



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2024 – 07:36 PM EST

PDB ID : 2DHH  
Title : Crystal structure of a multidrug transporter reveal a functionally rotating mechanism  
Authors : Murakami, S.; Nakashima, R.; Yamashita, E.; Matsumoto, T.  
Deposited on : 2006-03-23  
Resolution : 2.80 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

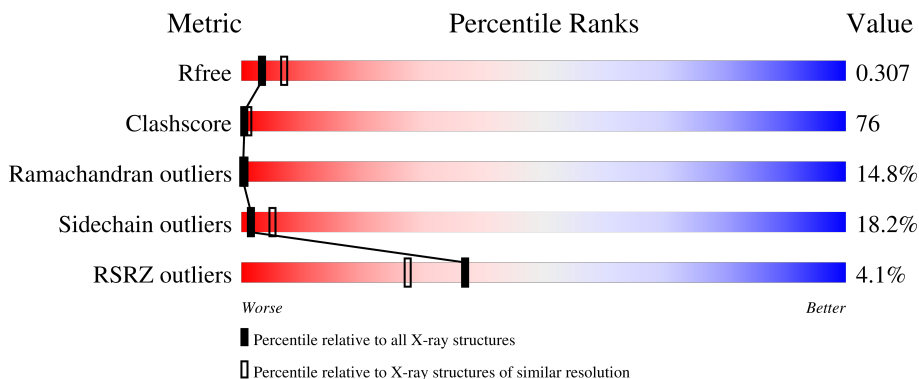
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	1053	 4% 23% 49% 20% 5% .
1	B	1053	 4% 19% 55% 21% . .
1	C	1053	 4% 18% 53% 22% 5% .

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 23378 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 ACRB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1022	7774	5003	1283	1444	44	0	0	0
1	B	1022	7774	5003	1283	1444	44	0	0	0
1	C	1022	7774	5003	1283	1444	44	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1050	HIS	-	expression tag	UNP P31224
A	1051	HIS	-	expression tag	UNP P31224
A	1052	HIS	-	expression tag	UNP P31224
A	1053	HIS	-	expression tag	UNP P31224
B	1050	HIS	-	expression tag	UNP P31224
B	1051	HIS	-	expression tag	UNP P31224
B	1052	HIS	-	expression tag	UNP P31224
B	1053	HIS	-	expression tag	UNP P31224
C	1050	HIS	-	expression tag	UNP P31224
C	1051	HIS	-	expression tag	UNP P31224
C	1052	HIS	-	expression tag	UNP P31224
C	1053	HIS	-	expression tag	UNP P31224

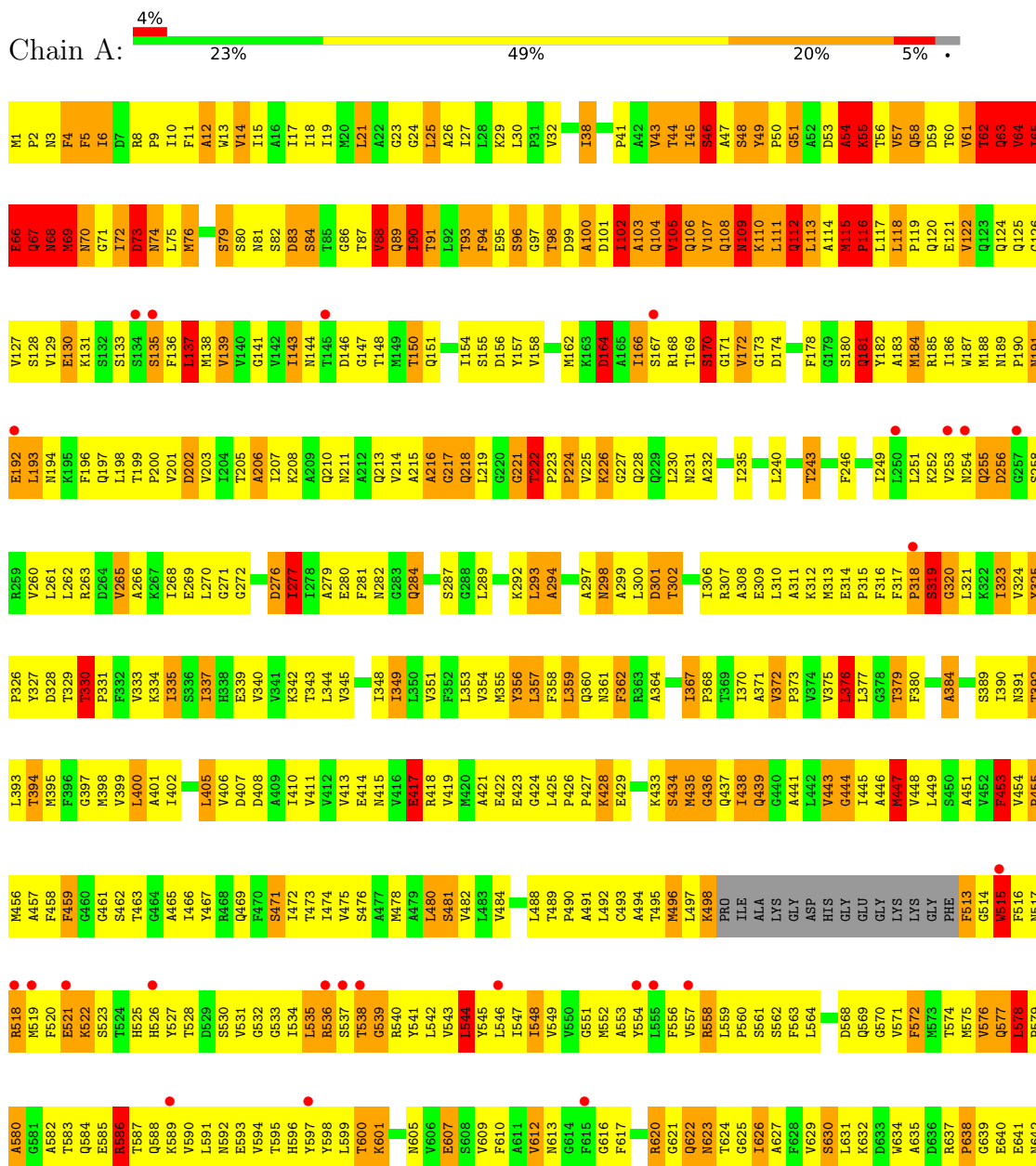
- Molecule 2 is water.

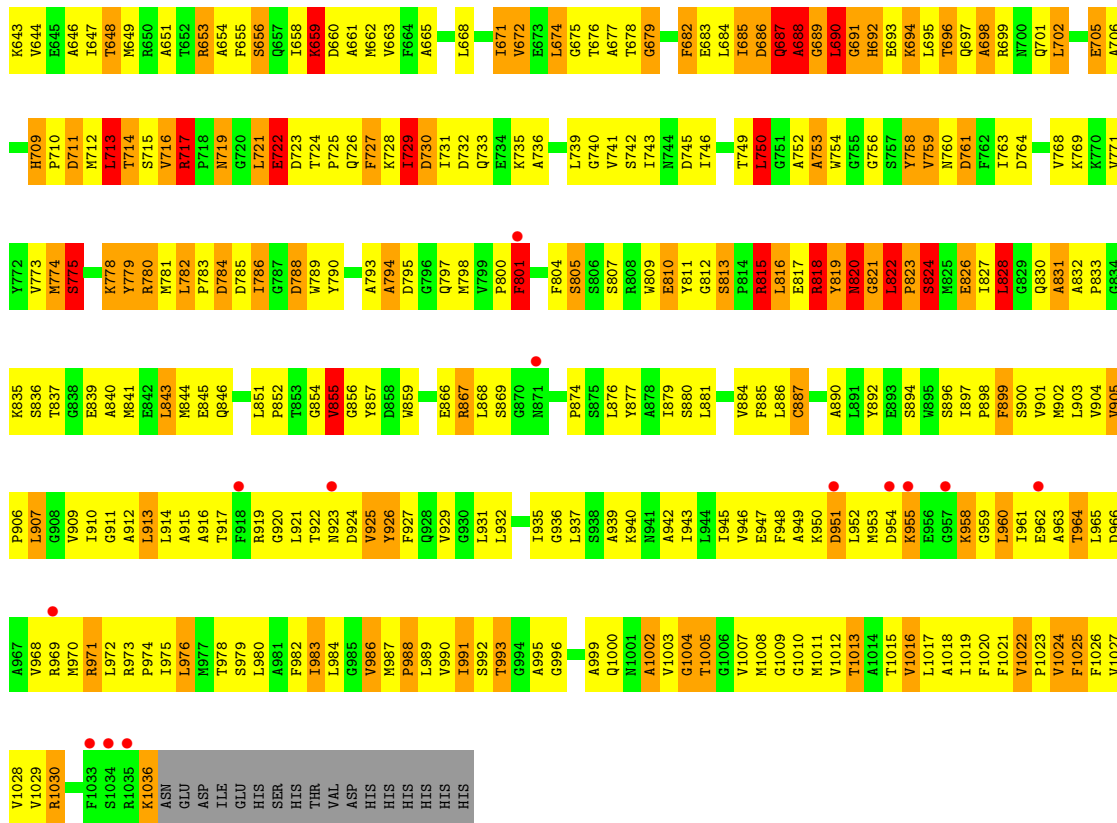
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	22	Total 22	O 22	0	0
2	B	8	Total 8	O 8	0	0
2	C	26	Total 26	O 26	0	0

### 3 Residue-property plots

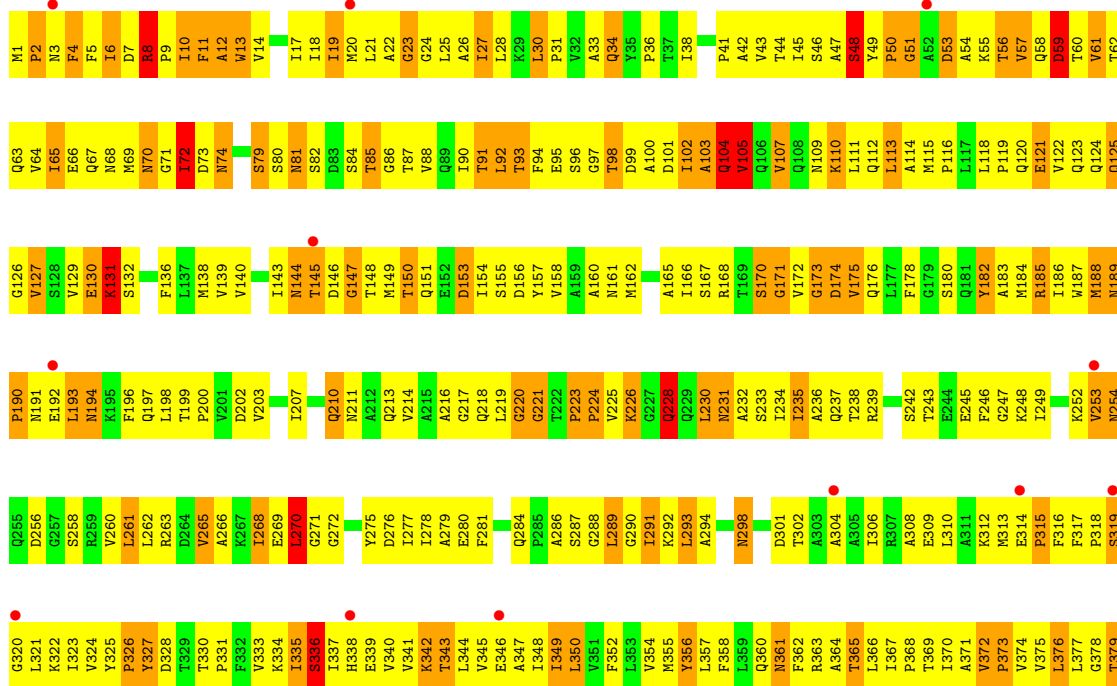
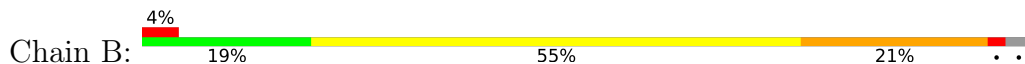
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

