.48
1:F:361:VAL:HG13	1:F:364:ASP:CG	2.38	0.48
1:F:548:ARG:NH1	1:F:548:ARG:HG2	2.28	0.48
1:F:566:ARG:O	1:F:569:LEU:HB3	2.13	0.48
1:A:233:GLY:O	1:A:236:ARG:CG	2.58	0.48
1:A:453:ARG:NH2	1:A:464:ARG:CZ	2.76	0.48
1:A:576:LEU:O	1:A:580:GLU:N	2.32	0.48
1:B:164:ALA:C	1:B:168:LEU:HD13	2.37	0.48
1:B:207:ARG:O	1:B:210:ALA:N	2.47	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:B:313:ARG:HG3	1:B:314:PRO:HG2	1.96	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:249:PRO:HB3	1:C:294:ALA:HB3	1.95	0.48
1:C:328:VAL:HG12	1:C:329:LYS:N	2.27	0.48
1:D:157:ASP:O	1:D:204:HIS:HE1	1.96	0.48
1:D:175:LEU:HD12	1:D:215:VAL:CG1	2.37	0.48
1:D:344:LEU:HB2	1:D:384:ILE:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:147:LEU:HD23	1:E:217:PHE:CB	2.43	0.48
1:E:212:GLU:N	1:E:214:ARG:CG	2.76	0.48
1:E:397:MET:HG3	1:E:406:VAL:CG1	2.43	0.48
1:E:443:ARG:O	1:E:443:ARG:HG2	2.14	0.48
1:F:517:VAL:CG1	1:F:519:TYR:OH	2.60	0.48
1:A:554:GLN:O	1:A:557:ARG:HB3	2.14	0.48
1:B:225:PHE:CD2	1:B:236:ARG:NE	2.81	0.48
1:C:520:ALA:HA	1:C:533:ARG:CG	2.43	0.48
1:D:165:LYS:CE	1:D:205:LEU:HG	2.43	0.48
1:D:180:ARG:NH1	1:D:184:MET:CE	2.76	0.48
1:D:242:GLU:CA	1:D:245:LYS:HB3	2.42	0.48
1:E:357:THR:C	1:E:360:PHE:HD1	2.21	0.48
1:E:462:ARG:CG	1:E:463:LYS:N	2.76	0.48
1:E:511:HIS:C	1:E:512:PRO:O	2.56	0.48
1:F:183:GLU:OE1	1:F:184:MET:HB3	2.14	0.48
1:F:376:ALA:HB1	1:F:381:ARG:CD	2.42	0.48
1:F:454:ARG:HH21	1:F:526:TYR:HA	1.78	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:A:447:LEU:HA	1:A:496:GLN:HE21	1.77	0.48
1:B:157:ASP:HB3	1:B:337:ILE:CD1	2.44	0.48
1:B:190:LYS:HG3	1:B:190:LYS:O	2.14	0.48
1:B:563:LEU:CD1	1:B:563:LEU:C	2.87	0.48
1:C:228:MET:CG	1:C:236:ARG:HH22	2.27	0.48
1:C:373:ALA:HA	1:C:384:ILE:CD1	2.43	0.48
1:C:445:ARG:O	1:C:447:LEU:N	2.47	0.48
1:D:174:PHE:CZ	1:D:294:ALA:CB	2.96	0.48
1:D:589:ARG:C	1:D:591:VAL:N	2.70	0.48
1:E:147:LEU:HB3	1:E:217:PHE:O	2.12	0.48
1:E:346:GLU:CD	1:E:347:ASP:N	2.71	0.48
1:F:397:MET:HA	1:F:400:PRO:HG2	1.95	0.48
1:F:563:LEU:O	1:F:566:ARG:CB	2.61	0.48
1:A:174:PHE:HB2	1:A:181:PHE:CE2	2.48	0.48
1:A:311:LEU:CG	1:A:316:ARG:HH22	2.25	0.48
1:B:428:PHE:C	1:B:428:PHE:HD1	2.21	0.48
1:B:564:GLU:O	1:B:566:ARG:N	2.47	0.48
1:C:467:ASP:O	1:C:471:VAL:HG23	2.13	0.48
1:D:228:MET:SD	1:D:232:VAL:CG1	3.01	0.48
1:D:286:MET:O	1:D:289:PHE:CD1	2.67	0.48
1:D:595:PRO:C	1:D:596:LEU:HD12	2.38	0.48
1:E:300:ALA:O	1:E:301:THR:CG2	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:414:ILE:HG22	1:E:415:THR:H	1.78	0.48
1:F:336:ARG:HD3	1:F:336:ARG:HA	1.50	0.48
1:F:388:ASP:OD1	1:F:388:ASP:N	2.46	0.48
1:F:389:LEU:O	1:F:390:GLU:C	2.56	0.48
1:F:400:PRO:HB2	1:F:404:SER:OG	2.14	0.48
1:F:476:ARG:NH1	1:F:487:THR:HG21	2.29	0.48
1:F:505:ILE:HG23	1:F:514:PHE:CD2	2.48	0.48
1:A:177:ASN:HD22	1:A:180:ARG:CD	2.25	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:B:468:GLN:O	1:B:471:VAL:N	2.45	0.48
1:C:274:GLU:HB3	1:C:275:ARG:H	1.43	0.48
1:D:149:GLU:O	1:D:150:ALA:C	2.57	0.48
1:D:302:ASN:ND2	1:D:443:ARG:NH2	2.55	0.48
1:D:397:MET:HA	1:D:400:PRO:HG2	1.95	0.48
1:D:410:ARG:O	1:D:413:ARG:CB	2.61	0.48
1:D:592:GLU:O	1:D:594:LEU:CB	2.61	0.48
1:E:215:VAL:HG21	1:E:250:CYS:CB	2.43	0.48
1:E:328:VAL:HG12	1:E:329:LYS:N	2.29	0.48
1:E:336:ARG:O	1:E:337:ILE:C	2.55	0.48
1:F:159:ALA:HB1	1:F:333:GLN:HG3	1.96	0.48
1:F:175:LEU:O	1:F:249:PRO:HG2	2.14	0.48
1:F:206:ALA:HA	1:F:298:MET:HE2	1.95	0.48
1:F:470:ALA:O	1:F:474:ALA:HB2	2.14	0.48
1:A:460:TRP:HD1	1:A:464:ARG:NH1	2.10	0.48
1:A:470:ALA:HB1	1:A:558:VAL:CG2	2.40	0.48
1:A:562:LEU:O	1:A:565:LYS:N	2.47	0.48
1:A:574:GLU:O	1:A:575:THR:C	2.57	0.48
1:B:336:ARG:HA	1:B:336:ARG:HD3	1.47	0.48
1:B:453:ARG:HA	1:B:456:ASP:OD2	2.14	0.48
1:B:478:ALA:O	1:B:479:GLU:C	2.57	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:479:GLU:OE2	1:C:488:THR:N	2.47	0.48
1:C:528:GLY:HA2	1:C:530:TYR:CE2	2.49	0.48
1:C:575:THR:HA	1:C:578:GLU:OE1	2.13	0.48
1:D:356:ARG:O	1:D:358:PRO:HD3	2.13	0.48
1:D:428:PHE:C	1:D:428:PHE:HD1	2.22	0.48
1:E:325:ALA:N	1:E:326:PRO:HD2	2.29	0.48
1:E:506:THR:CG2	1:E:543:ILE:HD13	2.44	0.48
1:E:570:GLU:O	1:E:571:ARG:C	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:159:ALA:HA	1:F:333:GLN:HE21	1.79	0.48
1:F:237:VAL:HG21	1:F:281:GLN:HG3	1.96	0.48
1:F:302:ASN:ND2	1:F:443:ARG:HH22	1.89	0.48
1:B:199:GLY:H	2:B:2001:ADP:PB	2.34	0.48
1:B:233:GLY:CA	1:B:236:ARG:NH2	2.59	0.48
1:B:233:GLY:C	1:B:236:ARG:HH22	2.22	0.48
1:B:374:LEU:HD23	1:B:374:LEU:C	2.38	0.48
1:B:387:LYS:HG3	1:B:388:ASP:N	2.26	0.48
1:B:488:THR:O	1:B:490:ALA:N	2.47	0.48
1:C:169:LYS:O	1:C:172:VAL:N	2.47	0.48
1:C:378:ARG:HG3	1:C:379:GLU:N	2.21	0.48
1:C:576:LEU:O	1:C:580:GLU:N	2.35	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: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:A:400:PRO:HG2	1:A:405:LEU:CD1	2.44	0.47
1:A:449:PHE:CE2	1:A:496:GLN:CD	2.92	0.47
1:A:587:PHE:CD2	1:A:587:PHE:C	2.92	0.47
1:A:594:LEU:HD12	1:A:595:PRO:O	2.13	0.47
1:B:170:GLU:CB	1:C:378:ARG:NH2	2.77	0.47
1:B:196:GLY:O	1:B:302:ASN:HA	2.14	0.47
1:B:338:HIS:CB	1:B:369:LEU:HD11	2.44	0.47
1:B:571:ARG:HH12	1:B:593:GLY:N	2.11	0.47
1:C:345:ALA:HB1	1:C:347:ASP:OD1	2.13	0.47
1:D:564:GLU:O	1:D:566:ARG:N	2.46	0.47
1:E:327:ASP:OD1	1:E:327:ASP:C	2.57	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:261:GLY:O	1:F:308:ASP:HB3	2.14	0.47
1:F:297:VAL:HG13	1:F:317:PHE:CZ	2.48	0.47
1:F:449:PHE:CE2	1:F:453:ARG:CZ	2.97	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:A:520:ALA:HA	1:A:533:ARG:CG	2.44	0.47
1:B:225:PHE:HA	1:B:236:ARG:CZ	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:460:TRP:CD1	1:B:464:ARG:HG2	2.49	0.47
1:C:483:PHE:C	1:C:485:ASP:H	2.23	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:D:428:PHE:C	1:D:428:PHE:CD1	2.92	0.47
1:D:517:VAL:CG1	1:D:519:TYR:OH	2.63	0.47
1:E:182:HIS:CD2	1:E:182:HIS:H	2.30	0.47
1:E:274:GLU:C	1:E:277:GLN:HB3	2.36	0.47
1:F:157:ASP:O	1:F:204:HIS:HE1	1.96	0.47
1:F:203:THR:OG1	2:F:2001:ADP:O1B	2.32	0.47
1:F:393:ALA:O	1:F:397:MET:HB3	2.15	0.47
1:F:563:LEU:O	1:F:566:ARG:HB3	2.14	0.47
1:F:585:GLU:O	1:F:586:GLU:C	2.55	0.47
1:A:191:GLY:CA	1:A:297:VAL:HG22	2.44	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:B:162:GLU:HA	1:B:162:GLU:OE1	2.15	0.47
1:B:215:VAL:HG21	1:B:249:PRO:C	2.38	0.47
1:B:241:PHE:HE2	1:B:285:GLU:OE2	1.90	0.47
1:D:388:ASP:OD1	1:D:388:ASP:N	2.42	0.47
1:D:438:VAL:CG2	1:D:439:THR:N	2.76	0.47
1:E:210:ALA:HB2	1:E:251:ILE:CD1	2.38	0.47
1:F:436:HIS:O	1:F:437:LYS:CG	2.61	0.47
1:A:336:ARG:O	1:A:337:ILE:C	2.58	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:B:409:PRO:O	1:B:413:ARG:HD3	2.14	0.47
1:B:517:VAL:CG2	1:B:518:ALA:N	2.76	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:C:479:GLU:OE2	1:C:487:THR:HA	2.15	0.47
1:D:157:ASP:O	1:D:204:HIS:CE1	2.67	0.47
1:D:225:PHE:CD2	1:D:236:ARG:CD	2.95	0.47
1:D:311:LEU:C	1:D:316:ARG:HG2	2.31	0.47
1:E:519:TYR:HB3	1:E:535:TYR:HD2	1.78	0.47
1:E:574:GLU:O	1:E:575:THR:C	2.57	0.47
1:F:290:GLU:CG	1:F:293:THR:HG23	2.29	0.47
1:F:589:ARG:CD	1:F:596:LEU:HD11	2.44	0.47
1:A:289:PHE:C	1:A:290:GLU:CD	2.83	0.47
1:B:186:ALA:HB1	1:C:374:LEU:CD1	2.44	0.47
1:B:376:ALA:HB1	1:B:381:ARG:HD3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:ILE:HG22	1:B:385:THR:N	2.30	0.47
1:B:538:GLU:C	1:B:540:ALA:N	2.72	0.47
1:C:548:ARG:NH2	1:C:552:GLU:OE1	2.43	0.47
1:C:589:ARG:HB3	1:C:589:ARG:HH11	1.73	0.47
1:D:169:LYS:O	1:D:172:VAL:HG22	2.14	0.47
1:D:247:HIS:O	1:D:249:PRO:O	2.33	0.47
1:D:571:ARG:HH12	1:D:593:GLY:H	1.61	0.47
1:E:159:ALA:HB1	1:E:333:GLN:HB3	1.96	0.47
1:E:172:VAL:CB	1:E:213:ALA:HB2	2.44	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:E:523:GLU:O	1:E:529:GLY:HA2	2.14	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
1:F:302:ASN:ND2	1:F:443:ARG:NH2	2.52	0.47
1:F:571:ARG:HH12	1:F:593:GLY:H	1.63	0.47
1:A:311:LEU:HD22	1:A:316:ARG:NH1	2.28	0.47
1:A:436:HIS:HB3	1:A:584:ALA:CB	2.45	0.47
1:A:456:ASP:CG	1:A:457:MET:H	2.13	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:D:274:GLU:HA	1:D:277:GLN:HE21	1.80	0.47
1:E:411:ASP:O	1:E:415:THR:OG1	2.31	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:238:ARG:O	1:F:239:ASP:C	2.56	0.47
1:F:262:ARG:CG	1:F:263:LYS:H	2.20	0.47
1:A:236:ARG:C	1:A:238:ARG:N	2.71	0.47
1:A:329:LYS:O	1:A:332:GLU:HB3	2.15	0.47
1:A:331:ARG:O	1:A:335:LEU:HG	2.14	0.47
1:A:454:ARG:HD3	1:A:454:ARG:C	2.39	0.47
1:A:458:LEU:C	1:A:458:LEU:HD12	2.39	0.47
1:B:155:PHE:O	1:B:156:LYS:C	2.57	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:C:169:LYS:O	1:C:172:VAL:CG1	2.61	0.47
1:C:192:VAL:N	1:C:297:VAL:O	2.39	0.47
1:C:210:ALA:HA	1:C:251:ILE:HD11	1.96	0.47
1:C:273:ASP:OD1	1:C:273:ASP:C	2.58	0.47
1:C:336:ARG:O	1:C:337:ILE:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:336:ARG:O	1:D:338:HIS:N	2.47	0.47
1:D:454:ARG:NH2	1:D:526:TYR:HA	2.29	0.47
1:D:505:ILE:HD13	1:D:547:VAL:HG23	1.95	0.47
1:D:510:MET:O	1:D:512:PRO:CD	2.61	0.47
1:D:563:LEU:CD1	1:D:563:LEU:C	2.87	0.47
1:E:174:PHE:O	1:E:177:ASN:C	2.58	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:E:207:ARG:HH21	1:E:217:PHE:HD2	1.61	0.47
1:E:331:ARG:O	1:E:335:LEU:HG	2.15	0.47
1:E:382:ARG:CG	1:E:383:LYS:N	2.75	0.47
1:E:589:ARG:HH22	1:E:596:LEU:N	2.13	0.47
1:F:158:VAL:HG22	1:F:204:HIS:ND1	2.29	0.47
1:F:215:VAL:O	1:F:216:PRO:C	2.56	0.47
1:F:301:THR:HG22	1:F:303:ARG:H	1.79	0.47
1:F:449:PHE:CZ	1:F:453:ARG:NH2	2.81	0.47
1:F:494:PHE:O	1:F:496:GLN:N	2.47	0.47
1:F:563:LEU:C	1:F:563:LEU:CD1	2.88	0.47
1:F:594:LEU:C	1:F:594:LEU:HD23	2.39	0.47
1:A:316:ARG:HG2	1:A:317:PHE:CD2	2.49	0.47
1:A:327:ASP:C	1:A:327:ASP:OD1	2.57	0.47
1:A:348:VAL:O	1:A:348:VAL:HG12	2.14	0.47
1:A:449:PHE:HZ	1:A:496:GLN:HG2	1.60	0.47
1:A:524:ASP:OD1	1:A:524:ASP:N	2.47	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:B:477:ALA:O	1:B:478:ALA:C	2.55	0.47
1:B:563:LEU:O	1:B:566:ARG:CB	2.62	0.47
1:D:400:PRO:O	1:D:403:LYS:N	2.48	0.47
1:D:414:ILE:O	1:D:415:THR:C	2.57	0.47
1:D:536:SER:OG	1:E:541:LYS:HA	2.15	0.47
1:E:206:ALA:CB	1:E:217:PHE:HZ	2.28	0.47
1:E:345:ALA:HB1	1:E:347:ASP:OD1	2.14	0.47
1:E:576:LEU:O	1:E:580:GLU:N	2.39	0.47
1:F:215:VAL:HG21	1:F:249:PRO:C	2.38	0.47
1:F:428:PHE:CZ	1:F:433:ASP:N	2.83	0.47
1:F:455:GLU:O	1:F:456:ASP:C	2.58	0.47
1:F:533:ARG:NH1	1:F:535:TYR:CD1	2.83	0.47
1:A:225:PHE:CE1	1:A:236:ARG:HG2	2.50	0.47
1:A:356:ARG:C	1:A:358:PRO:HD2	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:ALA:C	1:A:558:VAL:HG21	2.39	0.47
1:B:286:MET:HE3	1:B:286:MET:HB2	1.70	0.47
1:B:428:PHE:C	1:B:428:PHE:CD1	2.92	0.47
1:C:371:GLU:OE2	1:C:395:ARG:HD2	2.14	0.47
1:C:425:ALA:C	1:C:427:HIS:N	2.71	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:D:361:VAL:HG13	1:D:364:ASP:CG	2.40	0.47
1:D:559:LYS:O	1:D:563:LEU:HB2	2.15	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:E:365:LEU:O	1:E:368:LEU:HB3	2.14	0.47
1:E:413:ARG:HA	1:E:577:LEU:HD21	1.91	0.47
1:E:528:GLY:HA2	1:E:530:TYR:CE2	2.50	0.47
1:A:361:VAL:CG1	1:A:364:ASP:HB2	2.45	0.47
1:A:445:ARG:C	1:A:447:LEU:N	2.73	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:C:172:VAL:O	1:C:213:ALA:HB1	2.15	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: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:D:199:GLY:O	1:D:361:VAL:CG2	2.63	0.47
1:D:308:ASP:OD1	1:D:310:ALA:N	2.46	0.47
1:D:344:LEU:HA	1:D:383:LYS:CG	2.44	0.47
1:E:428:PHE:HE1	1:E:432:ALA:HA	1.67	0.47
1:F:319:ARG:CG	1:F:319:ARG:NH1	2.66	0.47
1:A:359:GLY:HA3	1:A:360:PHE:CG	2.50	0.46
1:A:450:MET:O	1:A:454:ARG:HB3	2.15	0.46
1:A:596:LEU:HG	1:A:597:GLU:H	1.80	0.46
1:B:225:PHE:CD2	1:B:225:PHE:N	2.81	0.46
1:C:300:ALA:O	1:C:301:THR:HG22	2.15	0.46
1:C:387:LYS:CA	1:C:390:GLU:HB2	2.44	0.46
1:D:241:PHE:C	1:D:243:THR:N	2.71	0.46
1:D:458:LEU:HD11	1:D:460:TRP:HB3	1.96	0.46
1:E:410:ARG:HA	1:E:413:ARG:HB3	1.97	0.46
1:E:449:PHE:CE2	1:E:496:GLN:NE2	2.83	0.46
1:F:567:GLU:O	1:F:568:VAL:C	2.59	0.46
1:A:292:ASP:OD2	1:B:227:GLU:OE1	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:ALA:HB1	1:F:181:PHE:CD1	2.50	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:B:336:ARG:O	1:B:339:ALA:N	2.23	0.46
1:B:469:ILE:HG23	1:B:497:ALA:HB1	1.98	0.46
1:B:505:ILE:HG23	1:B:514:PHE:CD2	2.50	0.46
1:B:506:THR:OG1	1:B:520:ALA:HB3	2.15	0.46
1:C:147:LEU:HD23	1:C:217:PHE:CB	2.44	0.46
1:C:182:HIS:CD2	1:C:182:HIS:H	2.32	0.46
1:C:210:ALA:O	1:C:214:ARG:HA	2.15	0.46
1:C:352:LEU:HD11	1:C:356:ARG:HH21	1.76	0.46
1:C:583:THR:HG22	1:C:586:GLU:OE1	2.15	0.46
1:D:345:ALA:CB	1:D:383:LYS:HE3	2.36	0.46
1:D:379:GLU:OE1	1:D:381:ARG:NE	2.48	0.46
1:D:452:PRO:O	1:D:456:ASP:CG	2.59	0.46
1:E:348:VAL:O	1:E:348:VAL:HG12	2.14	0.46
1:E:356:ARG:C	1:E:358:PRO:HD2	2.39	0.46
1:E:357:THR:HG1	1:E:360:PHE:CB	2.28	0.46
1:F:154:THR:HG23	1:F:156:LYS:HB3	1.96	0.46
1:F:355:LYS:HZ1	1:F:578:GLU:HG3	1.79	0.46
1:F:455:GLU:O	1:F:457:MET:N	2.48	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:A:358:PRO:CA	1:A:359:GLY:C	2.87	0.46
1:B:336:ARG:O	1:B:338:HIS:N	2.48	0.46
1:B:563:LEU:O	1:B:566:ARG:HB3	2.15	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:C:361:VAL:O	1:C:365:LEU:HG	2.16	0.46
1:D:200:VAL:HG12	1:D:325:ALA:HB2	1.98	0.46
1:D:311:LEU:HA	1:D:316:ARG:CZ	2.45	0.46
1:D:352:LEU:O	1:D:355:LYS:HB2	2.16	0.46
1:D:477:ALA:O	1:D:478:ALA:C	2.58	0.46
1:D:517:VAL:CG2	1:D:518:ALA:N	2.78	0.46
1:D:572:VAL:HG11	1:D:587:PHE:HE1	1.81	0.46
1:E:312:LEU:HD21	1:E:320:GLN:OE1	2.16	0.46
1:F:428:PHE:HD1	1:F:428:PHE:C	2.24	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:F:572:VAL:HG11	1:F:587:PHE:HE1	1.80	0.46
1:A:282:LEU:O	1:A:286:MET:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:ARG:HH12	1:F:170:GLU:HB2	1.80	0.46
1:A:507:GLU:HB2	1:A:520:ALA:HB3	1.98	0.46
1:B:215:VAL:O	1:B:216:PRO:C	2.55	0.46
1:B:297:VAL:CG1	1:B:317:PHE:CE1	2.98	0.46
1:B:332:GLU:CD	1:B:351:ALA:HA	2.41	0.46
1:B:469:ILE:HG22	1:B:473:LEU:HD12	1.96	0.46
1:C:282:LEU:HG	1:C:283:LEU:HD12	1.97	0.46
1:C:313:ARG:NH1	1:C:526:TYR:C	2.66	0.46
1:C:566:ARG:O	1:C:567:GLU:C	2.56	0.46
1:D:159:ALA:HA	1:D:333:GLN:HE21	1.80	0.46
1:D:411:ASP:O	1:D:414:ILE:HG13	2.16	0.46
1:D:571:ARG:HH12	1:D:593:GLY:N	2.13	0.46
1:E:249:PRO:HB3	1:E:294:ALA:HB3	1.98	0.46
1:E:289:PHE:C	1:E:290:GLU:CD	2.84	0.46
1:E:436:HIS:HB3	1:E:584:ALA:CB	2.45	0.46
1:F:412:ARG:O	1:F:413:ARG:C	2.59	0.46
1:F:467:ASP:O	1:F:471:VAL:HG13	2.16	0.46
1:A:253:PHE:HA	1:A:298:MET:O	2.16	0.46
1:A:373:ALA:HA	1:A:384:ILE:CD1	2.46	0.46
1:B:236:ARG:O	1:B:237:VAL:C	2.59	0.46
1:C:190:LYS:CD	1:C:289:PHE:CE1	2.87	0.46
1:C:361:VAL:CG1	1:C:364:ASP:HB2	2.45	0.46
1:D:399:LEU:O	1:D:402:LYS:HB3	2.16	0.46
1:D:476:ARG:NH1	1:D:487:THR:HG21	2.30	0.46
1:E:155:PHE:CZ	1:E:209:VAL:HG22	2.49	0.46
1:E:361:VAL:CG1	1:E:364:ASP:HB2	2.46	0.46
1:F:204:HIS:CD2	2:F:2001:ADP:H2'	2.50	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:A:449:PHE:HE2	1:A:496:GLN:HE21	1.60	0.46
1:A:481:ILE:HG22	1:A:482:VAL:N	2.31	0.46
1:B:228:MET:SD	1:B:232:VAL:CG1	3.04	0.46
1:B:494:PHE:O	1:B:496:GLN:N	2.48	0.46
1:C:218:ILE:HG12	1:C:218:ILE:H	1.64	0.46
1:C:407:LEU:HA	1:C:411:ASP:HB2	1.97	0.46
1:D:155:PHE:O	1:D:156:LYS:C	2.59	0.46
1:D:201:GLY:O	1:D:204:HIS:HB3	2.16	0.46
1:D:241:PHE:CZ	1:D:285:GLU:OE2	2.67	0.46
1:D:242:GLU:HA	1:D:245:LYS:CB	2.43	0.46
1:D:329:LYS:CG	1:D:330:GLY:N	2.78	0.46
1:D:349:ASP:C	1:D:351:ALA:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:242:GLU:HA	1:F:245:LYS:CB	2.45	0.46
1:F:438:VAL:CG2	1:F:439:THR:N	2.79	0.46
1:F:454:ARG:HH11	1:F:454:ARG:HA	1.80	0.46
1:A:215:VAL:HG22	1:A:216:PRO:N	2.30	0.46
1:A:357:THR:C	1:A:360:PHE:HD1	2.24	0.46
1:A:408:SER:HB2	1:A:409:PRO:CD	2.41	0.46
1:A:503:ARG:CG	1:A:508:TRP:CE3	2.99	0.46
1:B:328:VAL:HG22	1:B:355:LYS:CE	2.38	0.46
1:B:400:PRO:O	1:B:403:LYS:N	2.49	0.46
1:C:308:ASP:OD1	1:C:310:ALA:CB	2.64	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:C:549:ARG:O	1:C:550:LEU:C	2.58	0.46
1:D:202:LYS:N	2:D:2001:ADP:O1A	2.49	0.46
1:D:455:GLU:O	1:D:455:GLU:HG2	2.16	0.46
1:D:521:VAL:HG23	1:D:532:VAL:CG1	2.42	0.46
1:E:311:LEU:HD23	1:E:311:LEU:HA	1.68	0.46
1:F:256:GLU:O	1:F:256:GLU:CG	2.62	0.46
1:A:147:LEU:C	1:A:147:LEU:HD12	2.40	0.46
