



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 10:43 AM EDT

PDB ID : 2IPC  
Title : Crystal structure of the translocation ATPase SecA from *Thermus thermophilus* reveals a parallel, head-to-head dimer  
Authors : Vassilyev, D.G.; Mori, H.; Vassilyeva, M.N.; Tsukazaki, T.; Kimura, Y.; Tahir, T.H.; Ito, K.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2006-10-12  
Resolution : 2.80 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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 types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
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)	:	2.36.2

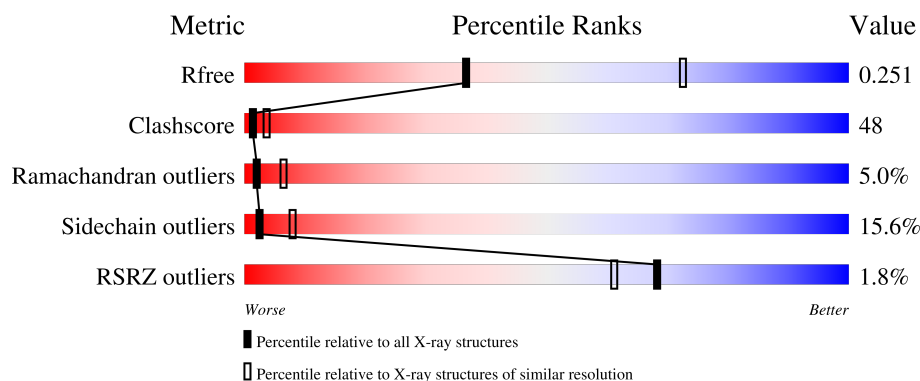
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*





The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	997	
1	B	997	
1	C	997	
1	D	997	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 31502 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 Preprotein translocase SecA subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	939	Total	C	N	O	S	0	0	0
			7551	4774	1354	1399	24			
1	B	934	Total	C	N	O	S	0	0	0
			7515	4749	1349	1394	23			
1	C	939	Total	C	N	O	S	0	0	0
			7551	4774	1354	1399	24			
1	D	934	Total	C	N	O	S	0	0	0
			7515	4749	1349	1394	23			

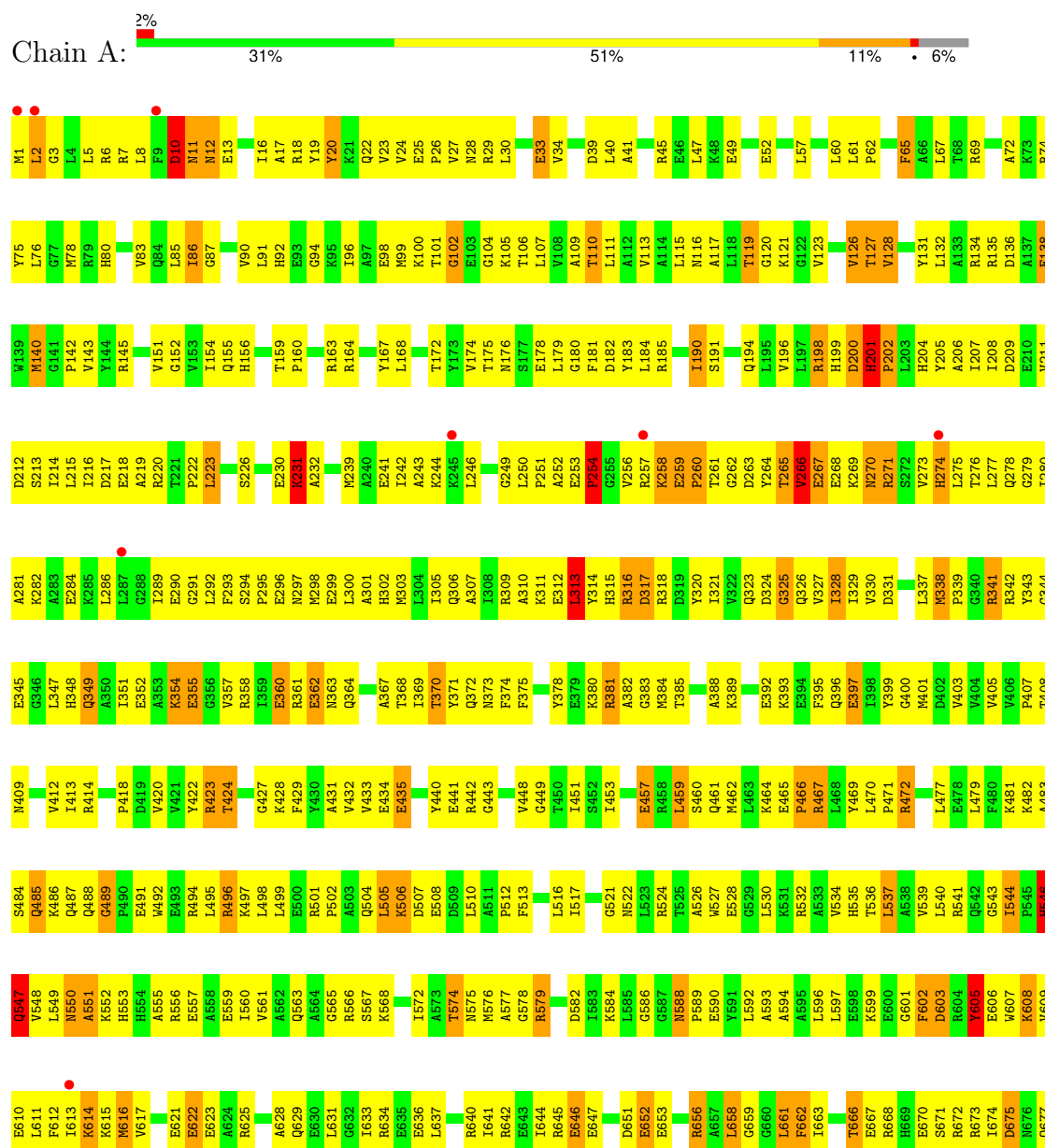
- Molecule 2 is water.

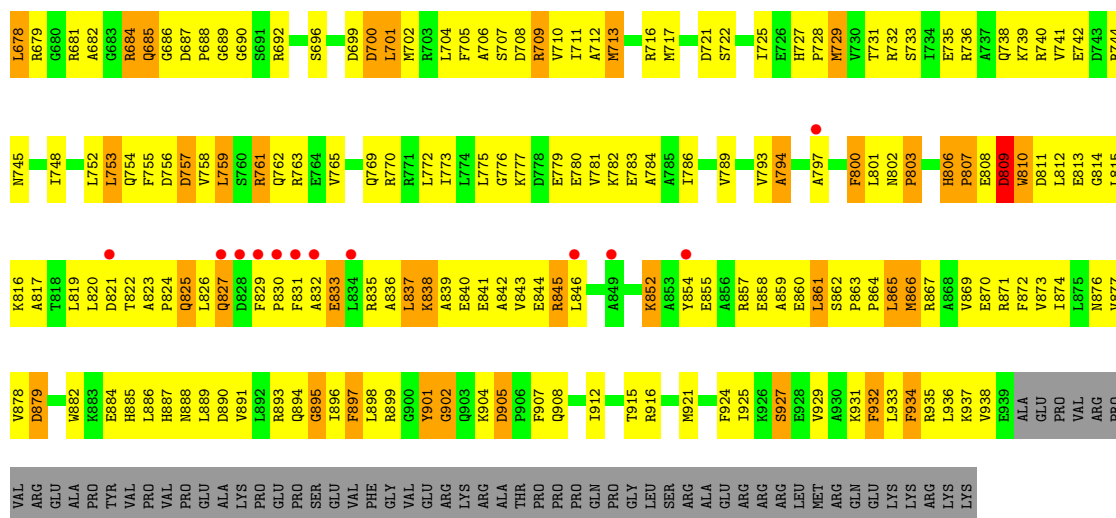
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	359	Total	O	0	0
			359	359		
2	B	320	Total	O	0	0
			320	320		
2	C	344	Total	O	0	0
			344	344		
2	D	347	Total	O	0	0
			347	347		

### 3 Residue-property plots

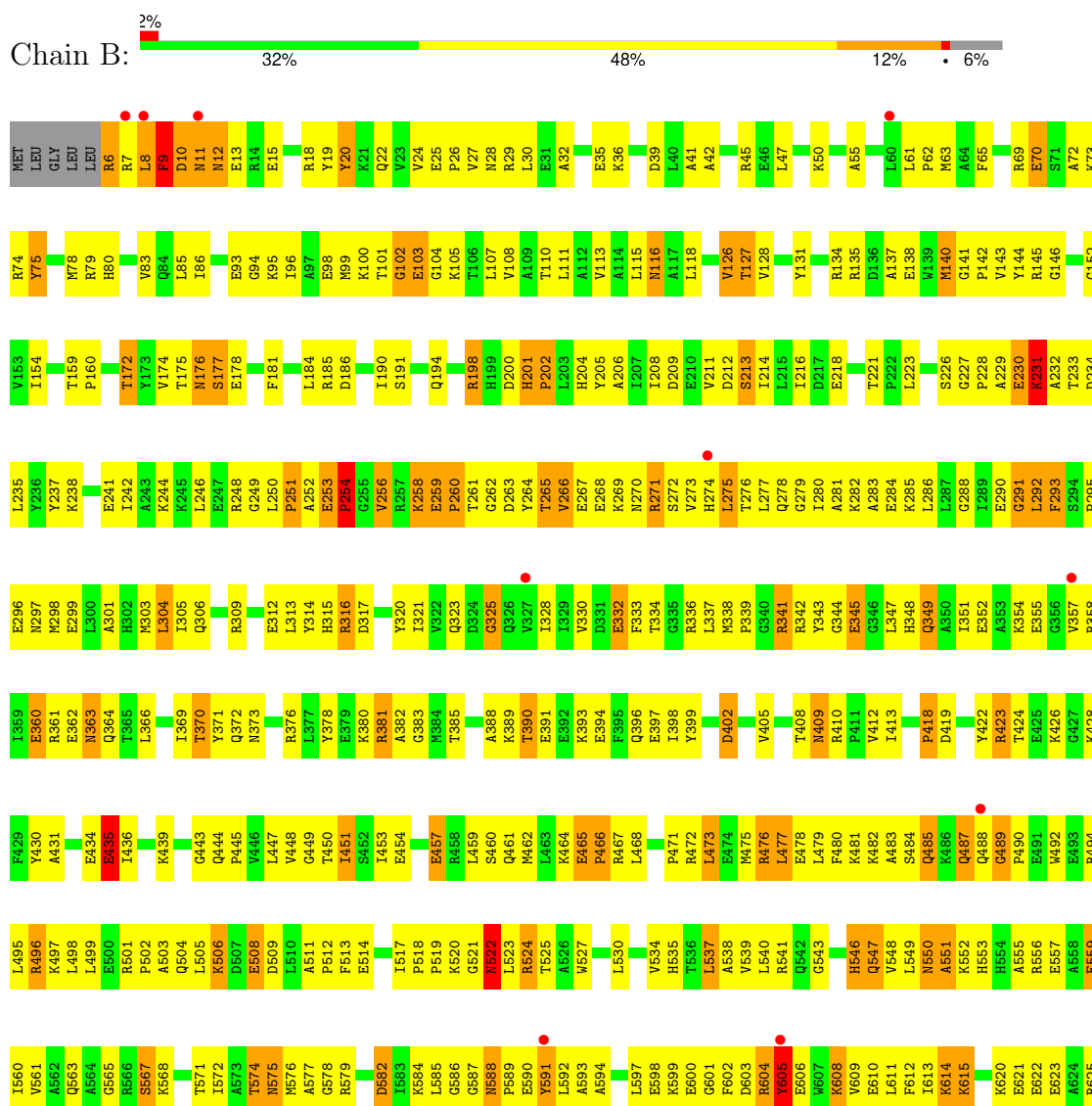
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

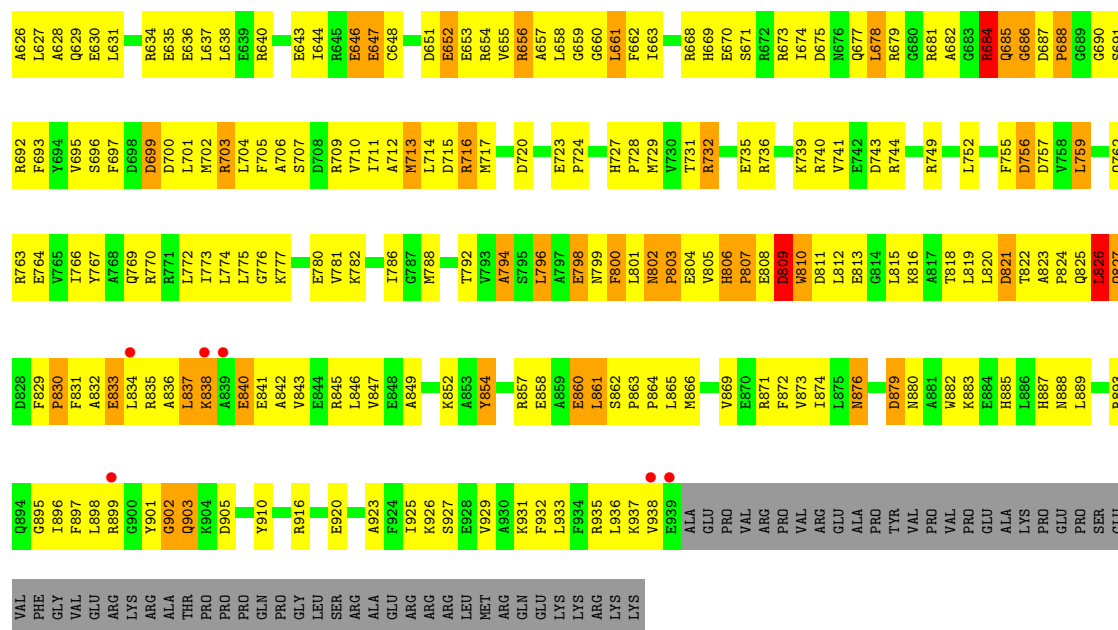
#### • Molecule 1: Preprotein translocase SecA subunit



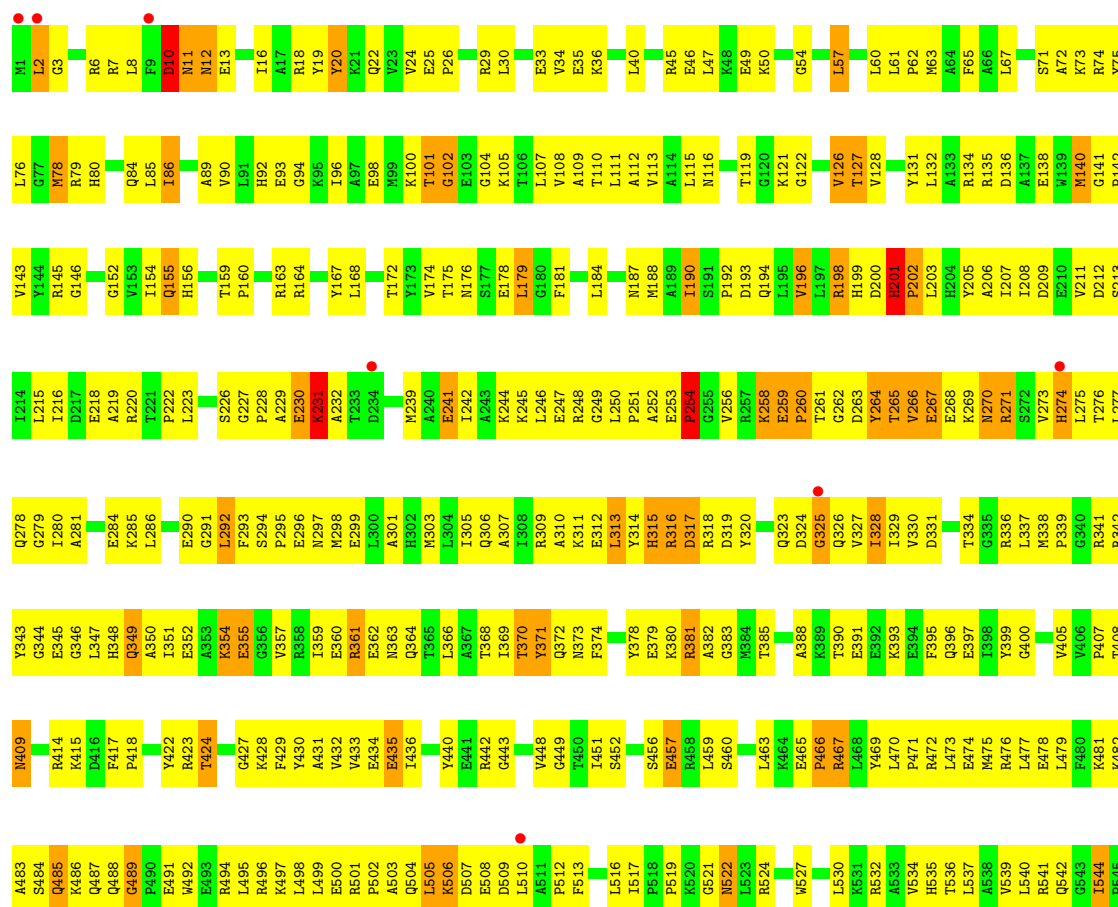


### • Molecule 1: Preprotein translocase SecA subunit





• Molecule 1: Preprotein translocase SecA subunit





GLU	F872	F806	K739	D675	V609	G543	L479
PRO	V873	P807	R740	R676	E610	I544	F480
VAL	L874	E809	V741	Q677	L611	P545	K481
ARG	N875	D809	E742	L678	F612	H546	K482
PRO	N876	N810	D743	R679	L613	O547	A483
VAL	N877	D811		G680	K614	Y548	S484
ARG	V878	L812	R749	R681	K615	L549	Q485
GLU	D879	E813	K750	A682	K616	N550	K486
ALA	N880	G814	Q751	G683	V617	A551	Q487
PRO	A881	L815	L752	Q684		K552	Q488
TYR	W882	K816	L753	Q685	K620	H553	Q489
VAL		A817	Q754	Q686	E621		
PRO	L886	T818	F755	D687	E622	R556	W492
VAL	H887	L819	D756	P688	E623	E557	E493
PRO		L820	D757	G689		A558	R494
GLU	R893	D821	V758	G690	A626	E559	L495
ALA	Q894	T822	R759	S691	L627	I560	R496
LYS	G895	A823	S760	R692	A628	V561	K497
PRO	I896	P824	R761	F693	O629	A562	L498
GLU	F897	Q825	Q762	V694	E630	Q563	L499
PRO	L898	L826	R763	V695	L631	A564	
SER	R899	Q827	E764	S696	G632	G565	P502
GLU	G900	D828	V765	F697	L633	H566	A503
VAL	Y901	F829	I766	D698	R634	S567	Q504
PHE	G902	P830	V767	D699			L505
GLY	Q903	F831	A768	D700	L637	I572	K506
VAL	R904	A832	Q769	L701	L638	A573	D507
GLU	D905	E833	R770	W702	E639	T574	E508
ARG	P906	L834		R703	R640	N575	D509
LYS	F907	R835	I773	L704	L641	N576	L510
ARG		A836	L774	F705	R642	A577	A511
ALA	Y910	L837	L775	A706	E643	G578	P512
THR		R838	Q776	S707	L644	R579	F513
PRO	E913	A839	K777	D708	R645	G580	E514
PRO	A914	E840	D778	R709	E646	T581	
PRO	T915	E841	E779	V710	E647	D582	I617
GLN		A842	E780	I711	C648	I583	P518
PRO	F918	V843	V781	A712		K584	P519
GLY	N919		K782	R713	E652	L585	K520
LEU	E920	L846	E783	L714	E653	G586	G521
SER	M921	V847		D715	R654	G587	N522
ARG	V922	E848	I786	R716	V655	N588	L523
ALA	A923		Q787		R656	P589	R524
GLU	F924	Y854	W788	F719	A657	E590	
ARG	I925				L658	V591	W527
ARG	K926	R857	E791	P724	G659	L592	E528
ARG	S927	E858	T792	I725	G660	A593	G529
LEU	E928	A859	V793	H726	L661	A594	L530
LEU	V929	E860	A794	H727	F662		K531
ARG	A930	L861	S795	P728	I663		R532
GLN	K931	S862	L796	W729		L597	R533
GLU	F932	P863	A797	V730	T666	E598	V534
LYS	L933	P864	E798	T731	E667	G600	H535
LYS	F934	L865	W799	R732	G668	G601	T536
ARG	R935	H866	F800	S733	H669	F602	L537
ARG	L936	R867	L801	I734	E670	D603	A538
LYS	K937	A868	H802	E735	S671	R604	V539
LYS	V938	V869	P803	R736	R672	V605	L540
	E939	E870	E804	A737	R673		R541
	ALA	R871	V805	Q738	L674	K608	Q542



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	168.62Å 168.62Å 149.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.80 37.02 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.4 (40.00-2.80) 97.5 (37.02-2.80)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.13 (at 2.81Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.221 , 0.255 0.215 , 0.251	Depositor DCC
$R_{free}$ test set	6730 reflections (5.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.4	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 33.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.038 for -h,-k,l 0.499 for h,-h-k,-l 0.039 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	31502	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

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	0.65	1/7682 (0.0%)	0.86	23/10350 (0.2%)
1	B	0.68	2/7646 (0.0%)	0.86	18/10302 (0.2%)
1	C	0.65	0/7682	0.85	19/10350 (0.2%)
1	D	0.66	1/7646 (0.0%)	0.86	21/10302 (0.2%)
All	All	0.66	4/30656 (0.0%)	0.86	81/41304 (0.2%)

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	B	0	1
1	C	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	716	ARG	CG-CD	8.29	1.72	1.51
1	D	716	ARG	CG-CD	8.19	1.72	1.51
1	B	804	GLU	CB-CG	-5.44	1.41	1.52
1	A	338	MET	CG-SD	5.10	1.94	1.81

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	201	HIS	C-N-CD	-13.17	91.63	120.60
1	B	201	HIS	C-N-CD	-12.87	92.30	120.60
1	A	201	HIS	C-N-CD	-12.44	93.22	120.60
1	C	201	HIS	C-N-CD	-11.34	95.65	120.60
1	D	809	ASP	N-CA-C	7.75	131.91	111.00
1	C	809	ASP	N-CA-C	7.59	131.50	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	423	ARG	NE-CZ-NH2	-7.45	116.57	120.30
1	A	10	ASP	N-CA-C	7.38	130.94	111.00
1	B	809	ASP	N-CA-C	7.28	130.66	111.00
1	A	809	ASP	N-CA-C	7.22	130.49	111.00
1	B	266	VAL	N-CA-C	-7.15	91.70	111.00
1	A	201	HIS	N-CA-C	7.09	130.16	111.00
1	A	423	ARG	NE-CZ-NH1	7.01	123.81	120.30
1	D	266	VAL	N-CA-C	-6.85	92.51	111.00
1	C	201	HIS	C-N-CA	6.81	150.62	122.00
1	A	201	HIS	C-N-CA	6.78	150.48	122.00
1	B	201	HIS	C-N-CA	6.76	150.40	122.00
1	C	201	HIS	N-CA-C	6.75	129.21	111.00
1	D	202	PRO	N-CA-C	-6.67	94.76	112.10
1	A	808	GLU	N-CA-C	6.64	128.92	111.00
1	A	266	VAL	N-CA-C	-6.55	93.32	111.00
1	C	10	ASP	N-CA-C	6.52	128.61	111.00
1	D	488	GLN	N-CA-C	6.46	128.45	111.00
1	C	266	VAL	N-CA-C	-6.44	93.61	111.00
1	B	808	GLU	N-CA-C	6.42	128.33	111.00
1	A	265	THR	N-CA-C	-6.39	93.75	111.00
1	D	506	LYS	N-CA-C	-6.36	93.82	111.00
1	D	265	THR	N-CA-C	-6.32	93.93	111.00
1	A	506	LYS	N-CA-C	-6.32	93.95	111.00
1	C	265	THR	N-CA-C	-6.32	93.95	111.00
1	C	506	LYS	N-CA-C	-6.31	93.96	111.00
1	D	838	LYS	N-CA-C	6.31	128.04	111.00
1	B	838	LYS	N-CA-C	6.31	128.03	111.00
1	A	838	LYS	N-CA-C	6.30	128.00	111.00
1	B	488	GLN	N-CA-C	6.22	127.81	111.00
1	B	506	LYS	N-CA-C	-6.22	94.19	111.00
1	D	101	THR	N-CA-C	6.22	127.79	111.00
1	A	223	LEU	N-CA-C	-6.21	94.22	111.00
1	A	837	LEU	CA-CB-CG	6.21	129.57	115.30
1	D	808	GLU	N-CA-C	6.18	127.68	111.00
1	C	808	GLU	N-CA-C	6.17	127.67	111.00
1	A	101	THR	N-CA-C	6.16	127.63	111.00
1	D	201	HIS	N-CA-C	6.11	127.50	111.00
1	C	837	LEU	CA-CB-CG	6.10	129.34	115.30
1	D	803	PRO	N-CA-C	6.08	127.92	112.10
1	C	101	THR	N-CA-C	6.06	127.37	111.00
1	B	265	THR	N-CA-C	-6.05	94.65	111.00
1	B	201	HIS	N-CA-C	6.05	127.34	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	435	GLU	CB-CG-CD	-6.02	97.96	114.20
1	D	837	LEU	CA-CB-CG	6.01	129.13	115.30
1	C	838	LYS	N-CA-C	5.87	126.84	111.00
1	C	488	GLN	N-CA-C	5.78	126.59	111.00
1	D	902	GLY	N-CA-C	5.75	127.48	113.10
1	B	101	THR	N-CA-C	5.75	126.52	111.00
1	D	759	LEU	CA-CB-CG	5.70	128.40	115.30
1	D	9	PHE	N-CA-C	5.66	126.29	111.00
1	A	10	ASP	CB-CG-OD1	-5.64	113.22	118.30
1	C	826	LEU	N-CA-C	-5.60	95.87	111.00
1	A	488	GLN	N-CA-C	5.56	126.01	111.00
1	B	902	GLY	N-CA-C	5.54	126.95	113.10
1	D	489	GLY	N-CA-C	5.52	126.90	113.10
1	B	100	LYS	N-CA-C	5.40	125.58	111.00
1	D	100	LYS	N-CA-C	5.37	125.49	111.00
1	B	837	LEU	CA-CB-CG	5.37	127.64	115.30
1	A	489	GLY	N-CA-C	5.36	126.49	113.10
1	D	201	HIS	C-N-CA	5.35	144.48	122.00
1	B	826	LEU	N-CA-C	-5.35	96.56	111.00
1	A	230	GLU	N-CA-C	-5.32	96.63	111.00
1	B	489	GLY	N-CA-C	5.32	126.40	113.10
1	C	902	GLY	N-CA-C	5.31	126.38	113.10
1	A	100	LYS	N-CA-C	5.31	125.33	111.00
1	C	230	GLU	N-CA-C	-5.31	96.67	111.00
1	A	902	GLY	N-CA-C	5.29	126.33	113.10
1	C	100	LYS	N-CA-C	5.25	125.17	111.00
1	C	10	ASP	CB-CG-OD1	-5.24	113.58	118.30
1	D	826	LEU	N-CA-C	-5.21	96.95	111.00
1	A	826	LEU	N-CA-C	-5.15	97.09	111.00
1	B	230	GLU	N-CA-C	-5.15	97.10	111.00
1	C	489	GLY	N-CA-C	5.10	125.85	113.10
1	A	313	LEU	CA-CB-CG	5.10	127.02	115.30
1	D	805	VAL	N-CA-C	-5.04	97.39	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	591	TYR	Sidechain
1	C	131	TYR	Sidechain

## 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	7551	0	7648	744	0
1	B	7515	0	7600	695	0
1	C	7551	0	7648	715	0
1	D	7515	0	7600	809	0
2	A	359	0	0	138	0
2	B	320	0	0	151	0
2	C	344	0	0	147	0
2	D	347	0	0	158	0
All	All	31502	0	30496	2909	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 48.