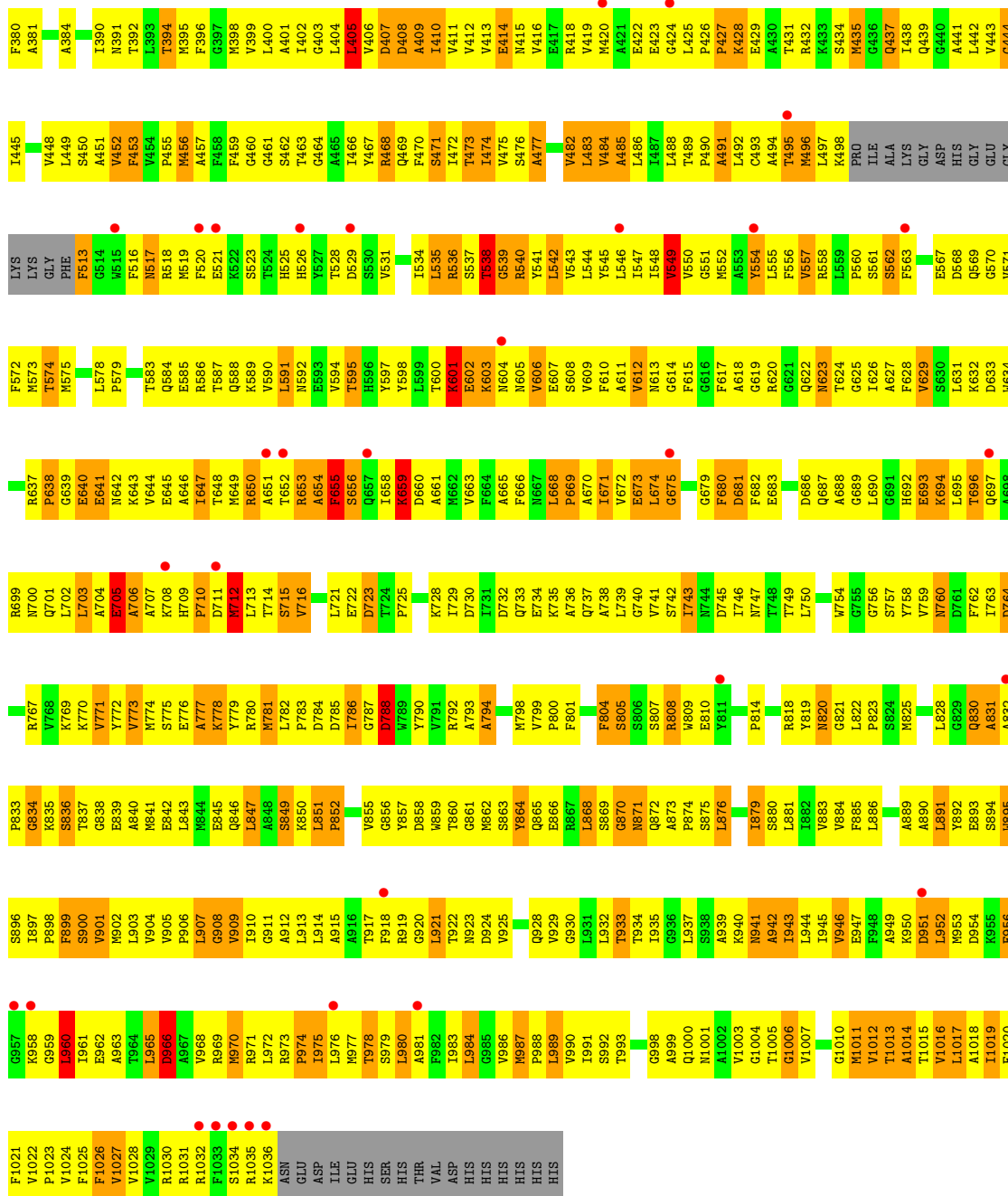
- Molecule 1: ACRB



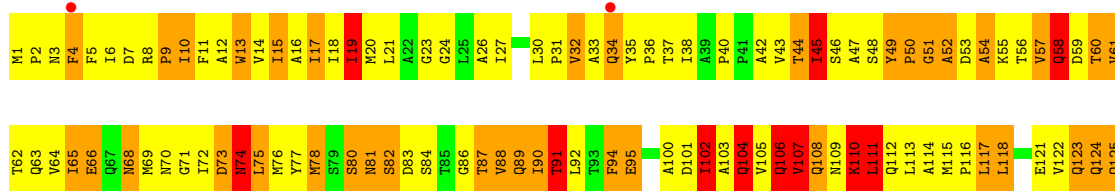
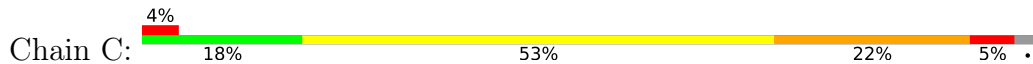


• Molecule 1: ACRB





● Molecule 1: ACRB



G126	V127	S134	S135	F136	L137	M138	V139	V140	G141	D201	D202	V203	M204	M144	T145	D146	G147	M148	T149	T150	N211	A212	Q213	D153	S155	D217	D156	V157	V158	A159	A160	M161	M162	K163	D164	A165	I166	S167	R168	Q229	L230	L230	M231	A232	S233	L234	I235	A236	Q237	T238	R239	L240	A303	A304	S242	T243	Y182	A183	M184	E244	E245	F246	G247						
M187	M188	M189	P190	L250	L251	K252	E192	L193	L194	K195	F196	R258	Q197	L198	T199	P200	V201	D202	V203	M204	M205	A206	L268	E269	Q210	N211	A212	Q213	V214	A215	A216	E217	Q218	L219	G220	G221	P223	P224	V225	K226	Q227	Q228	Q229	L230	M231	A232	S233	L234	I235	A236	Q237	T238	R239	L240	A303	A304	S242	T243	Y182	A183	M184	E244	E245	F246	G247				
K248	L249	L250	L251	K252	V253	M254	G257	S258	R259	V260	L261	L262	R263	D264	V265	A266	K267	L268	E269	Q270	M271	G272	E273	N274	L277	H278	A279	E280	F281	N282	L283	G284	P285	A286	S287	G288	L289	Q290	R291	Q292	L293	A294	T295	G296	A297	M298	L299	L300	D301	F302	A303	A304	S242	T243	Y182	A183	M184	E244	E245	F246	G247								
L310	A311	K312	M313	E314	P315	F316	F317	P318	S319	G320	L321	K322	L323	V324	Y325	P326	V327	D328	T329	T330	P331	F332	G333	K334	L335	S336	L337	H338	E339	A401	I402	V403	L404	T405	L406	D407	D408	A409	I410	V411	V412	G350	V351	F352	L353	V354	M355	Y356	L418	V419	M420	A421	L359	Q360	N361	F362	L426	A427	A364	A305	T365	L366	K428	A429	P490	A491	P368	L492	T369
L370	A371	P372	P373	V374	V375	L376	L377	G378	T379	F380	L383	F386	G387	F388	V389	A401	I402	V403	L404	T405	L406	D407	D408	A409	I410	V411	V412	G350	V351	F352	L353	V354	M355	Y356	L418	V419	M420	A421	L359	Q360	N361	F362	L426	A427	A364	A305	T365	L366	K428	A429	P490	A491	P368	L492	T369														
R432	K433	S434	M435	G436	L437	K438	Q439	G440	A441	L442	V443	G444	I445	A446	M447	V448	L449	S450	A451	V452	F453	V454	G455	A457	F458	F459	G460	A461	G462	T463	G464	A465	G283	L466	Y467	R468	Q469	F470	S471	I474	V475	S476	A477	M478	A479	L480	S481	V482	L483	V484	A485	L486	I487	A488	T489	P490	A491	P368	L492	T369									
C483	A484	T485	M486	L487	K488	P489	I489	ALA	LYS	GLY	ASP	HIS	GLY	GLU	GLY	LYS	LYS	GLY	PHE	F513	G514	W515	F516	M517	R518	M519	F520	E521	K522	S523	T524	H525	H526	T528	D529	S530	V531	G532	G533	L534	L535	Y541	L542	V543	L544	Y545	L546	I547	L548	V549	V550	G551	M552																
A553	L554	F555	F556	V557	R558	L559	F560	G561	S562	F563	L564	D568	Q569	G570	E571	V572	A573	T574	H575	V576	W577	L578	F579	R586	T587	Q588	K589	V590	L591	N592	L593	H594	T595	H596	Y597	L598	L599	T600	G601	X602	L603	V606	E607	S608	V609	F610	A611	V612	N613	G614	F615	G616	F617	A618	G619	R620													
G621	Q622	N623	L624	G625	I626	A627	F628	V629	K632	D633	V634	G639	E640	G641	N642	G643	V644	E645	A646	V576	I647	T648	M649	R650	R653	A654	F655	K656	Q657	L658	G659	A661	T662	H663	V664	F665	L666	P667	L668	P669	A670	L671	V672	S673	E674	L675	T678	G679	G680	D681	F682	G683	L684	I685	D686														
Q687	A688	G689	L690	G691	H692	E693	K694	L695	T696	D697	A698	R699	T700	Q701	L702	G703	A704	E705	A706	V711	K708	H709	P710	D711	M712	L713	T714	S715	V716	K717	F718	N719	G720	E722	A723	T724	F725	Q726	F727	K728	L729	D730	I731	D732	Q733	E734	K735	A738	S742	I743	N744	D745	I746	N747	T748	T749													
L750	G751	A752	A753	W754	G755	Y758	V759	L760	D761	F762	I763	D764	R765	G766	F767	V768	K769	K770	V771	Y772	W773	M774	S775	E776	A777	K778	Y779	R780	M781	L782	F783	D784	I786	G787	D788	W789	Y790	F791	R792	A793	G796	Q797	M798	W799	P800	F801	S802	A803	F804	S805	R806	Y926	F927	Q928	W929	G930	H931	Q872											
S813	P814	R815	L816	E817	R818	L819	M820	G821	L822	R823	S824	M825	E826	I827	L828	G829	Q830	A831	A832	P833	G834	K835	S836	G838	E839	S900	M841	E842	L843	M844	E845	F846	A848	G849	K850	L851	P852	T853	G854	V855	G856	Y857	D858	W859	R860	G861	M862	S863	Y864	Q865	G866	R867	Q928	W929	G930	H931	Q872												
A873	P874	S875	L876	Y877	A878	L879	S880	L881	L882	R883	V884	F885	L886	G887	L888	A889	K890	L891	Y892	E893	S894	W895	S896	L897	P898	F899	S900	M901	Q902	T903	L904	V904	D905	P906	G908	A909	S910	L911	G912	L913	L914	R915	A916	T917	F918	R919	G920	L921	T922	N923	D924	V925	N926	F927	Q928	W929	G930	H931	Q872										
T933	T934	T935	G936	L937	S938	A939	K940	R941	A942	R943	L944	T945	V946	E947	F948	A949	K950	D951	L952	R953	D954	G957	K958	G959	L960	T961	E962	A963	T964	L965	D966	A967	V968	R969	N970	R971	L972	R973	P974	L975	L976	N977	T978	S979	L980	A981	F982	L983	L984	G985	V986	N987	P988	L989	T993	G994													

S897	G898	A999	Q1000	V1003	G1004	V1007	M1008	G1009	G1010	M1011	V1012	T1013	A1014	T1015	V1016	L1017	A1018	I1019	F1020	F1021	V1022	P1023	V1024	F1025	F1026	V1027	V1028	V1029	R1030	R1031	R1032	F1033	S1034	R1035	K1036	ASN	GLU	ASP	ASP	ILE	GLU	HIS	SER	HIS	HIS	THR	VAL	ASP	HIS	HIS	HIS	HIS	HIS	HIS	HIS
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## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	225.87Å 134.42Å 163.19Å 90.00° 97.71° 90.00°	Depositor
Resolution (Å)	10.00 – 2.80 10.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.0 (10.00-2.80) 99.0 (10.00-2.80)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.40 (at 2.80Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.268 , 0.307 0.262 , 0.307	Depositor DCC
$R_{free}$ test set	5752 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	73.4	Xtrriage
Anisotropy	0.444	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 104.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	23378	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	93.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality 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	1.50	104/7920 (1.3%)	1.28	74/10756 (0.7%)
1	B	1.02	6/7920 (0.1%)	1.05	18/10756 (0.2%)
1	C	1.54	94/7920 (1.2%)	1.33	82/10756 (0.8%)
All	All	1.37	204/23760 (0.9%)	1.23	174/32268 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	2
1	C	0	6
All	All	0	12

