



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:34 PM UTC

PDB ID : 2IPC / pdb_00002ipc
Title : Crystal structure of the translocation ATPase SecA from *Thermus thermophilus* reveals a parallel, head-to-head dimer
Authors : Vassylyev, D.G.; Mori, H.; Vassylyeva, M.N.; Tsukazaki, T.; Kimura, Y.; Tahirov, 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.

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

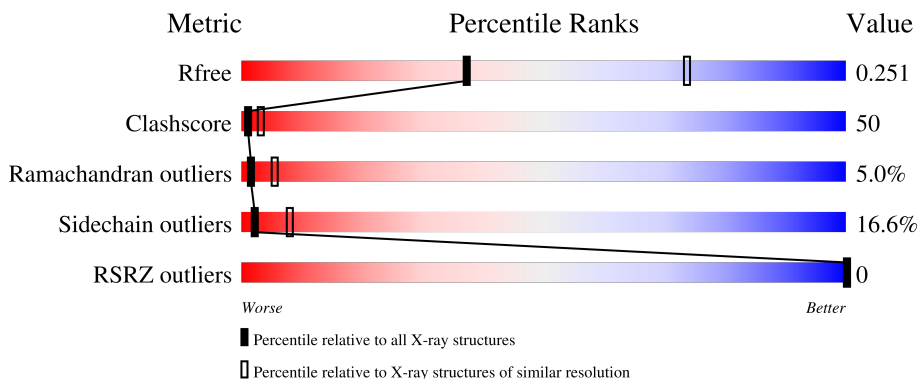
1 Overall quality at a glance

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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 ≥ 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	 28% 50% 14% • 6%
1	B	997	 29% 47% 14% • 6%
1	C	997	 28% 50% 14% • 6%
1	D	997	 27% 50% 14% • 6%

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.

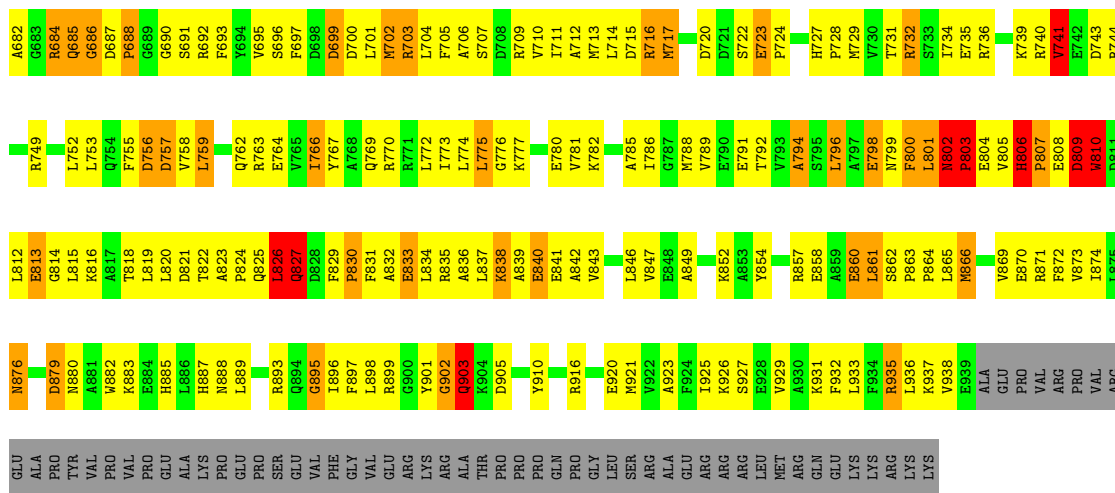
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Preprotein translocase SecA subunit.

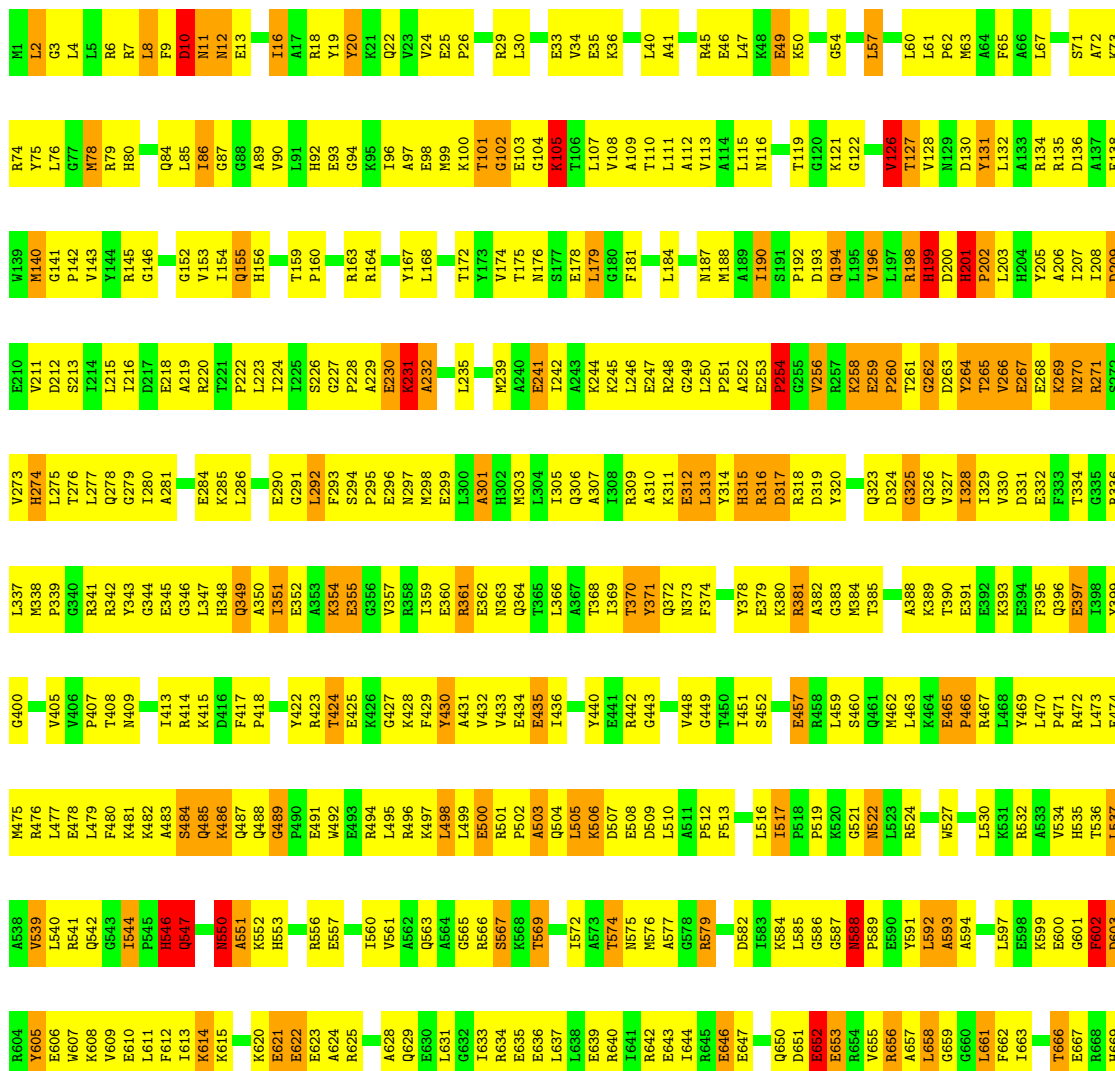
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	939	7551	4774	1354	1399	24	0	0	0
1	B	934	7515	4749	1349	1394	23	0	0	0
1	C	939	7551	4774	1354	1399	24	0	0	0
1	D	934	7515	4749	1349	1394	23	0	0	0

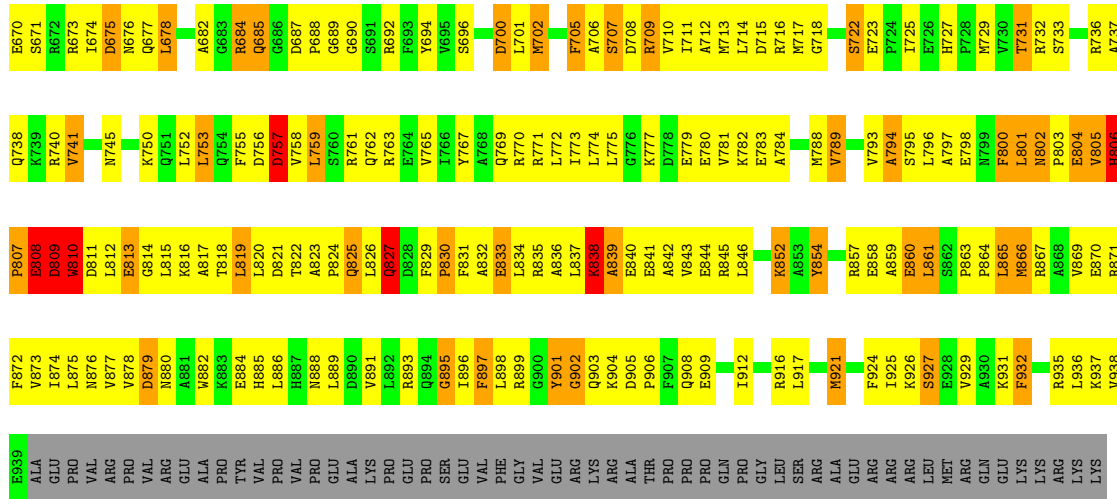
- Molecule 2 is water.