All (2909) 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:D:252:ALA:HB3	1:D:812:LEU:HD11	1.21	1.16
1:D:273:VAL:HG13	1:D:820:LEU:HB2	1.23	1.12
1:C:435:GLU:OE1	1:C:692:ARG:NH1	1.85	1.09
1:A:269:LYS:HD3	1:A:270:ASN:H	1.08	1.08
1:A:273:VAL:HG13	1:A:820:LEU:HB2	1.33	1.06
1:C:628:ALA:HA	1:C:633:ILE:HD12	1.39	1.04
1:C:476:ARG:HH22	1:C:723:GLU:HG2	1.26	0.99
1:C:269:LYS:HD3	1:C:270:ASN:H	1.28	0.98
1:A:206:ALA:HB3	2:A:1239:HOH:O	1.62	0.96
1:A:338:MET:HG2	1:A:341:ARG:HH11	1.27	0.96
1:C:861:LEU:HD13	1:C:938:VAL:HG21	1.45	0.95
1:A:269:LYS:HD3	1:A:270:ASN:N	1.81	0.95
1:A:628:ALA:HA	1:A:633:ILE:HD12	1.48	0.95
1:B:858:GLU:HG2	1:B:863:PRO:HG3	1.46	0.95
1:D:788:MET:HG2	1:D:926:LYS:HG2	1.45	0.94
1:A:354:LYS:HA	1:A:354:LYS:HE3	1.47	0.94
1:D:273:VAL:HG11	1:D:816:LYS:HG3	1.50	0.94
1:C:258:LYS:HE3	1:C:275:LEU:HD22	1.49	0.93
1:C:273:VAL:HG13	1:C:820:LEU:HB2	1.48	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:258:LYS:H	1:D:258:LYS:HD3	1.34	0.92
1:A:668:ARG:HH21	1:B:732:ARG:NH1	1.67	0.92
1:A:605:TYR:HB3	1:A:609:VAL:HG23	1.52	0.92
1:A:258:LYS:HE3	1:A:275:LEU:HD22	1.52	0.91
1:B:7:ARG:HA	1:B:13:GLU:HB3	1.49	0.91
1:C:277:LEU:HD23	1:C:280:ILE:HD12	1.52	0.91
1:C:605:TYR:HB3	1:C:609:VAL:HG23	1.48	0.91
1:D:295:PRO:HD3	1:D:937:LYS:HB2	1.52	0.91
1:A:258:LYS:HD2	1:A:816:LYS:HE2	1.49	0.91
1:D:670:GLU:HG2	1:D:741:VAL:HG11	1.53	0.91
1:C:476:ARG:NH2	1:C:723:GLU:HG2	1.85	0.91
1:C:716:ARG:HG2	1:D:6:ARG:HG3	1.53	0.90
1:D:190:ILE:HB	1:D:194:GLN:HE22	1.37	0.90
1:B:258:LYS:HD3	1:B:258:LYS:H	1.33	0.90
1:C:505:LEU:HG	2:C:1219:HOH:O	1.69	0.90
1:C:253:GLU:HB2	1:C:256:VAL:HG13	1.53	0.90
1:D:605:TYR:HB3	1:D:609:VAL:HG23	1.54	0.89
1:D:273:VAL:CG1	1:D:820:LEU:HB2	2.03	0.89
1:D:339:PRO:HA	2:D:1307:HOH:O	1.72	0.89
1:B:663:ILE:HD13	1:B:682:ALA:HB2	1.55	0.89
1:A:861:LEU:HD13	1:A:938:VAL:HG21	1.54	0.88
1:B:462:MET:HA	1:B:468:LEU:HD12	1.52	0.88
1:A:663:ILE:HD13	1:A:682:ALA:HB2	1.55	0.88
1:C:112:ALA:HA	2:C:1335:HOH:O	1.71	0.88
1:D:291:GLY:O	1:D:295:PRO:HD2	1.73	0.88
1:B:670:GLU:HG2	1:B:741:VAL:HG11	1.54	0.88
1:B:361:ARG:HD2	2:B:1275:HOH:O	1.72	0.88
1:C:338:MET:HG2	1:C:341:ARG:HH11	1.39	0.88
1:C:347:LEU:HD13	2:C:1050:HOH:O	1.73	0.88
1:D:663:ILE:HD13	1:D:682:ALA:HB2	1.55	0.88
1:A:253:GLU:HB2	1:A:256:VAL:HG13	1.53	0.88
1:C:819:LEU:HB3	2:C:1223:HOH:O	1.71	0.87
1:D:802:ASN:HA	1:D:839:ALA:CB	2.04	0.87
1:A:222:PRO:HG3	1:A:752:LEU:HD11	1.54	0.87
1:D:801:LEU:HD13	1:D:842:ALA:HB1	1.55	0.87
1:C:13:GLU:HB3	2:C:1218:HOH:O	1.75	0.87
1:A:320:TYR:HA	1:A:330:VAL:HG23	1.57	0.86
1:D:582:ASP:HB3	1:D:684:ARG:HH21	1.40	0.86
1:A:252:ALA:HB3	1:A:812:LEU:HD11	1.56	0.86
1:C:424:THR:HG23	1:C:427:GLY:H	1.40	0.85
1:A:249:GLY:HA2	1:A:260:PRO:HD2	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:739:LYS:HE2	2:B:1208:HOH:O	1.75	0.85
1:C:291:GLY:O	1:C:295:PRO:HD2	1.76	0.85
1:D:272:SER:O	1:D:820:LEU:HD22	1.76	0.85
1:A:716:ARG:HG3	1:B:6:ARG:HD2	1.57	0.85
1:B:190:ILE:HB	1:B:194:GLN:HE22	1.41	0.85
1:D:462:MET:HA	1:D:468:LEU:HD12	1.59	0.85
1:C:36:LYS:HE3	2:C:1225:HOH:O	1.75	0.85
1:A:894:GLN:HB2	2:A:1029:HOH:O	1.77	0.85
1:D:18:ARG:HH21	1:D:22:GLN:HE21	1.22	0.84
1:B:249:GLY:HA2	1:B:260:PRO:HD2	1.57	0.84
1:B:605:TYR:HB3	1:B:609:VAL:HG23	1.58	0.84
1:D:273:VAL:HG13	1:D:820:LEU:CB	2.07	0.84
1:A:517:ILE:HG21	1:A:524:ARG:HH11	1.41	0.84
1:D:857:ARG:HH12	1:D:936:LEU:H	1.26	0.84
1:D:364:GLN:HB2	2:D:1266:HOH:O	1.76	0.84
1:A:295:PRO:HD3	1:A:937:LYS:HB2	1.60	0.84
1:A:782:LYS:HG2	2:A:1264:HOH:O	1.78	0.84
1:D:550:ASN:ND2	1:D:550:ASN:H	1.71	0.84
1:A:932:PHE:HA	2:A:1109:HOH:O	1.76	0.83
1:B:589:PRO:HG2	1:B:614:LYS:NZ	1.93	0.83
1:C:190:ILE:O	1:C:774:LEU:HD21	1.78	0.83
1:C:823:ALA:HB2	1:C:935:ARG:HD3	1.59	0.83
1:A:602:PHE:HD1	1:A:603:ASP:H	1.22	0.83
1:B:260:PRO:HA	2:B:1066:HOH:O	1.77	0.83
1:B:256:VAL:HG12	2:B:1285:HOH:O	1.77	0.83
1:C:663:ILE:HD13	1:C:682:ALA:HB2	1.60	0.83
1:A:782:LYS:HE2	1:A:867:ARG:HB3	1.60	0.82
1:B:759:LEU:HB3	2:B:1122:HOH:O	1.77	0.82
1:D:249:GLY:HA2	1:D:260:PRO:HD2	1.59	0.82
1:D:269:LYS:HD3	1:D:270:ASN:H	1.45	0.82
1:C:602:PHE:HD1	1:C:603:ASP:H	1.26	0.82
1:D:580:GLY:HA2	2:D:1125:HOH:O	1.78	0.82
1:A:273:VAL:HA	1:A:820:LEU:HD13	1.62	0.82
1:C:812:LEU:HA	1:C:815:LEU:HD12	1.60	0.82
1:D:198:ARG:HD3	2:D:1116:HOH:O	1.79	0.81
1:D:791:GLU:HB2	2:D:1235:HOH:O	1.80	0.81
1:C:782:LYS:HE2	1:C:867:ARG:HB3	1.60	0.81
1:B:485:GLN:HG2	1:B:496:ARG:HH21	1.44	0.81
1:D:260:PRO:HB2	2:D:1088:HOH:O	1.80	0.81
1:D:257:ARG:HA	2:D:1237:HOH:O	1.79	0.81
1:B:131:TYR:HA	2:B:1094:HOH:O	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:759:LEU:HD21	1:C:889:LEU:HD13	1.62	0.81
1:C:898:LEU:HD23	2:C:1273:HOH:O	1.79	0.81
1:B:261:THR:HG23	1:B:279:GLY:HA3	1.62	0.81
1:D:257:ARG:HH22	1:D:825:GLN:HE22	1.27	0.81
1:D:459:LEU:HD13	1:D:572:ILE:HD13	1.63	0.81
1:D:430:TYR:HB3	1:D:472:ARG:HE	1.45	0.81
1:A:506:LYS:HE3	2:A:1356:HOH:O	1.80	0.80
1:D:857:ARG:HH22	1:D:936:LEU:HB3	1.45	0.80
1:B:777:LYS:HB2	2:B:1113:HOH:O	1.79	0.80
1:C:249:GLY:HA2	1:C:260:PRO:HD2	1.64	0.80
1:D:776:GLY:HA2	1:D:871:ARG:HH12	1.47	0.80
1:D:190:ILE:O	1:D:774:LEU:HD21	1.80	0.80
1:C:258:LYS:HD2	1:C:816:LYS:HE2	1.63	0.80
1:A:540:LEU:HA	1:A:544:ILE:HD11	1.61	0.80
1:C:54:GLY:HA2	2:C:1260:HOH:O	1.81	0.80
1:B:809:ASP:HB3	1:B:810:TRP:CD1	2.17	0.80
1:B:430:TYR:HB3	1:B:472:ARG:HE	1.46	0.80
1:C:262:GLY:HA3	2:C:1237:HOH:O	1.79	0.80
1:D:517:ILE:HG22	1:D:524:ARG:HD2	1.64	0.80
1:D:800:PHE:HA	2:D:1167:HOH:O	1.81	0.80
1:B:41:ALA:HB3	2:B:1184:HOH:O	1.80	0.79
1:A:486:LYS:HB3	1:A:487:GLN:HE22	1.45	0.79
1:D:517:ILE:HG21	1:D:524:ARG:HH11	1.47	0.79
1:A:732:ARG:HD2	2:A:1174:HOH:O	1.82	0.79
1:C:208:ILE:HB	1:C:211:VAL:HG12	1.64	0.79
1:C:269:LYS:HD3	1:C:270:ASN:N	1.97	0.79
1:D:591:TYR:HB2	2:D:1260:HOH:O	1.82	0.79
1:D:334:THR:HB	1:D:336:ARG:HG2	1.64	0.79
1:D:777:LYS:HD3	1:D:780:GLU:HG3	1.64	0.79
1:A:716:ARG:HG2	1:B:6:ARG:HG3	1.63	0.79
1:A:806:HIS:HB3	1:A:807:PRO:HD3	1.64	0.79
1:A:435:GLU:OE2	1:A:692:ARG:NH1	2.15	0.79
1:A:716:ARG:CG	1:B:6:ARG:HG3	2.13	0.79
1:B:18:ARG:HH21	1:B:22:GLN:HE21	1.31	0.79
1:A:296:GLU:HG2	2:A:1328:HOH:O	1.82	0.78
1:C:159:THR:O	1:C:163:ARG:HG3	1.84	0.78
1:D:347:LEU:HB2	2:D:1339:HOH:O	1.83	0.78
1:A:339:PRO:HD2	1:A:341:ARG:HH12	1.49	0.78
1:D:277:LEU:HD23	1:D:280:ILE:HD12	1.66	0.78
1:A:159:THR:HB	1:A:160:PRO:HD2	1.66	0.78
1:B:582:ASP:CB	1:B:684:ARG:HH21	1.95	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:761:ARG:HG2	2:A:1138:HOH:O	1.83	0.78
1:B:291:GLY:O	1:B:295:PRO:HD2	1.84	0.78
1:D:41:ALA:O	1:D:45:ARG:HG3	1.83	0.78
1:C:337:LEU:O	1:C:339:PRO:HD3	1.82	0.78
1:C:159:THR:HB	1:C:160:PRO:HD2	1.66	0.78
1:C:222:PRO:HG3	1:C:752:LEU:HD11	1.66	0.78
1:C:466:PRO:HG3	1:C:540:LEU:HB3	1.66	0.78
1:C:821:ASP:O	1:C:931:LYS:HA	1.84	0.78
1:A:276:THR:HB	2:A:1229:HOH:O	1.83	0.77
1:A:535:HIS:HB3	2:A:1294:HOH:O	1.84	0.77
1:B:246:LEU:HD11	1:B:261:THR:HG21	1.64	0.77
1:B:586:GLY:HA3	2:B:1241:HOH:O	1.84	0.77
1:D:313:LEU:HD11	2:D:1042:HOH:O	1.85	0.77
1:D:925:ILE:O	1:D:929:VAL:HG23	1.82	0.77
1:D:25:GLU:O	1:D:29:ARG:HG2	1.82	0.77
1:B:483:ALA:HB3	2:B:1012:HOH:O	1.84	0.77
1:B:484:SER:HB2	1:B:496:ARG:HH22	1.50	0.77
1:D:7:ARG:HA	1:D:13:GLU:HB3	1.65	0.77
1:A:18:ARG:HH21	1:A:22:GLN:HE21	1.30	0.77
1:B:825:GLN:HA	2:B:1201:HOH:O	1.85	0.76
1:B:430:TYR:CB	1:B:472:ARG:HE	1.98	0.76
1:B:18:ARG:HE	1:B:22:GLN:NE2	1.83	0.76
1:C:655:VAL:HA	1:C:658:LEU:HB2	1.68	0.76
1:C:707:SER:O	1:C:711:ILE:HG13	1.86	0.76
1:A:291:GLY:O	1:A:295:PRO:HD2	1.85	0.76
1:A:316:ARG:HD3	1:A:355:GLU:OE2	1.85	0.76
1:D:234:ASP:HB3	2:D:1226:HOH:O	1.85	0.76
1:A:131:TYR:HA	2:A:1338:HOH:O	1.84	0.76
1:B:430:TYR:O	1:B:434:GLU:HG3	1.86	0.76
1:D:444:GLN:HE21	1:D:660:GLY:H	1.34	0.76
1:D:517:ILE:CG2	1:D:524:ARG:HD2	2.15	0.76
1:D:662:PHE:HA	1:D:690:GLY:O	1.86	0.76
1:D:788:MET:HA	2:D:1235:HOH:O	1.86	0.76
1:A:277:LEU:HD23	1:A:280:ILE:HD12	1.68	0.76
1:C:266:VAL:CG2	1:C:269:LYS:HB2	2.16	0.76
1:A:775:LEU:HB3	2:A:1005:HOH:O	1.85	0.75
1:B:759:LEU:HD11	1:B:893:ARG:HH22	1.51	0.75
1:D:361:ARG:HA	2:D:1095:HOH:O	1.86	0.75
1:A:857:ARG:HE	1:A:861:LEU:HD21	1.51	0.75
1:A:606:GLU:HG2	1:A:610:GLU:OE2	1.85	0.75
1:B:413:ILE:HD12	1:B:686:GLY:O	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:GLY:HA3	2:C:1108:HOH:O	1.84	0.75
1:D:823:ALA:HB2	1:D:935:ARG:HD2	1.68	0.75
1:C:876:ASN:HA	2:C:1175:HOH:O	1.85	0.75
1:D:12:ASN:HD22	1:D:405:VAL:H	1.35	0.75
1:A:440:TYR:CD2	1:A:544:ILE:HG23	2.22	0.75
1:B:582:ASP:HB3	1:B:684:ARG:HH21	1.51	0.75
1:C:188:MET:HG2	2:C:1204:HOH:O	1.87	0.75
1:C:517:ILE:HG21	1:C:524:ARG:HH11	1.50	0.75
1:C:800:PHE:HB2	1:C:810:TRP:CG	2.22	0.75
1:B:41:ALA:O	1:B:45:ARG:HG3	1.86	0.74
1:C:709:ARG:HG3	1:D:389:LYS:HD3	1.69	0.74
1:D:191:SER:H	1:D:194:GLN:NE2	1.84	0.74
1:D:365:THR:HG22	1:D:886:LEU:HD13	1.69	0.74
1:A:298:MET:HE1	1:A:873:VAL:HA	1.69	0.74
1:A:622:GLU:HA	1:A:625:ARG:NE	2.01	0.74
1:C:76:LEU:HD13	1:C:142:PRO:HG2	1.69	0.74
1:C:342:ARG:HD2	1:C:891:VAL:HG21	1.68	0.74
1:B:663:ILE:CD1	1:B:682:ALA:HB2	2.17	0.74
1:D:301:ALA:HB3	1:D:932:PHE:HZ	1.50	0.74
1:A:524:ARG:HG2	2:A:1129:HOH:O	1.86	0.74
1:B:93:GLU:HA	2:B:1150:HOH:O	1.86	0.74
1:C:635:GLU:HB3	2:C:1031:HOH:O	1.86	0.74
1:D:184:LEU:HD11	1:D:369:ILE:HG22	1.69	0.74
1:A:337:LEU:O	1:A:339:PRO:HD3	1.88	0.74
1:C:320:TYR:HA	1:C:330:VAL:HG23	1.69	0.74
1:C:670:GLU:HG2	1:C:741:VAL:HG11	1.70	0.74
1:A:517:ILE:HG21	1:A:524:ARG:NH1	2.02	0.74
1:A:701:LEU:HA	2:A:1289:HOH:O	1.87	0.74
1:B:334:THR:HB	1:B:336:ARG:HG2	1.69	0.74
1:D:265:THR:HG22	1:D:271:ARG:O	1.88	0.74
1:D:345:GLU:HG2	2:D:1208:HOH:O	1.87	0.74
1:C:25:GLU:O	1:C:29:ARG:HG2	1.86	0.74
1:C:777:LYS:HB3	1:C:780:GLU:HB2	1.70	0.74
1:C:857:ARG:HA	1:C:860:GLU:HG3	1.70	0.74
1:D:754:GLN:HB3	1:D:907:PHE:CE1	2.23	0.74
1:D:876:ASN:O	1:D:880:ASN:HB2	1.88	0.74
1:A:354:LYS:HD2	2:A:1211:HOH:O	1.86	0.73
1:A:553:HIS:NE2	1:A:556:ARG:HD3	2.03	0.73
1:B:744:ARG:HG3	2:B:1207:HOH:O	1.87	0.73
1:C:563:GLN:HE21	1:C:587:GLY:HA3	1.52	0.73
1:C:716:ARG:CG	1:D:6:ARG:HG3	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:GLU:HG2	2:C:1290:HOH:O	1.86	0.73
1:D:364:GLN:HG2	1:D:887:HIS:CG	2.24	0.73
1:A:181:PHE:HA	1:A:184:LEU:HD12	1.70	0.73
1:C:18:ARG:HH21	1:C:22:GLN:HE21	1.35	0.73
1:D:532:ARG:HG3	2:D:1117:HOH:O	1.88	0.73
1:A:668:ARG:NH2	1:B:732:ARG:NH1	2.36	0.73
1:A:707:SER:O	1:A:711:ILE:HG13	1.89	0.73
1:A:121:LYS:C	1:A:198:ARG:HH21	1.92	0.73
1:D:778:ASP:HB2	2:D:1193:HOH:O	1.88	0.73
1:D:832:ALA:HB2	2:D:1310:HOH:O	1.87	0.73
1:B:262:GLY:HA2	2:B:1069:HOH:O	1.88	0.73
1:C:273:VAL:HG22	1:C:820:LEU:HD22	1.69	0.73
1:C:294:SER:OG	1:C:936:LEU:HA	1.89	0.73
1:C:800:PHE:CE1	1:C:813:GLU:HB2	2.24	0.73
1:C:904:LYS:HE3	1:C:908:GLN:HE22	1.54	0.73
1:D:550:ASN:H	1:D:550:ASN:HD22	1.36	0.73
1:D:773:ILE:HG22	2:D:1071:HOH:O	1.88	0.73
1:B:12:ASN:ND2	1:B:405:VAL:HG23	2.04	0.72
1:D:444:GLN:HE21	1:D:660:GLY:N	1.85	0.72
1:A:254:PRO:HG3	2:A:1176:HOH:O	1.88	0.72
1:A:412:VAL:HG12	2:A:1315:HOH:O	1.89	0.72
1:A:701:LEU:HD23	2:A:1289:HOH:O	1.88	0.72
1:C:852:LYS:HB2	1:C:852:LYS:NZ	2.04	0.72
1:A:814:GLY:HA2	2:A:1353:HOH:O	1.89	0.72
1:B:462:MET:CA	1:B:468:LEU:HD12	2.18	0.72
1:D:609:VAL:O	1:D:613:ILE:HG13	1.88	0.72
1:B:278:GLN:O	1:B:282:LYS:HG3	1.88	0.72
1:D:485:GLN:HG2	1:D:496:ARG:HH21	1.54	0.72
1:D:813:GLU:H	1:D:813:GLU:CD	1.93	0.72
1:A:305:ILE:HD12	2:A:1084:HOH:O	1.89	0.72
1:A:557:GLU:O	1:A:561:VAL:HG23	1.90	0.72
1:C:640:ARG:HE	1:C:644:ILE:HG13	1.52	0.72
1:D:198:ARG:O	1:D:202:PRO:HB3	1.90	0.72
1:C:146:GLY:HA2	2:C:1303:HOH:O	1.89	0.72
1:B:295:PRO:HD3	1:B:937:LYS:HB2	1.71	0.72
1:C:13:GLU:HG2	1:D:716:ARG:HH12	1.53	0.72
1:C:815:LEU:HD21	2:C:1239:HOH:O	1.89	0.72
1:C:115:LEU:HB3	2:C:1335:HOH:O	1.89	0.72
1:D:929:VAL:HG12	1:D:933:LEU:HD11	1.71	0.72
1:A:273:VAL:HG11	1:A:816:LYS:HG3	1.71	0.72
1:A:486:LYS:HB3	1:A:487:GLN:NE2	2.05	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:776:GLY:HA2	1:B:871:ARG:HH12	1.54	0.72
1:C:486:LYS:HB3	1:C:487:GLN:HE22	1.55	0.72
1:D:261:THR:HG23	1:D:279:GLY:HA3	1.72	0.72
1:D:816:LYS:HD3	2:D:1263:HOH:O	1.88	0.72
1:A:812:LEU:HA	1:A:815:LEU:HD12	1.71	0.71
1:B:517:ILE:HG22	1:B:524:ARG:HD2	1.72	0.71
1:C:265:THR:HG22	1:C:271:ARG:O	1.88	0.71
1:D:372:GLN:O	1:D:376:ARG:HG3	1.90	0.71
1:A:266:VAL:CG2	1:A:269:LYS:HB2	2.21	0.71
1:A:381:ARG:HA	2:A:1239:HOH:O	1.91	0.71
1:A:485:GLN:HB2	2:A:1236:HOH:O	1.89	0.71
1:B:381:ARG:HH11	1:B:381:ARG:H	1.38	0.71
1:D:18:ARG:HE	1:D:22:GLN:NE2	1.86	0.71
1:A:870:GLU:O	1:A:874:ILE:HG13	1.89	0.71
1:B:449:GLY:HA3	1:B:678:LEU:HD11	1.72	0.71
1:D:284:GLU:HG3	2:D:1256:HOH:O	1.89	0.71
1:B:252:ALA:HB3	1:B:812:LEU:HD21	1.72	0.71
1:B:254:PRO:HA	2:B:1272:HOH:O	1.90	0.71
1:D:582:ASP:CB	1:D:684:ARG:HH21	2.03	0.71
1:A:263:ASP:HB3	1:A:273:VAL:O	1.91	0.71
1:B:12:ASN:HD22	1:B:405:VAL:H	1.35	0.71
1:B:134:ARG:HD2	2:B:1215:HOH:O	1.88	0.71
1:B:485:GLN:HG2	1:B:496:ARG:NH2	2.05	0.71
1:C:119:THR:HG22	1:C:121:LYS:HG3	1.71	0.71
1:D:79:ARG:HD2	2:D:1046:HOH:O	1.90	0.71
1:D:252:ALA:HB3	1:D:812:LEU:CD1	2.13	0.71
1:A:102:GLY:N	1:A:105:LYS:HZ1	1.88	0.71
1:C:266:VAL:HG22	1:C:269:LYS:HB2	1.71	0.71
1:D:293:PHE:HZ	1:D:304:LEU:HD22	1.56	0.71
1:B:261:THR:HA	2:B:1059:HOH:O	1.90	0.71
1:C:712:ALA:HA	1:D:6:ARG:NH1	2.05	0.71
1:A:198:ARG:O	1:A:202:PRO:HB3	1.91	0.71
1:A:501:ARG:HG2	2:A:1150:HOH:O	1.89	0.71
1:B:876:ASN:O	1:B:880:ASN:HB2	1.90	0.71
1:D:273:VAL:CG1	1:D:816:LYS:HG3	2.20	0.71
1:B:96:ILE:HD12	1:B:211:VAL:HG21	1.72	0.71
1:B:561:VAL:HG21	1:B:578:GLY:HA3	1.73	0.71
1:D:712:ALA:O	1:D:716:ARG:HG3	1.90	0.71
1:D:857:ARG:HH12	1:D:936:LEU:N	1.87	0.71
1:A:18:ARG:HE	1:A:22:GLN:NE2	1.89	0.70
1:A:314:TYR:HE1	1:A:347:LEU:HD21	1.53	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:VAL:HG13	1:B:820:LEU:HD13	1.72	0.70
1:C:435:GLU:CD	1:C:692:ARG:NH1	2.44	0.70
1:D:413:ILE:HD12	1:D:686:GLY:O	1.91	0.70
1:D:794:ALA:O	1:D:798:GLU:HB3	1.90	0.70
1:A:127:THR:HG23	1:A:209:ASP:HB3	1.72	0.70
1:A:777:LYS:HB3	1:A:780:GLU:HB2	1.73	0.70
1:B:712:ALA:O	1:B:716:ARG:HG3	1.90	0.70
1:D:342:ARG:HH22	1:D:349:GLN:NE2	1.89	0.70
1:A:298:MET:CE	1:A:873:VAL:HA	2.21	0.70
1:B:517:ILE:HG21	1:B:524:ARG:HH11	1.57	0.70
1:D:8:LEU:HG	1:D:9:PHE:N	2.06	0.70
1:D:640:ARG:CZ	1:D:643:GLU:HG2	2.22	0.70
1:A:360:GLU:HA	2:A:1314:HOH:O	1.91	0.70
1:B:206:ALA:HB2	1:B:378:TYR:CE2	2.26	0.70
1:B:265:THR:HG22	1:B:271:ARG:O	1.92	0.70
1:B:589:PRO:HG2	1:B:614:LYS:HZ1	1.57	0.70
1:C:440:TYR:CD2	1:C:544:ILE:HG23	2.26	0.70
1:A:12:ASN:HD22	1:A:405:VAL:H	1.40	0.70
1:A:553:HIS:O	1:A:557:GLU:HG3	1.92	0.70
1:A:712:ALA:HA	1:B:6:ARG:NH1	2.07	0.70
1:D:597:LEU:HB2	2:D:1318:HOH:O	1.90	0.70
1:D:798:GLU:HB2	1:D:843:VAL:CG2	2.22	0.70
1:C:821:ASP:OD2	1:C:931:LYS:HE2	1.92	0.70
1:D:232:ALA:HB1	1:D:361:ARG:HH12	1.55	0.70
1:B:292:LEU:HB2	2:B:1125:HOH:O	1.92	0.69
1:B:501:ARG:HD3	2:B:1226:HOH:O	1.92	0.69
1:B:777:LYS:HD3	1:B:780:GLU:HG3	1.73	0.69
1:D:617:VAL:HA	1:D:645:ARG:HD2	1.74	0.69
1:C:229:ALA:HA	2:C:1236:HOH:O	1.90	0.69
1:A:670:GLU:HG2	1:A:741:VAL:HG11	1.72	0.69
1:D:663:ILE:CD1	1:D:682:ALA:HB2	2.21	0.69
1:D:370:THR:HG23	1:D:373:ASN:HB2	1.74	0.69
1:D:485:GLN:HG2	1:D:496:ARG:NH2	2.07	0.69
1:A:642:ARG:HD2	2:A:1146:HOH:O	1.91	0.69
1:B:275:LEU:HD11	1:B:935:ARG:HH12	1.58	0.69
1:B:336:ARG:HB2	2:B:1043:HOH:O	1.92	0.69
1:C:565:GLY:HA3	1:C:584:LYS:O	1.93	0.69
1:D:259:GLU:HB3	1:D:260:PRO:CD	2.23	0.69
1:A:857:ARG:HA	1:A:860:GLU:HG3	1.75	0.69
1:B:436:ILE:HD11	1:B:448:VAL:HG21	1.75	0.69
1:C:369:ILE:HA	1:C:763:ARG:NH1	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:LYS:H	1:A:258:LYS:HD3	1.58	0.69
1:C:219:ALA:HB1	1:C:372:GLN:NE2	2.08	0.69
1:C:899:ARG:HB2	2:C:1027:HOH:O	1.93	0.69
1:B:766:ILE:HD12	1:B:882:TRP:CE3	2.29	0.68
1:B:898:LEU:HB2	2:B:1065:HOH:O	1.92	0.68
1:C:772:LEU:HD11	1:C:780:GLU:HB3	1.75	0.68
1:A:659:GLY:O	1:A:688:PRO:HB2	1.94	0.68
1:B:266:VAL:HG23	2:B:1263:HOH:O	1.92	0.68
1:C:547:GLN:HG2	1:C:560:ILE:HG21	1.73	0.68
1:D:72:ALA:HA	1:D:143:VAL:HG22	1.75	0.68
1:D:274:HIS:N	1:D:820:LEU:HD13	2.08	0.68
1:D:199:HIS:HB2	2:D:1057:HOH:O	1.93	0.68
1:D:749:ARG:HG3	2:D:1188:HOH:O	1.93	0.68
1:A:865:LEU:HD13	1:A:938:VAL:HG11	1.75	0.68
1:D:34:VAL:HB	2:D:1099:HOH:O	1.93	0.68
1:B:191:SER:H	1:B:194:GLN:NE2	1.92	0.68
1:B:651:ASP:HB3	2:B:1241:HOH:O	1.94	0.68
1:C:143:VAL:HA	2:C:1265:HOH:O	1.92	0.68
1:C:486:LYS:HB3	1:C:487:GLN:NE2	2.08	0.68
1:D:599:LYS:HE3	1:D:637:LEU:HD21	1.75	0.68
1:B:32:ALA:HB1	2:B:1273:HOH:O	1.93	0.68
1:B:116:ASN:HD22	1:B:116:ASN:N	1.92	0.68
1:C:12:ASN:HD22	1:C:405:VAL:H	1.38	0.68
1:D:477:LEU:HD11	1:D:499:LEU:HD22	1.76	0.68
1:C:206:ALA:HB2	1:C:378:TYR:CE2	2.28	0.68
1:D:244:LYS:HD2	1:D:354:LYS:NZ	2.09	0.68
1:D:857:ARG:HH22	1:D:936:LEU:CB	2.07	0.68
1:A:759:LEU:HD21	1:A:889:LEU:HD13	1.75	0.68
1:B:198:ARG:O	1:B:202:PRO:HB3	1.94	0.68
1:C:925:ILE:O	1:C:929:VAL:HG23	1.94	0.68
1:D:320:TYR:HA	1:D:330:VAL:HG23	1.75	0.68
1:A:713:MET:HE2	2:A:1154:HOH:O	1.94	0.67
1:A:275:LEU:HD13	1:A:816:LYS:NZ	2.10	0.67
1:A:424:THR:HG23	1:A:427:GLY:H	1.59	0.67
1:B:567:SER:HB3	1:B:651:ASP:OD2	1.94	0.67
1:C:263:ASP:HB3	1:C:273:VAL:O	1.93	0.67
1:A:261:THR:HG23	1:A:279:GLY:HA3	1.77	0.67
1:B:552:LYS:HE3	2:B:1114:HOH:O	1.93	0.67
1:B:621:GLU:HA	2:B:1235:HOH:O	1.93	0.67
1:D:18:ARG:NH2	1:D:22:GLN:HE21	1.92	0.67
1:D:220:ARG:HB2	2:D:1063:HOH:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:MET:HA	1:A:306:GLN:HG2	1.77	0.67
1:B:259:GLU:HB3	1:B:260:PRO:CD	2.23	0.67
1:A:269:LYS:CD	1:A:270:ASN:H	1.98	0.67
1:A:772:LEU:HD11	1:A:780:GLU:HB3	1.75	0.67
1:B:7:ARG:HA	1:B:13:GLU:CB	2.21	0.67
1:C:18:ARG:HE	1:C:22:GLN:NE2	1.93	0.67
1:C:181:PHE:HA	1:C:184:LEU:HD12	1.76	0.67
1:C:273:VAL:HG11	1:C:816:LYS:HG3	1.76	0.67
1:C:424:THR:HG23	1:C:427:GLY:N	2.10	0.67
1:A:477:LEU:HD23	1:A:530:LEU:HD11	1.74	0.67
1:B:473:LEU:HD12	1:B:537:LEU:HD12	1.77	0.67
1:D:803:PRO:HB2	2:D:1080:HOH:O	1.94	0.67
1:B:253:GLU:HB2	1:B:256:VAL:HG13	1.77	0.67
1:D:859:ALA:HA	2:D:1149:HOH:O	1.93	0.67
1:B:213:SER:CB	1:B:579:ARG:HH22	2.07	0.67
1:C:547:GLN:HG2	1:C:560:ILE:CG2	2.25	0.67
1:C:732:ARG:HB3	2:C:1115:HOH:O	1.95	0.67
1:B:134:ARG:HB3	2:B:1094:HOH:O	1.95	0.67
1:B:281:ALA:O	1:B:285:LYS:HG3	1.95	0.67
1:C:76:LEU:HD22	1:C:143:VAL:HG23	1.77	0.67
1:D:829:PHE:HB2	2:D:1151:HOH:O	1.94	0.67
1:B:606:GLU:HG2	2:B:1031:HOH:O	1.94	0.66
1:D:256:VAL:HG21	2:D:1218:HOH:O	1.94	0.66
1:D:803:PRO:HB3	2:D:1340:HOH:O	1.94	0.66
1:A:347:LEU:HD13	2:A:1108:HOH:O	1.93	0.66
1:B:484:SER:O	1:B:487:GLN:HG3	1.95	0.66
1:B:662:PHE:HA	1:B:690:GLY:O	1.95	0.66
1:C:594:ALA:HA	1:C:597:LEU:HG	1.78	0.66
1:D:303:MET:HA	1:D:306:GLN:HG2	1.77	0.66
1:D:444:GLN:NE2	1:D:659:GLY:HA3	2.10	0.66
1:A:745:ASN:HB3	2:A:1116:HOH:O	1.95	0.66
1:D:551:ALA:HA	1:D:557:GLU:OE1	1.94	0.66
1:A:852:LYS:HB2	1:A:852:LYS:NZ	2.11	0.66
1:B:547:GLN:HG2	1:B:560:ILE:CG2	2.26	0.66
1:C:671:SER:HB3	1:C:674:ILE:HG13	1.78	0.66
1:A:709:ARG:HA	2:B:1027:HOH:O	1.94	0.66
1:D:189:ALA:HB2	2:D:1156:HOH:O	1.96	0.66
1:D:263:ASP:HB3	1:D:816:LYS:HG2	1.78	0.66
1:D:343:TYR:H	1:D:348:HIS:HB2	1.60	0.66
1:C:226:SER:HB2	1:C:363:ASN:HD22	1.59	0.66
1:C:761:ARG:H	1:C:761:ARG:HD2	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:263:ASP:HB2	1:D:273:VAL:O	1.96	0.66
1:C:220:ARG:O	1:C:752:LEU:HD22	1.95	0.66
1:D:311:LYS:HD3	2:D:1331:HOH:O	1.95	0.66
1:A:13:GLU:HG2	1:B:716:ARG:HH12	1.61	0.66
1:C:198:ARG:O	1:C:202:PRO:HB3	1.95	0.66
1:D:262:GLY:HA3	2:D:1179:HOH:O	1.95	0.66
1:A:821:ASP:OD2	1:A:931:LYS:HE2	1.96	0.66
1:B:522:ASN:HB2	2:B:1081:HOH:O	1.94	0.66
1:C:430:TYR:O	1:C:434:GLU:HG3	1.96	0.66
1:D:640:ARG:NH1	1:D:643:GLU:HG2	2.10	0.66
1:D:823:ALA:HB3	1:D:824:PRO:HD3	1.78	0.66
1:D:857:ARG:NH2	1:D:936:LEU:HB3	2.09	0.66
1:B:609:VAL:O	1:B:613:ILE:HG13	1.96	0.65
1:B:713:MET:HB3	1:B:729:MET:HE2	1.78	0.65
1:D:338:MET:HG2	1:D:341:ARG:HD2	1.78	0.65
1:D:423:ARG:HB2	2:D:1065:HOH:O	1.95	0.65
1:B:226:SER:HB3	2:B:1049:HOH:O	1.97	0.65
1:B:320:TYR:HA	1:B:330:VAL:HG23	1.78	0.65
1:D:257:ARG:HH22	1:D:825:GLN:NE2	1.91	0.65
1:D:770:ARG:HH12	1:D:879:ASP:CB	2.09	0.65
1:C:522:ASN:HA	2:C:1106:HOH:O	1.96	0.65
1:D:50:LYS:HG3	2:D:1315:HOH:O	1.94	0.65
1:A:159:THR:O	1:A:163:ARG:HG3	1.96	0.65
1:A:273:VAL:CG1	1:A:820:LEU:HB2	2.20	0.65
1:A:559:GLU:HG3	2:A:1194:HOH:O	1.96	0.65
1:A:663:ILE:CD1	1:A:682:ALA:HB2	2.24	0.65
1:A:709:ARG:HG3	1:B:389:LYS:HD3	1.78	0.65
1:B:80:HIS:CD2	1:B:107:LEU:HD21	2.32	0.65
1:B:269:LYS:HG3	2:B:1263:HOH:O	1.95	0.65
1:D:802:ASN:HA	1:D:839:ALA:HB1	1.76	0.65
1:A:145:ARG:HB2	1:A:607:TRP:CH2	2.31	0.65
1:A:865:LEU:O	1:A:869:VAL:HG23	1.96	0.65
1:D:484:SER:O	1:D:487:GLN:HG3	1.96	0.65
1:A:442:ARG:HD3	2:A:1074:HOH:O	1.97	0.65
1:B:812:LEU:HA	1:B:815:LEU:HD12	1.79	0.65
1:C:30:LEU:HD13	1:C:63:MET:HE2	1.79	0.65
1:D:12:ASN:ND2	1:D:405:VAL:HG23	2.11	0.65
1:D:213:SER:CB	1:D:579:ARG:HH22	2.10	0.65
1:D:742:GLU:HB3	2:D:1060:HOH:O	1.96	0.65
1:C:314:TYR:HE1	1:C:347:LEU:HD21	1.62	0.65
1:D:829:PHE:HD1	2:D:1310:HOH:O	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:LEU:HD13	1:A:142:PRO:HG2	1.77	0.65
1:A:206:ALA:HB2	1:A:378:TYR:CE2	2.31	0.65
1:A:338:MET:HG2	1:A:341:ARG:NH1	2.08	0.65
1:A:800:PHE:HB3	2:A:1042:HOH:O	1.96	0.65
1:B:547:GLN:HG2	1:B:560:ILE:HG21	1.79	0.65
1:D:368:THR:HG21	2:D:1270:HOH:O	1.96	0.65
1:D:821:ASP:OD2	1:D:931:LYS:HE2	1.97	0.65
1:A:25:GLU:O	1:A:29:ARG:HG2	1.97	0.65
1:A:662:PHE:HA	1:A:690:GLY:O	1.97	0.65
1:B:330:VAL:HG22	1:B:337:LEU:HD23	1.79	0.65
1:B:684:ARG:HG3	1:B:685:GLN:H	1.61	0.65
1:D:269:LYS:HG3	1:D:800:PHE:CE1	2.32	0.65
1:D:766:ILE:HD12	1:D:882:TRP:CE3	2.32	0.65
1:A:226:SER:HB2	1:A:363:ASN:HD22	1.62	0.65
1:A:825:GLN:HB3	2:A:1301:HOH:O	1.97	0.65
1:A:935:ARG:HB2	2:A:1139:HOH:O	1.97	0.65
1:B:823:ALA:HB3	1:B:824:PRO:HD3	1.79	0.65
1:C:303:MET:HA	1:C:306:GLN:HG2	1.79	0.65
1:C:369:ILE:HD12	1:C:763:ARG:NH1	2.12	0.65
1:D:585:LEU:HD22	1:D:655:VAL:HG11	1.79	0.65
1:A:363:ASN:HB3	2:A:1188:HOH:O	1.97	0.64
1:B:176:ASN:HD22	1:B:177:SER:H	1.43	0.64
1:B:625:ARG:O	1:B:629:GLN:HG2	1.97	0.64
1:B:813:GLU:H	1:B:813:GLU:CD	2.00	0.64
1:C:201:HIS:HB3	2:C:1246:HOH:O	1.97	0.64
1:C:211:VAL:HG11	1:C:383:GLY:HA3	1.78	0.64
1:C:102:GLY:N	1:C:105:LYS:HZ1	1.96	0.64
1:C:115:LEU:HD23	2:C:1335:HOH:O	1.96	0.64
1:D:99:MET:O	1:D:105:LYS:HE3	1.97	0.64
1:D:257:ARG:NH2	1:D:825:GLN:HE22	1.93	0.64
1:D:574:THR:HG22	1:D:575:ASN:N	2.11	0.64
1:C:369:ILE:HD12	1:C:763:ARG:CZ	2.27	0.64
1:D:85:LEU:HD23	1:D:111:LEU:HD11	1.79	0.64
1:A:754:GLN:HG2	1:A:907:PHE:CZ	2.32	0.64
1:C:369:ILE:HG12	1:C:374:PHE:HB2	1.78	0.64
1:C:393:LYS:HE3	2:C:1157:HOH:O	1.97	0.64
1:B:343:TYR:H	1:B:348:HIS:HB2	1.61	0.64
1:B:759:LEU:HD11	1:B:893:ARG:NH2	2.13	0.64
1:C:275:LEU:HD12	1:C:935:ARG:HH22	1.63	0.64
1:D:116:ASN:HD22	1:D:116:ASN:N	1.95	0.64
1:D:258:LYS:HB3	1:D:816:LYS:HE2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:464:LYS:HA	2:D:1328:HOH:O	1.97	0.64
1:D:798:GLU:OE1	1:D:843:VAL:HG11	1.98	0.64
1:A:119:THR:HG22	1:A:121:LYS:HG3	1.79	0.64
1:A:270:ASN:HA	2:A:1348:HOH:O	1.96	0.64
1:B:655:VAL:HA	1:B:658:LEU:HB2	1.79	0.64
1:C:92:HIS:CD2	1:C:116:ASN:HD21	2.16	0.64
1:C:339:PRO:HD2	1:C:341:ARG:HH12	1.63	0.64
1:C:557:GLU:O	1:C:561:VAL:HG23	1.97	0.64
1:D:141:GLY:HA3	2:D:1016:HOH:O	1.96	0.64
1:A:208:ILE:HB	1:A:211:VAL:HG12	1.78	0.64
1:B:277:LEU:HD23	1:B:280:ILE:HD12	1.79	0.64
1:C:636:GLU:HB3	2:C:1010:HOH:O	1.96	0.64
1:C:809:ASP:HB3	1:C:810:TRP:CD1	2.32	0.64
1:D:370:THR:HG22	1:D:756:ASP:OD1	1.98	0.64
1:A:306:GLN:HB2	2:A:1108:HOH:O	1.95	0.64
1:B:703:ARG:HD3	1:B:704:LEU:HG	1.79	0.64
1:B:830:PRO:HB3	1:B:834:LEU:HD12	1.80	0.64
1:C:622:GLU:HA	1:C:625:ARG:NE	2.13	0.64
1:D:274:HIS:HD1	1:D:274:HIS:H	1.44	0.64
1:A:904:LYS:HE3	1:A:908:GLN:HE22	1.63	0.64
1:C:192:PRO:HG3	1:C:774:LEU:HD22	1.79	0.64
1:D:514:GLU:O	1:D:517:ILE:HG12	1.98	0.64
1:A:354:LYS:NZ	1:D:634:ARG:HH22	1.97	0.63
1:C:231:LYS:HE2	1:C:232:ALA:H	1.63	0.63
1:D:494:ARG:HB2	1:D:513:PHE:HE2	1.63	0.63
1:A:266:VAL:HG22	1:A:269:LYS:HB2	1.78	0.63
1:C:275:LEU:HD11	1:C:935:ARG:HH12	1.62	0.63
1:D:547:GLN:HG2	1:D:560:ILE:CG2	2.27	0.63
1:A:250:LEU:H	1:A:259:GLU:HB3	1.64	0.63
1:B:258:LYS:HA	2:B:1078:HOH:O	1.99	0.63
1:D:152:GLY:O	1:D:172:THR:HA	1.98	0.63
1:D:242:ILE:HD12	1:D:286:LEU:HD12	1.79	0.63
1:A:325:GLY:O	1:A:326:GLN:HG3	1.98	0.63
1:A:806:HIS:CB	1:A:807:PRO:HD3	2.29	0.63
1:C:252:ALA:HB3	1:C:812:LEU:HD11	1.80	0.63
1:C:428:LYS:O	1:C:431:ALA:HB3	1.98	0.63
1:A:1:MET:N	1:A:5:LEU:HD12	2.14	0.63
1:A:326:GLN:HA	2:A:1023:HOH:O	1.99	0.63
1:A:823:ALA:HB2	1:A:935:ARG:HD3	1.81	0.63
1:B:451:ILE:HA	1:B:575:ASN:OD1	1.98	0.63
1:B:502:PRO:HG3	2:B:1282:HOH:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:736:ARG:HD3	1:D:739:LYS:HE3	1.79	0.63
1:D:295:PRO:CD	1:D:937:LYS:HB2	2.27	0.63
1:D:783:GLU:HG3	2:D:1047:HOH:O	1.99	0.63
1:C:184:LEU:HD11	1:C:369:ILE:HG22	1.81	0.63
1:C:230:GLU:HB3	2:C:1114:HOH:O	1.97	0.63
1:D:195:LEU:HB2	2:D:1231:HOH:O	1.98	0.63
1:A:12:ASN:ND2	1:A:405:VAL:H	1.97	0.63
1:B:72:ALA:HA	1:B:143:VAL:HG22	1.81	0.63
1:B:299:GLU:H	1:B:299:GLU:CD	2.01	0.63
1:C:800:PHE:HB2	1:C:810:TRP:CD1	2.32	0.63
1:B:39:ASP:HB3	2:B:1184:HOH:O	1.98	0.63
1:B:584:LYS:HE3	2:B:1178:HOH:O	1.99	0.63
1:C:25:GLU:HB3	2:C:1096:HOH:O	1.99	0.63
1:C:259:GLU:HB3	1:C:260:PRO:CD	2.29	0.63
1:D:70:GLU:OE2	1:D:73:LYS:HD3	1.97	0.63
1:D:80:HIS:NE2	1:D:107:LEU:HD11	2.12	0.63
1:A:673:ARG:O	1:A:677:GLN:HG3	1.97	0.63
1:A:727:HIS:O	1:A:731:THR:HG23	1.99	0.63
1:B:80:HIS:NE2	1:B:107:LEU:HD11	2.14	0.63
1:B:764:GLU:HA	2:B:1301:HOH:O	1.99	0.63
1:B:800:PHE:HB2	1:B:810:TRP:CD2	2.34	0.63
1:C:636:GLU:HG3	2:C:1001:HOH:O	1.96	0.63
1:A:389:LYS:HG3	1:A:405:VAL:CG2	2.30	0.62
1:A:574:THR:HG22	1:A:575:ASN:N	2.14	0.62
1:A:721:ASP:HB2	2:A:1161:HOH:O	1.99	0.62
1:B:141:GLY:O	1:B:145:ARG:HG3	1.98	0.62
1:D:266:VAL:HG22	1:D:813:GLU:CB	2.29	0.62
1:D:671:SER:OG	1:D:673:ARG:HG2	1.99	0.62
1:D:684:ARG:HG3	1:D:685:GLN:H	1.63	0.62
1:C:72:ALA:HA	1:C:143:VAL:HG22	1.81	0.62
1:C:663:ILE:CD1	1:C:682:ALA:HB2	2.29	0.62
1:D:561:VAL:HG21	1:D:578:GLY:HA3	1.80	0.62
1:A:772:LEU:HD11	1:A:780:GLU:CB	2.30	0.62
1:C:475:MET:O	1:C:479:LEU:HG	1.99	0.62
1:D:287:LEU:HA	2:D:1234:HOH:O	1.99	0.62
1:A:594:ALA:HA	1:A:597:LEU:HG	1.81	0.62
1:B:492:TRP:HB3	2:B:1112:HOH:O	1.98	0.62
1:B:703:ARG:HA	1:B:711:ILE:HD13	1.81	0.62
1:C:306:GLN:HA	2:C:1050:HOH:O	1.98	0.62
1:B:857:ARG:HE	1:B:861:LEU:HD21	1.64	0.62
1:A:265:THR:HG22	1:A:271:ARG:O	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:782:LYS:NZ	1:A:866:MET:SD	2.73	0.62
1:C:212:ASP:O	1:C:216:ILE:HB	1.98	0.62
1:C:265:THR:HG22	1:C:271:ARG:C	2.20	0.62
1:C:599:LYS:HE3	1:C:637:LEU:HD21	1.80	0.62
1:D:611:LEU:O	1:D:615:LYS:HB2	2.00	0.62
1:D:823:ALA:HB2	1:D:935:ARG:CD	2.30	0.62
1:D:860:GLU:HB2	1:D:861:LEU:HD23	1.82	0.62
1:A:215:LEU:HD22	1:A:399:TYR:CZ	2.35	0.62
1:A:344:GLY:O	1:A:345:GLU:HG2	1.99	0.62
1:A:535:HIS:O	1:A:539:VAL:HG23	1.99	0.62
1:C:504:GLN:HB2	2:C:1219:HOH:O	2.00	0.62
1:B:655:VAL:C	1:B:657:ALA:H	2.01	0.62
1:D:223:LEU:HD21	1:D:371:TYR:CZ	2.34	0.62
1:D:854:TYR:OH	1:D:933:LEU:HD13	2.00	0.62
1:A:927:SER:O	1:A:931:LYS:HG3	2.00	0.62
1:C:193:ASP:HB3	2:C:1078:HOH:O	1.99	0.62
1:C:435:GLU:OE2	1:C:694:TYR:OH	2.13	0.62
1:C:662:PHE:HA	1:C:690:GLY:O	1.99	0.62
1:B:104:GLY:O	1:B:108:VAL:HG23	1.98	0.62
1:B:430:TYR:OH	1:B:471:PRO:HB2	2.00	0.62
1:C:261:THR:HA	2:C:1076:HOH:O	2.00	0.62
1:D:370:THR:CG2	1:D:373:ASN:HD22	2.12	0.62
1:D:861:LEU:HD13	1:D:938:VAL:HG21	1.82	0.62
1:A:204:HIS:HB2	2:A:1126:HOH:O	1.99	0.61
1:A:231:LYS:HE2	1:A:232:ALA:H	1.65	0.61
1:B:794:ALA:O	1:B:798:GLU:HB3	1.98	0.61
1:C:247:GLU:HG2	2:C:1240:HOH:O	2.00	0.61
1:C:643:GLU:HG2	2:C:1104:HOH:O	2.00	0.61
1:C:673:ARG:O	1:C:677:GLN:HG3	2.00	0.61
1:D:145:ARG:HD2	2:D:1074:HOH:O	2.00	0.61
1:D:266:VAL:O	1:D:268:GLU:N	2.33	0.61
1:D:621:GLU:HA	2:D:1134:HOH:O	2.00	0.61
1:A:494:ARG:O	1:A:498:LEU:HG	1.99	0.61
1:A:732:ARG:HE	1:B:668:ARG:NH2	1.98	0.61
1:B:102:GLY:HA2	2:B:1006:HOH:O	2.00	0.61
1:B:494:ARG:HB2	1:B:513:PHE:HE2	1.66	0.61
1:B:842:ALA:O	1:B:846:LEU:HG	2.00	0.61
1:A:593:ALA:O	1:A:597:LEU:HG	2.00	0.61
1:C:343:TYR:H	1:C:348:HIS:HB2	1.65	0.61
1:C:806:HIS:CB	1:C:807:PRO:HD3	2.30	0.61
1:D:250:LEU:H	1:D:259:GLU:HB3	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:838:LYS:HA	2:D:1216:HOH:O	2.00	0.61
1:A:807:PRO:HB3	1:A:835:ARG:O	1.99	0.61
1:D:126:VAL:HA	1:D:174:VAL:O	2.00	0.61
1:B:250:LEU:H	1:B:259:GLU:HB3	1.65	0.61
1:B:453:ILE:HG12	1:B:550:ASN:HB3	1.81	0.61
1:C:795:SER:HB3	2:C:1095:HOH:O	1.99	0.61
1:D:176:ASN:HD22	1:D:177:SER:H	1.47	0.61
1:D:251:PRO:HA	2:D:1263:HOH:O	2.00	0.61
1:A:281:ALA:HA	1:A:284:GLU:CD	2.20	0.61
1:A:466:PRO:HG3	1:A:540:LEU:HB3	1.82	0.61
1:A:547:GLN:HG2	1:A:560:ILE:CG2	2.30	0.61
1:A:776:GLY:HA3	1:A:871:ARG:NH2	2.15	0.61
1:B:517:ILE:HG21	1:B:524:ARG:NH1	2.15	0.61
1:B:541:ARG:HA	2:B:1205:HOH:O	1.99	0.61
1:B:594:ALA:HA	1:B:597:LEU:HG	1.83	0.61
1:C:622:GLU:HA	1:C:625:ARG:HE	1.66	0.61
1:D:263:ASP:CG	1:D:816:LYS:HE3	2.21	0.61
1:D:364:GLN:HE21	1:D:887:HIS:CE1	2.19	0.61
1:D:575:ASN:O	1:D:576:MET:HB2	2.00	0.61
1:D:695:VAL:HG22	2:D:1024:HOH:O	2.00	0.61
1:D:812:LEU:HA	1:D:815:LEU:HD12	1.83	0.61
1:A:663:ILE:CG2	1:A:678:LEU:HD22	2.31	0.61
1:C:76:LEU:HD22	1:C:143:VAL:CG2	2.30	0.61
1:C:640:ARG:NE	1:C:644:ILE:HG13	2.15	0.61
1:D:663:ILE:HD13	1:D:682:ALA:CB	2.29	0.61
1:A:668:ARG:HH21	1:B:732:ARG:HH12	1.45	0.61
1:B:263:ASP:HB2	1:B:273:VAL:HB	1.81	0.61
1:C:18:ARG:NH2	1:C:22:GLN:HE21	1.98	0.61
1:C:298:MET:CE	1:C:873:VAL:HA	2.30	0.61
1:C:505:LEU:HD22	1:C:510:LEU:HD11	1.83	0.61
1:C:655:VAL:C	1:C:657:ALA:H	2.02	0.61
1:C:870:GLU:O	1:C:874:ILE:HG13	2.01	0.61
1:B:430:TYR:HB3	1:B:472:ARG:NE	2.16	0.61
1:B:744:ARG:HD2	2:B:1220:HOH:O	2.01	0.61
1:C:777:LYS:O	1:C:781:VAL:HG23	2.01	0.61
1:D:341:ARG:HD3	1:D:913:GLU:HG2	1.83	0.61
1:A:314:TYR:CE1	1:A:347:LEU:HD21	2.35	0.60
1:A:716:ARG:HG3	1:B:6:ARG:CD	2.30	0.60
1:B:419:ASP:OD1	1:B:693:PHE:HB2	2.01	0.60
1:C:19:TYR:HB3	1:C:86:ILE:HG12	1.83	0.60
1:D:370:THR:HG21	1:D:373:ASN:ND2	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:703:ARG:HD3	1:D:704:LEU:HG	1.82	0.60
1:A:428:LYS:O	1:A:431:ALA:HB3	2.00	0.60
1:A:471:PRO:HB3	2:A:1099:HOH:O	2.01	0.60
1:B:18:ARG:NH2	1:B:22:GLN:HE21	1.97	0.60
1:C:494:ARG:O	1:C:498:LEU:HG	2.01	0.60
1:D:96:ILE:HD12	1:D:211:VAL:HG21	1.83	0.60
1:D:181:PHE:CE1	1:D:223:LEU:HD22	2.35	0.60
1:D:338:MET:CG	1:D:341:ARG:HD2	2.31	0.60
1:D:393:LYS:HA	2:D:1096:HOH:O	2.01	0.60
1:A:47:LEU:HG	1:A:60:LEU:HD13	1.82	0.60
1:A:557:GLU:HA	1:A:560:ILE:HD12	1.81	0.60
1:A:752:LEU:HA	2:A:1335:HOH:O	2.01	0.60
1:B:303:MET:HA	1:B:306:GLN:HG2	1.82	0.60
1:B:550:ASN:ND2	1:B:550:ASN:H	1.98	0.60
1:B:800:PHE:O	1:B:810:TRP:CD1	2.54	0.60
1:C:408:THR:HG22	1:C:409:ASN:N	2.16	0.60
1:C:498:LEU:HB2	2:C:1130:HOH:O	2.02	0.60
1:D:373:ASN:HA	1:D:376:ARG:HD3	1.82	0.60
1:A:271:ARG:HH21	1:A:931:LYS:CE	2.13	0.60
1:C:258:LYS:HE3	1:C:275:LEU:CD2	2.30	0.60
1:C:415:LYS:HA	2:C:1101:HOH:O	2.01	0.60
1:A:552:LYS:HB3	2:A:1035:HOH:O	2.00	0.60
1:B:251:PRO:HA	2:B:1078:HOH:O	2.00	0.60
1:B:258:LYS:HD2	1:B:816:LYS:HE2	1.83	0.60
1:B:557:GLU:HA	1:B:560:ILE:HD12	1.82	0.60
1:C:215:LEU:HD22	1:C:399:TYR:CZ	2.37	0.60
1:C:927:SER:O	1:C:931:LYS:HG3	2.01	0.60
1:D:253:GLU:HG3	1:D:256:VAL:O	2.01	0.60
1:D:707:SER:OG	1:D:710:VAL:HG23	2.00	0.60
1:D:865:LEU:O	1:D:869:VAL:HG23	2.01	0.60
1:A:465:GLU:C	1:A:467:ARG:H	2.05	0.60
1:A:544:ILE:HD12	1:A:544:ILE:N	2.16	0.60
1:C:808:GLU:HG2	2:C:1021:HOH:O	2.01	0.60
1:D:213:SER:HB2	1:D:579:ARG:HH22	1.66	0.60
1:D:727:HIS:HD2	1:D:729:MET:H	1.48	0.60
1:A:259:GLU:HB3	1:A:260:PRO:CD	2.32	0.60
1:B:242:ILE:HD12	1:B:286:LEU:HD12	1.84	0.60
1:B:671:SER:OG	1:B:673:ARG:HG2	2.01	0.60
1:B:788:MET:HG2	1:B:926:LYS:HG2	1.83	0.60
1:C:258:LYS:HD3	1:C:258:LYS:H	1.66	0.60
1:C:298:MET:HE3	1:C:873:VAL:HA	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:GLY:HA3	2:A:1096:HOH:O	2.01	0.60
1:A:211:VAL:CG1	1:A:383:GLY:HA3	2.31	0.60
1:A:261:THR:HA	2:A:1229:HOH:O	2.01	0.60
1:B:12:ASN:ND2	1:B:405:VAL:H	2.00	0.60
1:B:25:GLU:O	1:B:29:ARG:HG2	2.00	0.60
1:B:805:VAL:HG11	1:B:809:ASP:OD1	2.01	0.60
1:C:132:LEU:HD23	1:C:135:ARG:HE	1.66	0.60
1:C:499:LEU:HG	2:C:1130:HOH:O	2.02	0.60