All (204) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	67	GLN	CB-CG	23.76	2.16	1.52
1	C	129	VAL	CB-CG2	21.03	1.97	1.52
1	C	167	SER	N-CA	20.35	1.87	1.46
1	A	818	ARG	CG-CD	20.25	2.02	1.51
1	C	166	ILE	CA-CB	20.11	2.01	1.54
1	A	68	ASN	CA-CB	16.05	1.94	1.53
1	C	164	ASP	C-O	15.81	1.53	1.23
1	C	161	ASN	N-CA	14.93	1.76	1.46
1	A	54	ALA	CA-CB	-14.74	1.21	1.52
1	C	45	ILE	CA-CB	14.56	1.88	1.54
1	C	128	SER	CA-CB	14.17	1.74	1.52
1	C	166	ILE	CA-C	-12.56	1.20	1.52
1	C	169	THR	CA-CB	12.51	1.85	1.53
1	C	160	ALA	CA-CB	-12.39	1.26	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	108	GLN	CB-CG	12.39	1.85	1.52
1	A	823	PRO	C-O	12.22	1.47	1.23
1	A	68	ASN	N-CA	12.03	1.70	1.46
1	A	819	TYR	CG-CD1	12.02	1.54	1.39
1	A	63	GLN	N-CA	-11.79	1.22	1.46
1	C	158	VAL	CB-CG2	11.70	1.77	1.52
1	C	157	TYR	C-O	11.57	1.45	1.23
1	A	69	MET	C-O	11.39	1.45	1.23
1	C	767	ARG	CZ-NH2	-11.12	1.18	1.33
1	C	46	SER	CA-CB	10.61	1.68	1.52
1	A	823	PRO	N-CA	-10.60	1.29	1.47
1	A	45	ILE	CA-CB	-10.55	1.30	1.54
1	C	164	ASP	CG-OD2	10.47	1.49	1.25
1	C	42	ALA	CA-CB	-10.25	1.30	1.52
1	C	157	TYR	CE2-CZ	-10.24	1.25	1.38
1	A	65	ILE	C-O	10.17	1.42	1.23
1	C	181	GLN	CD-OE1	10.08	1.46	1.24
1	A	65	ILE	CA-C	10.05	1.79	1.52
1	C	127	VAL	CA-CB	9.97	1.75	1.54
1	C	91	THR	CA-CB	9.49	1.78	1.53
1	A	43	VAL	CB-CG1	-9.27	1.33	1.52
1	A	67	GLN	CA-C	-8.97	1.29	1.52
1	C	161	ASN	CA-CB	-8.83	1.30	1.53
1	A	55	LYS	CD-CE	8.80	1.73	1.51
1	C	289	LEU	N-CA	-8.73	1.28	1.46
1	A	819	TYR	CE2-CZ	8.63	1.49	1.38
1	A	813	SER	CA-CB	8.50	1.65	1.52
1	C	157	TYR	CE1-CZ	-8.49	1.27	1.38
1	A	107	VAL	C-N	8.34	1.53	1.34
1	A	110	LYS	N-CA	-8.34	1.29	1.46
1	C	316	PHE	CG-CD1	-8.30	1.26	1.38
1	C	58	GLN	CB-CG	8.28	1.75	1.52
1	A	105	VAL	C-O	8.19	1.39	1.23
1	A	108	GLN	CA-C	-8.16	1.31	1.52
1	A	66	GLU	CA-C	8.09	1.74	1.52
1	A	819	TYR	CE1-CZ	8.08	1.49	1.38
1	A	61	VAL	CA-CB	7.84	1.71	1.54
1	A	819	TYR	CA-CB	-7.84	1.36	1.53
1	C	316	PHE	CG-CD2	-7.84	1.26	1.38
1	A	70	ASN	CA-C	7.80	1.73	1.52
1	C	104	GLN	CA-CB	7.79	1.71	1.53
1	A	46	SER	CA-CB	-7.77	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	104	GLN	CG-CD	7.74	1.68	1.51
1	A	688	ALA	CA-CB	7.72	1.68	1.52
1	A	73	ASP	CB-CG	7.69	1.68	1.51
1	A	66	GLU	CD-OE1	7.57	1.33	1.25
1	A	811	TYR	CE2-CZ	-7.53	1.28	1.38
1	C	165	ALA	C-O	7.52	1.37	1.23
1	C	772	TYR	CE2-CZ	-7.51	1.28	1.38
1	C	164	ASP	CG-OD1	7.43	1.42	1.25
1	C	166	ILE	N-CA	-7.41	1.31	1.46
1	B	107	VAL	CB-CG1	7.39	1.68	1.52
1	A	819	TYR	C-O	7.38	1.37	1.23
1	A	722	GLU	CB-CG	7.37	1.66	1.52
1	C	127	VAL	CB-CG1	7.32	1.68	1.52
1	A	855	VAL	CB-CG2	-7.29	1.37	1.52
1	C	164	ASP	CB-CG	7.27	1.67	1.51
1	A	69	MET	CB-CG	7.26	1.74	1.51
1	A	818	ARG	C-N	7.24	1.50	1.34
1	C	104	GLN	CG-CD	-7.21	1.34	1.51
1	A	816	LEU	N-CA	-7.19	1.31	1.46
1	C	94	PHE	CD2-CE2	-7.15	1.25	1.39
1	C	94	PHE	CD1-CE1	-7.14	1.25	1.39
1	C	297	ALA	CA-CB	-7.14	1.37	1.52
1	A	107	VAL	CA-C	-7.12	1.34	1.52
1	C	769	LYS	CA-C	7.00	1.71	1.52
1	A	70	ASN	CB-CG	-6.96	1.35	1.51
1	A	122	VAL	CB-CG2	-6.91	1.38	1.52
1	A	111	LEU	N-CA	6.89	1.60	1.46
1	C	128	SER	CB-OG	6.86	1.51	1.42
1	A	819	TYR	CB-CG	6.82	1.61	1.51
1	A	109	ASN	CB-CG	6.80	1.66	1.51
1	A	64	VAL	C-N	6.78	1.49	1.34
1	A	685	ILE	C-O	-6.78	1.10	1.23
1	A	821	GLY	N-CA	6.72	1.56	1.46
1	A	94	PHE	CG-CD1	6.71	1.48	1.38
1	A	79	SER	C-O	6.69	1.36	1.23
1	A	822	LEU	CA-CB	6.68	1.69	1.53
1	C	157	TYR	CD1-CE1	6.66	1.49	1.39
1	C	106	GLN	C-O	6.60	1.35	1.23
1	C	130	GLU	CG-CD	6.59	1.61	1.51
1	C	758	TYR	CE2-CZ	6.59	1.47	1.38
1	C	131	LYS	CE-NZ	6.57	1.65	1.49
1	A	57	VAL	CA-CB	-6.55	1.41	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	130	GLU	CD-OE2	6.55	1.32	1.25
1	C	169	THR	C-O	6.49	1.35	1.23
1	C	770	LYS	CD-CE	6.43	1.67	1.51
1	C	316	PHE	CB-CG	6.40	1.62	1.51
1	C	160	ALA	CA-C	-6.38	1.36	1.52
1	A	88	VAL	CB-CG1	6.30	1.66	1.52
1	A	66	GLU	C-O	-6.28	1.11	1.23
1	B	105	VAL	CA-CB	6.27	1.68	1.54
1	A	682	PHE	CE2-CZ	6.18	1.49	1.37
1	C	46	SER	CB-OG	6.18	1.50	1.42
1	C	168	ARG	CZ-NH2	6.17	1.41	1.33
1	A	696	THR	CA-CB	6.11	1.69	1.53
1	C	167	SER	CB-OG	6.10	1.50	1.42
1	A	65	ILE	CA-CB	-6.10	1.40	1.54
1	A	105	VAL	CA-CB	-6.09	1.42	1.54
1	C	139	VAL	CB-CG1	-6.09	1.40	1.52
1	C	767	ARG	C-O	6.08	1.34	1.23
1	A	698	ALA	CA-CB	-6.08	1.39	1.52
1	C	182	TYR	CE1-CZ	6.08	1.46	1.38
1	C	770	LYS	CG-CD	6.06	1.73	1.52
1	A	801	PHE	CB-CG	6.05	1.61	1.51
1	A	116	PRO	CA-C	-6.04	1.40	1.52
1	A	129	VAL	N-CA	-6.04	1.34	1.46
1	A	820	ASN	C-N	6.00	1.43	1.33
1	A	88	VAL	CB-CG2	-5.99	1.40	1.52
1	C	269	GLU	CD-OE1	5.99	1.32	1.25
1	C	182	TYR	CD2-CE2	5.97	1.48	1.39
1	A	725	PRO	C-O	5.95	1.35	1.23
1	A	66	GLU	CA-CB	5.92	1.67	1.53
1	A	67	GLN	C-O	5.87	1.34	1.23
1	A	55	LYS	CB-CG	5.86	1.68	1.52
1	B	773	VAL	CB-CG2	-5.82	1.40	1.52
1	C	44	THR	C-O	5.79	1.34	1.23
1	C	127	VAL	CB-CG2	-5.79	1.40	1.52
1	A	103	ALA	CA-CB	5.79	1.64	1.52
1	A	61	VAL	CA-C	5.78	1.68	1.52
1	C	764	ASP	N-CA	5.78	1.57	1.46
1	C	174	ASP	N-CA	5.76	1.57	1.46
1	C	324	VAL	CB-CG2	-5.75	1.40	1.52
1	C	772	TYR	CG-CD2	-5.75	1.31	1.39
1	C	212	ALA	CA-CB	5.75	1.64	1.52
1	C	180	SER	CB-OG	5.73	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	45	ILE	C-O	5.70	1.34	1.23
1	B	459	PHE	CB-CG	5.69	1.61	1.51
1	C	817	GLU	CB-CG	5.66	1.62	1.52
1	A	61	VAL	CB-CG1	5.64	1.64	1.52
1	A	94	PHE	CE1-CZ	5.64	1.48	1.37
1	A	817	GLU	CD-OE2	5.63	1.31	1.25
1	A	48	SER	CA-CB	-5.61	1.44	1.52
1	C	772	TYR	CD2-CE2	-5.58	1.30	1.39
1	A	41	PRO	CG-CD	5.56	1.69	1.50
1	C	136	PHE	CD2-CE2	-5.53	1.28	1.39
1	A	682	PHE	CD1-CE1	5.51	1.50	1.39
1	A	62	THR	N-CA	5.50	1.57	1.46
1	A	44	THR	C-O	5.47	1.33	1.23
1	A	45	ILE	N-CA	-5.45	1.35	1.46
1	A	69	MET	CG-SD	5.45	1.95	1.81
1	B	110	LYS	N-CA	5.45	1.57	1.46
1	C	178	PHE	CD1-CE1	5.44	1.50	1.39
1	A	72	ILE	C-O	5.43	1.33	1.23
1	C	107	VAL	CA-CB	5.43	1.66	1.54
1	A	100	ALA	CA-CB	-5.40	1.41	1.52
1	C	157	TYR	CG-CD1	-5.40	1.32	1.39
1	C	57	VAL	CB-CG1	-5.39	1.41	1.52
1	C	617	PHE	CE2-CZ	5.38	1.47	1.37
1	A	811	TYR	CA-CB	-5.35	1.42	1.53
1	C	273	GLU	CB-CG	-5.35	1.42	1.52
1	C	162	MET	CA-CB	5.35	1.65	1.53
1	A	106	GLN	N-CA	5.33	1.57	1.46
1	C	172	VAL	CB-CG1	5.33	1.64	1.52
1	A	826	GLU	CG-CD	5.31	1.59	1.51
1	C	887	CYS	CB-SG	-5.30	1.73	1.81
1	C	102	ILE	CA-CB	-5.29	1.42	1.54
1	A	94	PHE	CE2-CZ	5.29	1.47	1.37
1	C	266	ALA	CA-CB	-5.29	1.41	1.52
1	A	81	ASN	C-O	5.27	1.33	1.23
1	A	113	LEU	CG-CD1	5.26	1.71	1.51
1	A	111	LEU	CG-CD1	5.26	1.71	1.51
1	C	78	MET	CB-CG	5.25	1.68	1.51
1	A	93	THR	C-O	5.22	1.33	1.23
1	A	94	PHE	CD1-CE1	5.21	1.49	1.39
1	C	157	TYR	CG-CD2	-5.20	1.32	1.39
1	C	238	THR	CB-CG2	5.16	1.69	1.52
1	C	839	GLU	CG-CD	5.15	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	314	GLU	N-CA	5.14	1.56	1.46
1	C	156	ASP	CB-CG	5.13	1.62	1.51
1	A	815	ARG	NE-CZ	5.13	1.39	1.33
1	A	727	PHE	CA-C	-5.12	1.39	1.52
1	A	687	GLN	CA-CB	5.11	1.65	1.53
1	C	74	ASN	C-O	-5.09	1.13	1.23
1	A	112	GLN	N-CA	-5.09	1.36	1.46
1	A	688	ALA	N-CA	5.09	1.56	1.46
1	A	67	GLN	N-CA	-5.08	1.36	1.46
1	C	88	VAL	CB-CG2	-5.08	1.42	1.52
1	B	130	GLU	CB-CG	-5.07	1.42	1.52
1	C	572	PHE	CE1-CZ	5.07	1.47	1.37
1	C	291	ILE	CA-CB	-5.07	1.43	1.54
1	A	104	GLN	N-CA	5.04	1.56	1.46
1	C	273	GLU	C-O	-5.04	1.13	1.23
1	A	45	ILE	C-N	5.03	1.45	1.34
1	A	63	GLN	CD-NE2	5.03	1.45	1.32
1	C	220	GLY	C-O	-5.02	1.15	1.23
1	A	691	GLY	C-O	5.02	1.31	1.23
1	C	683	GLU	CG-CD	-5.01	1.44	1.51
1	A	55	LYS	CG-CD	5.01	1.69	1.52
1	C	158	VAL	CB-CG1	-5.00	1.42	1.52