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		

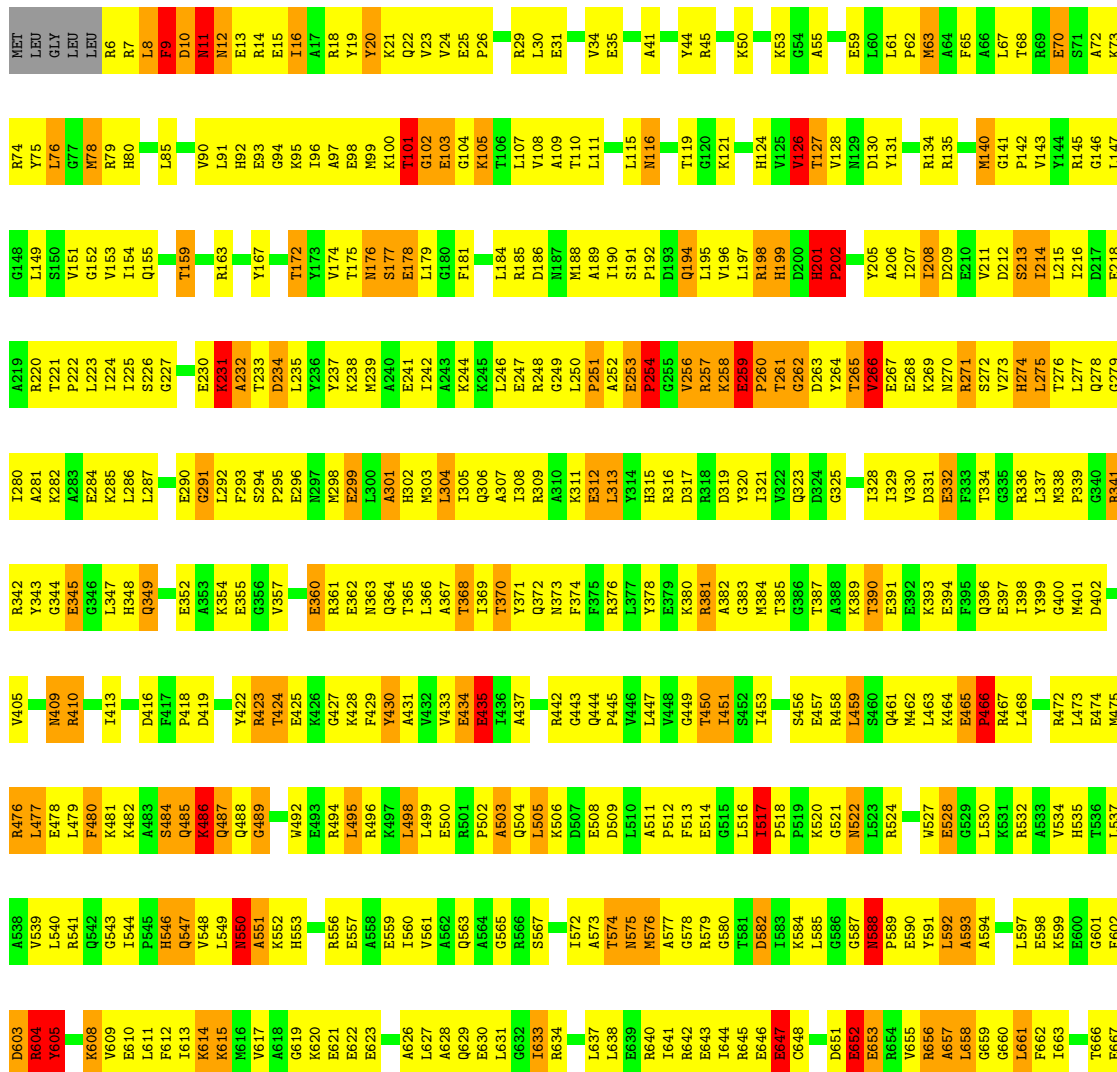


• Molecule 1: Preprotein translocase SecA subunit





● Molecule 1: Preprotein translocase SecA subunit



ARG	A930	L861	A797	T731	R668
GLN	K931	S662	E796	R732	H669
GLU	F932	P863	M799	S733	E670
LYS	L933	P864	F800	I734	S671
LYS	F934	L865	M802	R735	R672
ARG	R935	M866	R803	R736	R673
LYS	L936	R867	R804	A737	I674
LYS	K937	A868	E805	Q738	D675
LYS	V938	V869	V805	K739	N676
ALA	E939	R870	R806	V740	Q677
GLU	R871	F872	P807	V741	L678
PRD	F873	V874	D809	E742	R679
VAL	L874	L875	K810	D743	G680
ARG	L876	N877	D811		R681
PRD	V878	N879	L812	K749	A682
VAL	V879	V880	E813	R750	G683
GLU	D879	M880	G814	Q751	R684
ALA	M880	A881	L815	L752	Q685
PRO	A881	V882	L816	L753	G686
TYR	W882	L886	K817	Q754	D687
VAL	V882	H887	T818	F755	P688
VAL	V886		L819	D756	G689
VAL	H887		L820	D757	G690
PRO			D821	V759	S691
GLU			T822	S760	R692
ALA			A823	R761	F693
LYS			P824	V694	Y694
PRO			Q825	R762	V695
GLU			I826	R763	S696
PRO			F827	E764	F697
PRO			D828	V765	D698
SER			F829	I766	D699
GLU			P830	Y767	D700
VAL			F831	A768	L701
PHE			A832	Q769	M702
GLY			E833	R770	R703
VAL			L834		L704
GLU			R835	I773	F705
ARG			A836	L774	A706
LYS			L837	L775	S707
ARG			R838	G776	D708
ALA			A839	K777	R709
THR			E840	D778	V710
PRO			E841	E779	I711
PRO			A842	E780	A712
PRO			V843	V781	M713
GLN				K782	L714
GLY			L846	E783	D715
LEU			W847	A784	R716
SER			E848	A785	R716
ARG			L851	I786	F719
ALA			Y854	M788	E723
GLU			R857	E791	P724
ARG			E858	T792	I725
ARG			E928	V793	E726
LEU			V929	A794	H727
MET				S795	P728
				L796	M729
					V730

4 Data and refinement statistics i

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	168.62Å 168.62Å 149.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.80 40.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.4 (40.00-2.80) 97.5 (40.00-2.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.13 (at 2.81Å)	Xtrriage
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 ²)	52.4	Xtrriage
Anisotropy	0.061	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 49.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	0.038 for -h,-k,l 0.499 for h,-h-k,-l 0.039 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	31502	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

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	0.72	1/7682 (0.0%)	1.25	89/10350 (0.9%)
1	B	0.75	3/7646 (0.0%)	1.27	92/10302 (0.9%)
1	C	0.71	0/7682	1.25	83/10350 (0.8%)
1	D	0.73	3/7646 (0.0%)	1.27	88/10302 (0.9%)
All	All	0.73	7/30656 (0.0%)	1.26	352/41304 (0.9%)

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 (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	475	MET	SD-CE	6.99	1.97	1.79
1	B	716	ARG	CG-CD	6.74	1.72	1.52
1	D	716	ARG	CG-CD	6.66	1.72	1.52
1	D	434	GLU	C-N	-6.20	1.25	1.33
1	D	151	VAL	CA-CB	5.60	1.59	1.53
1	A	338	MET	CG-SD	5.46	1.94	1.80
1	B	803	PRO	C-N	-5.13	1.26	1.33