1:C:781:VAL:HG11	2:C:1113:HOH:O	2.01	0.60
1:A:614:LYS:HA	1:A:614:LYS:HE3	1.82	0.60
1:B:575:ASN:O	1:B:576:MET:HB2	2.01	0.60
1:B:589:PRO:HA	1:B:592:LEU:HD12	1.83	0.60
1:C:546:HIS:O	1:C:547:GLN:HB2	2.02	0.60
1:C:772:LEU:HD11	1:C:780:GLU:CB	2.31	0.60
1:D:246:LEU:HD21	1:D:261:THR:HG21	1.84	0.60
1:D:381:ARG:HH11	1:D:381:ARG:H	1.49	0.60
1:D:895:GLY:HA3	2:D:1323:HOH:O	2.01	0.60
1:B:301:ALA:O	1:B:305:ILE:HG13	2.02	0.60
1:A:18:ARG:NH2	1:A:22:GLN:HE21	1.99	0.59
1:A:211:VAL:HG11	1:A:383:GLY:HA3	1.84	0.59
1:A:369:ILE:CG1	1:A:374:PHE:HB2	2.31	0.59
1:A:777:LYS:O	1:A:781:VAL:HG23	2.02	0.59
1:A:777:LYS:HG2	1:A:780:GLU:HG3	1.84	0.59
1:B:230:GLU:HG3	2:B:1062:HOH:O	2.02	0.59
1:C:250:LEU:H	1:C:259:GLU:HB3	1.67	0.59
1:C:273:VAL:HG13	1:C:820:LEU:HD13	1.83	0.59
1:C:858:GLU:HG3	1:C:866:MET:CE	2.31	0.59
1:D:330:VAL:HG21	2:D:1186:HOH:O	2.01	0.59
1:D:498:LEU:HD22	1:D:509:ASP:OD2	2.02	0.59
1:A:13:GLU:CG	1:B:716:ARG:HH12	2.15	0.59
1:A:622:GLU:HA	1:A:625:ARG:HE	1.65	0.59
1:A:934:PHE:HA	2:A:1148:HOH:O	2.02	0.59
1:B:849:ALA:HA	1:B:852:LYS:HD2	1.83	0.59
1:C:807:PRO:HB3	1:C:835:ARG:O	2.02	0.59
1:D:330:VAL:HG22	2:D:1219:HOH:O	2.02	0.59
1:D:653:GLU:HB2	2:D:1053:HOH:O	2.02	0.59
1:D:770:ARG:HH12	1:D:879:ASP:HB2	1.66	0.59
1:A:599:LYS:HE3	1:A:637:LEU:HD21	1.85	0.59
1:B:126:VAL:HA	1:B:174:VAL:O	2.02	0.59
1:B:430:TYR:CD1	1:B:472:ARG:HG2	2.38	0.59
1:B:640:ARG:CZ	1:B:643:GLU:HG2	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:770:ARG:HH22	1:B:879:ASP:CB	2.15	0.59
1:B:806:HIS:CB	1:B:807:PRO:HD3	2.32	0.59
1:C:370:THR:HG23	1:C:373:ASN:HB2	1.83	0.59
1:D:428:LYS:O	1:D:431:ALA:HB3	2.02	0.59
1:D:444:GLN:HG3	1:D:445:PRO:HD2	1.84	0.59
1:A:820:LEU:HD12	1:A:935:ARG:NH2	2.17	0.59
1:B:152:GLY:O	1:B:172:THR:HA	2.02	0.59
1:C:30:LEU:HD13	1:C:63:MET:CE	2.32	0.59
1:C:407:PRO:HA	2:C:1122:HOH:O	2.02	0.59
1:C:574:THR:HG22	1:C:575:ASN:N	2.17	0.59
1:D:253:GLU:HB2	1:D:256:VAL:HG13	1.84	0.59
1:D:806:HIS:CB	1:D:807:PRO:HD3	2.32	0.59
1:B:244:LYS:HD2	1:B:354:LYS:NZ	2.17	0.59
1:B:269:LYS:HD3	1:B:270:ASN:H	1.67	0.59
1:B:271:ARG:HG3	2:B:1311:HOH:O	2.01	0.59
1:C:517:ILE:HG21	1:C:524:ARG:NH1	2.18	0.59
1:D:102:GLY:HA3	2:D:1308:HOH:O	2.03	0.59
1:D:295:PRO:HD3	1:D:937:LYS:CB	2.30	0.59
1:D:370:THR:HG21	1:D:373:ASN:HD22	1.67	0.59
1:D:663:ILE:HG12	1:D:678:LEU:O	2.02	0.59
1:A:20:TYR:CD2	1:A:24:VAL:HG21	2.38	0.59
1:B:663:ILE:HD13	1:B:682:ALA:CB	2.30	0.59
1:B:723:GLU:HB2	2:B:1204:HOH:O	2.02	0.59
1:C:865:LEU:O	1:C:869:VAL:HG23	2.02	0.59
1:D:679:ARG:NE	2:D:1104:HOH:O	2.34	0.59
1:A:253:GLU:HB2	1:A:256:VAL:CG1	2.29	0.59
1:B:266:VAL:O	1:B:268:GLU:N	2.35	0.59
1:B:816:LYS:HD3	2:B:1175:HOH:O	2.03	0.59
1:C:309:ARG:HA	1:C:313:LEU:HD23	1.84	0.59
1:C:832:ALA:O	1:C:836:ALA:HB3	2.03	0.59
1:D:311:LYS:HB3	2:D:1331:HOH:O	2.02	0.59
1:D:517:ILE:HG21	1:D:524:ARG:NH1	2.16	0.59
1:A:26:PRO:O	1:A:30:LEU:HG	2.03	0.59
1:C:343:TYR:CE1	1:C:351:ILE:HD12	2.37	0.59
1:D:321:ILE:HG23	2:D:1137:HOH:O	2.03	0.59
1:B:661:LEU:HD13	1:B:663:ILE:HD11	1.84	0.59
1:C:361:ARG:HD3	2:C:1159:HOH:O	2.02	0.59
1:C:504:GLN:HG3	2:C:1018:HOH:O	2.01	0.59
1:C:898:LEU:HA	2:C:1273:HOH:O	2.01	0.59
1:B:118:LEU:HB3	2:B:1197:HOH:O	2.03	0.59
1:B:453:ILE:HG23	1:B:550:ASN:OD1	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:295:PRO:HB3	1:D:937:LYS:O	2.03	0.59
1:D:323:GLN:NE2	1:D:328:ILE:HD12	2.17	0.59
1:D:833:GLU:O	1:D:837:LEU:HG	2.03	0.59
1:A:484:SER:HB3	1:A:496:ARG:HH12	1.69	0.58
1:A:589:PRO:HA	1:A:592:LEU:HD12	1.85	0.58
1:A:761:ARG:HD2	1:A:761:ARG:H	1.67	0.58
1:C:414:ARG:HD2	1:C:682:ALA:HB3	1.84	0.58
1:D:453:ILE:HG23	1:D:550:ASN:OD1	2.03	0.58
1:D:798:GLU:HB2	1:D:843:VAL:HG22	1.83	0.58
1:A:354:LYS:HE2	1:D:634:ARG:HH12	1.67	0.58
1:A:547:GLN:HG2	1:A:560:ILE:HG21	1.85	0.58
1:C:152:GLY:O	1:C:172:THR:HA	2.03	0.58
1:C:478:GLU:HB3	2:C:1183:HOH:O	2.01	0.58
1:D:273:VAL:HA	1:D:820:LEU:HD13	1.85	0.58
1:D:668:ARG:HG2	1:D:693:PHE:CD2	2.38	0.58
1:A:176:ASN:HB2	1:A:371:TYR:CE2	2.38	0.58
1:A:441:GLU:HG3	1:A:539:VAL:CG1	2.33	0.58
1:B:79:ARG:HG2	2:B:1166:HOH:O	2.03	0.58
1:B:770:ARG:HH12	1:B:879:ASP:CB	2.16	0.58
1:A:152:GLY:O	1:A:172:THR:HA	2.04	0.58
1:A:176:ASN:HB2	1:A:371:TYR:HE2	1.67	0.58
1:B:621:GLU:HG2	2:B:1041:HOH:O	2.02	0.58
1:B:707:SER:O	1:B:711:ILE:HG13	2.04	0.58
1:C:231:LYS:HE2	1:C:232:ALA:N	2.18	0.58
1:C:323:GLN:HG3	1:C:328:ILE:HD11	1.85	0.58
1:D:381:ARG:HG3	2:D:1048:HOH:O	2.02	0.58
1:A:281:ALA:HA	1:A:284:GLU:OE1	2.04	0.58
1:A:397:GLU:HG2	2:A:1102:HOH:O	2.03	0.58
1:A:414:ARG:HD2	1:A:682:ALA:HB3	1.85	0.58
1:B:295:PRO:O	1:B:296:GLU:HB2	2.04	0.58
1:B:468:LEU:O	1:B:471:PRO:HD2	2.04	0.58
1:B:807:PRO:HB3	1:B:835:ARG:O	2.04	0.58
1:C:716:ARG:HG3	1:D:6:ARG:HD2	1.85	0.58
1:A:606:GLU:HG2	1:A:610:GLU:CD	2.24	0.58
1:B:885:HIS:HA	2:B:1035:HOH:O	2.02	0.58
1:C:78:MET:HE3	2:C:1334:HOH:O	2.02	0.58
1:C:156:HIS:HA	1:C:178:GLU:OE1	2.03	0.58
1:C:611:LEU:O	1:C:615:LYS:HB2	2.04	0.58
1:C:861:LEU:CD1	1:C:938:VAL:HG21	2.27	0.58
1:D:12:ASN:ND2	1:D:405:VAL:H	2.01	0.58
1:D:35:GLU:HA	1:D:74:ARG:HH21	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:191:SER:H	1:D:194:GLN:HE21	1.51	0.58
1:D:705:PHE:CD2	1:D:741:VAL:HG13	2.39	0.58
1:A:212:ASP:O	1:A:216:ILE:HB	2.04	0.58
1:B:231:LYS:NZ	1:B:232:ALA:N	2.51	0.58
1:B:514:GLU:O	1:B:517:ILE:HG12	2.03	0.58
1:B:883:LYS:HD2	2:B:1221:HOH:O	2.03	0.58
1:C:491:GLU:HG2	1:C:516:LEU:HD21	1.85	0.58
1:C:796:LEU:HD21	1:C:817:ALA:HB3	1.84	0.58
1:D:250:LEU:HD23	1:D:259:GLU:OE1	2.03	0.58
1:D:269:LYS:CD	1:D:270:ASN:H	2.12	0.58
1:D:585:LEU:HD22	1:D:655:VAL:CG1	2.34	0.58
1:D:776:GLY:HA2	1:D:871:ARG:NH1	2.16	0.58
1:A:80:HIS:HE2	1:A:107:LEU:HD11	1.69	0.58
1:A:168:LEU:HA	1:A:198:ARG:HH11	1.68	0.58
1:A:263:ASP:CG	1:A:816:LYS:HG2	2.24	0.58
1:A:294:SER:HB3	1:A:295:PRO:CD	2.34	0.58
1:A:301:ALA:HB3	1:A:932:PHE:HZ	1.69	0.58
1:A:499:LEU:HD23	1:A:505:LEU:HD21	1.84	0.58
1:B:563:GLN:HG3	1:B:591:TYR:CE1	2.38	0.58
1:C:211:VAL:CG1	1:C:383:GLY:HA3	2.33	0.58
1:C:263:ASP:OD2	1:C:273:VAL:HB	2.04	0.58
1:D:104:GLY:O	1:D:108:VAL:HG23	2.03	0.58
1:A:220:ARG:O	1:A:752:LEU:HD22	2.04	0.58
1:B:258:LYS:H	1:B:258:LYS:CD	2.03	0.58
1:B:600:GLU:OE2	1:B:631:LEU:HD22	2.04	0.58
1:B:925:ILE:O	1:B:929:VAL:HG23	2.03	0.58
1:C:621:GLU:HB2	2:C:1111:HOH:O	2.04	0.58
1:C:803:PRO:HB2	1:C:805:VAL:O	2.04	0.58
1:C:806:HIS:HB3	1:C:807:PRO:HD3	1.86	0.58
1:A:843:VAL:HB	2:A:1237:HOH:O	2.04	0.58
1:B:810:TRP:CB	2:B:1243:HOH:O	2.51	0.58
1:C:154:ILE:HB	1:C:174:VAL:HG22	1.86	0.58
1:C:314:TYR:CE1	1:C:347:LEU:HD21	2.38	0.58
1:D:91:LEU:HD22	1:D:207:ILE:HD13	1.85	0.58
1:D:504:GLN:HG3	2:D:1092:HOH:O	2.04	0.58
1:D:563:GLN:HE22	1:D:587:GLY:HA3	1.69	0.58
1:A:47:LEU:HD11	1:A:60:LEU:HD22	1.86	0.57
1:A:271:ARG:HH21	1:A:931:LYS:NZ	2.02	0.57
1:A:343:TYR:H	1:A:348:HIS:HB2	1.68	0.57
1:A:551:ALA:HA	1:A:557:GLU:OE1	2.04	0.57
1:B:439:LYS:HE2	1:B:662:PHE:CD2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:822:THR:HG22	1:B:824:PRO:HD2	1.85	0.57
1:C:13:GLU:OE1	1:C:13:GLU:HA	2.04	0.57
1:C:329:ILE:HD12	1:C:341:ARG:O	2.04	0.57
1:D:589:PRO:HA	1:D:592:LEU:HB2	1.86	0.57
1:A:275:LEU:HD13	1:A:816:LYS:HZ1	1.69	0.57
1:A:477:LEU:HD21	1:A:499:LEU:HD22	1.84	0.57
1:A:860:GLU:HB2	1:A:861:LEU:HD23	1.84	0.57
1:B:548:VAL:O	1:B:549:LEU:HD23	2.05	0.57
1:B:705:PHE:CB	1:B:741:VAL:HG22	2.34	0.57
1:B:860:GLU:HB2	1:B:861:LEU:HD23	1.86	0.57
1:C:788:MET:HE1	1:C:929:VAL:HG11	1.86	0.57
1:D:192:PRO:HG3	1:D:774:LEU:HD22	1.86	0.57
1:D:295:PRO:O	1:D:296:GLU:HB2	2.04	0.57
1:D:547:GLN:HG2	1:D:560:ILE:HG21	1.85	0.57
1:A:408:THR:HG22	1:A:409:ASN:N	2.19	0.57
1:B:702:MET:O	1:B:706:ALA:HB3	2.04	0.57
1:C:593:ALA:O	1:C:597:LEU:HG	2.04	0.57
1:C:857:ARG:HE	1:C:861:LEU:HD21	1.69	0.57
1:D:337:LEU:O	1:D:339:PRO:HD3	2.04	0.57
1:A:25:GLU:HG3	2:A:1062:HOH:O	2.03	0.57
1:A:128:VAL:HG12	2:A:1072:HOH:O	2.04	0.57
1:A:651:ASP:HB3	2:A:1024:HOH:O	2.04	0.57
1:A:652:GLU:O	1:A:656:ARG:HB2	2.04	0.57
1:C:2:LEU:HG	1:D:716:ARG:HA	1.86	0.57
1:A:24:VAL:HG12	1:A:28:ASN:HD21	1.69	0.57
1:A:409:ASN:HB3	1:A:685:GLN:HE22	1.70	0.57
1:B:284:GLU:OE1	1:B:290:GLU:HB2	2.04	0.57
1:D:134:ARG:HD3	2:D:1286:HOH:O	2.03	0.57
1:D:265:THR:HG22	1:D:271:ARG:C	2.24	0.57
1:A:6:ARG:HD2	1:B:716:ARG:HH21	1.70	0.57
1:A:217:ASP:OD1	1:A:674:ILE:HD11	2.04	0.57
1:A:369:ILE:HA	1:A:763:ARG:NH1	2.19	0.57
1:A:801:LEU:C	1:A:803:PRO:HD3	2.24	0.57
1:B:769:GLN:O	1:B:773:ILE:HD13	2.04	0.57
1:C:552:LYS:HG2	2:C:1020:HOH:O	2.04	0.57
1:C:861:LEU:HB2	1:C:865:LEU:HB3	1.85	0.57
1:C:865:LEU:HD13	1:C:938:VAL:HG11	1.87	0.57
1:D:266:VAL:HG23	1:D:269:LYS:HB2	1.85	0.57
1:D:321:ILE:HG21	2:D:1213:HOH:O	2.04	0.57
1:A:266:VAL:O	1:A:268:GLU:N	2.37	0.57
1:B:110:THR:HG21	1:B:140:MET:HG2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:ARG:HH22	1:B:349:GLN:NE2	2.03	0.57
1:B:519:PRO:HA	2:B:1000:HOH:O	2.04	0.57
1:C:61:LEU:HB3	1:C:62:PRO:HD3	1.85	0.57
1:D:330:VAL:HG22	1:D:337:LEU:HD23	1.85	0.57
1:A:223:LEU:HD12	1:A:369:ILE:HG23	1.86	0.57
1:A:586:GLY:CA	2:A:1024:HOH:O	2.52	0.57
1:A:802:ASN:HA	1:A:839:ALA:HB2	1.86	0.57
1:B:551:ALA:HA	1:B:557:GLU:OE1	2.05	0.57
1:B:611:LEU:O	1:B:615:LYS:HB2	2.03	0.57
1:C:325:GLY:O	1:C:326:GLN:HG3	2.03	0.57
1:A:8:LEU:O	1:A:8:LEU:HD13	2.05	0.57
1:A:242:ILE:HD12	1:A:286:LEU:HD12	1.87	0.57
1:A:273:VAL:HG22	2:A:1243:HOH:O	2.04	0.57
1:C:852:LYS:HB2	1:C:852:LYS:HZ3	1.69	0.57
1:D:206:ALA:HB2	1:D:378:TYR:CE2	2.39	0.57
1:D:435:GLU:OE2	1:D:692:ARG:NH1	2.37	0.57
1:D:865:LEU:O	1:D:865:LEU:HD23	2.05	0.57
1:B:103:GLU:HG3	1:B:104:GLY:N	2.18	0.56
1:C:273:VAL:HA	1:C:820:LEU:HD13	1.87	0.56
1:C:524:ARG:NH1	1:C:527:TRP:HD1	2.03	0.56
1:C:777:LYS:HG2	1:C:780:GLU:HG3	1.86	0.56
1:D:95:LYS:HE2	1:D:402:ASP:HB2	1.87	0.56
1:D:590:GLU:HG3	1:D:591:TYR:CE1	2.40	0.56
1:D:797:ALA:CB	1:D:846:LEU:HD12	2.35	0.56
1:D:857:ARG:NH1	1:D:934:PHE:C	2.59	0.56
1:A:164:ARG:HG3	1:A:196:VAL:HA	1.87	0.56
1:A:179:LEU:HD23	1:A:374:PHE:CE2	2.40	0.56
1:A:231:LYS:HE2	1:A:232:ALA:N	2.19	0.56
1:A:857:ARG:HD3	2:A:1148:HOH:O	2.04	0.56
1:B:546:HIS:O	1:B:547:GLN:HB2	2.05	0.56
1:C:121:LYS:HA	2:C:1137:HOH:O	2.03	0.56
1:C:327:VAL:CG2	1:C:352:GLU:HG2	2.35	0.56
1:C:524:ARG:NH1	1:C:527:TRP:CD1	2.73	0.56
1:D:702:MET:O	1:D:706:ALA:HB3	2.06	0.56
1:A:61:LEU:HB3	1:A:62:PRO:HD3	1.88	0.56
1:A:576:MET:O	1:A:579:ARG:HB2	2.04	0.56
1:A:704:LEU:HD12	2:A:1037:HOH:O	2.05	0.56
1:B:75:TYR:CE1	1:B:146:GLY:HA3	2.40	0.56
1:B:190:ILE:O	1:B:774:LEU:HD21	2.04	0.56
1:B:422:TYR:O	1:B:696:SER:HA	2.05	0.56
1:B:620:LYS:HD2	1:B:623:GLU:OE1	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:640:ARG:NH1	1:B:643:GLU:HG2	2.20	0.56
1:C:779:GLU:O	1:C:783:GLU:HG2	2.04	0.56
1:C:909:GLU:HA	2:C:1309:HOH:O	2.05	0.56
1:D:85:LEU:HA	1:D:111:LEU:CD1	2.35	0.56
1:D:252:ALA:HB1	2:D:1237:HOH:O	2.05	0.56
1:D:363:ASN:HB3	2:D:1228:HOH:O	2.04	0.56
1:D:463:LEU:HD22	1:D:544:ILE:HD12	1.87	0.56
1:D:604:ARG:CZ	1:D:604:ARG:HB2	2.35	0.56
1:D:652:GLU:O	1:D:656:ARG:HB2	2.04	0.56
1:D:705:PHE:CB	1:D:741:VAL:HG22	2.35	0.56
1:A:704:LEU:HA	2:A:1034:HOH:O	2.05	0.56
1:B:45:ARG:HD3	2:B:1028:HOH:O	2.05	0.56
1:C:294:SER:HB3	1:C:295:PRO:CD	2.34	0.56
1:C:316:ARG:HA	1:C:320:TYR:CZ	2.40	0.56
1:C:589:PRO:HA	1:C:592:LEU:HD12	1.87	0.56
1:D:465:GLU:O	1:D:467:ARG:N	2.39	0.56
1:D:530:LEU:O	1:D:534:VAL:HG23	2.06	0.56
1:D:597:LEU:HD13	2:D:1324:HOH:O	2.05	0.56
1:A:449:GLY:O	1:A:666:THR:HB	2.05	0.56
1:A:784:ALA:HA	2:A:1276:HOH:O	2.06	0.56
1:B:517:ILE:CG2	1:B:524:ARG:HD2	2.36	0.56
1:B:776:GLY:HA2	1:B:871:ARG:NH1	2.19	0.56
1:D:281:ALA:HA	1:D:284:GLU:OE1	2.06	0.56
1:C:13:GLU:CG	1:D:716:ARG:HH12	2.18	0.56
1:C:284:GLU:OE1	1:C:290:GLU:HB3	2.06	0.56
1:C:563:GLN:HG3	1:C:591:TYR:CE1	2.40	0.56
1:A:797:ALA:HB1	1:A:801:LEU:HD12	1.86	0.56
1:A:801:LEU:O	1:A:803:PRO:HD3	2.06	0.56
1:B:7:ARG:HG2	1:B:13:GLU:CD	2.26	0.56
1:B:198:ARG:HG3	1:B:202:PRO:HA	1.86	0.56
1:B:299:GLU:HA	2:B:1218:HOH:O	2.06	0.56
1:B:523:LEU:O	1:B:523:LEU:HD23	2.06	0.56
1:B:770:ARG:HH22	1:B:879:ASP:HB2	1.71	0.56
1:C:219:ALA:HB1	1:C:372:GLN:HE22	1.68	0.56
1:C:788:MET:HG2	1:C:926:LYS:HG2	1.87	0.56
1:C:800:PHE:CD2	1:C:800:PHE:N	2.72	0.56
1:D:65:PHE:HE1	1:D:115:LEU:HD22	1.70	0.56
1:D:755:PHE:O	1:D:758:VAL:HB	2.05	0.56
1:A:422:TYR:O	1:A:696:SER:HA	2.05	0.56
1:A:732:ARG:NE	1:B:668:ARG:NH2	2.54	0.56
1:B:553:HIS:CE1	1:B:556:ARG:HD3	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:584:LYS:HG3	2:B:1178:HOH:O	2.06	0.56
1:B:865:LEU:O	1:B:865:LEU:HD23	2.06	0.56
1:C:231:LYS:HA	2:C:1156:HOH:O	2.06	0.56
1:C:292:LEU:HD23	2:C:1100:HOH:O	2.06	0.56
1:D:364:GLN:HG2	1:D:887:HIS:CB	2.36	0.56
1:D:459:LEU:HD13	1:D:572:ILE:CD1	2.35	0.56
1:A:770:ARG:NH1	1:A:879:ASP:HB2	2.21	0.56
1:B:574:THR:HG22	1:B:575:ASN:N	2.20	0.56
1:B:634:ARG:HB3	2:B:1032:HOH:O	2.06	0.56
1:C:242:ILE:HD12	1:C:286:LEU:HD12	1.87	0.56
1:C:517:ILE:HB	2:C:1211:HOH:O	2.05	0.56
1:A:65:PHE:CZ	1:A:111:LEU:HB3	2.41	0.56
1:A:72:ALA:HA	1:A:143:VAL:HG22	1.87	0.56
1:A:369:ILE:HG12	1:A:374:PHE:HB2	1.87	0.56
1:B:636:GLU:HB2	2:B:1228:HOH:O	2.05	0.56
1:B:833:GLU:O	1:B:837:LEU:HG	2.06	0.56
1:B:935:ARG:HD3	2:B:1103:HOH:O	2.06	0.56
1:C:96:ILE:HD12	1:C:395:PHE:CD1	2.41	0.56
1:C:551:ALA:HA	1:C:557:GLU:OE1	2.06	0.56
1:C:661:LEU:HD13	1:C:663:ILE:HD11	1.86	0.56
1:C:712:ALA:HA	1:D:6:ARG:HH11	1.71	0.56
1:D:802:ASN:HA	1:D:839:ALA:HB2	1.86	0.56
1:C:652:GLU:O	1:C:656:ARG:HB2	2.06	0.55
1:D:110:THR:CG2	1:D:140:MET:HG2	2.37	0.55
1:D:145:ARG:HB2	2:D:1121:HOH:O	2.05	0.55
1:D:774:LEU:HG	2:D:1071:HOH:O	2.05	0.55
1:D:857:ARG:HB2	2:D:1203:HOH:O	2.06	0.55
1:A:80:HIS:NE2	1:A:107:LEU:HD11	2.21	0.55
1:A:470:LEU:HD23	1:A:537:LEU:HD11	1.87	0.55
1:B:213:SER:HB2	1:B:579:ARG:HH22	1.71	0.55
1:C:227:GLY:HA3	1:C:366:LEU:HD11	1.87	0.55
1:C:576:MET:O	1:C:579:ARG:HB2	2.06	0.55
1:C:714:LEU:HD23	1:C:729:MET:HE3	1.88	0.55
1:D:110:THR:HG21	1:D:140:MET:HG2	1.87	0.55
1:D:663:ILE:HG23	1:D:678:LEU:HD22	1.88	0.55
1:D:858:GLU:HA	1:D:866:MET:HG3	1.87	0.55
1:A:441:GLU:HG3	1:A:539:VAL:HG13	1.87	0.55
1:A:616:MET:HG2	1:A:641:ILE:CG2	2.35	0.55
1:A:857:ARG:HH21	1:A:938:VAL:HG23	1.72	0.55
1:B:227:GLY:HA3	1:B:366:LEU:HD11	1.88	0.55
1:B:810:TRP:CD1	1:B:810:TRP:N	2.74	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:444:GLN:NE2	1:D:660:GLY:N	2.54	0.55
1:A:372:GLN:N	1:A:372:GLN:OE1	2.35	0.55
1:A:544:ILE:HD12	1:A:544:ILE:H	1.72	0.55
1:A:677:GLN:HG2	2:A:1342:HOH:O	2.06	0.55
1:A:820:LEU:HB3	2:A:1243:HOH:O	2.07	0.55
1:A:823:ALA:HB3	1:A:824:PRO:HD3	1.89	0.55
1:B:99:MET:O	1:B:105:LYS:HE3	2.07	0.55
1:C:442:ARG:NH1	1:C:658:LEU:HD23	2.22	0.55
1:D:301:ALA:O	1:D:305:ILE:HG13	2.06	0.55
1:D:422:TYR:O	1:D:696:SER:HA	2.06	0.55
1:A:457:GLU:O	1:A:460:SER:HB3	2.07	0.55
1:D:26:PRO:O	1:D:30:LEU:HG	2.07	0.55
1:D:227:GLY:HA3	1:D:366:LEU:HD11	1.88	0.55
1:A:782:LYS:HZ1	1:A:867:ARG:N	2.05	0.55
1:B:372:GLN:O	1:B:376:ARG:HG3	2.07	0.55
1:B:635:GLU:OE2	1:B:638:LEU:HD12	2.06	0.55
1:B:727:HIS:HD2	1:B:729:MET:H	1.54	0.55
1:C:127:THR:HG23	1:C:209:ASP:HB3	1.88	0.55
1:C:341:ARG:HE	1:C:896:ILE:HD11	1.71	0.55
1:D:410:ARG:HG3	1:D:685:GLN:HE21	1.72	0.55
1:A:885:HIS:HA	2:A:1179:HOH:O	2.06	0.55
1:B:306:GLN:HA	2:B:1290:HOH:O	2.06	0.55
1:B:444:GLN:HE21	1:B:660:GLY:N	2.04	0.55
1:B:475:MET:O	1:B:479:LEU:HG	2.06	0.55
1:B:589:PRO:HA	1:B:592:LEU:HB2	1.89	0.55
1:C:575:ASN:O	1:C:576:MET:HB2	2.07	0.55
1:D:131:TYR:CE2	1:D:135:ARG:HD3	2.41	0.55
1:D:474:GLU:HG2	2:D:1170:HOH:O	2.07	0.55
1:D:929:VAL:O	1:D:933:LEU:HG	2.06	0.55
1:A:151:VAL:HG23	2:A:1273:HOH:O	2.07	0.55
1:A:184:LEU:HD21	1:A:369:ILE:HG22	1.89	0.55
1:A:495:LEU:HD22	1:A:513:PHE:CD2	2.42	0.55
1:A:882:TRP:HE3	1:A:921:MET:HE1	1.70	0.55
1:B:292:LEU:HB3	1:B:297:ASN:ND2	2.22	0.55
1:B:604:ARG:HD3	1:B:605:TYR:H	1.72	0.55
1:B:705:PHE:CG	1:B:741:VAL:HG22	2.42	0.55
1:D:258:LYS:H	1:D:258:LYS:CD	2.06	0.55
1:D:832:ALA:O	1:D:836:ALA:HB3	2.06	0.55
1:C:261:THR:HG23	1:C:279:GLY:HA3	1.89	0.55
1:D:273:VAL:C	1:D:820:LEU:HD13	2.26	0.55
1:A:19:TYR:HB3	1:A:86:ILE:HG12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:GLU:CG	1:A:260:PRO:HD3	2.37	0.55
1:A:594:ALA:HB2	2:A:1215:HOH:O	2.06	0.55
1:B:801:LEU:C	1:B:803:PRO:HD3	2.28	0.55
1:C:275:LEU:CD1	2:C:1223:HOH:O	2.55	0.55
1:C:346:GLY:CA	1:C:884:GLU:HG2	2.37	0.55
1:C:535:HIS:O	1:C:539:VAL:HG23	2.07	0.55
1:A:451:ILE:HD12	1:A:667:GLU:CG	2.37	0.54
1:C:435:GLU:HG3	2:C:1315:HOH:O	2.07	0.54
1:C:904:LYS:HE3	1:C:908:GLN:NE2	2.20	0.54
1:D:7:ARG:HA	1:D:13:GLU:CB	2.34	0.54
1:A:479:LEU:HA	1:A:482:LYS:HE3	1.89	0.54
1:A:611:LEU:HD11	1:A:615:LYS:NZ	2.22	0.54
1:C:501:ARG:HB2	1:C:504:GLN:OE1	2.07	0.54
1:D:65:PHE:CE1	1:D:115:LEU:HD22	2.42	0.54
1:D:154:ILE:HD12	1:D:174:VAL:CG2	2.38	0.54
1:D:450:THR:HA	2:D:1107:HOH:O	2.07	0.54
1:D:453:ILE:HG12	1:D:550:ASN:HB3	1.90	0.54
1:A:842:ALA:O	1:A:846:LEU:HG	2.07	0.54
1:B:30:LEU:HD13	1:B:63:MET:HE2	1.87	0.54
1:B:498:LEU:HD22	1:B:509:ASP:OD2	2.07	0.54
1:C:26:PRO:O	1:C:30:LEU:HG	2.07	0.54
1:C:481:LYS:HA	1:C:496:ARG:NH2	2.23	0.54
1:C:589:PRO:HA	1:C:592:LEU:HB2	1.89	0.54
1:C:758:VAL:N	2:C:1084:HOH:O	2.39	0.54
1:A:354:LYS:CE	1:D:634:ARG:HH12	2.20	0.54
1:D:238:LYS:O	1:D:241:GLU:HG2	2.08	0.54
1:A:6:ARG:HD2	1:B:716:ARG:NH2	2.22	0.54
1:A:327:VAL:CG2	1:A:352:GLU:HG2	2.37	0.54
1:A:663:ILE:HG21	1:A:678:LEU:HD22	1.90	0.54
1:B:11:ASN:O	1:B:15:GLU:HB2	2.07	0.54
1:C:12:ASN:ND2	1:C:405:VAL:HG23	2.23	0.54
1:C:98:GLU:OE1	1:C:405:VAL:HG13	2.07	0.54
1:A:76:LEU:HD22	1:A:143:VAL:CG2	2.38	0.54
1:A:589:PRO:HA	1:A:592:LEU:HB2	1.90	0.54
1:B:176:ASN:HD22	1:B:177:SER:N	2.05	0.54
1:B:223:LEU:HD21	1:B:371:TYR:CE1	2.43	0.54
1:B:626:ALA:O	1:B:630:GLU:HG3	2.07	0.54
1:D:176:ASN:ND2	1:D:177:SER:H	2.06	0.54
1:D:585:LEU:HB2	1:D:652:GLU:HG2	1.89	0.54
1:D:589:PRO:HG2	1:D:614:LYS:NZ	2.21	0.54
1:A:273:VAL:CA	1:A:820:LEU:HD13	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:588:ASN:CB	1:A:589:PRO:HD3	2.38	0.54
1:A:925:ILE:O	1:A:929:VAL:HG23	2.07	0.54
1:B:370:THR:CG2	1:B:373:ASN:HD22	2.21	0.54
1:B:832:ALA:O	1:B:836:ALA:HB3	2.08	0.54
1:C:34:VAL:HG13	1:C:67:LEU:HD23	1.90	0.54
1:C:309:ARG:HB2	2:C:1050:HOH:O	2.08	0.54
1:C:796:LEU:HD21	1:C:817:ALA:CB	2.37	0.54
1:D:80:HIS:CD2	1:D:107:LEU:HD21	2.42	0.54
1:D:486:LYS:HE3	2:D:1224:HOH:O	2.08	0.54
1:A:179:LEU:HD23	1:A:374:PHE:HE2	1.72	0.54
1:A:302:HIS:HA	2:A:1084:HOH:O	2.07	0.54
1:A:677:GLN:HA	2:A:1342:HOH:O	2.08	0.54
1:B:268:GLU:HG3	2:B:1008:HOH:O	2.08	0.54
1:B:479:LEU:HA	1:B:482:LYS:HE3	1.88	0.54
1:B:559:GLU:HG3	1:B:590:GLU:CD	2.28	0.54
1:B:775:LEU:HD11	2:B:1109:HOH:O	2.07	0.54
1:C:499:LEU:HD23	1:C:505:LEU:HD21	1.88	0.54
1:C:606:GLU:HB2	2:C:1098:HOH:O	2.07	0.54
1:C:702:MET:O	1:C:706:ALA:HB3	2.08	0.54
1:D:546:HIS:O	1:D:547:GLN:HB2	2.08	0.54
1:A:249:GLY:CA	1:A:260:PRO:HD2	2.35	0.54
1:A:470:LEU:CD2	1:A:537:LEU:HD11	2.38	0.54
1:A:779:GLU:O	1:A:783:GLU:HG2	2.08	0.54
1:B:292:LEU:C	1:B:297:ASN:HD22	2.12	0.54
1:B:369:ILE:HD12	1:B:763:ARG:NH2	2.22	0.54
1:B:763:ARG:HD2	1:B:767:TYR:CE1	2.43	0.54
1:D:31:GLU:HA	2:D:1099:HOH:O	2.08	0.54
1:A:329:ILE:HD12	1:A:341:ARG:O	2.08	0.54
1:A:634:ARG:HB2	2:A:1050:HOH:O	2.07	0.54
1:B:893:ARG:HG2	1:B:910:TYR:CE1	2.42	0.54
1:C:309:ARG:HH12	1:C:924:PHE:HE1	1.54	0.54
1:D:190:ILE:HB	1:D:194:GLN:NE2	2.15	0.54
1:D:311:LYS:N	2:D:1098:HOH:O	2.40	0.54
1:A:168:LEU:HB3	2:A:1152:HOH:O	2.09	0.53
1:A:382:ALA:HA	1:A:401:MET:SD	2.48	0.53
1:B:284:GLU:OE2	1:B:290:GLU:HA	2.08	0.53
1:B:464:LYS:C	1:B:466:PRO:HD2	2.28	0.53
1:B:594:ALA:HB1	2:B:1307:HOH:O	2.09	0.53
1:C:231:LYS:HE2	1:C:231:LYS:HA	1.89	0.53
1:C:659:GLY:O	1:C:688:PRO:HB2	2.08	0.53
1:D:65:PHE:CD2	1:D:111:LEU:HD22	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:484:SER:HB2	1:D:496:ARG:HH22	1.74	0.53
1:D:628:ALA:HA	1:D:633:ILE:HD12	1.90	0.53
1:D:688:PRO:HB2	2:D:1241:HOH:O	2.07	0.53
1:D:802:ASN:HB2	1:D:839:ALA:HB1	1.90	0.53
1:D:858:GLU:HG3	1:D:866:MET:HG3	1.89	0.53
1:A:364:GLN:NE2	1:A:887:HIS:HA	2.22	0.53
1:A:451:ILE:HD12	1:A:667:GLU:HG3	1.89	0.53
1:A:783:GLU:HB3	2:A:1343:HOH:O	2.07	0.53
1:B:261:THR:O	1:B:274:HIS:HA	2.08	0.53
1:B:530:LEU:O	1:B:530:LEU:HD23	2.09	0.53
1:D:369:ILE:HG12	1:D:374:PHE:HB2	1.89	0.53
1:D:458:ARG:NH1	2:D:1175:HOH:O	2.41	0.53
1:D:511:ALA:HB3	1:D:512:PRO:HD3	1.91	0.53
1:A:80:HIS:CD2	1:A:107:LEU:HD21	2.43	0.53
1:B:35:GLU:HA	1:B:74:ARG:HH21	1.73	0.53
1:B:276:THR:N	2:B:1059:HOH:O	2.36	0.53
1:B:465:GLU:O	1:B:467:ARG:N	2.36	0.53
1:B:477:LEU:HD21	1:B:499:LEU:HB3	1.89	0.53
1:D:462:MET:CA	1:D:468:LEU:HD12	2.35	0.53
1:A:338:MET:SD	1:A:341:ARG:HD2	2.48	0.53
1:A:364:GLN:NE2	1:A:890:ASP:HB2	2.23	0.53
1:B:443:GLY:C	1:B:658:LEU:HD13	2.28	0.53
1:B:800:PHE:HB2	1:B:810:TRP:CE2	2.43	0.53
1:C:208:ILE:HB	1:C:211:VAL:CG1	2.36	0.53
1:C:266:VAL:O	1:C:268:GLU:N	2.40	0.53
1:C:788:MET:SD	1:C:929:VAL:HG21	2.49	0.53
1:C:861:LEU:HA	2:C:1161:HOH:O	2.09	0.53
1:D:475:MET:O	1:D:479:LEU:HG	2.09	0.53
1:A:370:THR:HG23	1:A:373:ASN:HB2	1.90	0.53
1:B:47:LEU:HD12	2:B:1277:HOH:O	2.09	0.53
1:B:154:ILE:HD12	1:B:174:VAL:CG2	2.38	0.53
1:B:337:LEU:O	1:B:339:PRO:HD3	2.08	0.53
1:C:2:LEU:HD12	1:D:423:ARG:HH22	1.74	0.53
1:C:253:GLU:HB2	1:C:256:VAL:CG1	2.32	0.53
1:C:717:MET:SD	1:C:729:MET:HE2	2.48	0.53
1:D:627:LEU:O	1:D:631:LEU:HG	2.07	0.53
1:D:815:LEU:O	1:D:819:LEU:HB2	2.09	0.53
1:A:492:TRP:HA	1:A:495:LEU:CD2	2.39	0.53
1:B:131:TYR:CE2	1:B:135:ARG:HD3	2.44	0.53
1:C:917:LEU:HD21	2:C:1330:HOH:O	2.08	0.53
1:A:244:LYS:HD3	1:D:629:GLN:HE22	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:VAL:HG12	1:B:175:THR:N	2.23	0.53
1:B:249:GLY:CA	1:B:260:PRO:HD2	2.33	0.53
1:B:655:VAL:O	1:B:657:ALA:N	2.41	0.53
1:B:684:ARG:HG3	1:B:684:ARG:HH11	1.74	0.53
1:B:916:ARG:HD3	2:B:1200:HOH:O	2.09	0.53
1:C:92:HIS:HD2	1:C:116:ASN:HD21	1.56	0.53
1:C:449:GLY:O	1:C:666:THR:HB	2.09	0.53
1:D:198:ARG:HG3	1:D:202:PRO:HA	1.90	0.53
1:D:272:SER:HB2	1:D:313:LEU:HD23	1.90	0.53
1:D:338:MET:SD	1:D:341:ARG:HD2	2.49	0.53
1:D:627:LEU:HD23	2:D:1062:HOH:O	2.08	0.53
1:B:858:GLU:HG2	1:B:863:PRO:CG	2.30	0.53
1:C:422:TYR:O	1:C:696:SER:HA	2.09	0.53
1:C:740:ARG:HH11	1:C:740:ARG:HG3	1.74	0.53
1:D:315:HIS:HA	2:D:1261:HOH:O	2.08	0.53
1:A:354:LYS:HE2	1:D:634:ARG:NH1	2.24	0.53
1:A:546:HIS:O	1:A:547:GLN:HB2	2.08	0.53
1:B:250:LEU:HD23	1:B:259:GLU:OE1	2.09	0.53
1:B:857:ARG:HG3	1:B:861:LEU:HD21	1.90	0.53
1:C:8:LEU:O	1:C:8:LEU:HD13	2.08	0.53
1:C:276:THR:HA	2:C:1292:HOH:O	2.09	0.53
1:C:316:ARG:HG3	1:C:320:TYR:CE1	2.44	0.53
1:C:319:ASP:HA	2:C:1217:HOH:O	2.08	0.53
1:C:825:GLN:HE21	1:C:827:GLN:NE2	2.06	0.53
1:D:857:ARG:HH11	1:D:934:PHE:C	2.12	0.53
1:A:485:GLN:HG2	1:A:496:ARG:NH2	2.24	0.53
1:B:369:ILE:HG13	1:B:370:THR:N	2.24	0.53
1:C:391:GLU:HG2	2:C:1166:HOH:O	2.09	0.53
1:D:274:HIS:NE2	1:D:305:ILE:HG12	2.23	0.53
1:A:29:ARG:HD3	2:A:1255:HOH:O	2.09	0.52
1:A:94:GLY:HA2	1:A:382:ALA:HB2	1.90	0.52
1:A:201:HIS:HD2	2:A:1135:HOH:O	1.91	0.52
1:A:501:ARG:HB2	1:A:504:GLN:OE1	2.09	0.52
1:B:110:THR:CG2	1:B:140:MET:HG2	2.38	0.52
1:B:266:VAL:HG12	2:B:1008:HOH:O	2.09	0.52
1:B:338:MET:HG2	1:B:341:ARG:HD2	1.90	0.52
1:C:263:ASP:OD2	1:C:816:LYS:HG2	2.10	0.52
1:C:477:LEU:HD23	1:C:530:LEU:HD11	1.90	0.52
1:C:820:LEU:HA	1:C:935:ARG:HH22	1.73	0.52
1:D:211:VAL:CG2	1:D:385:THR:HG22	2.40	0.52
1:D:416:ASP:HB2	2:D:1251:HOH:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:ARG:HB3	1:B:716:ARG:CZ	2.39	0.52
1:A:491:GLU:CG	1:A:516:LEU:HD11	2.39	0.52
1:A:575:ASN:O	1:A:576:MET:HB2	2.09	0.52
1:A:640:ARG:HE	1:A:644:ILE:HG13	1.74	0.52
1:C:301:ALA:O	1:C:305:ILE:HG13	2.09	0.52
1:C:508:GLU:N	2:C:1206:HOH:O	2.42	0.52
1:C:878:VAL:HG22	1:C:925:ILE:HG21	1.91	0.52
1:D:96:ILE:CD1	1:D:211:VAL:HG11	2.39	0.52
1:D:342:ARG:HH22	1:D:349:GLN:HE22	1.55	0.52
1:D:801:LEU:CD1	1:D:842:ALA:HB1	2.36	0.52
1:A:109:ALA:O	1:A:113:VAL:HG23	2.09	0.52
1:A:904:LYS:HE3	1:A:908:GLN:NE2	2.24	0.52
1:B:535:HIS:O	1:B:539:VAL:HG23	2.09	0.52
1:C:45:ARG:HD2	2:C:1171:HOH:O	2.08	0.52
1:C:435:GLU:CD	1:C:692:ARG:HH11	2.12	0.52
1:C:606:GLU:HG2	1:C:610:GLU:OE2	2.09	0.52
1:C:759:LEU:O	1:C:763:ARG:HG3	2.10	0.52
1:D:211:VAL:HG23	1:D:385:THR:HG22	1.90	0.52
1:D:713:MET:HB3	1:D:729:MET:HE1	1.90	0.52
1:A:1:MET:H1	1:A:5:LEU:HD12	1.74	0.52
1:A:858:GLU:HG3	1:A:866:MET:CE	2.39	0.52
1:B:321:ILE:HG13	1:B:330:VAL:HG21	1.91	0.52
1:C:190:ILE:HD12	1:C:194:GLN:HE22	1.74	0.52
1:D:281:ALA:HA	1:D:284:GLU:CD	2.30	0.52
1:A:85:LEU:HA	1:A:111:LEU:HD13	1.90	0.52
1:A:274:HIS:CE1	1:A:305:ILE:HA	2.44	0.52
1:B:95:LYS:HE2	1:B:402:ASP:HB2	1.92	0.52
1:B:223:LEU:HD21	1:B:371:TYR:CZ	2.45	0.52
1:B:663:ILE:HG12	1:B:678:LEU:O	2.09	0.52
1:C:12:ASN:ND2	1:C:405:VAL:H	2.04	0.52
1:C:563:GLN:NE2	1:C:587:GLY:HA3	2.22	0.52
1:C:908:GLN:HA	2:C:1341:HOH:O	2.09	0.52
1:D:103:GLU:HG3	1:D:104:GLY:N	2.23	0.52
1:D:290:GLU:HG2	1:D:937:LYS:NZ	2.24	0.52
1:D:589:PRO:HA	1:D:592:LEU:HD12	1.91	0.52
1:D:805:VAL:HG11	1:D:809:ASP:OD1	2.09	0.52
1:A:34:VAL:HG13	1:A:67:LEU:HD23	1.92	0.52
1:A:96:ILE:HD12	1:A:395:PHE:CD1	2.44	0.52
1:A:323:GLN:HG3	1:A:328:ILE:HD11	1.91	0.52
1:B:263:ASP:HB2	1:B:273:VAL:O	2.09	0.52
1:B:903:GLN:HB2	2:B:1164:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:ILE:HD13	1:C:211:VAL:HG21	1.91	0.52
1:C:295:PRO:HD3	1:C:937:LYS:HB2	1.92	0.52
1:D:201:HIS:HB2	2:D:1136:HOH:O	2.09	0.52
1:D:261:THR:O	1:D:274:HIS:HA	2.10	0.52
1:D:540:LEU:HD23	1:D:544:ILE:CD1	2.40	0.52
1:D:800:PHE:CZ	1:D:814:GLY:HA2	2.44	0.52
1:D:826:LEU:HD22	2:D:1113:HOH:O	2.10	0.52
1:A:663:ILE:HG12	1:A:678:LEU:O	2.10	0.52
1:B:640:ARG:HE	1:B:644:ILE:HG13	1.74	0.52
1:B:796:LEU:O	1:B:799:ASN:HB2	2.10	0.52
1:C:98:GLU:HA	1:C:385:THR:O	2.10	0.52
1:C:249:GLY:CA	1:C:260:PRO:HD2	2.38	0.52
1:C:553:HIS:O	1:C:557:GLU:HG3	2.10	0.52
1:C:585:LEU:HD13	1:C:656:ARG:HG3	1.91	0.52
1:C:909:GLU:HG3	2:C:1309:HOH:O	2.08	0.52
1:D:273:VAL:O	1:D:273:VAL:HG12	2.10	0.52
1:D:287:LEU:HD22	2:D:1325:HOH:O	2.08	0.52
1:D:661:LEU:HD13	1:D:663:ILE:HD11	1.91	0.52
1:D:807:PRO:HB3	1:D:835:ARG:O	2.10	0.52
1:A:40:LEU:HD13	1:A:75:TYR:HE1	1.75	0.52
1:A:263:ASP:OD2	1:A:816:LYS:HG2	2.09	0.52
1:A:448:VAL:HG11	1:A:459:LEU:HD11	1.91	0.52
1:A:770:ARG:HH12	1:A:879:ASP:HB2	1.75	0.52
1:A:794:ALA:HA	1:A:843:VAL:HG13	1.91	0.52
1:C:20:TYR:HA	1:C:24:VAL:CG2	2.40	0.52
1:C:205:TYR:CE1	1:C:380:LYS:HE3	2.44	0.52
1:D:91:LEU:HD22	1:D:207:ILE:CD1	2.40	0.52
1:A:275:LEU:O	1:A:275:LEU:HD23	2.10	0.52
1:B:347:LEU:HD13	2:B:1290:HOH:O	2.09	0.52
1:B:669:HIS:ND1	1:B:675:ASP:HB3	2.25	0.52
1:B:929:VAL:O	1:B:933:LEU:HG	2.09	0.52
1:C:126:VAL:HA	1:C:174:VAL:O	2.09	0.52
1:C:692:ARG:HG3	2:C:1069:HOH:O	2.08	0.52
1:C:789:VAL:HG21	1:C:854:TYR:CE1	2.44	0.52
1:D:321:ILE:HG13	1:D:330:VAL:HG21	1.92	0.52
1:D:550:ASN:HA	1:D:574:THR:HB	1.92	0.52
1:A:320:TYR:CD1	1:A:327:VAL:HG13	2.45	0.52
1:A:897:PHE:C	1:A:897:PHE:CD2	2.84	0.52
1:B:18:ARG:HE	1:B:22:GLN:HE21	1.56	0.52
1:B:265:THR:HG22	1:B:271:ARG:C	2.30	0.52
1:B:538:ALA:HB2	2:B:1057:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:GLN:CA	1:C:155:GLN:HE21	2.21	0.52
1:C:557:GLU:HA	1:C:560:ILE:HD12	1.92	0.52
1:D:59:GLU:HG3	2:D:1023:HOH:O	2.10	0.52
1:D:263:ASP:HB2	1:D:273:VAL:HB	1.92	0.52
1:D:677:GLN:NE2	2:D:1010:HOH:O	2.42	0.52
1:D:684:ARG:HG3	1:D:684:ARG:HH11	1.75	0.52
1:D:750:LYS:O	1:D:754:GLN:HG3	2.10	0.52
1:A:326:GLN:HG2	1:A:357:VAL:CG1	2.41	0.51
1:C:20:TYR:CD2	1:C:24:VAL:HG21	2.45	0.51
1:C:187:ASN:HA	2:C:1097:HOH:O	2.10	0.51
1:D:75:TYR:CE1	1:D:146:GLY:HA3	2.45	0.51
1:D:201:HIS:N	2:D:1136:HOH:O	2.42	0.51
1:D:829:PHE:N	1:D:830:PRO:CD	2.72	0.51
1:A:85:LEU:HA	1:A:111:LEU:CD1	2.40	0.51
1:A:98:GLU:HA	1:A:385:THR:O	2.09	0.51
1:A:277:LEU:HD12	2:A:1257:HOH:O	2.10	0.51
1:A:711:ILE:HG23	2:A:1143:HOH:O	2.09	0.51
1:B:226:SER:N	2:B:1049:HOH:O	2.42	0.51
1:B:589:PRO:HG2	1:B:614:LYS:HZ2	1.70	0.51
1:B:801:LEU:O	1:B:803:PRO:HD3	2.10	0.51
1:B:810:TRP:HB2	2:B:1243:HOH:O	2.09	0.51
1:C:414:ARG:HA	1:C:689:GLY:O	2.09	0.51
1:C:477:LEU:HD21	1:C:499:LEU:HD22	1.91	0.51
1:C:550:ASN:HA	1:C:574:THR:OG1	2.09	0.51
1:C:773:ILE:CD1	1:C:874:ILE:HG21	2.41	0.51
1:C:816:LYS:NZ	2:C:1223:HOH:O	2.43	0.51
1:A:497:LYS:HG3	2:A:1111:HOH:O	2.10	0.51
1:B:190:ILE:HD12	1:B:190:ILE:N	2.26	0.51
1:B:372:GLN:HA	1:B:399:TYR:OH	2.11	0.51
1:B:805:VAL:HG12	2:B:1009:HOH:O	2.10	0.51
1:C:278:GLN:HG3	2:C:1004:HOH:O	2.10	0.51
1:A:753:LEU:O	1:A:757:ASP:HB2	2.11	0.51
1:A:757:ASP:O	1:A:761:ARG:HD2	2.10	0.51
1:A:809:ASP:HB3	1:A:810:TRP:CD1	2.46	0.51
1:A:864:PRO:O	1:A:867:ARG:HG2	2.10	0.51
1:B:12:ASN:HB3	2:B:1247:HOH:O	2.09	0.51
1:B:94:GLY:HA2	1:B:382:ALA:HB2	1.91	0.51
1:B:298:MET:HG3	2:B:1179:HOH:O	2.10	0.51
1:B:647:GLU:HG2	1:B:648:CYS:N	2.25	0.51
1:C:457:GLU:O	1:C:460:SER:HB3	2.10	0.51
1:D:154:ILE:HD12	1:D:174:VAL:HG21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:451:ILE:HA	1:D:575:ASN:OD1	2.09	0.51
1:D:503:ALA:N	2:D:1195:HOH:O	2.42	0.51
1:A:338:MET:HG2	1:A:341:ARG:HG3	1.92	0.51
1:A:481:LYS:HA	1:A:496:ARG:NH2	2.26	0.51
1:A:508:GLU:O	1:A:512:PRO:HD3	2.11	0.51
1:A:616:MET:HG2	1:A:641:ILE:HG22	1.92	0.51
1:C:164:ARG:HG3	1:C:196:VAL:HA	1.92	0.51
1:C:443:GLY:O	1:C:658:LEU:HD13	2.10	0.51
1:D:68:THR:HA	1:D:147:LEU:HD11	1.92	0.51
1:D:181:PHE:HE1	1:D:223:LEU:HD22	1.75	0.51
1:C:94:GLY:HA2	1:C:382:ALA:HB2	1.93	0.51
1:C:344:GLY:O	1:C:345:GLU:HG2	2.10	0.51
1:C:622:GLU:CD	1:C:622:GLU:H	2.13	0.51
1:C:823:ALA:HB3	1:C:824:PRO:HD3	1.92	0.51
1:D:250:LEU:H	1:D:259:GLU:CB	2.24	0.51
1:D:373:ASN:O	1:D:376:ARG:HB2	2.10	0.51
1:D:640:ARG:HE	1:D:644:ILE:HG13	1.75	0.51
1:A:266:VAL:HG23	1:A:269:LYS:HB2	1.92	0.51
1:A:296:GLU:HG3	2:A:1112:HOH:O	2.10	0.51
1:B:36:LYS:HE3	2:B:1074:HOH:O	2.09	0.51
1:B:457:GLU:O	1:B:460:SER:HB3	2.10	0.51
1:B:576:MET:HA	1:B:681:ARG:HH12	1.74	0.51
1:B:815:LEU:O	1:B:819:LEU:HB2	2.11	0.51
1:C:620:LYS:HD3	1:C:623:GLU:OE1	2.10	0.51
1:C:634:ARG:HH11	1:C:634:ARG:HG3	1.76	0.51
1:D:609:VAL:HG12	1:D:613:ILE:HD11	1.92	0.51
1:A:13:GLU:OE1	1:A:13:GLU:HA	2.11	0.51
1:A:40:LEU:HD11	1:A:74:ARG:HH11	1.75	0.51
1:B:423:ARG:N	2:B:1002:HOH:O	2.44	0.51
1:B:604:ARG:HB2	1:B:604:ARG:CZ	2.39	0.51
1:C:893:ARG:HB3	2:C:1016:HOH:O	2.09	0.51
1:D:176:ASN:HD22	1:D:176:ASN:N	2.06	0.51
1:D:293:PHE:CZ	1:D:304:LEU:HD22	2.43	0.51
1:D:893:ARG:HG2	1:D:910:TYR:CE1	2.45	0.51
1:A:13:GLU:CG	1:B:716:ARG:NH1	2.74	0.51
1:A:126:VAL:HA	1:A:174:VAL:O	2.10	0.51
1:A:167:TYR:O	1:A:198:ARG:HD3	2.11	0.51
1:A:273:VAL:HG11	1:A:816:LYS:NZ	2.26	0.51
1:A:297:ASN:HA	1:A:299:GLU:OE2	2.11	0.51
1:A:342:ARG:HB2	1:A:888:ASN:ND2	2.26	0.51
1:A:364:GLN:HG2	1:A:887:HIS:CB	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:642:ARG:O	1:A:646:GLU:HB2	2.10	0.51
1:A:679:ARG:NH2	1:B:732:ARG:NH2	2.58	0.51
1:A:845:ARG:HG3	2:A:1226:HOH:O	2.11	0.51
1:B:865:LEU:O	1:B:869:VAL:HG23	2.10	0.51
1:C:369:ILE:HG13	1:C:370:THR:N	2.26	0.51
1:C:798:GLU:HB2	1:C:843:VAL:HG22	1.93	0.51
1:B:227:GLY:HA3	1:B:366:LEU:HD21	1.93	0.51
1:B:599:LYS:HE3	1:B:637:LEU:HD21	1.92	0.51
1:C:655:VAL:C	1:C:657:ALA:N	2.65	0.51
1:C:872:PHE:O	1:C:876:ASN:HB2	2.10	0.51
1:D:185:ARG:HA	2:D:1232:HOH:O	2.10	0.51
1:D:299:GLU:H	1:D:299:GLU:CD	2.14	0.51
1:D:737:ALA:O	1:D:741:VAL:HG23	2.11	0.51
1:A:102:GLY:O	1:A:105:LYS:NZ	2.44	0.50
1:A:364:GLN:HE21	1:A:887:HIS:HA	1.76	0.50
1:A:861:LEU:HB2	1:A:865:LEU:HB3	1.92	0.50
1:B:212:ASP:O	1:B:216:ILE:HB	2.12	0.50
1:B:325:GLY:HA3	2:B:1183:HOH:O	2.11	0.50
1:B:772:LEU:HD12	2:B:1113:HOH:O	2.10	0.50
1:C:155:GLN:HE21	1:C:155:GLN:HA	1.75	0.50
1:C:268:GLU:HA	2:C:1291:HOH:O	2.11	0.50
1:C:932:PHE:O	1:C:936:LEU:HB2	2.11	0.50
1:D:11:ASN:O	1:D:15:GLU:HB2	2.11	0.50
1:D:809:ASP:HB3	1:D:810:TRP:CD1	2.46	0.50
1:D:893:ARG:HD2	2:D:1264:HOH:O	2.10	0.50
1:A:244:LYS:HG3	1:A:311:LYS:NZ	2.26	0.50
1:A:485:GLN:HA	1:A:485:GLN:OE1	2.11	0.50
1:B:342:ARG:HG2	2:B:1297:HOH:O	2.11	0.50
1:B:530:LEU:O	1:B:534:VAL:HG23	2.12	0.50
1:C:13:GLU:CG	1:D:716:ARG:NH1	2.74	0.50
1:C:121:LYS:C	1:C:198:ARG:HH21	2.13	0.50
1:C:179:LEU:HD11	1:C:378:TYR:OH	2.11	0.50
1:C:187:ASN:ND2	1:C:767:TYR:HB3	2.26	0.50
1:C:508:GLU:O	1:C:512:PRO:HD3	2.10	0.50
1:C:759:LEU:HD23	1:C:893:ARG:HH21	1.76	0.50
1:C:797:ALA:O	1:C:801:LEU:HB2	2.11	0.50
1:D:20:TYR:HA	1:D:24:VAL:CG2	2.41	0.50
1:A:492:TRP:O	1:A:495:LEU:HD23	2.11	0.50
1:C:343:TYR:HB2	1:C:348:HIS:CA	2.42	0.50