All (174) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	164	ASP	CB-CG-OD1	-17.91	102.18	118.30
1	C	767	ARG	CD-NE-CZ	-16.19	100.94	123.60
1	C	168	ARG	N-CA-C	10.95	140.57	111.00
1	A	818	ARG	NE-CZ-NH2	9.96	125.28	120.30
1	A	111	LEU	CB-CA-C	-9.93	91.33	110.20
1	A	717	ARG	NE-CZ-NH2	-9.81	115.39	120.30
1	C	126	GLY	N-CA-C	-9.77	88.68	113.10
1	C	131	LYS	CD-CE-NZ	-9.68	89.43	111.70
1	A	818	ARG	CA-CB-CG	-9.66	92.14	113.40
1	A	68	ASN	N-CA-CB	-9.62	93.28	110.60
1	A	62	THR	CA-CB-CG2	-9.41	99.22	112.40
1	C	815	ARG	NE-CZ-NH2	-9.40	115.60	120.30
1	A	828	LEU	CB-CG-CD1	-9.39	95.03	111.00
1	A	70	ASN	N-CA-C	-9.26	85.99	111.00
1	C	166	ILE	O-C-N	9.18	137.39	122.70
1	A	818	ARG	CD-NE-CZ	-9.04	110.95	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	164	ASP	CB-CG-OD2	8.98	126.38	118.30
1	C	157	TYR	CA-CB-CG	-8.97	96.36	113.40
1	A	812	GLY	N-CA-C	-8.93	90.78	113.10
1	B	30	LEU	CA-CB-CG	8.58	135.04	115.30
1	C	767	ARG	NE-CZ-NH2	-8.35	116.12	120.30
1	B	230	LEU	CA-CB-CG	8.31	134.41	115.30
1	A	717	ARG	NE-CZ-NH1	8.28	124.44	120.30
1	C	168	ARG	CB-CA-C	-8.16	94.09	110.40
1	A	721	LEU	CB-CG-CD2	-8.04	97.33	111.00
1	C	239	ARG	NE-CZ-NH2	-7.99	116.30	120.30
1	C	425	LEU	CA-CB-CG	7.67	132.95	115.30
1	A	118	LEU	CB-CG-CD1	7.61	123.94	111.00
1	A	686	ASP	CB-CG-OD2	7.52	125.07	118.30
1	A	818	ARG	N-CA-CB	7.51	124.11	110.60
1	A	578	LEU	CA-CB-CG	7.50	132.54	115.30
1	A	65	ILE	CB-CG1-CD1	-7.36	93.29	113.90
1	B	989	LEU	CA-CB-CG	7.32	132.14	115.30
1	B	705	GLU	N-CA-C	-7.31	91.25	111.00
1	A	817	GLU	OE1-CD-OE2	7.26	132.01	123.30
1	C	167	SER	C-N-CA	-7.20	103.69	121.70
1	B	468	ARG	NE-CZ-NH1	-7.17	116.71	120.30
1	A	723	ASP	CB-CG-OD2	-7.16	111.86	118.30
1	C	73	ASP	CB-CG-OD1	-7.07	111.93	118.30
1	C	185	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	C	166	ILE	CB-CG1-CD1	-6.99	94.32	113.90
1	A	696	THR	N-CA-C	-6.96	92.20	111.00
1	B	289	LEU	CA-CB-CG	6.96	131.31	115.30
1	C	620	ARG	NE-CZ-NH1	-6.93	116.83	120.30
1	A	108	GLN	CB-CA-C	-6.88	96.65	110.40
1	A	723	ASP	CB-CG-OD1	6.83	124.45	118.30
1	C	239	ARG	NE-CZ-NH1	6.83	123.71	120.30
1	C	166	ILE	N-CA-CB	6.79	126.42	110.80
1	C	172	VAL	CA-CB-CG1	6.78	121.07	110.90
1	A	544	LEU	CA-CB-CG	6.78	130.88	115.30
1	B	4	PHE	N-CA-C	-6.76	92.75	111.00
1	C	66	GLU	OE1-CD-OE2	-6.74	115.21	123.30
1	B	952	LEU	CA-CB-CG	6.73	130.79	115.30
1	A	761	ASP	CB-CG-OD2	-6.67	112.29	118.30
1	C	127	VAL	CG1-CB-CG2	-6.53	100.46	110.90
1	C	160	ALA	N-CA-C	6.51	128.59	111.00
1	A	750	LEU	CA-CB-CG	6.48	130.21	115.30
1	A	44	THR	CA-CB-CG2	6.46	121.45	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	818	ARG	NH1-CZ-NH2	-6.45	112.31	119.40
1	A	57	VAL	CB-CA-C	-6.44	99.17	111.40
1	C	686	ASP	CB-CG-OD2	6.43	124.09	118.30
1	C	818	ARG	NE-CZ-NH2	6.38	123.49	120.30
1	C	68	ASN	N-CA-C	6.36	128.17	111.00
1	B	73	ASP	CB-CG-OD2	6.35	124.02	118.30
1	C	163	LYS	CD-CE-NZ	-6.34	97.12	111.70
1	C	131	LYS	CG-CD-CE	-6.33	92.91	111.90
1	C	45	ILE	CB-CA-C	-6.33	98.94	111.60
1	C	168	ARG	NE-CZ-NH1	-6.32	117.14	120.30
1	A	118	LEU	CA-CB-CG	-6.31	100.78	115.30
1	A	61	VAL	N-CA-C	6.30	128.00	111.00
1	A	67	GLN	N-CA-C	6.29	127.98	111.00
1	A	729	ILE	CG1-CB-CG2	-6.27	97.61	111.40
1	C	162	MET	CB-CG-SD	-6.26	93.62	112.40
1	A	724	THR	OG1-CB-CG2	-6.25	95.62	110.00
1	A	66	GLU	N-CA-CB	6.25	121.85	110.60
1	A	164	ASP	CB-CG-OD1	-6.15	112.76	118.30
1	C	620	ARG	NE-CZ-NH2	6.13	123.36	120.30
1	A	823	PRO	CA-N-CD	6.13	120.28	111.70
1	A	181	GLN	N-CA-C	-6.12	94.48	111.00
1	A	55	LYS	CD-CE-NZ	6.11	125.76	111.70
1	A	586	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	A	63	GLN	CA-CB-CG	6.09	126.80	113.40
1	B	220	GLY	N-CA-C	-6.00	98.10	113.10
1	A	115	MET	N-CA-CB	5.99	121.38	110.60
1	C	159	ALA	N-CA-CB	-5.99	101.72	110.10
1	C	166	ILE	CB-CA-C	5.99	123.57	111.60
1	A	821	GLY	N-CA-C	-5.92	98.31	113.10
1	A	276	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	A	69	MET	CG-SD-CE	5.91	109.65	100.20
1	A	819	TYR	CB-CA-C	5.88	122.17	110.40
1	C	792	ARG	NE-CZ-NH1	-5.87	117.36	120.30
1	C	239	ARG	CG-CD-NE	-5.87	99.47	111.80
1	C	127	VAL	N-CA-C	-5.86	95.18	111.00
1	A	674	LEU	CA-CB-CG	5.85	128.76	115.30
1	C	159	ALA	C-N-CA	-5.85	107.08	121.70
1	C	732	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	C	755	GLY	N-CA-C	-5.81	98.57	113.10
1	C	177	LEU	CB-CG-CD2	5.81	120.88	111.00
1	C	90	ILE	CB-CA-C	-5.80	100.00	111.60
1	C	157	TYR	CG-CD2-CE2	5.80	125.94	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	825	MET	CG-SD-CE	5.79	109.46	100.20
1	A	81	ASN	CB-CA-C	-5.78	98.84	110.40
1	A	118	LEU	CB-CG-CD2	-5.76	101.20	111.00
1	C	357	LEU	CA-CB-CG	5.76	128.55	115.30
1	C	87	THR	N-CA-C	5.76	126.55	111.00
1	C	164	ASP	N-CA-CB	-5.73	100.29	110.60
1	A	90	ILE	N-CA-C	-5.70	95.60	111.00
1	A	113	LEU	CB-CG-CD1	5.70	120.68	111.00
1	C	168	ARG	CG-CD-NE	-5.68	99.87	111.80
1	A	822	LEU	C-N-CD	-5.68	108.10	120.60
1	A	107	VAL	N-CA-C	-5.67	95.70	111.00
1	C	767	ARG	CG-CD-NE	-5.66	99.91	111.80
1	C	66	GLU	N-CA-CB	5.63	120.74	110.60
1	A	93	THR	O-C-N	5.60	131.66	122.70
1	A	62	THR	CA-C-N	-5.59	104.89	117.20
1	A	89	GLN	N-CA-C	-5.59	95.91	111.00
1	C	818	ARG	NE-CZ-NH1	-5.54	117.53	120.30
1	A	913	LEU	CA-CB-CG	5.52	128.00	115.30
1	C	156	ASP	CB-CG-OD1	5.51	123.25	118.30
1	C	681	ASP	CB-CG-OD2	5.51	123.26	118.30
1	C	972	LEU	CA-CB-CG	5.48	127.91	115.30
1	C	773	VAL	N-CA-C	-5.48	96.21	111.00
1	C	699	ARG	NE-CZ-NH1	-5.45	117.57	120.30
1	B	113	LEU	CB-CG-CD1	5.44	120.25	111.00
1	C	721	LEU	CA-CB-CG	5.44	127.81	115.30
1	A	68	ASN	N-CA-C	-5.44	96.32	111.00
1	C	166	ILE	CA-CB-CG1	-5.43	100.68	111.00
1	C	248	LYS	CD-CE-NZ	-5.43	99.22	111.70
1	A	109	ASN	CB-CA-C	-5.41	99.57	110.40
1	C	165	ALA	N-CA-CB	5.40	117.66	110.10
1	C	576	VAL	CB-CA-C	-5.40	101.14	111.40
1	A	818	ARG	CB-CG-CD	-5.39	97.58	111.60
1	B	350	LEU	CB-CG-CD1	-5.37	101.86	111.00
1	C	989	LEU	CA-CB-CG	5.36	127.63	115.30
1	A	788	ASP	CB-CG-OD1	-5.35	113.48	118.30
1	A	63	GLN	CA-C-N	-5.34	105.46	117.20
1	C	868	LEU	CA-CB-CG	5.34	127.57	115.30
1	A	64	VAL	C-N-CA	-5.33	108.36	121.70
1	B	650	ARG	NE-CZ-NH2	5.33	122.97	120.30
1	C	960	LEU	CA-CB-CG	5.32	127.54	115.30
1	C	822	LEU	CA-CB-CG	-5.30	103.11	115.30
1	C	772	TYR	CB-CG-CD1	5.29	124.17	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	GLU	CB-CA-C	-5.28	99.84	110.40
1	C	157	TYR	CA-C-N	-5.28	105.58	117.20
1	C	686	ASP	CB-CG-OD1	-5.28	113.55	118.30
1	A	867	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	B	72	ILE	CG1-CB-CG2	-5.26	99.83	111.40
1	B	998	GLY	N-CA-C	-5.25	99.98	113.10
1	C	125	GLN	CB-CA-C	5.25	120.89	110.40
1	A	816	LEU	N-CA-C	-5.23	96.87	111.00
1	C	129	VAL	CA-CB-CG1	-5.22	103.07	110.90
1	B	980	LEU	CA-CB-CG	5.20	127.27	115.30
1	C	720	GLY	N-CA-C	5.18	126.06	113.10
1	C	952	LEU	CA-CB-CG	5.17	127.20	115.30
1	A	721	LEU	CA-CB-CG	5.17	127.20	115.30
1	A	71	GLY	N-CA-C	-5.17	100.18	113.10
1	A	222	THR	N-CA-C	-5.17	97.05	111.00
1	C	104	GLN	CA-CB-CG	-5.17	102.04	113.40
1	B	376	LEU	CB-CG-CD1	-5.15	102.24	111.00
1	A	820	ASN	CB-CA-C	-5.14	100.11	110.40
1	C	765	ARG	CB-CA-C	-5.13	100.13	110.40
1	C	165	ALA	CA-C-N	-5.10	105.98	117.20
1	A	102	ILE	O-C-N	-5.10	114.54	122.70
1	C	157	TYR	CG-CD1-CE1	-5.09	117.23	121.30
1	C	123	GLN	N-CA-C	-5.08	97.29	111.00
1	C	172	VAL	N-CA-C	-5.07	97.32	111.00
1	C	815	ARG	CG-CD-NE	-5.06	101.17	111.80
1	A	67	GLN	CA-C-N	5.05	128.32	117.20
1	C	88	VAL	CB-CA-C	-5.05	101.81	111.40
1	C	167	SER	N-CA-C	-5.04	97.39	111.00
1	A	478	MET	CG-SD-CE	5.04	108.26	100.20
1	C	772	TYR	OH-CZ-CE2	-5.03	106.53	120.10
1	A	107	VAL	CB-CA-C	-5.01	101.87	111.40
1	A	824	SER	N-CA-C	5.00	124.51	111.00

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	62	THR	Mainchain
1	A	65	ILE	Mainchain
1	A	66	GLU	Peptide
1	A	818	ARG	Mainchain
1	B	102	ILE	Peptide

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Mol	Chain	Res	Type	Group
1	B	706	ALA	Peptide
1	C	104	GLN	Mainchain
1	C	160	ALA	Peptide,Mainchain
1	C	166	ILE	Peptide
1	C	168	ARG	Mainchain
1	C	45	ILE	Mainchain

## 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	7774	0	7931	1178	0
1	B	7774	0	7931	1189	0
1	C	7774	0	7931	1304	0
2	A	22	0	0	30	0
2	B	8	0	0	6	0
2	C	26	0	0	35	0
All	All	23378	0	23793	3559	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 76.