1:A:312:LEU:HD21	1:A:320:GLN:OE1	2.16	0.46
1:A:410:ARG:CG	1:A:411:ASP:N	2.77	0.46
1:A:523:GLU:O	1:A:529:GLY:HA2	2.16	0.46
1:B:314:PRO:HA	1:B:318:ASP:OD2	2.16	0.46
1:B:329:LYS:CG	1:B:330:GLY:N	2.78	0.46
1:B:384:ILE:CG2	1:B:385:THR:N	2.79	0.46
1:B:443:ARG:O	1:B:445:ARG:N	2.49	0.46
1:D:207:ARG:O	1:D:210:ALA:N	2.49	0.46
1:D:585:GLU:O	1:D:587:PHE:N	2.49	0.46
1:E:238:ARG:O	1:E:241:PHE:N	2.48	0.46
1:E:358:PRO:CA	1:E:359:GLY:C	2.88	0.46
1:E:469:ILE:HD11	1:E:500:LEU:HB3	1.98	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: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:F:571:ARG:O	1:F:575:THR:HG23	2.16	0.46
1:A:159:ALA:HB1	1:A:333:GLN:HB3	1.97	0.46
1:A:503:ARG:HG2	1:A:508:TRP:CE3	2.51	0.46
1:B:241:PHE:C	1:B:243:THR:N	2.71	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:GLU:HA	1:B:245:LYS:CB	2.42	0.46
1:B:454:ARG:HA	1:B:454:ARG:HH11	1.81	0.46
1:C:192:VAL:O	1:C:298:MET:HA	2.16	0.46
1:C:262:ARG:HG2	1:C:275:ARG:NH2	2.09	0.46
1:C:277:GLN:HG3	1:C:278:THR:N	2.28	0.46
1:C:445:ARG:C	1:C:447:LEU:N	2.74	0.46
1:C:462:ARG:HG3	1:C:466:LEU:HD11	1.97	0.46
1:D:165:LYS:NZ	1:D:168:LEU:CD2	2.79	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: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:207:ARG:CZ	1:E:207:ARG:CB	2.91	0.46
1:E:520:ALA:HA	1:E:533:ARG:HG2	1.96	0.46
1:E:538:GLU:O	1:E:539:THR:C	2.59	0.46
1:F:241:PHE:C	1:F:243:THR:N	2.72	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:A:570:GLU:O	1:A:571:ARG:C	2.58	0.46
1:B:165:LYS:HZ2	1:B:168:LEU:CD2	2.28	0.46
1:B:301:THR:HG23	1:B:303:ARG:H	1.81	0.46
1:C:212:GLU:C	1:C:214:ARG:HB2	2.41	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:D:349:ASP:C	1:D:350:LEU:HG	2.40	0.46
1:D:589:ARG:O	1:D:590:VAL:C	2.58	0.46
1:E:173:GLU:CA	1:E:176:LYS:HG3	2.36	0.46
1:E:441:VAL:O	1:E:441:VAL:CG1	2.61	0.46
1:F:236:ARG:O	1:F:237:VAL:C	2.58	0.46
1:F:274:GLU:O	1:F:275:ARG:C	2.59	0.46
1:F:329:LYS:CG	1:F:330:GLY:N	2.79	0.46
1:F:447:LEU:O	1:F:449:PHE:N	2.49	0.46
1:A:155:PHE:HZ	1:A:209:VAL:CG2	2.29	0.45
1:A:163:GLU:O	1:A:164:ALA:C	2.59	0.45
1:A:192:VAL:N	1:A:297:VAL:O	2.43	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:520:ALA:HA	1:A:533:ARG:HG2	1.98	0.45
1:B:468:GLN:O	1:B:469:ILE:C	2.59	0.45
1:B:567:GLU:O	1:B:568:VAL:C	2.59	0.45
1:C:228:MET:HG3	1:C:236:ARG:NH2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:289:PHE:C	1:C:290:GLU:CD	2.83	0.45
1:C:291:LYS:O	1:C:292:ASP:C	2.59	0.45
1:C:459:HIS:CE1	1:D:411:ASP:HB3	2.51	0.45
1:C:503:ARG:CD	1:C:508:TRP:CE2	2.95	0.45
1:D:476:ARG:CZ	1:D:487:THR:HG21	2.46	0.45
1:D:537:GLU:O	1:D:540:ALA:HB3	2.16	0.45
1:D:564:GLU:C	1:D:566:ARG:N	2.64	0.45
1:D:594:LEU:HD23	1:D:594:LEU:C	2.41	0.45
1:E:236:ARG:C	1:E:238:ARG:N	2.70	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:576:LEU:O	1:E:577:LEU:C	2.59	0.45
1:F:238:ARG:HA	1:F:241:PHE:HE2	1.81	0.45
1:F:441:VAL:O	1:F:442:PRO:C	2.58	0.45
1:A:328:VAL:HG12	1:A:329:LYS:N	2.30	0.45
1:B:175:LEU:O	1:B:249:PRO:HG2	2.15	0.45
1:B:523:GLU:OE2	1:C:264:ARG:NH2	2.50	0.45
1:C:346:GLU:CD	1:C:347:ASP:N	2.72	0.45
1:D:354:ALA:O	1:D:357:THR:HG23	2.15	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:F:384:ILE:HG22	1:F:385:THR:N	2.30	0.45
1:F:424:LEU:O	1:F:425:ALA:C	2.60	0.45
1:F:428:PHE:CD1	1:F:432:ALA:HB3	2.50	0.45
1:F:571:ARG:HH12	1:F:593:GLY:N	2.14	0.45
1:A:182:HIS:HD1	1:A:291:LYS:HB2	1.81	0.45
1:A:443:ARG:O	1:A:443:ARG:HG2	2.16	0.45
1:A:506:THR:CG2	1:A:543:ILE:HD13	2.46	0.45
1:B:470:ALA:O	1:B:474:ALA:HB2	2.16	0.45
1:B:492:ASN:O	1:B:493:ASP:C	2.59	0.45
1:C:300:ALA:O	1:C:301:THR:CG2	2.64	0.45
1:C:372:ALA:CB	1:C:389:LEU:HD23	2.47	0.45
1:D:215:VAL:HG21	1:D:249:PRO:C	2.41	0.45
1:D:379:GLU:OE1	1:D:381:ARG:CD	2.65	0.45
1:D:468:GLN:O	1:D:469:ILE:C	2.58	0.45
1:E:359:GLY:HA3	1:E:360:PHE:CG	2.51	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:E:469:ILE:HG13	1:E:500:LEU:HD23	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:517:VAL:HG23	1:F:498:THR:OG1	2.16	0.45
1:E:552:GLU:O	1:E:555:TYR:HB3	2.16	0.45
1:F:274:GLU:HA	1:F:277:GLN:HE21	1.80	0.45
1:F:336:ARG:O	1:F:337:ILE:C	2.58	0.45
1:F:357:THR:HB	1:F:360:PHE:CD2	2.52	0.45
1:F:511:HIS:O	1:F:512:PRO:O	2.34	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:B:230:VAL:C	1:B:232:VAL:H	2.24	0.45
1:B:459:HIS:HD1	1:B:459:HIS:C	2.15	0.45
1:B:483:PHE:C	1:B:485:ASP:H	2.24	0.45
1:B:589:ARG:CZ	1:B:596:LEU:HD22	2.46	0.45
1:C:171:ILE:O	1:C:172:VAL:C	2.59	0.45
1:C:198:PRO:HD3	1:C:302:ASN:HD21	1.81	0.45
1:C:222:GLY:O	1:C:225:PHE:HB2	2.17	0.45
1:C:410:ARG:O	1:C:411:ASP:C	2.58	0.45
1:C:438:VAL:HG22	1:C:582:LEU:HB2	1.99	0.45
1:D:155:PHE:C	1:D:157:ASP:N	2.69	0.45
1:D:261:GLY:O	1:D:308:ASP:HB3	2.16	0.45
1:D:449:PHE:CZ	1:D:496:GLN:OE1	2.69	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: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:165:LYS:O	1:F:167:GLU:N	2.50	0.45
1:F:165:LYS:NZ	1:F:205:LEU:CB	2.68	0.45
1:F:384:ILE:CG2	1:F:385:THR:N	2.79	0.45
1:A:218:ILE:HG12	1:A:218:ILE:H	1.65	0.45
1:A:449:PHE:N	1:A:449:PHE:HD2	2.11	0.45
1:A:528:GLY:HA2	1:A:530:TYR:CE2	2.52	0.45
1:B:184:MET:O	1:C:342:LYS:CD	2.63	0.45
1:B:241:PHE:CZ	1:B:285:GLU:OE2	2.69	0.45
1:B:329:LYS:O	1:B:332:GLU:HB3	2.16	0.45
1:B:410:ARG:O	1:B:413:ARG:CB	2.65	0.45
1:B:503:ARG:HG2	1:B:508:TRP:CZ2	2.51	0.45
1:C:381:ARG:CG	1:C:381:ARG:NH1	2.79	0.45
1:C:459:HIS:HE1	1:D:411:ASP:CB	2.29	0.45
1:C:464:ARG:O	1:C:465:LEU:C	2.57	0.45
1:C:491:GLU:O	1:C:492:ASN:C	2.58	0.45
1:C:519:TYR:CA	1:C:533:ARG:CZ	2.95	0.45
1:D:441:VAL:O	1:D:442:PRO:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:189:PRO:HD3	1:E:319:ARG:HH11	1.82	0.45
1:E:461:SER:O	1:E:462:ARG:C	2.60	0.45
1:F:260:VAL:C	1:F:279:LEU:HD11	2.38	0.45
1:F:381:ARG:NH2	1:F:388:ASP:OD2	2.50	0.45
1:F:538:GLU:C	1:F:540:ALA:N	2.72	0.45
1:A:422:HIS:O	1:A:423:ALA:C	2.59	0.45
1:A:574:GLU:OE1	1:A:575:THR:N	2.49	0.45
1:B:175:LEU:O	1:B:249:PRO:HB2	2.17	0.45
1:B:452:PRO:O	1:B:456:ASP:CG	2.60	0.45
1:B:454:ARG:HH21	1:B:526:TYR:HA	1.81	0.45
1:C:345:ALA:HA	1:C:383:LYS:HD3	1.97	0.45
1:D:257:ILE:O	1:D:258:ASP:C	2.60	0.45
1:D:350:LEU:O	1:D:353:LEU:N	2.50	0.45
1:E:200:VAL:N	2:E:1001:ADP:O1A	2.50	0.45
1:F:162:GLU:OE1	1:F:162:GLU:CA	2.64	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:460:TRP:CD1	1:F:464:ARG:HG2	2.52	0.45
1:F:523:GLU:O	1:F:530:TYR:N	2.43	0.45
1:F:582:LEU:CD2	1:F:590:VAL:HG21	2.42	0.45
1:A:212:GLU:O	1:A:214:ARG:CB	2.65	0.45
1:A:381:ARG:CG	1:A:381:ARG:NH1	2.80	0.45
1:A:464:ARG:NH1	1:A:464:ARG:HG2	2.32	0.45
1:B:342:LYS:HA	1:B:342:LYS:HD2	1.60	0.45
1:B:508:TRP:O	1:B:509:GLY:C	2.58	0.45
1:B:510:MET:O	1:B:512:PRO:CD	2.63	0.45
1:C:236:ARG:HG2	1:C:236:ARG:NH1	2.12	0.45
1:C:346:GLU:OE1	1:C:347:ASP:N	2.45	0.45
1:C:361:VAL:HG12	1:C:364:ASP:HB2	1.99	0.45
1:D:175:LEU:O	1:D:249:PRO:HB2	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:336:ARG:HD3	1:D:336:ARG:HA	1.51	0.45
1:D:393:ALA:O	1:D:397:MET:HB3	2.17	0.45
1:D:443:ARG:O	1:D:445:ARG:N	2.50	0.45
1:D:478:ALA:O	1:D:479:GLU:C	2.58	0.45
1:D:503:ARG:NH2	1:D:522:ARG:CZ	2.80	0.45
1:E:286:MET:CG	1:E:316:ARG:HG2	2.45	0.45
1:E:453:ARG:NH2	1:E:464:ARG:CZ	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:470:ALA:HB1	1:E:558:VAL:CG2	2.38	0.45
1:F:349:ASP:C	1:F:350:LEU:HG	2.41	0.45
1:A:236:ARG:HH11	1:A:236:ARG:CB	2.29	0.45
1:A:361:VAL:HG12	1:A:364:ASP:HB2	1.99	0.45
1:A:519:TYR:HB3	1:A:535:TYR:HD2	1.82	0.45
1:B:312:LEU:HD23	1:B:312:LEU:O	2.16	0.45
1:C:462:ARG:HH12	1:C:511:HIS:H	1.64	0.45
1:C:484:ASP:C	1:C:486:VAL:H	2.23	0.45
1:D:238:ARG:O	1:D:239:ASP:C	2.58	0.45
1:D:332:GLU:CD	1:D:351:ALA:HA	2.42	0.45
1:D:424:LEU:O	1:D:425:ALA:C	2.60	0.45
1:D:459:HIS:HD1	1:D:459:HIS:C	2.11	0.45
1:E:334:ILE:HD11	2:E:1001:ADP:N6	2.32	0.45
1:E:424:LEU:HD22	1:E:569:LEU:HA	1.99	0.45
1:E:447:LEU:HB2	1:E:496:GLN:HE22	1.82	0.45
1:E:572:VAL:O	1:E:573:ALA:C	2.60	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:F:428:PHE:CE1	1:F:433:ASP:N	2.84	0.45
1:F:459:HIS:HD1	1:F:459:HIS:C	2.17	0.45
1:A:352:LEU:HD11	1:A:356:ARG:HH21	1.74	0.45
1:B:428:PHE:HE1	1:B:432:ALA:C	2.23	0.45
1:B:438:VAL:CG2	1:B:439:THR:N	2.80	0.45
1:B:536:SER:HB2	1:C:537:GLU:OE2	2.17	0.45
1:B:585:GLU:C	1:B:587:PHE:N	2.71	0.45
1:B:594:LEU:HD23	1:B:594:LEU:C	2.42	0.45
1:C:159:ALA:HB1	1:C:333:GLN:HB3	1.99	0.45
1:C:174:PHE:O	1:C:177:ASN:C	2.60	0.45
1:C:191:GLY:CA	1:C:297:VAL:CG2	2.94	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:349:ASP:OD1	1:C:349:ASP:C	2.59	0.45
1:D:157:ASP:O	1:D:158:VAL:HG23	2.16	0.45
1:D:274:GLU:O	1:D:275:ARG:C	2.60	0.45
1:E:372:ALA:CB	1:E:389:LEU:HD23	2.47	0.45
1:E:407:LEU:H	1:E:407:LEU:HG	1.57	0.45
1:E:548:ARG:NH2	1:E:552:GLU:OE1	2.46	0.45
1:A:204:HIS:CD2	2:A:1001:ADP:C2	3.04	0.45
1:A:425:ALA:C	1:A:427:HIS:N	2.72	0.45
1:A:442:PRO:HG2	1:A:443:ARG:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:ARG:HG3	1:A:504:MET:N	2.28	0.45
1:A:527:LEU:HD12	1:A:527:LEU:O	2.16	0.45
1:A:534:GLN:N	1:A:534:GLN:CD	2.75	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:B:349:ASP:C	1:B:350:LEU:HG	2.41	0.45
1:B:517:VAL:HG13	1:B:519:TYR:CZ	2.52	0.45
1:B:569:LEU:O	1:B:570:GLU:C	2.60	0.45
1:C:163:GLU:O	1:C:164:ALA:C	2.59	0.45
1:C:271:GLY:O	1:C:275:ARG:NE	2.50	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:C:454:ARG:C	1:C:454:ARG:HD3	2.42	0.45
1:D:197:PRO:HD2	1:D:200:VAL:CG1	2.45	0.45
1:D:385:THR:O	1:D:386:MET:C	2.60	0.45
1:D:505:ILE:HG23	1:D:514:PHE:CD2	2.52	0.45
1:E:286:MET:CG	1:E:316:ARG:CG	2.94	0.45
1:E:291:LYS:O	1:E:292:ASP:C	2.60	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:F:428:PHE:C	1:F:428:PHE:CD1	2.93	0.45
1:F:468:GLN:O	1:F:471:VAL:N	2.49	0.45
1:F:508:TRP:O	1:F:510:MET:HG3	2.17	0.45
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:A:582:LEU:CD2	1:A:587:PHE:HA	2.34	0.44
1:B:150:ALA:HA	1:B:151:PRO:HD2	1.84	0.44
1:B:207:ARG:CB	1:B:217:PHE:CZ	2.96	0.44
1:B:241:PHE:CE2	1:B:285:GLU:CD	2.95	0.44
1:B:354:ALA:O	1:B:357:THR:HG23	2.17	0.44
1:C:337:ILE:CD1	1:C:338:HIS:CD2	3.00	0.44
1:C:458:LEU:C	1:C:458:LEU:HD12	2.42	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:D:307:LEU:CD1	1:D:307:LEU:H	2.31	0.44
1:D:332:GLU:HB2	1:D:354:ALA:HB2	1.98	0.44
1:D:334:ILE:C	1:D:336:ARG:N	2.75	0.44
1:E:153:VAL:HG13	1:E:157:ASP:CB	2.47	0.44
1:E:225:PHE:HZ	1:E:278:THR:HB	1.66	0.44
1:E:228:MET:HG3	1:E:236:ARG:NH2	2.31	0.44
1:E:236:ARG:O	1:E:239:ASP:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:237:VAL:HG11	1:E:281:GLN:CB	2.27	0.44
1:E:263:LYS:CG	1:E:264:ARG:H	2.28	0.44
1:E:371:GLU:CD	1:E:395:ARG:NH1	2.76	0.44
1:E:463:LYS:O	1:E:464:ARG:C	2.60	0.44
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:F:158:VAL:HG11	1:F:205:LEU:HD11	1.98	0.44
1:F:200:VAL:HA	1:F:361:VAL:HG23	1.99	0.44
1:F:314:PRO:HA	1:F:318:ASP:OD2	2.16	0.44
1:F:332:GLU:CD	1:F:351:ALA:HA	2.41	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:A:220:ALA:O	1:A:254:ILE:HA	2.16	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:A:382:ARG:CG	1:A:383:LYS:H	2.29	0.44
1:A:438:VAL:HG22	1:A:582:LEU:HB2	2.00	0.44
1:A:467:ASP:HA	1:A:557:ARG:NH2	2.32	0.44
1:B:334:ILE:O	1:B:335:LEU:C	2.60	0.44
1:B:441:VAL:O	1:B:442:PRO:C	2.59	0.44
1:B:523:GLU:CD	1:C:264:ARG:NH2	2.75	0.44
1:B:566:ARG:O	1:B:569:LEU:HB3	2.17	0.44
1:C:147:LEU:HB3	1:C:217:PHE:O	2.17	0.44
1:C:253:PHE:CD2	1:C:253:PHE:C	2.95	0.44
1:C:312:LEU:HD21	1:C:320:GLN:OE1	2.16	0.44
1:D:193:LEU:HB3	1:D:317:PHE:HD2	1.82	0.44
1:D:338:HIS:CB	1:D:369:LEU:HD11	2.47	0.44
1:D:525:THR:HG22	1:D:526:TYR:CD2	2.52	0.44
1:D:569:LEU:O	1:D:570:GLU:C	2.60	0.44
1:E:192:VAL:N	1:E:297:VAL:O	2.38	0.44
1:E:233:GLY:O	1:E:236:ARG:CG	2.61	0.44
1:E:387:LYS:CA	1:E:390:GLU:HB2	2.44	0.44
1:E:454:ARG:HG3	1:E:455:GLU:N	2.32	0.44
1:F:238:ARG:HH11	1:F:238:ARG:CG	2.30	0.44
1:F:238:ARG:C	1:F:240:LEU:N	2.74	0.44
1:F:385:THR:O	1:F:386:MET:C	2.60	0.44
1:A:147:LEU:HD23	1:A:217:PHE:CB	2.47	0.44
1:A:263:LYS:CG	1:A:264:ARG:H	2.27	0.44
1:A:305:ASP:OD2	1:A:447:LEU:HD13	2.16	0.44
1:B:184:MET:HE2	1:B:184:MET:HB2	1.91	0.44
1:B:343:PRO:HG2	1:B:383:LYS:CA	2.40	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:467:ASP:CG	1:C:557:ARG:HH22	2.24	0.44
1:D:170:GLU:HG2	1:D:171:ILE:N	2.32	0.44
1:D:428:PHE:CZ	1:D:433:ASP:N	2.85	0.44
1:D:428:PHE:CD1	1:D:432:ALA:HB3	2.52	0.44
1:D:452:PRO:O	1:D:456:ASP:CA	2.65	0.44
1:E:273:ASP:OD1	1:E:273:ASP:C	2.60	0.44
1:E:277:GLN:HG3	1:E:278:THR:N	2.31	0.44
1:E:587:PHE:CD2	1:E:588:GLN:N	2.85	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:F:312:LEU:O	1:F:312:LEU:HD23	2.17	0.44
1:A:182:HIS:CB	1:A:291:LYS:HD2	2.20	0.44
1:A:451:MET:HB2	1:A:452:PRO:CD	2.47	0.44
1:B:231:GLY:H	1:B:277:GLN:HE22	1.65	0.44
1:B:274:GLU:O	1:B:275:ARG:C	2.59	0.44
1:B:353:LEU:O	1:B:357:THR:CG2	2.65	0.44
1:B:548:ARG:NH1	1:B:548:ARG:HG2	2.32	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:HD2	1:C:533:ARG:HA	1.91	0.44
1:D:168:LEU:O	1:D:171:ILE:N	2.51	0.44
1:D:454:ARG:HA	1:D:454:ARG:HH11	1.83	0.44
1:D:533:ARG:HG3	1:D:533:ARG:NH1	2.21	0.44
1:E:198:PRO:HD3	1:E:302:ASN:HD21	1.82	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:F:311:LEU:C	1:F:311:LEU:CD1	2.87	0.44
1:F:382:ARG:HD2	1:F:382:ARG:HA	1.08	0.44
1:F:503:ARG:CG	1:F:508:TRP:CZ2	3.00	0.44
1:F:525:THR:CG2	1:F:526:TYR:CD2	2.98	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:A:340:ARG:C	1:A:342:LYS:N	2.57	0.44
1:A:548:ARG:NH1	1:F:513:GLU:O	2.50	0.44
1:B:238:ARG:NH1	1:B:239:ASP:CA	2.67	0.44
1:B:257:ILE:O	1:B:258:ASP:C	2.61	0.44
1:B:538:GLU:O	1:B:541:LYS:N	2.50	0.44
1:C:509:GLY:O	1:D:476:ARG:NH2	2.36	0.44
1:D:230:VAL:C	1:D:232:VAL:H	2.25	0.44
1:D:353:LEU:O	1:D:357:THR:CG2	2.65	0.44
1:E:225:PHE:CE1	1:E:233:GLY:HA3	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:410:ARG:O	1:E:411:ASP:C	2.60	0.44
1:F:147:LEU:HD13	1:F:149:GLU:OE1	2.18	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:F:476:ARG:CZ	1:F:487:THR:HG21	2.47	0.44
1:F:536:SER:O	1:F:537:GLU:C	2.61	0.44
1:A:236:ARG:O	1:A:239:ASP:N	2.51	0.44
1:A:324:ASP:C	1:A:326:PRO:HD2	2.43	0.44
1:A:503:ARG:CD	1:A:508:TRP:CE2	2.98	0.44
1:B:358:PRO:O	1:B:359:GLY:C	2.61	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:C:206:ALA:CB	1:C:217:PHE:HZ	2.31	0.44
1:C:382:ARG:HH11	1:C:383:LYS:HB2	1.83	0.44
1:C:465:LEU:CD2	1:C:508:TRP:CZ3	2.99	0.44
1:C:572:VAL:O	1:C:573:ALA:C	2.59	0.44
1:D:231:GLY:H	1:D:277:GLN:HE22	1.65	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: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: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:E:481:ILE:HG22	1:E:482:VAL:N	2.31	0.44
1:E:511:HIS:O	1:E:512:PRO:O	2.36	0.44
1:E:588:GLN:O	1:E:591:VAL:CB	2.55	0.44
1:F:286:MET:HE2	1:F:315:GLY:O	2.17	0.44
1:F:373:ALA:CA	1:F:384:ILE:HD11	2.45	0.44
1:F:526:TYR:O	1:F:528:GLY:CA	2.66	0.44
1:F:595:PRO:C	1:F:596:LEU:HD12	2.43	0.44
1:A:237:VAL:HG13	1:A:238:ARG:N	2.32	0.44
1:A:410:ARG:HA	1:A:413:ARG:HB3	2.00	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:B:263:LYS:HE2	1:C:228:MET:HE2	1.99	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:C:449:PHE:CE2	1:C:496:GLN:CD	2.95	0.44
1:C:534:GLN:N	1:C:534:GLN:CD	2.75	0.44
1:D:301:THR:HG22	1:D:303:ARG:H	1.82	0.44
1:D:374:LEU:HD23	1:D:375:LEU:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:506:THR:OG1	1:D:520:ALA:HB3	2.17	0.44
1:E:413:ARG:O	1:E:577:LEU:HD21	2.18	0.44
1:E:484:ASP:C	1:E:486:VAL:H	2.25	0.44
1:E:491:GLU:O	1:E:492:ASN:C	2.61	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:F:525:THR:HG22	1:F:526:TYR:N	2.33	0.44
1:F:589:ARG:C	1:F:591:VAL:N	2.75	0.44
1:B:161:ALA:O	1:B:164:ALA:HB3	2.18	0.44
1:B:162:GLU:OE1	1:B:162:GLU:CA	2.66	0.44
1:B:355:LYS:NZ	1:B:578:GLU:O	2.51	0.44
1:B:355:LYS:HZ3	1:B:578:GLU:HG3	1.83	0.44
1:B:476:ARG:O	1:B:479:GLU:N	2.51	0.44
1:B:500:LEU:O	1:B:501:ALA:C	2.61	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:C:422:HIS:O	1:C:423:ALA:C	2.61	0.44
1:F:178:PRO:O	1:F:182:HIS:CE1	2.71	0.44
1:F:355:LYS:NZ	1:F:578:GLU:O	2.51	0.44
1:F:542:ARG:O	1:F:543:ILE:C	2.61	0.44
1:F:569:LEU:O	1:F:570:GLU:C	2.61	0.44
1:F:589:ARG:CZ	1:F:596:LEU:HD11	2.45	0.44