1:D:675:ASP:HB2	1:D:693:PHE:CZ	2.47	0.50
1:D:808:GLU:HA	2:D:1018:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:875:LEU:HD21	2:D:1071:HOH:O	2.09	0.50
1:A:541:ARG:C	1:A:543:GLY:N	2.64	0.50
1:A:667:GLU:OE2	1:A:700:ASP:HB2	2.11	0.50
1:A:833:GLU:HG3	2:A:1226:HOH:O	2.11	0.50
1:B:447:LEU:HD12	1:B:571:THR:O	2.12	0.50
1:B:800:PHE:CZ	1:B:813:GLU:HB2	2.47	0.50
1:C:275:LEU:HD13	2:C:1223:HOH:O	2.10	0.50
1:C:338:MET:SD	1:C:341:ARG:HB2	2.52	0.50
1:D:234:ASP:O	1:D:238:LYS:HG3	2.12	0.50
1:D:252:ALA:O	1:D:812:LEU:HD21	2.12	0.50
1:A:265:THR:HA	2:A:1265:HOH:O	2.10	0.50
1:A:343:TYR:HB2	1:A:348:HIS:CA	2.41	0.50
1:A:358:ARG:HB2	2:A:1199:HOH:O	2.12	0.50
1:A:663:ILE:HD13	1:A:682:ALA:CB	2.35	0.50
1:A:797:ALA:O	1:A:801:LEU:HB2	2.11	0.50
1:B:184:LEU:HD11	1:B:369:ILE:HG22	1.94	0.50
1:C:231:LYS:HE2	1:C:231:LYS:CA	2.42	0.50
1:C:316:ARG:NH2	1:C:354:LYS:HG3	2.27	0.50
1:C:796:LEU:HD22	1:C:818:THR:OG1	2.11	0.50
1:D:285:LYS:HE3	2:D:1282:HOH:O	2.11	0.50
1:D:617:VAL:HA	1:D:645:ARG:CD	2.41	0.50
1:A:45:ARG:HG2	2:A:1120:HOH:O	2.11	0.50
1:A:343:TYR:CE1	1:A:351:ILE:HD12	2.46	0.50
1:A:553:HIS:CG	1:A:556:ARG:HB2	2.47	0.50
1:A:702:MET:O	1:A:706:ALA:HB3	2.11	0.50
1:A:820:LEU:HA	1:A:935:ARG:HH22	1.76	0.50
1:B:20:TYR:CD2	1:B:24:VAL:HG21	2.46	0.50
1:B:275:LEU:CD1	1:B:820:LEU:HD12	2.41	0.50
1:B:305:ILE:O	1:B:309:ARG:HG3	2.12	0.50
1:B:444:GLN:HE21	1:B:660:GLY:H	1.60	0.50
1:B:593:ALA:O	1:B:597:LEU:HG	2.12	0.50
1:B:655:VAL:O	1:B:658:LEU:N	2.35	0.50
1:B:775:LEU:HA	2:B:1182:HOH:O	2.11	0.50
1:C:266:VAL:O	1:C:269:LYS:N	2.42	0.50
1:C:569:THR:HG21	2:C:1053:HOH:O	2.10	0.50
1:D:258:LYS:HD2	1:D:816:LYS:HE2	1.92	0.50
1:D:266:VAL:HG22	1:D:813:GLU:HB3	1.94	0.50
1:D:397:GLU:HA	1:D:397:GLU:OE2	2.12	0.50
1:D:602:PHE:CD1	1:D:603:ASP:N	2.80	0.50
1:A:464:LYS:HE2	2:A:1073:HOH:O	2.12	0.50
1:A:565:GLY:HA3	1:A:584:LYS:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:837:LEU:HD12	1:A:837:LEU:O	2.11	0.50
1:B:477:LEU:HD11	1:B:499:LEU:HD22	1.93	0.50
1:B:518:PRO:O	1:B:524:ARG:HD3	2.12	0.50
1:C:3:GLY:O	1:C:7:ARG:HG3	2.11	0.50
1:C:669:HIS:O	1:C:738:GLN:NE2	2.42	0.50
1:C:782:LYS:NZ	1:C:866:MET:SD	2.85	0.50
1:C:788:MET:CE	1:C:929:VAL:HG11	2.42	0.50
1:D:666:THR:HB	2:D:1107:HOH:O	2.12	0.50
1:A:295:PRO:HB3	1:A:937:LYS:O	2.12	0.50
1:A:316:ARG:HD3	1:A:355:GLU:CD	2.32	0.50
1:B:293:PHE:HZ	1:B:304:LEU:HD22	1.77	0.50
1:B:553:HIS:NE2	1:B:556:ARG:HD3	2.27	0.50
1:B:813:GLU:CG	2:B:1243:HOH:O	2.58	0.50
1:B:829:PHE:N	1:B:830:PRO:CD	2.74	0.50
1:C:85:LEU:HA	1:C:111:LEU:HD13	1.93	0.50
1:C:102:GLY:CA	1:C:105:LYS:HZ1	2.25	0.50
1:C:239:MET:HG3	1:C:307:ALA:HB2	1.94	0.50
1:C:769:GLN:HB2	2:C:1253:HOH:O	2.12	0.50
1:D:239:MET:HE2	1:D:303:MET:CB	2.42	0.50
1:D:640:ARG:HD2	2:D:1223:HOH:O	2.11	0.50
1:D:830:PRO:HD3	2:D:1151:HOH:O	2.11	0.50
1:A:10:ASP:OD2	1:B:716:ARG:NH2	2.45	0.50
1:A:52:GLU:HG3	2:A:1006:HOH:O	2.11	0.50
1:A:208:ILE:HB	1:A:211:VAL:CG1	2.41	0.50
1:A:897:PHE:C	1:A:897:PHE:HD2	2.14	0.50
1:B:485:GLN:HG2	1:B:496:ARG:HE	1.76	0.50
1:B:935:ARG:HB2	2:B:1103:HOH:O	2.12	0.50
1:C:109:ALA:O	1:C:113:VAL:HG23	2.12	0.50
1:A:265:THR:HG22	1:A:271:ARG:C	2.31	0.49
1:A:584:LYS:NZ	2:A:1128:HOH:O	2.42	0.49
1:B:213:SER:O	1:B:218:GLU:HB2	2.12	0.49
1:B:266:VAL:O	1:B:269:LYS:N	2.43	0.49
1:B:565:GLY:O	1:B:585:LEU:HA	2.12	0.49
1:B:655:VAL:C	1:B:657:ALA:N	2.65	0.49
1:B:675:ASP:HB2	1:B:693:PHE:CZ	2.47	0.49
1:C:784:ALA:HA	2:C:1277:HOH:O	2.11	0.49
1:C:810:TRP:CD1	1:C:810:TRP:N	2.80	0.49
1:C:908:GLN:HG3	2:C:1341:HOH:O	2.11	0.49
1:D:141:GLY:N	1:D:142:PRO:HD2	2.27	0.49
1:D:921:MET:O	1:D:925:ILE:HG13	2.11	0.49
1:A:76:LEU:HD22	1:A:143:VAL:HG23	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:GLU:HG2	1:A:469:TYR:OH	2.12	0.49
1:A:442:ARG:NH1	1:A:658:LEU:HD23	2.27	0.49
1:A:717:MET:SD	1:A:729:MET:HE2	2.52	0.49
1:A:811:ASP:HB3	2:A:1187:HOH:O	2.11	0.49
1:B:69:ARG:NH1	2:B:1302:HOH:O	2.44	0.49
1:B:813:GLU:HG3	2:B:1243:HOH:O	2.10	0.49
1:C:273:VAL:CG1	1:C:820:LEU:HB2	2.32	0.49
1:C:897:PHE:C	1:C:897:PHE:CD2	2.86	0.49
1:D:801:LEU:HD22	1:D:842:ALA:HB1	1.94	0.49
1:A:134:ARG:HD2	2:A:1338:HOH:O	2.12	0.49
1:A:321:ILE:HB	1:A:337:LEU:HD21	1.93	0.49
1:C:316:ARG:NH1	2:C:1281:HOH:O	2.45	0.49
1:C:326:GLN:HG2	1:C:357:VAL:CG1	2.42	0.49
1:C:716:ARG:HG3	1:D:6:ARG:CD	2.41	0.49
1:C:770:ARG:NH1	1:C:879:ASP:HB2	2.28	0.49
1:A:145:ARG:HG2	2:A:1273:HOH:O	2.11	0.49
1:A:182:ASP:OD1	1:A:185:ARG:NH1	2.45	0.49
1:C:338:MET:HG2	1:C:341:ARG:HD2	1.94	0.49
1:D:176:ASN:HD22	1:D:177:SER:N	2.09	0.49
1:D:211:VAL:HG23	1:D:385:THR:CG2	2.42	0.49
1:A:213:SER:O	1:A:218:GLU:HB2	2.13	0.49
1:A:242:ILE:HD12	1:A:286:LEU:CD1	2.42	0.49
1:A:354:LYS:HE3	1:A:354:LYS:CA	2.31	0.49
1:B:134:ARG:CD	2:B:1094:HOH:O	2.61	0.49
1:B:248:ARG:NH1	1:B:312:GLU:HG3	2.27	0.49
1:B:250:LEU:H	1:B:259:GLU:CB	2.25	0.49
1:B:274:HIS:HE1	1:B:305:ILE:HG23	1.78	0.49
1:B:588:ASN:OD1	1:B:648:CYS:SG	2.71	0.49
1:C:134:ARG:HB2	1:C:155:GLN:OE1	2.12	0.49
1:C:135:ARG:NH2	1:C:136:ASP:OD1	2.45	0.49
1:C:431:ALA:O	1:C:434:GLU:HB2	2.12	0.49
1:C:467:ARG:HB2	2:C:1289:HOH:O	2.13	0.49
1:C:663:ILE:CG2	1:C:678:LEU:HD22	2.42	0.49
1:C:673:ARG:HD3	2:C:1166:HOH:O	2.13	0.49
1:D:12:ASN:HB3	2:D:1202:HOH:O	2.11	0.49
1:D:174:VAL:HA	2:D:1118:HOH:O	2.13	0.49
1:D:518:PRO:O	1:D:524:ARG:HD3	2.12	0.49
1:D:857:ARG:HH22	1:D:936:LEU:CA	2.25	0.49
1:A:102:GLY:CA	1:A:105:LYS:HZ1	2.25	0.49
1:A:553:HIS:CE1	1:A:556:ARG:HD3	2.48	0.49
1:A:710:VAL:HG11	1:A:733:SER:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:776:GLY:CA	1:A:871:ARG:NH2	2.75	0.49
1:A:895:GLY:N	2:A:1355:HOH:O	2.44	0.49
1:A:897:PHE:HD2	1:A:898:LEU:N	2.10	0.49
1:B:12:ASN:O	1:B:13:GLU:HG2	2.12	0.49
1:B:126:VAL:HG21	1:B:176:ASN:HB3	1.94	0.49
1:B:227:GLY:CA	1:B:366:LEU:HD11	2.43	0.49
1:B:806:HIS:HB2	1:B:807:PRO:HD3	1.93	0.49
1:C:261:THR:O	1:C:274:HIS:HA	2.12	0.49
1:C:338:MET:HG2	1:C:341:ARG:HG3	1.94	0.49
1:C:355:GLU:OE1	1:C:355:GLU:HA	2.13	0.49
1:C:381:ARG:NH1	2:C:1255:HOH:O	2.44	0.49
1:C:495:LEU:HD22	1:C:513:PHE:CD2	2.48	0.49
1:D:179:LEU:HD23	1:D:179:LEU:O	2.12	0.49
1:D:449:GLY:HA3	1:D:678:LEU:HD11	1.94	0.49
1:D:540:LEU:HD23	1:D:544:ILE:HD11	1.94	0.49
1:D:727:HIS:CD2	1:D:729:MET:H	2.28	0.49
1:A:266:VAL:O	1:A:269:LYS:N	2.41	0.49
1:A:424:THR:HG23	1:A:427:GLY:N	2.25	0.49
1:A:465:GLU:C	1:A:467:ARG:N	2.66	0.49
1:B:232:ALA:HB1	1:B:361:ARG:HH12	1.77	0.49
1:B:585:LEU:HD22	1:B:655:VAL:CG1	2.43	0.49
1:B:872:PHE:O	1:B:876:ASN:HB2	2.12	0.49
1:C:705:PHE:CB	1:C:741:VAL:HG22	2.43	0.49
1:C:827:GLN:HB2	2:C:1149:HOH:O	2.11	0.49
1:D:226:SER:HB2	1:D:363:ASN:HB2	1.93	0.49
1:D:485:GLN:HG2	1:D:496:ARG:NE	2.28	0.49
1:D:822:THR:HG22	1:D:824:PRO:HD2	1.95	0.49
1:A:39:ASP:OD2	1:A:41:ALA:HB3	2.12	0.49
1:A:216:ILE:HG21	1:A:673:ARG:NH2	2.27	0.49
1:A:364:GLN:HG2	1:A:887:HIS:CG	2.48	0.49
1:B:7:ARG:HA	1:B:13:GLU:CG	2.43	0.49
1:B:390:THR:HG22	1:B:391:GLU:OE2	2.13	0.49
1:C:253:GLU:HB3	1:C:254:PRO:HD2	1.93	0.49
1:C:563:GLN:HG3	1:C:591:TYR:HE1	1.75	0.49
1:C:653:GLU:HB2	2:C:1116:HOH:O	2.13	0.49
1:C:670:GLU:CG	1:C:741:VAL:HG11	2.41	0.49
1:C:822:THR:CG2	1:C:824:PRO:HD2	2.42	0.49
1:D:94:GLY:HA2	1:D:382:ALA:HB2	1.94	0.49
1:D:128:VAL:HG11	1:D:579:ARG:CZ	2.43	0.49
1:A:550:ASN:HA	1:A:574:THR:HB	1.95	0.49
1:B:261:THR:N	2:B:1169:HOH:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:679:ARG:HD3	1:B:691:SER:OG	2.12	0.49
1:B:776:GLY:HA2	1:B:871:ARG:HH22	1.78	0.49
1:B:777:LYS:O	1:B:781:VAL:HG23	2.13	0.49
1:C:422:TYR:HB3	2:C:1013:HOH:O	2.12	0.49
1:C:428:LYS:O	1:C:432:VAL:HG23	2.12	0.49
1:C:936:LEU:HD23	1:C:937:LYS:N	2.27	0.49
1:D:642:ARG:HB3	2:D:1341:HOH:O	2.12	0.49
1:D:777:LYS:O	1:D:781:VAL:HG23	2.12	0.49
1:A:259:GLU:HG2	1:A:260:PRO:HD3	1.95	0.49
1:B:83:VAL:HA	1:B:86:ILE:CD1	2.42	0.49
1:B:854:TYR:CZ	1:B:866:MET:HE1	2.48	0.49
1:C:530:LEU:O	1:C:534:VAL:HG23	2.13	0.49
1:C:663:ILE:HG12	1:C:678:LEU:O	2.12	0.49
1:D:7:ARG:HG2	1:D:13:GLU:CD	2.34	0.49
1:D:227:GLY:CA	1:D:366:LEU:HD11	2.42	0.49
1:D:444:GLN:HE22	1:D:659:GLY:HA3	1.76	0.49
1:D:762:GLN:HG3	1:D:918:PHE:CD1	2.48	0.49
1:A:17:ALA:HB3	2:A:1285:HOH:O	2.12	0.48
1:A:174:VAL:HG12	1:A:175:THR:N	2.28	0.48
1:A:294:SER:OG	1:A:936:LEU:HA	2.13	0.48
1:A:345:GLU:N	2:A:1009:HOH:O	2.41	0.48
1:C:47:LEU:HG	1:C:60:LEU:HD13	1.95	0.48
1:C:104:GLY:HA3	2:C:1266:HOH:O	2.13	0.48
1:C:553:HIS:NE2	1:C:556:ARG:HD3	2.28	0.48
1:C:805:VAL:HG12	1:C:808:GLU:OE1	2.12	0.48
1:C:833:GLU:O	1:C:837:LEU:HG	2.13	0.48
1:D:284:GLU:OE1	1:D:290:GLU:HB2	2.13	0.48
1:D:485:GLN:HG2	1:D:496:ARG:CZ	2.43	0.48
1:D:802:ASN:CA	1:D:839:ALA:HB1	2.43	0.48
1:A:261:THR:O	1:A:274:HIS:HA	2.13	0.48
1:A:330:VAL:HG22	1:A:337:LEU:HD23	1.95	0.48
1:A:832:ALA:O	1:A:836:ALA:HB3	2.13	0.48
1:B:190:ILE:HB	1:B:194:GLN:NE2	2.21	0.48
1:B:276:THR:N	2:B:1010:HOH:O	2.42	0.48
1:B:461:GLN:HA	1:B:464:LYS:HG2	1.94	0.48
1:C:491:GLU:CG	1:C:516:LEU:HD11	2.43	0.48
1:C:727:HIS:CE1	2:D:1251:HOH:O	2.65	0.48
1:C:801:LEU:HD11	1:C:834:LEU:HD13	1.94	0.48
1:C:840:GLU:OE2	1:C:841:GLU:HB2	2.13	0.48
1:D:20:TYR:CD2	1:D:24:VAL:HG21	2.48	0.48
1:D:174:VAL:HG12	1:D:175:THR:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:485:GLN:HG2	1:D:496:ARG:HE	1.77	0.48
1:D:563:GLN:NE2	1:D:587:GLY:HA3	2.27	0.48
1:A:40:LEU:HD11	1:A:74:ARG:NH1	2.28	0.48
1:A:295:PRO:O	1:A:296:GLU:HB2	2.12	0.48
1:A:371:TYR:HD2	1:A:375:PHE:CE1	2.31	0.48
1:B:85:LEU:HD23	1:B:111:LEU:HD11	1.96	0.48
1:B:338:MET:CG	1:B:341:ARG:HD2	2.43	0.48
1:B:338:MET:SD	1:B:341:ARG:HB3	2.53	0.48
1:C:40:LEU:HD13	1:C:75:TYR:HE1	1.79	0.48
1:D:275:LEU:HD11	1:D:819:LEU:O	2.13	0.48
1:D:341:ARG:HD3	1:D:913:GLU:CG	2.43	0.48
1:D:792:THR:O	1:D:796:LEU:HB2	2.13	0.48
1:A:92:HIS:CD2	1:A:116:ASN:HD21	2.31	0.48
1:A:132:LEU:HD23	1:A:135:ARG:HE	1.78	0.48
1:A:345:GLU:HB2	1:A:924:PHE:CE2	2.48	0.48
1:A:499:LEU:HD23	1:A:505:LEU:HD11	1.95	0.48
1:A:759:LEU:HD23	1:A:893:ARG:HH21	1.78	0.48
1:A:840:GLU:OE2	1:A:841:GLU:HB2	2.13	0.48
1:B:260:PRO:HB2	2:B:1169:HOH:O	2.13	0.48
1:C:484:SER:HB3	1:C:496:ARG:HH12	1.78	0.48
1:C:860:GLU:HB2	1:C:861:LEU:HD23	1.95	0.48
1:D:23:VAL:HG13	1:D:61:LEU:HD21	1.95	0.48
1:D:241:GLU:HG3	1:D:242:ILE:N	2.27	0.48
1:D:275:LEU:HG	1:D:820:LEU:HD12	1.96	0.48
1:D:364:GLN:HG2	1:D:887:HIS:ND1	2.27	0.48
1:D:857:ARG:HH22	1:D:936:LEU:C	2.17	0.48
1:A:297:ASN:HD22	1:A:300:LEU:CD2	2.27	0.48
1:B:428:LYS:NZ	1:B:699:ASP:HB3	2.27	0.48
1:B:565:GLY:HA3	1:B:584:LYS:O	2.13	0.48
1:C:179:LEU:HD23	1:C:374:PHE:CE2	2.48	0.48
1:D:273:VAL:HA	1:D:820:LEU:HD22	1.94	0.48
1:D:282:LYS:HG2	2:D:1282:HOH:O	2.14	0.48
1:D:390:THR:HG22	1:D:391:GLU:OE2	2.13	0.48
1:D:703:ARG:HA	1:D:711:ILE:HD13	1.94	0.48
1:A:663:ILE:HG23	1:A:678:LEU:HD22	1.95	0.48
1:B:314:TYR:CE1	1:B:347:LEU:HD21	2.48	0.48
1:B:385:THR:CG2	1:B:388:ALA:HB2	2.43	0.48
1:B:389:LYS:HE2	2:B:1245:HOH:O	2.14	0.48
1:B:459:LEU:HD13	1:B:572:ILE:HD13	1.94	0.48
1:C:269:LYS:CD	1:C:270:ASN:H	2.15	0.48
1:C:467:ARG:CB	2:C:1289:HOH:O	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:631:LEU:CD1	1:C:633:ILE:HD11	2.43	0.48
1:D:266:VAL:O	1:D:269:LYS:N	2.40	0.48
1:A:347:LEU:HB2	2:A:1108:HOH:O	2.13	0.48
1:A:622:GLU:HA	1:A:625:ARG:CZ	2.43	0.48
1:A:716:ARG:HG3	1:B:6:ARG:HG3	1.93	0.48
1:A:820:LEU:HD12	1:A:935:ARG:HH22	1.78	0.48
1:B:98:GLU:HA	1:B:385:THR:O	2.12	0.48
1:B:233:THR:HG23	1:B:237:TYR:CE1	2.48	0.48
1:C:448:VAL:HG11	1:C:459:LEU:HD11	1.96	0.48
1:C:594:ALA:CA	1:C:597:LEU:HG	2.44	0.48
1:C:614:LYS:HA	1:C:614:LYS:HE3	1.94	0.48
1:C:830:PRO:HB3	1:C:834:LEU:HD12	1.94	0.48
1:D:461:GLN:HA	1:D:464:LYS:HG2	1.96	0.48
1:D:862:SER:HB3	1:D:864:PRO:HD2	1.95	0.48
1:A:106:THR:HG23	1:A:136:ASP:OD2	2.13	0.48
1:A:226:SER:HA	1:A:364:GLN:O	2.13	0.48
1:A:244:LYS:HZ2	1:D:634:ARG:HE	1.61	0.48
1:A:271:ARG:NH2	1:A:931:LYS:NZ	2.61	0.48
1:A:434:GLU:OE2	1:A:472:ARG:NH1	2.47	0.48
1:A:759:LEU:O	1:A:763:ARG:HG3	2.14	0.48
1:C:396:GLN:O	1:C:400:GLY:HA2	2.14	0.48
1:D:227:GLY:HA3	1:D:366:LEU:HD21	1.95	0.48
1:D:273:VAL:CB	1:D:820:LEU:HB2	2.42	0.48
1:D:276:THR:HG23	2:D:1332:HOH:O	2.13	0.48
1:D:872:PHE:O	1:D:876:ASN:HB2	2.13	0.48
1:A:373:ASN:CB	1:A:763:ARG:HH22	2.27	0.48
1:A:882:TRP:CZ2	1:A:886:LEU:HD21	2.49	0.48
1:B:141:GLY:N	1:B:142:PRO:HD2	2.28	0.48
1:B:588:ASN:CB	1:B:589:PRO:HD3	2.44	0.48
1:C:259:GLU:CG	1:C:260:PRO:HD3	2.44	0.48
1:C:771:ARG:NH2	2:C:1089:HOH:O	2.40	0.48
1:C:861:LEU:HD22	1:C:938:VAL:HB	1.96	0.48
1:D:364:GLN:CG	1:D:887:HIS:HA	2.43	0.48
1:D:423:ARG:HG2	1:D:697:PHE:CD2	2.49	0.48
1:D:726:GLU:HA	2:D:1159:HOH:O	2.13	0.48
1:D:770:ARG:HH22	1:D:879:ASP:HB2	1.78	0.48
1:D:827:GLN:C	1:D:830:PRO:HD2	2.34	0.48
1:A:223:LEU:O	1:A:368:THR:HG23	2.14	0.48
1:A:339:PRO:HD2	1:A:341:ARG:NH1	2.25	0.48
1:A:707:SER:HB3	1:A:710:VAL:HG23	1.96	0.48
1:A:908:GLN:O	1:A:912:ILE:HG13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:GLY:HA3	2:B:1125:HOH:O	2.14	0.48
1:B:332:GLU:HG3	2:B:1108:HOH:O	2.14	0.48
1:B:550:ASN:HA	1:B:574:THR:CB	2.44	0.48
1:C:629:GLN:OE1	1:C:629:GLN:HA	2.14	0.48
1:C:811:ASP:OD1	1:C:812:LEU:N	2.47	0.48
1:C:837:LEU:HD13	1:C:841:GLU:HB3	1.96	0.48
1:D:184:LEU:O	1:D:188:MET:HG3	2.14	0.48
1:D:305:ILE:O	1:D:309:ARG:HG3	2.14	0.48
1:D:444:GLN:NE2	1:D:660:GLY:H	2.08	0.48
1:D:465:GLU:C	1:D:467:ARG:H	2.16	0.48
1:D:727:HIS:HB3	1:D:730:VAL:HG23	1.94	0.48
1:D:831:PHE:O	1:D:835:ARG:HB3	2.14	0.48
1:D:926:LYS:HD3	2:D:1235:HOH:O	2.14	0.48
1:A:142:PRO:HD3	1:A:606:GLU:OE1	2.14	0.47
1:A:309:ARG:HA	1:A:313:LEU:HD23	1.96	0.47
1:A:393:LYS:HE3	2:A:1102:HOH:O	2.13	0.47
1:A:806:HIS:CB	1:A:807:PRO:CD	2.91	0.47
1:A:833:GLU:O	1:A:837:LEU:HG	2.14	0.47
1:B:94:GLY:HA3	2:B:1124:HOH:O	2.14	0.47
1:D:465:GLU:N	1:D:466:PRO:HD2	2.29	0.47
1:D:597:LEU:HD22	2:D:1324:HOH:O	2.12	0.47
1:D:707:SER:O	1:D:711:ILE:HG13	2.14	0.47
1:A:75:TYR:HB3	1:A:607:TRP:HE1	1.79	0.47
1:A:218:GLU:HB3	2:A:1097:HOH:O	2.14	0.47
1:A:414:ARG:HA	1:A:689:GLY:O	2.14	0.47
1:A:894:GLN:C	2:A:1355:HOH:O	2.52	0.47
1:A:921:MET:O	1:A:925:ILE:HG13	2.14	0.47
1:C:301:ALA:HB3	1:C:932:PHE:HZ	1.79	0.47
1:C:379:GLU:N	2:C:1245:HOH:O	2.46	0.47
1:C:414:ARG:HD3	1:C:682:ALA:O	2.14	0.47
1:C:479:LEU:HA	1:C:482:LYS:HE3	1.95	0.47
1:C:706:ALA:O	1:C:711:ILE:HD11	2.14	0.47
1:D:285:LYS:HA	2:D:1155:HOH:O	2.14	0.47
1:D:430:TYR:O	1:D:434:GLU:HG3	2.14	0.47
1:D:727:HIS:HD2	1:D:729:MET:N	2.11	0.47
1:A:273:VAL:HA	1:A:820:LEU:HD22	1.96	0.47
1:A:837:LEU:CD1	1:A:841:GLU:HB3	2.44	0.47
1:B:176:ASN:HD22	1:B:176:ASN:N	2.11	0.47
1:B:305:ILE:HG22	1:B:309:ARG:HE	1.80	0.47
1:B:582:ASP:HB2	1:B:684:ARG:HH21	1.73	0.47
1:C:11:ASN:HB3	2:C:1209:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:ASN:HD21	1:C:771:ARG:HE	1.63	0.47
1:C:677:GLN:HB3	2:C:1269:HOH:O	2.14	0.47
1:C:741:VAL:HG12	1:C:745:ASN:ND2	2.30	0.47
1:D:101:THR:HG23	2:D:1308:HOH:O	2.14	0.47
1:D:141:GLY:O	1:D:145:ARG:HG3	2.14	0.47
1:D:176:ASN:ND2	1:D:177:SER:N	2.61	0.47
1:D:247:GLU:HB2	2:D:1039:HOH:O	2.14	0.47
1:D:281:ALA:O	1:D:285:LYS:HG3	2.14	0.47
1:D:770:ARG:HH22	1:D:879:ASP:CB	2.27	0.47
1:D:782:LYS:HB3	2:D:1031:HOH:O	2.13	0.47
1:A:428:LYS:O	1:A:432:VAL:HG23	2.15	0.47
1:A:878:VAL:HA	1:A:925:ILE:HD13	1.97	0.47
1:B:258:LYS:HD3	1:B:258:LYS:N	2.15	0.47
1:B:511:ALA:HB3	1:B:512:PRO:HD3	1.97	0.47
1:B:543:GLY:HA2	2:B:1013:HOH:O	2.13	0.47
1:B:568:LYS:HD3	2:B:1185:HOH:O	2.14	0.47
1:D:98:GLU:HA	1:D:385:THR:O	2.15	0.47
1:D:299:GLU:O	1:D:302:HIS:HB3	2.14	0.47
1:D:498:LEU:HA	2:D:1092:HOH:O	2.15	0.47
1:D:896:ILE:O	1:D:896:ILE:HG22	2.14	0.47
1:A:524:ARG:NH1	1:A:527:TRP:CD1	2.83	0.47
1:B:10:ASP:HA	2:B:1093:HOH:O	2.14	0.47
1:B:47:LEU:HA	2:B:1277:HOH:O	2.14	0.47
1:B:430:TYR:CG	1:B:472:ARG:HG2	2.48	0.47
1:C:179:LEU:HD23	1:C:374:PHE:HE2	1.80	0.47
1:C:226:SER:HB2	1:C:363:ASN:ND2	2.29	0.47
1:C:281:ALA:HA	1:C:284:GLU:CD	2.35	0.47
1:C:424:THR:CG2	1:C:427:GLY:H	2.20	0.47
1:C:663:ILE:HG23	1:C:678:LEU:HD22	1.94	0.47
1:C:842:ALA:O	1:C:846:LEU:HG	2.14	0.47
1:D:301:ALA:HB3	1:D:932:PHE:CZ	2.40	0.47
1:D:647:GLU:HG2	1:D:648:CYS:N	2.30	0.47
1:D:800:PHE:N	1:D:800:PHE:CD2	2.82	0.47
1:A:211:VAL:HG23	1:A:212:ASP:H	1.78	0.47
1:A:354:LYS:HZ3	1:D:634:ARG:HH22	1.60	0.47
1:B:208:ILE:HB	1:B:211:VAL:CG1	2.44	0.47
1:B:525:THR:HA	2:B:1249:HOH:O	2.14	0.47
1:C:800:PHE:CZ	1:C:813:GLU:HB2	2.50	0.47
1:C:825:GLN:NE2	1:C:827:GLN:NE2	2.63	0.47
1:A:273:VAL:HG22	1:A:820:LEU:HD22	1.96	0.47
1:A:277:LEU:HB2	2:A:1257:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:ASN:HB3	2:B:1163:HOH:O	2.14	0.47
1:B:412:VAL:HG12	2:B:1131:HOH:O	2.15	0.47
1:B:465:GLU:N	1:B:466:PRO:HD2	2.29	0.47
1:B:550:ASN:HA	1:B:574:THR:HB	1.97	0.47
1:B:705:PHE:CD2	1:B:741:VAL:HG13	2.49	0.47
1:B:770:ARG:HH12	1:B:879:ASP:HB2	1.78	0.47
1:C:61:LEU:HD13	1:C:115:LEU:CD2	2.45	0.47
1:C:119:THR:CG2	1:C:121:LYS:HE3	2.45	0.47
1:C:154:ILE:HD12	1:C:167:TYR:CZ	2.50	0.47
1:C:508:GLU:HB2	2:C:1162:HOH:O	2.14	0.47
1:C:624:ALA:HB2	2:C:1268:HOH:O	2.14	0.47
1:C:737:ALA:O	1:C:741:VAL:HG23	2.14	0.47
1:C:822:THR:HG22	1:C:824:PRO:HD2	1.97	0.47
1:D:16:ILE:HD13	2:D:1202:HOH:O	2.13	0.47
1:D:249:GLY:CA	1:D:260:PRO:HD2	2.38	0.47
1:D:275:LEU:CD1	1:D:820:LEU:HA	2.45	0.47
1:D:399:TYR:HD1	2:D:1048:HOH:O	1.97	0.47
1:D:464:LYS:C	1:D:466:PRO:HD2	2.35	0.47
1:D:588:ASN:CB	1:D:589:PRO:HD3	2.45	0.47
1:D:620:LYS:HD2	1:D:623:GLU:OE1	2.14	0.47
1:D:869:VAL:O	1:D:873:VAL:HG23	2.14	0.47
1:A:113:VAL:HG13	1:A:123:VAL:HG11	1.97	0.47
1:A:156:HIS:HA	1:A:178:GLU:OE1	2.15	0.47
1:A:861:LEU:HD22	1:A:938:VAL:HB	1.96	0.47
1:B:231:LYS:HD3	1:B:235:LEU:HD12	1.97	0.47
1:B:231:LYS:HE2	1:B:231:LYS:HA	1.97	0.47
1:B:272:SER:HB2	1:B:313:LEU:HD23	1.96	0.47
1:B:396:GLN:NE2	1:B:402:ASP:OD1	2.47	0.47
1:B:932:PHE:O	1:B:936:LEU:HB2	2.15	0.47
1:C:167:TYR:O	1:C:198:ARG:HD3	2.15	0.47
1:C:741:VAL:HG12	1:C:745:ASN:HD21	1.79	0.47
1:C:882:TRP:CZ2	1:C:886:LEU:HD21	2.49	0.47
1:D:231:LYS:HA	1:D:231:LYS:HE2	1.96	0.47
1:D:259:GLU:CB	1:D:260:PRO:CD	2.93	0.47
1:D:355:GLU:HB3	1:D:357:VAL:HG23	1.97	0.47
1:A:40:LEU:HD12	2:A:1058:HOH:O	2.15	0.47
1:A:465:GLU:O	1:A:467:ARG:N	2.48	0.47
1:A:716:ARG:NE	2:A:1154:HOH:O	2.47	0.47
1:B:116:ASN:N	1:B:116:ASN:ND2	2.61	0.47
1:C:174:VAL:HG12	1:C:175:THR:N	2.29	0.47
1:C:328:ILE:HD12	1:C:337:LEU:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:485:GLN:HG2	1:C:496:ARG:NH2	2.30	0.47
1:C:873:VAL:O	1:C:877:VAL:HG23	2.14	0.47
1:D:55:ALA:HA	2:D:1110:HOH:O	2.14	0.47
1:D:213:SER:O	1:D:218:GLU:HB2	2.15	0.47
1:D:224:ILE:HD13	1:D:368:THR:OG1	2.15	0.47
1:D:368:THR:O	1:D:763:ARG:NH1	2.48	0.47
1:D:401:MET:HA	2:D:1028:HOH:O	2.14	0.47
1:D:806:HIS:HB3	1:D:807:PRO:HD3	1.96	0.47
1:A:11:ASN:O	1:A:13:GLU:N	2.48	0.47
1:A:200:ASP:HB2	2:A:1135:HOH:O	2.15	0.47
1:A:262:GLY:HA3	2:A:1082:HOH:O	2.14	0.47
1:A:273:VAL:O	1:A:273:VAL:HG12	2.14	0.47
1:A:369:ILE:HD12	1:A:763:ARG:NH1	2.29	0.47
1:B:370:THR:HG22	1:B:756:ASP:OD1	2.15	0.47
1:C:369:ILE:CG1	1:C:374:PHE:HB2	2.43	0.47
1:C:644:ILE:HA	2:C:1104:HOH:O	2.15	0.47
1:C:831:PHE:CZ	1:C:835:ARG:HG2	2.50	0.47
1:D:801:LEU:HD21	1:D:834:LEU:HB3	1.96	0.47
1:D:842:ALA:O	1:D:846:LEU:HG	2.15	0.47
1:A:316:ARG:NE	1:A:355:GLU:HG2	2.29	0.46
1:A:872:PHE:O	1:A:876:ASN:HB2	2.15	0.46
1:B:61:LEU:HD12	1:B:115:LEU:CD2	2.45	0.46
1:B:291:GLY:O	1:B:293:PHE:N	2.48	0.46
1:B:321:ILE:HB	1:B:337:LEU:HD21	1.98	0.46
1:B:349:GLN:H	1:B:349:GLN:CD	2.17	0.46
1:B:646:GLU:HB3	2:B:1070:HOH:O	2.15	0.46
1:C:354:LYS:HA	1:C:354:LYS:HE3	1.97	0.46
1:C:370:THR:OG1	1:C:372:GLN:OE1	2.32	0.46
1:C:492:TRP:O	1:C:495:LEU:HD23	2.16	0.46
1:D:212:ASP:O	1:D:216:ILE:HB	2.15	0.46
1:A:219:ALA:HB1	1:A:372:GLN:NE2	2.29	0.46
1:A:275:LEU:HD13	1:A:816:LYS:HZ3	1.79	0.46
1:A:284:GLU:OE1	1:A:290:GLU:HB3	2.15	0.46
1:A:588:ASN:HB3	1:A:589:PRO:HD3	1.96	0.46
1:A:860:GLU:HG3	2:A:1140:HOH:O	2.15	0.46
1:B:96:ILE:CD1	1:B:211:VAL:HG11	2.44	0.46
1:B:205:TYR:CE1	1:B:380:LYS:HG2	2.50	0.46
1:B:397:GLU:HA	1:B:397:GLU:OE2	2.14	0.46
1:B:889:LEU:HD22	1:B:910:TYR:OH	2.16	0.46
1:C:492:TRP:HA	1:C:495:LEU:CD2	2.46	0.46
1:C:609:VAL:O	1:C:613:ILE:HG13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:VAL:HG13	1:D:67:LEU:HD23	1.96	0.46
1:D:116:ASN:N	1:D:116:ASN:ND2	2.63	0.46
1:D:154:ILE:HB	1:D:174:VAL:HG22	1.98	0.46
1:D:250:LEU:O	1:D:259:GLU:HB2	2.16	0.46
1:D:284:GLU:OE2	1:D:290:GLU:HA	2.15	0.46
1:D:298:MET:HA	1:D:932:PHE:CE1	2.50	0.46
1:D:779:GLU:HB2	2:D:1163:HOH:O	2.14	0.46
1:A:105:LYS:NZ	1:A:105:LYS:HB2	2.29	0.46
1:A:396:GLN:O	1:A:400:GLY:HA2	2.15	0.46
1:A:773:ILE:CD1	1:A:874:ILE:HG21	2.44	0.46
1:A:821:ASP:O	1:A:931:LYS:HA	2.14	0.46
1:A:822:THR:CG2	1:A:824:PRO:HD2	2.44	0.46
1:A:895:GLY:CA	2:A:1355:HOH:O	2.63	0.46
1:B:50:LYS:HD3	2:B:1277:HOH:O	2.14	0.46
1:B:226:SER:HB2	1:B:363:ASN:HB2	1.97	0.46
1:B:269:LYS:CD	1:B:270:ASN:H	2.28	0.46
1:C:266:VAL:HG23	1:C:269:LYS:HB2	1.93	0.46
1:D:208:ILE:HB	1:D:211:VAL:CG1	2.45	0.46
1:D:592:LEU:HD22	1:D:641:ILE:HG12	1.96	0.46
1:D:710:VAL:HG11	1:D:733:SER:HB2	1.96	0.46
1:D:782:LYS:O	1:D:786:ILE:HG13	2.15	0.46
1:A:191:SER:OG	1:A:194:GLN:HG3	2.16	0.46
1:A:608:LYS:HD2	2:A:1132:HOH:O	2.14	0.46
1:B:85:LEU:HA	1:B:111:LEU:HD13	1.97	0.46
1:B:246:LEU:CD1	1:B:261:THR:HG21	2.39	0.46
1:B:370:THR:HG21	1:B:373:ASN:ND2	2.30	0.46
1:B:671:SER:OG	1:B:673:ARG:NH1	2.48	0.46
1:C:102:GLY:O	1:C:105:LYS:NZ	2.48	0.46
1:C:259:GLU:CB	1:C:260:PRO:CD	2.94	0.46
1:C:588:ASN:CB	1:C:589:PRO:HD3	2.45	0.46
1:D:130:ASP:HB3	1:D:155:GLN:OE1	2.15	0.46
1:D:222:PRO:HA	2:D:1276:HOH:O	2.16	0.46
1:D:234:ASP:OD1	1:D:238:LYS:HE3	2.15	0.46
1:D:273:VAL:HA	1:D:820:LEU:HB2	1.98	0.46
1:D:541:ARG:C	1:D:543:GLY:N	2.69	0.46
1:D:766:ILE:HD12	1:D:882:TRP:CZ3	2.51	0.46
1:A:65:PHE:CE1	1:A:111:LEU:HB3	2.50	0.46
1:A:244:LYS:HG3	1:A:311:LYS:HZ3	1.79	0.46
1:A:253:GLU:HB3	1:A:254:PRO:HD2	1.97	0.46
1:A:289:ILE:HG22	1:A:291:GLY:H	1.81	0.46
1:A:549:LEU:HD22	1:A:557:GLU:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:563:GLN:HA	2:A:1287:HOH:O	2.15	0.46
1:A:594:ALA:HA	1:A:597:LEU:CD1	2.46	0.46
1:A:636:GLU:HB3	2:A:1050:HOH:O	2.15	0.46
1:A:640:ARG:NE	1:A:644:ILE:HG13	2.30	0.46
1:B:250:LEU:HB2	1:B:259:GLU:CD	2.35	0.46
1:B:485:GLN:HG2	1:B:496:ARG:NE	2.30	0.46
1:B:547:GLN:CG	1:B:560:ILE:HG21	2.44	0.46
1:D:498:LEU:HD23	2:D:1092:HOH:O	2.16	0.46
1:D:848:GLU:HG2	2:D:1061:HOH:O	2.16	0.46
1:D:915:THR:O	1:D:919:ASN:ND2	2.49	0.46
1:D:924:PHE:O	1:D:928:GLU:HB2	2.16	0.46
1:D:929:VAL:HG12	1:D:933:LEU:CD1	2.43	0.46
1:A:24:VAL:HG12	1:A:28:ASN:ND2	2.30	0.46
1:A:259:GLU:CB	1:A:260:PRO:CD	2.93	0.46
1:A:861:LEU:HD22	1:A:938:VAL:CG2	2.46	0.46
1:B:107:LEU:HA	1:B:140:MET:SD	2.55	0.46
1:B:408:THR:HG22	2:B:1229:HOH:O	2.14	0.46
1:B:485:GLN:OE1	1:B:485:GLN:HA	2.16	0.46
1:B:590:GLU:HG3	1:B:591:TYR:CE1	2.51	0.46
1:B:598:GLU:HA	2:B:1227:HOH:O	2.15	0.46
1:C:105:LYS:NZ	1:C:105:LYS:HB2	2.31	0.46
1:C:176:ASN:HB2	1:C:371:TYR:CE2	2.51	0.46
1:D:127:THR:HG22	1:D:128:VAL:H	1.81	0.46
1:D:174:VAL:CG1	1:D:178:GLU:HB3	2.45	0.46
1:D:633:ILE:HG22	1:D:638:LEU:HG	1.95	0.46
1:D:796:LEU:O	1:D:799:ASN:HB2	2.16	0.46
1:A:184:LEU:HD11	1:A:223:LEU:HB3	1.97	0.46
1:A:431:ALA:O	1:A:434:GLU:HB2	2.15	0.46
1:B:211:VAL:CG1	1:B:383:GLY:HA3	2.45	0.46
1:B:720:ASP:HB2	2:B:1204:HOH:O	2.16	0.46
1:B:820:LEU:CD1	1:B:935:ARG:HH22	2.28	0.46
1:C:11:ASN:O	1:C:13:GLU:N	2.47	0.46
1:C:275:LEU:HD11	2:C:1068:HOH:O	2.14	0.46
1:D:241:GLU:CG	1:D:242:ILE:N	2.79	0.46
1:D:253:GLU:CG	1:D:256:VAL:HG13	2.46	0.46
1:D:321:ILE:HG12	2:D:1119:HOH:O	2.14	0.46
1:D:410:ARG:HG3	1:D:685:GLN:NE2	2.31	0.46
1:B:293:PHE:HE2	1:B:301:ALA:HA	1.80	0.46
1:B:806:HIS:HB3	1:B:807:PRO:HD3	1.98	0.46
1:B:888:ASN:HB2	2:B:1035:HOH:O	2.16	0.46
1:C:104:GLY:O	1:C:108:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:599:LYS:HB3	1:C:600:GLU:H	1.62	0.46
1:D:354:LYS:HG2	2:D:1098:HOH:O	2.16	0.46
1:D:437:ALA:HB3	2:D:1085:HOH:O	2.16	0.46
1:D:548:VAL:O	1:D:549:LEU:HD23	2.15	0.46
1:A:672:ARG:HG2	1:A:742:GLU:OE2	2.16	0.46
1:B:20:TYR:HA	1:B:24:VAL:CG2	2.45	0.46
1:B:69:ARG:NH1	2:B:1186:HOH:O	2.40	0.46
1:B:258:LYS:HB3	2:B:1078:HOH:O	2.15	0.46
1:B:315:HIS:HE1	2:B:1299:HOH:O	1.99	0.46
1:C:101:THR:HG22	2:C:1017:HOH:O	2.15	0.46
1:C:640:ARG:HH21	1:C:644:ILE:HG12	1.81	0.46
1:C:761:ARG:HG2	1:C:761:ARG:HH11	1.81	0.46
1:C:801:LEU:HD22	1:C:842:ALA:HB1	1.97	0.46
1:D:479:LEU:HA	1:D:482:LYS:HE3	1.98	0.46
1:D:518:PRO:HD2	2:D:1058:HOH:O	2.13	0.46
1:D:763:ARG:O	1:D:767:TYR:HB2	2.16	0.46
1:A:609:VAL:O	1:A:613:ILE:HG13	2.16	0.46
1:B:448:VAL:HG11	1:B:459:LEU:HD11	1.98	0.46
1:B:462:MET:N	1:B:468:LEU:HD12	2.31	0.46
1:B:524:ARG:NH1	1:B:527:TRP:CD1	2.84	0.46
1:C:310:ALA:HB1	1:C:351:ILE:HG12	1.98	0.46
1:C:327:VAL:HG23	1:C:352:GLU:HG2	1.98	0.46
1:C:408:THR:CG2	1:C:409:ASN:N	2.79	0.46
1:C:829:PHE:N	1:C:830:PRO:CD	2.79	0.46
1:D:155:GLN:N	2:D:1301:HOH:O	2.49	0.46
1:D:231:LYS:NZ	1:D:232:ALA:N	2.64	0.46
1:D:291:GLY:O	1:D:293:PHE:N	2.49	0.46
1:D:861:LEU:HD13	1:D:869:VAL:HG21	1.97	0.46
1:A:360:GLU:HA	2:A:1048:HOH:O	2.15	0.45
1:A:492:TRP:HA	1:A:495:LEU:HD21	1.98	0.45
1:A:553:HIS:CD2	1:A:556:ARG:HD3	2.51	0.45
1:A:559:GLU:HB3	1:A:590:GLU:OE2	2.16	0.45
1:B:281:ALA:HA	1:B:284:GLU:CD	2.36	0.45
1:B:422:TYR:HB3	2:B:1002:HOH:O	2.15	0.45
1:B:477:LEU:HG	1:B:530:LEU:HD11	1.97	0.45
1:B:615:LYS:HG2	1:B:623:GLU:HB2	1.98	0.45
1:B:628:ALA:HB3	2:B:1138:HOH:O	2.15	0.45
1:B:929:VAL:HG12	1:B:933:LEU:HD11	1.98	0.45
1:C:429:PHE:O	1:C:433:VAL:HG23	2.16	0.45
1:C:452:SER:HB2	2:C:1080:HOH:O	2.16	0.45
1:C:656:ARG:HE	1:C:656:ARG:HB3	1.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:897:PHE:C	1:C:897:PHE:HD2	2.18	0.45
1:D:480:PHE:CE1	1:D:527:TRP:HE3	2.34	0.45
1:D:669:HIS:ND1	1:D:675:ASP:HB3	2.30	0.45
1:A:121:LYS:C	1:A:198:ARG:NH2	2.65	0.45
1:A:429:PHE:O	1:A:433:VAL:HG23	2.16	0.45
1:A:578:GLY:C	1:A:681:ARG:HH21	2.19	0.45
1:B:259:GLU:CB	1:B:260:PRO:CD	2.93	0.45
1:B:827:GLN:C	1:B:830:PRO:HD2	2.36	0.45
1:C:390:THR:HG22	1:C:391:GLU:OE2	2.15	0.45
1:C:509:ASP:O	1:C:512:PRO:HD2	2.16	0.45
1:C:819:LEU:C	2:C:1223:HOH:O	2.54	0.45
1:D:321:ILE:HB	1:D:337:LEU:HD21	1.97	0.45
1:D:659:GLY:O	1:D:688:PRO:HB2	2.16	0.45
1:A:33:GLU:HB3	2:A:1153:HOH:O	2.16	0.45
1:A:145:ARG:HD3	1:A:607:TRP:CZ3	2.51	0.45
1:A:408:THR:HB	2:A:1101:HOH:O	2.16	0.45
1:B:70:GLU:OE2	1:B:73:LYS:HD3	2.17	0.45
1:B:896:ILE:O	1:B:896:ILE:HG22	2.15	0.45
1:C:10:ASP:OD2	1:D:716:ARG:NH2	2.49	0.45
1:C:84:GLN:NE2	1:C:104:GLY:HA2	2.32	0.45
1:C:435:GLU:CD	1:C:694:TYR:HH	2.14	0.45
1:C:566:ARG:HG2	1:C:586:GLY:HA2	1.97	0.45
1:D:231:LYS:HD3	1:D:235:LEU:HD12	1.98	0.45
1:D:524:ARG:HG2	2:D:1038:HOH:O	2.16	0.45
1:D:593:ALA:O	1:D:597:LEU:HG	2.16	0.45
1:D:608:LYS:N	1:D:608:LYS:HD2	2.32	0.45
1:A:138:GLU:OE1	1:A:606:GLU:HG3	2.16	0.45
1:A:327:VAL:HG23	1:A:352:GLU:HG2	1.98	0.45
1:A:349:GLN:CD	1:A:349:GLN:H	2.19	0.45
1:A:392:GLU:OE1	1:A:403:VAL:HB	2.16	0.45
1:A:705:PHE:CB	1:A:741:VAL:HG22	2.47	0.45
1:A:810:TRP:CD1	1:A:810:TRP:N	2.85	0.45
1:B:198:ARG:H	1:B:198:ARG:HG2	1.57	0.45
1:B:281:ALA:HA	1:B:284:GLU:OE1	2.17	0.45
1:B:572:ILE:O	1:B:572:ILE:HG22	2.17	0.45
1:B:606:GLU:OE2	1:B:610:GLU:HG3	2.16	0.45
1:B:623:GLU:O	1:B:627:LEU:HG	2.17	0.45
1:B:861:LEU:HD23	1:B:861:LEU:H	1.80	0.45
1:D:927:SER:O	1:D:931:LYS:HG3	2.16	0.45
1:A:175:THR:HG21	2:A:1189:HOH:O	2.16	0.45
1:A:273:VAL:HA	1:A:820:LEU:CD1	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:ALA:O	1:A:305:ILE:HG13	2.16	0.45
1:A:483:ALA:HB2	2:A:1184:HOH:O	2.17	0.45
1:B:181:PHE:O	1:B:185:ARG:HG3	2.16	0.45
1:B:674:ILE:O	1:B:674:ILE:CG2	2.65	0.45
1:B:777:LYS:O	1:B:780:GLU:N	2.50	0.45
1:C:71:SER:HB2	2:C:1265:HOH:O	2.15	0.45
1:C:550:ASN:HA	1:C:574:THR:CB	2.47	0.45
1:C:636:GLU:HA	2:C:1307:HOH:O	2.16	0.45
1:C:794:ALA:HA	1:C:843:VAL:HG13	1.99	0.45
1:D:199:HIS:CD2	1:D:199:HIS:N	2.84	0.45
1:D:250:LEU:HB2	1:D:259:GLU:CD	2.35	0.45
1:D:517:ILE:HG23	2:D:1058:HOH:O	2.16	0.45
1:D:697:PHE:CZ	1:D:714:LEU:HD22	2.52	0.45
1:D:763:ARG:HD2	1:D:767:TYR:CE1	2.51	0.45
1:D:791:GLU:OE1	1:D:926:LYS:HD3	2.17	0.45
1:A:154:ILE:HD12	1:A:167:TYR:CZ	2.52	0.45
1:A:459:LEU:HA	1:A:462:MET:CE	2.47	0.45
1:A:622:GLU:HG2	1:A:623:GLU:HG3	1.99	0.45
1:B:485:GLN:HG2	1:B:496:ARG:CZ	2.46	0.45
1:C:274:HIS:CD2	1:C:274:HIS:H	2.33	0.45
1:C:359:ILE:HG23	2:C:1250:HOH:O	2.15	0.45
1:C:370:THR:O	1:C:372:GLN:N	2.50	0.45
1:C:537:LEU:O	1:C:541:ARG:HG3	2.16	0.45
1:D:175:THR:OG1	1:D:178:GLU:HB2	2.17	0.45
1:D:656:ARG:NH2	2:D:1150:HOH:O	2.48	0.45
1:D:695:VAL:CG1	1:D:696:SER:N	2.80	0.45
1:A:211:VAL:HG23	1:A:212:ASP:N	2.31	0.45
1:A:679:ARG:HH21	1:B:732:ARG:HH21	1.64	0.45
1:A:701:LEU:HD21	1:A:738:GLN:HA	1.99	0.45
1:A:829:PHE:N	1:A:830:PRO:CD	2.79	0.45
1:A:927:SER:OG	1:A:931:LYS:HE3	2.16	0.45
1:B:202:PRO:N	2:B:1283:HOH:O	2.50	0.45
1:B:250:LEU:O	1:B:259:GLU:HB2	2.17	0.45
1:B:274:HIS:H	1:B:274:HIS:HD1	1.64	0.45
1:B:389:LYS:HD2	1:B:405:VAL:HG21	1.98	0.45
1:B:409:ASN:HD22	1:B:409:ASN:HA	1.50	0.45
1:B:709:ARG:NH2	2:B:1142:HOH:O	2.49	0.45
1:B:755:PHE:HE2	1:B:893:ARG:HB3	1.81	0.45
1:B:854:TYR:CE1	1:B:866:MET:HE1	2.52	0.45
1:C:141:GLY:O	1:C:145:ARG:HG3	2.16	0.45
1:D:409:ASN:HD22	1:D:409:ASN:HA	1.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:792:THR:OG1	1:D:927:SER:HA	2.17	0.45
1:D:863:PRO:O	1:D:867:ARG:HG2	2.16	0.45
1:A:602:PHE:CD1	1:A:603:ASP:N	2.82	0.45
1:A:770:ARG:CZ	1:A:879:ASP:HB3	2.46	0.45
1:B:490:PRO:O	1:B:494:ARG:HG3	2.16	0.45
1:C:19:TYR:CE2	1:C:90:VAL:HG22	2.51	0.45
1:C:34:VAL:CG1	1:C:67:LEU:HD23	2.46	0.45
1:C:273:VAL:HA	1:C:820:LEU:HD22	1.98	0.45
1:C:278:GLN:HA	2:C:1190:HOH:O	2.16	0.45
1:C:594:ALA:HA	1:C:597:LEU:CD1	2.47	0.45
1:D:215:LEU:HD13	1:D:399:TYR:CE2	2.52	0.45
1:D:370:THR:HG22	1:D:756:ASP:CG	2.37	0.45
1:D:594:ALA:HA	1:D:597:LEU:HG	1.99	0.45
1:D:677:GLN:HG2	2:D:1182:HOH:O	2.16	0.45
1:D:806:HIS:HB2	1:D:807:PRO:HD3	1.98	0.45
1:D:857:ARG:O	1:D:861:LEU:HG	2.17	0.45
1:A:341:ARG:HH11	1:A:341:ARG:HG3	1.81	0.45
1:A:371:TYR:HD2	1:A:375:PHE:HE1	1.65	0.45
1:A:385:THR:CG2	1:A:388:ALA:HB2	2.46	0.45
1:A:443:GLY:O	1:A:658:LEU:HD13	2.17	0.45
1:B:85:LEU:HA	1:B:111:LEU:CD1	2.47	0.45
1:B:228:PRO:HA	2:B:1044:HOH:O	2.17	0.45
1:B:466:PRO:HG3	1:B:540:LEU:HB3	1.98	0.45
1:B:643:GLU:O	1:B:647:GLU:HB3	2.17	0.45
1:C:85:LEU:HA	1:C:111:LEU:CD1	2.47	0.45
1:C:269:LYS:HA	2:C:1286:HOH:O	2.17	0.45
1:C:789:VAL:O	1:C:793:VAL:HG23	2.17	0.45
1:C:804:GLU:HA	2:C:1033:HOH:O	2.17	0.45
1:D:19:TYR:HE1	1:D:93:GLU:OE2	2.00	0.45
1:D:87:GLY:HA3	1:D:99:MET:HE1	1.99	0.45
1:D:443:GLY:C	1:D:658:LEU:HD13	2.38	0.45
1:D:475:MET:HB3	2:D:1084:HOH:O	2.16	0.45
1:D:788:MET:SD	1:D:929:VAL:HG21	2.57	0.45
1:A:440:TYR:HE1	1:A:568:LYS:HB3	1.82	0.45
1:A:540:LEU:HD23	1:A:544:ILE:HD11	1.99	0.45
1:A:550:ASN:C	2:A:1125:HOH:O	2.56	0.45
1:A:661:LEU:HD13	1:A:663:ILE:HD11	1.98	0.45
1:A:684:ARG:HG3	1:A:685:GLN:H	1.81	0.45
1:A:852:LYS:HB2	1:A:852:LYS:HZ2	1.81	0.45
1:A:873:VAL:O	1:A:877:VAL:HG23	2.16	0.45
1:B:26:PRO:O	1:B:30:LEU:HG	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:GLN:HG3	1:B:399:TYR:OH	2.17	0.45
1:B:426:LYS:HB2	2:B:1276:HOH:O	2.16	0.45
1:B:688:PRO:HA	2:B:1067:HOH:O	2.16	0.45
1:B:773:ILE:HG12	1:B:874:ILE:HG21	1.98	0.45
1:C:40:LEU:HD11	1:C:74:ARG:HD2	1.99	0.45
1:C:73:LYS:HE3	1:C:79:ARG:CD	2.47	0.45
1:C:213:SER:O	1:C:218:GLU:HB2	2.17	0.45
1:C:223:LEU:O	1:C:368:THR:HG23	2.17	0.45
1:C:639:GLU:HB2	2:C:1307:HOH:O	2.16	0.45
1:C:640:ARG:N	2:C:1044:HOH:O	2.49	0.45
1:D:303:MET:HA	1:D:306:GLN:CG	2.47	0.45
1:D:634:ARG:HD3	1:D:634:ARG:HA	1.61	0.45
1:D:857:ARG:NH1	1:D:936:LEU:H	2.06	0.45
1:A:284:GLU:CD	1:A:290:GLU:HB3	2.37	0.44
1:A:290:GLU:O	1:A:293:PHE:HB3	2.17	0.44
1:A:294:SER:HB3	1:A:295:PRO:HD3	1.98	0.44
1:A:629:GLN:OE1	1:A:629:GLN:HA	2.17	0.44
1:A:675:ASP:OD2	1:A:675:ASP:C	2.55	0.44
1:A:739:LYS:HD2	1:B:736:ARG:HD3	2.00	0.44
1:A:897:PHE:N	2:A:1030:HOH:O	2.50	0.44
1:B:176:ASN:ND2	1:B:177:SER:H	2.10	0.44
1:C:343:TYR:HE2	2:C:1165:HOH:O	2.00	0.44
1:C:837:LEU:CD1	1:C:841:GLU:HB3	2.47	0.44
1:D:466:PRO:HG2	2:D:1295:HOH:O	2.16	0.44
1:D:547:GLN:CG	1:D:560:ILE:HG21	2.47	0.44
1:A:2:LEU:HG	1:B:716:ARG:HA	1.99	0.44
1:A:309:ARG:HH22	1:A:931:LYS:HZ2	1.65	0.44
1:A:355:GLU:OE1	1:A:355:GLU:HA	2.16	0.44
1:A:566:ARG:HA	1:A:651:ASP:OD1	2.17	0.44
1:B:127:THR:HG22	1:B:128:VAL:H	1.83	0.44
1:B:253:GLU:CB	1:B:256:VAL:HG13	2.44	0.44
1:B:821:ASP:CG	1:B:931:LYS:HG2	2.37	0.44
