



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 02:17 am BST

PDB ID : 4EIW
Title : Whole cytosolic region of atp-dependent metalloprotease FtsH (G399L)
Authors : Suno, R.; Niwa, H.; Tsuchiya, D.; Yoshida, M.; Morikawa, K.
Deposited on : 2012-04-06
Resolution : 3.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

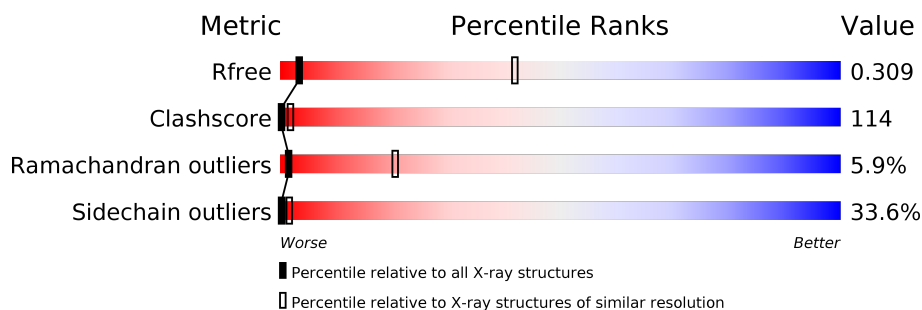
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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}	130704	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)

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

Mol	Chain	Length	Quality of chain
1	A	508	
1	B	508	
1	C	508	
1	D	508	
1	E	508	
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 crite-

ria:

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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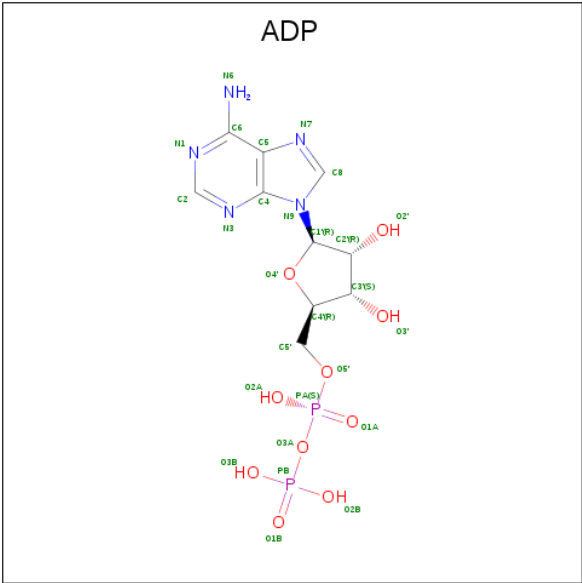
Chain	Residue	Modelled	Actual	Comment	Reference
B	124	GLY	-	EXPRESSION TAG	UNP Q5SI82
B	125	ALA	-	EXPRESSION TAG	UNP Q5SI82
B	399	LEU	GLY	ENGINEERED MUTATION	UNP Q5SI82
C	117	GLY	-	EXPRESSION TAG	UNP Q5SI82
C	118	PRO	-	EXPRESSION TAG	UNP Q5SI82
C	119	LEU	-	EXPRESSION TAG	UNP Q5SI82
C	120	GLY	-	EXPRESSION 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 (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).




GLY
ALA

- Molecule 1: ATP-dependent zinc metalloprotease FtsH

Chain D:  9% 52% 23% 12%

GLU	GLU	ARG	GLU	PRO	ARG	VAL	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY
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- Molecule 1: ATP-dependent zinc metalloprotease FtsH

Chain E:  17% 49% 22% 10%

M370	E371	A372	A373	L374	L375	A376	A377	R378	E379	G380	R381	R382	K383	I384	T385	P386	D387	K388	L389	E390	E391	A392	A393	R394	R395	V396	M397	H398	L399	P400	A401	K402	K403	S404	L405	L406	L407	S408	P409	R410	D411	A412	R413	I414	T415	R416	A417	H418	E419	G420	A421	H422	A423	L424	F428	E430	H431	A432	D433	G434	V435	H436	K437	V438	L439	I440	V441	P442	R443	G444	R445	A446	L447	G448	P449	M450	M451	P452	R453	R454	E455	D456	M457	L458	H459	A520	M460	S461	R462	R463	R464	L465	L466	D467	Q468	L469	A470	V471	A472	L473	A474	G475	R476	A477	A478	E479	E480	I481	V482	H483	D484	V485	L486	T487	G488	A489	E490	M491	D492	F493	R494	K495	A496	L497	L498	L499	L500	T501	E502	V503	G504	M505	H506	E507	V508	G509	M510	H511	E512	R513	F514	V515	A516	Y517	A518	E519	R520	E521	R522	E523	D524	T525	Y526	L527	G528	G529	Y530	D531	V532	R533	A534	Y535	S536	GLU	ALA	ARG																																																																																																																																																																																																																																																																																																																																																																																																																																																
D808	P809	A810	L811	L812	R813	R816	F817	D818	R819	Q820	R821	A822	I823	D824	A825	P826	D827	V828	K829	G830	R831	E832	Q833	I834	L835	R836	L837	H838	A839	R840	G841	K842	P843	L844	A845	E846	E847	V848	D849	L850	A851	L852	L853	A854	K855	R856	T857	P858	G859	F860	V861	D864	L865	E866	N867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935	L936	L937	L938	L939	L940	L941	L942	L943	L944	L945	L946	L947	L948	L949	L950	L951	L952	L953	L954	L955	L956	L957	L958	L959	L960	L961	L962	L963	L964	L965	L966	L967	L968	L969	L970	L971	L972	L973	L974	L975	L976	L977	L978	L979	L980	L981	L982	L983	L984	L985	L986	L987	L988	L989	L990	L991	L992	L993	L994	L995	L996	L997	L998	L999	L1000																																																																																																																																																																																																																																																																																																																																																																																																																										
S179	R180	F181	H182	E183	M184	I188	P189	K190	G191	V192	L193	L194	G195	G196	R662	K663	G199	V200	G201	K202	T203	H204	L205	A206	R207	A208	V209	A210	G211	E212	A213	R214	V215	P216	F217	L218	T219	A220	S221	G222	S223	D224	F225	V226	E227	M228	G233	A234	A235	A236	A300	T301	N302	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V237	R238	D239	L240	F241	N177	V2

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	146.15Å 146.15Å 349.06Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	71.53 – 3.90 71.53 – 3.90	Depositor EDS
% Data completeness (in resolution range)	97.1 (71.53-3.90) 97.1 (71.53-3.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.46 (at 3.89Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.299 , 0.312 0.298 , 0.309	Depositor DCC
R_{free} test set	1967 reflections (5.01%)	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)	0.17 , 19.0	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	0.78	EDS
Total number of atoms	21429	wwPDB-VP
Average B, all atoms (Å ²)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.60	3/3636 (0.1%)	0.95	16/4906 (0.3%)
1	B	0.63	3/3568 (0.1%)	1.01	18/4815 (0.4%)
1	C	0.59	2/3636 (0.1%)	1.03	24/4906 (0.5%)
1	D	0.60	2/3568 (0.1%)	0.98	17/4815 (0.4%)
1	E	0.61	6/3636 (0.2%)	0.96	13/4906 (0.3%)
1	F	0.58	2/3568 (0.1%)	0.96	12/4815 (0.2%)
All	All	0.60	18/21612 (0.1%)	0.98	100/29163 (0.3%)

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

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

All (18) bond length outliers are listed below:

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

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

All (100) bond angle outliers are listed below:

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

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

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

There are no chirality outliers.

All (20) planarity outliers are listed below:

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

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

5.2 Too-close contacts

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

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 114.