All (3559) 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:C:127:VAL:CA	1:C:127:VAL:CB	1.75	1.63
1:C:158:VAL:CB	1:C:158:VAL:CG2	1.77	1.60
1:A:69:MET:CB	1:A:69:MET:CG	1.74	1.60
1:C:58:GLN:CB	1:C:58:GLN:CG	1.74	1.55
1:A:68:ASN:N	1:A:68:ASN:CA	1.70	1.55
1:A:108:GLN:CG	1:A:108:GLN:CB	1.86	1.53
1:C:91:THR:CB	1:C:91:THR:CA	1.78	1.53
1:A:65:ILE:CA	1:A:65:ILE:C	1.79	1.51
1:C:169:THR:CA	1:C:169:THR:CB	1.85	1.50
1:C:45:ILE:CA	1:C:45:ILE:CB	1.88	1.49
1:C:161:ASN:N	1:C:161:ASN:CA	1.76	1.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:VAL:O	1:A:65:ILE:CG2	1.66	1.43
1:C:129:VAL:CB	1:C:129:VAL:CG2	1.97	1.43
1:A:68:ASN:CA	1:A:68:ASN:CB	1.94	1.42
1:C:167:SER:N	1:C:167:SER:CA	1.87	1.38
1:C:166:ILE:CA	1:C:166:ILE:CB	2.01	1.36
1:A:818:ARG:CG	1:A:818:ARG:CD	2.02	1.35
1:B:247:GLY:HA2	1:B:268:ILE:CD1	1.63	1.28
1:B:247:GLY:CA	1:B:268:ILE:HD13	1.67	1.23
1:A:67:GLN:CB	1:A:67:GLN:CG	2.16	1.22
1:A:61:VAL:O	1:A:65:ILE:HG22	1.09	1.22
1:C:115:MET:CE	1:C:118:LEU:HD22	1.70	1.22
1:C:159:ALA:HA	2:C:1078:HOH:O	1.05	1.21
1:C:950:LYS:NZ	1:C:1030:ARG:HD3	1.56	1.21
1:C:44:THR:HG22	1:C:91:THR:CB	1.70	1.20
1:A:66:GLU:HG2	2:A:1058:HOH:O	1.40	1.19
1:C:274:ASN:HB2	2:C:1060:HOH:O	1.43	1.19
1:A:108:GLN:HG3	1:B:112:GLN:OE1	1.38	1.18
1:A:686:ASP:HB3	2:A:1059:HOH:O	1.37	1.18
1:C:291:ILE:HD13	1:C:306:ILE:HD13	1.23	1.18
1:C:44:THR:CG2	1:C:91:THR:HB	1.74	1.17
1:B:456:MET:HG3	1:B:467:TYR:HB3	1.21	1.17
1:C:110:LYS:HA	1:C:113:LEU:HD12	1.28	1.16
1:C:82:SER:HB3	1:C:88:VAL:HA	1.26	1.15
1:B:1:MET:HB2	1:B:2:PRO:HD2	1.25	1.15
1:C:58:GLN:HB3	2:C:1079:HOH:O	1.45	1.15
1:A:344:LEU:HD23	1:A:402:ILE:HD13	1.15	1.15
1:B:544:LEU:HA	1:B:547:ILE:HD12	1.30	1.14
1:C:713:LEU:HG	1:C:832:ALA:O	1.47	1.14
1:C:166:ILE:HA	1:C:166:ILE:HD13	1.20	1.14
1:C:54:ALA:HB2	1:C:84:SER:HB2	1.30	1.14
1:B:1022:VAL:O	1:B:1024:VAL:O	1.66	1.14
1:A:531:VAL:HA	1:A:534:ILE:HD11	1.24	1.13
1:A:690:LEU:HD11	1:A:854:GLY:HA3	1.27	1.13
1:B:445:ILE:HG23	1:B:940:LYS:HG3	1.27	1.13
1:C:190:PRO:HD3	1:C:779:TYR:HD1	1.13	1.12
1:C:432:ARG:HH11	1:C:432:ARG:HG3	1.14	1.12
1:B:990:VAL:HG13	1:B:1005:THR:OG1	1.48	1.11
1:C:69:MET:CE	1:C:92:LEU:HD21	1.78	1.11
1:C:220:GLY:HA3	1:C:231:ASN:ND2	1.65	1.11
1:A:261:LEU:HD12	1:A:263:ARG:HH22	1.08	1.11
1:C:699:ARG:HG2	1:C:699:ARG:HH11	1.16	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:894:SER:HB3	1:B:897:ILE:HG12	1.33	1.10
1:C:358:PHE:HB3	1:C:977:MET:HE2	1.33	1.10
1:A:400:LEU:HD13	1:A:1003:VAL:HG13	1.27	1.10
1:A:686:ASP:O	1:A:688:ALA:N	1.84	1.09
1:A:713:LEU:HD22	1:A:714:THR:H	1.15	1.09
1:B:441:ALA:HB2	1:B:947:GLU:HG2	1.18	1.09
1:C:770:LYS:HG3	2:C:1070:HOH:O	1.48	1.09
1:C:699:ARG:HH11	1:C:699:ARG:CG	1.66	1.09
1:A:729:ILE:HG22	1:A:730:ASP:H	1.14	1.09
1:B:42:ALA:HB2	1:B:93:THR:HG22	1.34	1.08
1:C:847:LEU:HA	1:C:850:LYS:HD3	1.30	1.08
1:C:747:ASN:HA	2:C:1066:HOH:O	1.54	1.08
1:A:443:VAL:HG12	1:A:444:GLY:H	1.19	1.07
1:A:945:ILE:HG12	1:A:971:ARG:HG2	1.32	1.07
1:C:427:PRO:HA	1:C:498:LYS:HE3	1.22	1.07
1:A:66:GLU:HA	2:A:1056:HOH:O	1.54	1.06
1:C:1:MET:HB2	1:C:2:PRO:HD2	1.32	1.06
1:C:69:MET:HE2	1:C:92:LEU:CD2	1.86	1.06
1:C:166:ILE:HA	1:C:166:ILE:CD1	1.85	1.06
1:B:843:LEU:HD23	1:B:847:LEU:HD21	1.07	1.06
1:A:112:GLN:HA	1:A:112:GLN:HE21	1.15	1.05
1:A:713:LEU:HG	1:A:833:PRO:HD3	1.34	1.05
1:A:649:MET:HB3	1:A:653:ARG:HH21	1.22	1.05
1:C:167:SER:OG	1:C:168:ARG:N	1.85	1.05
1:C:163:LYS:O	1:C:166:ILE:N	1.89	1.04
1:A:54:ALA:HB1	1:A:816:LEU:HG	1.38	1.04
1:A:344:LEU:CD2	1:A:402:ILE:HD13	1.88	1.03
1:C:420:MET:SD	1:C:498:LYS:CE	2.46	1.03
1:A:400:LEU:CD1	1:A:1003:VAL:HG13	1.87	1.03
1:C:115:MET:HE2	1:C:118:LEU:HD22	1.08	1.03
1:B:574:THR:HG23	1:B:665:ALA:HB2	1.39	1.03
1:B:904:VAL:HG13	1:B:907:LEU:HD12	1.35	1.03
1:C:162:MET:HB3	1:C:313:MET:HE1	1.41	1.03
1:C:1022:VAL:HA	1:C:1025:PHE:HD2	1.22	1.03
1:C:713:LEU:HD11	1:C:834:GLY:HA3	1.35	1.03
1:B:431:THR:HG21	1:B:493:CYS:HB3	1.37	1.02
1:A:713:LEU:HB3	1:A:832:ALA:HA	1.37	1.02
1:A:959:GLY:HA3	1:A:962:GLU:HB2	1.41	1.02
1:C:712:MET:HB2	1:C:835:LYS:HG3	1.41	1.02
1:A:205:THR:HG22	1:A:205:THR:O	1.54	1.01
1:B:226:LYS:HA	1:B:226:LYS:HE3	1.40	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:THR:HG22	1:C:239:ARG:O	1.59	1.01
1:C:415:ASN:ND2	1:C:434:SER:HB2	1.74	1.01
1:B:876:LEU:HD13	1:B:932:LEU:HD11	1.43	1.00
1:C:901:VAL:O	1:C:904:VAL:HG23	1.59	1.00
1:A:713:LEU:O	1:A:714:THR:HG23	1.61	1.00
1:A:713:LEU:CB	1:A:832:ALA:HA	1.91	1.00
1:A:559:LEU:HD12	1:A:560:PRO:HD2	1.41	1.00
1:A:435:MET:HG2	1:A:490:PRO:HB3	1.44	0.99
1:A:536:ARG:HG2	1:A:537:SER:H	1.22	0.99
1:C:115:MET:CE	1:C:118:LEU:CD2	2.40	0.99
1:C:887:CYS:O	1:C:890:ALA:HB3	1.62	0.99
1:C:166:ILE:CB	1:C:166:ILE:HA	1.84	0.99
1:A:328:ASP:OD1	1:A:330:THR:HB	1.62	0.99
1:B:49:TYR:CD2	1:B:122:VAL:HA	1.98	0.99
1:C:159:ALA:O	1:C:161:ASN:N	1.94	0.99
1:B:144:ASN:HB2	1:B:320:GLY:O	1.62	0.99
1:C:143:ILE:HG23	1:C:284:GLN:NE2	1.77	0.98
1:A:819:TYR:H	1:A:824:SER:HB3	1.27	0.98
1:B:523:SER:HA	1:B:526:HIS:HD2	1.29	0.98
1:B:687:GLN:NE2	1:B:856:GLY:HA3	1.79	0.98
1:B:549:VAL:HG22	1:B:550:VAL:N	1.79	0.97
1:C:162:MET:HG2	1:C:313:MET:CE	1.94	0.97
1:A:818:ARG:HD3	1:A:821:GLY:O	1.64	0.97
1:C:729:ILE:HD11	1:C:786:ILE:HD13	1.46	0.97
1:A:687:GLN:NE2	1:A:856:GLY:HA3	1.78	0.97
1:A:251:LEU:HD11	1:A:262:LEU:HA	1.46	0.97
1:A:690:LEU:HD11	1:A:854:GLY:CA	1.96	0.96
1:C:588:GLN:HG2	1:C:613:ASN:HD22	1.25	0.96
1:C:111:LEU:HB3	2:C:1056:HOH:O	1.64	0.96
1:C:674:LEU:HD11	1:C:862:MET:HA	1.46	0.96
1:B:704:ALA:O	1:B:705:GLU:HG3	1.66	0.96
1:C:684:LEU:HG	1:C:684:LEU:O	1.64	0.96
1:B:361:ASN:O	1:B:365:THR:HB	1.64	0.96
1:C:164:ASP:O	1:C:167:SER:OG	1.84	0.95
1:A:105:VAL:O	1:A:109:ASN:N	1.99	0.95
1:C:372:VAL:HG13	1:C:373:PRO:HD3	1.48	0.95
1:B:742:SER:HB3	1:B:745:ASP:OD2	1.66	0.95
1:B:843:LEU:CD2	1:B:847:LEU:HD21	1.96	0.95
1:B:537:SER:HB2	1:B:540:ARG:HG2	1.47	0.95
1:B:714:THR:HG21	1:B:833:PRO:HD2	1.49	0.95
1:A:389:SER:O	1:A:394:THR:HG21	1.67	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:790:TYR:HE1	1:A:800:PRO:HG3	1.30	0.95
1:B:712:MET:HB3	1:B:713:LEU:HD12	1.46	0.95
1:A:108:GLN:HG3	1:B:112:GLN:CD	1.86	0.95
1:A:214:VAL:HG12	1:A:215:ALA:N	1.79	0.95
1:A:979:SER:OG	1:A:1015:THR:HG21	1.66	0.95
1:B:172:VAL:O	1:B:172:VAL:HG12	1.64	0.94
1:B:1022:VAL:HG23	1:B:1023:PRO:HD3	1.48	0.94
1:C:420:MET:SD	1:C:498:LYS:HE2	2.06	0.94
1:A:76:MET:HG2	1:A:95:GLU:OE2	1.66	0.94
1:B:431:THR:HG21	1:B:493:CYS:CB	1.96	0.94
1:B:988:PRO:O	1:B:989:LEU:HB3	1.65	0.94
1:C:162:MET:HB3	1:C:313:MET:CE	1.96	0.94
1:C:162:MET:CB	1:C:313:MET:CE	2.45	0.94
1:A:66:GLU:CG	2:A:1058:HOH:O	2.02	0.94