1:B:920:GLU:O	1:B:923:ALA:HB3	2.17	0.44
1:C:167:TYR:O	1:C:198:ARG:NH1	2.49	0.44
1:C:901:TYR:HD2	1:C:901:TYR:HA	1.66	0.44
1:D:176:ASN:HB3	1:D:214:ILE:HD13	2.00	0.44
1:D:238:LYS:HA	1:D:241:GLU:OE1	2.17	0.44
1:D:253:GLU:CB	1:D:256:VAL:HG13	2.45	0.44
1:D:626:ALA:O	1:D:630:GLU:HG3	2.17	0.44
1:A:423:ARG:HB2	1:A:725:ILE:HD11	2.00	0.44
1:A:532:ARG:HE	1:A:532:ARG:HB2	1.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:905:ASP:OD2	1:A:908:GLN:HB2	2.17	0.44
1:B:231:LYS:HZ1	1:B:232:ALA:HB3	1.82	0.44
1:B:428:LYS:O	1:B:431:ALA:HB3	2.17	0.44
1:B:480:PHE:O	1:B:484:SER:OG	2.34	0.44
1:B:519:PRO:HD3	2:B:1250:HOH:O	2.15	0.44
1:B:893:ARG:HG2	1:B:910:TYR:CZ	2.52	0.44
1:C:211:VAL:HG23	1:C:212:ASP:N	2.32	0.44
1:C:246:LEU:CD2	1:C:261:THR:HG21	2.47	0.44
1:C:248:ARG:HD2	1:C:264:TYR:CE2	2.53	0.44
1:C:663:ILE:HD13	1:C:682:ALA:CB	2.39	0.44
1:C:777:LYS:O	1:C:781:VAL:N	2.50	0.44
1:C:837:LEU:HD12	1:C:837:LEU:O	2.16	0.44
1:D:244:LYS:HD2	1:D:354:LYS:HZ1	1.79	0.44
1:D:615:LYS:HD3	1:D:623:GLU:HB3	1.98	0.44
1:A:40:LEU:HD12	1:A:40:LEU:H	1.82	0.44
1:A:86:ILE:O	1:A:90:VAL:HG23	2.18	0.44
1:A:117:ALA:HA	2:A:1017:HOH:O	2.18	0.44
1:A:198:ARG:H	1:A:198:ARG:HG2	1.62	0.44
1:A:827:GLN:HE21	1:A:827:GLN:HB2	1.54	0.44
1:B:211:VAL:HG11	1:B:383:GLY:HA3	1.99	0.44
1:B:454:GLU:HG3	2:B:1007:HOH:O	2.16	0.44
1:B:766:ILE:HD12	1:B:882:TRP:CZ3	2.52	0.44
1:B:858:GLU:HG3	1:B:863:PRO:HA	2.00	0.44
1:C:7:ARG:HG2	2:C:1218:HOH:O	2.16	0.44
1:C:102:GLY:CA	1:C:105:LYS:NZ	2.80	0.44
1:C:192:PRO:CG	1:C:774:LEU:HD22	2.47	0.44
1:C:858:GLU:HG3	1:C:866:MET:HE3	1.98	0.44
1:D:159:THR:O	1:D:163:ARG:HG3	2.17	0.44
1:D:175:THR:HG23	2:D:1118:HOH:O	2.16	0.44
1:D:394:GLU:HG3	1:D:398:ILE:HD12	1.98	0.44
1:D:576:MET:HA	1:D:681:ARG:HH12	1.82	0.44
1:D:727:HIS:CD2	1:D:728:PRO:HD2	2.52	0.44
1:A:369:ILE:HG13	1:A:374:PHE:HB2	1.98	0.44
1:A:459:LEU:HA	1:A:462:MET:HE3	1.98	0.44
1:A:770:ARG:NH1	1:A:879:ASP:CB	2.81	0.44
1:A:827:GLN:C	1:A:830:PRO:HD2	2.38	0.44
1:B:39:ASP:CB	2:B:1184:HOH:O	2.62	0.44
1:B:198:ARG:CG	1:B:202:PRO:HA	2.46	0.44
1:B:275:LEU:HD21	1:B:935:ARG:NH1	2.33	0.44
1:B:370:THR:CG2	1:B:373:ASN:ND2	2.80	0.44
1:B:435:GLU:OE1	1:B:692:ARG:NH1	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:599:LYS:HE2	1:B:599:LYS:HB2	1.75	0.44
1:C:119:THR:CG2	1:C:121:LYS:HG3	2.44	0.44
1:C:727:HIS:O	1:C:731:THR:HG23	2.17	0.44
1:C:732:ARG:NH2	1:D:679:ARG:HH21	2.16	0.44
1:D:6:ARG:O	1:D:13:GLU:HG3	2.18	0.44
1:D:271:ARG:NE	1:D:821:ASP:OD2	2.50	0.44
1:D:338:MET:SD	1:D:341:ARG:HB3	2.58	0.44
1:D:450:THR:HG21	1:D:456:SER:HA	1.99	0.44
1:D:502:PRO:HB2	2:D:1195:HOH:O	2.18	0.44
1:D:565:GLY:HA3	1:D:584:LYS:O	2.17	0.44
1:A:120:GLY:O	1:A:198:ARG:NH2	2.51	0.44
1:A:205:TYR:HD1	1:A:380:LYS:O	2.01	0.44
1:B:364:GLN:HG2	1:B:887:HIS:CG	2.52	0.44
1:B:373:ASN:O	1:B:376:ARG:HB2	2.17	0.44
1:B:594:ALA:HA	1:B:597:LEU:CD1	2.48	0.44
1:C:532:ARG:HE	1:C:532:ARG:HB2	1.54	0.44
1:C:884:GLU:HG3	2:C:1173:HOH:O	2.18	0.44
1:D:447:LEU:HD11	1:D:573:ALA:HB2	1.99	0.44
1:D:710:VAL:C	1:D:712:ALA:H	2.20	0.44
1:A:263:ASP:HB3	1:A:273:VAL:HB	2.00	0.44
1:A:328:ILE:HD12	1:A:337:LEU:HD13	1.99	0.44
1:A:381:ARG:CB	2:A:1239:HOH:O	2.66	0.44
1:A:550:ASN:HA	1:A:574:THR:CB	2.47	0.44
1:A:612:PHE:CE1	1:A:633:ILE:HD13	2.53	0.44
1:A:817:ALA:HA	2:A:1243:HOH:O	2.18	0.44
1:A:822:THR:HG22	1:A:824:PRO:HD2	2.00	0.44
1:A:840:GLU:HB2	2:A:1110:HOH:O	2.17	0.44
1:B:497:LYS:NZ	2:B:1064:HOH:O	2.43	0.44
1:B:759:LEU:H	1:B:759:LEU:HD23	1.83	0.44
1:C:18:ARG:HH21	1:C:22:GLN:NE2	2.09	0.44
1:C:244:LYS:HE3	1:C:311:LYS:HZ3	1.82	0.44
1:C:246:LEU:HG	1:C:261:THR:HG21	1.99	0.44
1:C:294:SER:HB3	1:C:295:PRO:HD3	2.00	0.44
1:C:363:ASN:ND2	2:C:1087:HOH:O	2.50	0.44
1:C:483:ALA:HB1	2:C:1091:HOH:O	2.18	0.44
1:C:732:ARG:HD3	2:C:1115:HOH:O	2.17	0.44
1:D:278:GLN:O	1:D:282:LYS:HG3	2.17	0.44
1:D:399:TYR:HB3	2:D:1048:HOH:O	2.17	0.44
1:D:550:ASN:ND2	1:D:550:ASN:N	2.48	0.44
1:D:572:ILE:O	1:D:572:ILE:HG22	2.18	0.44
1:D:858:GLU:HB3	2:D:1014:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:GLU:H	1:A:299:GLU:CD	2.20	0.44
1:A:616:MET:HG2	1:A:641:ILE:HG21	2.00	0.44
1:A:732:ARG:HG2	1:B:735:GLU:OE2	2.17	0.44
1:B:269:LYS:HB3	2:B:1030:HOH:O	2.18	0.44
1:B:381:ARG:NH1	1:B:381:ARG:HG2	2.33	0.44
1:B:428:LYS:HD3	1:B:695:VAL:C	2.38	0.44
1:B:524:ARG:NH1	1:B:527:TRP:HD1	2.16	0.44
1:B:772:LEU:HD11	1:B:780:GLU:HB3	1.99	0.44
1:C:316:ARG:HD3	1:C:355:GLU:OE2	2.18	0.44
1:C:349:GLN:CD	1:C:349:GLN:H	2.21	0.44
1:C:485:GLN:OE1	1:C:485:GLN:HA	2.18	0.44
1:C:684:ARG:HB3	2:C:1054:HOH:O	2.17	0.44
1:C:763:ARG:O	1:C:767:TYR:HB2	2.17	0.44
1:D:271:ARG:NH2	1:D:821:ASP:OD2	2.51	0.44
1:D:478:GLU:HA	1:D:481:LYS:HB2	1.99	0.44
1:D:487:GLN:HB2	1:D:492:TRP:CE2	2.53	0.44
1:D:769:GLN:O	1:D:773:ILE:HD13	2.17	0.44
1:D:865:LEU:HD13	1:D:938:VAL:HG11	1.99	0.44
1:A:586:GLY:HA3	2:A:1024:HOH:O	2.16	0.44
1:B:27:VAL:HG12	2:B:1302:HOH:O	2.18	0.44
1:B:69:ARG:O	1:B:72:ALA:HB3	2.17	0.44
1:B:127:THR:HG23	1:B:209:ASP:HB3	2.00	0.44
1:B:271:ARG:HH21	1:B:931:LYS:CE	2.31	0.44
1:B:685:GLN:HE21	1:B:685:GLN:HB3	1.59	0.44
1:B:695:VAL:HG12	1:B:696:SER:N	2.33	0.44
1:C:667:GLU:OE2	1:C:700:ASP:HB2	2.18	0.44
1:C:710:VAL:HG11	1:C:733:SER:HB2	2.00	0.44
1:C:777:LYS:C	1:C:781:VAL:HG23	2.37	0.44
1:C:802:ASN:HA	1:C:839:ALA:HB2	2.00	0.44
1:D:239:MET:HE2	1:D:303:MET:HB3	2.00	0.44
1:D:428:LYS:HZ2	1:D:667:GLU:HB3	1.83	0.44
1:D:550:ASN:HD22	1:D:550:ASN:N	2.11	0.44
1:D:615:LYS:HG2	1:D:623:GLU:HB2	2.00	0.44
1:D:663:ILE:O	1:D:691:SER:HA	2.18	0.44
1:D:873:VAL:O	1:D:877:VAL:HG23	2.18	0.44
1:A:180:GLY:O	1:A:183:TYR:HB3	2.17	0.43
1:A:594:ALA:CA	1:A:597:LEU:HG	2.47	0.43
1:B:668:ARG:HH12	1:B:735:GLU:CD	2.21	0.43
1:C:102:GLY:N	1:C:105:LYS:NZ	2.65	0.43
1:C:241:GLU:O	1:C:245:LYS:HG2	2.17	0.43
1:D:257:ARG:HH11	1:D:258:LYS:HZ3	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:422:TYR:CZ	1:D:431:ALA:HB2	2.53	0.43
1:D:462:MET:HA	1:D:468:LEU:CD1	2.41	0.43
1:D:551:ALA:HB2	1:D:577:ALA:HA	2.00	0.43
1:D:638:LEU:O	1:D:642:ARG:HG3	2.18	0.43
1:A:223:LEU:HB2	1:A:369:ILE:O	2.18	0.43
1:A:469:TYR:CZ	1:A:536:THR:HG21	2.53	0.43
1:A:559:GLU:H	1:A:559:GLU:HG2	1.67	0.43
1:A:755:PHE:O	1:A:758:VAL:HB	2.19	0.43
1:B:42:ALA:HB2	2:B:1129:HOH:O	2.18	0.43
1:B:134:ARG:HD2	2:B:1094:HOH:O	2.18	0.43
1:B:204:HIS:N	2:B:1283:HOH:O	2.51	0.43
1:B:360:GLU:CG	1:B:362:GLU:HG2	2.48	0.43
1:B:360:GLU:HG3	1:B:362:GLU:HG2	1.99	0.43
1:B:695:VAL:CG1	1:B:696:SER:N	2.81	0.43
1:B:773:ILE:O	1:B:871:ARG:NH1	2.51	0.43
1:B:792:THR:O	1:B:796:LEU:HB2	2.17	0.43
1:B:861:LEU:HD12	1:B:866:MET:N	2.33	0.43
1:C:6:ARG:HB3	1:D:716:ARG:CZ	2.48	0.43
1:C:89:ALA:O	1:C:93:GLU:HG3	2.18	0.43
1:C:102:GLY:HA3	1:C:582:ASP:OD1	2.17	0.43
1:C:316:ARG:NE	1:C:355:GLU:HG2	2.33	0.43
1:C:369:ILE:HD12	1:C:763:ARG:NH2	2.33	0.43
1:C:563:GLN:NE2	1:C:587:GLY:O	2.51	0.43
1:C:882:TRP:HE3	1:C:921:MET:HE1	1.83	0.43
1:D:44:TYR:HE2	1:D:149:LEU:HD21	1.83	0.43
1:D:239:MET:HG3	1:D:307:ALA:HB2	1.99	0.43
1:D:517:ILE:HA	2:D:1058:HOH:O	2.17	0.43
1:D:604:ARG:CG	1:D:605:TYR:H	2.32	0.43
1:D:719:PHE:HB3	2:D:1065:HOH:O	2.17	0.43
1:A:34:VAL:CG1	1:A:67:LEU:HD23	2.48	0.43
1:A:310:ALA:HB1	1:A:351:ILE:HG12	1.98	0.43
1:A:495:LEU:O	1:A:499:LEU:HG	2.18	0.43
1:A:706:ALA:O	1:A:711:ILE:HD11	2.18	0.43
1:B:208:ILE:CG2	1:B:214:ILE:HD12	2.48	0.43
1:B:476:ARG:HH11	1:B:476:ARG:HG3	1.84	0.43
1:B:546:HIS:N	1:B:546:HIS:ND1	2.66	0.43
1:C:45:ARG:NH1	2:C:1171:HOH:O	2.52	0.43
1:C:277:LEU:HD23	1:C:280:ILE:CD1	2.34	0.43
1:C:295:PRO:O	1:C:296:GLU:HB2	2.18	0.43
1:C:417:PHE:HB3	2:C:1069:HOH:O	2.17	0.43
1:C:806:HIS:N	2:C:1194:HOH:O	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:199:HIS:CE1	2:D:1336:HOH:O	2.72	0.43
1:D:225:ILE:HD12	1:D:367:ALA:HB3	2.00	0.43
1:D:370:THR:CG2	1:D:373:ASN:ND2	2.77	0.43
1:D:685:GLN:HE21	1:D:685:GLN:HB3	1.58	0.43
1:A:784:ALA:CA	2:A:1276:HOH:O	2.66	0.43
1:B:113:VAL:HG11	1:B:144:TYR:CZ	2.53	0.43
1:C:181:PHE:CE2	1:C:223:LEU:HB3	2.53	0.43
1:C:400:GLY:N	2:C:1131:HOH:O	2.52	0.43
1:D:344:GLY:O	1:D:345:GLU:HG3	2.19	0.43
1:A:119:THR:CG2	1:A:121:LYS:HG3	2.47	0.43
1:A:184:LEU:HD22	1:A:367:ALA:O	2.18	0.43
1:A:408:THR:CG2	1:A:409:ASN:N	2.81	0.43
1:A:510:LEU:N	1:A:510:LEU:HD12	2.33	0.43
1:A:549:LEU:CD1	1:A:561:VAL:HG22	2.49	0.43
1:A:611:LEU:O	1:A:615:LYS:HB2	2.18	0.43
1:B:621:GLU:O	1:B:625:ARG:HG2	2.18	0.43
1:B:865:LEU:HD13	1:B:938:VAL:HG11	2.00	0.43
1:C:463:LEU:HB2	1:C:546:HIS:NE2	2.33	0.43
1:C:469:TYR:CZ	1:C:536:THR:HG21	2.52	0.43
1:D:208:ILE:HB	1:D:211:VAL:HG13	1.99	0.43
1:D:365:THR:HB	1:D:886:LEU:HB3	2.00	0.43
1:D:442:ARG:NH1	1:D:658:LEU:HD23	2.33	0.43
1:D:777:LYS:O	1:D:780:GLU:N	2.51	0.43
1:A:481:LYS:HE3	2:A:1306:HOH:O	2.19	0.43
1:A:712:ALA:HB3	2:B:1027:HOH:O	2.18	0.43
1:A:773:ILE:HD11	1:A:874:ILE:HG21	1.99	0.43
1:B:551:ALA:HB2	1:B:577:ALA:HA	2.01	0.43
1:B:602:PHE:N	2:B:1242:HOH:O	2.52	0.43
1:C:49:GLU:HB3	2:C:1081:HOH:O	2.17	0.43
1:C:540:LEU:HA	1:C:544:ILE:HD11	1.99	0.43
1:D:273:VAL:CA	1:D:820:LEU:HD13	2.48	0.43
1:D:349:GLN:HA	1:D:352:GLU:OE1	2.19	0.43
1:D:364:GLN:OE1	1:D:364:GLN:HA	2.19	0.43
1:D:423:ARG:HH12	1:D:715:ASP:HA	1.83	0.43
1:D:895:GLY:O	1:D:898:LEU:HG	2.18	0.43
1:A:735:GLU:OE2	1:A:735:GLU:HA	2.19	0.43
1:A:811:ASP:O	1:A:815:LEU:HG	2.19	0.43
1:A:831:PHE:O	1:A:835:ARG:HB3	2.19	0.43
1:B:83:VAL:HA	1:B:86:ILE:HG13	2.01	0.43
1:B:200:ASP:HB2	2:B:1087:HOH:O	2.17	0.43
1:B:238:LYS:HA	1:B:241:GLU:OE1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:GLU:HG3	1:B:256:VAL:O	2.19	0.43
1:C:80:HIS:CD2	1:C:107:LEU:HD21	2.54	0.43
1:C:675:ASP:C	1:C:675:ASP:OD2	2.57	0.43
1:C:801:LEU:HD22	1:C:842:ALA:CB	2.49	0.43
1:C:852:LYS:HB2	1:C:852:LYS:HZ2	1.83	0.43
1:C:871:ARG:N	2:C:1113:HOH:O	2.52	0.43
1:D:119:THR:HB	1:D:121:LYS:HG3	2.01	0.43
1:D:273:VAL:HG21	1:D:816:LYS:O	2.18	0.43
1:D:294:SER:HB2	1:D:295:PRO:CD	2.49	0.43
1:D:381:ARG:NH1	2:D:1056:HOH:O	2.48	0.43
1:A:205:TYR:CE1	1:A:380:LYS:HE3	2.54	0.43
1:A:441:GLU:OE2	1:A:539:VAL:HG22	2.18	0.43
1:A:524:ARG:NH1	1:A:527:TRP:HD1	2.16	0.43
1:A:605:TYR:HA	2:A:1132:HOH:O	2.17	0.43
1:A:716:ARG:HG3	1:B:6:ARG:CG	2.49	0.43
1:C:105:LYS:HB2	1:C:105:LYS:HZ3	1.84	0.43
1:C:222:PRO:HB2	1:C:368:THR:CG2	2.49	0.43
1:C:242:ILE:HD12	1:C:286:LEU:CD1	2.49	0.43
1:C:473:LEU:HD13	1:C:473:LEU:C	2.38	0.43
1:C:912:ILE:HD12	2:C:1309:HOH:O	2.19	0.43
1:D:75:TYR:CD1	1:D:146:GLY:HA3	2.53	0.43
1:D:273:VAL:CG1	1:D:816:LYS:NZ	2.82	0.43
1:D:655:VAL:C	1:D:657:ALA:H	2.21	0.43
1:D:660:GLY:HA2	2:D:1241:HOH:O	2.19	0.43
1:D:777:LYS:O	1:D:781:VAL:N	2.51	0.43
1:D:803:PRO:CD	1:D:839:ALA:HB2	2.49	0.43
1:A:631:LEU:CD1	1:A:633:ILE:HD11	2.48	0.43
1:A:679:ARG:NH2	1:B:732:ARG:HH21	2.17	0.43
1:B:25:GLU:HB2	1:B:26:PRO:HD3	2.01	0.43
1:B:369:ILE:HD12	1:B:763:ARG:CZ	2.49	0.43
1:B:506:LYS:HG2	2:B:1057:HOH:O	2.17	0.43
1:C:206:ALA:HB2	1:C:378:TYR:CD2	2.54	0.43
1:D:107:LEU:HA	1:D:140:MET:SD	2.59	0.43
1:D:329:ILE:HD13	1:D:343:TYR:CE2	2.54	0.43
1:D:663:ILE:CG2	1:D:678:LEU:HD22	2.48	0.43
1:D:759:LEU:HD11	1:D:893:ARG:NH2	2.33	0.43
1:A:761:ARG:HD3	2:A:1142:HOH:O	2.18	0.43
1:A:777:LYS:C	1:A:781:VAL:HG23	2.39	0.43
1:A:858:GLU:HG3	1:A:866:MET:HE2	2.00	0.43
1:B:208:ILE:HG22	1:B:214:ILE:HD12	1.99	0.43
1:B:338:MET:HG2	1:B:341:ARG:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:THR:HG23	1:B:373:ASN:HB2	2.01	0.43
1:C:168:LEU:HA	1:C:198:ARG:HH11	1.84	0.43
1:C:732:ARG:HD2	2:C:1012:HOH:O	2.17	0.43
1:D:90:VAL:HG13	1:D:95:LYS:HB2	2.01	0.43
1:D:360:GLU:CG	1:D:362:GLU:HG2	2.48	0.43
1:D:364:GLN:HG3	1:D:887:HIS:HA	2.01	0.43
1:D:369:ILE:CG1	1:D:374:PHE:HB2	2.48	0.43
1:A:3:GLY:O	1:A:7:ARG:HG3	2.19	0.42
1:A:190:ILE:HD12	1:A:194:GLN:HE22	1.83	0.42
1:A:253:GLU:O	1:A:254:PRO:C	2.57	0.42
1:A:282:LYS:HD2	2:A:1223:HOH:O	2.18	0.42
1:A:303:MET:CA	1:A:306:GLN:HG2	2.48	0.42
1:A:381:ARG:CA	2:A:1239:HOH:O	2.60	0.42
1:A:420:VAL:HG12	1:A:422:TYR:CE1	2.54	0.42
1:A:590:GLU:HB2	2:A:1039:HOH:O	2.18	0.42
1:A:896:ILE:O	1:A:896:ILE:HG22	2.19	0.42
1:B:8:LEU:HG	1:B:9:PHE:N	2.33	0.42
1:B:131:TYR:CE1	1:B:555:ALA:HA	2.54	0.42
1:B:154:ILE:HD12	1:B:174:VAL:HG22	1.99	0.42
1:B:176:ASN:ND2	1:B:177:SER:N	2.67	0.42
1:B:559:GLU:HG3	1:B:590:GLU:OE2	2.19	0.42
1:B:697:PHE:CZ	1:B:714:LEU:HD22	2.54	0.42
1:C:215:LEU:HD13	1:C:399:TYR:CE2	2.54	0.42
1:C:315:HIS:CE1	2:C:1234:HOH:O	2.71	0.42
1:C:424:THR:HG23	1:C:427:GLY:CA	2.49	0.42
1:C:615:LYS:HE3	1:C:623:GLU:OE1	2.19	0.42
1:C:838:LYS:HG2	1:C:839:ALA:N	2.34	0.42
1:D:194:GLN:C	2:D:1156:HOH:O	2.57	0.42
1:D:735:GLU:HA	1:D:735:GLU:OE2	2.19	0.42
1:D:801:LEU:HD22	1:D:842:ALA:CB	2.49	0.42
1:A:96:ILE:HD13	1:A:211:VAL:HG21	2.02	0.42
1:A:123:VAL:HG23	2:A:1017:HOH:O	2.19	0.42
1:A:326:GLN:HG2	2:A:1199:HOH:O	2.19	0.42
1:A:526:ALA:HB1	2:A:1326:HOH:O	2.19	0.42
1:B:279:GLY:N	2:B:1079:HOH:O	2.50	0.42
1:B:840:GLU:OE2	1:B:841:GLU:HG3	2.18	0.42
1:C:65:PHE:CZ	1:C:111:LEU:HB3	2.54	0.42
1:C:379:GLU:HB2	2:C:1245:HOH:O	2.18	0.42
1:C:522:ASN:N	2:C:1106:HOH:O	2.52	0.42
1:C:821:ASP:CB	1:C:931:LYS:HG2	2.49	0.42
1:D:61:LEU:HG	1:D:65:PHE:CE1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:GLU:OE1	1:D:178:GLU:HA	2.17	0.42
1:D:466:PRO:CG	2:D:1295:HOH:O	2.67	0.42
1:D:609:VAL:O	1:D:612:PHE:HB3	2.19	0.42
1:D:759:LEU:HD11	1:D:893:ARG:HH22	1.84	0.42
1:D:820:LEU:O	1:D:820:LEU:HG	2.18	0.42
1:A:91:LEU:HD22	1:A:207:ILE:HG23	2.00	0.42
1:A:309:ARG:HH22	1:A:931:LYS:NZ	2.16	0.42
1:A:740:ARG:HH11	1:A:740:ARG:HG3	1.85	0.42
1:A:858:GLU:O	1:A:863:PRO:HD3	2.19	0.42
1:B:229:ALA:N	2:B:1044:HOH:O	2.44	0.42
1:B:349:GLN:HA	1:B:352:GLU:OE1	2.20	0.42
1:B:594:ALA:HA	1:B:597:LEU:CG	2.50	0.42
1:B:599:LYS:HB3	1:B:600:GLU:H	1.50	0.42
1:C:355:GLU:HB3	1:C:357:VAL:HG23	1.99	0.42
1:C:370:THR:C	1:C:372:GLN:N	2.73	0.42
1:C:503:ALA:CB	2:C:1317:HOH:O	2.67	0.42
1:D:273:VAL:CA	1:D:820:LEU:HB2	2.49	0.42
1:D:308:ILE:H	1:D:308:ILE:HG13	1.69	0.42
1:D:372:GLN:HA	1:D:399:TYR:OH	2.19	0.42
1:D:387:THR:HB	1:D:673:ARG:HB2	2.01	0.42
1:D:550:ASN:HA	1:D:574:THR:CB	2.48	0.42
1:D:592:LEU:HD23	1:D:592:LEU:HA	1.87	0.42
1:D:863:PRO:HB2	1:D:864:PRO:HD3	2.01	0.42
1:D:920:GLU:O	1:D:923:ALA:HB3	2.19	0.42
1:A:208:ILE:CG2	1:A:214:ILE:HD12	2.48	0.42
1:B:134:ARG:O	1:B:137:ALA:HB3	2.19	0.42
1:B:727:HIS:CD2	1:B:728:PRO:HD2	2.54	0.42
1:C:65:PHE:HE2	1:C:85:LEU:O	2.02	0.42
1:C:190:ILE:HG13	1:C:194:GLN:OE1	2.19	0.42
1:C:253:GLU:O	1:C:254:PRO:C	2.58	0.42
1:C:449:GLY:HA3	1:C:678:LEU:HD11	2.00	0.42
1:C:451:ILE:HD12	1:C:667:GLU:HG3	2.01	0.42
1:C:594:ALA:HA	1:C:597:LEU:CG	2.47	0.42
1:C:801:LEU:O	1:C:801:LEU:HD23	2.19	0.42
1:C:852:LYS:HB3	2:C:1079:HOH:O	2.19	0.42
1:D:276:THR:HG22	1:D:278:GLN:H	1.84	0.42
1:D:679:ARG:HD3	1:D:691:SER:OG	2.19	0.42
1:A:61:LEU:HD13	1:A:115:LEU:CD2	2.50	0.42
1:A:453:ILE:HG13	2:A:1047:HOH:O	2.19	0.42
1:A:492:TRP:NE1	1:A:516:LEU:HD13	2.34	0.42
1:A:732:ARG:O	1:A:736:ARG:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:ILE:HD12	1:B:174:VAL:HG21	2.01	0.42
1:B:550:ASN:H	1:B:550:ASN:HD22	1.64	0.42
1:B:688:PRO:CA	2:B:1067:HOH:O	2.67	0.42
1:C:187:ASN:HB3	1:C:767:TYR:CD2	2.55	0.42
1:C:202:PRO:CD	1:C:203:LEU:N	2.80	0.42
1:C:205:TYR:CE2	1:C:207:ILE:HD11	2.54	0.42
1:C:274:HIS:CE1	1:C:305:ILE:HA	2.54	0.42
1:C:284:GLU:CD	1:C:290:GLU:HB3	2.40	0.42
1:D:273:VAL:HG21	1:D:816:LYS:C	2.40	0.42
1:D:381:ARG:HD3	1:D:381:ARG:N	2.34	0.42
1:D:430:TYR:CB	1:D:472:ARG:HE	2.24	0.42
1:A:772:LEU:HD12	2:A:1005:HOH:O	2.19	0.42
1:B:476:ARG:HG3	1:B:476:ARG:NH1	2.35	0.42
1:C:576:MET:SD	1:C:579:ARG:NH2	2.92	0.42
1:C:753:LEU:O	1:C:757:ASP:HB2	2.19	0.42
1:C:865:LEU:HG	2:C:1238:HOH:O	2.19	0.42
1:D:258:LYS:CB	1:D:816:LYS:HE2	2.50	0.42
1:D:631:LEU:CD1	1:D:633:ILE:HD11	2.49	0.42
1:D:779:GLU:HG2	2:D:1047:HOH:O	2.18	0.42
1:D:840:GLU:OE2	1:D:841:GLU:HG3	2.20	0.42
1:A:274:HIS:CE1	1:A:305:ILE:HG23	2.55	0.42
1:A:555:ALA:O	1:A:559:GLU:HG2	2.19	0.42
1:A:754:GLN:HG2	1:A:907:PHE:CE1	2.54	0.42
1:A:887:HIS:O	1:A:891:VAL:HG23	2.19	0.42
1:B:104:GLY:HA3	2:B:1161:HOH:O	2.19	0.42
1:B:305:ILE:HG22	1:B:309:ARG:NE	2.34	0.42
1:B:652:GLU:O	1:B:656:ARG:N	2.41	0.42
1:B:679:ARG:HG2	1:B:691:SER:CB	2.50	0.42
1:C:50:LYS:HG3	2:C:1066:HOH:O	2.19	0.42
1:C:465:GLU:HG2	2:C:1289:HOH:O	2.20	0.42
1:C:470:LEU:N	1:C:471:PRO:CD	2.83	0.42
1:C:494:ARG:HB2	1:C:513:PHE:HE2	1.85	0.42
1:C:857:ARG:HH22	1:C:936:LEU:C	2.23	0.42
1:D:419:ASP:OD2	1:D:668:ARG:HD2	2.18	0.42
1:D:802:ASN:CB	1:D:839:ALA:HB1	2.49	0.42
1:A:179:LEU:HD11	1:A:378:TYR:OH	2.20	0.42
1:A:364:GLN:HG2	1:A:887:HIS:HB2	2.02	0.42
1:A:464:LYS:HB3	1:A:546:HIS:CE1	2.54	0.42
1:A:685:GLN:C	1:A:687:ASP:H	2.23	0.42
1:A:769:GLN:NE2	2:A:1106:HOH:O	2.47	0.42
1:A:915:THR:HG23	2:A:1244:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:478:GLU:HA	1:B:481:LYS:HB2	2.02	0.42
1:B:508:GLU:N	1:B:508:GLU:OE1	2.53	0.42
1:B:776:GLY:CA	1:B:871:ARG:HH22	2.32	0.42
1:B:777:LYS:HE2	2:B:1052:HOH:O	2.19	0.42
1:B:862:SER:HB2	1:B:864:PRO:HD2	2.01	0.42
1:C:85:LEU:HD23	1:C:111:LEU:HD11	2.01	0.42
1:C:260:PRO:HB3	2:C:1026:HOH:O	2.19	0.42
1:C:506:LYS:HB3	2:C:1206:HOH:O	2.20	0.42
1:C:818:THR:O	1:C:822:THR:HB	2.20	0.42
1:D:205:TYR:CE1	1:D:380:LYS:HG2	2.55	0.42
1:D:764:GLU:HG2	2:D:1101:HOH:O	2.19	0.42
1:D:798:GLU:HB2	1:D:843:VAL:HG21	2.00	0.42
1:A:274:HIS:NE2	1:A:305:ILE:HG12	2.34	0.42
1:A:354:LYS:CD	1:D:634:ARG:HH12	2.33	0.42
1:A:381:ARG:CZ	2:A:1046:HOH:O	2.67	0.42
1:A:517:ILE:CG2	1:A:524:ARG:HD2	2.50	0.42
1:A:670:GLU:CG	1:A:741:VAL:HG11	2.46	0.42
1:A:710:VAL:C	1:A:712:ALA:H	2.23	0.42
1:A:901:TYR:HD2	1:A:901:TYR:HA	1.68	0.42
2:A:1313:HOH:O	1:B:709:ARG:NH1	2.52	0.42
1:B:216:ILE:HG23	1:B:749:ARG:CZ	2.49	0.42
1:B:674:ILE:O	1:B:674:ILE:HG22	2.19	0.42
1:B:685:GLN:HA	2:B:1123:HOH:O	2.18	0.42
1:B:888:ASN:ND2	2:B:1035:HOH:O	2.53	0.42
1:C:298:MET:HA	2:C:1077:HOH:O	2.19	0.42
1:C:491:GLU:HA	1:C:494:ARG:HD2	2.02	0.42
1:C:519:PRO:HA	2:C:1228:HOH:O	2.18	0.42
1:D:313:LEU:HD12	1:D:313:LEU:O	2.19	0.42
1:D:431:ALA:O	1:D:434:GLU:HB2	2.20	0.42
1:D:710:VAL:C	1:D:712:ALA:N	2.73	0.42
1:A:276:THR:HG22	1:A:278:GLN:H	1.85	0.42
1:A:494:ARG:HB2	1:A:513:PHE:HE2	1.85	0.42
1:B:12:ASN:HA	2:B:1143:HOH:O	2.19	0.42
1:B:373:ASN:HA	1:B:376:ARG:HD3	2.02	0.42
1:B:590:GLU:HG3	1:B:591:TYR:CD1	2.55	0.42
1:B:685:GLN:C	1:B:687:ASP:H	2.23	0.42
1:B:782:LYS:O	1:B:786:ILE:HG13	2.20	0.42
1:B:802:ASN:CG	1:B:802:ASN:O	2.57	0.42
1:C:75:TYR:HD1	2:C:1265:HOH:O	2.03	0.42
1:C:327:VAL:HG21	1:C:352:GLU:HG2	2.02	0.42
1:C:572:ILE:O	1:C:572:ILE:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:635:GLU:HB2	2:C:1214:HOH:O	2.18	0.42
1:C:896:ILE:HG22	1:C:896:ILE:O	2.18	0.42
1:A:199:HIS:CD2	1:A:199:HIS:N	2.87	0.41
1:B:6:ARG:O	1:B:13:GLU:HG3	2.20	0.41
1:B:271:ARG:HH21	1:B:931:LYS:HE2	1.84	0.41
1:B:389:LYS:CE	2:B:1245:HOH:O	2.66	0.41
1:C:284:GLU:OE2	1:C:290:GLU:HA	2.20	0.41
1:C:297:ASN:HA	1:C:299:GLU:OE2	2.20	0.41
1:C:350:ALA:HB1	2:C:1338:HOH:O	2.19	0.41
1:C:474:GLU:O	1:C:477:LEU:HB2	2.19	0.41
1:D:7:ARG:HG2	1:D:13:GLU:OE1	2.20	0.41
1:D:126:VAL:HG23	1:D:176:ASN:N	2.35	0.41
1:D:184:LEU:HB3	1:D:225:ILE:HD11	2.02	0.41
1:D:589:PRO:HG2	1:D:614:LYS:HZ2	1.83	0.41
1:D:777:LYS:HB3	1:D:780:GLU:CG	2.50	0.41
1:A:110:THR:CG2	1:A:140:MET:HG2	2.50	0.41
1:A:316:ARG:NH2	1:A:354:LYS:HG3	2.35	0.41
1:B:45:ARG:N	2:B:1135:HOH:O	2.53	0.41
1:B:283:ALA:O	1:B:286:LEU:HG	2.20	0.41
1:B:549:LEU:O	1:B:577:ALA:CB	2.69	0.41
1:B:634:ARG:HA	1:B:634:ARG:HD3	1.83	0.41
1:B:792:THR:OG1	1:B:927:SER:HA	2.20	0.41
1:B:800:PHE:CG	2:B:1243:HOH:O	2.70	0.41
1:C:226:SER:HA	1:C:364:GLN:O	2.19	0.41
1:C:228:PRO:HD3	2:C:1040:HOH:O	2.20	0.41
1:C:385:THR:CG2	1:C:388:ALA:HB2	2.50	0.41
1:C:642:ARG:O	1:C:646:GLU:HB2	2.20	0.41
1:D:253:GLU:O	1:D:254:PRO:C	2.58	0.41
1:D:424:THR:HG23	1:D:427:GLY:H	1.84	0.41
1:D:472:ARG:HH11	1:D:476:ARG:NH1	2.18	0.41
1:D:753:LEU:O	1:D:753:LEU:HD22	2.20	0.41
1:D:826:LEU:HD23	1:D:830:PRO:HG3	2.01	0.41
1:A:91:LEU:CD2	1:A:207:ILE:HG23	2.49	0.41
1:A:442:ARG:HG2	1:A:658:LEU:CD2	2.50	0.41
1:A:530:LEU:O	1:A:534:VAL:HG23	2.21	0.41
1:A:656:ARG:HE	1:A:656:ARG:HB3	1.46	0.41
1:A:729:MET:HE2	1:A:729:MET:HB3	1.87	0.41
1:A:744:ARG:HG2	1:A:748:ILE:HD11	2.02	0.41
1:B:18:ARG:NE	1:B:22:GLN:HE21	2.17	0.41
1:B:293:PHE:O	1:B:293:PHE:HD2	2.03	0.41
1:B:465:GLU:C	1:B:467:ARG:H	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:553:HIS:O	1:B:557:GLU:HG3	2.21	0.41
1:C:92:HIS:C	1:C:94:GLY:H	2.23	0.41
1:C:274:HIS:CE1	1:C:305:ILE:HG23	2.55	0.41
1:C:609:VAL:O	1:C:612:PHE:HB3	2.20	0.41
1:C:740:ARG:HG3	1:C:740:ARG:NH1	2.34	0.41
1:C:821:ASP:CG	1:C:931:LYS:HE2	2.41	0.41
1:D:601:GLY:CA	2:D:1022:HOH:O	2.67	0.41
1:A:242:ILE:O	1:A:246:LEU:HB2	2.20	0.41
1:A:254:PRO:HD2	2:A:1297:HOH:O	2.20	0.41
1:A:551:ALA:HB2	1:A:577:ALA:HA	2.03	0.41
1:A:782:LYS:O	1:A:786:ILE:HG13	2.20	0.41
1:B:276:THR:HB	2:B:1079:HOH:O	2.19	0.41
1:B:355:GLU:HB3	1:B:357:VAL:HG23	2.03	0.41
1:B:608:LYS:HD2	1:B:608:LYS:N	2.35	0.41
1:B:705:PHE:CE2	1:B:741:VAL:HG13	2.55	0.41
1:C:436:ILE:HD11	1:C:448:VAL:HG21	2.02	0.41
1:C:770:ARG:HG3	1:C:875:LEU:CD2	2.50	0.41
1:D:198:ARG:H	1:D:198:ARG:HG2	1.49	0.41
1:D:258:LYS:HD3	1:D:258:LYS:N	2.17	0.41
1:D:643:GLU:O	1:D:647:GLU:HB3	2.20	0.41
1:D:805:VAL:N	2:D:1080:HOH:O	2.50	0.41
1:A:75:TYR:HB3	1:A:607:TRP:NE1	2.36	0.41
1:A:271:ARG:HG2	2:A:1243:HOH:O	2.21	0.41
1:A:303:MET:HA	1:A:306:GLN:CG	2.49	0.41
1:A:382:ALA:CA	1:A:401:MET:SD	3.09	0.41
1:A:679:ARG:HH21	1:B:732:ARG:NH2	2.18	0.41
1:A:857:ARG:O	1:A:861:LEU:HG	2.19	0.41
1:B:61:LEU:HB3	1:B:62:PRO:HD3	2.03	0.41
1:B:237:TYR:OH	1:B:358:ARG:HA	2.19	0.41
1:B:253:GLU:CG	1:B:256:VAL:HG13	2.51	0.41
1:B:323:GLN:NE2	1:B:328:ILE:HD12	2.35	0.41
1:B:333:PHE:HD2	2:B:1055:HOH:O	2.02	0.41
1:B:673:ARG:HG3	1:B:674:ILE:N	2.35	0.41
1:B:826:LEU:HD23	1:B:830:PRO:HG3	2.02	0.41
1:C:121:LYS:C	1:C:198:ARG:NH2	2.74	0.41
1:C:539:VAL:O	1:C:542:GLN:HB3	2.20	0.41
1:D:319:ASP:O	1:D:330:VAL:HB	2.20	0.41
1:D:396:GLN:O	1:D:400:GLY:HA2	2.21	0.41
1:D:476:ARG:HD2	1:D:476:ARG:HA	1.79	0.41
1:D:695:VAL:HG12	1:D:696:SER:N	2.35	0.41
1:D:801:LEU:O	1:D:839:ALA:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:GLY:CA	1:A:105:LYS:NZ	2.83	0.41
1:A:218:GLU:HG2	2:A:1333:HOH:O	2.20	0.41
1:A:409:ASN:HB3	1:A:685:GLN:NE2	2.33	0.41
1:A:501:ARG:HA	1:A:502:PRO:HD3	1.90	0.41
1:A:837:LEU:HD13	1:A:841:GLU:HB3	2.03	0.41
1:B:75:TYR:CD1	1:B:146:GLY:HA3	2.55	0.41
1:B:604:ARG:CD	1:B:605:TYR:H	2.32	0.41
1:C:75:TYR:CD2	1:C:607:TRP:HZ2	2.39	0.41
1:C:199:HIS:CD2	1:C:199:HIS:N	2.89	0.41
1:C:338:MET:HG2	1:C:341:ARG:CG	2.51	0.41
1:C:435:GLU:CG	2:C:1315:HOH:O	2.64	0.41
1:C:484:SER:O	1:C:487:GLN:OE1	2.39	0.41
1:C:503:ALA:HB3	2:C:1317:HOH:O	2.20	0.41
1:C:716:ARG:CG	1:D:6:ARG:CG	2.96	0.41
1:D:535:HIS:O	1:D:539:VAL:HG23	2.21	0.41
1:D:631:LEU:HD12	1:D:633:ILE:HD11	2.02	0.41
1:D:671:SER:HG	1:D:673:ARG:HG2	1.86	0.41
1:D:810:TRP:CD1	1:D:810:TRP:N	2.88	0.41
1:A:87:GLY:HA3	1:A:99:MET:HE2	2.03	0.41
1:A:243:ALA:HB3	2:A:1211:HOH:O	2.21	0.41
1:A:279:GLY:HA2	2:A:1223:HOH:O	2.20	0.41
1:A:428:LYS:NZ	1:A:699:ASP:HB3	2.36	0.41
1:A:548:VAL:HG22	1:A:572:ILE:HD12	2.02	0.41
1:A:789:VAL:O	1:A:793:VAL:HG23	2.20	0.41
1:A:855:GLU:HB2	2:A:1207:HOH:O	2.20	0.41
1:B:7:ARG:HG2	1:B:13:GLU:OE2	2.21	0.41
1:B:19:TYR:HB3	1:B:86:ILE:HG23	2.03	0.41
1:B:65:PHE:CD2	1:B:111:LEU:HD22	2.55	0.41
1:B:131:TYR:CD2	1:B:131:TYR:C	2.94	0.41
1:B:344:GLY:O	1:B:345:GLU:HG3	2.20	0.41
1:B:563:GLN:NE2	1:B:590:GLU:HB3	2.36	0.41
1:B:759:LEU:HD21	1:B:893:ARG:NH1	2.35	0.41
1:B:869:VAL:O	1:B:873:VAL:HG23	2.20	0.41
1:C:211:VAL:HG23	1:C:212:ASP:H	1.84	0.41
1:C:281:ALA:O	1:C:285:LYS:HG3	2.21	0.41
1:C:349:GLN:NE2	2:C:1323:HOH:O	2.52	0.41
1:C:602:PHE:CD1	1:C:603:ASP:N	2.84	0.41
1:C:797:ALA:HB1	1:C:801:LEU:HD12	2.01	0.41
1:C:820:LEU:HA	1:C:935:ARG:NH2	2.36	0.41
1:D:30:LEU:O	1:D:34:VAL:HG23	2.20	0.41
1:D:233:THR:HG23	1:D:237:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:252:ALA:CB	2:D:1237:HOH:O	2.67	0.41
1:D:273:VAL:HA	1:D:820:LEU:CB	2.51	0.41
1:D:349:GLN:CD	1:D:349:GLN:H	2.17	0.41
1:D:368:THR:HG22	1:D:369:ILE:N	2.36	0.41
1:D:477:LEU:HD21	1:D:499:LEU:HB3	2.03	0.41
1:D:835:ARG:O	1:D:835:ARG:HD3	2.20	0.41
1:D:921:MET:SD	1:D:925:ILE:HD11	2.61	0.41
1:A:145:ARG:CB	1:A:607:TRP:CH2	3.01	0.41
1:A:596:LEU:HD12	1:A:613:ILE:HD11	2.02	0.41
1:A:617:VAL:HA	1:A:645:ARG:HD2	2.03	0.41
1:B:22:GLN:NE2	2:B:1130:HOH:O	2.54	0.41
1:B:41:ALA:CB	2:B:1184:HOH:O	2.55	0.41
1:B:503:ALA:O	1:B:504:GLN:C	2.59	0.41
1:B:563:GLN:CG	1:B:591:TYR:HE1	2.34	0.41
1:C:259:GLU:HG2	1:C:260:PRO:HD3	2.00	0.41
1:C:553:HIS:CG	1:C:556:ARG:HB2	2.56	0.41
1:C:685:GLN:HE21	1:C:685:GLN:HB3	1.62	0.41
1:D:195:LEU:HA	2:D:1156:HOH:O	2.21	0.41
1:D:248:ARG:NH1	1:D:312:GLU:HG3	2.36	0.41
1:D:503:ALA:C	1:D:505:LEU:N	2.74	0.41
1:D:770:ARG:NH1	1:D:770:ARG:HG3	2.36	0.41
1:D:803:PRO:CB	2:D:1080:HOH:O	2.63	0.41
1:A:69:ARG:O	1:A:72:ALA:HB3	2.21	0.41
1:A:83:VAL:O	1:A:86:ILE:HB	2.21	0.41
1:A:127:THR:HG23	1:A:209:ASP:CB	2.46	0.41
1:A:327:VAL:HG21	1:A:352:GLU:HG2	2.03	0.41
1:A:362:GLU:HB3	2:A:1204:HOH:O	2.21	0.41
1:A:492:TRP:CD1	1:A:516:LEU:HD13	2.55	0.41
1:B:32:ALA:O	1:B:35:GLU:HG2	2.21	0.41
1:B:159:THR:CB	1:B:160:PRO:HD2	2.51	0.41
1:B:227:GLY:CA	1:B:366:LEU:HD21	2.50	0.41
1:B:237:TYR:HE1	2:B:1097:HOH:O	2.04	0.41
1:B:275:LEU:HD12	1:B:816:LYS:HZ2	1.85	0.41
1:B:316:ARG:HA	1:B:320:TYR:CZ	2.56	0.41
1:B:364:GLN:HA	1:B:364:GLN:OE1	2.21	0.41
1:B:444:GLN:NE2	1:B:659:GLY:HA3	2.36	0.41
1:C:76:LEU:HD21	1:C:140:MET:HE2	2.03	0.41
1:C:269:LYS:HG3	2:C:1127:HOH:O	2.20	0.41
1:C:271:ARG:HH21	1:C:931:LYS:NZ	2.18	0.41
1:C:273:VAL:CG1	1:C:820:LEU:HD13	2.50	0.41
1:C:293:PHE:HE2	1:C:301:ALA:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:423:ARG:HB2	1:C:725:ILE:HD11	2.03	0.41
1:C:497:LYS:HA	1:C:500:GLU:HB2	2.02	0.41
1:C:710:VAL:HG11	1:C:733:SER:CB	2.50	0.41
1:C:714:LEU:HA	1:C:729:MET:HE1	2.03	0.41
1:C:716:ARG:C	1:C:718:GLY:N	2.74	0.41
1:D:76:LEU:HD12	1:D:142:PRO:HG2	2.01	0.41
1:D:76:LEU:HD13	1:D:143:VAL:HG23	2.03	0.41
1:D:126:VAL:HG21	1:D:176:ASN:HB3	2.02	0.41
1:D:175:THR:N	2:D:1118:HOH:O	2.54	0.41
1:D:294:SER:O	1:D:936:LEU:HD12	2.21	0.41
1:D:503:ALA:O	1:D:504:GLN:C	2.59	0.41
1:D:550:ASN:O	1:D:552:LYS:N	2.54	0.41
1:D:657:ALA:HB2	2:D:1190:HOH:O	2.21	0.41
1:D:801:LEU:HD11	1:D:834:LEU:HD13	2.01	0.41
1:A:16:ILE:HG12	1:A:407:PRO:HD3	2.02	0.41
1:A:20:TYR:HA	1:A:24:VAL:CG2	2.50	0.41
1:A:164:ARG:HB2	1:A:164:ARG:CZ	2.51	0.41
1:A:373:ASN:HB3	1:A:763:ARG:HH22	1.86	0.41
1:A:752:LEU:HD12	2:A:1286:HOH:O	2.20	0.41
1:B:394:GLU:HG3	1:B:398:ILE:HD12	2.03	0.41
1:B:520:LYS:NZ	2:B:1145:HOH:O	2.54	0.41
1:B:585:LEU:HD22	1:B:655:VAL:HG12	2.03	0.41
1:B:609:VAL:O	1:B:612:PHE:HB3	2.21	0.41
1:B:843:VAL:O	1:B:847:VAL:HG23	2.21	0.41
1:C:96:ILE:HA	1:C:383:GLY:O	2.21	0.41
1:C:239:MET:HG3	1:C:307:ALA:CB	2.51	0.41
1:C:338:MET:SD	1:C:341:ARG:CB	3.09	0.41
1:C:465:GLU:O	1:C:467:ARG:N	2.54	0.41
1:C:715:ASP:HB2	1:D:6:ARG:CZ	2.51	0.41
1:C:753:LEU:HB3	2:C:1071:HOH:O	2.21	0.41
1:C:770:ARG:NH1	2:C:1226:HOH:O	2.53	0.41
1:C:805:VAL:HG23	2:C:1090:HOH:O	2.21	0.41
1:D:79:ARG:HB2	2:D:1046:HOH:O	2.21	0.41
1:D:211:VAL:CG1	1:D:383:GLY:HA3	2.50	0.41
1:D:381:ARG:NH1	1:D:381:ARG:HG2	2.36	0.41
1:D:458:ARG:NE	2:D:1127:HOH:O	2.54	0.41
1:D:520:LYS:HA	1:D:520:LYS:HD3	1.93	0.41
1:D:553:HIS:CE1	1:D:556:ARG:HD3	2.56	0.41
1:D:770:ARG:NH1	1:D:879:ASP:HB2	2.33	0.41
1:A:250:LEU:HD23	2:A:1015:HOH:O	2.21	0.40
1:A:461:GLN:O	1:A:465:GLU:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:LYS:C	1:A:466:PRO:HD3	2.42	0.40
1:A:540:LEU:CD2	1:A:544:ILE:HD11	2.52	0.40
1:A:727:HIS:HA	1:A:728:PRO:HD3	1.95	0.40
1:A:857:ARG:C	1:A:859:ALA:H	2.23	0.40
1:A:870:GLU:HA	1:A:933:LEU:HD21	2.03	0.40
2:A:1051:HOH:O	1:B:728:PRO:HA	2.21	0.40
1:B:684:ARG:CG	1:B:685:GLN:H	2.29	0.40
1:C:16:ILE:HG12	1:C:407:PRO:HD3	2.02	0.40
1:C:281:ALA:HA	1:C:284:GLU:OE1	2.20	0.40
1:C:576:MET:SD	1:C:579:ARG:CZ	3.09	0.40
1:D:176:ASN:ND2	1:D:176:ASN:N	2.69	0.40
1:D:294:SER:HB2	1:D:937:LYS:HD2	2.03	0.40
1:D:369:ILE:HG13	1:D:370:THR:N	2.35	0.40
1:D:381:ARG:HD2	2:D:1249:HOH:O	2.21	0.40
1:D:433:VAL:HG13	1:D:463:LEU:HD23	2.02	0.40
1:D:524:ARG:NH2	2:D:1277:HOH:O	2.53	0.40
1:D:575:ASN:HA	2:D:1220:HOH:O	2.21	0.40
1:D:582:ASP:HB3	1:D:684:ARG:NH2	2.21	0.40
1:D:598:GLU:HB3	2:D:1236:HOH:O	2.19	0.40
1:D:753:LEU:O	1:D:753:LEU:HD13	2.21	0.40
1:D:932:PHE:O	1:D:936:LEU:HB2	2.21	0.40
1:A:263:ASP:OD2	1:A:273:VAL:HB	2.21	0.40
1:B:35:GLU:HA	1:B:74:ARG:NH2	2.36	0.40
1:B:288:GLY:HA3	2:B:1127:HOH:O	2.19	0.40
1:B:418:PRO:HB2	2:B:1037:HOH:O	2.21	0.40
1:C:429:PHE:O	1:C:430:TYR:C	2.59	0.40
1:C:435:GLU:CD	1:C:694:TYR:OH	2.58	0.40
1:C:800:PHE:HE1	1:C:813:GLU:HB2	1.84	0.40
1:C:833:GLU:HA	1:C:837:LEU:HG	2.03	0.40
1:C:882:TRP:CZ3	1:C:885:HIS:HD2	2.39	0.40
1:D:7:ARG:HA	1:D:13:GLU:CG	2.51	0.40
1:D:61:LEU:HB3	1:D:62:PRO:HD3	2.02	0.40
1:D:167:TYR:O	1:D:198:ARG:NH1	2.51	0.40
1:D:253:GLU:HG3	1:D:256:VAL:HG13	2.02	0.40
1:D:271:ARG:HB3	2:D:1032:HOH:O	2.21	0.40
1:D:530:LEU:O	1:D:530:LEU:HD23	2.21	0.40
1:D:700:ASP:HB2	2:D:1051:HOH:O	2.20	0.40
1:D:861:LEU:HD12	1:D:866:MET:HA	2.02	0.40
1:A:23:VAL:O	1:A:27:VAL:HG23	2.22	0.40
1:A:259:GLU:CB	1:A:260:PRO:HD3	2.51	0.40
1:A:269:LYS:HD3	1:A:271:ARG:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:ILE:HG23	1:A:293:PHE:CE1	2.56	0.40
1:A:291:GLY:O	1:A:293:PHE:N	2.55	0.40
1:A:449:GLY:HA3	1:A:678:LEU:HD11	2.03	0.40
1:A:572:ILE:O	1:A:572:ILE:HG22	2.20	0.40
1:A:777:LYS:O	1:A:780:GLU:N	2.54	0.40
1:B:55:ALA:N	2:B:1084:HOH:O	2.54	0.40
1:B:295:PRO:HB3	1:B:937:LYS:O	2.21	0.40
1:B:408:THR:HG22	1:B:409:ASN:N	2.37	0.40
1:B:517:ILE:HA	1:B:518:PRO:HD2	1.92	0.40
1:B:710:VAL:C	1:B:712:ALA:H	2.23	0.40
1:C:78:MET:CE	2:C:1334:HOH:O	2.67	0.40
1:C:119:THR:HG21	1:C:121:LYS:HE3	2.03	0.40
1:C:309:ARG:HG2	1:C:313:LEU:CD2	2.50	0.40
1:C:805:VAL:HG12	2:C:1194:HOH:O	2.22	0.40
1:C:864:PRO:O	1:C:867:ARG:HG2	2.22	0.40
1:D:273:VAL:HG11	1:D:816:LYS:O	2.22	0.40
1:D:305:ILE:HG22	1:D:309:ARG:HE	1.85	0.40
1:D:355:GLU:HA	1:D:355:GLU:OE1	2.21	0.40
1:D:599:LYS:HB2	1:D:599:LYS:HE2	1.87	0.40
1:D:705:PHE:HB3	1:D:741:VAL:HG22	2.03	0.40
1:A:99:MET:O	1:A:105:LYS:HE3	2.21	0.40
1:A:239:MET:HG3	1:A:307:ALA:HB2	2.04	0.40
1:A:457:GLU:O	1:A:460:SER:N	2.55	0.40
1:A:674:ILE:O	1:A:674:ILE:HG22	2.22	0.40
1:A:777:LYS:O	1:A:781:VAL:N	2.54	0.40
1:A:800:PHE:CD2	1:A:800:PHE:N	2.88	0.40
1:B:206:ALA:HB2	1:B:378:TYR:CD2	2.56	0.40
1:B:253:GLU:O	1:B:254:PRO:C	2.60	0.40
1:B:343:TYR:CD1	1:B:351:ILE:HD12	2.56	0.40
1:B:347:LEU:O	1:B:347:LEU:HG	2.21	0.40
1:B:445:PRO:O	1:B:661:LEU:O	2.39	0.40
1:B:502:PRO:HD3	2:B:1203:HOH:O	2.21	0.40
1:B:654:ARG:O	1:B:658:LEU:HB2	2.20	0.40
1:C:334:THR:HB	1:C:336:ARG:HG2	2.02	0.40
1:C:390:THR:HA	1:D:709:ARG:NH1	2.36	0.40
1:C:481:LYS:HA	1:C:496:ARG:HH22	1.87	0.40
1:C:694:TYR:CD1	1:C:694:TYR:N	2.90	0.40
1:C:816:LYS:HA	1:C:819:LEU:HB2	2.02	0.40
1:D:124:HIS:CE1	2:D:1116:HOH:O	2.74	0.40
1:D:130:ASP:O	1:D:131:TYR:C	2.60	0.40
1:D:233:THR:H	1:D:361:ARG:NH1	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:274:HIS:N	1:D:274:HIS:ND1	2.60	0.40
1:D:458:ARG:HH11	1:D:458:ARG:HG3	1.86	0.40
1:D:479:LEU:O	1:D:482:LYS:HG2	2.21	0.40
1:D:840:GLU:HG3	1:D:841:GLU:N	2.36	0.40
1:A:119:THR:CG2	1:A:121:LYS:HE3	2.51	0.40
1:A:820:LEU:O	1:A:935:ARG:NH2	2.54	0.40
1:A:878:VAL:HG22	1:A:925:ILE:HG21	2.03	0.40
1:B:79:ARG:N	2:B:1166:HOH:O	2.46	0.40
1:B:563:GLN:OE1	1:B:587:GLY:HA3	2.22	0.40
1:B:749:ARG:HH11	1:B:749:ARG:HD2	1.77	0.40
1:B:837:LEU:HD12	1:B:837:LEU:O	2.21	0.40
1:C:57:LEU:O	1:C:115:LEU:HD11	2.22	0.40
1:C:164:ARG:HG3	1:C:196:VAL:O	2.22	0.40
1:C:198:ARG:H	1:C:198:ARG:HG2	1.59	0.40
1:D:9:PHE:HB2	2:D:1055:HOH:O	2.22	0.40
1:D:130:ASP:HB2	2:D:1033:HOH:O	2.21	0.40
1:D:196:VAL:HG23	1:D:197:LEU:N	2.37	0.40
1:D:304:LEU:O	1:D:308:ILE:HG13	2.22	0.40
1:D:369:ILE:HD12	1:D:763:ARG:NH2	2.37	0.40
1:D:549:LEU:O	1:D:577:ALA:CB	2.70	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	937/997 (94%)	789 (84%)	101 (11%)	47 (5%)	2	6
1	B	932/997 (94%)	778 (84%)	108 (12%)	46 (5%)	2	7
1	C	937/997 (94%)	784 (84%)	108 (12%)	45 (5%)	2	7
1	D	932/997 (94%)	777 (83%)	107 (12%)	48 (5%)	2	6
All	All	3738/3988 (94%)	3128 (84%)	424 (11%)	186 (5%)	2	6