1:A:163:GLU:H	1:A:163:GLU:CD	2.08	0.44
1:A:192:VAL:O	1:A:298:MET:HA	2.18	0.44
1:A:378:ARG:NH2	1:F:170:GLU:HB2	2.28	0.44
1:A:397:MET:SD	1:A:406:VAL:HG11	2.58	0.44
1:A:467:ASP:O	1:A:471:VAL:HG23	2.18	0.44
1:A:493:ASP:O	1:A:496:GLN:CB	2.65	0.44
1:B:187:ARG:N	1:C:374:LEU:HD11	2.27	0.44
1:B:307:LEU:HD12	1:B:307:LEU:N	2.33	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:D:165:LYS:HZ2	1:D:168:LEU:HD23	1.83	0.44
1:D:236:ARG:O	1:D:237:VAL:C	2.60	0.44
1:D:286:MET:HG3	1:D:287:ASP:OD1	2.18	0.44
1:D:385:THR:H	1:D:388:ASP:CG	2.26	0.44
1:E:282:LEU:HG	1:E:283:LEU:HD12	2.00	0.44
1:E:298:MET:HE2	1:E:298:MET:HB3	1.75	0.44
1:E:450:MET:HG3	1:E:451:MET:H	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:301:THR:HG23	1:F:303:ARG:H	1.81	0.44
1:A:228:MET:CG	1:A:236:ARG:HH22	2.31	0.43
1:A:234:ALA:O	1:A:235:ALA:C	2.61	0.43
1:A:282:LEU:HG	1:A:283:LEU:HD12	2.00	0.43
1:A:349:ASP:OD1	1:A:349:ASP:C	2.61	0.43
1:A:462:ARG:HG3	1:A:466:LEU:HD11	1.99	0.43
1:A:566:ARG:O	1:A:569:LEU:N	2.51	0.43
1:B:155:PHE:C	1:B:157:ASP:N	2.74	0.43
1:B:174:PHE:CZ	1:B:294:ALA:CB	3.00	0.43
1:B:297:VAL:CG1	1:B:317:PHE:CZ	3.01	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:517:VAL:CG1	1:B:519:TYR:CZ	3.01	0.43
1:B:582:LEU:CD2	1:B:590:VAL:HG21	2.43	0.43
1:C:252:VAL:O	1:C:297:VAL:HA	2.18	0.43
1:C:311:LEU:HA	1:C:311:LEU:HD23	1.68	0.43
1:C:462:ARG:O	1:C:465:LEU:N	2.51	0.43
1:C:527:LEU:HD12	1:C:527:LEU:O	2.18	0.43
1:D:210:ALA:O	1:D:214:ARG:HA	2.18	0.43
1:D:286:MET:HB2	1:D:286:MET:HE3	1.77	0.43
1:D:355:LYS:HZ1	1:D:578:GLU:C	2.26	0.43
1:D:414:ILE:H	1:D:414:ILE:HG12	1.65	0.43
1:D:511:HIS:O	1:D:512:PRO:C	2.57	0.43
1:E:171:ILE:O	1:E:172:VAL:C	2.61	0.43
1:E:370:ASN:OD1	1:E:374:LEU:HD13	2.18	0.43
1:E:445:ARG:C	1:E:447:LEU:N	2.75	0.43
1:E:449:PHE:CB	1:E:468:GLN:HE21	2.28	0.43
1:F:343:PRO:HG2	1:F:383:LYS:CA	2.43	0.43
1:F:411:ASP:O	1:F:414:ILE:HG13	2.18	0.43
1:A:301:THR:C	1:A:303:ARG:H	2.26	0.43
1:B:159:ALA:HB1	1:B:333:GLN:HG3	1.98	0.43
1:B:352:LEU:HD21	1:B:386:MET:CE	2.48	0.43
1:C:153:VAL:HG13	1:C:157:ASP:CB	2.48	0.43
1:C:511:HIS:C	1:C:512:PRO:O	2.61	0.43
1:C:586:GLU:HG2	1:C:587:PHE:N	2.32	0.43
1:D:158:VAL:HG11	1:D:205:LEU:HD11	2.00	0.43
1:D:196:GLY:O	1:D:302:ASN:HA	2.17	0.43
1:D:297:VAL:CG1	1:D:317:PHE:CZ	3.01	0.43
1:D:370:ASN:OD1	1:D:370:ASN:C	2.61	0.43
1:D:412:ARG:O	1:D:413:ARG:C	2.60	0.43
1:D:538:GLU:HB2	1:E:541:LYS:NZ	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:567:GLU:O	1:D:568:VAL:C	2.60	0.43
1:D:585:GLU:C	1:D:587:PHE:N	2.75	0.43
1:E:503:ARG:CD	1:E:508:TRP:CE2	3.00	0.43
1:E:574:GLU:OE1	1:E:575:THR:N	2.51	0.43
1:F:358:PRO:O	1:F:359:GLY:C	2.61	0.43
1:F:453:ARG:HH12	1:F:495:ARG:NH2	2.08	0.43
1:F:562:LEU:O	1:F:563:LEU:C	2.60	0.43
1:A:397:MET:HG3	1:A:406:VAL:CG1	2.47	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:A:541:LYS:HD3	1:F:538:GLU:CB	2.48	0.43
1:A:587:PHE:HD2	1:A:588:GLN:N	2.15	0.43
1:B:237:VAL:HG21	1:B:281:GLN:HG3	1.98	0.43
1:B:261:GLY:O	1:B:308:ASP:HB3	2.18	0.43
1:B:393:ALA:O	1:B:397:MET:HB3	2.18	0.43
1:C:174:PHE:HB2	1:C:181:PHE:CZ	2.53	0.43
1:C:200:VAL:HG11	1:C:323:ILE:HG13	2.00	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:C:408:SER:O	1:C:410:ARG:N	2.45	0.43
1:D:194:LEU:HD23	1:D:323:ILE:CD1	2.49	0.43
1:D:307:LEU:HD12	1:D:307:LEU:N	2.32	0.43
1:D:352:LEU:HD21	1:D:386:MET:CE	2.48	0.43
1:E:196:GLY:C	1:E:202:LYS:NZ	2.76	0.43
1:F:194:LEU:HD23	1:F:323:ILE:CD1	2.48	0.43
1:F:241:PHE:CE2	1:F:285:GLU:CD	2.96	0.43
1:F:360:PHE:CE1	1:F:364:ASP:HB3	2.54	0.43
1:A:371:GLU:OE2	1:A:395:ARG:HD2	2.17	0.43
1:A:453:ARG:NH1	1:A:460:TRP:NE1	2.66	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:B:235:ALA:HA	1:B:238:ARG:NE	2.33	0.43
1:B:355:LYS:C	1:B:357:THR:N	2.76	0.43
1:B:436:HIS:O	1:B:437:LYS:CG	2.64	0.43
1:B:452:PRO:O	1:B:456:ASP:CA	2.67	0.43
1:C:292:ASP:HB2	1:D:227:GLU:CD	2.41	0.43
1:C:411:ASP:O	1:C:415:THR:OG1	2.28	0.43
1:C:443:ARG:O	1:C:443:ARG:HG2	2.18	0.43
1:C:574:GLU:O	1:C:575:THR:C	2.62	0.43
1:C:585:GLU:O	1:C:588:GLN:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:586:GLU:HA	1:C:589:ARG:CB	2.49	0.43
1:D:204:HIS:CD2	2:D:2001:ADP:H2'	2.53	0.43
1:D:391:GLU:O	1:D:392:ALA:C	2.60	0.43
1:D:468:GLN:O	1:D:471:VAL:N	2.51	0.43
1:D:508:TRP:O	1:D:509:GLY:C	2.62	0.43
1:D:589:ARG:CD	1:D:596:LEU:HD11	2.48	0.43
1:E:408:SER:O	1:E:410:ARG:N	2.48	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:F:173:GLU:O	1:F:174:PHE:C	2.60	0.43
1:F:175:LEU:O	1:F:249:PRO:CG	2.66	0.43
1:F:179:SER:HA	1:F:182:HIS:NE2	2.33	0.43
1:F:180:ARG:HH12	1:F:184:MET:CE	2.31	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:A:147:LEU:O	1:A:216:PRO:HB3	2.19	0.43
1:A:425:ALA:O	1:A:426:ALA:C	2.61	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:B:385:THR:O	1:B:386:MET:C	2.61	0.43
1:B:428:PHE:CZ	1:B:433:ASP:N	2.87	0.43
1:B:455:GLU:O	1:B:455:GLU:HG2	2.19	0.43
1:C:145:ARG:CB	1:C:145:ARG:HH11	2.30	0.43
1:C:327:ASP:OD1	1:C:329:LYS:N	2.51	0.43
1:C:382:ARG:HG3	1:C:383:LYS:CA	2.48	0.43
1:D:248:ALA:HB1	1:D:294:ALA:HB3	2.00	0.43
1:D:285:GLU:O	1:D:286:MET:C	2.58	0.43
1:D:428:PHE:CE1	1:D:433:ASP:N	2.87	0.43
1:D:558:VAL:HG12	1:D:559:LYS:N	2.32	0.43
1:E:228:MET:CG	1:E:236:ARG:HH22	2.31	0.43
1:E:327:ASP:OD1	1:E:329:LYS:N	2.51	0.43
1:F:230:VAL:C	1:F:232:VAL:H	2.26	0.43
1:F:334:ILE:O	1:F:335:LEU:C	2.61	0.43
1:F:342:LYS:HA	1:F:342:LYS:HD2	1.66	0.43
1:F:559:LYS:O	1:F:563:LEU:HB2	2.18	0.43
1:F:568:VAL:HG13	1:F:591:VAL:HA	2.00	0.43
1:A:227:GLU:CG	1:F:263:LYS:NZ	2.67	0.43
1:A:346:GLU:OE1	1:A:347:ASP:N	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:GLU:HG2	1:B:171:ILE:N	2.33	0.43
1:B:247:HIS:O	1:B:249:PRO:O	2.36	0.43
1:B:391:GLU:O	1:B:395:ARG:CB	2.66	0.43
1:B:559:LYS:O	1:B:563:LEU:HB2	2.18	0.43
1:C:188:ILE:HG22	1:C:190:LYS:H	1.84	0.43
1:C:344:LEU:HB3	1:C:348:VAL:HG11	2.00	0.43
1:C:357:THR:O	1:C:360:PHE:CD1	2.72	0.43
1:C:596:LEU:HG	1:C:597:GLU:N	2.34	0.43
1:D:155:PHE:C	1:D:155:PHE:CD1	2.96	0.43
1:D:177:ASN:OD1	1:D:180:ARG:CB	2.65	0.43
1:D:200:VAL:HA	1:D:361:VAL:HG23	2.01	0.43
1:E:361:VAL:O	1:E:365:LEU:HG	2.18	0.43
1:E:361:VAL:HG12	1:E:364:ASP:HB2	1.99	0.43
1:F:155:PHE:C	1:F:157:ASP:N	2.71	0.43
1:A:145:ARG:CB	1:A:145:ARG:HH11	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:A:462:ARG:O	1:A:463:LYS:C	2.61	0.43
1:B:399:LEU:O	1:B:402:LYS:HB3	2.19	0.43
1:C:162:GLU:O	1:C:163:GLU:C	2.62	0.43
1:C:462:ARG:HH11	1:C:510:MET:HB3	1.84	0.43
1:D:184:MET:HE2	1:D:184:MET:HB2	1.89	0.43
1:D:350:LEU:O	1:D:351:ALA:C	2.62	0.43
1:D:428:PHE:CE1	1:D:432:ALA:HB3	2.52	0.43
1:E:234:ALA:O	1:E:235:ALA:C	2.61	0.43
1:E:261:GLY:O	1:E:262:ARG:HB2	2.19	0.43
1:E:349:ASP:OD1	1:E:349:ASP:C	2.62	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: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:228:MET:SD	1:F:232:VAL:CG1	3.04	0.43
1:F:297:VAL:CG1	1:F:317:PHE:CZ	3.01	0.43
1:F:355:LYS:HD2	1:F:355:LYS:HA	1.46	0.43
1:A:189:PRO:C	1:A:191:GLY:H	2.27	0.43
1:A:332:GLU:O	1:A:335:LEU:HB2	2.19	0.43
1:A:408:SER:O	1:A:410:ARG:N	2.47	0.43
1:A:471:VAL:O	1:A:474:ALA:HB3	2.19	0.43
1:A:480:GLU:OE1	1:A:555:TYR:OH	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:MET:HE1	1:B:236:ARG:HD3	2.01	0.43
1:B:257:ILE:HG22	1:B:261:GLY:H	1.83	0.43
1:B:597:GLU:O	1:B:599:PRO:CD	2.66	0.43
1:C:462:ARG:O	1:C:463:LYS:C	2.62	0.43
1:C:503:ARG:HD2	1:C:508:TRP:CD2	2.52	0.43
1:D:334:ILE:O	1:D:335:LEU:C	2.61	0.43
1:D:342:LYS:HA	1:D:342:LYS:HD2	1.66	0.43
1:D:417:TYR:CZ	1:D:482:VAL:HG21	2.54	0.43
1:D:583:THR:HG22	1:D:586:GLU:OE1	2.19	0.43
1:E:177:ASN:HA	1:E:178:PRO:HD2	1.91	0.43
1:E:372:ALA:O	1:E:375:LEU:HB3	2.19	0.43
1:E:462:ARG:O	1:E:463:LYS:C	2.61	0.43
1:E:503:ARG:CG	1:E:508:TRP:CE3	3.02	0.43
1:E:541:LYS:O	1:E:542:ARG:C	2.59	0.43
1:F:376:ALA:C	1:F:381:ARG:CG	2.91	0.43
1:F:478:ALA:O	1:F:479:GLU:C	2.59	0.43
1:F:503:ARG:HA	1:F:503:ARG:HD3	1.58	0.43
1:F:570:GLU:O	1:F:571:ARG:C	2.62	0.43
1:A:196:GLY:C	1:A:202:LYS:NZ	2.77	0.43
1:A:200:VAL:HG13	1:A:323:ILE:HG13	2.00	0.43
1:A:378:ARG:NH2	1:F:170:GLU:CA	2.80	0.43
1:B:165:LYS:CE	1:B:205:LEU:HG	2.48	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:B:307:LEU:CD1	1:B:307:LEU:H	2.31	0.43
1:B:338:HIS:HB3	1:B:369:LEU:HD12	2.00	0.43
1:B:449:PHE:HZ	1:B:496:GLN:OE1	2.01	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:371:GLU:CG	1:C:392:ALA:HB1	2.40	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:D:235:ALA:HA	1:D:238:ARG:HD3	2.00	0.43
1:D:255:ASP:OD1	1:D:256:GLU:N	2.52	0.43
1:D:355:LYS:HA	1:D:355:LYS:HD2	1.44	0.43
1:D:568:VAL:HG11	1:D:591:VAL:HG13	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:344:LEU:HB3	1:E:348:VAL:HG11	1.99	0.43
1:E:438:VAL:HG22	1:E:582:LEU:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:445:ARG:O	1:E:447:LEU:N	2.52	0.43
1:E:549:ARG:O	1:E:550:LEU:C	2.62	0.43
1:F:349:ASP:C	1:F:351:ALA:H	2.27	0.43
1:F:458:LEU:HD11	1:F:460:TRP:HB3	2.01	0.43
1:F:477:ALA:O	1:F:478:ALA:C	2.61	0.43
1:F:585:GLU:O	1:F:587:PHE:N	2.52	0.43
1:A:337:ILE:CD1	1:A:338:HIS:CD2	3.01	0.43
1:A:372:ALA:CB	1:A:389:LEU:HD23	2.48	0.43
1:A:411:ASP:O	1:A:415:THR:OG1	2.29	0.43
1:A:453:ARG:NH1	1:A:460:TRP:HE1	2.16	0.43
1:B:169:LYS:O	1:B:172:VAL:HG22	2.19	0.43
1:B:215:VAL:CG2	1:B:216:PRO:CD	2.87	0.43
1:B:238:ARG:HH11	1:B:238:ARG:CB	2.32	0.43
1:B:238:ARG:O	1:B:239:ASP:C	2.59	0.43
1:B:382:ARG:HA	1:B:382:ARG:HD2	1.08	0.43
1:B:413:ARG:O	1:B:414:ILE:C	2.62	0.43
1:B:539:THR:O	1:B:543:ILE:HG13	2.18	0.43
1:C:348:VAL:O	1:C:348:VAL:HG12	2.18	0.43
1:C:460:TRP:HD1	1:C:464:ARG:NH1	2.13	0.43
1:C:480:GLU:OE1	1:C:555:TYR:OH	2.31	0.43
1:C:500:LEU:O	1:C:504:MET:HG2	2.19	0.43
1:D:203:THR:HG23	1:D:253:PHE:CE1	2.53	0.43
1:D:422:HIS:CD2	1:D:475:GLY:CA	3.02	0.43
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:E:163:GLU:O	1:E:164:ALA:C	2.60	0.43
1:E:400:PRO:HG2	1:E:405:LEU:CD1	2.44	0.43
1:E:479:GLU:OE2	1:E:487:THR:HA	2.19	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:A:171:ILE:O	1:A:172:VAL:C	2.60	0.42
1:A:308:ASP:OD1	1:A:310:ALA:CB	2.67	0.42
1:A:399:LEU:N	1:A:400:PRO:CD	2.83	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:188:ILE:HD13	1:B:188:ILE:HA	1.80	0.42
1:B:411:ASP:O	1:B:414:ILE:HG13	2.18	0.42
1:B:428:PHE:CE1	1:B:433:ASP:N	2.87	0.42
1:B:449:PHE:CE2	1:B:453:ARG:CZ	3.01	0.42
1:B:554:GLN:OE1	1:B:554:GLN:HA	2.19	0.42
1:C:263:LYS:CG	1:C:264:ARG:H	2.29	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:ARG:HD2	1:C:266:SER:CB	2.49	0.42
1:C:297:VAL:HG23	1:C:317:PHE:CE1	2.54	0.42
1:C:350:LEU:H	1:C:350:LEU:HG	1.48	0.42
1:C:371:GLU:CD	1:C:395:ARG:NH1	2.77	0.42
1:D:173:GLU:O	1:D:176:LYS:N	2.51	0.42
1:D:253:PHE:HA	1:D:298:MET:CB	2.46	0.42
1:D:518:ALA:CB	1:E:495:ARG:HA	2.48	0.42
1:E:147:LEU:HD21	1:E:151:PRO:CG	2.45	0.42
1:E:346:GLU:OE1	1:E:347:ASP:N	2.45	0.42
1:E:355:LYS:HA	1:E:355:LYS:HD3	1.88	0.42
1:E:493:ASP:N	1:E:493:ASP:OD1	2.50	0.42
1:E:527:LEU:O	1:E:530:TYR:OH	2.30	0.42
1:F:190:LYS:CD	1:F:289:PHE:CZ	3.02	0.42
1:F:301:THR:HG23	1:F:302:ASN:N	2.34	0.42
1:F:353:LEU:O	1:F:357:THR:CG2	2.66	0.42
1:A:153:VAL:HG13	1:A:157:ASP:CB	2.48	0.42
1:A:168:LEU:C	1:A:171:ILE:CD1	2.79	0.42
1:A:313:ARG:NH1	1:A:526:TYR:C	2.70	0.42
1:B:147:LEU:HD13	1:B:149:GLU:OE1	2.19	0.42
1:B:216:PRO:HG3	1:B:247:HIS:CE1	2.53	0.42
1:B:253:PHE:HA	1:B:298:MET:CB	2.47	0.42
1:B:321:ILE:HD12	1:B:321:ILE:HA	1.82	0.42
1:C:172:VAL:HG22	1:C:173:GLU:N	2.34	0.42
1:C:236:ARG:O	1:C:239:ASP:N	2.52	0.42
1:C:236:ARG:C	1:C:238:ARG:N	2.71	0.42
1:C:334:ILE:HD11	2:C:1001:ADP:N6	2.34	0.42
1:C:358:PRO:CA	1:C:359:GLY:C	2.84	0.42
1:C:410:ARG:CG	1:C:411:ASP:N	2.79	0.42
1:C:508:TRP:HD1	1:D:491:GLU:HG2	1.84	0.42
1:D:159:ALA:CA	1:D:333:GLN:HE21	2.32	0.42
1:D:187:ARG:H	1:E:374:LEU:HD11	1.82	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:E:480:GLU:OE1	1:E:555:TYR:OH	2.29	0.42
1:F:175:LEU:O	1:F:249:PRO:HB2	2.19	0.42
1:F:180:ARG:HH12	1:F:184:MET:HE1	1.83	0.42
1:F:257:ILE:HG22	1:F:261:GLY:H	1.84	0.42
1:F:455:GLU:O	1:F:455:GLU:HG2	2.19	0.42
1:F:536:SER:O	1:F:538:GLU:N	2.51	0.42
1:A:286:MET:CE	1:A:297:VAL:HG21	2.46	0.42
1:A:394:ASP:O	1:A:395:ARG:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:PHE:C	1:B:155:PHE:CD1	2.97	0.42
1:B:397:MET:O	1:B:400:PRO:CD	2.68	0.42
1:C:157:ASP:OD1	1:C:157:ASP:N	2.51	0.42
1:C:234:ALA:HB1	1:C:281:GLN:HG2	2.01	0.42
1:C:237:VAL:HG13	1:C:238:ARG:N	2.34	0.42
1:D:488:THR:O	1:D:490:ALA:N	2.53	0.42
1:E:157:ASP:N	1:E:157:ASP:OD1	2.51	0.42
1:E:168:LEU:O	1:E:171:ILE:CG1	2.67	0.42
1:E:189:PRO:C	1:E:191:GLY:H	2.27	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:E:416:ALA:HB2	1:E:577:LEU:CD2	2.11	0.42
1:E:424:LEU:HD12	1:E:424:LEU:HA	1.83	0.42
1:F:193:LEU:HB3	1:F:317:PHE:CD2	2.54	0.42
1:F:205:LEU:HA	1:F:208:ALA:HB3	2.02	0.42
1:F:286:MET:SD	1:F:316:ARG:HG3	2.59	0.42
1:F:506:THR:OG1	1:F:520:ALA:HB3	2.19	0.42
1:F:532:VAL:HG13	1:F:532:VAL:O	2.19	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
1:A:372:ALA:O	1:A:375:LEU:HB3	2.20	0.42
1:A:583:THR:H	1:A:586:GLU:CD	2.25	0.42
1:B:159:ALA:CA	1:B:333:GLN:HE21	2.32	0.42
1:B:173:GLU:O	1:B:174:PHE:C	2.61	0.42
1:B:228:MET:O	1:B:229:PHE:HB2	2.20	0.42
1:B:256:GLU:CG	1:B:256:GLU:O	2.67	0.42
1:B:417:TYR:CZ	1:B:482:VAL:HG21	2.55	0.42
1:C:471:VAL:O	1:C:474:ALA:HB3	2.20	0.42
1:D:225:PHE:CG	1:D:236:ARG:NH1	2.88	0.42
1:D:328:VAL:HG21	1:D:579:ARG:HA	2.01	0.42
1:E:200:VAL:HG11	1:E:323:ILE:HG13	2.01	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:257:ILE:O	1:F:258:ASP:C	2.62	0.42
1:F:319:ARG:NH1	1:F:319:ARG:HB3	2.35	0.42
1:F:348:VAL:CG2	1:F:352:LEU:CD1	2.98	0.42
1:A:344:LEU:HB3	1:A:348:VAL:HG11	2.01	0.42
1:A:350:LEU:H	1:A:350:LEU:HG	1.47	0.42
1:A:463:LYS:HB2	1:B:486:VAL:HG11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:GLU:O	1:A:492:ASN:C	2.62	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
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:C:527:LEU:O	1:C:530:TYR:OH	2.31	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:D:147:LEU:HD13	1:D:149:GLU:OE1	2.19	0.42
1:D:178:PRO:O	1:D:182:HIS:CE1	2.72	0.42
1:D:241:PHE:O	1:D:242:GLU:C	2.62	0.42
1:D:373:ALA:CA	1:D:384:ILE:HD11	2.49	0.42
1:E:264:ARG:HB3	1:E:265:GLY:H	1.50	0.42
1:E:302:ASN:HB3	1:E:443:ARG:NH1	2.35	0.42
1:E:582:LEU:HA	1:E:586:GLU:OE2	2.20	0.42
2:E:1001:ADP:N3	2:E:1001:ADP:H2'	2.35	0.42
1:F:203:THR:HG23	1:F:253:PHE:CE1	2.54	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:328:VAL:HG22	1:F:355:LYS:CD	2.49	0.42
1:F:334:ILE:C	1:F:336:ARG:N	2.75	0.42
1:F:399:LEU:O	1:F:402:LYS:HB3	2.20	0.42
1:A:188:ILE:CG2	1:A:189:PRO:HD2	2.50	0.42
1:A:378:ARG:HG2	1:A:379:GLU:N	2.22	0.42
1:B:193:LEU:HB3	1:B:317:PHE:CD2	2.54	0.42
1:B:199:GLY:O	1:B:361:VAL:HG22	2.19	0.42
1:B:352:LEU:HD23	1:B:352:LEU:C	2.43	0.42
1:B:476:ARG:O	1:B:477:ALA:C	2.62	0.42
1:B:476:ARG:HD3	1:B:494:PHE:HZ	1.85	0.42
1:B:530:TYR:CD1	1:B:530:TYR:C	2.95	0.42
1:B:562:LEU:O	1:B:563:LEU:C	2.63	0.42
1:D:355:LYS:C	1:D:357:THR:N	2.75	0.42
1:E:586:GLU:CA	1:E:589:ARG:HG3	2.41	0.42
1:F:171:ILE:O	1:F:172:VAL:C	2.63	0.42
1:F:344:LEU:CG	1:F:346:GLU:OE1	2.67	0.42
1:F:464:ARG:O	1:F:467:ASP:N	2.53	0.42
1:F:517:VAL:CG2	1:F:518:ALA:N	2.81	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:338:HIS:ND1	1:A:366:GLU:HB2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:GLU:CD	1:A:395:ARG:NH1	2.78	0.42
1:A:408:SER:CB	1:A:409:PRO:HD2	2.45	0.42
1:A:462:ARG:O	1:A:466:LEU:HD12	2.19	0.42
1:A:561:LEU:O	1:A:564:GLU:HB3	2.19	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:B:558:VAL:O	1:B:559:LYS:C	2.60	0.42
1:C:155:PHE:HZ	1:C:209:VAL:CG2	2.31	0.42
1:C:189:PRO:C	1:C:191:GLY:H	2.28	0.42
1:D:155:PHE:HB2	1:D:158:VAL:HB	2.01	0.42
1:D:173:GLU:O	1:D:174:PHE:C	2.63	0.42
1:D:260:VAL:C	1:D:279:LEU:HD11	2.39	0.42
1:E:449:PHE:CD1	1:E:468:GLN:NE2	2.87	0.42
1:F:355:LYS:C	1:F:357:THR:N	2.77	0.42
1:A:155:PHE:CZ	1:A:209:VAL:CG2	3.03	0.42
1:A:162:GLU:O	1:A:163:GLU:C	2.61	0.42
1:A:381:ARG:CG	1:A:382:ARG:N	2.81	0.42
1:A:582:LEU:HA	1:A:586:GLU:OE2	2.19	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
1:C:194:LEU:H	1:C:194:LEU:HD12	1.85	0.42