1:A:742:SER:OG	1:A:745:ASP:HB2	1.68	0.94
1:A:818:ARG:HD3	1:A:821:GLY:C	1.88	0.94
1:B:807:SER:O	1:B:808:ARG:HG3	1.68	0.94
1:B:930:GLY:O	1:B:934:THR:HG23	1.68	0.94
1:C:69:MET:HE2	1:C:92:LEU:HD21	0.94	0.94
1:C:535:LEU:HB2	2:C:1076:HOH:O	1.68	0.94
1:A:418:ARG:HD3	1:A:970:MET:HG3	1.46	0.94
1:C:190:PRO:HD3	1:C:779:TYR:CD1	2.02	0.93
1:A:578:LEU:CD2	1:A:587:THR:HG23	1.98	0.93
1:C:58:GLN:HG3	1:C:62:THR:OG1	1.67	0.93
1:B:987:MET:HA	1:B:987:MET:HE3	1.49	0.93
1:B:225:VAL:HG22	1:C:781:MET:CE	1.98	0.93
1:C:548:ILE:HD12	1:C:549:VAL:N	1.84	0.93
1:B:962:GLU:O	1:B:966:ASP:HB2	1.69	0.93
1:C:979:SER:O	1:C:983:ILE:HG13	1.68	0.93
1:A:560:PRO:HB2	1:A:922:THR:HG22	1.50	0.92
1:C:222:THR:HB	1:C:223:PRO:HD3	1.50	0.92
1:C:115:MET:HE2	1:C:118:LEU:CD2	1.96	0.92
1:C:162:MET:CG	1:C:313:MET:CE	2.48	0.92
1:C:3:ASN:HD21	1:C:432:ARG:HD3	1.35	0.92
1:A:965:LEU:O	1:A:969:ARG:HG3	1.69	0.92
1:A:919:ARG:HG3	1:A:920:GLY:H	1.33	0.92
1:A:57:VAL:HG12	1:A:58:GLN:N	1.84	0.92
1:B:406:VAL:O	1:B:408:ASP:O	1.88	0.92
1:A:214:VAL:HG12	1:A:215:ALA:H	1.32	0.92
1:B:549:VAL:HG22	1:B:550:VAL:H	1.33	0.92
1:C:950:LYS:H	1:C:953:MET:HE2	1.35	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:PHE:HB3	1:C:8:ARG:HH22	1.34	0.91
1:C:143:ILE:HG23	1:C:284:GLN:HE22	1.35	0.91
1:C:1022:VAL:HA	1:C:1025:PHE:CD2	2.05	0.91
1:A:919:ARG:CG	1:A:920:GLY:H	1.82	0.91
1:A:443:VAL:O	1:A:445:ILE:N	2.03	0.91
1:A:495:THR:O	1:A:496:MET:HB2	1.71	0.91
1:C:1025:PHE:O	1:C:1029:VAL:HG23	1.71	0.91
1:A:5:PHE:CD1	1:A:12:ALA:HB2	2.05	0.91
1:A:781:MET:HB3	1:C:228:GLN:OE1	1.70	0.91
1:A:901:VAL:O	1:A:904:VAL:HG23	1.70	0.91
1:B:81:ASN:O	1:B:81:ASN:ND2	2.02	0.91
1:A:585:GLU:OE2	1:C:227:GLY:HA2	1.71	0.91
1:A:128:SER:HB2	1:B:113:LEU:CD2	2.01	0.91
1:A:571:VAL:HG12	1:A:630:SER:HA	1.53	0.91
1:C:459:PHE:H	1:C:459:PHE:HD2	1.13	0.91
1:C:417:GLU:HA	1:C:417:GLU:OE2	1.70	0.91
1:C:188:MET:CE	1:C:200:PRO:HB3	2.01	0.90
1:C:431:THR:HG21	1:C:494:ALA:HB2	1.51	0.90
1:B:115:MET:HE1	1:B:127:VAL:HG21	1.53	0.90
1:A:578:LEU:HD21	1:A:587:THR:HA	1.52	0.90
1:A:968:VAL:CG2	1:A:1023:PRO:HB3	2.00	0.90
1:C:185:ARG:HG3	1:C:271:GLY:HA3	1.54	0.90
1:C:314:GLU:HB2	1:C:315:PRO:HD3	1.54	0.90
1:A:552:MET:HE1	1:A:906:PRO:HA	1.51	0.90
1:B:51:GLY:O	1:B:53:ASP:OD2	1.90	0.90
1:B:911:GLY:HA3	1:B:1013:THR:HG21	1.51	0.90
1:A:418:ARG:HG2	1:A:970:MET:HE3	1.53	0.90
1:A:277:ILE:HG23	1:A:277:ILE:O	1.70	0.89
1:C:44:THR:HG22	1:C:91:THR:HB	0.91	0.89
1:B:441:ALA:O	1:B:445:ILE:HG13	1.72	0.89
1:C:418:ARG:O	1:C:420:MET:N	2.04	0.89
1:C:214:VAL:HG12	1:C:215:ALA:N	1.88	0.89
1:A:139:VAL:CG1	1:A:327:TYR:HB3	2.02	0.89
1:B:49:TYR:CE1	1:B:122:VAL:HG13	2.06	0.89
1:A:190:PRO:HG3	1:A:789:TRP:CE2	2.08	0.89
1:A:968:VAL:HG21	1:A:1023:PRO:HB3	1.52	0.89
1:B:1:MET:CB	1:B:2:PRO:HD2	2.01	0.89
1:B:184:MET:HG3	1:B:184:MET:O	1.71	0.89
1:C:950:LYS:HZ1	1:C:1030:ARG:HD3	1.30	0.89
1:A:909:VAL:HG12	1:A:913:LEU:HD21	1.55	0.89
1:B:456:MET:HG3	1:B:467:TYR:CB	2.02	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:423:GLU:HB3	1:C:426:PRO:HG3	1.54	0.89
1:B:171:GLY:HA3	1:B:302:THR:CG2	2.03	0.88
1:B:225:VAL:H	1:C:781:MET:HE2	1.34	0.88
1:B:242:SER:HB2	1:B:245:GLU:OE2	1.72	0.88
1:A:818:ARG:HD2	2:A:1054:HOH:O	1.72	0.88
1:C:131:LYS:O	1:C:295:THR:HG22	1.72	0.88
1:A:1024:VAL:HG12	1:A:1025:PHE:H	1.37	0.88
1:B:247:GLY:HA2	1:B:268:ILE:HD13	0.88	0.88
1:C:291:ILE:HD13	1:C:306:ILE:CD1	2.03	0.88
1:C:1017:LEU:O	1:C:1017:LEU:HD23	1.73	0.88
1:B:47:ALA:HB3	1:B:88:VAL:HB	1.56	0.88
1:A:64:VAL:O	1:A:65:ILE:C	2.12	0.88
1:B:103:ALA:O	1:B:107:VAL:HG23	1.73	0.88
1:C:444:GLY:O	1:C:448:VAL:HG23	1.74	0.88
1:B:171:GLY:HA3	1:B:302:THR:HG22	1.56	0.87
1:B:14:VAL:HG11	1:C:890:ALA:HB2	1.54	0.87
1:A:355:MET:CE	1:A:410:ILE:HG12	2.03	0.87
1:A:909:VAL:HG12	1:A:913:LEU:CD2	2.03	0.87
1:C:950:LYS:NZ	1:C:1030:ARG:CD	2.36	0.87
1:A:105:VAL:O	1:A:108:GLN:HB3	1.75	0.87
1:A:228:GLN:HG2	1:B:781:MET:HG2	1.54	0.87
1:C:452:VAL:O	1:C:932:LEU:HD13	1.73	0.87
1:A:214:VAL:CG1	1:A:215:ALA:H	1.87	0.87
1:A:1009:GLY:O	1:A:1011:MET:N	2.08	0.87
1:C:396:PHE:O	1:C:400:LEU:HD23	1.73	0.87
1:A:528:THR:HG21	1:A:969:ARG:HE	1.38	0.86
1:B:3:ASN:H	1:B:6:ILE:HG12	1.39	0.86
1:C:141:GLY:HA3	1:C:324:VAL:HG22	1.56	0.86
1:C:162:MET:HG2	1:C:313:MET:HE2	1.57	0.86
1:C:291:ILE:CD1	1:C:306:ILE:HD13	2.04	0.86
1:B:590:VAL:O	1:B:594:VAL:HG23	1.75	0.86
1:A:819:TYR:N	1:A:824:SER:HB3	1.89	0.86
1:B:42:ALA:CB	1:B:93:THR:HG22	2.05	0.86
1:B:919:ARG:HG3	1:B:1005:THR:CG2	2.05	0.86
1:A:32:VAL:HG22	1:A:390:ILE:HB	1.57	0.86
1:A:261:LEU:HD12	1:A:263:ARG:NH2	1.89	0.86
1:B:49:TYR:CD1	1:B:122:VAL:HG22	2.10	0.86
1:C:513:PHE:HA	1:C:516:PHE:HB3	1.57	0.86
1:C:950:LYS:HZ3	1:C:1030:ARG:HD3	1.34	0.86
1:B:714:THR:HG22	1:B:831:ALA:HA	1.57	0.86
1:B:729:ILE:HG13	1:B:730:ASP:N	1.90	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:804:PHE:HD1	1:B:804:PHE:O	1.58	0.86
1:C:181:GLN:OE1	1:C:767:ARG:NE	2.08	0.86
1:B:226:LYS:HA	1:B:226:LYS:CE	2.06	0.86
1:C:743:ILE:H	1:C:743:ILE:HD12	1.38	0.86
1:B:225:VAL:HG22	1:C:781:MET:HE3	1.54	0.86
1:B:517:ASN:HB3	1:B:521:GLU:OE1	1.75	0.86
1:C:872:GLN:HB2	1:C:875:SER:HB3	1.55	0.86
1:A:756:GLY:HA2	1:A:774:MET:HB2	1.56	0.85
1:A:809:TRP:O	1:A:810:GLU:HB3	1.73	0.85
1:C:686:ASP:OD1	1:C:690:LEU:HB2	1.76	0.85
1:A:355:MET:HE1	1:A:410:ILE:HG12	1.58	0.85
1:A:729:ILE:HG22	1:A:730:ASP:N	1.88	0.85
1:B:690:LEU:HB2	1:B:694:LYS:HB2	1.57	0.85
1:A:139:VAL:HG13	1:A:327:TYR:HB3	1.58	0.85
1:C:314:GLU:HB2	1:C:315:PRO:CD	2.06	0.85
1:C:927:PHE:O	1:C:931:LEU:HB2	1.74	0.85
1:C:43:VAL:HA	1:C:130:GLU:O	1.74	0.85
1:A:513:PHE:HD1	1:A:517:ASN:ND2	1.73	0.85
1:A:911:GLY:HA3	1:A:1013:THR:HG21	1.56	0.85
1:C:432:ARG:HG3	1:C:432:ARG:NH1	1.79	0.85
1:A:113:LEU:HD21	1:C:128:SER:HA	1.56	0.85
1:C:62:THR:HG23	1:C:90:ILE:HD11	1.56	0.85
1:A:520:PHE:H	1:A:522:LYS:HE3	1.42	0.84
1:A:632:LYS:O	1:A:637:ARG:HD3	1.76	0.84
1:B:431:THR:CG2	1:B:493:CYS:HB3	2.06	0.84
1:B:552:MET:SD	1:B:909:VAL:HG23	2.17	0.84
1:A:10:ILE:HD11	1:B:895:TRP:HB2	1.58	0.84
1:B:605:ASN:HD21	1:B:642:ASN:ND2	1.75	0.84
1:A:103:ALA:O	1:A:107:VAL:HG23	1.76	0.84
1:A:454:VAL:O	1:A:456:MET:O	1.95	0.84
1:A:687:GLN:HG2	1:C:316:PHE:CG	2.13	0.84
1:B:150:THR:H	1:B:153:ASP:HB3	1.41	0.84
1:C:951:ASP:C	1:C:953:MET:H	1.79	0.84
1:B:190:PRO:HG2	1:B:779:TYR:CD1	2.12	0.84
1:B:659:LYS:HD3	1:B:660:ASP:N	1.92	0.84
1:C:162:MET:CG	1:C:313:MET:HE3	2.06	0.84
1:C:685:ILE:HD11	1:C:687:GLN:HA	1.59	0.84
1:A:186:ILE:HB	1:A:773:VAL:HG23	1.60	0.84
1:B:49:TYR:CG	1:B:122:VAL:HA	2.12	0.84
1:C:759:VAL:O	1:C:760:ASN:HB3	1.78	0.84
1:A:441:ALA:O	1:A:445:ILE:HG23	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:PRO:HD2	1:B:749:THR:HG22	1.58	0.84