All (186) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	11	ASN
1	A	12	ASN
1	A	231	LYS
1	A	254	PRO
1	A	259	GLU
1	A	267	GLU
1	A	316	ARG
1	A	547	GLN
1	A	551	ALA
1	A	574	THR
1	A	684	ARG
1	A	806	HIS
1	A	809	ASP
1	A	838	LYS
1	A	902	GLY
1	B	231	LYS
1	B	254	PRO
1	B	259	GLU
1	B	267	GLU
1	B	316	ARG
1	B	466	PRO
1	B	547	GLN
1	B	551	ALA
1	B	574	THR
1	B	603	ASP
1	B	684	ARG
1	B	806	HIS
1	B	809	ASP
1	B	838	LYS
1	B	902	GLY
1	C	2	LEU
1	C	11	ASN
1	C	12	ASN
1	C	231	LYS
1	C	254	PRO
1	C	259	GLU
1	C	267	GLU
1	C	316	ARG
1	C	547	GLN
1	C	551	ALA
1	C	574	THR

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Mol	Chain	Res	Type
1	C	684	ARG
1	C	806	HIS
1	C	809	ASP
1	C	838	LYS
1	D	9	PHE
1	D	231	LYS
1	D	254	PRO
1	D	259	GLU
1	D	267	GLU
1	D	316	ARG
1	D	466	PRO
1	D	547	GLN
1	D	551	ALA
1	D	574	THR
1	D	684	ARG
1	D	806	HIS
1	D	809	ASP
1	D	838	LYS
1	D	902	GLY
1	A	260	PRO
1	A	489	GLY
1	A	603	ASP
1	B	102	GLY
1	B	260	PRO
1	B	292	LEU
1	B	489	GLY
1	B	522	ASN
1	B	601	GLY
1	B	656	ARG
1	B	860	GLU
1	C	260	PRO
1	C	371	TYR
1	C	489	GLY
1	C	522	ASN
1	C	603	ASP
1	C	902	GLY
1	D	102	GLY
1	D	202	PRO
1	D	260	PRO
1	D	292	LEU
1	D	489	GLY
1	D	505	LEU