All (4895) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:416:ALA:CB	1:E:577:LEU:HD23	1.18	1.63
1:A:416:ALA:HB3	1:A:577:LEU:CD2	1.33	1.58
1:A:416:ALA:CB	1:A:577:LEU:HD23	1.15	1.55
1:F:376:ALA:CA	1:F:381:ARG:HD2	1.31	1.55
1:E:416:ALA:HB3	1:E:577:LEU:CD2	1.35	1.55
1:B:376:ALA:CA	1:B:381:ARG:HD2	1.18	1.54
1:B:376:ALA:HA	1:B:381:ARG:CD	1.38	1.54
1:A:286:MET:HG3	1:A:316:ARG:CD	1.39	1.49
1:B:313:ARG:CD	1:B:314:PRO:HD2	1.42	1.49
1:B:283:LEU:CD1	1:B:316:ARG:NH2	1.77	1.46
1:D:313:ARG:CD	1:D:314:PRO:HD2	1.40	1.46
1:A:586:GLU:HB2	1:A:589:ARG:NH2	1.18	1.46
1:F:311:LEU:HA	1:F:316:ARG:NH1	1.17	1.46
1:A:286:MET:CG	1:A:316:ARG:HD3	1.43	1.45
1:B:283:LEU:CD1	1:B:316:ARG:HH21	1.28	1.45
1:F:313:ARG:CD	1:F:314:PRO:HD2	1.45	1.44
1:E:589:ARG:NH2	1:E:596:LEU:CB	1.82	1.42
1:A:316:ARG:NH1	1:A:317:PHE: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:NH1	1:E:303:ARG:HB2	1.50	1.25
1:A:303:ARG:HB2	1:A:303:ARG:NH1	1.48	1.25
1:A:416:ALA:CB	1:A:577:LEU:CD2	1.98	1.22
1: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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:416:ALA:CB	1:C:577:LEU:HD23	1.78	1.13
1:C:524:ASP:HA	1:C:529:GLY:HA2	1.14	1.13
1:F:395:ARG:HH11	1:F:395:ARG:HG2	1.08	1.12
1:E:524:ASP:HA	1:E:529:GLY:HA2	1.13	1.12
1:A:416:ALA:HB3	1:A:577:LEU:HD21	1.21	1.12
1:E:236:ARG:HG3	1:E:237:VAL:N	1.50	1.12
1:A:413:ARG:HA	1:A:577:LEU:HD22	1.31	1.12
1:F:165:LYS:HD3	1:F:168:LEU:HD22	1.20	1.12
1:A:170:GLU:O	1:A:174:PHE:HB3	1.49	1.12
1:A:342:LYS:NZ	1:F:184:MET:SD	2.23	1.12
1:B:171:ILE:HD11	1:B:296:VAL:HG11	1.16	1.11
1:C:236:ARG:HG3	1:C:237:VAL:N	1.48	1.11
1:C:182:HIS:HB2	1:C:291:LYS:HD2	1.31	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: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:A:286:MET:HG3	1:A:316:ARG:HD2	1.27	1.11
1:E:283:LEU:HG	1:E:316:ARG:NH1	1.64	1.11
1:F:286:MET:HE1	1:F:316:ARG:HA	1.11	1.11
1:D:190:LYS:HE3	1:D:289:PHE:CZ	1.85	1.10
1:E:172:VAL:HG23	1:E:213:ALA:HB2	1.24	1.10
1:D:290:GLU:HG2	1:D:293:THR:HG23	1.28	1.10
1:D:171:ILE:HD11	1:D:296:VAL:HG11	1.15	1.10
1:B:286:MET:HE1	1:B:316:ARG:HA	1.17	1.10
1:C:172:VAL:HG23	1:C:213:ALA:HB2	1.28	1.10
1:A:416:ALA:HB2	1:A:577:LEU:HD23	1.15	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:C:264:ARG:HG3	1:C:266:SER:H	1.08	1.10
1:B:290:GLU:HG2	1:B:293:THR:HG23	1.33	1.10
1:E:182:HIS:HB2	1:E:291:LYS:HD2	1.31	1.10
1: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:F:165:LYS:HE2	1:F:205:LEU:HD23	1.24	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:412:ARG:HH12	1:F:440:ILE:HG21	1.16	1.09
1:E:174:PHE:CE1	1:E:188:ILE:HD11	1.86	1.09
1:B:190:LYS:NZ	1:B:289:PHE:HE2	1.49	1.09
1:D:280:ASN:O	1:D:284:VAL:HG12	1.51	1.09
1:A:311:LEU:HD23	1:A:316:ARG:NH2	1.68	1.09
1:A:428:PHE:CE1	1:A:432:ALA:HA	1.86	1.09
1:F:280:ASN:O	1:F:284:VAL:HG12	1.51	1.09
1:D:376:ALA:HA	1:D:381:ARG:HG3	1.33	1.09
1:E:145:ARG:NH2	1:E:219:THR:OG1	1.84	1.09
1:D:589:ARG:HE	1:D:594:LEU:HD21	1.09	1.09
1:A:378:ARG:HH22	1:F:170:GLU:HB3	1.06	1.09
1:A:286:MET:CB	1:A:316:ARG:HD3	1.81	1.09
1:C:264:ARG:CG	1:C:266:SER:H	1.66	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: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:262:ARG:HB3	1:C:275:ARG:HH12	1.10	1.08
1:D:286:MET:HE1	1:D:316:ARG:HA	1.23	1.08
1:D:413:ARG:HG2	1:D:413:ARG:HH11	1.08	1.08
1:C:174:PHE:CE1	1:C:188:ILE:HD11	1.87	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:F:238:ARG:NH1	1:F:239:ASP:N	2.02	1.08
1:B:382:ARG:HH11	1:B:382:ARG:HG3	1.10	1.08
1:F:238:ARG:NH1	1:F:239:ASP:H	1.50	1.08
1:C:170:GLU:O	1:C:174:PHE:HB3	1.50	1.07
1:A:182:HIS:HB2	1:A:291:LYS:HD2	1.27	1.07
1:D:316:ARG:HH11	1:D:316:ARG:HG3	0.99	1.07
1:D:318:ASP:O	1:D:319:ARG:HB2	1.48	1.07
1: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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:LYS:HD2	1:A:276:GLU:CD	1.77	1.04
1:C:263:LYS:NZ	1:C:276:GLU:CD	2.10	1.04
1:E:533:ARG:NH2	1:E:534:GLN:O	1.91	1.04
1:F:313:ARG:HD2	1:F:314:PRO:HD2	1.05	1.04
1:A:263:LYS:NZ	1:A:276:GLU:CD	2.11	1.03
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:E:152:LYS:HG3	1:E:153:VAL:HG23	1.39	1.03
1:A:225:PHE:HE1	1:A:233:GLY:CA	1.71	1.03
1:F:482:VAL:HG13	1:F:483:PHE:HD2	1.24	1.03
1:B:482:VAL:HG13	1:B:483:PHE:HD2	1.21	1.03
1:B:376:ALA:CA	1:B:381:ARG:CD	2.10	1.03
1:E:263:LYS:HD2	1:E:276:GLU:CD	1.79	1.03
1:A:342:LYS:HD3	1:F:184:MET:O	1.58	1.03
1:E:147:LEU:HD21	1:E:151:PRO:CB	1.88	1.03
1:B:337:ILE:HD12	1:B:340:ARG:HH12	1.19	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:263:LYS:NZ	1:E:276:GLU:CD	2.12	1.02
1:E:449:PHE:CE2	1:E:496:GLN:HG2	1.93	1.02
1:A:374:LEU:HD11	1:F:187:ARG:H	1.24	1.02
1:C:218:ILE:HD11	1:C:250:CYS:SG	2.00	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: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:C:147:LEU:HD21	1:C:151:PRO:CB	1.88	1.01
1:B:165:LYS:HE2	1:B:205:LEU:HD23	1.38	1.01
1:A:533:ARG:NH2	1:A:534:GLN:O	1.94	1.01
1:B:459:HIS:O	1:B:459:HIS:ND1	1.92	1.01
1:C:152:LYS:HG3	1:C:153:VAL:HG23	1.42	1.01
1: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:PRO:HB3	1:B:360:PHE:O	1.60	1.01
1:C:589:ARG:HB3	1:C:589:ARG:NH1	1.76	1.01
1:D:453:ARG:CZ	1:D:495:ARG:HH21	1.73	1.01
1: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:NH1	1:D:382:ARG:HG3	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:E:286:MET:HG3	1:E:316:ARG:HD2	1.40	1.00
1:B:439:THR:HG23	1:B:445:ARG:HH22	1.25	1.00
1: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:E:212:GLU:C	1:E:214:ARG:HG3	1.82	0.99
1:A:378:ARG:HH22	1:F:170:GLU:CB	1.75	0.99
1:B:348:VAL:CG2	1:B:352:LEU:HD22	1.92	0.99
1:D:439:THR:HG23	1:D:445:ARG:HH22	1.23	0.99
1:A:166:GLU:HA	1:A:169:LYS:HG2	1.42	0.99
1:E:173:GLU:HA	1:E:176:LYS:CG	1.92	0.99
1:B: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:D:381:ARG:HH22	1:D:388:ASP:CG	1.66	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
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:O	1:F:459:HIS:ND1	1.94	0.98
1:A:311:LEU:CA	1:A:316:ARG:HH22	1.75	0.98
1: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:286:MET:CG	1:C:316:ARG:CD	2.41	0.98
1:C:190:LYS:HD2	1:C:289:PHE:CE1	1.98	0.98
1:E: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: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: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:A:378:ARG:HA	1:F:173:GLU:OE1	1.63	0.97
1:F:171:ILE:CD1	1:F:296:VAL:HG11	1.93	0.97
1:D:337:ILE:HD12	1:D:340:ARG:HH12	1.29	0.97
1: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:166:GLU:HB2	1:A:169:LYS:HZ2	1.31	0.95
1:D:439:THR:HG23	1:D:445:ARG:NH2	1.80	0.95
1:B:578:GLU:HG2	1:B:579:ARG:N	1.81	0.95
1:E:263:LYS:NZ	1:E:276:GLU:OE1	1.99	0.95
1: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: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
1:B:310:ALA:C	1:B:316:ARG:NH1	2.21	0.94
1:E:511:HIS:NE2	1:E:516:PRO:HD3	1.81	0.94
1:F:319:ARG:HH11	1:F:319:ARG:HG2	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:VAL:O	1:D:279:LEU:HD11	1.68	0.94
1:B:203:THR:OG1	2:B:2001:ADP:O2A	1.84	0.94
1:D:190:LYS:NZ	1:D:289:PHE:HE2	1.65	0.94
1:D:453:ARG:NH1	1:D:495:ARG:HH21	1.65	0.94
1:A:413:ARG:HA	1:A:577:LEU:CD2	1.98	0.94
1: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: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:A:511:HIS:NE2	1:A:516:PRO:HD3	1.83	0.94
1:C:533:ARG:NH2	1:C:534:GLN:O	2.01	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:291:LYS:HG3	1:D:292:ASP:N	1.81	0.93
1:E:236:ARG:HH11	1:E:236:ARG:HG2	1.32	0.93
1: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:E:286:MET:HE1	1:E:297:VAL:HG11	1.50	0.92
1:F:215:VAL:CG2	1:F:216:PRO:HD2	1.99	0.92
1:A:262:ARG:CB	1:A:275:ARG:HH12	1.82	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:CE	1:D:289:PHE:CZ	2.51	0.92
1:D:190:LYS:NZ	1:D:289:PHE:CE2	2.37	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
1:A:453:ARG:HH11	1:A:453:ARG:HG3	1.34	0.91
1:A:453:ARG:NH1	1:A:460:TRP:HZ2	1.67	0.91
1:B:460:TRP:HE3	1:B:460:TRP:H	1.18	0.91
1:C:286:MET:HE1	1:C:297:VAL:HG11	1.51	0.91
1:F:233:GLY:CA	1:F:236:ARG:HH22	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:439:THR:HG23	1:F:445:ARG:HH22	1.34	0.91
1:C: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:NH1	1:D:316:ARG:HG3	1.83	0.91
1:F:233:GLY:CA	1:F:236:ARG:NH2	2.32	0.91
1:D:257:ILE:O	1:D:260:VAL:N	2.03	0.91
1:F:313:ARG:HD2	1:F:314:PRO:CD	1.97	0.91
1:C:274:GLU:O	1:C:277:GLN:HB3	1.70	0.91
1:A:174:PHE:CZ	1:A:188:ILE:HD11	2.05	0.91
1:C: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: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: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:A:313:ARG:HH22	1:A:526:TYR:C	1.75	0.90
1:B:412:ARG:HH12	1:B:440:ILE:CG2	1.85	0.90
1: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:A:201:GLY:N	2:A:1001:ADP:O1A	2.03	0.90
1:A:168:LEU:HB2	1:A:171:ILE:CD1	2.01	0.90
1:B:376:ALA:CB	1:B:381:ARG:HD2	2.01	0.90
1:B:376:ALA:HA	1:B:381:ARG:NE	1.87	0.89
1:E:262:ARG:CB	1:E:275:ARG:HH12	1.83	0.89
1:F:487:THR:HG22	1:F:488:THR:H	1.36	0.89
1:C:286:MET:CB	1:C:316:ARG:CG	2.47	0.89
1: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:NH1	1:B:395:ARG:HG2	1.83	0.89
1:C:292:ASP:HB2	1:D:227:GLU:OE2	1.72	0.89
1:A:236:ARG:CG	1:A:237:VAL:N	2.35	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:ARG:NH1	1:B:413:ARG:HG2	1.78	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:D:352:LEU:HD21	1:D:386:MET:HE1	1.55	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:HE3	1:D:460:TRP:H	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:C:263:LYS:CD	1:C:276:GLU:CD	2.40	0.89
1:E:533:ARG:HD2	1:E:534:GLN:H	1.36	0.89
1:F:257:ILE:O	1:F:260:VAL:N	2.05	0.89
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
1:D:327:ASP:OD1	1:D:328:VAL:N	2.06	0.88
1:A:166:GLU:HB2	1:A:169:LYS:NZ	1.89	0.88
1:C: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:C:313:ARG:HH22	1:C:526:TYR:C	1.77	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:CG	1:B:356:ARG:HH11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:LYS:HE2	1:B:578:GLU:O	1.72	0.88
1:C:412:ARG:NH1	1:C:577:LEU:O	2.06	0.88
1:E:211:GLY:O	1:E:214:ARG:HD2	1.72	0.88
1:E:176:LYS:HD3	1:E:213:ALA:HA	1.54	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:B:382:ARG:NH1	1:B:382:ARG:HG3	1.74	0.88
1:D:165:LYS:CD	1:D:168:LEU:HD22	2.03	0.88
1:D:168:LEU:O	1:D:171:ILE:HG22	1.73	0.88
1:D:173:GLU:O	1:D:176:LYS:HG2	1.74	0.88
1:A:311:LEU:CD2	1:A:316:ARG:HH22	1.88	0.87
1:A:453:ARG:HH22	1:A:464:ARG:HH12	1.23	0.87
1:B:482:VAL:HG13	1:B:483:PHE:CD2	2.09	0.87
1:F:302:ASN:HD21	1:F:443:ARG:NH2	1.71	0.87
1:C:384:ILE:HG23	1:C:388:ASP:HB2	1.56	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:A:263:LYS:CD	1:A:276:GLU:CD	2.42	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
1:F:165:LYS:CD	1:F:168:LEU:HD22	2.04	0.87
1:F:159:ALA:HB3	1:F:334:ILE:HG13	1.57	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:NH1	1:F:395:ARG:HG2	1.81	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:H	1:F:460:TRP:HE3	1.19	0.87
1:F:470:ALA:O	1:F:558:VAL:HG21	1.74	0.87
1:C:410:ARG:O	1:C:413:ARG:N	2.07	0.87
1:E:313:ARG:HH22	1:E:526:TYR:C	1.77	0.87
1:D: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:338:HIS:ND1	1:D:366:GLU:HG3	1.90	0.87
1:F:286:MET:HE1	1:F:316:ARG:CA	2.03	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:301:THR:HG21	1:B:307:LEU:HD11	1.57	0.86
1:B:283:LEU:HD12	1:B:316:ARG:NH2	1.86	0.86
1:C:536:SER:OG	1:D:544:ASP:OD2	1.94	0.86
1:D:164:ALA:O	1:D:168:LEU:HD13	1.73	0.86
1:D:370:ASN:OD1	1:D:371:GLU:N	2.08	0.86
1:F:370:ASN:OD1	1:F:371:GLU:N	2.08	0.86
1:A:342:LYS:CD	1:A:343:PRO:HD2	2.04	0.86
1:A:313:ARG:CZ	1:A:526:TYR:HA	2.05	0.86
1:C:308:ASP:OD1	1:C:310:ALA:N	2.09	0.86
1:E:263:LYS:CD	1:E:276:GLU:CD	2.44	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:346:GLU:HG2	1:F:348:VAL:H	1.41	0.85
1:F:382:ARG:NH1	1:F:382:ARG:HG3	1.73	0.85
1:A:155:PHE:CZ	1:A:168:LEU:HD11	2.11	0.85
1: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: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:F:526:TYR:O	1:F:527:LEU:C	2.15	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:311:LEU:O	1:D:316:ARG:CG	2.25	0.85
1:D:159:ALA:HB3	1:D:334:ILE:HG13	1.56	0.85
1:E:173:GLU:HA	1:E:176:LYS:HG2	1.59	0.85
1:F:168:LEU:O	1:F:171:ILE:HG22	1.74	0.85
1:A: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:CZ	1:C:589:ARG:HB3	2.07	0.85
1:D:356:ARG:CG	1:D:356:ARG:HH11	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:NH1	1:B:356:ARG:HG3	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:384:ILE:CG2	1:A:388:ASP:HB2	2.08	0.84
1:B:352:LEU:HD21	1:B:386:MET:HE1	1.59	0.84
1:B:460:TRP:HE3	1:B:460:TRP:N	1.74	0.84
1:C:509:GLY:C	1:D:476:ARG:HH22	1.80	0.84
1:D:470:ALA:O	1:D:558:VAL:HG21	1.77	0.84
1:B:345:ALA:HB2	1:B:383:LYS:HE3	1.57	0.84
1:E:163:GLU:OE1	1:E:163:GLU:N	2.11	0.84
1:A:202:LYS:HD2	1:A:300:ALA:HB1	1.59	0.84
1: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:NH1	1:D:395:ARG:HG2	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:263:LYS:HZ2	1:A:276:GLU:CD	1.79	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:A:151:PRO:HD2	1:A:211:GLY:HA2	1.59	0.84
1:F:214:ARG:HH11	1:F:214:ARG:HG3	1.38	0.84
1:A:263:LYS:CE	1:A:276:GLU:CD	2.46	0.84
1:A:428:PHE:CD1	1:A:432:ALA:HA	2.13	0.84
1:F:356:ARG:CG	1:F:356:ARG:HH11	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:NH1	1:F:356:ARG:HG3	1.83	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:A:509:GLY:C	1:B:476:ARG:HH22	1.81	0.83
1:C:470:ALA:HB1	1:C:558:VAL:HG23	1.59	0.83
1:B:526:TYR:O	1:B:527:LEU:C	2.17	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
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:HD12	1:D:257:ILE:H	1.43	0.83
1:E:215:VAL:CG2	1:E:250:CYS:HA	2.09	0.83
1:F:253:PHE:HE2	1:F:255:ASP:HB2	1.42	0.83
1: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:D:526:TYR:O	1:D:527:LEU:C	2.16	0.82
1:E:223:SER:O	1:E:225:PHE:N	2.11	0.82
1:F:345:ALA:HB2	1:F:383:LYS:CE	2.08	0.82
1: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:376:ALA:C	1:D:381:ARG:HG3	1.99	0.82
1:E:197:PRO:HD2	1:E:200:VAL:HG21	1.61	0.82
1: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:HB2	1:E:207:ARG:CZ	2.10	0.82
1:C:197:PRO:HD2	1:C:200:VAL:HG21	1.59	0.82
1:C:263:LYS:CE	1:C:276:GLU:CD	2.47	0.82
1: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:C:460:TRP:O	1:D:488:THR:HA	1.80	0.82
1:E:223:SER:C	1:E:225:PHE:H	1.81	0.82
1:A:377:ALA:HB1	1:F:181:PHE:CE1	2.15	0.82
1:F:262:ARG:HG3	1:F:263:LYS:H	1.45	0.82
1: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:B:313:ARG:HG3	1:B:314:PRO:CD	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:286:MET:CE	1:F:316:ARG:HA	2.04	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:337:ILE:HD12	1:B:340:ARG:NH1	1.96	0.81
1:F:579:ARG:O	1:F:579:ARG:HG2	1.78	0.81
1:A:207:ARG:CZ	1:A:207:ARG:HB2	2.10	0.81
1:A:352:LEU:HD12	1:A:356:ARG:HH21	1.45	0.81
1:B:209:VAL:HG13	1:B:210:ALA:H	1.44	0.81
1:D:378:ARG:C	1:D:380:GLY:H	1.84	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: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:E:352:LEU:HD21	1:E:386:MET:SD	2.21	0.81
1:E:371:GLU:HG3	1:E:392:ALA:HB1	1.62	0.81
1: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:N	1:F:460:TRP:HE3	1.77	0.81
1:A:178:PRO:HB3	1:A:294:ALA:HB2	1.62	0.80
1:B:430:GLU:OE1	1:B:430:GLU:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:223:SER:C	1:C:225:PHE:H	1.84	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:CG	1:E:236:ARG:HH11	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:168:LEU:C	1:A:171:ILE:HD13	2.02	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:D:286:MET:CE	1:D:316:ARG:HA	2.09	0.80
1:E:215:VAL:HG11	1:E:250:CYS:HA	1.64	0.80
1:E:352:LEU:CD1	1:E:356:ARG:HH21	1.95	0.80
1:A:225:PHE:HE1	1:A:233:GLY:HA2	1.44	0.80
1:A:233:GLY:HA2	1:A:236:ARG:NH1	1.96	0.80
1:A:339:ALA:HA	1:A:369:LEU:HD21	1.63	0.80
1: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:A:223:SER:C	1:A:225:PHE:H	1.85	0.80
1:F:450:MET:HA	1:F:453:ARG:HD2	1.63	0.80
1:E:210:ALA:HB2	1:E:251:ILE:HD12	1.63	0.79
1:F:468:GLN:O	1:F:471:VAL:HG22	1.82	0.79
1:F:449:PHE:CE2	1:F:453:ARG:NH2	2.50	0.79
1: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:286:MET:HE1	1:D:316:ARG:CA	2.08	0.79
1:F:325:ALA:HB3	1:F:326:PRO:HD3	1.65	0.79
1:B:165:LYS:HA	1:B:168:LEU:HD22	1.64	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:E:509:GLY:C	1:F:476:ARG:HH22	1.85	0.79
1:A:461:SER:HA	1:B:487:THR:O	1.82	0.79
1:C:354:ALA:O	1:C:357:THR:HG23	1.83	0.79
1:F:376:ALA:C	1:F:381:ARG:HD2	2.03	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:E:263:LYS:CE	1:E:276:GLU:CD	2.50	0.78
1:F:241:PHE:O	1:F:244:ALA:N	2.16	0.78
1:A:236:ARG:CG	1:A:236:ARG:HH11	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:F:378:ARG:C	1:F:380:GLY:H	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:286:MET:CB	1:E:316:ARG:CG	2.45	0.78
1:C:396:VAL:O	1:C:400:PRO:HD3	1.83	0.78
1:D:199:GLY:N	2:D:2001:ADP:O2B	2.15	0.78
1:A:215:VAL:CG2	1:A:250:CYS:HA	2.14	0.78
1: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: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:CG	1:D:319:ARG:HH11	1.96	0.78
1:D:382:ARG:NH1	1:D:382:ARG:CG	2.17	0.78
1:F:236:ARG:HG2	1:F:237:VAL:N	1.97	0.78
1:C:346:GLU:OE1	1:C:346:GLU:N	2.17	0.78
1:E:233:GLY:O	1:E:236:ARG:HG2	1.82	0.78
1:E:533:ARG:HD2	1:E:534:GLN:N	1.99	0.78
1:B:313:ARG:NE	1:B:314:PRO:HD2	1.99	0.78
1: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
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:263:LYS:HD2	1:A:276:GLU:OE1	1.79	0.77
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:F:352:LEU:HD11	1:F:386:MET:HE1	1.65	0.77
1:A:346:GLU:N	1:A:346:GLU:OE1	2.17	0.77
1:B:155:PHE:CD2	1:B:212:GLU:OE2	2.36	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:582:LEU:HD21	1:B:590:VAL:HG21	1.65	0.77
1:E:346:GLU:OE1	1:E:346:GLU:N	2.18	0.77
1:E:357:THR:HG1	1:E:360:PHE:HD1	1.33	0.77
1:F:165:LYS:HA	1:F:168:LEU:HD22	1.66	0.77
1:F:215:VAL:HG21	1:F:249:PRO:O	1.84	0.77
1:A:418:HIS:O	1:A:421:GLY:N	2.18	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: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:CG	1:B:413:ARG:HH11	1.95	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: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
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:453:ARG:HH11	1:E:453:ARG:HG3	1.50	0.76
1:E:449:PHE:CE2	1:E:496:GLN:CG	2.67	0.76
1:B:276:GLU:HA	1:B:279:LEU:CD1	2.15	0.76
1:C:503:ARG:HD2	1:C:508:TRP:CE2	2.20	0.76
1:C:313:ARG:HH22	1:C:526:TYR:HA	1.50	0.76
1: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:348:VAL:HG21	1:B:352:LEU:CD2	2.15	0.76
1:B:331:ARG:NH2	1:B:580:GLU:OE1	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:CE3	1:B:460:TRP:N	2.52	0.75
1:D:588:GLN:O	1:D:591:VAL:HB	1.86	0.75
1:E:339:ALA:CA	1:E:369:LEU:HD21	2.15	0.75
1: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:F:451:MET:HB3	1:F:452:PRO:HD3	1.69	0.75
1:A:219:THR:HB	1:A:253:PHE:HD2	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:PRO:HD2	1:B:200:VAL:HG11	1.69	0.75
1: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
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: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:B:451:MET:HB3	1:B:452:PRO:HD3	1.69	0.74
1:D:412:ARG:HH22	1:D:440:ILE:HB	1.49	0.74
1: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:381:ARG:HG3	1:C:381:ARG:HH11	1.52	0.74
1:C:313:ARG:CZ	1:C:526:TYR:O	2.34	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:310:ALA:C	1:B:316:ARG:HH12	1.86	0.74
1:B:503:ARG:HH12	1:B:522:ARG:HH21	1.35	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:LEU:HD11	1:B:569:LEU:HA	1.69	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: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:236:ARG:O	1:A:237:VAL:C	2.26	0.74
1:A:264:ARG:HG3	1:A:265:GLY:N	2.02	0.74
1:A:249:PRO:HA	1:A:294:ALA:O	1.87	0.74
1:F:331:ARG:NH1	1:F:357:THR:O	2.19	0.74
1:B:378:ARG:C	1:B:380:GLY:H	1.89	0.74
1:C:342:LYS:HD2	1:C:343:PRO:CD	2.16	0.74
1:E:465:LEU:HD22	1:E:508:TRP:CZ3	2.22	0.74
1:A:165:LYS:O	1:A:168:LEU:HG	1.87	0.74
1:C:449:PHE:CE2	1:C:496:GLN:CG	2.68	0.74
1:F:458:LEU:HD12	1:F:459:HIS:H	1.53	0.74
1:A:390:GLU:O	1:A:393:ALA:HB3	1.88	0.74