1:C:361:VAL:HG22	1:C:362:GLY:N	2.35	0.42
1:C:589:ARG:HH22	1:C:596:LEU:N	2.17	0.42
1:D:307:LEU:H	1:D:307:LEU:HD12	1.85	0.42
1:E:145:ARG:CB	1:E:145:ARG:HH11	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:E:509:GLY:C	1:F:476:ARG:NH2	2.64	0.42
1:F:417:TYR:CZ	1:F:482:VAL:HG21	2.55	0.42
1:A:180:ARG:H	1:A:180:ARG:HG2	1.50	0.42
1:A:252:VAL:HB	1:A:297:VAL:HA	2.01	0.42
1:A:374:LEU:HD21	1:F:187:ARG:C	2.29	0.42
1:A:407:LEU:HA	1:A:411:ASP:HB2	2.02	0.42
1:A:461:SER:O	1:A:462:ARG:C	2.63	0.42
1:B:157:ASP:O	1:B:204:HIS:CE1	2.73	0.42
1:B:533:ARG:HG3	1:B:533:ARG:NH1	2.31	0.42
1:C:216:PRO:HG2	1:C:247:HIS:CD2	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:456:ASP:CG	1:C:457:MET:H	2.15	0.42
1:D:162:GLU:OE1	1:D:162:GLU:CA	2.68	0.42
1:D:200:VAL:HG12	1:D:325:ALA:CB	2.50	0.42
1:D:238:ARG:NH1	1:D:239:ASP:CA	2.69	0.42
1:D:238:ARG:HA	1:D:241:PHE:HE2	1.84	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: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:566:ARG:O	1:D:567:GLU:C	2.63	0.42
1:E:175:LEU:O	1:E:175:LEU:HD12	2.20	0.42
1:E:204:HIS:CD2	2:E:1001:ADP:C2	3.07	0.42
1:E:253:PHE:HA	1:E:298:MET:O	2.20	0.42
1:E:566:ARG:O	1:E:567:GLU:C	2.62	0.42
1:E:587:PHE:CD2	1:E:587:PHE:C	2.97	0.42
1:F:172:VAL:O	1:F:175:LEU:HB2	2.20	0.42
1:F:173:GLU:O	1:F:176:LYS:N	2.50	0.42
1:F:253:PHE:HA	1:F:298:MET:CB	2.45	0.42
1:F:307:LEU:N	1:F:307:LEU:HD12	2.35	0.42
1:F:400:PRO:O	1:F:403:LYS:N	2.52	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:A:545:GLU:O	1:A:546:ALA:C	2.61	0.42
1:B:157:ASP:O	1:B:204:HIS:HE1	2.03	0.42
1:B:168:LEU:O	1:B:171:ILE:N	2.52	0.42
1:B:349:ASP:C	1:B:351:ALA:H	2.28	0.42
1:B:388:ASP:OD1	1:B:388:ASP:N	2.48	0.42
1:B:570:GLU:O	1:B:571:ARG:C	2.63	0.42
1:B:589:ARG:CZ	1:B:596:LEU:CD2	2.97	0.42
1:C:196:GLY:C	1:C:202:LYS:NZ	2.76	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:C:252:VAL:HB	1:C:297:VAL:HA	2.02	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: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:D:233:GLY:O	1:D:236:ARG:NH2	2.52	0.42
1:D:376:ALA:O	1:D:377:ALA:C	2.62	0.42
1:D:449:PHE:HZ	1:D:496:GLN:OE1	2.03	0.42
1:D:453:ARG:CZ	1:D:495:ARG:NH2	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:544:ASP:O	1:D:545:GLU:C	2.62	0.42
1:E:174:PHE:HZ	1:E:294:ALA:HB1	1.85	0.42
1:E:180:ARG:H	1:E:180:ARG:HG2	1.51	0.42
1:E:461:SER:OG	1:F:486:VAL:HG11	2.19	0.42
1:E:571:ARG:O	1:E:575:THR:HG23	2.20	0.42
1:F:333:GLN:O	1:F:336:ARG:CB	2.65	0.42
1:F:585:GLU:C	1:F:587:PHE:N	2.77	0.42
1:A:172:VAL:HG22	1:A:173:GLU:N	2.35	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:A:382:ARG:HG2	1:A:383:LYS:H	1.84	0.41
1:A:464:ARG:NH1	1:A:464:ARG:CG	2.80	0.41
1:A:566:ARG:O	1:A:567:GLU:C	2.63	0.41
1:B:163:GLU:O	1:B:164:ALA:C	2.63	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:B:536:SER:O	1:B:538:GLU:N	2.53	0.41
1:C:163:GLU:H	1:C:163:GLU:CD	2.09	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
1:C:447:LEU:CB	1:C:496:GLN:HE22	2.33	0.41
1:C:586:GLU:HA	1:C:589:ARG:HB2	2.02	0.41
1:D:206:ALA:O	1:D:209:VAL:CG1	2.67	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:E:454:ARG:C	1:E:454:ARG:HD3	2.45	0.41
1:E:468:GLN:O	1:E:471:VAL:HB	2.20	0.41
1:F:241:PHE:O	1:F:242:GLU:C	2.63	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:A:414:ILE:O	1:A:415:THR:C	2.63	0.41
1:B:301:THR:HG23	1:B:302:ASN:N	2.35	0.41
1:B:500:LEU:O	1:B:503:ARG:CB	2.68	0.41
1:C:236:ARG:HH11	1:C:236:ARG:CB	2.32	0.41
1:C:462:ARG:O	1:C:466:LEU:HD12	2.20	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:589:ARG:HH22	1:E:596:LEU:CA	2.30	0.41
1:F:158:VAL:HG13	1:F:205:LEU:HD11	2.02	0.41
1:F:307:LEU:CD1	1:F:307:LEU:H	2.32	0.41
1:F:344:LEU:CD1	1:F:346:GLU:OE1	2.68	0.41
1:F:500:LEU:O	1:F:503:ARG:CB	2.67	0.41
1:A:345:ALA:CB	1:A:347:ASP:OD1	2.69	0.41
1:A:495:ARG:HD2	1:F:521:VAL:CG1	2.50	0.41
1:A:517:VAL:HG21	1:B:547:VAL:HG12	2.02	0.41
1:B:202:LYS:O	1:B:203:THR:C	2.63	0.41
1:B:235:ALA:O	1:B:238:ARG:NH1	2.53	0.41
1:B:412:ARG:O	1:B:413:ARG:C	2.63	0.41
1:C:210:ALA:CB	1:C:217:PHE:CD1	3.04	0.41
1:C:234:ALA:O	1:C:237:VAL:CG1	2.65	0.41
1:C:512:PRO:HB2	1:C:514:PHE:CD2	2.52	0.41
1:D:205:LEU:HA	1:D:208:ALA:HB3	2.01	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:D:346:GLU:OE2	1:D:348:VAL:HG12	2.20	0.41
1:D:562:LEU:O	1:D:563:LEU:C	2.62	0.41
1:E:226:VAL:HG22	1:E:274:GLU:HG2	2.03	0.41
1:E:381:ARG:CG	1:E:381:ARG:NH1	2.80	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:E:458:LEU:C	1:E:458:LEU:HD12	2.45	0.41
1:E:462:ARG:HG3	1:E:463:LYS:N	2.28	0.41
1:E:569:LEU:O	1:E:570:GLU:C	2.63	0.41
1:F:228:MET:O	1:F:229:PHE:HB2	2.20	0.41
1:F:336:ARG:O	1:F:338:HIS:N	2.53	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:253:PHE:CD2	1:A:253:PHE:C	2.98	0.41
1:A:279:LEU:HD11	1:A:311:LEU:HD11	2.02	0.41
1:A:448:GLY:O	1:A:452:PRO:CD	2.51	0.41
1:B:154:THR:HG23	1:B:156:LYS:N	2.33	0.41
1:B:173:GLU:CD	1:C:378:ARG:HA	2.44	0.41
1:B:190:LYS:CD	1:B:289:PHE:CZ	3.04	0.41
1:B:353:LEU:O	1:B:357:THR:HG23	2.20	0.41
1:B:405:LEU:O	1:B:405:LEU:HD12	2.20	0.41
1:B:538:GLU:O	1:B:540:ALA:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:574:GLU:O	1:B:575:THR:C	2.63	0.41
1:C:253:PHE:HA	1:C:298:MET:O	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:566:ARG:HG2	1:C:567:GLU:N	2.35	0.41
1:D:171:ILE:O	1:D:172:VAL:C	2.64	0.41
1:D:172:VAL:CG2	1:D:173:GLU:N	2.82	0.41
1:D:249:PRO:O	1:D:250:CYS:HB3	2.20	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:E:188:ILE:HG22	1:E:189:PRO:CD	2.50	0.41
1:E:425:ALA:C	1:E:427:HIS:N	2.76	0.41
1:E:466:LEU:HG	1:E:504:MET:HE1	2.03	0.41
1:F:280:ASN:O	1:F:283:LEU:HB3	2.19	0.41
1:F:418:HIS:O	1:F:419:GLU:C	2.63	0.41
1:B:206:ALA:O	1:B:209:VAL:CG1	2.69	0.41
1:B:391:GLU:O	1:B:392:ALA:C	2.62	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:B:453:ARG:HH12	1:B:495:ARG:NH2	2.12	0.41
1:B:508:TRP:O	1:B:510:MET:HG3	2.20	0.41
1:C:277:GLN:CG	1:C:278:THR:N	2.81	0.41
1:C:286:MET:HA	1:C:289:PHE:CE2	2.54	0.41
1:C:519:TYR:O	1:C:533:ARG:HG2	2.19	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:D:301:THR:HG23	1:D:302:ASN:N	2.36	0.41
1:D:413:ARG:O	1:D:414:ILE:C	2.63	0.41
1:E:575:THR:HA	1:E:578:GLU:OE1	2.20	0.41
1:F:176:LYS:HB3	1:F:176:LYS:HE2	1.83	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:A:519:TYR:O	1:A:533:ARG:HG2	2.20	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:B:428:PHE:CD1	1:B:432:ALA:HB3	2.56	0.41
1:C:264:ARG:HG2	1:C:267:GLY:H	1.85	0.41
1:C:302:ASN:HB3	1:C:443:ARG:NH1	2.35	0.41
1:C:375:LEU:HD12	1:C:375:LEU:C	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:396:VAL:CG1	1:C:397:MET:N	2.83	0.41
1:C:424:LEU:HD22	1:C:569:LEU:HA	2.02	0.41
1:C:468:GLN:O	1:C:471:VAL:HB	2.20	0.41
1:C:523:GLU:O	1:C:529:GLY:HA2	2.21	0.41
1:D:162:GLU:OE1	1:D:162:GLU:HA	2.19	0.41
1:D:283:LEU:HD13	1:D:316:ARG:HH21	1.82	0.41
1:D:500:LEU:O	1:D:503:ARG:CB	2.69	0.41
1:E:425:ALA:O	1:E:426:ALA:C	2.64	0.41
1:E:596:LEU:HG	1:E:597:GLU:N	2.36	0.41
1:F:178:PRO:O	1:F:179:SER:C	2.63	0.41
1:F:243:THR:CA	1:F:246:ARG:HH21	2.26	0.41
1:F:301:THR:CG2	1:F:302:ASN:N	2.83	0.41
1:F:350:LEU:O	1:F:351:ALA:C	2.63	0.41
1:F:428:PHE:CE1	1:F:432:ALA:HB3	2.52	0.41
1:F:530:TYR:CD1	1:F:530:TYR:C	2.98	0.41
1:A:168:LEU:HA	1:A:171:ILE:HD12	2.02	0.41
1:A:174:PHE:CG	1:A:175:LEU:N	2.85	0.41
1:A:234:ALA:HB1	1:A:281:GLN:HG2	2.02	0.41
1:A:273:ASP:OD1	1:A:273:ASP:C	2.63	0.41
1:B:202:LYS:CD	2:B:2001:ADP:O2B	2.68	0.41
1:B:303:ARG:O	1:B:304:PRO:C	2.62	0.41
1:B:327:ASP:HB3	1:B:330:GLY:H	1.86	0.41
1:B:335:LEU:HD23	1:B:365:LEU:HB3	2.00	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:508:TRP:HD1	1:C:491:GLU:HG2	1.85	0.41
1:C:168:LEU:O	1:C:171:ILE:CG1	2.68	0.41
1:C:191:GLY:O	1:C:317:PHE:HA	2.21	0.41
1:C:324:ASP:C	1:C:326:PRO:HD2	2.45	0.41
1:C:372:ALA:O	1:C:375:LEU:HB3	2.20	0.41
1:D:184:MET:SD	1:E:342:LYS:CE	3.08	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:D:597:GLU:O	1:D:599:PRO:CD	2.66	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
1:E:503:ARG:CZ	1:E:522:ARG:CZ	2.99	0.41
1:E:570:GLU:O	1:E:573:ALA:HB3	2.21	0.41
1:F:150:ALA:HA	1:F:151:PRO:HD2	1.85	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:248:ALA:HB1	1:F:294:ALA:HB3	2.02	0.41
1:F:249:PRO:O	1:F:250:CYS:HB3	2.21	0.41
1:F:303:ARG:O	1:F:304:PRO:C	2.64	0.41
1:F:452:PRO:O	1:F:456:ASP:CA	2.68	0.41
1:F:551:ILE:HG22	1:F:552:GLU:N	2.35	0.41
1:A:203:THR:OG1	2:A:1001:ADP:O2A	2.20	0.41
1:A:214:ARG:NH1	1:A:214:ARG:CG	2.78	0.41
1:A:218:ILE:CD1	1:A:250:CYS:SG	2.92	0.41
1:A:550:LEU:O	1:A:551:ILE:C	2.63	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:B:422:HIS:CD2	1:B:475:GLY:CA	3.04	0.41
1:B:447:LEU:C	1:B:449:PHE:N	2.78	0.41
1:C:200:VAL:HG13	1:C:323:ILE:HG13	2.03	0.41
1:C:234:ALA:O	1:C:235:ALA:C	2.62	0.41
1:C:423:ALA:HB1	1:C:436:HIS:HE1	1.85	0.41
1:D:387:LYS:O	1:D:390:GLU:HB3	2.20	0.41
1:D:422:HIS:CD2	1:D:475:GLY:HA3	2.56	0.41
1:E:274:GLU:HB3	1:E:275:ARG:H	1.56	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:E:447:LEU:CA	1:E:496:GLN:NE2	2.82	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:A:157:ASP:OD1	1:A:157:ASP:N	2.53	0.41
1:A:305:ASP:O	1:A:306:ILE:C	2.63	0.41
1:A:549:ARG:O	1:A:550:LEU:C	2.62	0.41
1:B:178:PRO:O	1:B:179:SER:C	2.64	0.41
1:B:285:GLU:O	1:B:286:MET:C	2.62	0.41
1:B:307:LEU:HD12	1:B:307:LEU:H	1.86	0.41
1:B:327:ASP:O	1:B:331:ARG:NH2	2.54	0.41
1:B:521:VAL:HG12	1:C:495:ARG:HD2	2.03	0.41
1:B:572:VAL:HG11	1:B:587:PHE:HE1	1.86	0.41
1:B:589:ARG:C	1:B:591:VAL:N	2.75	0.41
1:B:589:ARG:CD	1:B:596:LEU:HD21	2.50	0.41
1:C:180:ARG:H	1:C:180:ARG:HG2	1.53	0.41
1:C:215:VAL:CG2	1:C:216:PRO:CD	2.97	0.41
1:C:286:MET:CE	1:C:297:VAL:HG21	2.50	0.41
1:C:463:LYS:H	1:D:486:VAL:CG1	2.34	0.41
1:C:513:GLU:O	1:D:548:ARG:CZ	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:212:GLU:O	1:D:214:ARG:HG3	2.21	0.41
1:D:228:MET:O	1:D:229:PHE:HB2	2.20	0.41
1:D:257:ILE:HD11	1:D:299:ALA:HB1	2.03	0.41
1:D:280:ASN:HA	1:D:283:LEU:CD2	2.51	0.41
1:D:357:THR:HB	1:D:360:PHE:CD2	2.56	0.41
1:D:374:LEU:C	1:D:376:ALA:N	2.76	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:D:408:SER:C	1:D:410:ARG:N	2.79	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:D:527:LEU:HD11	1:E:226:VAL:CG1	2.51	0.41
1:E:153:VAL:CG1	1:E:157:ASP:HB2	2.51	0.41
1:E:177:ASN:OD1	1:E:177:ASN:N	2.54	0.41
1:E:196:GLY:CA	1:E:202:LYS:NZ	2.84	0.41
1:E:210:ALA:HB2	1:E:217:PHE:CD1	2.56	0.41
1:E:337:ILE:CD1	1:E:338:HIS:CD2	3.03	0.41
1:E:408:SER:CB	1:E:409:PRO:HD2	2.49	0.41
1:E:451:MET:CB	1:E:452:PRO:HD3	2.51	0.41
1:F:207:ARG:CB	1:F:217:PHE:CZ	2.95	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:392:ALA:C	2.62	0.41
1:F:391:GLU:O	1:F:395:ARG:CB	2.69	0.41
1:F:509:GLY:O	1:F:510:MET:HG2	2.21	0.41
1:A:182:HIS:CD2	1:A:182:HIS:N	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:A:378:ARG:HA	1:F:173:GLU:OE2	2.20	0.41
1:A:513:GLU:O	1:B:548:ARG:CZ	2.68	0.41
1:B:179:SER:HA	1:B:182:HIS:NE2	2.36	0.41
1:B:238:ARG:C	1:B:240:LEU:N	2.76	0.41
1:B:334:ILE:C	1:B:336:ARG:N	2.76	0.41
1:B:412:ARG:NH2	1:B:440:ILE:HB	2.28	0.41
1:B:467:ASP:O	1:B:471:VAL:HG13	2.20	0.41
1:C:226:VAL:HG22	1:C:274:GLU:HG2	2.02	0.41
1:C:372:ALA:HB3	1:C:389:LEU:HD23	2.03	0.41
1:C:373:ALA:HA	1:C:384:ILE:HD11	2.02	0.41
1:C:550:LEU:O	1:C:551:ILE:C	2.62	0.41
1:D:180:ARG:NH2	1:E:377:ALA:HA	2.36	0.41
1:D:376:ALA:HB1	1:D:381:ARG:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:594:LEU:HD23	1:D:594:LEU:O	2.20	0.41
1:E:199:GLY:HA2	2:E:1001:ADP:PA	2.61	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:E:541:LYS:C	1:E:543:ILE:N	2.76	0.41
1:F:199:GLY:O	1:F:361:VAL:CG2	2.69	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:298:MET:HE2	1:A:298:MET:HB3	1.79	0.40
1:A:423:ALA:HB1	1:A:587:PHE:CE1	2.57	0.40
1:A:569:LEU:O	1:A:570:GLU:C	2.63	0.40
1:A:571:ARG:O	1:A:575:THR:HG23	2.20	0.40
1:B:168:LEU:O	1:B:169:LYS:C	2.64	0.40
1:B:568:VAL:HG13	1:B:591:VAL:HA	2.02	0.40
1:C:147:LEU:HD12	1:C:148:THR:N	2.36	0.40
1:C:210:ALA:HB2	1:C:217:PHE:CD1	2.56	0.40
1:C:514:PHE:HB3	1:C:519:TYR:OH	2.20	0.40
1:D:178:PRO:O	1:D:179:SER:C	2.64	0.40
1:E:408:SER:C	1:E:410:ARG:N	2.79	0.40
1:E:561:LEU:O	1:E:564:GLU:HB3	2.21	0.40
1:F:155:PHE:O	1:F:156:LYS:C	2.63	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:A:382:ARG:HG3	1:A:383:LYS:CA	2.51	0.40
1:A:407:LEU:H	1:A:407:LEU:HG	1.57	0.40
1:A:413:ARG:O	1:A:577:LEU:HD21	2.21	0.40
1:A:445:ARG:O	1:A:446:ALA:C	2.64	0.40
1:B:360:PHE:CE1	1:B:364:ASP:HB3	2.55	0.40
1:B:414:ILE:O	1:B:415:THR:C	2.63	0.40
1:C:316:ARG:O	1:C:318:ASP:N	2.54	0.40
1:C:331:ARG:NH2	1:C:358:PRO:HG3	2.36	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:D:373:ALA:C	1:D:376:ALA:HB3	2.46	0.40
1:D:500:LEU:O	1:D:501:ALA:C	2.64	0.40
1:D:542:ARG:O	1:D:543:ILE:C	2.64	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:E:396:VAL:CG1	1:E:397:MET:N	2.84	0.40
1:E:449:PHE:CE2	1:E:496:GLN:CD	2.98	0.40
1:F:155:PHE:HB2	1:F:158:VAL:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:184:MET:HE2	1:F:184:MET:HB2	1.90	0.40
1:F:192:VAL:O	1:F:317:PHE:HE2	2.04	0.40
1:F:238:ARG:N	1:F:281:GLN:HE21	2.20	0.40
1:F:303:ARG:HA	1:F:304:PRO:HD2	1.90	0.40
1:F:307:LEU:HD12	1:F:307:LEU:H	1.86	0.40
1:F:538:GLU:O	1:F:540:ALA:N	2.54	0.40
1:A:374:LEU:O	1:A:375:LEU:C	2.64	0.40
1:A:497:ALA:O	1:A:498:THR:C	2.64	0.40
1:B:188:ILE:HD12	1:B:189:PRO:HD3	2.03	0.40
1:B:235:ALA:O	1:B:238:ARG:NE	2.51	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:B:441:VAL:C	1:B:443:ARG:N	2.80	0.40
1:B:460:TRP:HD1	1:B:464:ARG:HG2	1.86	0.40
1:B:531:ASP:OD1	1:B:531:ASP:N	2.55	0.40
1:B:567:GLU:O	1:B:570:GLU:HB3	2.21	0.40
1:C:153:VAL:CG1	1:C:157:ASP:HB2	2.51	0.40
1:C:176:LYS:HG2	1:C:176:LYS:H	1.76	0.40
1:D:238:ARG:C	1:D:240:LEU:N	2.75	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:D:472:ALA:C	1:D:474:ALA:N	2.79	0.40
1:D:508:TRP:O	1:D:510:MET:HG3	2.22	0.40
1:D:536:SER:HB2	1:E:537:GLU:OE2	2.20	0.40
1:E:202:LYS:O	1:E:203:THR:C	2.64	0.40
1:E:228:MET:HE3	1:E:236:ARG:NH2	2.36	0.40
1:E:375:LEU:HD12	1:E:375:LEU:C	2.46	0.40
1:E:450:MET:O	1:E:454:ARG:HB3	2.21	0.40
1:E:582:LEU:HD21	1:E:590:VAL:HG11	2.02	0.40
1:F:414:ILE:O	1:F:415:THR:C	2.63	0.40
1:F:566:ARG:O	1:F:567:GLU:C	2.64	0.40
1:A:173:GLU:CA	1:A:176:LYS:HG3	2.43	0.40
1:A:263:LYS:CG	1:A:264:ARG:N	2.83	0.40
1:A:287:ASP:OD1	1:A:287:ASP:N	2.51	0.40
1:A:314:PRO:HA	1:A:318:ASP:HB3	2.04	0.40
1:A:355:LYS:HA	1:A:355:LYS:HD3	1.90	0.40
1:A:511:HIS:C	1:A:512:PRO:O	2.65	0.40
1:B:260:VAL:C	1:B:279:LEU:HD11	2.40	0.40
1:B:313:ARG:O	1:B:316:ARG:HB2	2.21	0.40
1:B:346:GLU:OE2	1:B:348:VAL:HG12	2.22	0.40
1:B:417:TYR:O	1:B:420:ALA:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:HIS:CD2	1:B:475:GLY:HA3	2.57	0.40
1:C:462:ARG:CG	1:C:463:LYS:N	2.83	0.40
1:D:193:LEU:HD12	1:D:194:LEU:H	1.86	0.40
1:D:464:ARG:O	1:D:467:ASP:N	2.55	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:D:568:VAL:HG13	1:D:591:VAL:HA	2.02	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: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:F:468:GLN:O	1:F:469:ILE:C	2.63	0.40
1:F:469:ILE:HG23	1:F:497:ALA:HB1	2.02	0.40
1:F:478:ALA:O	1:F:482:VAL:HG12	2.21	0.40
1:F:597:GLU:O	1:F:599:PRO:CD	2.68	0.40
1:A:173:GLU:O	1:A:174:PHE:C	2.64	0.40
1:A:194:LEU:HD12	1:A:194:LEU:H	1.87	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:249:PRO:O	1:B:250:CYS:HB3	2.21	0.40
1:B:260:VAL:O	1:B:262:ARG:N	2.47	0.40
1:B:387:LYS:O	1:B:390:GLU:HB3	2.21	0.40
1:B:525:THR:HG22	1:B:526:TYR:N	2.34	0.40
1:B:589:ARG:O	1:B:590:VAL:C	2.64	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:173:GLU:OE1	1:E:378:ARG:HA	2.21	0.40
1:D:447:LEU:C	1:D:449:PHE:N	2.78	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:E:162:GLU:O	1:E:163:GLU:C	2.65	0.40
1:E:182:HIS:HD1	1:E:291:LYS:HB2	1.86	0.40
1:E:252:VAL:HB	1:E:297:VAL:HA	2.03	0.40
1:E:397:MET:SD	1:E:406:VAL:HG11	2.62	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:F:494:PHE:C	1:F:496:GLN:N	2.80	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:224:ASP:OD2	1:E:180:ARG:NH2[6_665]	2.17	0.03
1:B:238:ARG:CZ	1:F:378:ARG:NH2[6_665]	2.17	0.03