1:A:1024:VAL:O	1:A:1026:PHE:N	2.11	0.84
1:B:26:ALA:O	1:B:30:LEU:HD22	1.78	0.84
1:C:72:ILE:HG22	1:C:94:PHE:CE2	2.13	0.84
1:A:154:ILE:HG22	1:A:287:SER:HB3	1.60	0.83
1:A:1029:VAL:HG12	1:A:1030:ARG:H	1.43	0.83
1:B:831:ALA:CB	1:B:840:ALA:HB2	2.08	0.83
1:A:46:SER:O	1:A:127:VAL:HG13	1.78	0.83
1:A:406:VAL:HG13	1:A:407:ASP:N	1.92	0.83
1:A:1020:PHE:O	1:A:1024:VAL:HG23	1.77	0.83
1:B:555:LEU:HB2	1:B:913:LEU:HD23	1.59	0.83
1:A:63:GLN:O	1:A:66:GLU:N	2.10	0.83
1:B:945:ILE:HD12	1:B:1026:PHE:HE2	1.42	0.83
1:C:247:GLY:HA2	1:C:268:ILE:HD13	1.59	0.83
1:C:713:LEU:HD11	1:C:834:GLY:CA	2.07	0.83
1:C:190:PRO:CD	1:C:779:TYR:HD1	1.89	0.83
1:C:699:ARG:HD2	1:C:703:LEU:HD11	1.60	0.83
1:A:649:MET:HB3	1:A:653:ARG:NH2	1.93	0.83
1:C:4:PHE:CB	1:C:8:ARG:HH22	1.92	0.83
1:B:158:VAL:HA	1:B:162:MET:HG2	1.58	0.83
1:B:187:TRP:CZ3	1:B:774:MET:HE3	2.13	0.83
1:C:420:MET:SD	1:C:498:LYS:NZ	2.52	0.83
1:C:568:ASP:OD1	1:C:634:TRP:NE1	2.10	0.83
1:A:902:MET:O	1:A:905:VAL:HG23	1.79	0.83
1:B:528:THR:O	1:B:531:VAL:HG12	1.79	0.83
1:B:894:SER:CB	1:B:897:ILE:HG12	2.07	0.83
1:B:563:PHE:O	1:B:925:VAL:HG12	1.78	0.83
1:C:164:ASP:O	1:C:168:ARG:HG2	1.78	0.83
1:C:418:ARG:C	1:C:420:MET:H	1.81	0.83
1:B:493:CYS:O	1:B:494:ALA:HB3	1.79	0.82
1:B:613:ASN:HD22	1:B:614:GLY:N	1.75	0.82
1:B:713:LEU:HD12	1:B:713:LEU:H	1.44	0.82
1:B:892:TYR:CB	1:B:897:ILE:HD11	2.09	0.82
1:C:164:ASP:CG	2:C:1058:HOH:O	2.15	0.82
1:C:165:ALA:HA	1:C:168:ARG:HG3	1.59	0.82
1:C:950:LYS:HZ1	1:C:1030:ARG:CD	1.92	0.82
1:A:106:GLN:O	1:A:107:VAL:O	1.97	0.82
1:B:104:GLN:HG3	1:B:105:VAL:N	1.93	0.82
1:A:405:LEU:HD22	1:A:406:VAL:N	1.93	0.82
1:B:987:MET:HA	1:B:987:MET:CE	2.09	0.82
1:C:699:ARG:HG2	1:C:699:ARG:NH1	1.93	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:ALA:H	1:C:57:VAL:HG23	1.44	0.82
1:C:562:SER:O	1:C:924:ASP:HA	1.79	0.82
1:B:45:ILE:HD12	1:B:90:ILE:HB	1.61	0.82
1:C:55:LYS:HE2	1:C:59:ASP:OD1	1.79	0.82
1:C:686:ASP:HB3	1:C:823:PRO:HG2	1.61	0.82
1:A:342:LYS:HG3	1:A:343:THR:H	1.43	0.82
1:A:820:ASN:O	1:C:168:ARG:NH2	2.13	0.82
1:C:144:ASN:HB3	2:C:1077:HOH:O	1.80	0.82
1:C:962:GLU:O	1:C:965:LEU:HB3	1.79	0.82
1:B:245:GLU:HA	1:B:248:LYS:HG2	1.62	0.82
1:A:115:MET:HA	1:A:115:MET:HE3	1.60	0.82
1:A:443:VAL:HG12	1:A:444:GLY:N	1.95	0.82
1:C:115:MET:CE	1:C:115:MET:HA	2.10	0.82
1:C:166:ILE:CD1	2:C:1075:HOH:O	2.27	0.82
1:A:69:MET:HG2	2:A:1056:HOH:O	1.77	0.82
1:A:498:LYS:O	1:A:498:LYS:NZ	2.11	0.82
1:A:545:TYR:HB2	1:A:1021:PHE:CE1	2.14	0.82
1:A:722:GLU:HG3	2:A:1060:HOH:O	1.78	0.82
1:B:1:MET:HB2	1:B:2:PRO:CD	2.09	0.82
1:A:713:LEU:CD2	1:A:714:THR:H	1.92	0.81
1:A:276:ASP:HB3	1:C:222:THR:HG23	1.62	0.81
1:A:419:VAL:O	1:A:424:GLY:HA3	1.81	0.81
1:B:104:GLN:CG	1:B:105:VAL:N	2.42	0.81
1:B:276:ASP:O	1:B:614:GLY:HA3	1.81	0.81
1:B:880:SER:O	1:B:884:VAL:HG23	1.81	0.81
1:A:45:ILE:HG22	1:A:45:ILE:O	1.81	0.81
1:A:223:PRO:HD3	1:B:275:TYR:CD2	2.16	0.81
1:B:213:GLN:HE21	1:B:239:ARG:HD2	1.45	0.81
1:B:92:LEU:HD22	1:B:92:LEU:N	1.94	0.81
1:C:164:ASP:O	1:C:168:ARG:CG	2.28	0.81
1:C:644:VAL:HG11	1:C:667:ASN:HD22	1.45	0.81
1:C:888:LEU:HB3	1:C:898:PRO:HB3	1.62	0.81
1:B:674:LEU:HD23	1:B:675:GLY:N	1.94	0.81
1:B:859:TRP:HB3	1:B:863:SER:HB2	1.61	0.81
1:C:38:ILE:HG21	1:C:466:ILE:HD11	1.61	0.81
1:A:214:VAL:CG1	1:A:215:ALA:N	2.44	0.81
1:A:536:ARG:HG2	1:A:537:SER:N	1.95	0.81
1:A:314:GLU:HA	2:A:1061:HOH:O	1.79	0.81
1:B:405:LEU:HD12	1:B:406:VAL:N	1.96	0.81
1:A:205:THR:O	1:A:205:THR:CG2	2.27	0.81
1:A:413:VAL:HG23	1:A:493:CYS:HB2	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:713:LEU:HB3	1:A:832:ALA:CA	2.11	0.81
1:B:70:ASN:O	1:B:70:ASN:ND2	2.14	0.81
1:B:399:VAL:O	1:B:402:ILE:HG22	1.81	0.81
1:B:314:GLU:H	1:B:315:PRO:HD2	1.44	0.81
1:B:623:ASN:HD22	1:B:623:ASN:C	1.82	0.81
1:A:253:VAL:HG23	1:A:258:SER:O	1.80	0.80
1:A:467:TYR:CE1	1:A:925:VAL:HG22	2.16	0.80
1:B:350:LEU:HB3	1:B:984:LEU:HD12	1.61	0.80
1:C:350:LEU:HD13	1:C:984:LEU:CD2	2.11	0.80
1:C:713:LEU:HD21	1:C:835:LYS:H	1.46	0.80
1:A:605:ASN:OD1	1:A:637:ARG:HG2	1.82	0.80
1:A:634:TRP:CE3	1:A:995:ALA:HB1	2.16	0.80
1:B:100:ALA:O	1:B:103:ALA:HB3	1.81	0.80
1:B:416:VAL:HG11	1:B:431:THR:HG22	1.64	0.80
1:B:456:MET:CG	1:B:467:TYR:HB3	2.09	0.80
1:B:879:ILE:O	1:B:883:VAL:HG23	1.82	0.80
1:C:184:MET:HA	1:C:184:MET:HE3	1.62	0.80
1:C:702:LEU:HB2	1:C:851:LEU:HD21	1.62	0.80
1:A:801:PHE:CD2	1:A:805:SER:OG	2.34	0.80
1:A:951:ASP:O	1:A:955:LYS:HB2	1.81	0.80
1:B:157:TYR:HA	1:B:161:ASN:ND2	1.97	0.80
1:A:298:ASN:HD22	1:A:298:ASN:C	1.84	0.80
1:B:646:ALA:O	1:B:648:THR:N	2.13	0.80
1:B:849:SER:O	1:B:850:LYS:HD3	1.81	0.80
1:A:372:VAL:HB	1:A:373:PRO:HD3	1.62	0.80
1:A:949:ALA:HB1	1:A:1026:PHE:CE2	2.17	0.80
1:B:11:PHE:O	1:B:14:VAL:HB	1.81	0.80
1:B:945:ILE:HD11	1:B:1022:VAL:HB	1.64	0.80
1:C:188:MET:HE1	1:C:200:PRO:HB3	1.62	0.80
1:C:346:GLU:OE1	1:C:988:PRO:HG3	1.82	0.80
1:C:190:PRO:CD	1:C:779:TYR:CD1	2.64	0.80
1:A:406:VAL:HG13	1:A:407:ASP:H	1.45	0.79
1:B:568:ASP:OD1	1:B:644:VAL:HG22	1.82	0.79
1:C:536:ARG:HH11	1:C:961:ILE:HD11	1.47	0.79
1:A:66:GLU:OE2	2:A:1058:HOH:O	1.99	0.79
1:B:230:LEU:HD21	1:C:809:TRP:CH2	2.16	0.79
1:B:830:GLN:H	1:B:830:GLN:HE21	1.30	0.79
1:B:912:ALA:HB2	1:B:1010:GLY:HA3	1.65	0.79
1:C:169:THR:HB	1:C:172:VAL:HG21	1.63	0.79
1:A:105:VAL:O	1:A:108:GLN:CB	2.30	0.79
1:A:685:ILE:HG22	1:A:687:GLN:H	1.48	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:986:VAL:C	1:A:988:PRO:HD2	2.02	0.79
1:C:162:MET:HG2	1:C:313:MET:HE3	1.63	0.79
1:C:350:LEU:HD12	1:C:985:GLY:HA2	1.64	0.79
1:A:61:VAL:O	1:A:65:ILE:HG23	1.77	0.79
1:A:112:GLN:HE21	1:A:112:GLN:CA	1.95	0.79
1:B:2:PRO:HD3	1:B:486:LEU:HD12	1.65	0.79
1:B:972:LEU:HD13	1:B:976:LEU:HD23	1.64	0.79
1:A:590:VAL:O	1:A:594:VAL:HG23	1.83	0.79
1:C:423:GLU:HB3	1:C:426:PRO:CG	2.12	0.79
1:A:568:ASP:OD2	1:A:637:ARG:NH1	2.16	0.79
1:C:183:ALA:O	1:C:185:ARG:HG2	1.82	0.79
1:C:427:PRO:CA	1:C:498:LYS:HE3	2.09	0.79
1:C:728:LYS:HG3	1:C:729:ILE:N	1.97	0.79
1:A:255:GLN:H	1:A:255:GLN:CD	1.85	0.79
1:B:358:PHE:HZ	1:B:976:LEU:HD12	1.47	0.79
1:C:158:VAL:O	1:C:162:MET:N	2.15	0.79
1:C:778:LYS:HD2	1:C:779:TYR:HE2	1.48	0.79
1:A:584:GLN:H	1:A:622:GLN:HB3	1.48	0.78
1:B:452:VAL:O	1:B:453:PHE:HB2	1.82	0.78
1:C:685:ILE:HG12	1:C:687:GLN:OE1	1.82	0.78
1:A:60:THR:HG21	1:A:119:PRO:HG3	1.65	0.78
1:C:911:GLY:HA3	1:C:1013:THR:HG21	1.63	0.78
1:A:781:MET:HE1	1:C:225:VAL:H	1.49	0.78
1:B:531:VAL:HG13	1:B:965:LEU:HD21	1.64	0.78
1:C:61:VAL:HG12	2:C:1064:HOH:O	1.81	0.78
1:C:252:LYS:O	1:C:260:VAL:HG12	1.82	0.78
1:C:352:PHE:HA	1:C:369:THR:HG21	1.65	0.78
1:B:538:THR:N	1:B:540:ARG:HH21	1.81	0.78