1:A:313:ARG:NH2	1:A:526:TYR:O	2.20	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: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: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:381:ARG:HG3	1:A:381:ARG:HH11	1.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:376:ALA:C	1:B:381:ARG:HB2	2.08	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
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:358:PRO:HA	1:C:359:GLY:C	2.08	0.73
1:C:474:ALA:HA	1:C:558:VAL:HG11	1.70	0.73
1:A:441:VAL:O	1:A:441:VAL:HG12	1.88	0.73
1: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:HA	1:D:430:GLU:OE1	1.88	0.73
1:D:439:THR:CG2	1:D:445:ARG:HH22	2.00	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: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: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:155:PHE:HA	1:D:158:VAL:HG23	1.71	0.73
1:D:153:VAL:HB	1:D:207:ARG:HH11	1.54	0.73
1:E:382:ARG:HG3	1:E:383:LYS:H	1.51	0.73
1: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HH11	1:F:316:ARG:HG2	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
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:OE1	1:B:163:GLU:N	2.22	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:331:ARG:NH1	1:C:354:ALA:O	2.22	0.72
1:D:173:GLU:HA	1:D:176:LYS:HE3	1.71	0.72
1:D:215:VAL:HG21	1:D:249:PRO:O	1.89	0.72
1:D:171:ILE:HG13	1:D:296:VAL:HG21	1.70	0.72
1:D:283:LEU:CD1	1:D:316:ARG:HH21	2.01	0.72
1:D:454:ARG:HH21	1:D:526:TYR:C	1.93	0.72
1:C: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:392:ALA:O	1:F:396:VAL:HG12	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:SER:O	1:A:464:ARG:HB3	1.89	0.72
1:C:224:ASP:HA	1:C:227:GLU:OE2	1.89	0.72
1:E:236:ARG:O	1:E:237:VAL:C	2.27	0.72
1:E:441:VAL:HG12	1:E:441:VAL:O	1.89	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:B:454:ARG:HH21	1:B:526:TYR:C	1.91	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:F:466:LEU:HD11	1:F:504:MET:HE1	1.72	0.72
1:A:382:ARG:HG3	1:A:383:LYS:CB	2.20	0.72
1:B:286:MET:HE1	1:B:316:ARG:CA	2.09	0.72
1:B:286:MET:O	1:B:289:PHE:CB	2.37	0.72
1:D:214:ARG:HB3	1:D:214:ARG:HH11	1.54	0.72
1:F:376:ALA:C	1:F:381:ARG:HB2	2.10	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: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: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:B:184:MET:O	1:C:342:LYS:HD3	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:358:PRO:HA	1:A:359:GLY:C	2.11	0.71
1:B:352:LEU:O	1:B:355:LYS:HB2	1.90	0.71
1: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:N	1:F:163:GLU:OE1	2.24	0.71
1:A:467:ASP:OD1	1:A:557:ARG:NH2	2.24	0.71
1:A:488:THR:O	1:A:490:ALA:N	2.21	0.71
1:A:474:ALA:HA	1:A:558:VAL:HG11	1.70	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:465:LEU:O	1:D:469:ILE:HG13	1.89	0.71
1:D:424:LEU:HD11	1:D:569:LEU:HA	1.72	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:HG3	1:B:533:ARG:HH11	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:C:236:ARG:O	1:C:237:VAL:C	2.29	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:HA	1:E:419:GLU:OE1	1.92	0.70
1:A:340:ARG:C	1:A:342:LYS:H	1.92	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: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:376:ALA:C	1:D:381:ARG:CG	2.60	0.70
1:D:389:LEU:O	1:D:392:ALA:N	2.25	0.70
1: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:GLU:HG3	1:F:263:LYS:HZ3	1.57	0.70
1:A:224:ASP:HA	1:A:227:GLU:OE2	1.91	0.70
1:A:196:GLY:HA2	1:A:443:ARG:HH21	1.55	0.70
1:C:333:GLN:HG3	1:C:336:ARG:NH1	2.06	0.70
1:C:340:ARG:C	1:C:342:LYS:H	1.95	0.70
1:D:165:LYS:O	1:D:168:LEU:HB2	1.91	0.70
1:D:220:ALA:O	1:D:254:ILE:HA	1.91	0.70
1: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:E:215:VAL:CG1	1:E:250:CYS:HA	2.22	0.70
1:E:286:MET:O	1:E:289:PHE:CZ	2.45	0.70
1:A:381:ARG:N	1:F:180:ARG:NH2	2.40	0.70
1: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:340:ARG:C	1:E:342:LYS:H	1.93	0.69
1:E:453:ARG:NH2	1:E:460:TRP:NE1	2.35	0.69
1:F:394:ASP:HA	1:F:397:MET:CE	2.22	0.69
1:F:454:ARG:HH21	1:F:526:TYR:C	1.94	0.69
1:F:355:LYS:CE	1:F:578:GLU:O	2.40	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:CD2	1:E:449:PHE:N	2.60	0.69
1:E:503:ARG:HD2	1:E:508:TRP:CE2	2.27	0.69
1:A:215:VAL:HG21	1:A:250:CYS:CA	2.21	0.69
1:A:286:MET:HE1	1:A:297:VAL:HG11	1.74	0.69
1: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:D:564:GLU:C	1:D:566:ARG:H	1.95	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:173:GLU:HA	1:F:176:LYS:HE3	1.74	0.69
1:F:158:VAL:HG22	1:F:204:HIS:CE1	2.26	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:358:PRO:HA	1:E:359:GLY:C	2.11	0.69
1:E:382:ARG:HD3	1:E:383:LYS:HB3	1.74	0.69
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:286:MET:CE	1:B:316:ARG:HA	2.09	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:424:LEU:O	1:D:427:HIS:N	2.23	0.69
1:D:355:LYS:CE	1:D:578:GLU:O	2.41	0.69
1:E:303:ARG:HH11	1:E:303:ARG:HB2	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:584:ALA:O	1:A:587:PHE:HB3	1.92	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:F:242:GLU:HA	1:F:245:LYS:HB3	1.73	0.69
1:A:469:ILE:HG23	1:A:497:ALA:HB1	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:234:ALA:HB1	1:E:281:GLN:NE2	2.08	0.69
1:E:340:ARG:O	1:E:342:LYS:N	2.25	0.69
1:F:365:LEU:O	1:F:368:LEU:HB3	1.93	0.69
1:A:486:VAL:HG21	1:F:463:LYS:HE3	1.73	0.69
1:C:357:THR:OG1	1:C:360:PHE:CD1	2.46	0.69
1:D:503:ARG:HH22	1:D:522:ARG:NH2	1.91	0.69
1: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:215:VAL:CG2	1:B:249:PRO:O	2.41	0.69
1:B:193:LEU:HA	1:B:299:ALA:O	1.92	0.69
1:C:178:PRO:HB3	1:C:294:ALA:CB	2.23	0.69
1:C:286:MET:O	1:C:289:PHE:CZ	2.46	0.69
1: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:NH1	1:E:453:ARG:HG3	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:235:ALA:HA	1:B:238:ARG:CD	2.23	0.68
1:B:220:ALA:O	1:B:254:ILE:HA	1.94	0.68
1:D:263:LYS:HZ3	1:E:227:GLU:HG3	1.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:319:ARG:HH21	1:B:402:LYS:HZ1	1.39	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:F:564:GLU:C	1:F:566:ARG:H	1.95	0.68
1:B:201:GLY:O	1:B:205:LEU:HD13	1.94	0.68
1:B: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:245:LYS:C	1:B:247:HIS:H	1.97	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:245:LYS:C	1:F:247:HIS:H	1.97	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
1:D:174:PHE:CZ	1:D:294:ALA:HB1	2.29	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:B:466:LEU:HD11	1:B:504:MET:HE1	1.75	0.67
1:C:313:ARG:HH12	1:C:526:TYR:C	1.97	0.67
1: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:CG	1:B:395:ARG:HH11	1.98	0.67
1:C:168:LEU:O	1:C:171:ILE:HD12	1.95	0.67
1:C:263:LYS:HZ1	1:C:276:GLU:CD	1.98	0.67
1:D:188:ILE:HG23	1:D:189:PRO:CD	2.24	0.67
1:D:376:ALA:C	1:D:381:ARG:HB2	2.15	0.67
1:F:174:PHE:CZ	1:F:294:ALA:HB1	2.28	0.67
1:B:564:GLU:C	1:B:566:ARG:H	1.95	0.67
1:C:519:TYR:HA	1:C:533:ARG:NH2	2.09	0.67
1:D:253:PHE:HA	1:D:298:MET:HB3	1.76	0.67
1:D:236:ARG:HH12	1:D:278:THR:HG22	1.59	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:334:ILE:HD13	2:E:1001:ADP:C6	2.30	0.67
1:E:331:ARG:HD2	1:E:357:THR:HG23	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:263:LYS:HZ2	1:E:276:GLU:CD	1.80	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:E:357:THR:OG1	1:E:360:PHE:CD1	2.48	0.67
1:D:452:PRO:HG3	1:E:402:LYS:HE3	1.77	0.67
1:F:190:LYS:HE3	1:F:289:PHE:CZ	2.30	0.67
1:A:378:ARG:HA	1:F:173:GLU:CD	2.14	0.67
1:A:523:GLU:N	1:A:523:GLU:OE1	2.27	0.67
1:C:449:PHE:CB	1:C:468:GLN:HE22	2.08	0.67
1:D:154:THR:HG23	1:D:156:LYS:HB3	1.77	0.67
1:C:517:VAL:HG23	1:D:498:THR:OG1	1.95	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:273:ASP:OD1	1:C:274:GLU:N	2.28	0.67
1:C:196:GLY:O	1:C:302:ASN:HA	1.95	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:238:ARG:HG2	1:D:281:GLN:HE22	1.59	0.66
1:D:193:LEU:HA	1:D:299:ALA:O	1.93	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:311:LEU:C	1:F:311:LEU:HD12	2.14	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:245:LYS:C	1:D:247:HIS:H	1.98	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:HG2	1:A:580:GLU:O	1.94	0.66
1:B:228:MET:SD	1:B:232:VAL:HG12	2.35	0.66
1:D:394:ASP:HA	1:D:397:MET:HE3	1.77	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
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: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:A:453:ARG:NH2	1:A:464:ARG:HH22	1.93	0.66
1:C:207:ARG:HH21	1:C:217:PHE:HD2	1.42	0.66
1:C:207:ARG:NH2	1:C:217:PHE:HD2	1.93	0.66
1:D:241:PHE:CD2	1:D:285:GLU:HG3	2.31	0.66
1:D:225:PHE:HB3	1:D:278:THR:HG21	1.77	0.66
1: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:OE1	1:C:523:GLU:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:D:241:PHE:CE2	1:D:285:GLU:HG3	2.31	0.66
1:A:381:ARG:O	1:F:180:ARG:NH2	2.29	0.66
1:A:155:PHE:HZ	1:A:168:LEU:HD11	1.59	0.66
1:C:585:GLU:O	1:C:588:GLN:HG2	1.94	0.66
1:D:200:VAL:HG22	1:D:202:LYS:HD2	1.78	0.66
1:F:428:PHE:CE1	1:F:432:ALA:HB1	2.30	0.66
1: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:A:225:PHE:HE1	1:A:233:GLY:C	1.98	0.65
1:B:178:PRO:HG3	1:B:249:PRO:HG3	1.78	0.65
1:B:589:ARG:HB3	1:B:594:LEU:CD2	2.26	0.65
1: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:500:LEU:O	1:C:503:ARG:HB3	1.96	0.65
1:D:343:PRO:HG2	1:D:383:LYS:HA	1.79	0.65
1:D:466:LEU:HD11	1:D:504:MET:HE1	1.77	0.65
1:E:155:PHE:HZ	1:E:168:LEU:HD11	1.58	0.65
1:D:508:TRP:HD1	1:E:491:GLU:HG2	1.61	0.65
1:A:169:LYS:O	1:A:172:VAL:HG13	1.96	0.65
1:A:202:LYS:HB2	2:A:1001:ADP:O1B	1.96	0.65
1:A:316:ARG:HG2	1:A:317:PHE:N	2.11	0.65
1:A:357:THR:OG1	1:A:360:PHE:CD1	2.49	0.65
1:A:196:GLY:CA	1:A:443:ARG:NH2	2.60	0.65
1:B:263:LYS:HZ3	1:C:227:GLU:HG3	1.59	0.65
1: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:D:487:THR:HG22	1:D:488:THR:N	2.07	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:273:ASP:CG	1:C:274:GLU:N	2.49	0.65
1:C:333:GLN:HA	1:C:336:ARG:CZ	2.26	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:E:225:PHE:HE1	1:E:233:GLY:C	2.00	0.65
1:E:313:ARG:HH12	1:E:526:TYR:C	1.99	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:202:LYS:HG2	2:F:2001:ADP:O1A	1.97	0.65
1:F:160:GLY:H	1:F:333:GLN:NE2	1.95	0.65
1:A:275:ARG:O	1:A:279:LEU:HB2	1.96	0.65
1:A:419:GLU:HA	1:A:419:GLU:OE1	1.97	0.65
1:B:188:ILE:HG23	1:B:189:PRO:CD	2.24	0.65
1:B:311:LEU:HD12	1:B:311:LEU:C	2.16	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:352:LEU:O	1:D:355:LYS:N	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:F:463:LYS:O	1:F:466:LEU:N	2.30	0.65
1:B:514:PHE:HB3	1:B:519:TYR:HE1	1.62	0.65
1: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:D:263:LYS:HZ2	1:E:227:GLU:HG3	1.60	0.65
1:E:233:GLY:HA2	1:E:236:ARG:HH12	1.61	0.65
1:E:195:VAL:HG11	1:E:304:PRO:HD3	1.78	0.65
1:E:510:MET:O	1:E:512:PRO:CD	2.44	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:344:LEU:HD22	1:D:346:GLU:OE1	1.97	0.64
1:D:328:VAL:HG23	1:D:580:GLU:HG3	1.79	0.64
1:E:580:GLU:HG2	1:E:580:GLU:O	1.97	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:263:LYS:HZ1	1:E:276:GLU:CD	1.99	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:394:ASP:HA	1:B:397:MET:CE	2.27	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:HG2	1:C:580:GLU:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:N	1:D:273:ASP:OD1	2.29	0.64
1:D:474:ALA:HA	1:D:558:VAL:CG1	2.21	0.64
1:E:533:ARG:CD	1:E:534:GLN:N	2.60	0.64
1:E:470:ALA:O	1:E:558:VAL:HG21	1.98	0.64
1:B:257:ILE:N	1:B:257:ILE:HD12	2.13	0.64
1:B:237:VAL:HG22	1:B:281:GLN:HG3	1.79	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:453:ARG:NH2	1:A:464:ARG:NH2	2.46	0.64
1:D:209:VAL:HG13	1:D:210:ALA:N	2.10	0.64
1:D:207:ARG:HB2	1:D:217:PHE:CE1	2.31	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:A:313:ARG:HH12	1:A:526:TYR:C	2.01	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:OD1	1:F:273:ASP:N	2.31	0.64
1:F:465:LEU:O	1:F:469:ILE:HG13	1.98	0.64
1: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
1:C:449:PHE:N	1:C:449:PHE:CD2	2.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:453:ARG:CG	1:C:453:ARG:HH11	2.10	0.64
1:D:258:ASP:N	1:D:258:ASP:OD1	2.28	0.64
1:C:518:ALA:CB	1:D:495:ARG:HA	2.27	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: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: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:N	1:F:257:ILE:HD12	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: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:292:ASP:OD1	1:E:292:ASP:C	2.36	0.63
1:E:523:GLU:N	1:E:523:GLU:OE1	2.31	0.63
1:F:214:ARG:HH11	1:F:214:ARG:CG	2.11	0.63
1:F:396:VAL:O	1:F:400:PRO:HD2	1.98	0.63
1: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:328:VAL:CG2	1:B:355:LYS:CE	2.76	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:D:526:TYR:HE2	1:E:256:GLU:OE2	1.81	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:D:215:VAL:CG2	1:D:249:PRO:O	2.45	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:292:ASP:OD1	1:C:292:ASP:C	2.37	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: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:E:215:VAL:HG23	1:E:216:PRO:CD	2.26	0.63
1:E:273:ASP:CG	1:E:274:GLU:N	2.51	0.63
1: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:539:THR:O	1:A:543:ILE:HG13	1.99	0.63
1:B:209:VAL:HG13	1:B:210:ALA:N	2.14	0.63
1:B:159:ALA:HB3	1:B:334:ILE:CG1	2.29	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:B:318:ASP:OD1	2.24	0.62
1:D:317:PHE:HD1	1:D:317:PHE:N	1.97	0.62
1:E: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: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: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
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:F:258:ASP:N	1:F:258:ASP:OD1	2.31	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:HG2	1:C:214:ARG:O	1.98	0.62
1:D:586:GLU:O	1:D:589:ARG:HB2	2.00	0.62
1: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:ASP:N	1:B:258:ASP:OD1	2.31	0.62
1:C:524:ASP:CA	1:C:529:GLY:HA2	2.09	0.62
1:E:153:VAL:HA	1:E:157:ASP:OD2	1.99	0.62
1: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: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:NH1	1:A:236:ARG:CG	2.59	0.62
1:A:428:PHE:O	1:A:432:ALA:HB2	2.00	0.62
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: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: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: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:F:190:LYS:HZ1	1:F:289:PHE:HE2	0.70	0.61
1:F:378:ARG:C	1:F:380:GLY:N	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:255:ASP:O	1:F:256:GLU:HG2	1.99	0.61
1:A:292:ASP:OD1	1:A:292:ASP:C	2.37	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:D:511:HIS:C	1:D:512:PRO:O	2.38	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:166:GLU:CB	1:A:169:LYS:HZ2	2.08	0.61
1:A:440:ILE:HG22	1:A:441:VAL:HG23	1.83	0.61
1:B:241:PHE:CD1	1:B:242:GLU:N	2.68	0.61
1:D:382:ARG:HG2	1:D:382:ARG:NH1	2.11	0.61
1:D:344:LEU:HA	1:D:383:LYS:HG3	1.83	0.61
1:E:338:HIS:CE1	1:E:366:GLU:HG3	2.36	0.61
1:F:241:PHE:CD1	1:F:242:GLU:N	2.68	0.61
1:F:159:ALA:HB1	1:F:333:GLN:CG	2.31	0.61
1: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:D:314:PRO:C	1:D:316:ARG:H	2.02	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:382:ARG:HB3	1:F:383:LYS:HB2	1.82	0.61
1:F:394:ASP:HA	1:F:397:MET:HE3	1.81	0.61
1: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:367:ASN:C	1:B:367:ASN:OD1	2.39	0.61
1:B:391:GLU:O	1:B:395:ARG:HB3	2.01	0.61
1:B:501:ALA:O	1:B:505:ILE:HD12	2.00	0.61
1:C:225:PHE:HE1	1:C:233:GLY:C	2.03	0.61
1: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:313:ARG:NH2	1:A:526:TYR:C	2.51	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:378:ARG:C	1:B:380:GLY:N	2.54	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:E:223:SER:C	1:E:225:PHE:N	2.48	0.61
1:F:348:VAL:HG21	1:F:352:LEU:CD1	2.31	0.61
1:F:352:LEU:CD1	1:F:353:LEU:N	2.64	0.61
1: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: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: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:F:369:LEU:O	1:F:372:ALA:N	2.33	0.60
1:F:394:ASP:O	1:F:397:MET:HG2	2.01	0.60
1:F:328:VAL:HG23	1:F:580:GLU:HG3	1.83	0.60
1:A:263:LYS:HZ1	1:A:276:GLU:CD	2.02	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:D:327:ASP:O	1:D:331:ARG:CZ	2.49	0.60
1:A:347:ASP:N	1:A:347:ASP:OD1	2.34	0.60
1: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:D:367:ASN:C	1:D:367:ASN:OD1	2.40	0.60
1:E:371:GLU:OE1	1:E:395:ARG:NH1	2.34	0.60
1:E:196:GLY:CA	1:E:443:ARG:NH2	2.65	0.60
1:E:488:THR:O	1:E:490:ALA:N	2.29	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:367:ASN:OD1	1:F:367:ASN:C	2.39	0.60
1:F:577:LEU:HG	1:F:578:GLU:N	2.15	0.60
1:A:150:ALA:HB2	1:A:214:ARG:NH1	2.17	0.60
1:A:225:PHE:CE1	1:A:233:GLY:C	2.74	0.60
1:B:317:PHE:N	1:B:317:PHE: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: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: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
1:E:166:GLU:O	1:E:169:LYS:HG2	2.01	0.60
1:F:294:ALA:C	1:F:295:ILE:HG12	2.21	0.60
1: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:266:SER:C	1:C:268:VAL:H	2.05	0.60
1:C:387:LYS:O	1:C:390:GLU:HB2	2.02	0.60
1:D: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:319:ARG:C	1:D:320:GLN:OE1	2.40	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:211:GLY:C	1:A:214:ARG:HE	2.05	0.60
1:A:331:ARG:HD2	1:A:357:THR:HG23	1.83	0.60
1:B:237:VAL:HG22	1:B:281:GLN:CG	2.31	0.60
1:B:159:ALA:HB1	1:B:333: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:HG3	1:A:275:ARG:NH1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:394:ASP:HA	1:B:397:MET:HE2	1.84	0.60
1:C:519:TYR:HA	1:C:533:ARG:CZ	2.31	0.60
1:D:311:LEU:C	1:D:311:LEU:HD12	2.22	0.60
1:E:166:GLU:O	1:E:169:LYS:CG	2.50	0.60
1:E:346:GLU:CD	1:E:347:ASP:H	2.04	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:D:410:ARG:O	1:D:413:ARG:N	2.34	0.60
1:E:264:ARG:HE	1:E:266:SER:HB2	1.65	0.60
1:A:191:GLY:HA2	1:A:297:VAL:CG2	2.32	0.59
1:A:286:MET:HB3	1:A:316:ARG:HD3	1.80	0.59
1: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:A:346:GLU:CD	1:A:347:ASP:H	2.05	0.59
1:B:165:LYS:HZ2	1:B:168:LEU:HD23	1.67	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:294:ALA:C	1:D:295:ILE:HG12	2.23	0.59
1:E:357:THR:N	1:E:358:PRO:HD2	2.17	0.59
1: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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:597:GLU:O	1:F:599:PRO:HD3	2.03	0.59
1:B:157:ASP:OD1	1:B:157:ASP:N	2.34	0.59
1:B:171:ILE:CG1	1:B:296:VAL:HG21	2.33	0.59
1: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:266:SER:C	1:E:268:VAL:H	2.05	0.59
1:F:257:ILE:CD1	1:F:257:ILE:H	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
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:376:ALA:HA	1:F:381:ARG:CZ	2.32	0.59
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: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: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:196:GLY:CA	1:C:443:ARG:NH2	2.66	0.58
1:C:453:ARG:NH2	1:C:464:ARG:HH12	1.98	0.58
1:D:182:HIS:N	1:D:182:HIS:ND1	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:B:511:HIS:C	1:B:512:PRO:O	2.41	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:E:145:ARG:NH2	1:E:219:THR:HG1	1.98	0.58
1:F:192:VAL:O	1:F:317:PHE:CE2	2.56	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:286:MET:O	1:A:289:PHE:CE1	2.56	0.58
1:B:376:ALA:CB	1:B:381:ARG:HD3	2.33	0.58
1:A:513:GLU:O	1:B:548:ARG:NH2	2.37	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: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:346:GLU:CD	1:C:347:ASP:H	2.06	0.58
1:D:257:ILE:CD1	1:D:257:ILE:H	2.14	0.58
1:E:337:ILE:HD12	1:E:338:HIS:CD2	2.39	0.58
1:E:507:GLU:CD	1:E:522:ARG:HE	2.07	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:336:ARG:O	1:A:339:ALA:N	2.37	0.58
1:A:509:GLY:C	1:B:476:ARG:NH2	2.56	0.58
1:B:239:ASP:HA	1:B:242:GLU:OE1	2.03	0.58
1:C:438:VAL:HG23	1:C:439:THR:N	2.19	0.58
1:D:463:LYS:O	1:D:464:ARG:C	2.41	0.58
1:E:264:ARG:NE	1:E:266:SER:HB2	2.19	0.58
1: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:A:276:GLU:OE2	1:A:527:LEU:HD11	2.03	0.58
1:E:155:PHE:HZ	1:E:209:VAL:HG22	1.69	0.58
1:E:238:ARG:CZ	1:E:238:ARG:HB2	2.34	0.58
1: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:340:ARG:C	1:A:342:LYS:N	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:333:GLN:O	1:D:336:ARG:HB3	2.04	0.58
1:F:245:LYS:CG	1:F:246:ARG:N	2.66	0.58
1:A:503:ARG:HG2	1:A:508:TRP:CH2	2.39	0.58