All (352) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	10	ASP	N-CA-C	13.84	130.94	110.46
1	D	100	LYS	N-CA-C	13.48	125.49	111.07
1	B	100	LYS	N-CA-C	13.41	125.58	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	201	HIS	C-N-CD	-13.17	91.63	120.60
1	B	266	VAL	N-CA-C	-13.09	91.70	109.37
1	C	10	ASP	N-CA-C	12.96	128.61	109.95
1	B	201	HIS	C-N-CD	-12.87	92.30	120.60
1	D	266	VAL	N-CA-C	-12.49	92.51	109.37
1	A	201	HIS	C-N-CD	-12.44	93.22	120.60
1	A	266	VAL	N-CA-C	-11.89	93.32	109.37
1	D	488	GLN	N-CA-C	11.87	128.45	112.90
1	D	101	THR	N-CA-C	11.86	127.79	108.34
1	A	101	THR	N-CA-C	11.76	127.63	108.34
1	A	100	LYS	N-CA-C	11.73	125.33	111.02
1	C	266	VAL	N-CA-C	-11.67	93.61	109.37
1	C	100	LYS	N-CA-C	11.60	125.17	111.02
1	D	484	SER	N-CA-C	11.48	123.53	111.14
1	B	488	GLN	N-CA-C	11.38	127.81	112.90
1	C	484	SER	N-CA-C	11.36	123.41	111.14
1	B	484	SER	N-CA-C	11.34	123.39	111.14
1	C	201	HIS	C-N-CD	-11.34	95.65	120.60
1	A	265	THR	N-CA-C	-11.31	93.75	110.48
1	D	265	THR	N-CA-C	-11.18	93.93	110.48
1	C	265	THR	N-CA-C	-11.17	93.95	110.48
1	C	101	THR	N-CA-C	11.01	127.37	108.76
1	B	265	THR	N-CA-C	-10.69	94.65	110.48
1	B	101	THR	N-CA-C	10.51	126.52	108.76
1	C	488	GLN	N-CA-C	10.46	126.59	112.90
1	A	484	SER	N-CA-C	10.43	124.13	111.40
1	C	232	ALA	N-CA-C	10.31	123.63	110.33
1	D	506	LYS	N-CA-C	-10.21	93.82	109.96
1	A	506	LYS	N-CA-C	-10.13	93.95	109.96
1	C	506	LYS	N-CA-C	-10.13	93.96	109.96
1	A	488	GLN	N-CA-C	10.01	126.01	112.90
1	B	506	LYS	N-CA-C	-9.98	94.19	109.96
1	D	809	ASP	N-CA-C	9.91	131.91	110.80
1	C	201	HIS	CA-C-N	9.84	150.62	127.00
1	C	201	HIS	C-N-CA	9.84	150.62	127.00
1	A	201	HIS	CA-C-N	9.78	150.48	127.00
1	A	201	HIS	C-N-CA	9.78	150.48	127.00
1	B	201	HIS	CA-C-N	9.75	150.40	127.00
1	B	201	HIS	C-N-CA	9.75	150.40	127.00
1	C	809	ASP	N-CA-C	9.72	131.50	110.80
1	D	517	ILE	N-CA-C	9.65	117.50	107.76
1	C	804	GLU	N-CA-C	-9.48	100.28	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	517	ILE	N-CA-C	9.44	117.29	107.76
1	B	809	ASP	N-CA-C	9.32	130.66	110.80
1	A	809	ASP	N-CA-C	9.25	130.49	110.80
1	A	223	LEU	N-CA-C	-9.22	94.22	109.07
1	A	201	HIS	N-CA-C	9.21	130.16	109.81
1	A	199	HIS	N-CA-C	-9.07	102.36	113.97
1	A	651	ASP	N-CA-C	-8.99	101.12	112.90
1	A	804	GLU	N-CA-C	-8.98	102.48	113.97
1	C	230	GLU	N-CA-C	-8.79	96.67	109.59
1	C	201	HIS	N-CA-C	8.78	129.21	109.81
1	C	199	HIS	N-CA-C	-8.78	102.74	113.97
1	B	804	GLU	N-CA-C	-8.75	102.04	112.89
1	A	860	GLU	N-CA-C	-8.74	101.71	111.07
1	B	801	LEU	N-CA-C	-8.72	102.35	113.16
1	A	230	GLU	N-CA-C	-8.70	96.63	109.15
1	B	435	GLU	CB-CG-CD	-8.61	97.96	112.60
1	A	808	GLU	N-CA-C	8.51	128.92	110.80
1	B	230	GLU	N-CA-C	-8.50	97.10	109.59
1	D	486	LYS	N-CA-C	-8.43	102.98	113.18
1	B	14	ARG	N-CA-C	-8.41	102.06	111.82
1	D	839	ALA	N-CA-C	8.37	123.62	113.41
1	B	808	GLU	N-CA-C	8.23	128.33	110.80
1	A	757	ASP	N-CA-C	-8.18	102.19	112.90
1	C	651	ASP	N-CA-C	-8.13	102.25	112.90
1	D	838	LYS	N-CA-C	8.10	128.04	110.80
1	B	838	LYS	N-CA-C	8.09	128.03	110.80
1	A	838	LYS	N-CA-C	8.07	128.00	110.80
1	D	503	ALA	N-CA-C	8.01	120.09	111.36
1	D	201	HIS	N-CA-C	8.00	127.50	109.81
1	B	201	HIS	N-CA-C	7.93	127.34	109.81
1	D	808	GLU	N-CA-C	7.92	127.68	110.80
1	D	230	GLU	N-CA-C	-7.92	97.74	109.15
1	C	808	GLU	N-CA-C	7.92	127.67	110.80
1	A	503	ALA	N-CA-C	7.86	119.93	111.36
1	B	10	ASP	N-CA-C	7.86	119.93	110.19
1	B	11	ASN	N-CA-C	-7.85	102.66	111.14
1	C	503	ALA	N-CA-C	7.81	119.79	111.28
1	B	503	ALA	N-CA-C	7.77	119.83	111.36
1	D	592	LEU	N-CA-C	-7.75	101.67	112.45
1	C	757	ASP	N-CA-C	-7.72	101.72	112.45
1	A	542	GLN	N-CA-C	-7.69	103.00	112.38
1	C	517	ILE	N-CA-C	7.67	115.51	107.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	592	LEU	N-CA-C	-7.61	101.87	112.45
1	A	517	ILE	N-CA-C	7.61	115.44	107.76
1	B	903	GLN	N-CA-C	7.60	119.56	111.28
1	B	486	LYS	N-CA-C	-7.58	104.00	113.18
1	C	838	LYS	N-CA-C	7.53	126.84	110.80
1	D	803	PRO	N-CA-C	7.50	127.92	112.47
1	C	839	ALA	N-CA-C	7.42	123.01	113.88
1	C	486	LYS	N-CA-C	-7.36	104.27	113.18
1	D	271	ARG	N-CA-C	7.33	121.41	109.76
1	D	14	ARG	N-CA-C	-7.31	103.34	111.82
1	C	592	LEU	N-CA-C	-7.29	102.31	112.45
1	D	201	HIS	CA-C-N	7.29	144.48	127.00
1	D	201	HIS	C-N-CA	7.29	144.48	127.00
1	D	9	PHE	N-CA-C	7.27	126.29	110.80
1	D	10	ASP	N-CA-C	7.25	120.69	109.60
1	A	467	ARG	N-CA-C	-7.24	103.39	111.28
1	A	486	LYS	N-CA-C	-7.18	104.49	113.18
1	B	806	HIS	CA-C-N	-7.17	110.88	119.84
1	B	806	HIS	C-N-CA	-7.17	110.88	119.84
1	B	826	LEU	N-CA-C	-7.17	96.56	108.32
1	B	199	HIS	N-CA-C	-7.14	104.83	113.97
1	D	489	GLY	N-CA-C	7.14	126.90	112.34
1	D	194	GLN	N-CA-C	-7.14	105.19	114.04
1	C	126	VAL	N-CA-C	7.11	119.31	108.71
1	C	271	ARG	N-CA-C	7.01	120.91	109.76
1	D	805	VAL	N-CA-C	-7.01	97.39	107.98
1	C	826	LEU	N-CA-C	-7.01	95.87	108.48
1	D	11	ASN	N-CA-C	-6.98	103.11	111.69
1	A	775	LEU	N-CA-C	-6.98	104.03	112.54
1	B	489	GLY	CA-C-N	6.97	126.22	118.97
1	B	489	GLY	C-N-CA	6.97	126.22	118.97
1	B	810	TRP	N-CA-C	6.97	119.77	108.41
1	D	199	HIS	N-CA-C	-6.96	105.06	113.97
1	D	652	GLU	N-CA-C	-6.96	103.62	111.07
1	B	702	MET	N-CA-C	6.96	121.36	113.01
1	C	194	GLN	N-CA-C	-6.94	105.43	114.04
1	A	489	GLY	N-CA-C	6.94	126.49	112.34
1	D	826	LEU	N-CA-C	-6.93	96.95	108.32
1	A	839	ALA	N-CA-C	6.91	122.38	113.88
1	B	271	ARG	N-CA-C	6.91	120.75	109.76
1	B	489	GLY	N-CA-C	6.89	126.40	112.34
1	B	312	GLU	N-CA-C	6.85	119.76	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	741	VAL	CB-CA-C	-6.84	103.21	111.97
1	B	10	ASP	CA-C-N	6.83	129.73	120.44
1	B	10	ASP	C-N-CA	6.83	129.73	120.44
1	C	775	LEU	N-CA-C	-6.83	104.20	112.54
1	A	4	LEU	N-CA-C	6.82	119.72	111.40
1	D	860	GLU	N-CA-C	-6.81	102.94	111.11
1	C	903	GLN	N-CA-C	6.80	119.56	111.33
1	A	805	VAL	N-CA-C	-6.80	97.71	107.37
1	D	435	GLU	CB-CG-CD	-6.77	101.09	112.60
1	D	757	ASP	N-CA-C	-6.76	103.38	111.69
1	A	271	ARG	N-CA-C	6.74	120.48	109.76
1	D	202	PRO	N-CA-C	-6.67	94.76	112.10
1	D	702	MET	N-CA-C	6.66	120.67	112.54
1	A	194	GLN	N-CA-C	-6.66	105.78	114.04
1	C	489	GLY	N-CA-C	6.62	125.85	112.34
1	C	9	PHE	N-CA-C	6.62	123.40	110.56
1	D	312	GLU	N-CA-C	6.61	119.46	111.40
1	B	592	LEU	N-CA-C	-6.60	103.28	112.45
1	D	903	GLN	N-CA-C	6.56	119.27	111.33
1	A	810	TRP	N-CA-C	6.53	119.17	108.52
1	A	312	GLU	N-CA-C	6.51	119.70	111.69
1	B	658	LEU	N-CA-C	-6.48	105.13	113.16
1	C	806	HIS	CA-C-N	-6.48	111.74	119.84
1	C	806	HIS	C-N-CA	-6.48	111.74	119.84
1	A	903	GLN	N-CA-C	6.46	119.15	111.33
1	A	126	VAL	N-CA-C	6.44	117.86	108.53
1	D	676	ASN	N-CA-C	-6.39	105.45	113.18
1	C	425	GLU	N-CA-C	-6.38	104.37	111.71
1	D	775	LEU	N-CA-C	-6.38	104.37	111.71
1	C	550	ASN	N-CA-C	-6.38	99.97	109.15
1	D	105	LYS	N-CA-C	6.38	117.89	111.07
1	A	500	GLU	N-CA-C	-6.38	105.08	112.92
1	C	224	ILE	N-CA-C	6.37	117.48	108.17
1	B	194	GLN	N-CA-C	-6.36	106.15	114.04
1	C	602	PHE	N-CA-C	6.34	119.42	111.24
1	B	789	VAL	N-CA-C	-6.33	104.33	110.72
1	A	826	LEU	N-CA-C	-6.33	97.09	108.48
1	B	775	LEU	N-CA-C	-6.32	104.67	112.38
1	B	757	ASP	N-CA-C	-6.31	103.67	112.45
1	D	550	ASN	N-CA-C	-6.31	100.06	109.15
1	C	312	GLU	N-CA-C	6.30	119.43	111.69
1	B	676	ASN	N-CA-C	-6.28	105.58	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	839	ALA	N-CA-C	6.27	121.99	113.97
1	C	262	GLY	N-CA-C	6.27	121.86	110.95
1	A	758	VAL	N-CA-C	-6.26	104.41	110.42
1	B	9	PHE	N-CA-C	6.26	124.14	110.80