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Mol	Chain	Res	Type
1	D	522	ASN
1	D	603	ASP
1	A	292	LEU
1	A	317	ASP
1	A	522	ASN
1	A	567	SER
1	A	605	TYR
1	B	9	PHE
1	B	251	PRO
1	B	317	ASP
1	B	485	GLN
1	B	505	LEU
1	B	521	GLY
1	B	567	SER
1	B	700	ASP
1	B	794	ALA
1	B	899	ARG
1	C	292	LEU
1	C	466	PRO
1	C	505	LEU
1	C	521	GLY
1	C	567	SER
1	C	756	ASP
1	C	794	ALA
1	D	12	ASN
1	D	317	ASP
1	D	485	GLN
1	D	521	GLY
1	D	567	SER
1	D	604	ARG
1	D	605	TYR
1	D	794	ALA
1	D	899	ARG
1	A	102	GLY
1	A	202	PRO
1	A	257	ARG
1	A	485	GLN
1	A	505	LEU
1	A	521	GLY
1	A	546	HIS
1	A	794	ALA
1	A	899	ARG

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Mol	Chain	Res	Type
1	B	12	ASN
1	B	202	PRO
1	B	605	TYR
1	C	102	GLY
1	C	251	PRO
1	C	317	ASP
1	C	605	TYR
1	D	251	PRO
1	D	700	ASP
1	D	807	PRO
1	A	201	HIS
1	A	251	PRO
1	A	588	ASN
1	A	601	GLY
1	A	662	PHE
1	B	201	HIS
1	B	686	GLY
1	B	807	PRO
1	C	201	HIS
1	C	418	PRO
1	C	485	GLN
1	C	546	HIS
1	C	577	ALA
1	C	588	ASN
1	C	601	GLY
1	C	807	PRO
1	D	201	HIS
1	D	418	PRO
1	D	588	ASN
1	A	325	GLY
1	A	466	PRO
1	B	325	GLY
1	B	418	PRO
1	D	257	ARG
1	D	325	GLY
1	D	656	ARG
1	D	803	PRO
1	A	862	SER
1	A	895	GLY
1	C	765	VAL
1	C	895	GLY
1	D	895	GLY