1:B:237:VAL:HA	1:B:240:LEU:HD12	1.86	0.58
1:C:349:ASP:O	1:C:349:ASP:OD1	2.22	0.58
1:C:400:PRO:O	1:C:405:LEU:HD11	2.03	0.58
1:D:233:GLY:C	1:D:236:ARG:HH22	2.07	0.58
1:D:526:TYR:O	1:D:528:GLY:N	2.37	0.58
1:E:236:ARG:NH1	1:E:236:ARG:CB	2.67	0.58
1:F:463:LYS:O	1:F:464:ARG:C	2.41	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:E:189:PRO:O	1:E:190:LYS:HG2	2.04	0.58
1:E:225:PHE:CE1	1:E:233:GLY:C	2.76	0.58
1:D:526:TYR:CE2	1:E:256:GLU:OE2	2.57	0.58
1: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: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:N	1:C:514:PHE:CD2	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: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:373:ALA:O	1:F:376:ALA:HB3	2.05	0.57
1:A:318:ASP:OD1	1:A:318:ASP:N	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
1:D:348:VAL:HG13	1:D:350:LEU:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:501:ALA:O	1:D:505:ILE:HD12	2.05	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:B:549:ARG:O	1:B:550:LEU:C	2.42	0.57
1:C:191:GLY:HA2	1:C:297:VAL:CG2	2.35	0.57
1:D:549:ARG:O	1:D:550:LEU:C	2.42	0.57
1:E:247:HIS:O	1:E:250:CYS:HB2	2.04	0.57
1:F:165:LYS:O	1:F:168:LEU:CA	2.51	0.57
1:F:233:GLY:C	1:F:236:ARG:HH22	2.07	0.57
1:F:238:ARG:CG	1:F:281:GLN:HE22	2.15	0.57
1:F:244:ALA:O	1:F:250:CYS:SG	2.62	0.57
1: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: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:B:308:ASP:OD1	1:B:308:ASP:C	2.42	0.57
1:B:463:LYS:O	1:B:464:ARG:C	2.41	0.57
1:C:225:PHE:CE1	1:C:233:GLY:C	2.78	0.57
1:E:334:ILE:CD1	2:E:1001:ADP:C6	2.86	0.57
1:E:211:GLY:C	1:E:214:ARG:CG	2.72	0.57
1:D:523:GLU:CD	1:E:264:ARG:NH2	2.58	0.57
1:E:394:ASP:O	1:E:397:MET:N	2.37	0.57
1:E:313:ARG:NH2	1:E:526:TYR:C	2.52	0.57
1:A:378:ARG:CA	1:F:173:GLU:OE1	2.45	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:223:SER:C	1:C:225:PHE:N	2.51	0.57
1:E:275:ARG:HG3	1:E:275:ARG:NH1	2.19	0.57
1:E:382:ARG:HD3	1:E:383:LYS:CB	2.34	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:A:196:GLY:C	1:A:443:ARG:NH2	2.58	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:235:ALA:C	1:D:238:ARG:HG3	2.25	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: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:433:ASP:OD1	1:D:433:ASP:N	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: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: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: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:A:507:GLU:CD	1:A:522:ARG:HE	2.09	0.56
1:A:583:THR:HG22	1:A:586:GLU:CD	2.26	0.56
1:C:263:LYS:HD2	1:C:276:GLU:CG	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:308:ASP:OD1	1:D:308:ASP:C	2.42	0.56
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: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:245:LYS:C	1:F:247:HIS:N	2.58	0.56
1:F:467:ASP:O	1:F:470:ALA:HB3	2.06	0.56
1:A:407:LEU:O	1:A:407:LEU:HD12	2.05	0.56
1:B:245:LYS:C	1:B:247:HIS:N	2.58	0.56
1:C:219:THR:HA	1:C:253:PHE:O	2.06	0.56
1:D:245:LYS:CG	1:D:246:ARG:N	2.68	0.56
1:C:516:PRO:HB2	1:D:494:PHE:CD1	2.40	0.56
1:F:210:ALA:O	1:F:214:ARG:N	2.38	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: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: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:D:261:GLY:O	1:D:308:ASP:N	2.34	0.56
1:D:286:MET:HE2	1:D:315:GLY:O	2.05	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:525:THR:HG22	1:F:526:TYR:H	1.71	0.56
1:B:165:LYS:HE2	1:B:205:LEU:CG	2.36	0.56
1:B:391:GLU:O	1:B:394:ASP:OD1	2.23	0.56
1:B:449:PHE:CE2	1:B:492:ASN:HB3	2.37	0.56
1:B:477:ALA:O	1:B:481:ILE:HG13	2.06	0.56
1:C:263:LYS:HZ2	1:C:276:GLU:CD	1.80	0.56
1:F:447:LEU:O	1:F:450:MET:HG3	2.06	0.56
1:A:238:ARG:CZ	1:A:238:ARG:HB2	2.35	0.56
1:C:407:LEU:HD12	1:C:407:LEU:O	2.05	0.56
1:D:245:LYS:C	1:D:247:HIS:N	2.59	0.56
1:F:180:ARG:NH1	1:F:184:MET:HE1	2.20	0.56
1:F:235:ALA:C	1:F:238:ARG:HG3	2.26	0.56
1: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: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:A:459:HIS:HB2	1:B:488:THR:HB	1.87	0.56
1:C:166:GLU:C	1:C:169:LYS:HG2	2.26	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: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:F:192:VAL:C	1:F:317:PHE:CE2	2.79	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:308:ASP:OD1	1:E:308:ASP:C	2.43	0.56
1:E:407:LEU:O	1:E:407:LEU:HD12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:519:TYR:C	1:C:533:ARG:NE	2.59	0.56
1:C:585:GLU:CD	1:C:586:GLU:N	2.59	0.56
1:C:589:ARG:CZ	1:C:596:LEU:HB2	2.28	0.56
1: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
1:A:438:VAL:HG11	1:A:587:PHE:CD1	2.41	0.56
1:A:536:SER:O	1:A:537:GLU:C	2.44	0.56
1:C:177:ASN:HD22	1:C:180:ARG:CD	2.17	0.56
1:C:234:ALA:HB1	1:C:281:GLN:CD	2.26	0.56
1:C:238:ARG:HB2	1:C:238:ARG:CZ	2.35	0.56
1: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: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:E:166:GLU:C	1:E:169:LYS:HG2	2.26	0.56
1:F:344:LEU:HA	1:F:383:LYS:HG3	1.88	0.56
1:B: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:308:ASP:OD1	1:C:308:ASP:C	2.43	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:308:ASP:OD1	1:F:308:ASP:C	2.45	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:B:286:MET:HA	1:B:289:PHE:CD1	2.41	0.55
1:B:286:MET:O	1:B:289:PHE:CD1	2.59	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:ALA:HB1	1:B:381:ARG:CD	2.36	0.55
1:D:316:ARG:NH1	1:D:316:ARG:CG	2.42	0.55
1:D:461:SER:O	1:D:464:ARG:HB3	2.06	0.55
1:F:319:ARG:C	1:F:320:GLN:OE1	2.44	0.55
1:A:194:LEU:HA	1:A:321:ILE:O	2.06	0.55
1:A:223:SER:C	1:A:225:PHE:N	2.51	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
1:D:165:LYS:O	1:D:168:LEU:CB	2.54	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:168:LEU:O	1:A:169:LYS:C	2.45	0.55
1:A:262:ARG:HG2	1:A:275:ARG:NH2	2.06	0.55
1: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:C:196:GLY:H	1:C:202:LYS:HZ1	1.55	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:319:ARG:NH2	1:B:402:LYS:HZ3	2.04	0.55
1:A:531:ASP:C	1:A:531:ASP:OD1	2.45	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:237:VAL:C	1:D:240:LEU:HB3	2.27	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:E:340:ARG:C	1:E:342:LYS:N	2.58	0.55
1:F:233:GLY:C	1:F:236:ARG:NH2	2.60	0.55
1:A:495:ARG:HD2	1:F:521:VAL:HG12	1.88	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:B:494:PHE:O	1:B:495:ARG:C	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:197:PRO:C	1:E:302:ASN:OD1	2.45	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: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:414:ILE:HG22	1:C:415:THR:H	1.71	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:233:GLY:C	1:D:236:ARG:NH2	2.60	0.55
1:D:236:ARG:O	1:D:239:ASP:OD1	2.25	0.55
1:E:219:THR:HA	1:E:253:PHE:O	2.07	0.55
1:F:241:PHE:CE2	1:F:285:GLU:CG	2.90	0.55
1:F:344:LEU:HG	1:F:346:GLU:OE1	2.06	0.55
1:F:348:VAL:HG21	1:F:386:MET:HE2	1.89	0.55
1: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: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:334:ILE:HD13	2:E:1001:ADP:N1	2.22	0.55
1:E:174:PHE:CD2	1:E:175:LEU:N	2.74	0.55
1:F:154:THR:HG23	1:F:156:LYS:H	1.71	0.55
1: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:ALA:O	1:B:237:VAL:HG13	2.07	0.54
1:B:235:ALA:C	1:B:238:ARG:HG3	2.28	0.54
1:B:525:THR:HG22	1:B:526:TYR:H	1.73	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:D:253:PHE:CD2	1:D:253:PHE:C	2.80	0.54
1:C:463:LYS:HD2	1:D:486:VAL:CG2	2.37	0.54
1:E:199:GLY:O	1:E:361:VAL:HG22	2.06	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:A:234:ALA:HB1	1:A:281:GLN:CD	2.27	0.54
1:C:197:PRO:C	1:C:302:ASN:OD1	2.46	0.54
1:C:336:ARG:CG	1:C:337:ILE:N	2.69	0.54
1:C:336:ARG:O	1:C:339:ALA:N	2.38	0.54
1:D:430:GLU:CA	1:D:430:GLU:OE1	2.54	0.54
1:F: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:394:ASP:HA	1:F:397:MET:HE2	1.88	0.54
1:F:433:ASP:OD1	1:F:433:ASP:N	2.39	0.54
1:A:199:GLY:O	1:A:361:VAL:HG22	2.07	0.54
1:A:197:PRO:C	1:A:302:ASN:OD1	2.45	0.54
1:A:283:LEU:CD1	1:A:311:LEU:HD21	2.36	0.54
1:A:339:ALA:N	1:A:369:LEU:HD21	2.22	0.54
1:A:381:ARG:CG	1:A:381:ARG:HH11	2.21	0.54
1:B:348:VAL:HG13	1:B:350:LEU:H	1.72	0.54
1:C:334:ILE:HD13	2:C:1001:ADP:N1	2.23	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: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:D:193:LEU:C	1:D:194:LEU:HD12	2.28	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:C:516:PRO:HB2	1:D:494:PHE:CE1	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:234:ALA:HB1	1:E:281:GLN:CD	2.27	0.54
1:E:283:LEU:O	1:E:286:MET:HB2	2.07	0.54
1:E:174:PHE:CZ	1:E:294:ALA:HB1	2.41	0.54
1:E:189:PRO:HD3	1:E:319:ARG:NH1	2.23	0.54
1:F:311:LEU:O	1:F:311:LEU:HD12	2.07	0.54
1:A:174:PHE:CZ	1:A:294:ALA:HB1	2.42	0.54
1:A:353:LEU:O	1:A:357:THR:HG22	2.06	0.54
1:B:192:VAL:C	1:B:317:PHE:CE2	2.80	0.54
1:B:433:ASP:OD1	1:B:433:ASP:N	2.41	0.54
1:C:353:LEU:O	1:C:357:THR:HG22	2.08	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:A:149:GLU:O	1:A:150:ALA:CB	2.53	0.54
1:A:179:SER:C	1:A:181:PHE:H	2.10	0.54
1: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:C:196:GLY:C	1:C:443:ARG:NH2	2.61	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:180:ARG:NH1	1:D:184:MET:HE1	2.22	0.54
1:D:190:LYS:NZ	1:D:289:PHE:CZ	2.73	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:F:237:VAL:C	1:F:240:LEU:HB3	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:NH1	1:B:319:ARG:CG	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:438:VAL:HG23	1:E:439:THR:N	2.23	0.54
1:E:512:PRO:HB2	1:E:514:PHE:HD2	1.72	0.54
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: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: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:319:ARG:C	1:C:320:GLN:NE2	2.61	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:334:ILE:O	1:E:335:LEU:C	2.47	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:236:ARG:O	1:B:239:ASP:OD1	2.26	0.54
1:B:170:GLU:CB	1:C:378:ARG:HH22	2.20	0.54
1:D:285:GLU:O	1:D:288:GLY:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1: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:375:LEU:CD1	1:F:388:ASP:HB3	2.36	0.54
1:F:511:HIS:C	1:F:512:PRO:O	2.45	0.54
1:F:454:ARG:NH2	1:F:528:GLY:C	2.61	0.54
1:A:196:GLY:O	1:A:302:ASN:OD1	2.25	0.53
1:A:367:ASN:O	1:A:371:GLU:HB3	2.07	0.53
1:B:334:ILE:O	1:B:337:ILE:HG22	2.09	0.53
1:C:551:ILE:O	1:C:552:GLU:C	2.46	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:166:GLU:C	1:A:169:LYS:HG2	2.28	0.53
1:A:218:ILE:HG12	1:A:251:ILE:O	2.08	0.53
1:A:311:LEU:HB3	1:A:316:ARG:HH22	1.73	0.53
1:A:336:ARG:CG	1:A:337:ILE:N	2.72	0.53
1:B:165:LYS:CD	1:B:168:LEU:CD2	2.76	0.53
1:B:328:VAL:HG21	1:B:355:LYS:HE3	1.88	0.53
1:D: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:517:VAL:HG11	1:D:519:TYR:CZ	2.43	0.53
1:D:480:GLU:OE1	1:D:555:TYR:OH	2.26	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: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:253:PHE:CD2	1:B:253:PHE:C	2.82	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:D:467:ASP:O	1:D:470:ALA:HB3	2.08	0.53
1:C:461:SER:HA	1:D:487:THR:O	2.08	0.53
1:E:177:ASN:ND2	1:E:180:ARG:HD3	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:448:GLY:O	1:A:449:PHE:C	2.46	0.53
1:A:493:ASP:OD1	1:A:493:ASP:N	2.41	0.53
1:A:465:LEU:CD2	1:A:508:TRP:CZ3	2.92	0.53
1:A:313:ARG:NH1	1:A:526:TYR:HA	2.24	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:196:GLY:C	1:E:443:ARG:NH2	2.61	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:507:GLU:CD	1:C:522:ARG:HE	2.12	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: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:585:GLU:CD	1:A:586:GLU:N	2.62	0.53
1:B:201:GLY:N	2:B:2001:ADP:O1A	2.39	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:477:ALA:O	1:F:481:ILE:HG13	2.09	0.53
1:F:467:ASP:OD1	1:F:557:ARG:NH2	2.42	0.53
1:A:334:ILE:O	1:A:335:LEU:C	2.46	0.53
1:A:368:LEU:HD13	1:A:393:ALA:HA	1.91	0.53
1: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:ILE:HG23	1:D:172:VAL:N	2.23	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:E:585:GLU:CD	1:E:586:GLU:N	2.62	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:253:PHE:C	1:F:253:PHE:CD2	2.82	0.53
1:F:331:ARG:HD2	1:F:354:ALA:O	2.09	0.53
1:F:494:PHE:O	1:F:495:ARG:C	2.45	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: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:D:277:GLN:HA	1:D:280:ASN:HD21	1.74	0.53
1:D:592:GLU:O	1:D:594:LEU:N	2.42	0.53
1:E:319:ARG:O	1:E:320:GLN:NE2	2.41	0.53
1:E:343:PRO:C	1:E:344:LEU:HD13	2.28	0.53
1:E:349:ASP:O	1:E:349:ASP:OD1	2.26	0.53
1:E:514:PHE:CD2	1:E:514:PHE:N	2.77	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:227:GLU:HG3	1:F:263:LYS:HZ1	1.68	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:C:169:LYS:HA	1:C:172:VAL:CG1	2.38	0.53
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:168:LEU:O	1:E:169:LYS:C	2.47	0.53
1:F:186:ALA:O	1:F:187:ARG:HB3	2.08	0.53
1:E:461:SER:HA	1:F:487:THR:O	2.09	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:C:343:PRO:C	1:C:344:LEU:HD13	2.30	0.52
1:D:459:HIS:O	1:D:459:HIS:CG	2.56	0.52
1:D:421:GLY:HA2	1:D:562:LEU:HD11	1.90	0.52
1:E:179:SER:C	1:E:181:PHE:H	2.13	0.52
1:F:165:LYS:HZ1	1:F:205:LEU:CB	2.21	0.52
1:F:479:GLU:OE2	1:F:488:THR:HG23	2.09	0.52
1:F:526:TYR:N	1:F:526:TYR:CD2	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:460:TRP:HB3	1:C:465:LEU:HD11	1.91	0.52
1:D:263:LYS:HE2	1:E:228:MET:HE1	1.91	0.52
1:D:335:LEU:HD21	1:D:365:LEU:HB3	1.90	0.52
1:E:240:LEU:O	1:E:243:THR:OG1	2.22	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: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:E:178:PRO:O	1:E:182:HIS:CD2	2.62	0.52
1:E:177:ASN:HD22	1:E:180:ARG:CD	2.22	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:D:187:ARG:O	1:E:374:LEU:HD21	2.08	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
1:F:356:ARG:O	1:F:358:PRO:HD3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:LEU:HD13	1:A:393:ALA:CA	2.39	0.52
1: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:C:451:MET:HB2	1:C:452:PRO:HD3	1.92	0.52
1:B:463:LYS:HE3	1:C:486:VAL:HG21	1.90	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:273:ASP:CG	1:A:274:GLU:N	2.63	0.52
1:B:171:ILE:HG23	1:B:172:VAL:N	2.23	0.52
1:B:180:ARG:NH1	1:B:184:MET:HE1	2.24	0.52
1:B:571:ARG:HH12	1:B:593:GLY:H	1.57	0.52
1:C:463:LYS:HD2	1:D:486:VAL:HG22	1.90	0.52
1:D:216:PRO:HG2	1:D:250:CYS:CB	2.39	0.52
1:D:331:ARG:HH22	1:D:580:GLU:CD	2.10	0.52
1:D:376:ALA:C	1:D:381:ARG:CB	2.77	0.52
1: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:A:374:LEU:CD1	1:F:187:ARG:H	2.11	0.52
1:A:343:PRO:C	1:A:344:LEU:HD13	2.29	0.52
1:A:451:MET:HB2	1:A:452:PRO:HD3	1.92	0.52
1:A:574:GLU:C	1:A:574:GLU:OE1	2.48	0.52
1:A:583:THR:N	1:A:586:GLU:OE2	2.36	0.52
1: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:286:MET:HE3	1:A:297:VAL:HG21	1.90	0.52
1:B:190:LYS:HD2	1:B:289:PHE:HZ	1.73	0.52
1:B:297:VAL:HG13	1:B:317:PHE:HZ	1.75	0.52
1: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:179:SER:C	1:C:181:PHE:H	2.13	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:378:ARG:C	1:D:380:GLY:N	2.51	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:B:180:ARG:HH12	1:B:184:MET:HE1	1.75	0.52
1:C:334:ILE:CD1	2:C:1001:ADP:N6	2.73	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: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:C:241:PHE:O	1:C:244:ALA:N	2.43	0.52
1:D:180:ARG:HH12	1:D:184:MET:HE1	1.73	0.52
1: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:C:539:THR:OG1	1:D:544:ASP:OD2	2.25	0.52
1:F:237:VAL:CG2	1:F:281:GLN:CG	2.88	0.52
1:F:453:ARG:HA	1:F:456:ASP:OD2	2.10	0.52
1:A:334:ILE:HD13	2:A:1001:ADP:N1	2.26	0.51
1:A:206:ALA:HB1	1:A:217:PHE:HZ	1.75	0.51
1:A:238:ARG:O	1:A:241:PHE:N	2.43	0.51
1:A:346:GLU:OE1	1:A:347:ASP:OD1	2.28	0.51
1:B:174:PHE:HZ	1:B:294:ALA:HA	1.76	0.51
1:B:376:ALA:C	1:B:381:ARG:CD	2.61	0.51
1: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:B:173:GLU:OE1	1:C:378:ARG:HA	2.10	0.51
1:D:366:GLU:O	1:D:369:LEU:HB2	2.09	0.51
1:E:345:ALA:O	1:E:348:VAL:HB	2.10	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:O	1:A:594:LEU:HG	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:B:583:THR:O	1:B:584:ALA:C	2.48	0.51
1:C:174:PHE:HB2	1:C:181:PHE:CE2	2.46	0.51
1:C:368:LEU:HG	1:C:369:LEU:N	2.25	0.51
1:D:192:VAL:O	1:D:317:PHE:CE2	2.64	0.51
1:D:352:LEU:O	1:D:353:LEU:C	2.48	0.51
1:D:338:HIS:CE1	1:D:366:GLU:HG3	2.44	0.51
1:D:376:ALA:O	1:D:381:ARG:HG2	2.10	0.51
1: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:376:ALA:HA	1:F:381:ARG:HH11	1.74	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
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: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:241:PHE:O	1:C:242:GLU:C	2.49	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:523:GLU:OE1	1:C:264:ARG:NH2	2.43	0.51
1:C:334:ILE:O	1:C:335:LEU:C	2.48	0.51
1:C:397:MET:SD	1:C:406:VAL:CG1	2.98	0.51
1:C:525:THR:OG1	1:C:528:GLY:HA3	2.11	0.51
1: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:354:ALA:HA	1:A:357:THR:CG2	2.40	0.51
1:A:313:ARG:NH1	1:A:526:TYR:CA	2.73	0.51
1:C:338:HIS:ND1	1:C:366:GLU:HG3	2.25	0.51
1:D:175:LEU:O	1:D:249:PRO:CB	2.58	0.51
1:E:196:GLY:H	1:E:202:LYS:HZ1	1.55	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:CG	1:A:464:ARG:HH11	2.23	0.51
1:B:175:LEU:O	1:B:249:PRO:CB	2.58	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:B:355:LYS:HZ3	1:B:578:GLU:HG3	1.74	0.51
1:C:236:ARG:NH1	1:C:236:ARG:CB	2.73	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: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:F:428:PHE:CE1	1:F:432:ALA:C	2.84	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
1:C:292:ASP:OD1	1:C:293:THR:N	2.43	0.51
1:D:327:ASP:O	1:D:331:ARG:NH2	2.43	0.51
1:D:514:PHE:HB3	1:D:519:TYR:HE1	1.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:181:PHE:HA	1:C:184:MET:HE2	1.91	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: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: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:C:459:HIS:HE1	1:D:411:ASP:HB3	1.76	0.51
1:E:166:GLU:HB2	1:E:169:LYS:HZ1	1.75	0.51
1:D:521:VAL:HG12	1:E:495:ARG:HD2	1.93	0.51
1:E:513:GLU:O	1:F:548:ARG:NH2	2.44	0.51
1:E:566:ARG:O	1:E:569:LEU:N	2.44	0.51
1:E:583:THR:HG22	1:E:586:GLU:CD	2.31	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: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
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:292:ASP:OD1	1:E:293:THR:N	2.43	0.51
1:E:346:GLU:OE1	1:E:347:ASP:OD1	2.28	0.51
1:E:524:ASP:OD1	1:E:524:ASP:N	2.43	0.51
1:E:589:ARG:HH21	1:E:596:LEU:CB	1.74	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:PHE:O	1:A:242:GLU:C	2.48	0.51
1:A:316:ARG:O	1:A:317:PHE:C	2.50	0.51
1:A:331:ARG:CZ	1:A:358:PRO:HD3	2.40	0.51
1:A:586:GLU:HG2	1:A:587:PHE:N	2.26	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: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: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:331:ARG:HH22	1:F:580:GLU:CD	2.13	0.51
1:F:332:GLU:HB2	1:F:354:ALA:HB2	1.93	0.51
1:F:381:ARG:HH22	1:F:388:ASP:CG	2.15	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:397:MET:O	1:D:400:PRO:HG2	2.11	0.50
1:D:428:PHE:CE1	1:D:432:ALA:C	2.85	0.50
1:D:538:GLU:O	1:D:541:LYS:N	2.44	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: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:454:ARG:HH21	1:D:526:TYR:CA	2.23	0.50
1:D:355:LYS:NZ	1:D:578:GLU:HG3	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:378:ARG:HG3	1:C:379:GLU:N	2.21	0.50
1:D:236:ARG:NH1	1:D:237:VAL:HG12	2.27	0.50
1:D:262:ARG:CG	1:D:263:LYS:H	2.19	0.50
1:D:325:ALA:CB	1:D:326:PRO:HD3	2.37	0.50
1:E:300:ALA:O	1:E:301:THR:HG22	2.11	0.50
1:D:508:TRP:CD1	1:E:491:GLU:HG2	2.45	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:357:THR:OG1	1:A:360:PHE:HB2	2.12	0.50
1:A:479:GLU:OE2	1:A:488:THR:N	2.45	0.50
1:A:313:ARG:HH12	1:A:526:TYR:CA	2.25	0.50
1:B:174:PHE:HZ	1:B:294:ALA:CA	2.24	0.50
1:C:168:LEU:O	1:C:169:LYS:C	2.47	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:B:538:GLU:HB2	1:C:541:LYS:NZ	2.26	0.50
1:D:451:MET:HB3	1:D:452:PRO:CD	2.38	0.50
1:D:479:GLU:OE2	1:D:488:THR:HG23	2.11	0.50
1:E:368:LEU:HG	1:E:369:LEU:N	2.25	0.50