1	A	702	MET	N-CA-C	6.25	120.17	112.54
1	A	806	HIS	CA-C-N	-6.24	112.04	119.84
1	A	806	HIS	C-N-CA	-6.24	112.04	119.84
1	C	806	HIS	N-CA-C	6.23	123.58	109.81
1	D	827	GLN	N-CA-C	6.22	124.06	110.80
1	C	652	GLU	N-CA-C	-6.20	104.21	110.97
1	C	4	LEU	N-CA-C	6.19	119.31	111.69
1	C	500	GLU	N-CA-C	-6.16	105.34	112.92
1	A	880	ASN	N-CA-C	-6.15	104.84	112.90
1	B	550	ASN	N-CA-C	-6.14	100.30	109.15
1	D	259	GLU	CA-C-N	-6.12	112.19	119.84
1	D	259	GLU	C-N-CA	-6.12	112.19	119.84
1	A	550	ASN	N-CA-C	-6.12	100.34	109.15
1	D	214	ILE	N-CA-C	6.11	116.27	110.53
1	B	105	LYS	N-CA-C	6.10	117.60	111.07
1	C	465	GLU	CA-C-N	6.08	127.44	119.84
1	C	465	GLU	C-N-CA	6.08	127.44	119.84
1	C	802	ASN	CA-C-N	-6.07	112.25	119.84
1	C	802	ASN	C-N-CA	-6.07	112.25	119.84
1	B	758	VAL	N-CA-C	-6.05	104.43	110.30
1	D	489	GLY	CA-C-N	6.03	125.25	118.97
1	D	489	GLY	C-N-CA	6.03	125.25	118.97
1	D	902	GLY	N-CA-C	6.03	127.48	113.18
1	C	805	VAL	N-CA-C	-6.03	98.81	107.37
1	D	153	VAL	N-CA-C	6.03	116.55	107.75
1	D	810	TRP	N-CA-C	6.02	118.33	108.52
1	D	806	HIS	CA-C-N	-6.00	112.34	119.84
1	D	806	HIS	C-N-CA	-6.00	112.34	119.84
1	D	425	GLU	N-CA-C	-6.00	104.74	111.28
1	B	232	ALA	N-CA-C	5.99	123.56	110.80
1	B	100	LYS	CA-C-N	-5.99	113.52	122.74
1	B	100	LYS	C-N-CA	-5.99	113.52	122.74
1	A	652	GLU	N-CA-C	-5.99	104.67	111.07
1	A	827	GLN	N-CA-C	5.97	123.72	114.64
1	B	651	ASP	N-CA-C	-5.96	104.36	111.69
1	D	232	ALA	N-CA-C	5.96	123.50	110.80
1	D	576	MET	N-CA-C	-5.95	105.32	112.58
1	B	126	VAL	N-CA-C	5.95	117.15	108.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	588	ASN	N-CA-C	5.94	122.93	109.81
1	D	806	HIS	N-CA-C	5.93	122.91	109.81
1	C	827	GLN	N-CA-C	5.91	123.38	110.80
1	B	652	GLU	N-CA-C	-5.88	104.78	111.07
1	A	232	ALA	N-CA-C	5.84	123.24	110.80
1	B	827	GLN	N-CA-C	5.83	123.23	110.80
1	D	368	THR	N-CA-C	5.83	118.98	109.24
1	B	262	GLY	N-CA-C	5.82	121.07	110.95
1	B	902	GLY	N-CA-C	5.81	126.95	113.18
1	C	702	MET	N-CA-C	5.80	119.62	112.54
1	C	41	ALA	N-CA-C	-5.79	104.87	111.07
1	D	516	LEU	CA-C-N	-5.79	118.42	122.59
1	D	516	LEU	C-N-CA	-5.79	118.42	122.59
1	B	741	VAL	CB-CA-C	-5.78	104.57	111.97
1	C	209	ASP	N-CA-C	5.78	118.52	111.82
1	A	528	GLU	N-CA-C	-5.75	105.15	111.82
1	A	153	VAL	N-CA-C	5.75	116.27	107.77
1	A	498	LEU	N-CA-C	-5.72	105.18	111.82
1	D	801	LEU	N-CA-C	-5.72	106.07	113.16
1	B	313	LEU	N-CA-C	5.72	119.56	112.59
1	B	228	PRO	N-CA-C	-5.70	103.24	111.22
1	C	810	TRP	N-CA-C	5.68	117.78	108.52
1	B	53	LYS	N-CA-C	-5.67	106.36	113.28
1	A	741	VAL	CB-CA-C	-5.65	104.75	111.81
1	A	425	GLU	N-CA-C	-5.64	105.21	111.36
1	D	126	VAL	N-CA-C	5.64	116.71	108.53
1	B	593	ALA	N-CA-C	-5.63	105.28	111.82
1	B	397	GLU	N-CA-C	5.63	117.50	111.36
1	C	332	GLU	N-CA-C	-5.62	106.40	113.20
1	D	657	ALA	N-CA-C	-5.61	105.39	114.09
1	D	498	LEU	N-CA-C	-5.60	105.32	111.82
1	C	676	ASN	N-CA-C	-5.60	106.41	113.18
1	B	498	LEU	N-CA-C	-5.58	105.29	111.71
1	C	902	GLY	N-CA-C	5.57	126.38	113.18
1	A	602	PHE	N-CA-C	5.57	118.42	111.24
1	D	500	GLU	N-CA-C	-5.56	106.08	112.92
1	B	576	MET	N-CA-C	-5.55	105.81	112.58
1	A	902	GLY	N-CA-C	5.55	126.33	113.18
1	B	435	GLU	CA-CB-CG	-5.54	103.01	114.10
1	C	650	GLN	N-CA-CB	-5.54	101.76	110.46
1	D	100	LYS	CA-C-N	-5.53	114.97	122.77
1	D	100	LYS	C-N-CA	-5.53	114.97	122.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	153	VAL	N-CA-C	5.53	115.95	107.77
1	C	801	LEU	N-CA-C	-5.53	106.54	113.28
1	B	259	GLU	CA-C-N	-5.53	112.93	119.84
1	B	259	GLU	C-N-CA	-5.53	112.93	119.84
1	A	100	LYS	CA-C-N	-5.52	114.99	122.77
1	A	100	LYS	C-N-CA	-5.52	114.99	122.77
1	C	906	PRO	N-CA-C	-5.51	105.53	113.75
1	D	647	GLU	N-CA-C	-5.50	104.92	111.69
1	B	802	ASN	CA-C-N	-5.50	112.97	119.84
1	B	802	ASN	C-N-CA	-5.50	112.97	119.84
1	C	397	GLU	N-CA-C	5.50	117.35	111.36
1	C	880	ASN	N-CA-C	-5.50	105.70	112.90
1	A	105	LYS	N-CA-C	5.48	116.94	111.07
1	B	516	LEU	CA-C-N	-5.48	118.64	122.59
1	B	516	LEU	C-N-CA	-5.48	118.64	122.59
1	D	528	GLU	N-CA-C	-5.48	105.46	111.82
1	B	459	LEU	N-CA-C	-5.46	105.22	111.07
1	A	588	ASN	N-CA-C	5.45	121.86	109.81
1	C	588	ASN	N-CA-C	5.45	121.86	109.81
1	C	860	GLU	N-CA-C	-5.45	105.24	111.07
1	A	722	SER	N-CA-C	5.44	120.01	112.45
1	A	9	PHE	N-CA-C	5.43	122.36	110.80
1	B	554	HIS	N-CA-C	5.43	117.90	111.33
1	A	34	VAL	N-CA-C	5.42	116.15	110.62
1	A	658	LEU	N-CA-C	-5.41	106.36	113.17
1	D	301	ALA	N-CA-C	-5.39	105.40	111.28
1	C	8	LEU	N-CA-C	-5.39	106.55	113.23
1	A	301	ALA	N-CA-C	-5.37	105.42	111.28
1	A	676	ASN	N-CA-C	-5.36	106.69	113.18
1	C	593	ALA	N-CA-C	-5.36	105.44	111.28
1	A	705	PHE	N-CA-C	5.36	120.48	113.30
1	A	332	GLU	N-CA-C	-5.33	106.75	113.20
1	C	430	TYR	N-CA-C	-5.33	104.88	111.33
1	C	863	PRO	N-CA-C	5.32	117.19	110.70
1	A	41	ALA	N-CA-C	-5.31	105.39	111.07
1	D	678	LEU	N-CA-C	-5.31	105.50	111.28
1	A	544	ILE	CA-C-N	5.30	126.47	119.84
1	A	544	ILE	C-N-CA	5.30	126.47	119.84
1	D	741	VAL	CB-CA-C	-5.30	105.18	111.97
1	B	657	ALA	N-CA-C	-5.30	105.88	114.09
1	A	214	ILE	N-CA-C	5.29	115.51	110.53
1	D	633	ILE	N-CA-C	5.29	114.93	106.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	430	TYR	N-CA-C	-5.29	104.93	111.33
1	A	807	PRO	N-CA-C	5.29	123.37	112.47
1	A	633	ILE	N-CA-C	5.28	114.90	106.88
1	D	231	LYS	N-CA-C	5.27	122.03	110.80
1	A	567	SER	N-CA-C	5.27	122.02	110.80
1	B	679	ARG	N-CA-C	-5.27	105.71	111.82
1	D	262	GLY	N-CA-C	5.27	120.11	110.95
1	C	722	SER	N-CA-C	5.25	119.75	112.45
1	C	498	LEU	N-CA-C	-5.25	105.73	111.82
1	A	8	LEU	N-CA-C	-5.24	106.04	112.90
1	B	723	GLU	CA-C-N	5.22	125.22	119.89
1	B	723	GLU	C-N-CA	5.22	125.22	119.89
1	D	53	LYS	N-CA-C	-5.21	106.92	113.28
1	A	72	ALA	N-CA-C	-5.20	105.70	111.36
1	B	500	GLU	N-CA-C	-5.20	106.53	112.92
1	C	105	LYS	N-CA-C	5.19	116.63	111.07
1	C	480	PHE	N-CA-C	-5.19	105.62	111.28
1	C	814	GLY	N-CA-C	-5.19	108.23	114.66
1	B	214	ILE	N-CA-C	5.16	115.38	110.53
1	D	588	ASN	N-CA-C	5.15	121.19	109.81
1	D	723	GLU	CA-C-N	5.14	126.27	119.84
1	D	723	GLU	C-N-CA	5.14	126.27	119.84
1	D	593	ALA	N-CA-C	-5.13	105.80	111.71
1	D	651	ASP	N-CA-C	-5.13	105.77	112.23
1	B	332	GLU	N-CA-C	-5.13	107.00	113.20
1	D	480	PHE	N-CA-C	-5.12	105.70	111.28
1	B	722	SER	N-CA-C	5.11	119.39	112.04
1	D	313	LEU	N-CA-C	5.09	118.80	112.59
1	A	262	GLY	N-CA-C	5.08	119.80	110.95
1	A	259	GLU	CA-C-N	-5.08	113.49	119.84
1	A	259	GLU	C-N-CA	-5.08	113.49	119.84
1	C	153	VAL	N-CA-C	5.08	115.28	107.77
1	C	789	VAL	N-CA-C	-5.07	105.59	110.72
1	A	906	PRO	N-CA-C	-5.07	106.20	113.75
1	B	425	GLU	N-CA-C	-5.06	105.95	111.82
1	A	517	ILE	CB-CA-C	-5.06	105.30	110.71
1	A	398	ILE	N-CA-C	5.05	116.51	111.00
1	A	801	LEU	N-CA-C	-5.05	107.11	113.28
1	D	332	GLU	N-CA-C	-5.05	107.08	113.20
1	D	679	ARG	N-CA-C	-5.05	105.96	111.82
1	C	301	ALA	N-CA-C	-5.04	105.79	111.28
1	B	275	LEU	N-CA-C	5.04	120.81	114.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	528	GLU	N-CA-C	-5.04	105.98	111.82
1	B	814	GLY	N-CA-C	-5.04	108.42	114.66
1	D	261	THR	N-CA-C	5.03	116.85	111.36
1	A	384	MET	N-CA-C	5.03	116.89	108.99
1	C	705	PHE	N-CA-C	5.03	120.03	113.30
1	D	430	TYR	N-CA-C	-5.02	105.08	111.11
1	A	806	HIS	N-CA-C	5.01	120.89	109.81
1	B	678	LEU	N-CA-C	-5.01	105.90	111.36
1	C	567	SER	N-CA-C	5.01	121.47	110.80
1	B	278	GLN	N-CA-C	-5.01	105.71	111.07
1	A	789	VAL	N-CA-C	-5.01	105.66	110.72
1	C	100	LYS	CA-C-N	-5.00	115.04	122.74
1	C	100	LYS	C-N-CA	-5.00	115.04	122.74