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	456/508 (90%)	323 (71%)	111 (24%)	22 (5%)	2	18
1	B	442/508 (87%)	289 (65%)	125 (28%)	28 (6%)	1	15
1	C	456/508 (90%)	323 (71%)	112 (25%)	21 (5%)	2	19
1	D	442/508 (87%)	288 (65%)	121 (27%)	33 (8%)	1	12
1	E	456/508 (90%)	324 (71%)	110 (24%)	22 (5%)	2	18
1	F	442/508 (87%)	288 (65%)	120 (27%)	34 (8%)	1	12
All	All	2694/3048 (88%)	1835 (68%)	699 (26%)	160 (6%)	1	15

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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%)	229 (63%)	136 (37%)	0	1
1	B	361/402 (90%)	224 (62%)	137 (38%)	0	1
1	C	365/402 (91%)	225 (62%)	140 (38%)	0	1
1	D	361/402 (90%)	222 (62%)	139 (38%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	365/402 (91%)	228 (62%)	137 (38%)	0	1
1	F	361/402 (90%)	225 (62%)	136 (38%)	0	1
All	All	2178/2412 (90%)	1353 (62%)	825 (38%)	0	1

All (825) 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	152	LYS
1	A	153	VAL
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	182	HIS
1	A	183	GLU
1	A	188	ILE
1	A	192	VAL
1	A	194	LEU
1	A	200	VAL
1	A	207	ARG
1	A	215	VAL
1	A	218	ILE
1	A	219	THR
1	A	221	SER
1	A	223	SER
1	A	226	VAL
1	A	230	VAL
1	A	236	ARG
1	A	237	VAL
1	A	242	GLU
1	A	245	LYS
1	A	251	ILE