1:E:381:ARG:CG	1:E:381:ARG:HH11	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:F:564:GLU:C	1:F:566:ARG:N	2.65	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:C:574:GLU:C	1:C:574:GLU:OE1	2.49	0.50
1:D:278:THR:O	1:D:281:GLN:HB3	2.12	0.50
1:D:285:GLU:C	1:D:288:GLY:H	2.14	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:329:LYS:O	1:D:332:GLU:HB3	2.12	0.50
1:E:325:ALA:N	1:E:326:PRO:CD	2.74	0.50
1:E:334:ILE:O	1:E:337:ILE:HG13	2.10	0.50
1:E:397:MET:SD	1:E:406:VAL:CG1	2.99	0.50
1:E:302:ASN:HB3	1:E:443:ARG:HH12	1.76	0.50
1:E:507:GLU:HB2	1:E:520:ALA:HB3	1.92	0.50
1:E:536:SER:O	1:E:537:GLU:C	2.49	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:F:549:ARG:O	1:F:550:LEU:C	2.49	0.50
1:A:279:LEU:O	1:A:282:LEU:N	2.45	0.50
1:A:325:ALA:N	1:A:326:PRO:HD2	2.27	0.50
1: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: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
1:C:408:SER:C	1:C:410:ARG:H	2.14	0.50
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:319:ARG:C	1:E:320:GLN:NE2	2.65	0.50
1:F:297:VAL:HG13	1:F:317:PHE:HZ	1.77	0.50
1: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:285:GLU:C	1:B:288:GLY:H	2.15	0.50
1:B:345:ALA:CB	1:B:383:LYS:HE3	2.37	0.50
1:C:493:ASP:N	1:C:493:ASP:OD1	2.44	0.50
1:C:449:PHE:HE2	1:C:496:GLN:NE2	2.10	0.50
1:C:524:ASP:OD1	1:C:524:ASP:N	2.44	0.50
1:C:313:ARG:NH1	1:C:526:TYR:CA	2.75	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:241:PHE:O	1:E:242:GLU:C	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:585:GLU:O	1:B:586:GLU:C	2.50	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:389:LEU:O	1:D:390:GLU:C	2.50	0.50
1:D:447:LEU:O	1:D:450:MET:HG3	2.11	0.50
1:E:210:ALA:HA	1:E:251:ILE:HD11	1.94	0.50
1:E:448:GLY:O	1:E:449:PHE:C	2.51	0.50
1:A:211:GLY:HA2	1:A:214:ARG:NE	2.25	0.50
1:A:319:ARG:C	1:A:320:GLN:NE2	2.65	0.50
1: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:D:238:ARG:NH1	1:D:239:ASP:HB3	2.16	0.50
1:D:313:ARG:O	1:D:316:ARG:HB3	2.12	0.50
1:D:313:ARG:HG3	1:D:314:PRO:HG2	1.94	0.50
1:C:463:LYS:HB2	1:D:486:VAL:HG11	1.94	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:428:PHE:HE1	1:A:432:ALA:HA	1.66	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:531:ASP:C	1:C:531:ASP:OD1	2.51	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: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: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: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:357:THR:N	1:C:358:PRO:CD	2.74	0.49
1:C:302:ASN:HB3	1:C:443:ARG:HH12	1.76	0.49
1:C:448:GLY:O	1:C:449:PHE:C	2.50	0.49
1:C:539:THR:O	1:C:543:ILE:HG13	2.13	0.49
1:C:594:LEU:HD12	1:C:595:PRO:O	2.12	0.49
1:D:186:ALA:O	1:D:187:ARG:HB3	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:F:193:LEU:C	1:F:194:LEU:HD12	2.33	0.49
1:F:338:HIS:CE1	1:F:366:GLU:HG3	2.47	0.49
1:F:443:ARG:O	1:F:445:ARG:N	2.45	0.49
1:F:454:ARG:HH21	1:F:526:TYR:CA	2.25	0.49
1:E:537:GLU:N	1:F:537:GLU:OE2	2.41	0.49
1:A:147:LEU:HD23	1:A:217:PHE:HB3	1.93	0.49
1:A:453:ARG:HH21	1:A:464:ARG:HH22	1.55	0.49
1:A:449:PHE:CE2	1:A:496:GLN:NE2	2.79	0.49
1:B:336:ARG:C	1:B:338:HIS:N	2.62	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:D:454:ARG:NH2	1:D:528:GLY:C	2.66	0.49
1:D:564:GLU:C	1:D:566:ARG:N	2.64	0.49
1:E:195:VAL:HG22	1:E:301:THR:O	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:ASP:OD1	1:B:310:ALA:N	2.43	0.49
1:B:454:ARG:NH2	1:B:528:GLY:C	2.66	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:E:470:ALA:C	1:E:558:VAL:HG21	2.32	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:D:566:ARG:O	1:D:569:LEU:HB3	2.13	0.49
1:E:580:GLU:CG	1:E:580:GLU:O	2.60	0.49
1:F:239:ASP:O	1:F:242:GLU:OE2	2.30	0.49
2:A:1001:ADP:N3	2:A:1001:ADP:H2'	2.27	0.49
1:A:219:THR:HB	1:A:253:PHE:CD2	2.40	0.49
1:B:174:PHE:C	1:B:174:PHE:CD2	2.86	0.49
1:B: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: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:B:334:ILE:HG21	1:B:365:LEU:HD12	1.94	0.49
1:B:567:GLU:O	1:B:570:GLU:CB	2.61	0.49
2:C:1001:ADP:N3	2:C:1001:ADP:H2'	2.28	0.49
1:C:155:PHE:CZ	1:C:209:VAL:HG22	2.47	0.49
1:C:583:THR:HG22	1:C:586:GLU:CD	2.32	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:A:378:ARG:NH1	1:F:170:GLU:HB2	2.28	0.49
1:F:175:LEU:O	1:F:249:PRO:CB	2.61	0.49
1:F:319:ARG:O	1:F:320:GLN:HB3	2.11	0.49
1:F:336:ARG:C	1:F:338:HIS:N	2.64	0.49
1:F:352:LEU:O	1:F:353:LEU:C	2.49	0.49
1:F:360:PHE:HE1	1:F:364:ASP:HB3	1.77	0.49
1:F:335:LEU:HD13	1:F:365:LEU:HB3	1.93	0.49
1:B:278:THR:O	1:B:281:GLN:HB3	2.13	0.49
1:C:329:LYS:O	1:C:332:GLU:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:174:PHE:CD2	1:D:174:PHE:C	2.85	0.49
1:D:525:THR:HG22	1:D:526:TYR:H	1.77	0.49
1:E:236:ARG:NH1	1:E:236:ARG:HG2	2.11	0.49
1:E:220:ALA:O	1:E:254:ILE:HA	2.13	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
1:A:203:THR:OG1	2:A:1001:ADP:O2A	2.20	0.49
1:A:260:VAL:HG23	1:A:261:GLY:H	1.76	0.49
1:A:408:SER:C	1:A:410:ARG:H	2.15	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: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: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:369:LEU:O	1:B:370:ASN:C	2.51	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:E:574:GLU:OE1	1:E:574:GLU:C	2.52	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:210:ALA:HB2	1:A:251:ILE:CD1	2.42	0.48
1:A:198:PRO:HD3	1:A:302:ASN:ND2	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:580:GLU:O	1:C:580:GLU:CG	2.61	0.48
1:D:159:ALA:H	2:D:2001:ADP:HN62	1.61	0.48
1:D:225:PHE:N	1:D:225:PHE:CD2	2.80	0.48
1:D:175:LEU:O	1:D:249:PRO:HG2	2.13	0.48
1:D:312:LEU:HD23	1:D:312:LEU:O	2.13	0.48
1:D:336:ARG:C	1:D:338:HIS:N	2.61	0.48
1:D:548:ARG:NH1	1:D:548:ARG:HG2	2.28	0.48
1:E:181:PHE:HA	1:E:184:MET:HE2	1.95	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:483:PHE:C	1:E:485:ASP:H	2.17	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: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:260:VAL:HG23	1:C:261:GLY:H	1.78	0.48
1:C:273:ASP:CG	1:C:274:GLU:H	2.17	0.48
1:E:236:ARG:HH11	1:E:236:ARG:CB	2.26	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: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:193:LEU:C	1:B:194:LEU:HD12	2.34	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:249:PRO:HB3	1:C:294:ALA:HB3	1.95	0.48
1:C:196:GLY:O	1:C:302:ASN:OD1	2.31	0.48
1:C:328:VAL:HG12	1:C:329:LYS:N	2.27	0.48
1: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:344:LEU:HB2	1:D:384:ILE:O	2.13	0.48
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:HG2	1:E:443:ARG:O	2.14	0.48
1:F:311:LEU:C	1:F:316:ARG:NH1	2.66	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:B:313:ARG:CG	1:B:314:PRO:N	2.74	0.48
1:B:394:ASP:HA	1:B:397:MET:HE3	1.94	0.48
1:C:520:ALA:HA	1:C:533:ARG:CG	2.43	0.48
1:D:180:ARG:NH1	1:D:184:MET:CE	2.76	0.48
1:D:165:LYS:CE	1:D:205:LEU:HG	2.43	0.48
1:D:242:GLU:CA	1:D:245:LYS:HB3	2.42	0.48
1:E:462:ARG:CG	1:E:463:LYS:N	2.76	0.48
1:A:380:GLY:C	1:F:180:ARG:NH2	2.66	0.48
1:F:183:GLU:OE1	1:F:184:MET:HB3	2.14	0.48
1: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:O	1:B:190:LYS:HG3	2.14	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:E:147:LEU:HB3	1:E:217:PHE:O	2.12	0.48
1:F:397:MET:HA	1:F:400:PRO:HG2	1.95	0.48
1: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:179:SER:C	1:A:181:PHE:N	2.65	0.48
1:A:311:LEU:CG	1:A:316:ARG:HH22	2.25	0.48
1:B:564:GLU:O	1:B:566:ARG:N	2.47	0.48
1:C:280:ASN:O	1:C:281:GLN:C	2.52	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:369:LEU:O	1:D:370:ASN:C	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:238:ARG:O	1:E:239:ASP:C	2.51	0.48
1:E:300:ALA:O	1:E:301:THR:CG2	2.62	0.48
1:E:414:ILE:HG22	1:E:415:THR:H	1.78	0.48
1:E:519:TYR:C	1:E:533:ARG:NE	2.67	0.48
1:F:285:GLU:C	1:F:288:GLY:H	2.16	0.48
1:F:336:ARG:HD3	1:F:336:ARG:HA	1.50	0.48
1:F:388:ASP:N	1:F:388:ASP:OD1	2.46	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:A:280:ASN:O	1:A:281:GLN:C	2.50	0.48
1:B:222:GLY:N	1:B:255:ASP:O	2.43	0.48
1:B:311:LEU:HD12	1:B:311:LEU:O	2.13	0.48
1:B:468:GLN:O	1:B:471:VAL:N	2.45	0.48
1:C:179:SER:C	1:C:181:PHE:N	2.67	0.48
1:C:274:GLU:HB3	1:C:275:ARG:H	1.43	0.48
1:D:397:MET:HA	1:D:400:PRO:HG2	1.95	0.48
1:D:410:ARG:O	1:D:413:ARG:CB	2.61	0.48
1:D:302:ASN:ND2	1:D:443:ARG:NH2	2.55	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:531:ASP:OD1	1:E:531:ASP:C	2.52	0.48
1:F:175:LEU:O	1:F:249:PRO:HG2	2.14	0.48
1:F:159:ALA:HB1	1:F:333:GLN:HG3	1.96	0.48
1: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:B:336:ARG:HA	1:B:336:ARG:HD3	1.47	0.48
1:B:428:PHE:CE1	1:B:432:ALA:C	2.87	0.48
1:B:453:ARG:HA	1:B:456:ASP:OD2	2.14	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:374:LEU:C	1:D:374:LEU:HD23	2.34	0.48
1:E:179:SER:C	1:E:181:PHE:N	2.67	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:237:VAL:HG21	1:F:281:GLN:HG3	1.96	0.48
1:F:159:ALA:HA	1:F:333:GLN:HE21	1.79	0.48
1: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:286:MET:HE2	1:B:315:GLY:O	2.14	0.48
1:B:314:PRO:C	1:B:316:ARG:H	2.16	0.48
1: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:B:564:GLU:C	1:B:566:ARG:N	2.64	0.48
1:C:169:LYS:O	1:C:172:VAL:N	2.47	0.48
1:C:576:LEU:O	1:C:580:GLU:N	2.35	0.48
1:D:159:ALA:HB1	1:D:333:GLN:HG3	1.96	0.48
1:D:158:VAL:CG1	1:D:205:LEU:HD11	2.44	0.48
1:D:154:THR:OG1	1:D:212:GLU:OE2	2.32	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:594:LEU:HD12	1:A:595:PRO:O	2.13	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:B:170:GLU:CB	1:C:378:ARG:NH2	2.77	0.47
1:C:470:ALA:C	1:C:558:VAL:HG21	2.35	0.47
1:D:564:GLU:O	1:D:566:ARG:N	2.46	0.47
1:F: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:B:517:VAL:CG2	1:B:518:ALA:N	2.76	0.47
1:C:357:THR:C	1:C:360:PHE:HD1	2.17	0.47
1:C:536:SER:O	1:C:537:GLU:C	2.51	0.47
1:D: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: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: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:452:PRO:O	1:F:456:ASP:CG	2.53	0.47
1:F:563:LEU:O	1:F:566:ARG:HB3	2.14	0.47
1:A:191:GLY:CA	1:A:297:VAL:HG22	2.44	0.47
1: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:241:PHE:HE2	1:B:285:GLU:OE2	1.90	0.47
1:D:388:ASP:N	1:D:388:ASP:OD1	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:D:263:LYS:HE2	1:E:228:MET:CE	2.43	0.47
1:F:436:HIS:O	1:F:437:LYS:CG	2.61	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: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:E:519:TYR:HB3	1:E:535:TYR:HD2	1.78	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:238:ARG:O	1:A:239:ASP:C	2.51	0.47
1:B:376:ALA:HB1	1:B:381:ARG:HD3	1.95	0.47
1:B:384:ILE:HG22	1:B:385:THR:N	2.30	0.47
1:B:186:ALA:HB1	1:C:374:LEU:CD1	2.44	0.47
1:C:548:ARG:NH2	1:C:552:GLU:OE1	2.43	0.47
1:C:589:ARG:HH11	1:C:589:ARG:HB3	1.73	0.47
1:D:169:LYS:O	1:D:172:VAL:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:172:VAL:CB	1:E:213:ALA:HB2	2.44	0.47
1:E:159:ALA:HB1	1:E:333:GLN:HB3	1.96	0.47
1:E:462:ARG:HH12	1:E:511:HIS:H	1.62	0.47
1:E:449:PHE:HE2	1:E:496:GLN:HE21	1.63	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:B:165:LYS:HZ2	1:B:168:LEU:CD2	2.27	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:F:169:LYS:O	1:F:172:VAL:HG22	2.15	0.47
1:F:235:ALA:O	1:F:238:ARG:NH1	2.48	0.47
1:F:262:ARG:CG	1:F:263:LYS:H	2.20	0.47
1: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:B:332:GLU:HB2	1:B:354:ALA:HB2	1.95	0.47
1:B:159:ALA:CB	1:B:334:ILE:HG13	2.36	0.47
1:C:169:LYS:O	1:C:172:VAL:CG1	2.61	0.47
1:C:210:ALA:HA	1:C:251:ILE:HD11	1.96	0.47
1:C:192:VAL:N	1:C:297:VAL:O	2.39	0.47
1:D:510:MET:O	1:D:512:PRO:CD	2.61	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:589:ARG:HH22	1:E:596:LEU:N	2.13	0.47
1:F:494:PHE:O	1:F:496:GLN:N	2.47	0.47
1:B:397:MET:HA	1:B:400:PRO:HG2	1.95	0.47
1:B:455:GLU:O	1:B:456:ASP:C	2.53	0.47
1:D:336:ARG:O	1:D:338:HIS:N	2.47	0.47
1:D:381:ARG:NH2	1:D:388:ASP:CG	2.47	0.47
1: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:E:188:ILE:CG2	1:E:189:PRO:HD2	2.45	0.47
1:E:192:VAL:O	1:E:298:MET:HA	2.14	0.47
1:E:191:GLY:CA	1:E:297:VAL:CG2	2.93	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:382:ARG:CG	1:E:383:LYS:N	2.75	0.47
1:F:158:VAL:HG22	1:F:204:HIS:ND1	2.29	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:A:316:ARG:HG2	1:A:317:PHE:CD2	2.49	0.47
1:A:348:VAL:HG12	1:A:348:VAL:O	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:331:ARG:HH22	1:B:580:GLU:CD	2.14	0.47
1:B:159:ALA:HA	1:B:333:GLN:HE21	1.79	0.47
1:B:338:HIS:CE1	1:B:366:GLU:HG3	2.50	0.47
1:B:410:ARG:O	1:B:411:ASP:C	2.53	0.47
1:B:563:LEU:O	1:B:566:ARG:CB	2.62	0.47
1:C:277:GLN:HG3	1:C:278:THR:N	2.28	0.47
1:D:400:PRO:O	1:D:403:LYS:N	2.48	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:408:SER:C	1:E:410:ARG:H	2.17	0.47
1:E:576:LEU:O	1:E:580:GLU:N	2.39	0.47
1:F:314:PRO:C	1:F:316:ARG:H	2.18	0.47
1:F:428:PHE:CZ	1:F:433:ASP:N	2.83	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:C:272:ASN:OD1	1:C:272:ASN:C	2.53	0.47
1:C:371:GLU:OE2	1:C:395:ARG:HD2	2.14	0.47
1:D:175:LEU:HB3	1:D:213:ALA:HB1	1.97	0.47
1:D:238:ARG:HA	1:D:241:PHE:CE2	2.50	0.47
1:D:237:VAL:HG21	1:D:281:GLN:HG3	1.95	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:F:369:LEU:O	1:F:370:ASN:C	2.53	0.47
1:A:361:VAL:CG1	1:A:364:ASP:HB2	2.45	0.47
1:B:154:THR:OG1	1:B:212:GLU:OE2	2.33	0.47
1:B:194:LEU:HD23	1:B:323:ILE:CD1	2.45	0.47
1:C:189:PRO:HG3	1:C:319:ARG:NH1	2.31	0.47
1:C:172:VAL:O	1:C:213:ALA:HB1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:199:GLY:O	1:D:361:VAL:CG2	2.63	0.47
1:E:428:PHE:HE1	1:E:432:ALA:HA	1.67	0.47
1:F:319:ARG:NH1	1:F:319:ARG:CG	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:147:LEU:C	1:C:147:LEU:HD12	2.36	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:C:387:LYS:C	1:C:390:GLU:HB2	2.35	0.46
1:D:458:LEU:HD11	1:D:460:TRP:HB3	1.96	0.46
1:E:147:LEU:C	1:E:147:LEU:HD12	2.35	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:A:292:ASP:OD2	1:B:227:GLU:OE1	2.33	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:157:ASP:HB3	1:B:337:ILE:CG1	2.45	0.46
1:B:469:ILE:HG23	1:B:497:ALA:HB1	1.98	0.46
1:B:506:THR:OG1	1:B:520:ALA:HB3	2.15	0.46
1:B:505:ILE:HG23	1:B:514:PHE:CD2	2.50	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:147:LEU:HD23	1:C:217:PHE:CB	2.44	0.46
1:C:238:ARG:O	1:C:239:ASP:C	2.52	0.46
1:C:316:ARG:O	1:C:317:PHE:C	2.54	0.46
1: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:379:GLU:OE1	1:D:381:ARG:NE	2.48	0.46
1:D:345:ALA:CB	1:D:383:LYS:HE3	2.36	0.46
1:D:455:GLU:O	1:D:456:ASP:C	2.54	0.46
1:E:348:VAL:HG12	1:E:348:VAL:O	2.14	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:A:377:ALA:HB1	1:F:181:PHE:CD1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:410:ARG:O	1:F:411:ASP:C	2.53	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: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:C:570:GLU:O	1:C:571:ARG:C	2.54	0.46
1:D:311:LEU:HA	1:D:316:ARG:CZ	2.45	0.46
1:D:200:VAL:HG12	1:D:325:ALA:HB2	1.98	0.46
1:D:352:LEU:O	1:D:355:LYS:HB2	2.16	0.46
1: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: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
1:A:507:GLU:HB2	1:A:520:ALA:HB3	1.98	0.46
1:B:297:VAL:CG1	1:B:317:PHE:CE1	2.98	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: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:436:HIS:HB3	1:E:584:ALA:CB	2.45	0.46
1:A:378:ARG:HH12	1:F:170:GLU:HB2	1.80	0.46
1:F:467:ASP:O	1:F:471:VAL:HG13	2.16	0.46
1:A:212:GLU:C	1:A:214:ARG:HB2	2.34	0.46
1:A:253:PHE:HA	1:A:298:MET:O	2.16	0.46
1:A:373:ALA:HA	1:A:384:ILE:CD1	2.46	0.46
1:A:551:ILE:O	1:A:552:GLU:C	2.52	0.46
1:B:384:ILE:CG2	1:B:385:THR:N	2.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:361:VAL:CG1	1:E:364:ASP:HB2	2.46	0.46
1:F:204:HIS:CD2	2:F:2001:ADP:H2'	2.50	0.46
1:F:256:GLU:CG	1:F:256:GLU:O	2.62	0.46
1: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:305:ASP:C	1:A:307:LEU:N	2.68	0.46
1:A:449:PHE:HE2	1:A:496:GLN:HE21	1.60	0.46
1: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:H	1:C:218:ILE:HG12	1.64	0.46
1:C:407:LEU:HA	1:C:411:ASP:HB2	1.97	0.46
1:D:201:GLY:O	1:D:204:HIS:HB3	2.16	0.46
1:D:242:GLU:HA	1:D:245:LYS:CB	2.43	0.46
1:D:241:PHE:CZ	1:D:285:GLU:OE2	2.67	0.46
1:D:329:LYS:CG	1:D:330:GLY:N	2.78	0.46
1:D:454:ARG:HH21	1:D:526:TYR:HA	1.80	0.46
1:E:225:PHE:CE1	1:E:236:ARG:HG2	2.51	0.46
1:F:174:PHE:CD2	1:F:174:PHE:C	2.89	0.46
1:F:242:GLU:HA	1:F:245:LYS:CB	2.45	0.46
1:F:374:LEU:HD23	1:F:374:LEU:C	2.36	0.46
1:F:438:VAL:CG2	1:F:439:THR:N	2.79	0.46
1:F:454:ARG:HA	1:F:454:ARG:HH11	1.80	0.46
1:A:215:VAL:HG22	1:A:216:PRO:N	2.30	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:149:GLU:O	1:B:150:ALA:C	2.54	0.46
1:B:336:ARG:O	1:B:337:ILE:C	2.54	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:D:164:ALA:C	1:D:168:LEU:HD13	2.35	0.46
1:D:202:LYS:N	2:D:2001:ADP:O1A	2.49	0.46
1:D:455:GLU:HG2	1:D:455:GLU:O	2.16	0.46
1:D:521:VAL:HG23	1:D:532:VAL:CG1	2.42	0.46
1:E:311:LEU:HD23	1:E:311:LEU:HA	1.68	0.46
1:E:316:ARG:O	1:E:317:PHE:C	2.51	0.46
1:A:272:ASN:C	1:A:272:ASN:OD1	2.54	0.46
1:A:312:LEU:HD21	1:A:320:GLN:OE1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1: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:443:ARG:O	1:B:445:ARG:N	2.49	0.46
1:C:340:ARG:C	1:C:342:LYS:N	2.59	0.46
1:D:192:VAL:C	1:D:317:PHE:CE2	2.89	0.46
1:D:207:ARG:O	1:D:210:ALA:N	2.49	0.46
1:D:286:MET:HB2	1:D:286:MET:HE3	1.82	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:280:ASN:O	1:E:281:GLN:C	2.54	0.46
1:E:469:ILE:HD11	1:E:500:LEU:HB3	1.98	0.46
1:F:238:ARG:HH12	1:F:239:ASP:H	1.43	0.46
1:F:199:GLY:O	1:F:361:VAL:HG22	2.14	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:242:GLU:HA	1:B:245:LYS:CB	2.42	0.46
1:B:389:LEU:O	1:B:390:GLU:C	2.54	0.46
1:B:454:ARG:HH11	1:B:454:ARG:HA	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: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:CB	1:E:207:ARG:CZ	2.91	0.46
1:E:370:ASN:C	1:E:370:ASN:OD1	2.55	0.46
1:E:520:ALA:HA	1:E:533:ARG:HG2	1.96	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:B:228:MET:HE3	1:B:236:ARG:HD3	1.98	0.46
1:B:301:THR:HG23	1:B:303:ARG:H	1.81	0.46
1:C:305:ASP:C	1:C:307:LEU:N	2.69	0.46
1:C:356:ARG:C	1:C:358:PRO:HD2	2.37	0.46
1:D:297:VAL:HG13	1:D:317:PHE:HZ	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:314:PRO:HA	1:D:318:ASP:OD2	2.16	0.46
1:E:173:GLU:CA	1:E:176:LYS:HG3	2.36	0.46
1:E:441:VAL:O	1:E:441:VAL:CG1	2.61	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:174:PHE:O	1:A:177:ASN:C	2.55	0.45
1:A:206:ALA:CB	1:A:217:PHE:HZ	2.29	0.45
1:A:237:VAL:O	1:A:240:LEU:HB3	2.16	0.45
1:A:192:VAL:N	1:A:297:VAL:O	2.43	0.45
1:A:410:ARG:O	1:A:411:ASP:C	2.54	0.45
1:A:520:ALA:HA	1:A:533:ARG:HG2	1.98	0.45
1:B:352:LEU:O	1:B:353:LEU:C	2.53	0.45
1:C:228:MET:HG3	1:C:236:ARG:NH2	2.31	0.45
1:C:450:MET:HE2	1:C:451:MET:SD	2.56	0.45
1:C:503:ARG:CD	1:C:508:TRP:CE2	2.95	0.45
1:C:459:HIS:CE1	1:D:411:ASP:HB3	2.51	0.45
1:D:428:PHE:HE1	1:D:432:ALA:C	2.19	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:E:168:LEU:C	1:E:168:LEU:HD12	2.36	0.45
1:E:462:ARG:HG3	1:E:466:LEU:HD11	1.98	0.45
1:E:506:THR:HA	1:E:519:TYR:HD1	1.80	0.45
1:E:534:GLN:N	1:E:534:GLN:CD	2.70	0.45
1:F:238:ARG:HA	1:F:241:PHE:HE2	1.81	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:D:354:ALA:O	1:D:357:THR:HG23	2.15	0.45
1:D:410:ARG:O	1:D:411:ASP:C	2.54	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: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:274:GLU:C	1:A:277:GLN:HB3	2.37	0.45
1:A:443:ARG:HG2	1:A:443:ARG:O	2.16	0.45
1:A:503:ARG:HG3	1:A:504:MET:N	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:336:ARG:O	1:D:337:ILE:C	2.53	0.45
1:D:379:GLU:OE1	1:D:381:ARG:CD	2.65	0.45
1: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
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: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:589:ARG:CZ	1:B:596:LEU:HD22	2.46	0.45
1:C:222:GLY:O	1:C:225:PHE:HB2	2.17	0.45
1:C:198:PRO:HD3	1:C:302:ASN:HD21	1.81	0.45
1:C:438:VAL:HG22	1:C:582:LEU:HB2	1.99	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:NZ	1:F:205:LEU:CB	2.68	0.45
1:F:165:LYS:O	1:F:167:GLU:N	2.50	0.45
1:F:384:ILE:CG2	1:F:385:THR:N	2.79	0.45
1:A:218:ILE:H	1:A:218:ILE:HG12	1.65	0.45
1:A:449:PHE:HD2	1:A:449:PHE:N	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:NH1	1:C:381:ARG:CG	2.79	0.45
1:C:519:TYR:CA	1:C:533:ARG:CZ	2.95	0.45
1:C:459:HIS:HE1	1:D:411:ASP:CB	2.29	0.45