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7551	0	7648	771	0
1	B	7515	0	7600	724	0
1	C	7551	0	7648	745	0
1	D	7515	0	7600	835	0
2	A	359	0	0	138	0
2	B	320	0	0	154	0
2	C	344	0	0	149	0
2	D	347	0	0	160	0
All	All	31502	0	30496	3021	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 50.

All (3021) 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:298:MET:HE1	1:A:873:VAL:HA	1.26	1.09
1:A:269:LYS:HD3	1:A:270:ASN:H	1.08	1.08
1:C:298:MET:HE1	1:C:873:VAL:HA	1.35	1.06
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:C:858:GLU:HG3	1:C:866:MET:HE3	1.44	0.97
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:339:PRO:HA	2:D:1307:HOH:O	1.72	0.89
1:A:858:GLU:HG3	1:A:866:MET:HE3	1.51	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:121:LYS:C	1:A:198:ARG:HH21	1.92	0.78
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:99:MET:HE1	1:D:108:VAL:HG11	1.66	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:813:GLU:H	1:D:813:GLU:CD	1.93	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:C:435:GLU:CD	1:C:692:ARG:NH1	2.44	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
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:A:459:LEU:HA	1:A:462:MET:HE3	1.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:365:THR:HG22	1:D:886:LEU:HD13	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:102:GLY:N	1:A:105:LYS:HZ1	1.84	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:78:MET:HE2	2:C:1039:HOH:O	1.89	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:B:273:VAL:HG13	1:B:820:LEU:HD13	1.72	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:B:517:ILE:HG21	1:B:524:ARG:HH11	1.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:813:GLU:H	1:B:813:GLU:CD	2.00	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
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:99:MET:HE1	1:B:108:VAL:HG11	1.73	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:1:MET:H1	1:A:5:LEU:HD12	1.58	0.68
1:A:865:LEU:HD13	1:A:938:VAL:HG11	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:LEU:HG	1:D:9:PHE:N	2.06	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:B:299:GLU:H	1:B:299:GLU:CD	2.01	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:LYS:HZ1	1:D:634:ARG:HH22	1.42	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:A:717:MET:CE	1:A:729:MET:HE2	2.24	0.67
1:B:213:SER:CB	1:B:579:ARG:HH22	2.07	0.67
1:C:265:THR:HG22	1:C:271:ARG:C	2.20	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:B:655:VAL:C	1:B:657:ALA:H	2.01	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
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:A:281:ALA:HA	1:A:284:GLU:CD	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:263:ASP:CG	1:D:816:LYS:HE3	2.21	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: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:C:298:MET:HE2	1:C:872:PHE:CE2	2.30	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:C:655:VAL:C	1:C:657:ALA:H	2.02	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:465:GLU:C	1:A:467:ARG:H	2.05	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: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:A:76:LEU:HD21	1:A:140:MET:HE2	1.79	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:ALA:HA	1:B:143:VAL:HG22	1.81	0.63
1:C:800:PHE:HB2	1:C:810:TRP:CD1	2.32	0.63
1:A:606:GLU:HG2	1:A:610:GLU:CD	2.24	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:63:MET:HE2	1:D:63:MET:HA	1.80	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:263:ASP:CG	1:A:816:LYS:HG2	2.24	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:1:MET:N	1:A:5:LEU:HD12	2.14	0.62
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:354:LYS:NZ	1:D:634:ARG:HH22	1.97	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
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:599:LYS:HE3	1:C:637:LEU:HD21	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:223:LEU:HD21	1:D:371:TYR:CZ	2.34	0.62
1:D:265:THR:HG22	1:D:271:ARG:C	2.24	0.62
1:D:854:TYR:OH	1:D:933:LEU:HD13	2.00	0.62
1:A:801:LEU:C	1:A:803:PRO:HD3	2.24	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:244:LYS:HD2	1:D:354:LYS:HZ3	1.64	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:76:LEU:HD21	1:C:140:MET:HE2	1.83	0.61
1:C:622:GLU:HA	1:C:625:ARG:HE	1.66	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:505:LEU:HD22	1:C:510:LEU:HD11	1.83	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:7:ARG:HG2	1:B:13:GLU:CD	2.26	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:857:ARG:NH1	1:D:934:PHE:C	2.59	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:800:PHE:O	1:B:810:TRP:CD1	2.54	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:99:MET:HE1	1:A:108:VAL:HG11	1.83	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: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:550:ASN:ND2	1:B:550:ASN:H	1.98	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:399:TYR:CB	1:D:401:MET:HE2	2.32	0.60
1:D:399:TYR:HB2	1:D:401:MET:HE2	1.83	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:B:717:MET:SD	1:B:729:MET:HE3	2.41	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:717:MET:SD	1:A:729:MET:HE2	2.42	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:408:THR:HG22	1:C:409:ASN:N	2.16	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:273:VAL:C	1:D:820:LEU:HD13	2.26	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:B:801:LEU:C	1:B:803:PRO:HD3	2.28	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:A:298:MET:HE2	1:A:872:PHE:CE2	2.38	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:399:TYR:CB	1:B:401:MET:HE2	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:852:LYS:HB2	1:A:852:LYS:HZ3	1.68	0.58
1:C:414:ARG:HD2	1:C:682:ALA:HB3	1.84	0.58
1:C:714:LEU:HD23	1:C:729:MET:HE1	1.83	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:239:MET:HE3	1:D:304:LEU:N	2.18	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:292:LEU:C	1:B:297:ASN:HD22	2.12	0.58
1:B:770:ARG:HH12	1:B:879:ASP:CB	2.16	0.58
1:D:331:ASP:OD1	1:D:338:MET:HE2	2.03	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:559:GLU:HG3	1:B:590:GLU:CD	2.28	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:C:852:LYS:HB2	1:C:852:LYS:HZ3	1.67	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:464:LYS:C	1:B:466:PRO:HD2	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:885:HIS:HA	2:B:1035: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
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: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:443:GLY:C	1:B:658:LEU:HD13	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:30:LEU:HD13	1:C:63:MET:HE3	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:B:63:MET:HE2	1:B:63:MET:HA	1.85	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:C:435:GLU:CD	1:C:692:ARG:HH11	2.12	0.57
1:D:134:ARG:HD3	2:D:1286:HOH:O	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:ILE:HA	1:A:763:ARG:NH1	2.19	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
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:D:281:ALA:HA	1:D:284:GLU:CD	2.30	0.57
1:D:298:MET:HE1	1:D:873:VAL:HA	1.87	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: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:524:ARG:HH12	1:C:527:TRP:CD1	2.22	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:30:LEU:HD13	1:B:63:MET:HE3	1.88	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:265:THR:HG22	1:B:271:ARG:C	2.30	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
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:435:GLU:CD	1:C:694:TYR:HH	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:897:PHE:C	1:A:897:PHE:CD2	2.84	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
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:D:857:ARG:HH11	1:D:934:PHE:C	2.12	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:622:GLU:CD	1:C:622:GLU:H	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:D:299:GLU:H	1:D:299:GLU:CD	2.14	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:121:LYS:C	1:C:198:ARG:HH21	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:121:LYS:C	1:A:198:ARG:NH2	2.65	0.55
1:C:261:THR:HG23	1:C:279:GLY:HA3	1.89	0.55
1:A:19:TYR:HB3	1:A:86:ILE:HG12	1.89	0.55
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: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:316:ARG:HD3	1:A:355:GLU:CD	2.32	0.54
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:A:897:PHE:C	1:A:897:PHE:HD2	2.14	0.54
1:C:501:ARG:HB2	1:C:504:GLN:OE1	2.07	0.54
1:C:885:HIS:HB2	1:C:921:MET:HE2	1.90	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:265:THR:HG22	1:A:271:ARG:C	2.31	0.54
1:A:842:ALA:O	1:A:846:LEU:HG	2.07	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:LYS:CE	1:D:634:ARG:HH12	2.20	0.54
1:C:882:TRP:HE3	1:C:921:MET:HE1	1.72	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:D:78:MET:HE3	1:D:103:GLU:OE1	2.08	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:C:897:PHE:C	1:C:897:PHE:CD2	2.86	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
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:78:MET:HE3	2:C:1334:HOH:O	2.07	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:541:ARG:C	1:A:543:GLY:N	2.64	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:465:GLU:C	1:A:467:ARG:N	2.66	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: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
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:714:LEU:HD23	1:A:729:MET:HE1	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:7:ARG:HG2	1:D:13:GLU:CD	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:D:857:ARG:HH22	1:D:936:LEU:C	2.17	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
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:349:GLN:H	1:B:349:GLN:CD	2.17	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:655:VAL:C	1:C:657:ALA:N	2.65	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:TYR:HB2	1:B:401:MET:HE2	1.91	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: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:D:827:GLN:C	1:D:830:PRO:HD2	2.34	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