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Mol	Chain	Res	Type
1	A	252	VAL
1	A	262	ARG
1	A	273	ASP
1	A	274	GLU
1	A	275	ARG
1	A	277	GLN
1	A	281	GLN
1	A	282	LEU
1	A	287	ASP
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
1	A	323	ILE
1	A	327	ASP
1	A	334	ILE
1	A	344	LEU
1	A	346	GLU
1	A	347	ASP
1	A	348	VAL
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	370	ASN
1	A	371	GLU
1	A	375	LEU
1	A	378	ARG

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Mol	Chain	Res	Type
1	A	381	ARG
1	A	382	ARG
1	A	383	LYS
1	A	384	ILE
1	A	388	ASP
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	438	VAL
1	A	447	LEU
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	463	LYS
1	A	464	ARG
1	A	465	LEU
1	A	482	VAL
1	A	484	ASP
1	A	487	THR
1	A	491	GLU
1	A	493	ASP
1	A	500	LEU
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	534	GLN
1	A	535	TYR

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Mol	Chain	Res	Type
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	562	LEU
1	A	569	LEU
1	A	574	GLU
1	A	576	LEU
1	A	578	GLU
1	A	579	ARG
1	A	580	GLU
1	A	585	GLU
1	A	594	LEU
1	A	596	LEU
1	B	152	LYS
1	B	153	VAL
1	B	157	ASP
1	B	162	GLU
1	B	166	GLU
1	B	167	GLU
1	B	170	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
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

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Mol	Chain	Res	Type
1	B	217	PHE
1	B	223	SER
1	B	227	GLU
1	B	230	VAL
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	247	HIS
1	B	251	ILE
1	B	252	VAL
1	B	253	PHE
1	B	255	ASP
1	B	256	GLU
1	B	257	ILE
1	B	258	ASP
1	B	260	VAL
1	B	263	LYS
1	B	273	ASP
1	B	274	GLU
1	B	276	GLU
1	B	284	VAL
1	B	290	GLU
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	321	ILE
1	B	323	ILE
1	B	328	VAL
1	B	332	GLU
1	B	344	LEU

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Mol	Chain	Res	Type
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	361	VAL
1	B	367	ASN
1	B	374	LEU
1	B	375	LEU
1	B	378	ARG
1	B	382	ARG
1	B	386	MET
1	B	387	LYS
1	B	388	ASP
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	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	463	LYS
1	B	476	ARG
1	B	484	ASP
1	B	485	ASP
1	B	486	VAL
1	B	499	GLU

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Mol	Chain	Res	Type
1	B	500	LEU
1	B	503	ARG
1	B	505	ILE
1	B	506	THR
1	B	517	VAL
1	B	521	VAL
1	B	522	ARG
1	B	523	GLU
1	B	531	ASP
1	B	533	ARG
1	B	535	TYR
1	B	539	THR
1	B	547	VAL
1	B	548	ARG
1	B	558	VAL
1	B	563	LEU
1	B	564	GLU
1	B	570	GLU
1	B	575	THR
1	B	577	LEU
1	B	578	GLU
1	B	581	THR
1	B	582	LEU
1	B	583	THR
1	B	586	GLU
1	B	590	VAL
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	152	LYS
1	C	154	THR
1	C	157	ASP
1	C	166	GLU
1	C	171	ILE
1	C	172	VAL
1	C	173	GLU
1	C	174	PHE
1	C	175	LEU
1	C	177	ASN

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Mol	Chain	Res	Type
1	C	179	SER
1	C	182	HIS
1	C	183	GLU
1	C	188	ILE
1	C	192	VAL
1	C	194	LEU
1	C	200	VAL
1	C	207	ARG
1	C	215	VAL
1	C	218	ILE
1	C	219	THR
1	C	221	SER
1	C	223	SER
1	C	226	VAL
1	C	230	VAL
1	C	236	ARG
1	C	237	VAL
1	C	242	GLU
1	C	245	LYS
1	C	251	ILE
1	C	262	ARG
1	C	273	ASP
1	C	274	GLU
1	C	275	ARG
1	C	277	GLN
1	C	281	GLN
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	311	LEU
1	C	312	LEU
1	C	318	ASP
1	C	320	GLN
1	C	323	ILE

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Mol	Chain	Res	Type
1	C	327	ASP
1	C	334	ILE
1	C	340	ARG
1	C	344	LEU
1	C	346	GLU
1	C	347	ASP
1	C	348	VAL
1	C	349	ASP
1	C	350	LEU
1	C	352	LEU
1	C	355	LYS
1	C	357	THR
1	C	360	PHE
1	C	364	ASP
1	C	368	LEU
1	C	370	ASN
1	C	371	GLU
1	C	375	LEU
1	C	378	ARG
1	C	381	ARG
1	C	382	ARG
1	C	384	ILE
1	C	388	ASP
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	418	HIS
1	C	419	GLU
1	C	433	ASP
1	C	436	HIS
1	C	437	LYS
1	C	438	VAL
1	C	447	LEU
1	C	449	PHE
1	C	453	ARG
1	C	454	ARG

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Mol	Chain	Res	Type
1	C	459	HIS
1	C	461	SER
1	C	462	ARG
1	C	463	LYS
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	498	THR
1	C	500	LEU
1	C	502	ARG
1	C	511	HIS
1	C	514	PHE
1	C	524	ASP
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	553	GLU
1	C	558	VAL
1	C	561	LEU
1	C	562	LEU
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	580	GLU
1	C	585	GLU
1	C	586	GLU
1	C	589	ARG
1	C	590	VAL

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Mol	Chain	Res	Type
1	C	594	LEU
1	D	152	LYS
1	D	153	VAL
1	D	157	ASP
1	D	162	GLU
1	D	166	GLU
1	D	167	GLU
1	D	170	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	209	VAL
1	D	214	ARG
1	D	217	PHE
1	D	223	SER
1	D	227	GLU
1	D	230	VAL
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	247	HIS
1	D	251	ILE
1	D	252	VAL
1	D	253	PHE
1	D	255	ASP

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Mol	Chain	Res	Type
1	D	256	GLU
1	D	257	ILE
1	D	258	ASP
1	D	260	VAL
1	D	263	LYS
1	D	273	ASP
1	D	274	GLU
1	D	276	GLU
1	D	284	VAL
1	D	285	GLU
1	D	289	PHE
1	D	290	GLU
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	316	ARG
1	D	318	ASP
1	D	319	ARG
1	D	321	ILE
1	D	323	ILE
1	D	328	VAL
1	D	332	GLU
1	D	344	LEU
1	D	347	ASP
1	D	348	VAL
1	D	350	LEU
1	D	352	LEU
1	D	355	LYS
1	D	356	ARG
1	D	357	THR
1	D	360	PHE
1	D	361	VAL
1	D	367	ASN
1	D	374	LEU
1	D	375	LEU
1	D	378	ARG
1	D	382	ARG
1	D	385	THR

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Mol	Chain	Res	Type
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	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	463	LYS
1	D	476	ARG
1	D	484	ASP
1	D	485	ASP
1	D	486	VAL
1	D	499	GLU
1	D	500	LEU
1	D	503	ARG
1	D	505	ILE
1	D	506	THR
1	D	517	VAL
1	D	521	VAL
1	D	522	ARG
1	D	523	GLU
1	D	531	ASP
1	D	533	ARG
1	D	535	TYR
1	D	539	THR
1	D	547	VAL

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Mol	Chain	Res	Type
1	D	548	ARG
1	D	558	VAL
1	D	563	LEU
1	D	567	GLU
1	D	570	GLU
1	D	575	THR
1	D	577	LEU
1	D	578	GLU
1	D	581	THR
1	D	582	LEU
1	D	583	THR
1	D	590	VAL
1	D	592	GLU
1	D	600	GLU
1	E	145	ARG
1	E	146	VAL
1	E	147	LEU
1	E	152	LYS
1	E	154	THR
1	E	157	ASP
1	E	166	GLU
1	E	171	ILE
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	182	HIS
1	E	183	GLU
1	E	188	ILE
1	E	192	VAL
1	E	194	LEU
1	E	200	VAL
1	E	207	ARG
1	E	215	VAL
1	E	218	ILE
1	E	219	THR
1	E	221	SER
1	E	223	SER
1	E	226	VAL
1	E	230	VAL

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Mol	Chain	Res	Type
1	E	236	ARG
1	E	237	VAL
1	E	242	GLU
1	E	245	LYS
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	281	GLN
1	E	282	LEU
1	E	287	ASP
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	311	LEU
1	E	312	LEU
1	E	318	ASP
1	E	320	GLN
1	E	323	ILE
1	E	327	ASP
1	E	334	ILE
1	E	344	LEU
1	E	346	GLU
1	E	347	ASP
1	E	348	VAL
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

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Mol	Chain	Res	Type
1	E	370	ASN
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	384	ILE
1	E	388	ASP
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	438	VAL
1	E	439	THR
1	E	447	LEU
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	463	LYS
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	500	LEU
1	E	502	ARG
1	E	504	MET
1	E	511	HIS

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Mol	Chain	Res	Type
1	E	514	PHE
1	E	524	ASP
1	E	530	TYR
1	E	532	VAL
1	E	534	GLN
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
1	E	562	LEU
1	E	569	LEU
1	E	574	GLU
1	E	576	LEU
1	E	578	GLU
1	E	579	ARG
1	E	580	GLU
1	E	585	GLU
1	E	586	GLU
1	E	589	ARG
1	E	590	VAL
1	E	594	LEU
1	F	152	LYS
1	F	153	VAL
1	F	157	ASP
1	F	162	GLU
1	F	166	GLU
1	F	167	GLU
1	F	170	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

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Mol	Chain	Res	Type
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	214	ARG
1	F	217	PHE
1	F	223	SER
1	F	227	GLU
1	F	230	VAL
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	247	HIS
1	F	251	ILE
1	F	252	VAL
1	F	253	PHE
1	F	255	ASP
1	F	256	GLU
1	F	257	ILE
1	F	258	ASP
1	F	260	VAL
1	F	263	LYS
1	F	273	ASP
1	F	274	GLU
1	F	276	GLU
1	F	284	VAL
1	F	290	GLU
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

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Mol	Chain	Res	Type
1	F	318	ASP
1	F	319	ARG
1	F	321	ILE
1	F	323	ILE
1	F	328	VAL
1	F	332	GLU
1	F	335	LEU
1	F	344	LEU
1	F	347	ASP
1	F	348	VAL
1	F	350	LEU
1	F	352	LEU
1	F	355	LYS
1	F	356	ARG
1	F	357	THR
1	F	360	PHE
1	F	361	VAL
1	F	367	ASN
1	F	374	LEU
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
1	F	405	LEU
1	F	407	LEU
1	F	414	ILE
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

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Mol	Chain	Res	Type
1	F	459	HIS
1	F	460	TRP
1	F	463	LYS
1	F	476	ARG
1	F	484	ASP
1	F	485	ASP
1	F	486	VAL
1	F	499	GLU
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	523	GLU
1	F	526	TYR
1	F	531	ASP
1	F	533	ARG
1	F	535	TYR
1	F	539	THR
1	F	547	VAL
1	F	548	ARG
1	F	558	VAL
1	F	563	LEU
1	F	564	GLU
1	F	570	GLU
1	F	575	THR
1	F	577	LEU
1	F	578	GLU
1	F	581	THR
1	F	582	LEU
1	F	583	THR
1	F	590	VAL
1	F	592	GLU
1	F	600	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	177	ASN
1	A	182	HIS
1	A	204	HIS