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Mol	Chain	Res	Type
1	A	418	PRO
1	A	803	PRO
1	A	807	PRO
1	B	588	ASN
1	B	803	PRO
1	B	895	GLY
1	D	291	GLY
1	D	862	SER
1	A	765	VAL
1	B	291	GLY
1	B	465	GLU
1	C	325	GLY
1	D	465	GLU
1	D	765	VAL
1	A	686	GLY
1	D	686	GLY
1	C	202	PRO
1	C	502	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	788/840 (94%)	667 (85%)	121 (15%)	2	8
1	B	784/840 (93%)	660 (84%)	124 (16%)	2	8
1	C	788/840 (94%)	672 (85%)	116 (15%)	3	9
1	D	784/840 (93%)	655 (84%)	129 (16%)	2	7
All	All	3144/3360 (94%)	2654 (84%)	490 (16%)	2	8

All (490) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASP
1	A	20	TYR
1	A	33	GLU

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Mol	Chain	Res	Type
1	A	49	GLU
1	A	57	LEU
1	A	65	PHE
1	A	78	MET
1	A	86	ILE
1	A	110	THR
1	A	119	THR
1	A	126	VAL
1	A	127	THR
1	A	128	VAL
1	A	138	GLU
1	A	140	MET
1	A	155	GLN
1	A	190	ILE
1	A	198	ARG
1	A	200	ASP
1	A	231	LYS
1	A	241	GLU
1	A	254	PRO
1	A	258	LYS
1	A	264	TYR
1	A	266	VAL
1	A	267	GLU
1	A	270	ASN
1	A	271	ARG
1	A	274	HIS
1	A	312	GLU
1	A	313	LEU
1	A	315	HIS
1	A	317	ASP
1	A	318	ARG
1	A	324	ASP
1	A	328	ILE
1	A	331	ASP
1	A	341	ARG
1	A	349	GLN
1	A	354	LYS
1	A	355	GLU
1	A	360	GLU
1	A	361	ARG
1	A	362	GLU
1	A	370	THR

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Mol	Chain	Res	Type
1	A	381	ARG
1	A	384	MET
1	A	397	GLU
1	A	413	ILE
1	A	424	THR
1	A	435	GLU
1	A	457	GLU
1	A	459	LEU
1	A	467	ARG
1	A	472	ARG
1	A	496	ARG
1	A	507	ASP
1	A	528	GLU
1	A	537	LEU
1	A	544	ILE
1	A	546	HIS
1	A	547	GLN
1	A	550	ASN
1	A	579	ARG
1	A	582	ASP
1	A	602	PHE
1	A	605	TYR
1	A	608	LYS
1	A	614	LYS
1	A	616	MET
1	A	621	GLU
1	A	622	GLU
1	A	646	GLU
1	A	647	GLU
1	A	652	GLU
1	A	653	GLU
1	A	656	ARG
1	A	658	LEU
1	A	661	LEU
1	A	666	THR
1	A	671	SER
1	A	675	ASP
1	A	678	LEU
1	A	685	GLN
1	A	700	ASP
1	A	701	LEU
1	A	708	ASP

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Mol	Chain	Res	Type
1	A	709	ARG
1	A	713	MET
1	A	722	SER
1	A	729	MET
1	A	753	LEU
1	A	756	ASP
1	A	757	ASP
1	A	759	LEU
1	A	761	ARG
1	A	762	GLN
1	A	800	PHE
1	A	809	ASP
1	A	810	TRP
1	A	813	GLU
1	A	819	LEU
1	A	825	GLN
1	A	827	GLN
1	A	833	GLU
1	A	844	GLU
1	A	845	ARG
1	A	852	LYS
1	A	854	TYR
1	A	861	LEU
1	A	865	LEU
1	A	866	MET
1	A	879	ASP
1	A	884	GLU
1	A	897	PHE
1	A	901	TYR
1	A	905	ASP
1	A	916	ARG
1	A	927	SER
1	A	932	PHE
1	A	934	PHE
1	B	6	ARG
1	B	8	LEU
1	B	9	PHE
1	B	10	ASP
1	B	11	ASN
1	B	20	TYR
1	B	70	GLU
1	B	75	TYR

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Mol	Chain	Res	Type
1	B	78	MET
1	B	103	GLU
1	B	116	ASN
1	B	126	VAL
1	B	127	THR
1	B	138	GLU
1	B	140	MET
1	B	172	THR
1	B	176	ASN
1	B	177	SER
1	B	178	GLU
1	B	186	ASP
1	B	198	ARG
1	B	213	SER
1	B	221	THR
1	B	231	LYS
1	B	234	ASP
1	B	253	GLU
1	B	254	PRO
1	B	256	VAL
1	B	258	LYS
1	B	264	TYR
1	B	271	ARG
1	B	275	LEU
1	B	293	PHE
1	B	304	LEU
1	B	332	GLU
1	B	341	ARG
1	B	345	GLU
1	B	349	GLN
1	B	360	GLU
1	B	363	ASN
1	B	370	THR
1	B	381	ARG
1	B	390	THR
1	B	393	LYS
1	B	402	ASP
1	B	409	ASN
1	B	410	ARG
1	B	423	ARG
1	B	424	THR
1	B	435	GLU

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Mol	Chain	Res	Type
1	B	450	THR
1	B	451	ILE
1	B	457	GLU
1	B	473	LEU
1	B	476	ARG
1	B	477	LEU
1	B	487	GLN
1	B	495	LEU
1	B	496	ARG
1	B	508	GLU
1	B	522	ASN
1	B	524	ARG
1	B	537	LEU
1	B	546	HIS
1	B	550	ASN
1	B	559	GLU
1	B	575	ASN
1	B	582	ASP
1	B	604	ARG
1	B	605	TYR
1	B	608	LYS
1	B	614	LYS
1	B	615	LYS
1	B	622	GLU
1	B	646	GLU
1	B	647	GLU
1	B	652	GLU
1	B	653	GLU
1	B	661	LEU
1	B	677	GLN
1	B	678	LEU
1	B	684	ARG
1	B	685	GLN
1	B	688	PRO
1	B	699	ASP
1	B	701	LEU
1	B	703	ARG
1	B	713	MET
1	B	715	ASP
1	B	717	MET
1	B	724	PRO
1	B	731	THR

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Mol	Chain	Res	Type
1	B	732	ARG
1	B	740	ARG
1	B	743	ASP
1	B	752	LEU
1	B	756	ASP
1	B	757	ASP
1	B	759	LEU
1	B	762	GLN
1	B	796	LEU
1	B	798	GLU
1	B	800	PHE
1	B	802	ASN
1	B	809	ASP
1	B	810	TRP
1	B	811	ASP
1	B	818	THR
1	B	821	ASP
1	B	826	LEU
1	B	827	GLN
1	B	830	PRO
1	B	831	PHE
1	B	833	GLU
1	B	840	GLU
1	B	845	ARG
1	B	854	TYR
1	B	861	LEU
1	B	876	ASN
1	B	879	ASP
1	B	897	PHE
1	B	901	TYR
1	B	903	GLN
1	B	905	ASP
1	C	10	ASP
1	C	20	TYR
1	C	33	GLU
1	C	35	GLU
1	C	57	LEU
1	C	78	MET
1	C	86	ILE
1	C	110	THR
1	C	126	VAL
1	C	127	THR

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Mol	Chain	Res	Type
1	C	128	VAL
1	C	138	GLU
1	C	140	MET
1	C	155	GLN
1	C	179	LEU
1	C	190	ILE
1	C	196	VAL
1	C	198	ARG
1	C	200	ASP
1	C	231	LYS
1	C	241	GLU
1	C	254	PRO
1	C	258	LYS
1	C	264	TYR
1	C	267	GLU
1	C	270	ASN
1	C	271	ARG
1	C	274	HIS
1	C	312	GLU
1	C	313	LEU
1	C	315	HIS
1	C	317	ASP
1	C	318	ARG
1	C	324	ASP
1	C	328	ILE
1	C	331	ASP
1	C	349	GLN
1	C	354	LYS
1	C	355	GLU
1	C	360	GLU
1	C	361	ARG
1	C	362	GLU
1	C	370	THR
1	C	381	ARG
1	C	397	GLU
1	C	409	ASN
1	C	424	THR
1	C	435	GLU
1	C	456	SER
1	C	457	GLU
1	C	467	ARG
1	C	472	ARG

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Mol	Chain	Res	Type
1	C	507	ASP
1	C	544	ILE
1	C	546	HIS
1	C	547	GLN
1	C	550	ASN
1	C	569	THR
1	C	579	ARG
1	C	599	LYS
1	C	602	PHE
1	C	605	TYR
1	C	607	TRP
1	C	608	LYS
1	C	614	LYS
1	C	621	GLU
1	C	646	GLU
1	C	652	GLU
1	C	653	GLU
1	C	656	ARG
1	C	658	LEU
1	C	661	LEU
1	C	666	THR
1	C	675	ASP
1	C	678	LEU
1	C	685	GLN
1	C	700	ASP
1	C	701	LEU
1	C	707	SER
1	C	708	ASP
1	C	709	ARG
1	C	713	MET
1	C	715	ASP
1	C	722	SER
1	C	731	THR
1	C	753	LEU
1	C	756	ASP
1	C	757	ASP
1	C	759	LEU
1	C	761	ARG
1	C	762	GLN
1	C	800	PHE
1	C	809	ASP
1	C	810	TRP

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Mol	Chain	Res	Type
1	C	813	GLU
1	C	819	LEU
1	C	825	GLN
1	C	827	GLN
1	C	830	PRO
1	C	833	GLU
1	C	844	GLU
1	C	845	ARG
1	C	852	LYS
1	C	854	TYR
1	C	861	LEU
1	C	865	LEU
1	C	866	MET
1	C	879	ASP
1	C	897	PHE
1	C	901	TYR
1	C	905	ASP
1	C	916	ARG
1	C	921	MET
1	C	927	SER
1	C	932	PHE
1	C	934	PHE
1	D	6	ARG
1	D	8	LEU
1	D	9	PHE
1	D	10	ASP
1	D	11	ASN
1	D	20	TYR
1	D	21	LYS
1	D	70	GLU
1	D	75	TYR
1	D	78	MET
1	D	82	ASP
1	D	103	GLU
1	D	116	ASN
1	D	126	VAL
1	D	127	THR
1	D	140	MET
1	D	172	THR
1	D	176	ASN
1	D	177	SER
1	D	178	GLU

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Mol	Chain	Res	Type
1	D	186	ASP
1	D	198	ARG
1	D	213	SER
1	D	221	THR
1	D	231	LYS
1	D	234	ASP
1	D	253	GLU
1	D	254	PRO
1	D	256	VAL
1	D	258	LYS
1	D	264	TYR
1	D	266	VAL
1	D	275	LEU
1	D	293	PHE
1	D	298	MET
1	D	304	LEU
1	D	332	GLU
1	D	341	ARG
1	D	345	GLU
1	D	349	GLN
1	D	360	GLU
1	D	370	THR
1	D	381	ARG
1	D	390	THR
1	D	402	ASP
1	D	409	ASN
1	D	410	ARG
1	D	423	ARG
1	D	424	THR
1	D	450	THR
1	D	451	ILE
1	D	457	GLU
1	D	459	LEU
1	D	473	LEU
1	D	476	ARG
1	D	477	LEU
1	D	486	LYS
1	D	487	GLN
1	D	495	LEU
1	D	496	ARG
1	D	508	GLU
1	D	522	ASN

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Mol	Chain	Res	Type
1	D	528	GLU
1	D	537	LEU
1	D	546	HIS
1	D	550	ASN
1	D	559	GLU
1	D	575	ASN
1	D	582	ASP
1	D	599	LYS
1	D	604	ARG
1	D	605	TYR
1	D	608	LYS
1	D	610	GLU
1	D	614	LYS
1	D	615	LYS
1	D	622	GLU
1	D	646	GLU
1	D	647	GLU
1	D	652	GLU
1	D	653	GLU
1	D	658	LEU
1	D	661	LEU
1	D	671	SER
1	D	677	GLN
1	D	678	LEU
1	D	684	ARG
1	D	685	GLN
1	D	699	ASP
1	D	701	LEU
1	D	703	ARG
1	D	713	MET
1	D	715	ASP
1	D	724	PRO
1	D	731	THR
1	D	732	ARG
1	D	741	VAL
1	D	743	ASP
1	D	750	LYS
1	D	752	LEU
1	D	757	ASP
1	D	759	LEU
1	D	760	SER
1	D	762	GLN

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Mol	Chain	Res	Type
1	D	791	GLU
1	D	796	LEU
1	D	798	GLU
1	D	800	PHE
1	D	801	LEU
1	D	802	ASN
1	D	809	ASP
1	D	810	TRP
1	D	811	ASP
1	D	818	THR
1	D	821	ASP
1	D	826	LEU
1	D	827	GLN
1	D	831	PHE
1	D	833	GLU
1	D	840	GLU
1	D	861	LEU
1	D	876	ASN
1	D	879	ASP
1	D	897	PHE
1	D	901	TYR
1	D	903	GLN
1	D	905	ASP
1	D	921	MET
1	D	935	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (96) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	12	ASN
1	A	22	GLN
1	A	28	ASN
1	A	92	HIS
1	A	187	ASN
1	A	199	HIS
1	A	297	ASN
1	A	306	GLN
1	A	363	ASN
1	A	409	ASN
1	A	487	GLN
1	A	550	ASN

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Mol	Chain	Res	Type
1	A	685	GLN
1	A	825	GLN
1	A	827	GLN
1	A	887	HIS
1	A	903	GLN
1	A	908	GLN
1	B	11	ASN
1	B	12	ASN
1	B	22	GLN
1	B	28	ASN
1	B	92	HIS
1	B	116	ASN
1	B	176	ASN
1	B	194	GLN
1	B	199	HIS
1	B	297	ASN
1	B	323	GLN
1	B	348	HIS
1	B	409	ASN
1	B	444	GLN
1	B	487	GLN
1	B	504	GLN
1	B	522	ASN
1	B	547	GLN
1	B	685	GLN
1	B	727	HIS
1	B	827	GLN
1	B	880	ASN
1	B	888	ASN
1	B	903	GLN
1	C	11	ASN
1	C	12	ASN
1	C	22	GLN
1	C	92	HIS
1	C	155	GLN
1	C	187	ASN
1	C	199	HIS
1	C	297	ASN
1	C	306	GLN
1	C	363	ASN
1	C	409	ASN
1	C	487	GLN

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Mol	Chain	Res	Type
1	C	522	ASN
1	C	563	GLN
1	C	685	GLN
1	C	727	HIS
1	C	745	ASN
1	C	825	GLN
1	C	827	GLN
1	C	888	ASN
1	C	903	GLN
1	C	908	GLN
1	D	11	ASN
1	D	12	ASN
1	D	22	GLN
1	D	92	HIS
1	D	124	HIS
1	D	176	ASN
1	D	187	ASN
1	D	194	GLN
1	D	199	HIS
1	D	297	ASN
1	D	323	GLN
1	D	348	HIS
1	D	364	GLN
1	D	373	ASN
1	D	409	ASN
1	D	444	GLN
1	D	461	GLN
1	D	487	GLN
1	D	542	GLN
1	D	550	ASN
1	D	563	GLN
1	D	629	GLN
1	D	650	GLN
1	D	677	GLN
1	D	685	GLN
1	D	727	HIS
1	D	745	ASN
1	D	825	GLN
1	D	827	GLN
1	D	903	GLN
1	D	919	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	939/997 (94%)	-0.30	20 (2%) 63 54	18, 61, 86, 103	0
1	B	934/997 (93%)	-0.35	16 (1%) 70 63	16, 59, 85, 112	0
1	C	939/997 (94%)	-0.30	17 (1%) 68 61	20, 61, 88, 102	0
1	D	934/997 (93%)	-0.36	13 (1%) 75 70	21, 59, 87, 112	0
All	All	3746/3988 (93%)	-0.33	66 (1%) 68 61	16, 60, 87, 112	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	274	HIS	5.7
1	A	832	ALA	4.9
1	B	11	ASN	4.5
1	D	938	VAL	4.5
1	D	600	GLU	4.5
1	B	834	LEU	4.4
1	B	327	VAL	4.2
1	C	831	PHE	4.1
1	A	1	MET	4.0
1	C	834	LEU	3.8
1	C	234	ASP	3.7
1	A	2	LEU	3.7
1	A	245	LYS	3.6
1	C	821	ASP	3.6
1	A	834	LEU	3.6
1	A	274	HIS	3.5
1	A	828	ASP	3.4
1	A	9	PHE	3.3
1	B	274	HIS	3.3
1	D	902	GLY	3.2
1	A	821	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	1	MET	3.1
1	B	938	VAL	3.1
1	C	2	LEU	3.0
1	B	839	ALA	3.0
1	D	901	TYR	3.0
1	C	846	LEU	2.9
1	D	61	LEU	2.9
1	C	811	ASP	2.9
1	B	939	GLU	2.9
1	C	9	PHE	2.8
1	B	7	ARG	2.8
1	D	320	TYR	2.8
1	D	488	GLN	2.8
1	A	827	GLN	2.6
1	C	633	ILE	2.6
1	A	830	PRO	2.6
1	B	60	LEU	2.5
1	D	274	HIS	2.5
1	B	357	VAL	2.5
1	A	829	PHE	2.5
1	B	8	LEU	2.5
1	C	325	GLY	2.4
1	A	831	PHE	2.4
1	D	903	GLN	2.3
1	B	838	LYS	2.3
1	C	510	LEU	2.3
1	D	939	GLU	2.3
1	B	899	ARG	2.3
1	A	257	ARG	2.3
1	C	900	GLY	2.3
1	C	829	PHE	2.3
1	D	9	PHE	2.3
1	A	854	TYR	2.3
1	B	488	GLN	2.2
1	D	14	ARG	2.2
1	D	304	LEU	2.2
1	A	797	ALA	2.2
1	A	613	ILE	2.1
1	C	605	TYR	2.1
1	A	846	LEU	2.1
1	C	609	VAL	2.1
1	B	591	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	605	TYR	2.0
1	A	849	ALA	2.0
1	A	287	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.