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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:F:381:ARG:NH2	1:F:388:ASP:OD2	2.50	0.45
1:A:286:MET:CE	1:A:297:VAL:HG21	2.46	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: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:350:LEU:O	1:D:353:LEU:N	2.50	0.45
1:D:583:THR:O	1:D:584:ALA:C	2.55	0.45
1:E:200:VAL:N	2:E:1001:ADP:O1A	2.50	0.45
1: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:460:TRP:CD1	1:F:464:ARG:HG2	2.52	0.45
1:F:449:PHE:HZ	1:F:496:GLN:OE1	2.00	0.45
1:F:523:GLU:O	1:F:530:TYR:N	2.43	0.45
1:F:582:LEU:CD2	1:F:590:VAL:HG21	2.42	0.45
1:A:196:GLY:C	1:A:202:LYS:HZ1	2.18	0.45
1:A:212:GLU:O	1:A:214:ARG:CB	2.65	0.45
1:A:381:ARG:CG	1:A:381:ARG:NH1	2.80	0.45
1:A:387:LYS:C	1:A:390:GLU:HB2	2.37	0.45
1:A:464:ARG:NH1	1:A:464:ARG:HG2	2.32	0.45
1:A:483:PHE:C	1:A:485:ASP:H	2.20	0.45
1:A:519:TYR:C	1:A:533:ARG:NE	2.68	0.45
1:B:342:LYS:HA	1:B:342:LYS:HD2	1.60	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:274:GLU:C	1:C:277:GLN:HB3	2.34	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:336:ARG:HA	1:D:336:ARG:HD3	1.51	0.45
1:D:393:ALA:O	1:D:397:MET:HB3	2.17	0.45
1:D:302:ASN:ND2	1:D:443:ARG:HH22	1.91	0.45
1:D:443:ARG:O	1:D:445:ARG:N	2.50	0.45
1: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
1:E:470:ALA:HB1	1:E:558:VAL:CG2	2.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:352:LEU:HD11	1:F:386:MET:CE	2.40	0.45
1:A:236:ARG:CB	1:A:236:ARG:HH11	2.29	0.45
1:A:361:VAL:HG12	1:A:364:ASP:HB2	1.99	0.45
1:A:519:TYR:HB3	1:A:535:TYR:HD2	1.82	0.45
1:B:312:LEU:O	1:B:312:LEU:HD23	2.16	0.45
1:C:462:ARG:HH12	1:C:511:HIS:H	1.64	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: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:A:168:LEU:C	1:A:168:LEU:HD12	2.38	0.45
1:A:352:LEU:HD11	1:A:356:ARG:HH21	1.74	0.45
1:B:286:MET:HB2	1:B:286:MET:HE3	1.87	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:C:159:ALA:HB1	1:C:333:GLN:HB3	1.99	0.45
1:C:233:GLY:O	1:C:236:ARG:CG	2.62	0.45
1:C:236:ARG:CG	1:C:237:VAL:H	2.18	0.45
1:C:238:ARG:O	1:C:241:PHE:N	2.50	0.45
1:C:191:GLY:CA	1:C:297:VAL:CG2	2.94	0.45
1:D:157:ASP:O	1:D:158:VAL:HG23	2.16	0.45
1:E:305:ASP:C	1:E:307:LEU:N	2.70	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:442:PRO:HG2	1:A:443:ARG:H	1.81	0.45
1:A:527:LEU:O	1:A:527:LEU:HD12	2.16	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:517:VAL:HG13	1:B:519:TYR:CZ	2.52	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:D:197:PRO:HD2	1:D:200:VAL:CG1	2.45	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:465:LEU:O	1:A:469:ILE:HG13	2.17	0.44
1:A:447:LEU:HB2	1:A:496:GLN:HE22	1.80	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: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: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:E:153:VAL:HG13	1:E:157:ASP:CB	2.47	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
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:225:PHE:HZ	1:E:278:THR:HB	1.66	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:314:PRO:HA	1:F:318:ASP:OD2	2.16	0.44
1:F:338:HIS:HB3	1:F:369:LEU:HD12	1.99	0.44
1:F:344:LEU:HA	1:F:383:LYS:CG	2.47	0.44
1:F:200:VAL:HA	1:F:361:VAL:HG23	1.99	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:467:ASP:HA	1:A:557:ARG:NH2	2.32	0.44
1:A:438:VAL:HG22	1:A:582:LEU:HB2	2.00	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:312:LEU:HD21	1:C:320:GLN:OE1	2.16	0.44
1:C:370:ASN:C	1:C:370:ASN:OD1	2.55	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:E:211:GLY:C	1:E:214:ARG:HG2	2.37	0.44
1:E:233:GLY:O	1:E:236:ARG:CG	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:277:GLN:HG3	1:E:278:THR:N	2.31	0.44
1:E:192:VAL:N	1:E:297:VAL:O	2.38	0.44
1: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:149:GLU:O	1:F:150:ALA:C	2.56	0.44
1:F:238:ARG:HH11	1:F:238:ARG:CG	2.30	0.44
1:F:376:ALA:C	1:F:381:ARG:CB	2.84	0.44
1:F:583:THR:O	1:F:584:ALA:C	2.56	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:343:PRO:HG2	1:B:383:LYS:CA	2.40	0.44
1:D:170:GLU:HG2	1:D:171:ILE:N	2.32	0.44
1:D:428:PHE:CD1	1:D:432:ALA:HB3	2.52	0.44
1:D:428:PHE:CZ	1:D:433:ASP:N	2.85	0.44
1:D:452:PRO:O	1:D:456:ASP:CA	2.65	0.44
1:E:266:SER:C	1:E:268:VAL:N	2.71	0.44
1: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:HD23	1:F:312:LEU:O	2.17	0.44
1:A:182:HIS:CB	1:A:291:LYS:HD2	2.20	0.44
1:A:291:LYS:O	1:A:292:ASP:C	2.56	0.44
1: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:353:LEU:O	1:B:357:THR:CG2	2.65	0.44
1:B:361:VAL:HG13	1:B:364:ASP:CG	2.38	0.44
1: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:HA	1:C:533:ARG:HD2	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:NH1	1:D:533:ARG:HG3	2.21	0.44
1:E:273:ASP:CG	1:E:274:GLU:H	2.20	0.44
1:E:198:PRO:HD3	1:E:302:ASN:HD21	1.82	0.44
1:E:387:LYS:C	1:E:390:GLU:HB2	2.38	0.44
1: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:266:SER:C	1:A:268:VAL:N	2.70	0.44
1:A:318:ASP:O	1:A:319:ARG:HG3	2.18	0.44
1:B:238:ARG:NH1	1:B:239:ASP:CA	2.67	0.44
1:B:538:GLU:O	1:B:541:LYS:N	2.50	0.44
1:C:168:LEU:C	1:C:168:LEU:HD12	2.38	0.44
1:C:327:ASP:OD1	1:C:327:ASP:C	2.56	0.44
1:C:509:GLY:O	1:D:476:ARG:NH2	2.36	0.44
1:C:519:TYR:C	1:C:533:ARG:CZ	2.86	0.44
1:D:215:VAL:O	1:D:216:PRO:C	2.56	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
1:E:464:ARG:O	1:E:465:LEU:C	2.56	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:A:548:ARG:NH1	1:F:513:GLU:O	2.50	0.44
1:A:236:ARG:O	1:A:239:ASP:N	2.51	0.44
1:A:370:ASN:OD1	1:A:370:ASN:C	2.55	0.44
1:A:503:ARG:CD	1:A:508:TRP:CE2	2.98	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:586:GLU:HG2	1:C:587:PHE:N	2.32	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: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:A:237:VAL:HG13	1:A:238:ARG:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:ARG:HG2	1:A:379:GLU:N	2.22	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: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: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
1:D:506:THR:OG1	1:D:520:ALA:HB3	2.17	0.44
1:D:585:GLU:O	1:D:586:GLU:C	2.56	0.44
1:E:413:ARG:O	1:E:577:LEU:HD21	2.18	0.44
1:E:551:ILE:O	1:E:552:GLU:C	2.56	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:B:162:GLU:CA	1:B:162:GLU:OE1	2.66	0.44
1:B:161:ALA:O	1:B:164:ALA:HB3	2.18	0.44
1:B:476:ARG:O	1:B:479:GLU:N	2.51	0.44
1:B:355:LYS:HZ1	1:B:578:GLU:HG3	1.83	0.44
1:B:355:LYS:NZ	1:B:578:GLU:O	2.51	0.44
1:B:585:GLU:C	1:B:587:PHE:N	2.71	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:266:SER:C	1:C:268:VAL:N	2.70	0.44
1:C:290:GLU:CD	1:D:226:VAL:HG11	2.37	0.44
1:E:272:ASN:OD1	1:E:272:ASN:C	2.55	0.44
1:F:178:PRO:O	1:F:182:HIS:CE1	2.71	0.44
1:A:381:ARG:C	1:F:180:ARG:HH22	2.18	0.44
1:F:355:LYS:NZ	1:F:578:GLU:O	2.51	0.44
1:F:589:ARG:CZ	1:F:596:LEU:HD11	2.45	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:307:LEU:HD12	1:B:307:LEU:N	2.33	0.44
1:B:187:ARG:N	1:C:374:LEU:HD11	2.27	0.44
1:D:165:LYS:HZ2	1:D:168:LEU:HD23	1.83	0.44
1:D:286:MET:HG3	1:D:287:ASP:OD1	2.18	0.44
1:D:494:PHE:O	1:D:495:ARG:C	2.56	0.44
1:C:518:ALA:HB2	1:D:495:ARG:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:518:ALA:HB3	1:D:495:ARG:HA	2.00	0.44
1:E:282:LEU:HG	1:E:283:LEU:HD12	2.00	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
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:282:LEU:HG	1:A:283:LEU:HD12	2.00	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: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:O	1:C:527:LEU:HD12	2.18	0.43
1:D:210:ALA:O	1:D:214:ARG:HA	2.18	0.43
1:D:414:ILE:H	1:D:414:ILE:HG12	1.65	0.43
1:D:558:VAL:HG12	1:D:559:LYS:N	2.32	0.43
1:E:370:ASN:OD1	1:E:374:LEU:HD13	2.18	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:F:428:PHE:HE1	1:F:432:ALA:C	2.20	0.43
1:A:180:ARG:O	1:A:184:MET:HE2	2.18	0.43
1:B:159:ALA:HB1	1:B:333:GLN:HG3	1.98	0.43
1:B:348:VAL:HG21	1:B:386:MET:HE2	2.00	0.43
1:B:563:LEU:CD1	1:B:563:LEU:C	2.87	0.43
1:C:153:VAL:HG13	1:C:157:ASP:CB	2.48	0.43
1:D:158:VAL:HG11	1:D:205:LEU:HD11	2.00	0.43
1:D:297:VAL:CG1	1:D:317:PHE:CZ	3.01	0.43
1:D:196:GLY:O	1:D:302:ASN:HA	2.17	0.43
1:E:357:THR:C	1:E:360:PHE:HD1	2.21	0.43
1:E:503:ARG:CD	1:E:508:TRP:CE2	3.00	0.43
1:D:538:GLU:HB2	1:E:541:LYS:NZ	2.34	0.43
1:E:574:GLU:OE1	1:E:575:THR:N	2.51	0.43
1:F:361:VAL:HG13	1:F:364:ASP:CG	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:389:LEU:O	1:F:390:GLU:C	2.56	0.43
1:F:453:ARG:HH12	1:F:495:ARG:NH2	2.08	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:587:PHE:HD2	1:A:588:GLN:N	2.15	0.43
1:B:261:GLY:O	1:B:308:ASP:HB3	2.18	0.43
1:B:237:VAL:HG21	1:B:281:GLN:HG3	1.98	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:307:LEU:HD12	1:D:307:LEU:N	2.32	0.43
1:D:194:LEU:HD23	1:D:323:ILE:CD1	2.49	0.43
1:D:589:ARG:C	1:D:591:VAL:N	2.70	0.43
1:D:595:PRO:C	1:D:596:LEU:HD12	2.38	0.43
1:E:346:GLU:CD	1:E:347:ASP:N	2.71	0.43
1:E:511:HIS:C	1:E:512:PRO:O	2.56	0.43
1:F:194:LEU:HD23	1:F:323:ILE:CD1	2.48	0.43
1:F:360:PHE:CE1	1:F:364:ASP:HB3	2.54	0.43
1:A:541:LYS:HD3	1:F:538:GLU:CB	2.48	0.43
1:A:371:GLU:OE2	1:A:395:ARG:HD2	2.17	0.43
1:A:425:ALA:C	1:A:427:HIS:N	2.72	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:428:PHE:C	1:B:428:PHE:HD1	2.21	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: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:586:GLU:HA	1:C:589:ARG:CB	2.49	0.43
1:C:585:GLU:O	1:C:588:GLN:N	2.51	0.43
1:D:204:HIS:CD2	2:D:2001:ADP:H2'	2.53	0.43
1:D:468:GLN:O	1:D:471:VAL:N	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:493:ASP:O	1:E:496:GLN:CB	2.65	0.43
1:F:179:SER:HA	1:F:182:HIS:NE2	2.33	0.43
1:F:175:LEU:O	1:F:249:PRO:CG	2.66	0.43
1:F:297:VAL:CG1	1:F:317:PHE:CE1	3.02	0.43
1:F:325:ALA:CB	1:F:326:PRO:HD3	2.42	0.43
1:F:397:MET:O	1:F:400:PRO:CD	2.66	0.43
1:E:516:PRO:HB2	1:F:494:PHE:CE1	2.53	0.43
1:A:147:LEU:O	1:A:216:PRO:HB3	2.19	0.43
1:A:346:GLU:CD	1:A:347:ASP:N	2.71	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: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:HH11	1:C:145:ARG:CB	2.30	0.43
1:C:327:ASP:OD1	1:C:329:LYS:N	2.51	0.43
1:C:358:PRO:CA	1:C:359:GLY:C	2.84	0.43
1:C:382:ARG:HG3	1:C:383:LYS:CA	2.48	0.43
1:D:149:GLU:O	1:D:150:ALA:C	2.57	0.43
1:D:248:ALA:HB1	1:D:294:ALA:HB3	2.00	0.43
1:D:428:PHE:CE1	1:D:433:ASP:N	2.87	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:E:336:ARG:O	1:E:337:ILE:C	2.55	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:346:GLU:OE1	1:A:347:ASP:N	2.44	0.43
1:A:574:GLU:O	1:A:575:THR:C	2.57	0.43
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:478:ALA:O	1:B:479:GLU:C	2.57	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:428:PHE:C	1:D:428:PHE:HD1	2.22	0.43
1:E:361:VAL:HG12	1:E:364:ASP:HB2	1.99	0.43
1:E:361:VAL:O	1:E:365:LEU:HG	2.18	0.43
1:E:570:GLU:O	1:E:571:ARG:C	2.57	0.43
1:A:227:GLU:CG	1:F:263:LYS:NZ	2.67	0.43
1:A:145:ARG:HH11	1:A:145:ARG:CB	2.32	0.43
1:A:228:MET:SD	1:A:236:ARG:NH2	2.89	0.43
1:A:225:PHE:CE1	1:A:233:GLY:O	2.72	0.43
1:A:286:MET:HA	1:A:289:PHE:CE2	2.54	0.43
1:B:374:LEU:HD23	1:B:374:LEU:C	2.38	0.43
1:B:399:LEU:O	1:B:402:LYS:HB3	2.19	0.43
1:C:462:ARG:HH11	1:C:510:MET:HB3	1.84	0.43
1:D:241:PHE:C	1:D:243:THR:N	2.71	0.43
1:D:428:PHE:CE1	1:D:432:ALA:HB3	2.52	0.43
1:E:261:GLY:O	1:E:262:ARG:HB2	2.19	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:228:MET:SD	1:F:232:VAL:CG1	3.04	0.43
1:F:225:PHE:CG	1:F:236:ARG:NH1	2.86	0.43
1:F:297:VAL:CG1	1:F:317:PHE:CZ	3.01	0.43
1:F:355:LYS:HD2	1:F:355:LYS:HA	1.46	0.43
1:A:287:ASP:OD1	1:A:287:ASP:N	2.51	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:449:PHE:CE2	1:A:496:GLN:CD	2.92	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
1:A:587:PHE:C	1:A:587:PHE:CD2	2.92	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:503:ARG:HD2	1:C:508:TRP:CD2	2.52	0.43
1:D:342:LYS:HD2	1:D:342:LYS:HA	1.66	0.43
1:D:394:ASP:HA	1:D:397:MET:HE2	1.98	0.43
1:D:417:TYR:CZ	1:D:482:VAL:HG21	2.54	0.43
1:D:428:PHE:C	1:D:428:PHE:CD1	2.92	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:327:ASP:OD1	1:E:327:ASP:C	2.57	0.43
1:E:372:ALA:O	1:E:375:LEU:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:503:ARG:CG	1:E:508:TRP:CE3	3.02	0.43
1:F:503:ARG:HA	1:F:503:ARG:HD3	1.58	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:164:ALA:C	1:B:168:LEU:HD13	2.37	0.43
1:B:178:PRO:O	1:B:182:HIS:CE1	2.72	0.43
1:B:165:LYS:CE	1:B:205:LEU:HG	2.48	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:204:HIS:CD2	2:C:1001:ADP:C2	3.07	0.43
1:C:203:THR:OG1	1:C:204:HIS:N	2.52	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:C:483:PHE:C	1:C:485:ASP:H	2.23	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:HD2	1:D:355:LYS:HA	1.44	0.43
1:D:568:VAL:HG11	1:D:591:VAL:HG13	2.00	0.43
1:E:252:VAL:O	1:E:297:VAL:HA	2.19	0.43
1:E:274:GLU:C	1:E:277:GLN:HB3	2.36	0.43
1:E:234:ALA:HB1	1:E:281:GLN:HG2	2.01	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
1:E:445:ARG:O	1:E:447:LEU:N	2.52	0.43
1:F:458:LEU:HD11	1:F:460:TRP:HB3	2.01	0.43
1:F:585:GLU:O	1:F:586:GLU:C	2.55	0.43
1:F:585:GLU:O	1:F:587:PHE:N	2.52	0.43
1:F:594:LEU:C	1:F:594:LEU:HD23	2.39	0.43
1: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:CB	1:B:238:ARG:HH11	2.32	0.43
1:B:382:ARG:HA	1:B:382:ARG:HD2	1.08	0.43
1:B:539:THR:O	1:B:543:ILE:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:HA	1:B:188:ILE:HD13	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:HA	1:B:554:GLN:OE1	2.19	0.42
1:C:263:LYS:CG	1:C:264:ARG:H	2.29	0.42
1:C:264:ARG:HD2	1:C:266:SER:CB	2.49	0.42
1:C:297:VAL:HG23	1:C:317:PHE:CE1	2.54	0.42
1:C:350:LEU:HG	1:C:350:LEU:H	1.48	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:188:ILE:O	1:E:190:LYS:NZ	2.42	0.42
1:E:346:GLU:OE1	1:E:347:ASP:N	2.45	0.42
1:E:355:LYS:HD3	1:E:355:LYS:HA	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:E:574:GLU:O	1:E:575:THR:C	2.57	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:336:ARG:O	1:A:337:ILE:C	2.58	0.42
1:B:147:LEU:HD13	1:B:149:GLU:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	1:B:321:ILE:HD12	1.82	0.42
1:B:538:GLU:C	1:B:540:ALA:N	2.72	0.42
1:C:334:ILE:HD11	2:C:1001:ADP:N6	2.34	0.42
1:C: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:410:ARG:CG	1:C:411:ASP:N	2.79	0.42
1:D:159:ALA:CA	1:D:333:GLN:HE21	2.32	0.42
1:D:352:LEU:HD11	1:D:356:ARG:NH1	2.33	0.42
1:D:376:ALA:HA	1:D:381:ARG:NH1	2.34	0.42
1:C:508:TRP:HD1	1:D:491:GLU:HG2	1.84	0.42
1:D:187:ARG:H	1:E:374:LEU:HD11	1.82	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: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:B:215:VAL:HG21	1:B:249:PRO:C	2.38	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:237:VAL:HG13	1:C:238:ARG:N	2.34	0.42
1:C:234:ALA:HB1	1:C:281:GLN:HG2	2.01	0.42
1: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: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:E:462:ARG:HG3	1:E:463:LYS:N	2.28	0.42
1:F:205:LEU:HA	1:F:208:ALA:HB3	2.02	0.42
1:F:238:ARG:O	1:F:239:ASP:C	2.56	0.42
1:F:286:MET:SD	1:F:316:ARG:HG3	2.59	0.42
1:F:193:LEU:HB3	1:F:317:PHE:CD2	2.54	0.42
1:F:506:THR:OG1	1:F:520:ALA:HB3	2.19	0.42
1:F:532:VAL:O	1:F:532:VAL:HG13	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:147:LEU:HB3	1:A:217:PHE:O	2.19	0.42
1:A:236:ARG:CG	1:A:237:VAL:H	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:ARG:C	1:A:238:ARG:N	2.71	0.42
1:A:372:ALA:O	1:A:375:LEU:HB3	2.20	0.42
1:A:458:LEU:HD12	1:A:458:LEU:C	2.39	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:159:ALA:CA	1:B:333:GLN:HE21	2.32	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:215:VAL:O	1:F:216:PRO:C	2.56	0.42
1:F:319:ARG:HB3	1:F:319:ARG:NH1	2.35	0.42
1:F:348:VAL:CG2	1:F:352:LEU:CD1	2.98	0.42
1:F:563:LEU:C	1:F:563:LEU:CD1	2.88	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:445:ARG:C	1:A:447:LEU:N	2.73	0.42
1:A:454:ARG:HD3	1:A:454:ARG:C	2.39	0.42
1: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:A:463:LYS:HB2	1:B:486:VAL:HG11	2.00	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:336:ARG:O	1:C:337:ILE:C	2.57	0.42
1:C:425:ALA:C	1:C:427:HIS:N	2.71	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:311:LEU:C	1:D:316:ARG:HG2	2.31	0.42
1:D:373:ALA:CA	1:D:384:ILE:HD11	2.49	0.42
2:E:1001:ADP:H2'	2:E:1001:ADP:N3	2.35	0.42
1:E:174:PHE:O	1:E:177:ASN:C	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:155:PHE:O	1:B:156:LYS:C	2.57	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:215:VAL:O	1:B:216:PRO:C	2.55	0.42
1:B:476:ARG:HD3	1:B:494:PHE:HZ	1.85	0.42
1:B:477:ALA:O	1:B:478:ALA:C	2.55	0.42
1:C:273:ASP:OD1	1:C:273:ASP:C	2.58	0.42
1:D:414:ILE:O	1:D:415:THR:C	2.57	0.42
1:E:586:GLU:CA	1:E:589:ARG:HG3	2.41	0.42
1:F:215:VAL:HG21	1:F:249:PRO:C	2.38	0.42
1:F:344:LEU:CG	1:F:346:GLU:OE1	2.67	0.42
1:F:357:THR:HG1	1:F:360:PHE:HD2	1.65	0.42
1:F:455:GLU:O	1:F:456:ASP:C	2.58	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:327:ASP:C	1:A:327:ASP:OD1	2.57	0.42
1:A:338:HIS:ND1	1:A:366:GLU:HB2	2.35	0.42
1: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:470:ALA:C	1:A:558:VAL:HG21	2.39	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:428:PHE:CD1	1:B:428:PHE:C	2.92	0.42
1:C:155:PHE:HZ	1:C:209:VAL:CG2	2.31	0.42
1:D:155:PHE:HB2	1:D:158:VAL:HB	2.01	0.42
1:D:361:VAL:HG13	1:D:364:ASP:CG	2.40	0.42
1:E:449:PHE:CD1	1:E:468:GLN:NE2	2.87	0.42
1:F:529:GLY:O	1:F:530:TYR:CB	2.58	0.42
1:A:155:PHE:CZ	1:A:209:VAL:CG2	3.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD12	1:D:307:LEU:H	1.85	0.42
1:D:563:LEU:CD1	1:D:563:LEU:C	2.87	0.42
1:D:355:LYS:HZ3	1:D:578:GLU:HG3	1.85	0.42
1:E:145:ARG:HH11	1:E:145:ARG:CB	2.32	0.42
1:E:147:LEU:HD12	1:E:148:THR:N	2.35	0.42
1:E:222:GLY:O	1:E:225:PHE:HB2	2.20	0.42
1:F:164:ALA:C	1:F:168:LEU:HD13	2.36	0.42
1:F:236:ARG:O	1:F:237:VAL:C	2.58	0.42
1:F:417:TYR:CZ	1:F:482:VAL:HG21	2.55	0.42
1:A:180:ARG:HG2	1:A:180:ARG:H	1.50	0.42
1:A:252:VAL:HB	1:A:297:VAL:HA	2.01	0.42
1:A:356:ARG:C	1:A:358:PRO:HD2	2.40	0.42
1:A:407:LEU:HA	1:A:411:ASP:HB2	2.02	0.42
1:B:157:ASP:O	1:B:204:HIS:CE1	2.73	0.42
1:B:376:ALA:C	1:B:381:ARG:CB	2.84	0.42
1: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
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:HA	1:D:241:PHE:HE2	1.84	0.42
1:D:238:ARG:NH1	1:D:239:ASP:CA	2.69	0.42
1: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:E:204:HIS:CD2	2:E:1001:ADP:C2	3.07	0.42
1:E:163:GLU:H	1:E:163:GLU:CD	2.08	0.42
1:E:175:LEU:HD12	1:E:175:LEU:O	2.20	0.42
1:E:253:PHE:HA	1:E:298:MET:O	2.20	0.42
1:F:173:GLU:O	1:F:176:LYS:N	2.50	0.42
1:F:172:VAL:O	1:F:175:LEU:HB2	2.20	0.42
1:F:253:PHE:HA	1:F:298:MET:CB	2.45	0.42
1:F:307:LEU:N	1:F:307:LEU:HD12	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:400:PRO:O	1:F:403:LYS:N	2.52	0.42
1:F:567:GLU:O	1:F:568:VAL:C	2.59	0.42
1:A:277:GLN:CG	1:A:278:THR:N	2.83	0.42
1:A:311:LEU:HD23	1:A:316:ARG:HH21	1.75	0.42
1:B:168:LEU:O	1:B:171:ILE:N	2.52	0.42
1:B:157:ASP:O	1:B:204:HIS:HE1	2.03	0.42
1:B:388:ASP:N	1:B:388:ASP:OD1	2.48	0.42
1:B:589:ARG:CZ	1:B:596:LEU:CD2	2.97	0.42
1:C:215:VAL:HG21	1:C:250:CYS:CB	2.49	0.42
1:C:264:ARG:HD2	1:C:266:SER:HB2	2.00	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: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:452:PRO:O	1:D:456:ASP:CG	2.59	0.42
1:D:453:ARG:CZ	1:D:495:ARG:NH2	2.57	0.42
1:D:449:PHE:HZ	1:D:496:GLN:OE1	2.03	0.42
1:E:180:ARG:H	1:E:180:ARG:HG2	1.51	0.42
1:E:180:ARG:O	1:E:184:MET:HE2	2.19	0.42
1:E:174:PHE:HZ	1:E:294:ALA:HB1	1.85	0.42
1: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:A:172:VAL:HG22	1:A:173:GLU:N	2.35	0.41
1:A:174:PHE:CG	1:A:175:LEU:N	2.85	0.41
1:A:203:THR:OG1	1:A:204:HIS:N	2.52	0.41
1:A:222:GLY:O	1:A:225:PHE:HB2	2.19	0.41
1:A:361:VAL:HG22	1:A:362:GLY:N	2.35	0.41
1:A:382:ARG:HG2	1:A:383:LYS:H	1.84	0.41
1:A:464:ARG:CG	1:A:464:ARG:NH1	2.80	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: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:D:477:ALA:O	1:D:478:ALA:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:356:ARG:C	1:E:358:PRO:HD2	2.39	0.41
1:E:468:GLN:O	1:E:471:VAL:HB	2.20	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:B:301:THR:HG23	1:B:302:ASN:N	2.35	0.41
1:B:332:GLU:CD	1:B:351:ALA:HA	2.41	0.41
1:B:500:LEU:O	1:B:503:ARG:CB	2.68	0.41
1:B:508:TRP:O	1:B:509:GLY:C	2.58	0.41
1:C:236:ARG:HH11	1:C:236:ARG:CB	2.32	0.41
1:C:313:ARG:NH1	1:C:526:TYR:C	2.66	0.41
1:C:462:ARG:O	1:C:466:LEU:HD12	2.20	0.41
1:C:566:ARG:O	1:C:567:GLU:C	2.56	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:349:ASP:C	1:D:350:LEU:HG	2.40	0.41
1:D:525:THR:HG22	1:D:526:TYR:HD2	1.84	0.41
1:E:200:VAL:HG13	1:E:323:ILE:HG13	2.01	0.41
1:E:442:PRO:CG	1:E:443:ARG:H	2.33	0.41
1:E: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:412:ARG:O	1:F:413:ARG:C	2.59	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:235:ALA:O	1:B:238:ARG:NH1	2.53	0.41
1:B:236:ARG:O	1:B:237:VAL:C	2.59	0.41
1: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:391:GLU:HG3	1:C:391:GLU:O	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:HD12	1:B:405:LEU:O	2.20	0.41
1:B:538:GLU:O	1:B:540:ALA:N	2.53	0.41
1:C:196:GLY:C	1:C:202:LYS:HZ1	2.19	0.41
1:C:253:PHE:HA	1:C:298:MET:O	2.19	0.41
1:C:445:ARG:O	1:C:448:GLY:N	2.51	0.41
1:C:305:ASP:OD2	1:C:447:LEU:HD13	2.20	0.41
1:C:462:ARG:CG	1:C:463:LYS:N	2.83	0.41
1:C:566:ARG:HG2	1:C:567:GLU:N	2.35	0.41
1:D:155:PHE:O	1:D:156:LYS:C	2.59	0.41
1:D:172:VAL:CG2	1:D:173:GLU:N	2.82	0.41
1: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:F:280:ASN:O	1:F:283:LEU:HB3	2.19	0.41
1:A:357:THR:C	1:A:360:PHE:HD1	2.24	0.41
1:B:206:ALA:O	1:B:209:VAL:CG1	2.69	0.41
1:B:400:PRO:HB2	1:B:404:SER:OG	2.21	0.41
1:B:402:LYS:HE3	1:B:403:LYS:HG3	2.03	0.41
1: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:491:GLU:O	1:C:492:ASN:C	2.58	0.41
1:C:519:TYR:O	1:C:533:ARG:HG2	2.19	0.41
1:C:549:ARG:O	1:C:550:LEU:C	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:301:THR:HG23	1:D:302:ASN:N	2.36	0.41
1:D:529:GLY:O	1:D:530:TYR:CB	2.55	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:181:PHE:HA	1:C:184:MET:CE	2.51	0.41
1:C:236:ARG:C	1:C:238:ARG:N	2.71	0.41
1: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: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:HA	1:D:162:GLU:OE1	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:596:LEU:HG	1:E:597:GLU:N	2.36	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:286:MET:HE2	1:F:315:GLY:O	2.21	0.41
1:F:428:PHE:CE1	1:F:432:ALA:HB3	2.52	0.41
1:A:147:LEU:C	1:A:147:LEU:HD12	2.40	0.41
1:A:168:LEU:HA	1:A:171:ILE:HD12	2.02	0.41
1:A:234:ALA:HB1	1:A:281:GLN:HG2	2.02	0.41
1:B:202:LYS:CD	2:B:2001:ADP:O2B	2.68	0.41
1:B:241:PHE:C	1:B:243:THR:N	2.71	0.41
1:B:327:ASP:HB3	1:B:330:GLY:H	1.86	0.41
1:B:338:HIS:HB3	1:B:369:LEU:HD11	2.03	0.41
1:B:343:PRO:O	1:B:344:LEU:CB	2.68	0.41
1:B:335:LEU:HD23	1:B:365:LEU:HB3	2.00	0.41
1: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:372:ALA:O	1:C:375:LEU:HB3	2.20	0.41
1:B:508:TRP:HD1	1:C:491:GLU:HG2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:538:GLU:O	1:E:539:THR:C	2.59	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
1:F:172:VAL:CG2	1:F:173:GLU:N	2.84	0.41
1:F:241:PHE:C	1:F:243:THR:N	2.72	0.41
1:F:249:PRO:O	1:F:250:CYS:HB3	2.21	0.41
1:F:248:ALA:HB1	1:F:294:ALA:HB3	2.02	0.41
1:F:428:PHE:C	1:F:428:PHE:HD1	2.24	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:214:ARG:CG	1:A:214:ARG:NH1	2.78	0.41
1:A:218:ILE:CD1	1:A:250:CYS:SG	2.92	0.41
1:A:570:GLU:O	1:A:571:ARG:C	2.58	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:C:180:ARG:O	1:C:184:MET:HE2	2.21	0.41
1:C:212:GLU:C	1:C:214:ARG:HB2	2.41	0.41
1:C:200:VAL:HG13	1:C:323:ILE:HG13	2.03	0.41
1:C:346:GLU:CD	1:C:347:ASP:N	2.72	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:D:589:ARG:O	1:D:590:VAL:C	2.58	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:163:GLU:O	1:A:164:ALA:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:GLU:HG2	1:A:167:GLU:N	2.34	0.41
1:B:327:ASP:O	1:B:331:ARG:NH2	2.54	0.41
1:B:567:GLU:O	1:B:568:VAL:C	2.59	0.41
1:B:572:VAL:HG11	1:B:587:PHE:HE1	1.86	0.41
1:C:180:ARG:HG2	1:C:180:ARG:H	1.53	0.41
1:C:291:LYS:O	1:C:292:ASP:C	2.59	0.41
1:B:521:VAL:HG12	1:C:495:ARG:HD2	2.03	0.41
1:C:509:GLY:C	1:D:476:ARG:NH2	2.61	0.41
1:C:513:GLU:O	1:D:548:ARG:CZ	2.69	0.41
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: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:D:594:LEU:C	1:D:594:LEU:HD23	2.41	0.41
1:E:153:VAL:CG1	1:E:157:ASP:HB2	2.51	0.41
1:E:210:ALA:HB2	1:E:217:PHE:CD1	2.56	0.41
1:E:236:ARG:C	1:E:238:ARG:N	2.70	0.41
1:E:576:LEU:O	1:E:577:LEU:C	2.59	0.41
1:F:155:PHE:C	1:F:157:ASP:N	2.71	0.41
1:F:274:GLU:O	1:F:275:ARG:C	2.59	0.41
1:F:441:VAL:O	1:F:442:PRO:C	2.58	0.41
1:B:307:LEU:HD12	1:B:307:LEU:H	1.86	0.41
1:B:468:GLN:O	1:B:469:ILE:C	2.59	0.41
1:B:589:ARG:CD	1:B:596:LEU:HD21	2.50	0.41
1:C:163:GLU:O	1:C:164:ALA:C	2.59	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:D:280:ASN:HA	1:D:283:LEU:CD2	2.51	0.41
1:D:257:ILE:HD11	1:D:299:ALA:HB1	2.03	0.41
1:D:357:THR:HB	1:D:360:PHE:CD2	2.56	0.41
1:D:376:ALA:CA	1:D:381:ARG:CG	2.80	0.41
1:D:381:ARG:NH1	1:D:384:ILE:HA	2.35	0.41
1:E:177:ASN:N	1:E:177:ASN:OD1	2.54	0.41
1:E:196:GLY:CA	1:E:202:LYS:NZ	2.84	0.41
1:E:337:ILE:CD1	1:E:338:HIS:CD2	3.03	0.41
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:286:MET:HB2	1:F:286:MET:HE3	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:311:LEU:C	1:F:311:LEU:CD1	2.87	0.41
1:F:353:LEU:O	1:F:357:THR:HG23	2.21	0.41
1:F:354:ALA:O	1:F:357:THR:HG23	2.20	0.41
1:F:391:GLU:O	1:F:395:ARG:CB	2.69	0.41
1:F:424:LEU:O	1:F:425:ALA:C	2.60	0.41
1:F:509:GLY:O	1:F:510:MET:HG2	2.21	0.41
1:A:182:HIS:N	1:A:182:HIS:CD2	2.89	0.41
1:A:225:PHE:HB3	1:A:226:VAL:H	1.77	0.41
1:A:352:LEU:CD1	1:A:356:ARG:NH2	2.72	0.41
1: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:428:PHE:HE1	1:B:432:ALA:C	2.23	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:B:492:ASN:O	1:B:493:ASP:C	2.59	0.41
1:C:226:VAL:HG22	1:C:274:GLU:HG2	2.02	0.41
1:C:373:ALA:HA	1:C:384:ILE:HD11	2.02	0.41
1:C:372:ALA:HB3	1:C:389:LEU:HD23	2.03	0.41
1:D:180:ARG:NH2	1:E:377:ALA:HA	2.36	0.41
1:D:215:VAL:HG21	1:D:249:PRO:C	2.41	0.41
1:D:376:ALA:HB1	1:D:381:ARG:CB	2.51	0.41
1:D:468:GLN:O	1:D:469:ILE:C	2.58	0.41
1:D:594:LEU:O	1:D:594:LEU:HD23	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:F:199:GLY:O	1:F:361:VAL:CG2	2.69	0.41
1:F:336:ARG:O	1:F:337:ILE:C	2.58	0.41
1:A:248:ALA:HA	1:A:249:PRO:HA	1.92	0.40
1:A:252:VAL:O	1:A:297:VAL:HA	2.21	0.40
1:A:423:ALA:HB1	1:A:587:PHE:CE1	2.57	0.40
1:A:571:ARG:O	1:A:575:THR:HG23	2.20	0.40
1:B:230:VAL:C	1:B:232:VAL:H	2.24	0.40
1:B:459:HIS:C	1:B:459:HIS:HD1	2.15	0.40
1:B:483:PHE:C	1:B:485:ASP:H	2.24	0.40
1: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:171:ILE:O	1:C:172:VAL:C	2.59	0.40
1:C:210:ALA:HB2	1:C:217:PHE:CD1	2.56	0.40
1:C:410:ARG:O	1:C:411:ASP:C	2.58	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:445:ARG:C	1:C:447:LEU:N	2.74	0.40
1:C:514:PHE:HB3	1:C:519:TYR:OH	2.20	0.40
1:E:561:LEU:O	1:E:564:GLU:HB3	2.21	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:HG	1:A:407:LEU:H	1.57	0.40
1:A:413:ARG:O	1:A:577:LEU:HD21	2.21	0.40
1:B:360:PHE:CE1	1:B:364:ASP:HB3	2.55	0.40
1:C: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:256:GLU:CG	1:D:256:GLU:O	2.69	0.40
1:D:441:VAL:O	1:D:442:PRO:C	2.59	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:411:ASP:O	1:E:415:THR:OG1	2.31	0.40
1:E:461:SER:O	1:E:462:ARG:C	2.60	0.40
1:F:155:PHE:HB2	1:F:158:VAL:HB	2.03	0.40
1:F:192:VAL:O	1:F:317:PHE:HE2	2.04	0.40
1:F:260:VAL:C	1:F:279:LEU:HD11	2.38	0.40
1:F:238:ARG:N	1:F:281:GLN:HE21	2.20	0.40
1:F:303:ARG:HA	1:F:304:PRO:HD2	1.90	0.40
1:F:307:LEU:H	1:F:307:LEU:HD12	1.86	0.40
1:F:538:GLU:O	1:F:540:ALA:N	2.54	0.40
1:A:422:HIS:O	1:A:423:ALA:C	2.59	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:452:PRO:O	1:B:456:ASP:CG	2.60	0.40
1:B:460:TRP:HD1	1:B:464:ARG:HG2	1.86	0.40
1:B:531:ASP:N	1:B:531:ASP:OD1	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:C:464:ARG:O	1:C:465:LEU:C	2.57	0.40
1:C:484:ASP:C	1:C:486:VAL:H	2.23	0.40
1:D:155:PHE:C	1:D:157:ASP:N	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:257:ILE:O	1:D:258:ASP:C	2.60	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: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: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:349:ASP:C	1:F:350:LEU:HG	2.41	0.40
1:F:538:GLU:C	1:F:540:ALA:N	2.72	0.40
1:A:166:GLU:HB2	1:A:169:LYS:HZ1	1.82	0.40
1:A:173:GLU:CA	1:A:176:LYS:HG3	2.43	0.40
1:A:263:LYS:CG	1:A:264:ARG:N	2.83	0.40
1:A:314:PRO:HA	1:A:318:ASP:HB3	2.04	0.40
1:A:355:LYS:HD3	1:A:355:LYS:HA	1.90	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
1:B:422:HIS:CD2	1:B:475:GLY:HA3	2.57	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:478:ALA:O	1:D:479:GLU:C	2.58	0.40
1:D:518:ALA:HB3	1:E:495:ARG:HA	2.03	0.40
1:D:505:ILE:HG21	1:D:543:ILE:HG12	2.04	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:180:ARG:HH12	1:F:184:MET:CE	2.31	0.40
1:F:241:PHE:O	1:F:243:THR:N	2.54	0.40
1:F:263:LYS:HA	1:F:263:LYS:HD2	1.38	0.40
1:F:478:ALA:O	1:F:482:VAL:HG12	2.21	0.40
1:F:469:ILE:HG23	1:F:497:ALA:HB1	2.02	0.40
1:F:597:GLU:O	1:F:599:PRO:CD	2.68	0.40
1: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:349:ASP:C	1:B:350:LEU:HG	2.41	0.40
1:B:387:LYS:O	1:B:390:GLU:HB3	2.21	0.40
1:B:525:THR:HG22	1:B:526:TYR:N	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:PHE:HB3	1:C:226:VAL:H	1.73	0.40
1:D:161:ALA:O	1:D:164:ALA:HB3	2.21	0.40
1:D:332:GLU:CD	1:D:351:ALA:HA	2.42	0.40
1:D:424:LEU:O	1:D:425:ALA:C	2.60	0.40
1:D:467:ASP:O	1:D:471:VAL:HG13	2.21	0.40
1:D:514:PHE:HB3	1:D:519:TYR:CE1	2.56	0.40
1:E:174:PHE:CG	1:E:175:LEU:N	2.85	0.40
1:E:252:VAL:HB	1:E:297:VAL:HA	2.03	0.40
1:E:182:HIS:HD1	1:E:291:LYS:HB2	1.86	0.40
1:D:173:GLU:OE1	1:E:378:ARG:HA	2.21	0.40
1:E:397:MET:SD	1:E:406:VAL:HG11	2.62	0.40
1:E:572:VAL:O	1:E:573:ALA:C	2.60	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