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Mol	Chain	Res	Type
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	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	177	ASN
1	E	204	HIS
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
1	F	338	HIS
1	F	431	HIS
1	F	511	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	D	2001	-	28,29,29	1.54	6 (21%)	43,45,45	2.03	10 (23%)
2	ADP	B	2001	-	28,29,29	1.53	5 (17%)	43,45,45	1.87	11 (25%)
2	ADP	F	2001	-	28,29,29	1.54	5 (17%)	43,45,45	1.94	12 (27%)
2	ADP	E	1001	-	28,29,29	1.47	4 (14%)	43,45,45	1.87	9 (20%)
2	ADP	A	1001	-	28,29,29	1.52	4 (14%)	43,45,45	1.93	10 (23%)
2	ADP	C	1001	-	28,29,29	1.51	4 (14%)	43,45,45	2.07	10 (23%)

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	D	2001	-	-	2/16/32/32	0/3/3/3
2	ADP	B	2001	-	-	3/16/32/32	0/3/3/3
2	ADP	F	2001	-	-	2/16/32/32	0/3/3/3
2	ADP	E	1001	-	-	2/16/32/32	0/3/3/3
2	ADP	A	1001	-	-	1/16/32/32	0/3/3/3
2	ADP	C	1001	-	-	2/16/32/32	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	ADP	C5-C4	5.16	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2001	ADP	C5-C4	5.12	1.48	1.39
2	E	1001	ADP	C5-C4	5.08	1.48	1.39
2	C	1001	ADP	C5-C4	4.92	1.47	1.39
2	B	2001	ADP	C5-C4	4.88	1.47	1.39
2	D	2001	ADP	C5-C4	4.62	1.47	1.39
2	C	1001	ADP	C5-C6	3.25	1.50	1.41
2	A	1001	ADP	C5-C6	3.07	1.49	1.41
2	F	2001	ADP	C5-C6	3.06	1.49	1.41
2	D	2001	ADP	PA-O3A	3.04	1.62	1.59
2	D	2001	ADP	C5-C6	2.91	1.49	1.41
2	B	2001	ADP	C5-C6	2.89	1.49	1.41
2	E	1001	ADP	C5-C6	2.81	1.48	1.41
2	F	2001	ADP	PA-O3A	2.80	1.62	1.59
2	B	2001	ADP	PA-O3A	2.68	1.62	1.59
2	D	2001	ADP	C5-N7	-2.67	1.34	1.39
2	B	2001	ADP	C5-N7	-2.42	1.34	1.39
2	C	1001	ADP	C8-N7	2.41	1.36	1.31
2	F	2001	ADP	C8-N7	2.39	1.36	1.31
2	D	2001	ADP	C8-N9	-2.32	1.33	1.37
2	B	2001	ADP	C8-N7	2.32	1.36	1.31
2	E	1001	ADP	C5-N7	-2.30	1.34	1.39
2	A	1001	ADP	C5-N7	-2.30	1.34	1.39
2	A	1001	ADP	C8-N7	2.28	1.36	1.31
2	D	2001	ADP	C8-N7	2.25	1.36	1.31
2	E	1001	ADP	C8-N7	2.16	1.35	1.31
2	F	2001	ADP	C5-N7	-2.02	1.35	1.39
2	C	1001	ADP	C5-N7	-2.00	1.35	1.39

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2001	ADP	C5-C4-N3	-6.87	117.26	126.72
2	C	1001	ADP	C5-C4-N3	-6.36	117.95	126.72
2	A	1001	ADP	C5-C4-N3	-6.11	118.30	126.72
2	E	1001	ADP	C5-C4-N3	-5.92	118.56	126.72
2	F	2001	ADP	C5-C4-N3	-5.86	118.64	126.72
2	B	2001	ADP	C5-C4-N3	-5.57	119.05	126.72
2	C	1001	ADP	N3-C4-N9	5.19	136.00	127.17
2	D	2001	ADP	N3-C4-N9	5.14	135.91	127.17
2	A	1001	ADP	N3-C4-N9	5.09	135.83	127.17
2	E	1001	ADP	N3-C4-N9	5.02	135.70	127.17
2	F	2001	ADP	N3-C4-N9	4.74	135.22	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2001	ADP	N3-C4-N9	4.65	135.07	127.17
2	D	2001	ADP	C4-C5-N7	-4.33	105.63	110.58
2	C	1001	ADP	C2-N3-C4	4.26	122.23	111.83
2	D	2001	ADP	C2-N3-C4	4.01	121.62	111.83
2	C	1001	ADP	C4-C5-N7	-3.88	106.15	110.58
2	C	1001	ADP	N3-C2-N1	-3.78	122.86	128.58
2	F	2001	ADP	C4-C5-N7	-3.77	106.27	110.58
2	A	1001	ADP	C2-N3-C4	3.75	121.00	111.83
2	F	2001	ADP	C2-N3-C4	3.65	120.74	111.83
2	A	1001	ADP	C4-C5-N7	-3.60	106.46	110.58
2	B	2001	ADP	C2-N3-C4	3.54	120.47	111.83
2	B	2001	ADP	C4-C5-N7	-3.54	106.54	110.58
2	E	1001	ADP	C2-N3-C4	3.49	120.36	111.83
2	E	1001	ADP	C4-C5-N7	-3.47	106.61	110.58
2	F	2001	ADP	C2'-C1'-N9	-3.33	105.02	113.30
2	B	2001	ADP	N3-C2-N1	-3.17	123.78	128.58
2	D	2001	ADP	N3-C2-N1	-3.14	123.83	128.58
2	A	1001	ADP	N3-C2-N1	-3.10	123.89	128.58
2	D	2001	ADP	C5-N7-C8	3.08	108.29	103.45
2	F	2001	ADP	N3-C2-N1	-3.07	123.93	128.58
2	B	2001	ADP	C4-N9-C8	3.01	108.90	105.74
2	E	1001	ADP	C4-N9-C8	3.01	108.90	105.74
2	C	1001	ADP	C4-N9-C8	3.01	108.89	105.74
2	C	1001	ADP	C5-N7-C8	3.00	108.16	103.45
2	F	2001	ADP	C4-N9-C8	2.97	108.85	105.74
2	B	2001	ADP	C5-N7-C8	2.83	107.90	103.45
2	A	1001	ADP	C4-N9-C8	2.81	108.69	105.74
2	C	1001	ADP	C2'-C1'-N9	-2.81	106.33	113.30
2	E	1001	ADP	N3-C2-N1	-2.77	124.39	128.58
2	F	2001	ADP	C5-N7-C8	2.73	107.74	103.45
2	E	1001	ADP	C5-N7-C8	2.70	107.69	103.45
2	A	1001	ADP	C2'-C1'-N9	-2.66	106.69	113.30
2	A	1001	ADP	C5-N7-C8	2.66	107.63	103.45
2	B	2001	ADP	C2'-C1'-N9	-2.57	106.93	113.30
2	F	2001	ADP	C3'-C2'-C1'	2.56	106.30	101.46
2	C	1001	ADP	C6-C5-N7	2.55	137.01	132.09
2	B	2001	ADP	C3'-C2'-C1'	2.30	105.81	101.46
2	C	1001	ADP	N9-C8-N7	-2.25	110.75	113.94
2	A	1001	ADP	C3'-C2'-C1'	2.24	105.69	101.46
2	B	2001	ADP	N9-C8-N7	-2.22	110.78	113.94
2	D	2001	ADP	C4-N9-C8	2.20	108.05	105.74
2	D	2001	ADP	O3B-PB-O2B	2.19	116.03	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	ADP	C6-C5-N7	2.18	136.30	132.09
2	E	1001	ADP	C3'-C2'-C1'	2.09	105.42	101.46
2	F	2001	ADP	C6-C5-N7	2.07	136.08	132.09
2	F	2001	ADP	N9-C8-N7	-2.07	111.00	113.94
2	D	2001	ADP	C3'-C2'-C1'	2.04	105.32	101.46
2	E	1001	ADP	N9-C8-N7	-2.03	111.06	113.94
2	F	2001	ADP	C2-N1-C6	2.02	122.06	118.73
2	B	2001	ADP	C2-N1-C6	2.02	122.05	118.73
2	D	2001	ADP	C6-C5-N7	2.02	135.98	132.09

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	ADP	C5'-O5'-PA-O1A
2	B	2001	ADP	C5'-O5'-PA-O2A
2	C	1001	ADP	C5'-O5'-PA-O1A
2	C	1001	ADP	C5'-O5'-PA-O3A
2	D	2001	ADP	C5'-O5'-PA-O3A
2	E	1001	ADP	C5'-O5'-PA-O1A
2	E	1001	ADP	C5'-O5'-PA-O3A
2	F	2001	ADP	C5'-O5'-PA-O3A
2	B	2001	ADP	C5'-O5'-PA-O1A
2	B	2001	ADP	C5'-O5'-PA-O3A
2	D	2001	ADP	C5'-O5'-PA-O1A
2	F	2001	ADP	C5'-O5'-PA-O1A

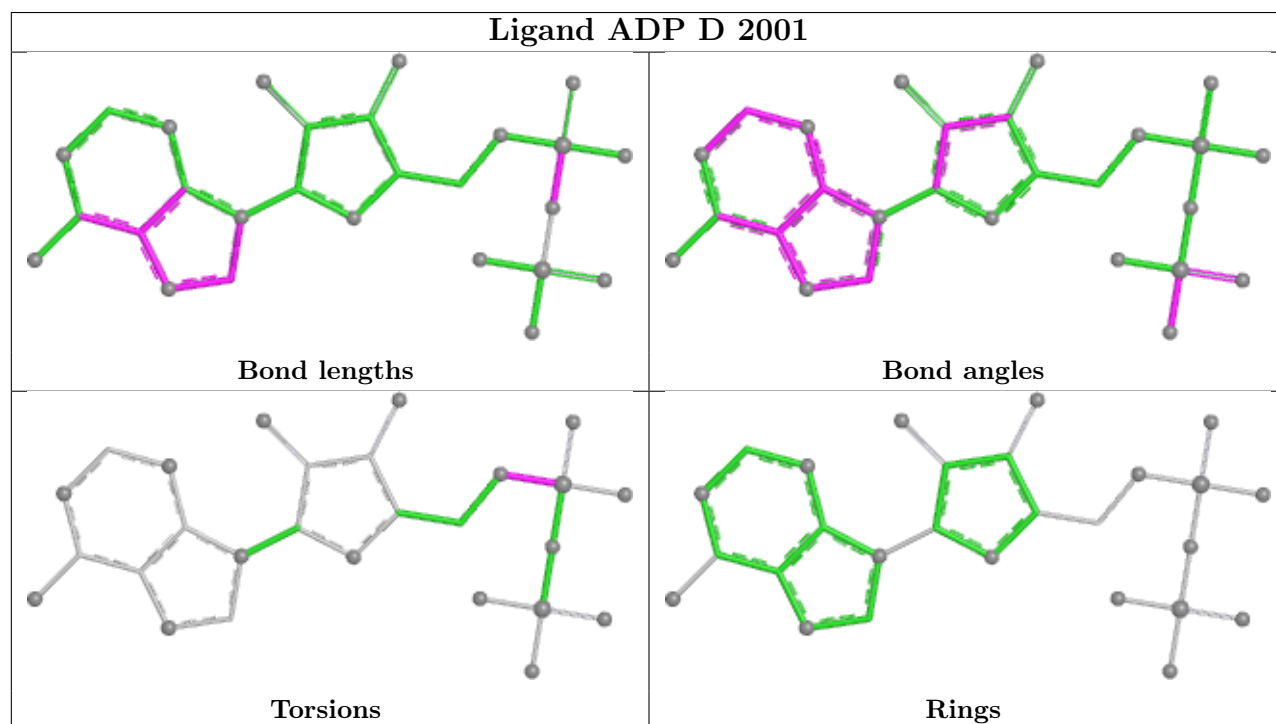
There are no ring outliers.

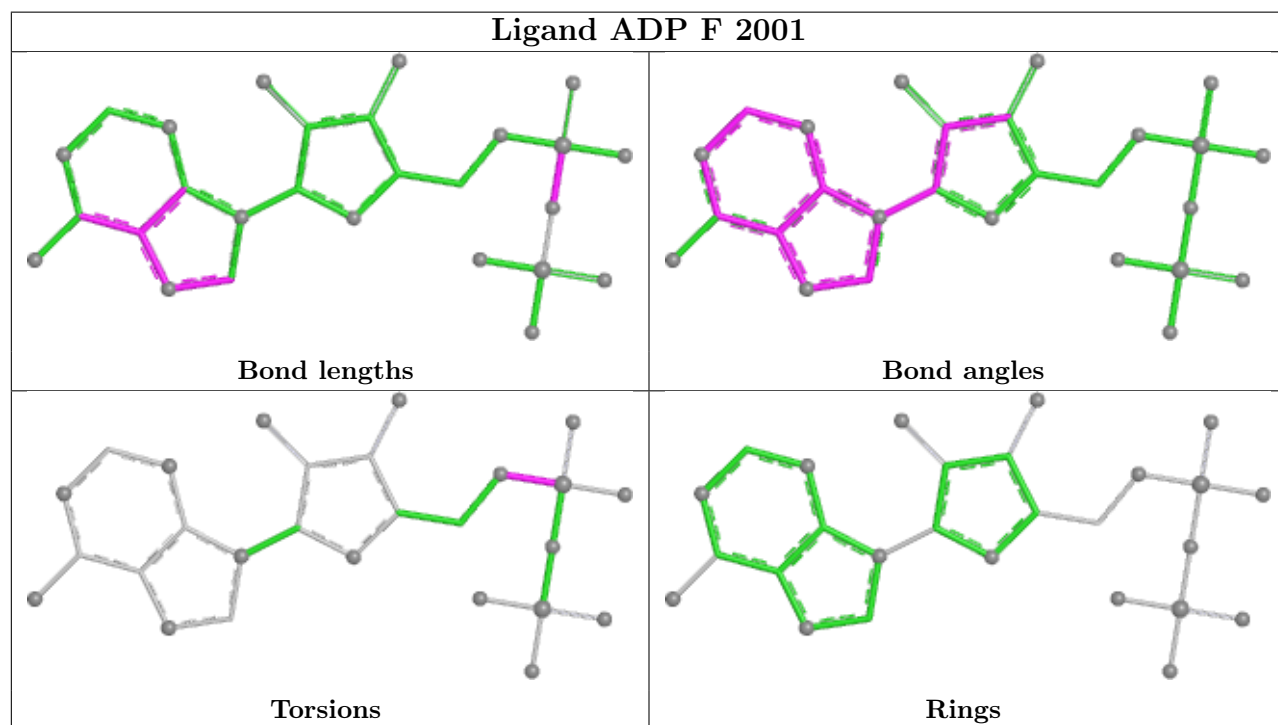
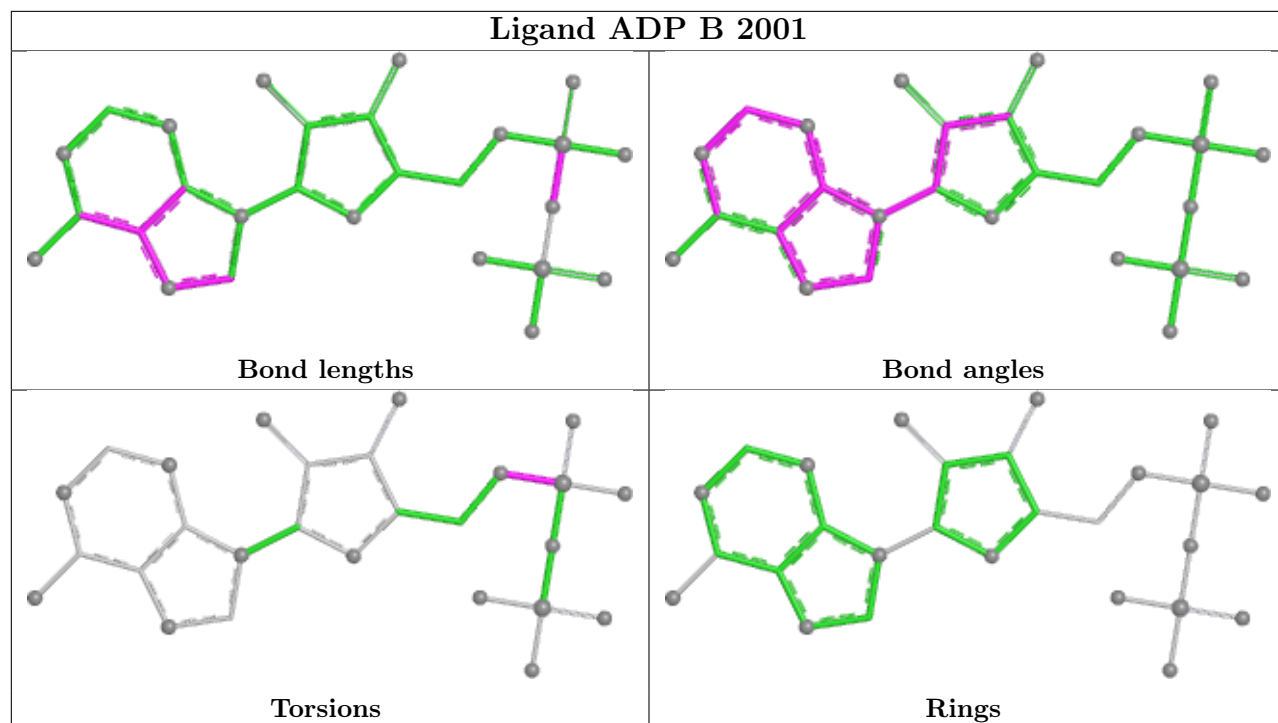
6 monomers are involved in 57 short contacts:

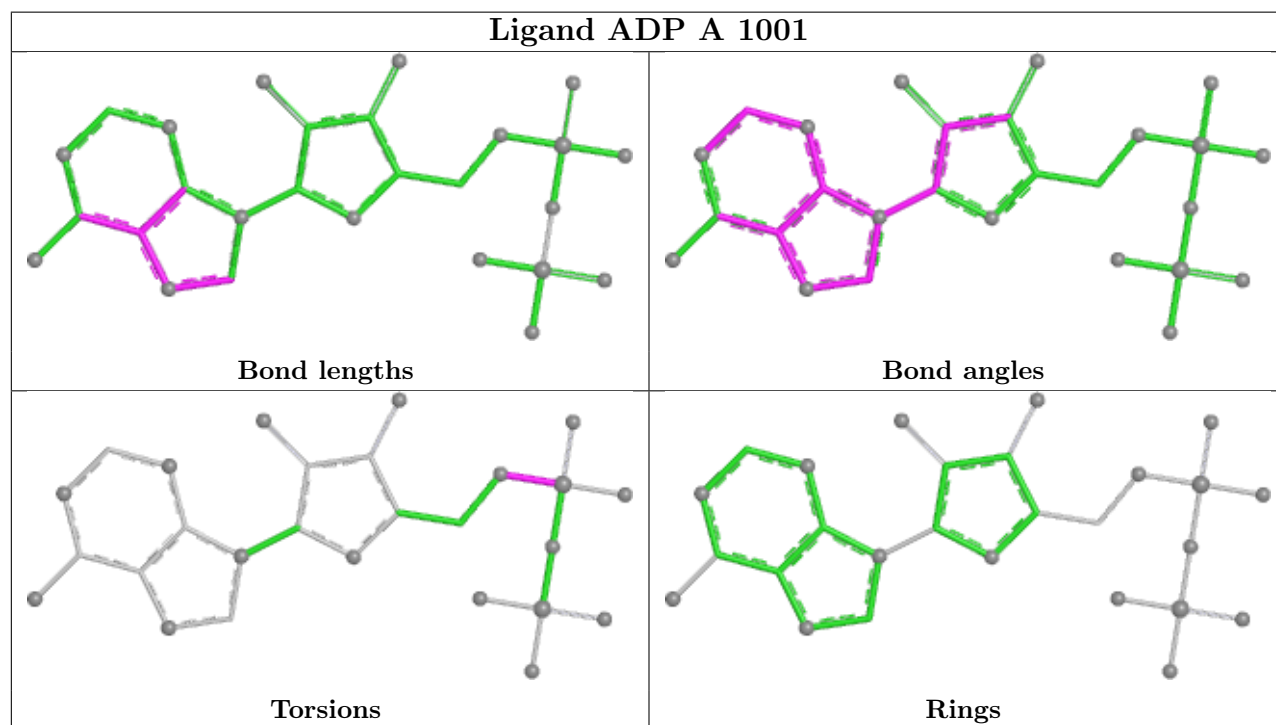
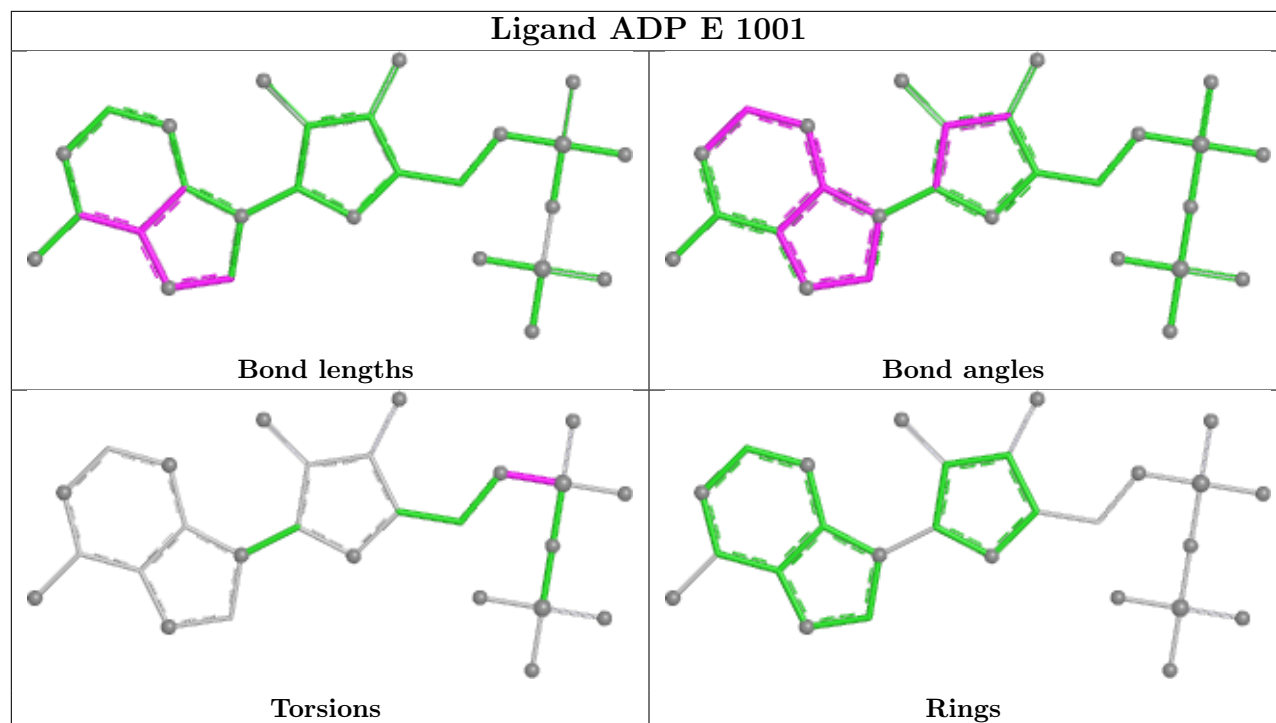
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2001	ADP	9	0
2	B	2001	ADP	9	0
2	F	2001	ADP	10	0
2	E	1001	ADP	11	0
2	A	1001	ADP	8	0
2	C	1001	ADP	10	0

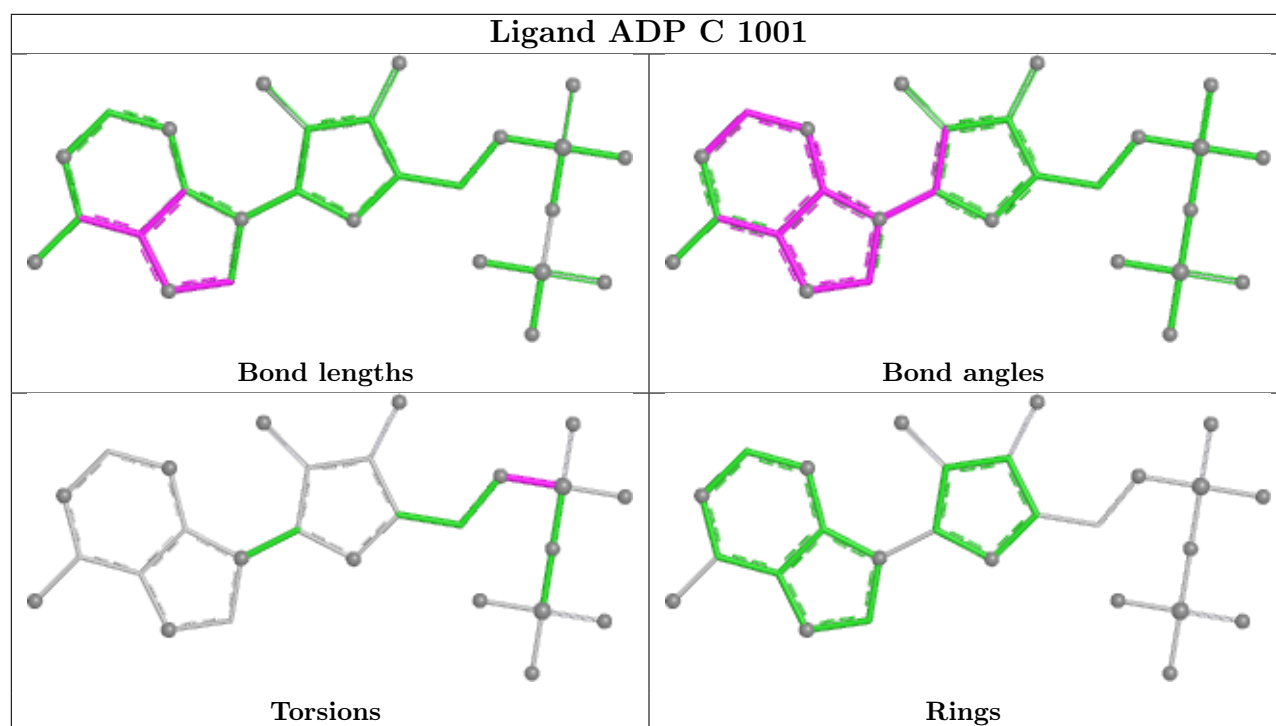
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.31	1 (0%) 91 81	21, 118, 174, 229	0
1	B	446/508 (87%)	-0.29	1 (0%) 91 81	16, 125, 176, 241	0
1	C	458/508 (90%)	-0.21	0 100 100	21, 129, 184, 237	0
1	D	446/508 (87%)	-0.28	2 (0%) 88 74	23, 103, 173, 241	0
1	E	458/508 (90%)	-0.22	1 (0%) 91 81	24, 130, 179, 223	0
1	F	446/508 (87%)	-0.23	1 (0%) 91 81	21, 128, 173, 261	0
All	All	2712/3048 (88%)	-0.25	6 (0%) 91 81	16, 124, 177, 261	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	600	GLU	2.8
1	A	528	GLY	2.4
1	B	382	ARG	2.4
1	D	443	ARG	2.3
1	E	270	GLY	2.2
1	D	377	ALA	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](#)

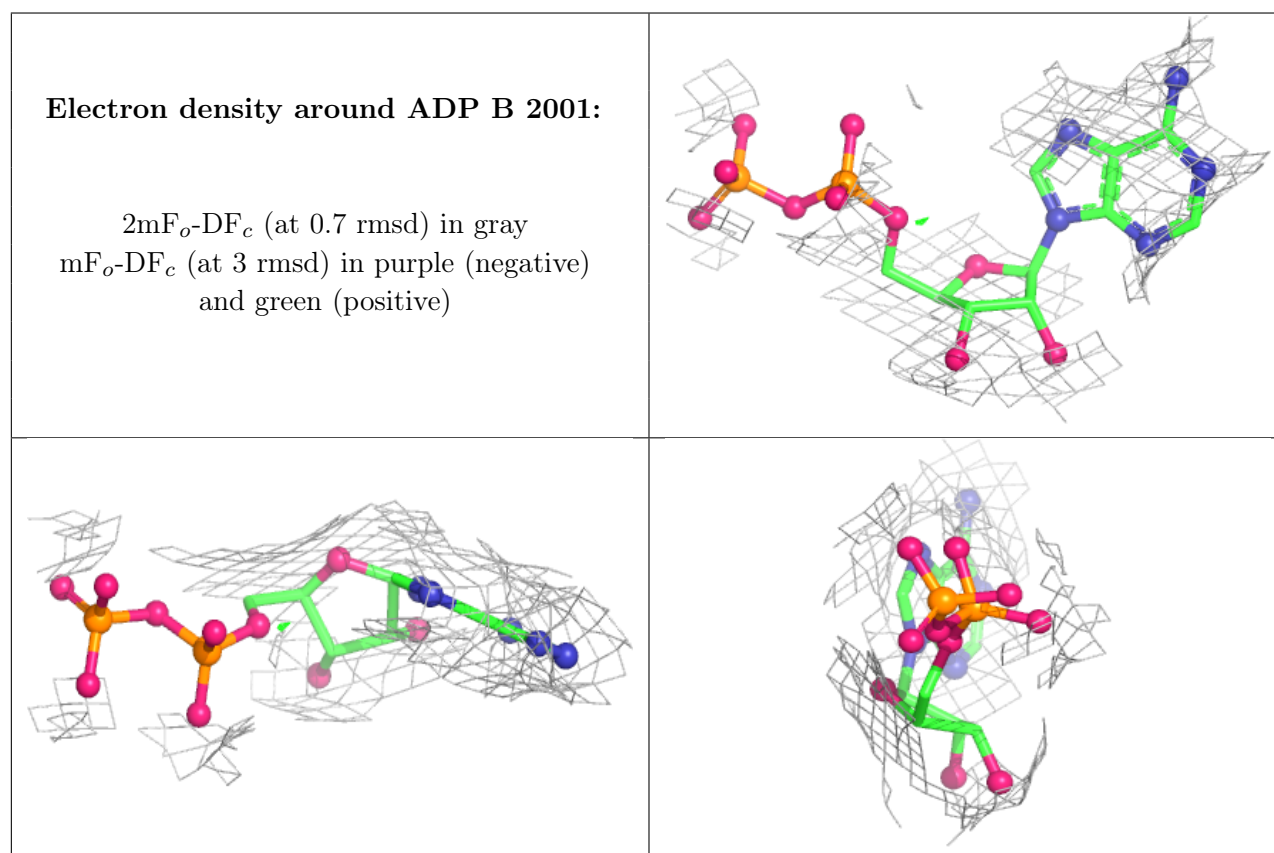
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

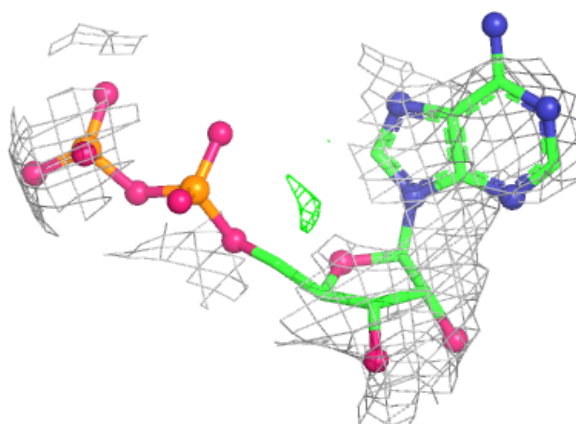
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ADP	B	2001	27/27	0.97	0.06	65,72,75,79	0
2	ADP	C	1001	27/27	0.97	0.07	70,73,74,76	0
2	ADP	F	2001	27/27	0.97	0.07	64,69,74,74	0
2	ADP	E	1001	27/27	0.98	0.07	66,70,72,73	0
2	ADP	A	1001	27/27	0.98	0.06	63,66,70,71	0
2	ADP	D	2001	27/27	0.99	0.07	58,64,74,74	0

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

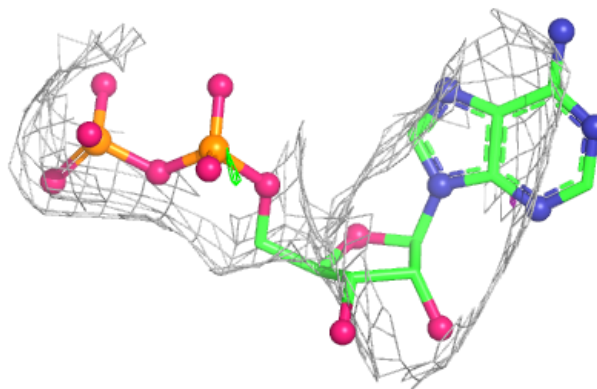


Electron density around ADP C 1001:

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

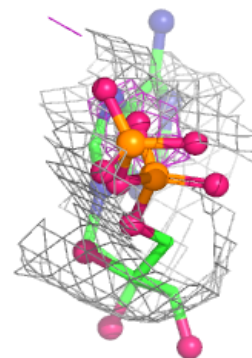
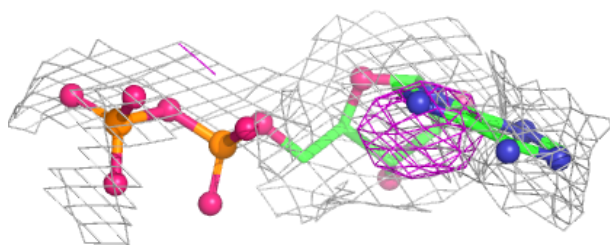
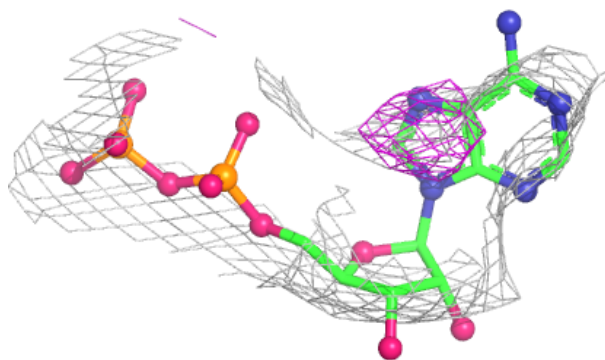
**Electron density around ADP F 2001:**

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

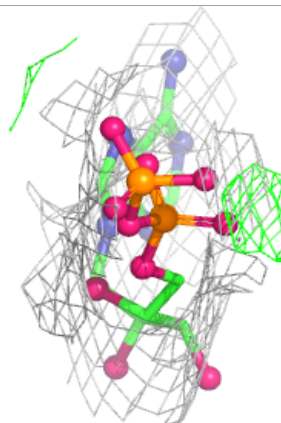
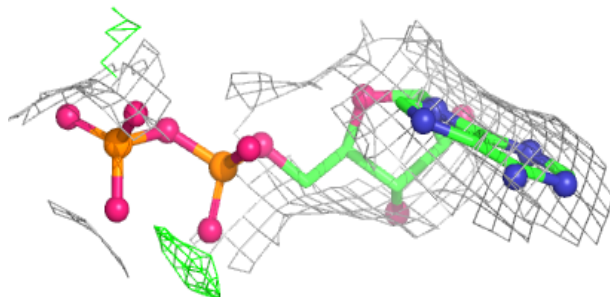
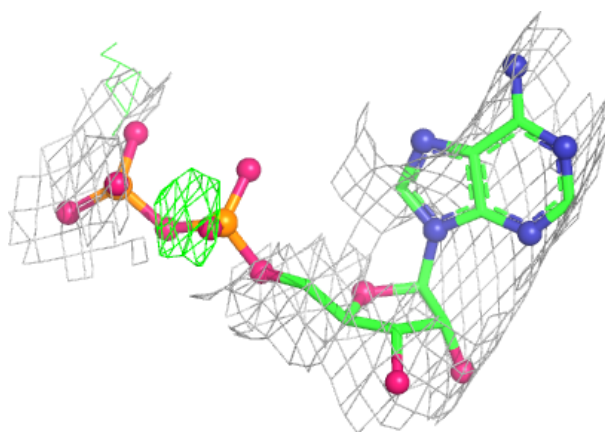


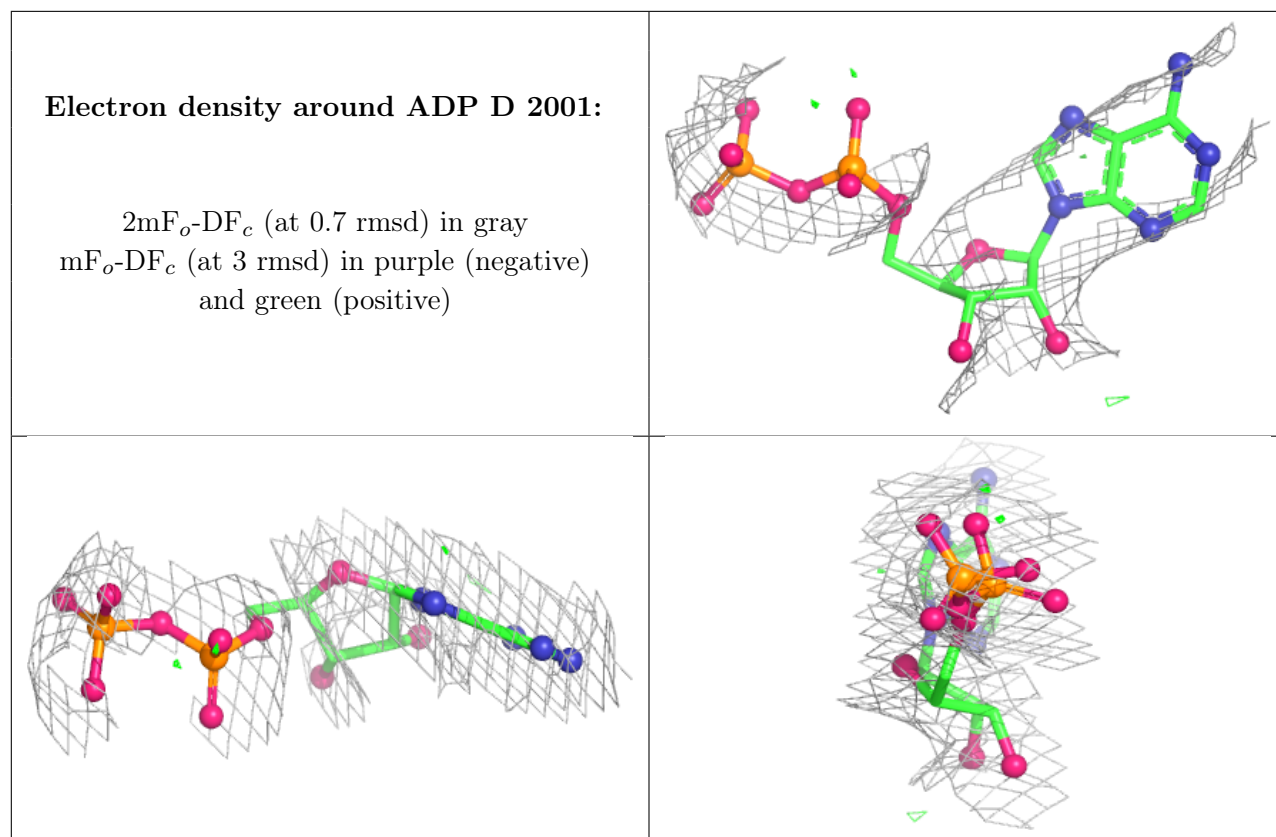
Electron density around ADP E 1001:

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

**Electron density around ADP A 1001:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.