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:465:GLU:C	1:D:467:ARG:H	2.16	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:211:VAL:HG23	1:D:385:THR:HG22	1.90	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: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:A:524:ARG:HH12	1:A:527:TRP:CD1	2.28	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
1:C:96:ILE:HD13	1:C:211:VAL:HG21	1.91	0.52
1:C:281:ALA:HA	1:C:284:GLU:CD	2.35	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:A:717:MET:HE1	1:A:729:MET:HE2	1.91	0.52
1:A:894:GLN:C	2:A:1355:HOH:O	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:349:GLN:CD	1:D:349:GLN:H	2.17	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:298:MET:HE2	1:C:872:PHE:CD2	2.44	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:464:LYS:C	1:D:466:PRO:HD2	2.35	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:B:18:ARG:HE	1:B:22:GLN:HE21	1.56	0.52
1:B:538:ALA:HB2	2:B:1057:HOH:O	2.10	0.52
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:298:MET:HE2	1:A:872:PHE:CD2	2.45	0.51
1:A:326:GLN:HG2	1:A:357:VAL:CG1	2.41	0.51
1:B:250:LEU:HB2	1:B:259:GLU:CD	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:ASP:OD2	1:A:816:LYS:HG2	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:D:97:ALA:HB1	1:D:99:MET:HE2	1.92	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:239:MET:HE3	1:B:304:LEU:N	2.25	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
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:B:281:ALA:HA	1:B:284:GLU:CD	2.36	0.51
1:B:655:VAL:C	1:B:657:ALA:N	2.65	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:866:MET:HE1	1:B:870:GLU:OE2	2.10	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:250:LEU:HB2	1:D:259:GLU:CD	2.35	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: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: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:A:578:GLY:C	1:A:681:ARG:HH21	2.19	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
1:D:875:LEU:HD21	2:D:1071:HOH:O	2.09	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:C:897:PHE:C	1:C:897:PHE:HD2	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:827:GLN:C	1:B:830:PRO:HD2	2.36	0.50
1:C:63:MET:HE2	1:C:63:MET:HA	1.93	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:C:819:LEU:C	2:C:1223:HOH:O	2.54	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:541:ARG:C	1:D:543:GLY:N	2.69	0.50
1:D:602:PHE:CD1	1:D:603:ASP:N	2.80	0.50
1:A:349:GLN:CD	1:A:349:GLN:H	2.19	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:485:GLN:HA	1:A:485:GLN:OE1	2.11	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:284:GLU:CD	1:A:290:GLU:HB3	2.37	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: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
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: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:D:801:LEU:HD22	1:D:842:ALA:HB1	1.94	0.49
1:A:102:GLY:CA	1:A:105:LYS:HZ1	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:370:THR:HG22	1:D:756:ASP:CG	2.37	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:A:550:ASN:C	2:A:1125:HOH:O	2.56	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:A:675:ASP:OD2	1:A:675:ASP:C	2.55	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:B:821:ASP:CG	1:B:931:LYS:HG2	2.37	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:MET:HG2	1:C:341:ARG:HG3	1.94	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: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:349:GLN:CD	1:C:349:GLN:H	2.21	0.49
1:C:705:PHE:CB	1:C:741:VAL:HG22	2.43	0.49
1:C:777:LYS:C	1:C:781:VAL:HG23	2.37	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:443:GLY:C	1:D:658:LEU:HD13	2.38	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:A:827:GLN:C	1:A:830:PRO:HD2	2.38	0.49
1:B:261:THR:N	2:B:1169:HOH:O	2.45	0.49
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:B:785:ALA:HA	1:B:788:MET:HE3	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:710:VAL:C	1:D:712:ALA:H	2.20	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:299:GLU:H	1:A:299:GLU:CD	2.20	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:428:LYS:HD3	1:B:695:VAL:C	2.38	0.48
1:B:668:ARG:HH12	1:B:735:GLU:CD	2.21	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: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:C:675:ASP:C	1:C:675:ASP:OD2	2.57	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:777:LYS:C	1:A:781:VAL:HG23	2.39	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:97:ALA:HB1	1:C:99:MET:HE2	1.95	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:355:GLU:OE1	1:C:355:GLU:HA	2.13	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: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
1:B:288:GLY:HA3	2:B:1125:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:655:VAL:C	1:D:657:ALA:H	2.21	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:244:LYS:HG3	1:A:311:LYS:HZ3	1.78	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:C:473:LEU:HD13	1:C:473:LEU:C	2.38	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: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:209:ASP:OD1	1:B:384:MET:HE3	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:ASN:HB3	2:C:1209:HOH:O	2.13	0.47
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: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:194:GLN:C	2:D:1156:HOH:O	2.57	0.47
1:D:209:ASP:OD1	1:D:384:MET:HE3	2.15	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:LEU:HB2	2:A:1257:HOH:O	2.14	0.47
1:A:858:GLU:CG	1:A:866:MET:HE3	2.35	0.47
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:284:GLU:CD	1:C:290:GLU:HB3	2.40	0.47
1:C:370:THR:C	1:C:372:GLN:N	2.73	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:273:VAL:HG21	1:D:816:LYS:C	2.40	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: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:857:ARG:HH22	1:C:936:LEU:C	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:A:685:GLN:C	1:A:687:ASP:H	2.23	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: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:253:GLU:O	1:A:254:PRO:C	2.57	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:710:VAL:C	1:A:712:ALA:H	2.23	0.46
1:A:860:GLU:HG3	2:A:1140:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:685:GLN:C	1:B:687:ASP:H	2.23	0.46
1:B:802:ASN:CG	1:B:802:ASN:O	2.57	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
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:92:HIS:C	1:C:94:GLY:H	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:234:ASP:OD1	1:D:238:LYS:HE3	2.15	0.46
1:D:253:GLU:O	1:D:254:PRO:C	2.58	0.46
1:D:273:VAL:HA	1:D:820:LEU:HB2	1.98	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: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
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:465:GLU:C	1:B:467:ARG:H	2.21	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:C:253:GLU:O	1:C:254:PRO:C	2.58	0.46
1:C:821:ASP:CG	1:C:931:LYS:HE2	2.41	0.46
1:D:498:LEU:HD23	2:D:1092:HOH:O	2.16	0.46
1:D:710:VAL:C	1:D:712:ALA:N	2.73	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:A:857:ARG:C	1:A:859:ALA:H	2.23	0.46
1:B:211:VAL:CG1	1:B:383:GLY:HA3	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:121:LYS:C	1:C:198:ARG:NH2	2.74	0.46
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:131:TYR:C	1:B:131:TYR:CD2	2.94	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:503:ALA:O	1:B:504:GLN:C	2.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:D:480:PHE:CE1	1:D:527:TRP:HE3	2.34	0.45
1:D:503:ALA:O	1:D:504:GLN:C	2.59	0.45
1:D:669:HIS:ND1	1:D:675:ASP:HB3	2.30	0.45
1:A:429:PHE:O	1:A:433:VAL:HG23	2.16	0.45
1:A:464:LYS:C	1:A:466:PRO:HD3	2.42	0.45
1:B:259:GLU:CB	1:B:260:PRO:CD	2.93	0.45
1:B:810:TRP:CD1	1:B:810:TRP:H	2.34	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:D:109:ALA:HB2	1:D:384:MET:HE1	1.98	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: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:392:GLU:OE1	1:A:403:VAL:HB	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:702:MET:HE2	1:B:734:ILE:HG12	1.99	0.45
1:B:861:LEU:HD23	1:B:861:LEU:H	1.80	0.45
1:C:429:PHE:O	1:C:430:TYR:C	2.59	0.45
1:C:435:GLU:CD	1:C:694:TYR:OH	2.58	0.45
1:C:885:HIS:CB	1:C:921:MET:HE2	2.47	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
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: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:622:GLU:HG2	1:A:623:GLU:HG3	1.99	0.45
1:B:253:GLU:O	1:B:254:PRO:C	2.60	0.45
1:B:485:GLN:HG2	1:B:496:ARG:CZ	2.46	0.45
1:B:710:VAL:C	1:B:712:ALA:H	2.23	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:130:ASP:O	1:D:131:TYR:C	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:804:GLU:HA	2:C:1033:HOH:O	2.17	0.45
1:C:858:GLU:HG3	1:C:866:MET:CE	2.31	0.45
1:D:19:TYR:HE1	1:D:93:GLU:OE2	2.00	0.45
1:D:345:GLU:CD	2:D:1339:HOH:O	2.60	0.45
1:D:475:MET:HB3	2:D:1084:HOH:O	2.16	0.45
1:D:685:GLN:C	1:D:687:ASP:H	2.25	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: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: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
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: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:729:MET:HE3	1:A:729:MET:HB3	1.84	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:GLU:CB	1:B:256:VAL:HG13	2.44	0.44
1:B:920:GLU:O	1:B:923:ALA:HB3	2.17	0.44
1:C:86:ILE:O	1:C:87:GLY:C	2.60	0.44
1:C:130:ASP:O	1:C:131:TYR:C	2.60	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:602:PHE:O	1:D:603:ASP:C	2.61	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
1:A:905:ASP:OD2	1:A:908:GLN:HB2	2.17	0.44
1:B:92:HIS:C	1:B:94:GLY:H	2.26	0.44