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

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	456/508 (90%)	323 (71%)	111 (24%)	22 (5%)	2	24
1	B	442/508 (87%)	289 (65%)	125 (28%)	28 (6%)	1	19
1	C	456/508 (90%)	323 (71%)	112 (25%)	21 (5%)	2	25
1	D	442/508 (87%)	288 (65%)	121 (27%)	33 (8%)	1	16
1	E	456/508 (90%)	324 (71%)	110 (24%)	22 (5%)	2	24
1	F	442/508 (87%)	288 (65%)	120 (27%)	34 (8%)	1	16
All	All	2694/3048 (88%)	1835 (68%)	699 (26%)	160 (6%)	1	20

All (160) Ramachandran outliers are listed below:

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

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

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

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

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	365/402 (91%)	240 (66%)	125 (34%)	0	1
1	B	361/402 (90%)	242 (67%)	119 (33%)	0	1
1	C	365/402 (91%)	240 (66%)	125 (34%)	0	1
1	D	361/402 (90%)	241 (67%)	120 (33%)	0	1
1	E	365/402 (91%)	244 (67%)	121 (33%)	0	1
1	F	361/402 (90%)	240 (66%)	121 (34%)	0	1
All	All	2178/2412 (90%)	1447 (66%)	731 (34%)	0	1

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ADP	D	2001	-	24,29,29	1.03	3 (12%)	29,45,45	1.45	5 (17%)
2	ADP	C	1001	-	24,29,29	1.10	3 (12%)	29,45,45	1.56	4 (13%)
2	ADP	E	1001	-	24,29,29	1.06	2 (8%)	29,45,45	1.45	4 (13%)
2	ADP	B	2001	-	24,29,29	1.05	2 (8%)	29,45,45	1.49	4 (13%)
2	ADP	A	1001	-	24,29,29	1.10	2 (8%)	29,45,45	1.50	4 (13%)
2	ADP	F	2001	-	24,29,29	1.01	1 (4%)	29,45,45	1.52	4 (13%)

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	-	-	2/12/32/32	0/3/3/3
2	ADP	C	1001	-	-	2/12/32/32	0/3/3/3
2	ADP	E	1001	-	-	2/12/32/32	0/3/3/3
2	ADP	B	2001	-	-	3/12/32/32	0/3/3/3
2	ADP	A	1001	-	-	2/12/32/32	0/3/3/3
2	ADP	F	2001	-	-	2/12/32/32	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	ADP	C5-C4	2.78	1.48	1.40
2	F	2001	ADP	C5-C4	2.76	1.48	1.40
2	E	1001	ADP	C5-C4	2.73	1.48	1.40
2	C	1001	ADP	C5-C4	2.62	1.47	1.40
2	B	2001	ADP	C5-C4	2.59	1.47	1.40
2	D	2001	ADP	C5-C4	2.42	1.47	1.40
2	A	1001	ADP	C2-N3	2.24	1.35	1.32
2	E	1001	ADP	C2-N3	2.23	1.35	1.32
2	C	1001	ADP	O4'-C1'	2.19	1.44	1.41
2	C	1001	ADP	C2-N3	2.17	1.35	1.32
2	D	2001	ADP	O4'-C1'	2.08	1.44	1.41
2	B	2001	ADP	O4'-C1'	2.06	1.43	1.41
2	D	2001	ADP	C2-N3	2.05	1.35	1.32

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	ADP	PA-O3A-PB	-4.26	118.21	132.83
2	C	1001	ADP	PA-O3A-PB	-4.20	118.40	132.83
2	E	1001	ADP	PA-O3A-PB	-4.05	118.92	132.83
2	B	2001	ADP	PA-O3A-PB	-3.99	119.13	132.83
2	C	1001	ADP	N3-C2-N1	-3.72	122.86	128.68
2	F	2001	ADP	PA-O3A-PB	-3.69	120.17	132.83
2	D	2001	ADP	C4-C5-N7	-3.61	105.63	109.40
2	F	2001	ADP	C3'-C2'-C1'	3.54	106.30	100.98
2	B	2001	ADP	C3'-C2'-C1'	3.21	105.81	100.98
2	B	2001	ADP	N3-C2-N1	-3.13	123.78	128.68
2	A	1001	ADP	C3'-C2'-C1'	3.13	105.69	100.98
2	C	1001	ADP	C4-C5-N7	-3.12	106.15	109.40
2	D	2001	ADP	N3-C2-N1	-3.10	123.83	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	ADP	N3-C2-N1	-3.06	123.89	128.68
2	F	2001	ADP	N3-C2-N1	-3.04	123.93	128.68
2	F	2001	ADP	C4-C5-N7	-3.01	106.27	109.40
2	E	1001	ADP	C3'-C2'-C1'	2.95	105.42	100.98
2	D	2001	ADP	C3'-C2'-C1'	2.88	105.32	100.98
2	A	1001	ADP	C4-C5-N7	-2.82	106.46	109.40
2	D	2001	ADP	PA-O3A-PB	-2.75	123.39	132.83
2	B	2001	ADP	C4-C5-N7	-2.74	106.54	109.40
2	E	1001	ADP	N3-C2-N1	-2.74	124.39	128.68
2	E	1001	ADP	C4-C5-N7	-2.67	106.61	109.40
2	C	1001	ADP	C3'-C2'-C1'	2.57	104.85	100.98
2	D	2001	ADP	O3B-PB-O2B	2.20	116.03	107.64

There are no chirality outliers.

All (13) torsion outliers are listed below:

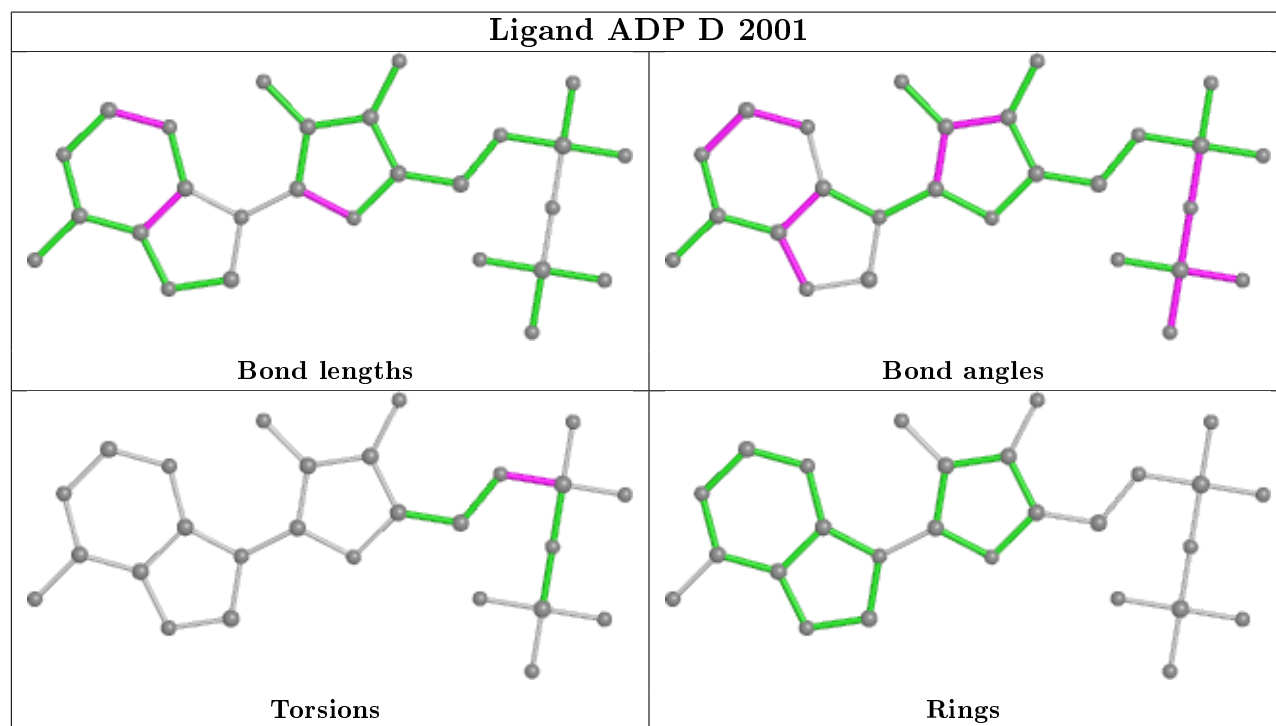
Mol	Chain	Res	Type	Atoms
2	D	2001	ADP	C5'-O5'-PA-O3A
2	C	1001	ADP	C5'-O5'-PA-O1A
2	C	1001	ADP	C5'-O5'-PA-O3A
2	E	1001	ADP	C5'-O5'-PA-O1A
2	B	2001	ADP	C5'-O5'-PA-O3A
2	A	1001	ADP	C5'-O5'-PA-O1A
2	F	2001	ADP	C5'-O5'-PA-O3A
2	E	1001	ADP	C5'-O5'-PA-O3A
2	D	2001	ADP	C5'-O5'-PA-O1A
2	B	2001	ADP	C5'-O5'-PA-O1A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

There are no ring outliers.