1:B:130:ASP:O	1:B:131:TYR:C	2.60	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: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:244:LYS:HE3	1:C:311:LYS:HZ2	1.82	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:273:VAL:HG12	1:D:816:LYS:HZ1	1.81	0.44
1:D:615:LYS:HD3	1:D:623:GLU:HB3	1.98	0.44
1:A:11:ASN:C	1:A:13:GLU:H	2.26	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:130:ASP:O	1:A:131:TYR:C	2.60	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:523:LEU:HD23	1:B:523:LEU:C	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:316:ARG:HD3	1:C:355:GLU:CD	2.43	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:429:PHE:O	1:A:430:TYR:C	2.60	0.44
1:A:716:ARG:C	1:A:718:GLY:N	2.76	0.44
1:A:770:ARG:NH1	1:A:879:ASP:CB	2.81	0.44
1:B:39:ASP:CB	2:B:1184:HOH:O	2.62	0.44
1:B:109:ALA:HB2	1:B:384:MET:HE1	1.99	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
1:B:599:LYS:HE2	1:B:599:LYS:HB2	1.75	0.44
1:B:710:VAL:C	1:B:712:ALA:N	2.75	0.44
1:C:103:GLU:HG2	1:C:582:ASP:CG	2.43	0.44
1:C:119:THR:CG2	1:C:121:LYS:HG3	2.44	0.44
1:C:717:MET:CE	1:C:729:MET:HE2	2.48	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:A:309:ARG:HH22	1:A:931:LYS:HZ2	1.66	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:298:MET:HE3	1:C:876:ASN:CB	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:447:LEU:HD11	1:D:573:ALA:HB2	1.99	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:A:857:ARG:HH22	1:A:936:LEU:C	2.25	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: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
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: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: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:C:893:ARG:C	1:C:895:GLY:H	2.25	0.44
1:D:271:ARG:NH2	1:D:821:ASP:OD2	2.51	0.44
1:D:429:PHE:O	1:D:430:TYR:C	2.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:163:ARG:HH11	1:B:182:ASP:CG	2.26	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:802:ASN:HA	1:C:839:ALA:HB2	2.00	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:495:LEU:C	1:B:495:LEU:HD12	2.43	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
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:D:893:ARG:C	1:D:895:GLY:H	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:30:LEU:HD13	1:D:63:MET:HE3	1.99	0.43
1:D:44:TYR:HE2	1:D:149:LEU:HD21	1.83	0.43
1:D:92:HIS:C	1:D:94:GLY:H	2.26	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: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
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:B:893:ARG:C	1:B:895:GLY:H	2.26	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:C:485:GLN:OE1	1:C:485:GLN:HA	2.18	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:11:ASN:C	1:C:13:GLU:H	2.27	0.43
1:C:463:LEU:HB2	1:C:546:HIS:NE2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:788:MET:HE1	1:D:874:ILE:CD1	2.48	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
1:B:253:GLU:HG3	1:B:256:VAL:O	2.19	0.43
1:B:887:HIS:C	1:B:887:HIS:CD2	2.97	0.43
1:C:80:HIS:CD2	1:C:107:LEU:HD21	2.54	0.43
1:C:788:MET:HE1	1:C:874:ILE:HG23	2.00	0.43
1:C:801:LEU:HD22	1:C:842:ALA:CB	2.49	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:92:HIS:C	1:A:94:GLY:H	2.26	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:A:918:PHE:O	1:A:919:ASN:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:503:ALA:C	1:B:505:LEU:N	2.73	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:716:ARG:C	1:C:718:GLY:N	2.74	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: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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:480:PHE:CD2	1:B:480:PHE:C	2.97	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:714:LEU:CD2	1:C:729:MET:HE1	2.47	0.42
1:C:755:PHE:C	1:C:757:ASP:H	2.27	0.42
1:C:838:LYS:HG2	1:C:839:ALA:N	2.34	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:503:ALA:C	1:A:505:LEU:N	2.76	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:506:LYS:C	2:C:1206:HOH:O	2.62	0.42
1:C:522:ASN:N	2:C:1106:HOH:O	2.52	0.42
1:C:685:GLN:C	1:C:687:ASP:H	2.27	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
1:D:178:GLU:OE1	1:D:178:GLU:HA	2.17	0.42
1:D:428:LYS:HZ2	1:D:667:GLU:HB3	1.84	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: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:217:ASP:C	2:B:1017:HOH:O	2.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:599:LYS:HB3	1:B:600:GLU:H	1.50	0.42
1:C:295:PRO:O	1:C:296:GLU:HB2	2.18	0.42
1:C:355:GLU:HB3	1:C:357:VAL:HG23	1.99	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:A:503:ALA:O	1:A:504:GLN:C	2.62	0.42
1:A:893:ARG:C	1:A:895:GLY:H	2.26	0.42
1:B:134:ARG:O	1:B:137:ALA:HB3	2.19	0.42
1:B:298:MET:HE1	1:B:873:VAL:HA	2.02	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: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:473:LEU:HD13	1:A:473:LEU:C	2.44	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
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:235:LEU:HD13	1:C:303:MET:HE1	2.02	0.42
1:C:274:HIS:CE1	1:C:305:ILE:HA	2.54	0.42
1:C:714:LEU:HA	1:C:729:MET:HE1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:MET:HE1	1:D:366:LEU:HB2	2.00	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:741:VAL:O	1:A:742:GLU:C	2.63	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:813:GLU:CD	1:D:813:GLU:N	2.70	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:503:ALA:O	1:C:504:GLN:C	2.62	0.42
1:C:796:LEU:HD23	1:C:796:LEU:C	2.45	0.42
1:D:419:ASP:OD2	1:D:668:ARG:HD2	2.18	0.42
1:D:619:GLY:C	1:D:620:LYS:HG2	2.44	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: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
1:B:78:MET:HE3	1:B:103:GLU:OE1	2.20	0.42
1:B:390:THR:HG22	1:B:391:GLU:CD	2.45	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:459:LEU:HA	1:C:462:MET:HE3	2.01	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:D:808:GLU:H	1:D:808:GLU:CD	2.28	0.42
1:A:220:ARG:C	1:A:752:LEU:HD22	2.45	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:N	2.77	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:866:MET:HB3	1:B:866:MET:HE3	1.75	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: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:782:LYS:O	1:B:786:ILE:HG13	2.20	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
1:C:602:PHE:O	1:C:603:ASP:C	2.63	0.42
1:C:635:GLU:HB2	2:C:1214:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:896:ILE:HG22	1:C:896:ILE:O	2.18	0.42
1:D:541:ARG:C	1:D:543:GLY:H	2.26	0.42
1:A:199:HIS:CD2	1:A:199:HIS:N	2.87	0.41
1:A:428:LYS:HZ3	1:A:699:ASP:HB3	1.85	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:C:852:LYS:HB2	1:C:852:LYS:HZ2	1.85	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: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:553:HIS:O	1:B:557:GLU:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:602:PHE:O	1:B:603:ASP:C	2.63	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:810:TRP:CD1	1:C:810:TRP:H	2.38	0.41
1:C:827:GLN:C	1:C:830:PRO:HD2	2.46	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:C:857:ARG:C	1:C:859:ALA:H	2.28	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:116:ASN:N	1:B:116:ASN:ND2	2.61	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:801:LEU:O	1:D:839:ALA:HA	2.20	0.41
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:A:889:LEU:O	1:A:890:ASP:C	2.64	0.41
1:B:6:ARG:C	1:B:13:GLU:HG3	2.44	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:495:LEU:C	1:D:495:LEU:HD12	2.45	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:63:MET:HE2	1:A:63:MET:HA	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:92:HIS:O	1:B:380:LYS:NZ	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:103:GLU:O	1:B:104:GLY:C	2.64	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: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:441:GLU:CD	1:A:539:VAL:HG22	2.46	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:316:ARG:HA	1:B:320:TYR:CZ	2.56	0.41
1:B:444:GLN:NE2	1:B:659:GLY:HA3	2.36	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:813:GLU:CD	1:C:813:GLU:N	2.78	0.41
1:D:76:LEU:HD13	1:D:143:VAL:HG23	2.03	0.41
1:D:76:LEU:HD12	1:D:142:PRO:HG2	2.01	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:257:ARG:HH22	1:D:825:GLN:CD	2.28	0.41
1:D:294:SER:O	1:D:936:LEU:HD12	2.21	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:753:LEU:HD13	1:D:753:LEU:C	2.46	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:460:SER:O	1:A:461:GLN:C	2.64	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:710:VAL:C	1:C:712:ALA:H	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:217:ASP:CG	1:B:674:ILE:HD11	2.46	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:251:PRO:C	2:B:1078:HOH:O	2.63	0.40
1:B:265:THR:O	1:B:266:VAL:C	2.62	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:103:GLU:O	1:C:104:GLY:C	2.62	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:503:ALA:C	1:D:505:LEU:N	2.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:343:TYR:C	1:C:888:ASN:HD21	2.29	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:D:713:MET:HB3	1:D:729:MET:CE	2.51	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:A:810:TRP:CD1	1:A:810:TRP:H	2.38	0.40
1:B:201:HIS:C	2:B:1283:HOH:O	2.65	0.40
1:B:206:ALA:HB2	1:B:378:TYR:CD2	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:233:THR:H	1:D:361:ARG:NH1	2.19	0.40
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:103:GLU:O	1:A:104:GLY:C	2.65	0.40
1:A:119:THR:CG2	1:A:121:LYS:HE3	2.51	0.40
1:A:487:GLN:CD	1:A:487:GLN:N	2.79	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:A:885:HIS:HB2	1:A:921:MET:HE2	2.04	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:248:ARG:C	2:D:1088:HOH:O	2.65	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
1:D:785:ALA:HA	1:D:788:MET:HE3	2.02	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%)	1	5
1	B	932/997 (94%)	778 (84%)	108 (12%)	46 (5%)	1	6
1	C	937/997 (94%)	784 (84%)	108 (12%)	45 (5%)	2	6
1	D	932/997 (94%)	777 (83%)	107 (12%)	48 (5%)	1	5
All	All	3738/3988 (94%)	3128 (84%)	424 (11%)	186 (5%)	1	5