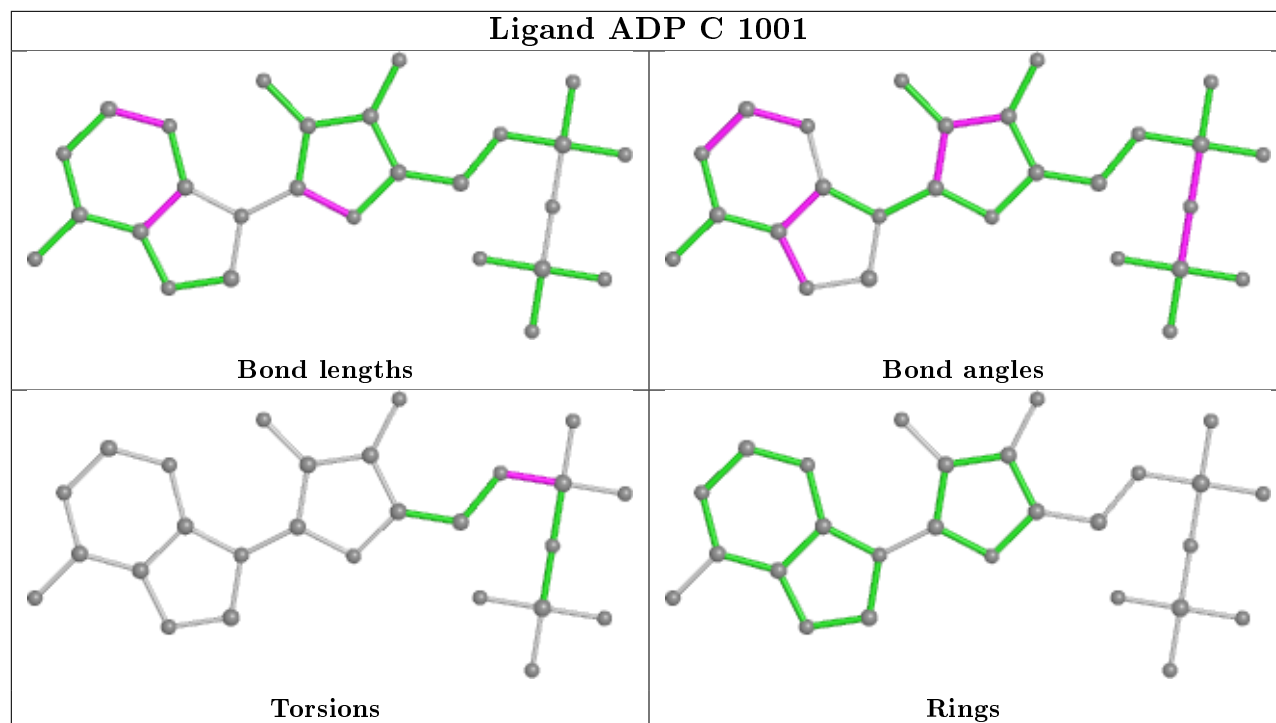
6 monomers are involved in 57 short contacts:

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

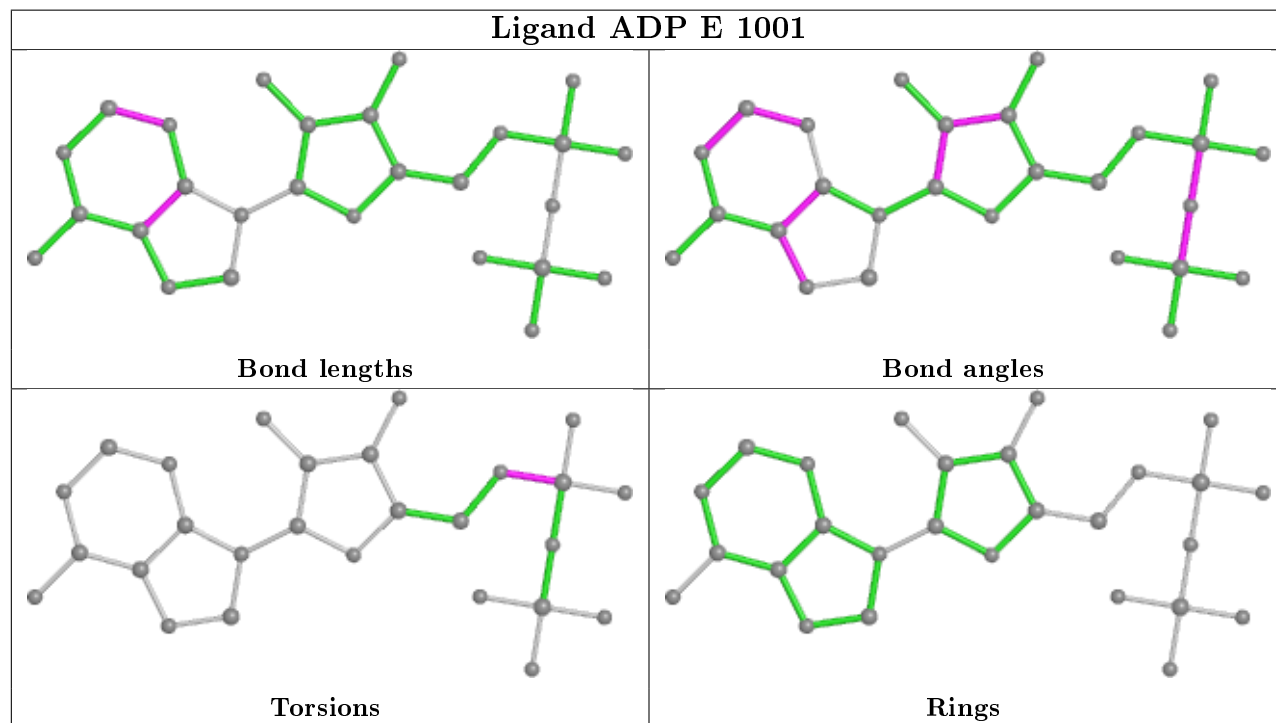
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



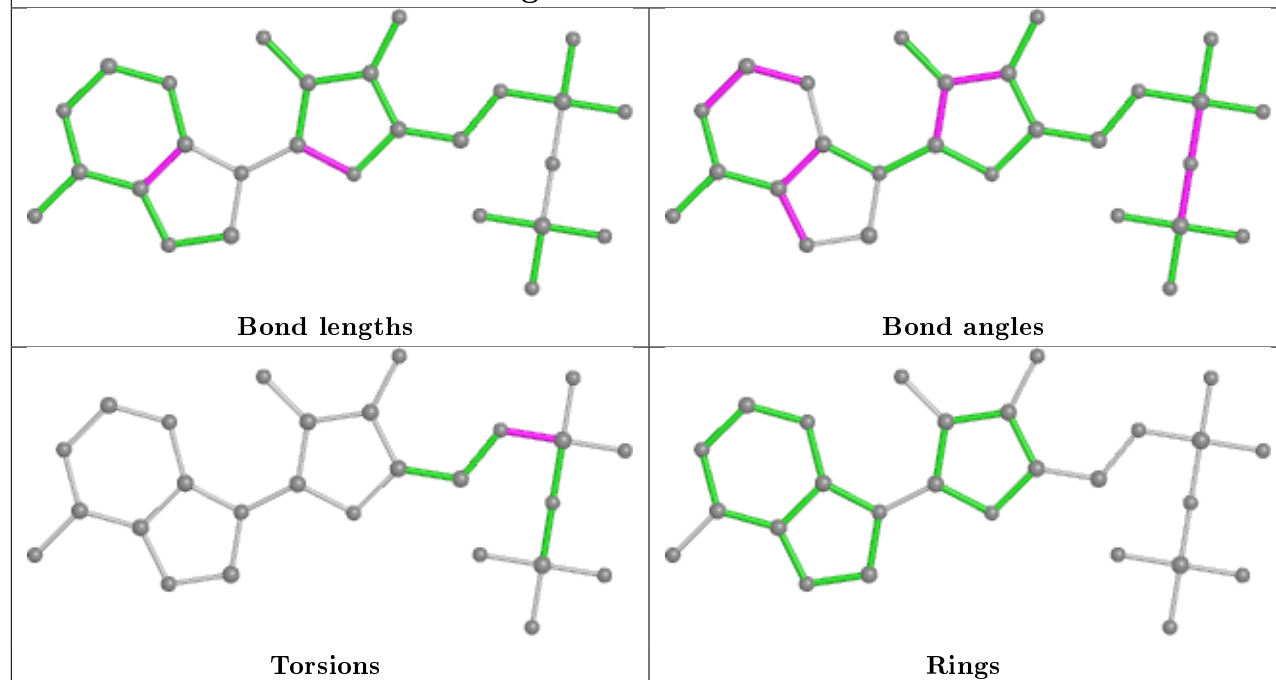
Ligand ADP C 1001



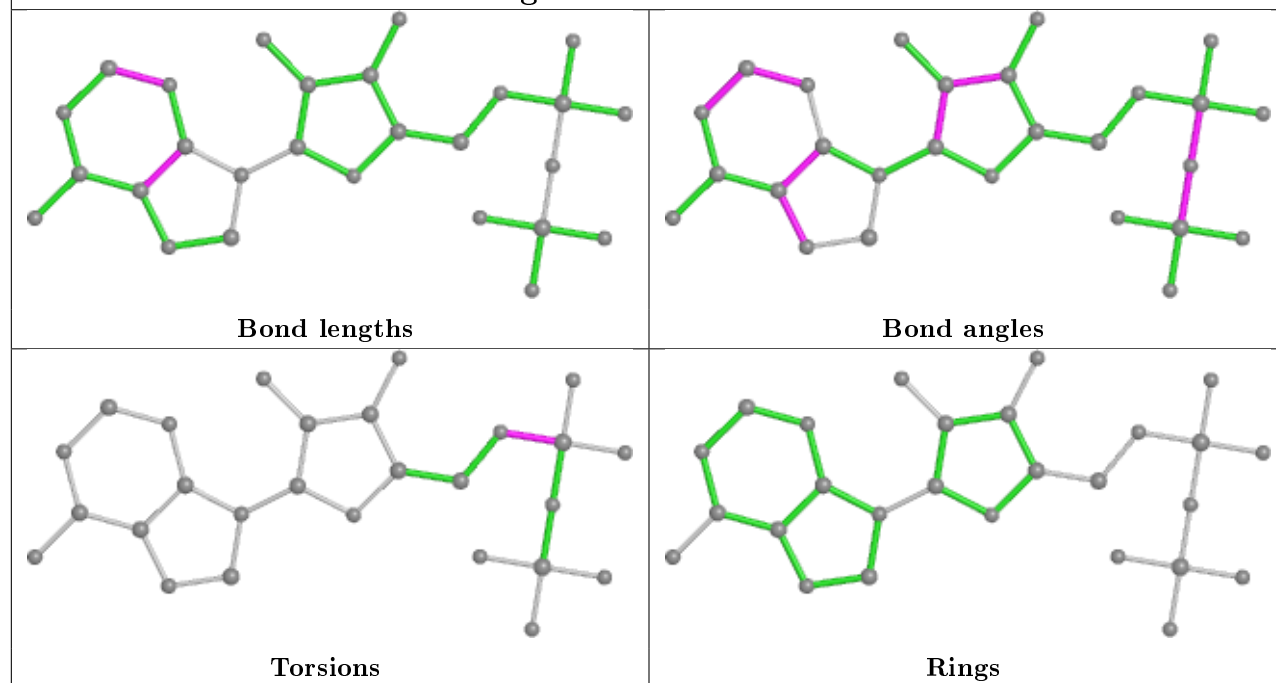
Ligand ADP E 1001

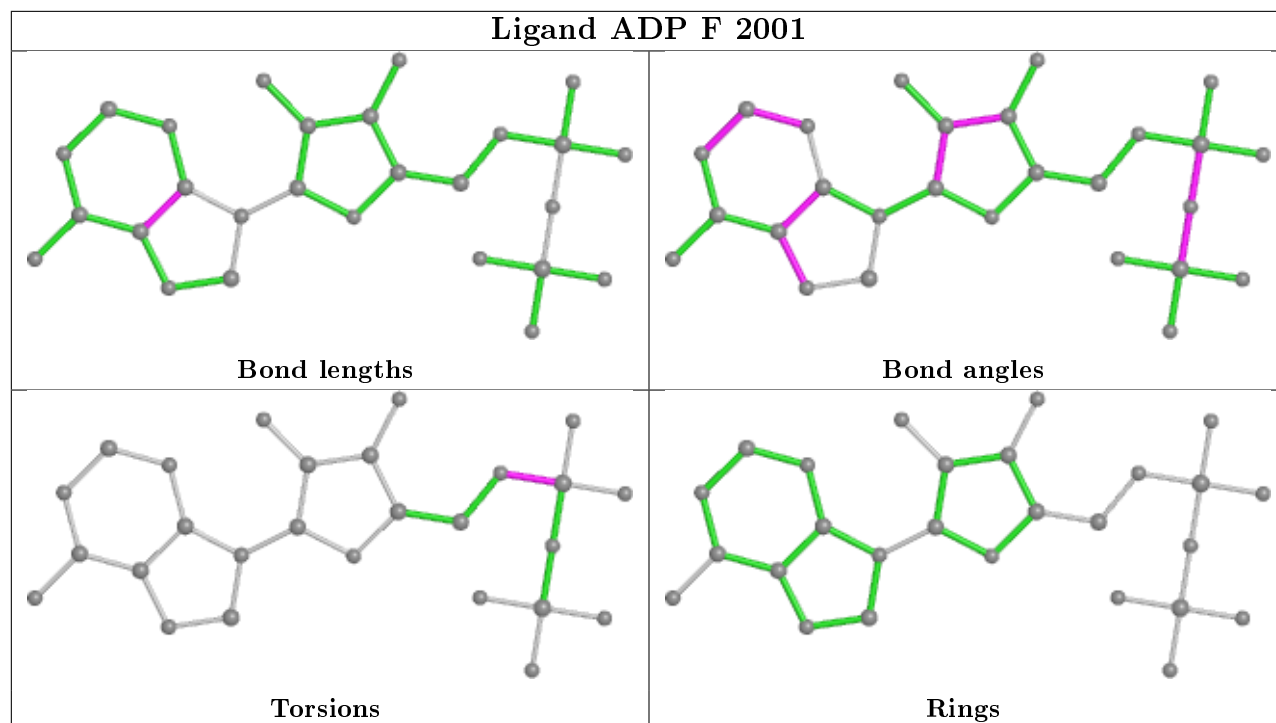


Ligand ADP B 2001



Ligand ADP A 1001





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

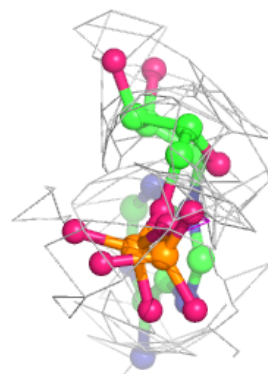
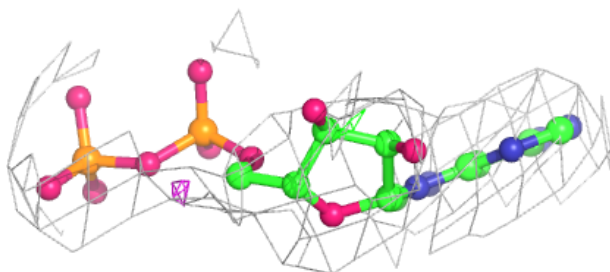
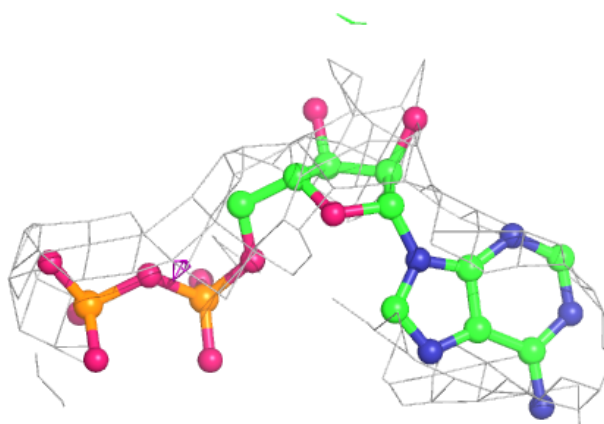
6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

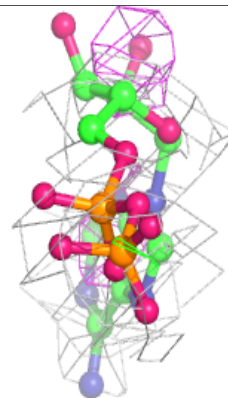
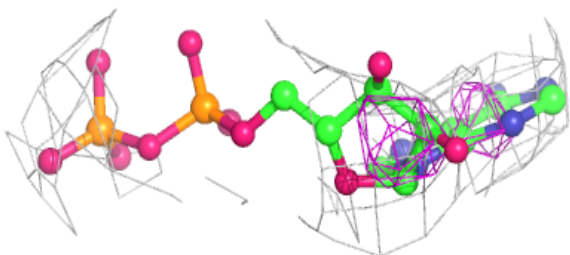
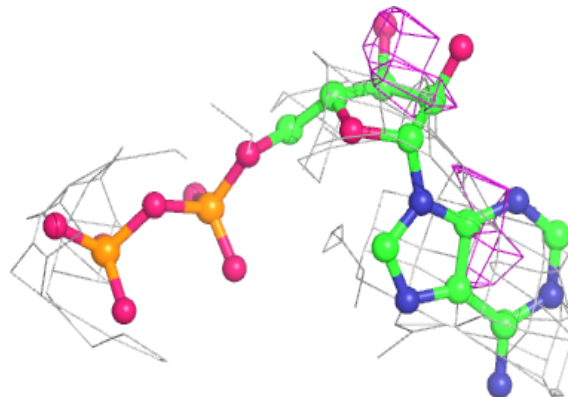
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP D 2001:

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

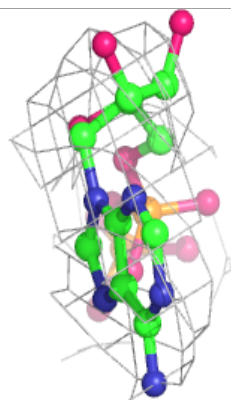
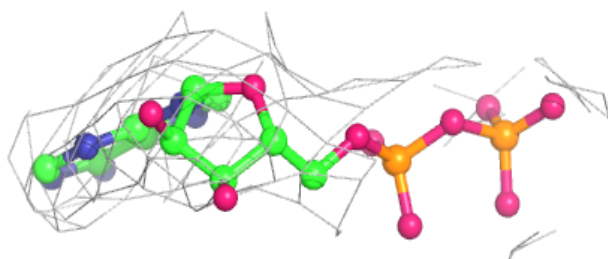
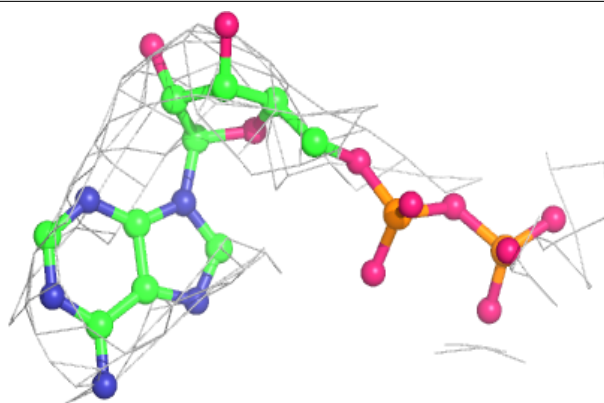
**Electron density around ADP C 1001:**

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

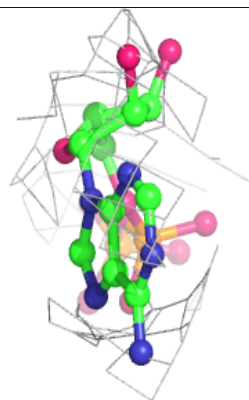
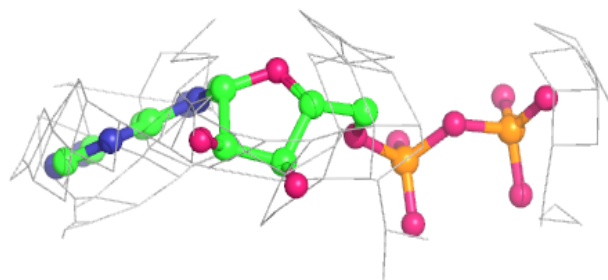
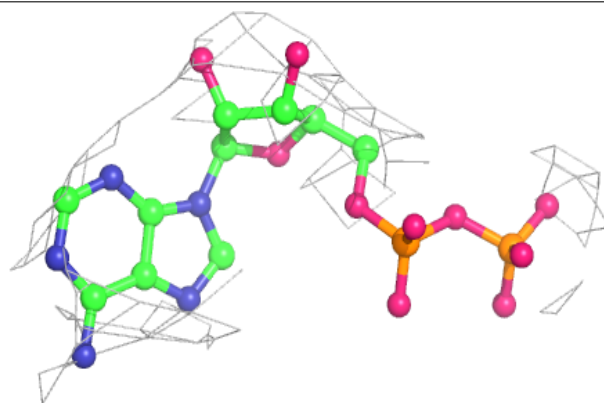


Electron density around ADP E 1001:

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

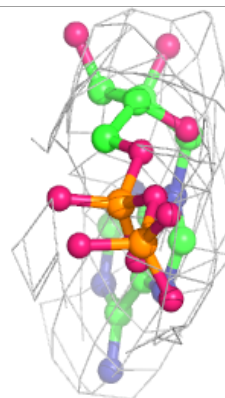
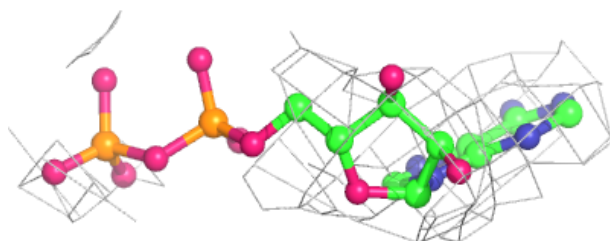
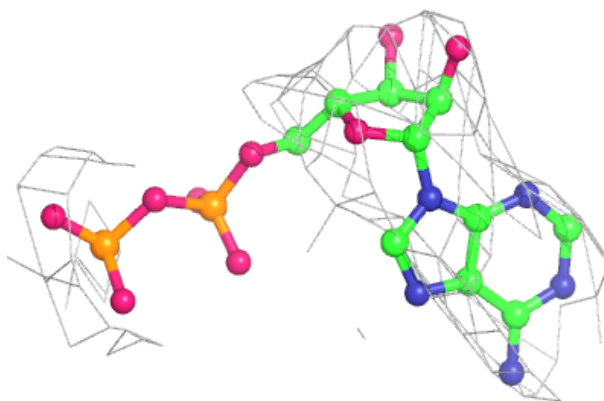
**Electron density around ADP B 2001:**

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

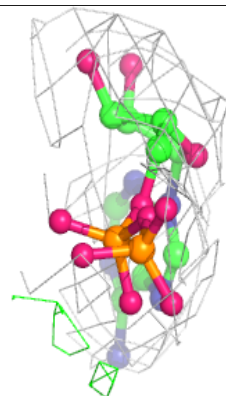
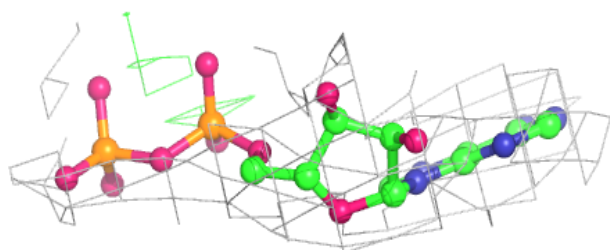
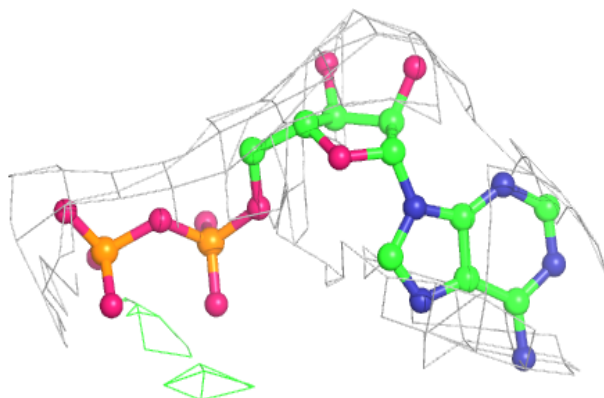


Electron density around ADP A 1001:

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

**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)



6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.