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 [i](#)

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%)	656 (83%)	132 (17%)	2 8
1	B	784/840 (93%)	648 (83%)	136 (17%)	2 7
1	C	788/840 (94%)	668 (85%)	120 (15%)	3 10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	784/840 (93%)	649 (83%)	135 (17%)	2	7
All	All	3144/3360 (94%)	2621 (83%)	523 (17%)	2	8

All (523) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASP
1	A	15	GLU
1	A	16	ILE
1	A	20	TYR
1	A	33	GLU
1	A	35	GLU
1	A	49	GLU
1	A	57	LEU
1	A	63	MET
1	A	78	MET
1	A	86	ILE
1	A	105	LYS
1	A	106	THR
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	199	HIS
1	A	200	ASP
1	A	231	LYS
1	A	241	GLU
1	A	246	LEU
1	A	254	PRO
1	A	256	VAL
1	A	258	LYS
1	A	264	TYR
1	A	266	VAL
1	A	267	GLU
1	A	270	ASN
1	A	274	HIS

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Mol	Chain	Res	Type
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	349	GLN
1	A	351	ILE
1	A	354	LYS
1	A	355	GLU
1	A	360	GLU
1	A	361	ARG
1	A	362	GLU
1	A	370	THR
1	A	381	ARG
1	A	384	MET
1	A	389	LYS
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	466	PRO
1	A	472	ARG
1	A	507	ASP
1	A	530	LEU
1	A	537	LEU
1	A	539	VAL
1	A	544	ILE
1	A	546	HIS
1	A	547	GLN
1	A	559	GLU
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

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Mol	Chain	Res	Type
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	675	ASP
1	A	678	LEU
1	A	685	GLN
1	A	700	ASP
1	A	701	LEU
1	A	708	ASP
1	A	709	ARG
1	A	713	MET
1	A	722	SER
1	A	729	MET
1	A	731	THR
1	A	741	VAL
1	A	750	LYS
1	A	753	LEU
1	A	756	ASP
1	A	757	ASP
1	A	759	LEU
1	A	762	GLN
1	A	782	LYS
1	A	800	PHE
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

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Mol	Chain	Res	Type
1	A	866	MET
1	A	875	LEU
1	A	884	GLU
1	A	892	LEU
1	A	897	PHE
1	A	901	TYR
1	A	904	LYS
1	A	905	ASP
1	A	916	ARG
1	A	921	MET
1	A	927	SER
1	A	934	PHE
1	B	8	LEU
1	B	9	PHE
1	B	10	ASP
1	B	11	ASN
1	B	16	ILE
1	B	70	GLU
1	B	75	TYR
1	B	78	MET
1	B	101	THR
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	159	THR
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	253	GLU
1	B	254	PRO
1	B	256	VAL
1	B	258	LYS
1	B	259	GLU

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Mol	Chain	Res	Type
1	B	264	TYR
1	B	265	THR
1	B	275	LEU
1	B	299	GLU
1	B	304	LEU
1	B	332	GLU
1	B	334	THR
1	B	341	ARG
1	B	345	GLU
1	B	347	LEU
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	407	PRO
1	B	409	ASN
1	B	410	ARG
1	B	423	ARG
1	B	424	THR
1	B	435	GLU
1	B	436	ILE
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	486	LYS
1	B	487	GLN
1	B	490	PRO
1	B	495	LEU
1	B	508	GLU
1	B	517	ILE
1	B	522	ASN
1	B	524	ARG
1	B	528	GLU
1	B	537	LEU
1	B	546	HIS
1	B	550	ASN
1	B	559	GLU

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Mol	Chain	Res	Type
1	B	575	ASN
1	B	582	ASP
1	B	604	ARG
1	B	605	TYR
1	B	608	LYS
1	B	610	GLU
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	672	ARG
1	B	677	GLN
1	B	678	LEU
1	B	681	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
1	B	732	ARG
1	B	740	ARG
1	B	741	VAL
1	B	743	ASP
1	B	752	LEU
1	B	753	LEU
1	B	756	ASP
1	B	757	ASP
1	B	759	LEU
1	B	762	GLN
1	B	766	ILE
1	B	791	GLU
1	B	796	LEU
1	B	798	GLU

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Mol	Chain	Res	Type
1	B	800	PHE
1	B	802	ASN
1	B	810	TRP
1	B	813	GLU
1	B	818	THR
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	854	TYR
1	B	861	LEU
1	B	866	MET
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	B	921	MET
1	B	935	ARG
1	C	10	ASP
1	C	16	ILE
1	C	20	TYR
1	C	33	GLU
1	C	35	GLU
1	C	49	GLU
1	C	57	LEU
1	C	78	MET
1	C	86	ILE
1	C	105	LYS
1	C	110	THR
1	C	126	VAL
1	C	127	THR
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

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Mol	Chain	Res	Type
1	C	198	ARG
1	C	199	HIS
1	C	200	ASP
1	C	231	LYS
1	C	241	GLU
1	C	254	PRO
1	C	256	VAL
1	C	258	LYS
1	C	264	TYR
1	C	267	GLU
1	C	269	LYS
1	C	270	ASN
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	351	ILE
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	384	MET
1	C	389	LYS
1	C	397	GLU
1	C	413	ILE
1	C	424	THR
1	C	435	GLU
1	C	457	GLU
1	C	472	ARG
1	C	507	ASP
1	C	537	LEU
1	C	539	VAL
1	C	544	ILE

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Mol	Chain	Res	Type
1	C	546	HIS
1	C	547	GLN
1	C	550	ASN
1	C	569	THR
1	C	579	ARG
1	C	602	PHE
1	C	608	LYS
1	C	614	LYS
1	C	621	GLU
1	C	622	GLU
1	C	646	GLU
1	C	647	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	722	SER
1	C	731	THR
1	C	750	LYS
1	C	753	LEU
1	C	757	ASP
1	C	759	LEU
1	C	762	GLN
1	C	800	PHE
1	C	808	GLU
1	C	810	TRP
1	C	813	GLU
1	C	819	LEU
1	C	825	GLN
1	C	827	GLN
1	C	830	PRO

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Mol	Chain	Res	Type
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	D	8	LEU
1	D	9	PHE
1	D	10	ASP
1	D	11	ASN
1	D	16	ILE
1	D	20	TYR
1	D	21	LYS
1	D	63	MET
1	D	70	GLU
1	D	76	LEU
1	D	78	MET
1	D	101	THR
1	D	103	GLU
1	D	116	ASN
1	D	126	VAL
1	D	127	THR
1	D	140	MET
1	D	159	THR
1	D	172	THR
1	D	176	ASN
1	D	177	SER
1	D	178	GLU
1	D	186	ASP
1	D	198	ARG
1	D	208	ILE
1	D	213	SER

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Mol	Chain	Res	Type
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	259	GLU
1	D	264	TYR
1	D	266	VAL
1	D	274	HIS
1	D	275	LEU
1	D	299	GLU
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	409	ASN
1	D	410	ARG
1	D	423	ARG
1	D	424	THR
1	D	435	GLU
1	D	450	THR
1	D	451	ILE
1	D	457	GLU
1	D	459	LEU
1	D	466	PRO
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	508	GLU
1	D	517	ILE
1	D	522	ASN
1	D	528	GLU

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Mol	Chain	Res	Type
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	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	670	GLU
1	D	671	SER
1	D	672	ARG
1	D	677	GLN
1	D	678	LEU
1	D	681	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	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
1	D	766	ILE

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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	813	GLU
1	D	818	THR
1	D	826	LEU
1	D	827	GLN
1	D	831	PHE
1	D	833	GLU
1	D	840	GLU
1	D	851	LEU
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 (98) 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	156	HIS
1	A	199	HIS
1	A	297	ASN
1	A	306	GLN
1	A	323	GLN
1	A	363	ASN
1	A	409	ASN
1	A	487	GLN

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Mol	Chain	Res	Type
1	A	685	GLN
1	A	769	GLN
1	A	799	ASN
1	A	825	GLN
1	A	827	GLN
1	A	903	GLN
1	A	908	GLN
1	B	11	ASN
1	B	12	ASN
1	B	22	GLN
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	348	HIS
1	B	364	GLN
1	B	396	GLN
1	B	409	ASN
1	B	444	GLN
1	B	487	GLN
1	B	504	GLN
1	B	650	GLN
1	B	677	GLN
1	B	685	GLN
1	B	727	HIS
1	B	827	GLN
1	B	887	HIS
1	B	888	ASN
1	B	903	GLN
1	B	908	GLN
1	C	11	ASN
1	C	22	GLN
1	C	92	HIS
1	C	155	GLN
1	C	187	ASN
1	C	199	HIS
1	C	201	HIS
1	C	274	HIS
1	C	297	ASN
1	C	302	HIS

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Mol	Chain	Res	Type
1	C	306	GLN
1	C	363	ASN
1	C	409	ASN
1	C	487	GLN
1	C	563	GLN
1	C	575	ASN
1	C	650	GLN
1	C	685	GLN
1	C	727	HIS
1	C	745	ASN
1	C	769	GLN
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	297	ASN
1	D	323	GLN
1	D	364	GLN
1	D	409	ASN
1	D	444	GLN
1	D	487	GLN
1	D	542	GLN
1	D	550	ASN
1	D	563	GLN
1	D	629	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	908	GLN

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Mol	Chain	Res	Type
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 oligosaccharides 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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	939/997 (94%)	-1.61	0 100 100	18, 61, 86, 103	0
1	B	934/997 (93%)	-1.60	0 100 100	16, 59, 85, 112	0
1	C	939/997 (94%)	-1.61	0 100 100	20, 61, 88, 102	0
1	D	934/997 (93%)	-1.61	0 100 100	21, 59, 87, 112	0
All	All	3746/3988 (93%)	-1.61	0 100 100	16, 60, 87, 112	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.