1:B:729:ILE:HG13	1:B:730:ASP:H	1.46	0.78
1:A:61:VAL:HG13	1:A:118:LEU:HD22	1.64	0.78
1:A:210:GLN:HG3	1:A:249:ILE:HG23	1.63	0.78
1:A:298:ASN:ND2	1:A:300:LEU:H	1.80	0.78
1:B:525:HIS:HA	1:B:528:THR:HG22	1.64	0.78
1:A:400:LEU:HD13	1:A:1003:VAL:CG1	2.11	0.78
1:B:587:THR:O	1:B:591:LEU:HB2	1.83	0.78
1:A:166:ILE:HD13	1:A:166:ILE:N	1.96	0.78
1:A:578:LEU:HD23	1:A:587:THR:HG23	1.66	0.78
1:A:836:SER:OG	1:A:839:GLU:HG2	1.84	0.78
1:A:886:LEU:HD21	1:C:17:ILE:HG21	1.63	0.78
1:B:157:TYR:HA	1:B:161:ASN:HD22	1.49	0.78
1:C:410:ILE:HG22	1:C:411:VAL:N	1.98	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:463:THR:O	1:C:465:ALA:N	2.17	0.78
1:A:520:PHE:N	1:A:522:LYS:HE3	1.99	0.78
1:A:314:GLU:N	1:A:315:PRO:CD	2.47	0.78
1:A:467:TYR:HE1	1:A:925:VAL:HG22	1.46	0.78
1:A:719:ASN:HD22	1:A:719:ASN:C	1.85	0.78
1:A:783:PRO:HD3	1:C:219:LEU:HD13	1.65	0.78
1:B:562:SER:O	1:B:924:ASP:HA	1.84	0.78
1:B:602:GLU:OE2	1:B:650:ARG:HD2	1.82	0.78
1:B:448:VAL:O	1:B:452:VAL:HG22	1.84	0.77
1:C:115:MET:N	1:C:116:PRO:CD	2.47	0.77
1:C:143:ILE:HD11	1:C:286:ALA:HB2	1.67	0.77
1:C:578:LEU:HB3	1:C:579:PRO:HD2	1.65	0.77
1:A:168:ARG:O	1:A:168:ARG:HG3	1.84	0.77
1:A:843:LEU:HA	1:A:846:GLN:NE2	1.98	0.77
1:A:909:VAL:O	1:A:912:ALA:HB3	1.84	0.77
1:B:6:ILE:HD12	1:B:490:PRO:HB2	1.64	0.77
1:B:699:ARG:HG2	1:B:700:ASN:H	1.49	0.77
1:A:54:ALA:CB	1:A:816:LEU:HG	2.15	0.77
1:A:108:GLN:CG	1:B:112:GLN:OE1	2.28	0.77
1:A:495:THR:O	1:A:495:THR:HG22	1.83	0.77
1:B:346:GLU:OE1	1:B:988:PRO:HB3	1.84	0.77
1:B:345:VAL:HA	1:B:348:ILE:HD12	1.67	0.77
1:B:983:ILE:HD13	1:B:1012:VAL:HG12	1.66	0.77
1:C:220:GLY:CA	1:C:231:ASN:ND2	2.46	0.77
1:C:754:TRP:CZ2	1:C:786:ILE:HG13	2.20	0.77
1:A:522:LYS:N	1:A:522:LYS:HE2	2.00	0.77
1:A:1018:ALA:O	1:A:1022:VAL:HG13	1.85	0.77
1:B:674:LEU:HD13	1:B:860:THR:HG21	1.66	0.77
1:A:57:VAL:O	1:A:57:VAL:HG13	1.81	0.77
1:A:596:HIS:O	1:A:598:TYR:N	2.18	0.77
1:A:687:GLN:HE21	1:A:856:GLY:HA3	1.47	0.77
1:A:514:GLY:O	1:A:518:ARG:HB2	1.84	0.77
1:B:714:THR:HG21	1:B:833:PRO:CD	2.14	0.77
1:C:127:VAL:CA	1:C:127:VAL:CG2	2.60	0.77
1:B:945:ILE:CD1	1:B:1026:PHE:HE2	1.98	0.76
1:C:62:THR:CA	2:C:1064:HOH:O	2.33	0.76
1:A:728:LYS:NZ	1:C:235:ILE:HG22	2.00	0.76
1:C:717:ARG:HH12	1:C:829:GLY:HA2	1.50	0.76
1:A:48:SER:HA	1:A:86:GLY:O	1.85	0.76
1:A:543:VAL:O	1:A:544:LEU:HB3	1.86	0.76
1:A:885:PHE:HD2	1:A:886:LEU:HD12	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:VAL:O	1:B:438:ILE:HG12	1.86	0.76
1:B:707:ALA:O	1:B:708:LYS:HB3	1.83	0.76
1:C:72:ILE:HG22	1:C:94:PHE:HE2	1.49	0.76
1:C:162:MET:CB	1:C:313:MET:HE1	2.11	0.76
1:C:975:ILE:HG21	1:C:1019:ILE:HD13	1.65	0.76
1:B:517:ASN:O	1:B:521:GLU:HG3	1.85	0.76
1:B:520:PHE:HA	1:B:523:SER:OG	1.85	0.76
1:C:82:SER:HB3	1:C:88:VAL:CA	2.13	0.76
1:C:972:LEU:H	1:C:974:PRO:HD2	1.49	0.76
1:A:539:GLY:HA2	1:A:542:LEU:HB2	1.67	0.76
1:B:418:ARG:HG3	1:B:970:MET:CE	2.16	0.76
1:C:190:PRO:O	1:C:191:ASN:C	2.23	0.76
1:A:522:LYS:HE2	1:A:522:LYS:H	1.50	0.76
1:C:259:ARG:HH11	1:C:259:ARG:HB2	1.46	0.76
1:C:407:ASP:OD2	1:C:940:LYS:NZ	2.17	0.76
1:C:391:ASN:H	1:C:394:THR:CG2	1.97	0.76
1:C:527:TYR:OH	1:C:968:VAL:HG12	1.86	0.76
1:B:136:PHE:HE1	1:B:617:PHE:CZ	2.04	0.76
1:B:420:MET:HE2	1:B:425:LEU:HD23	1.68	0.76
1:A:60:THR:HG22	1:A:119:PRO:HD3	1.68	0.76
1:A:818:ARG:HA	1:A:824:SER:H	1.49	0.76
1:B:690:LEU:HB2	1:B:694:LYS:CB	2.14	0.76
1:B:894:SER:HB3	1:B:897:ILE:CG1	2.15	0.76
1:A:472:ILE:HD12	1:A:472:ILE:N	1.98	0.76
1:C:713:LEU:HD22	1:C:713:LEU:H	1.51	0.76
1:B:221:GLY:HA3	1:C:780:ARG:NH1	2.02	0.75
1:B:234:ILE:HG22	1:B:234:ILE:O	1.87	0.75
1:B:269:GLU:O	1:B:270:LEU:HB2	1.86	0.75
1:A:1:MET:N	1:A:2:PRO:HD2	2.01	0.75
1:A:472:ILE:HD12	1:A:472:ILE:H	1.48	0.75
1:B:418:ARG:HG3	1:B:970:MET:HE1	1.66	0.75
1:C:156:ASP:O	1:C:157:TYR:C	2.22	0.75
1:A:227:GLY:HA2	1:B:585:GLU:OE1	1.87	0.75
1:A:282:ASN:HD21	1:A:609:VAL:H	1.31	0.75
1:A:515:TRP:HA	1:A:519:MET:SD	2.26	0.75
1:B:328:ASP:HB2	2:B:1059:HOH:O	1.86	0.75
1:A:890:ALA:HB1	1:C:11:PHE:CD1	2.22	0.75
1:B:610:PHE:O	1:B:627:ALA:HB1	1.86	0.75
1:B:804:PHE:O	1:B:804:PHE:CD1	2.39	0.75
1:A:713:LEU:HD22	1:A:714:THR:N	1.97	0.75
1:A:790:TYR:CE1	1:A:800:PRO:HG3	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:818:ARG:CB	1:A:818:ARG:HE	1.98	0.75
1:C:459:PHE:CD2	1:C:459:PHE:N	2.48	0.75
1:A:61:VAL:HG13	1:A:118:LEU:CD2	2.16	0.75
1:B:1022:VAL:HG23	1:B:1023:PRO:CD	2.16	0.75
1:A:534:ILE:HB	1:A:540:ARG:NH1	2.01	0.75
1:A:661:ALA:O	1:A:663:VAL:HG23	1.87	0.75
1:B:549:VAL:CG2	1:B:550:VAL:N	2.49	0.75
1:A:112:GLN:HA	1:A:112:GLN:NE2	1.97	0.74
1:B:560:PRO:HB2	1:B:836:SER:HB3	1.69	0.74
1:A:73:ASP:HB3	1:A:106:GLN:HE22	1.51	0.74
1:A:781:MET:HE1	1:C:225:VAL:N	2.02	0.74
1:C:489:THR:O	1:C:493:CYS:HB3	1.88	0.74
1:A:599:LEU:O	1:A:600:THR:HB	1.86	0.74
1:A:1023:PRO:O	1:A:1027:VAL:HG23	1.87	0.74
1:C:32:VAL:O	1:C:32:VAL:HG12	1.87	0.74
1:C:975:ILE:HG22	1:C:976:LEU:N	2.00	0.74
1:C:73:ASP:O	1:C:74:ASN:O	2.06	0.74
1:C:424:GLY:HA2	2:C:1073:HOH:O	1.86	0.74
1:C:457:ALA:HB1	1:C:468:ARG:HA	1.67	0.74
1:C:577:GLN:HB3	1:C:624:THR:HG22	1.69	0.74
1:C:643:LYS:O	1:C:647:ILE:HG13	1.87	0.74
1:A:559:LEU:HD12	1:A:560:PRO:CD	2.15	0.74
1:A:578:LEU:HD21	1:A:587:THR:HG23	1.69	0.74
1:B:946:VAL:HG22	1:B:1026:PHE:CZ	2.23	0.74
1:C:158:VAL:CG2	1:C:158:VAL:CG1	2.62	0.74
1:C:655:PHE:C	1:C:657:GLN:H	1.91	0.74
1:B:262:LEU:HB3	1:B:268:ILE:HD11	1.69	0.74
1:C:166:ILE:HG12	2:C:1075:HOH:O	1.88	0.74
1:C:513:PHE:HA	1:C:516:PHE:CB	2.18	0.74
1:C:588:GLN:HG2	1:C:613:ASN:ND2	2.03	0.74
1:C:643:LYS:HG2	1:C:645:GLU:H	1.52	0.74
1:C:655:PHE:HA	1:C:659:LYS:HD3	1.70	0.74
1:A:44:THR:O	1:A:45:ILE:HG13	1.88	0.74
1:A:44:THR:O	1:A:45:ILE:CG1	2.36	0.74
1:A:68:ASN:N	1:A:68:ASN:C	2.41	0.74
1:A:701:GLN:OE1	1:A:852:PRO:HD3	1.87	0.74
1:B:686:ASP:HB3	1:B:823:PRO:O	1.87	0.74
1:B:973:ARG:HG2	1:B:974:PRO:HD3	1.70	0.74
1:A:568:ASP:HB3	1:A:634:TRP:HZ3	1.53	0.74
1:C:592:ASN:HD22	1:C:592:ASN:N	1.84	0.74
1:A:919:ARG:HG3	1:A:920:GLY:N	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:184:MET:HG2	1:C:246:PHE:CD1	2.23	0.73
1:A:578:LEU:O	1:A:623:ASN:ND2	2.20	0.73
1:A:749:THR:O	1:A:753:ALA:HB2	1.88	0.73
1:B:704:ALA:O	1:B:705:GLU:CG	2.35	0.73
1:C:69:MET:CE	1:C:92:LEU:CD2	2.54	0.73
1:C:879:ILE:O	1:C:883:VAL:HG23	1.88	0.73
1:C:950:LYS:O	1:C:954:ASP:HB2	1.88	0.73
1:A:69:MET:C	1:A:70:ASN:HD22	1.91	0.73
1:A:736:ALA:O	1:A:741:VAL:HG13	1.88	0.73
1:A:993:THR:HG21	1:A:1000:GLN:OE1	1.87	0.73
1:B:945:ILE:CD1	1:B:1026:PHE:CE2	2.72	0.73
1:C:62:THR:HA	2:C:1064:HOH:O	1.86	0.73
1:A:832:ALA:HB3	1:A:835:LYS:HB2	1.70	0.73
1:B:291:ILE:HG21	1:B:306:ILE:HD11	1.69	0.73
1:C:87:THR:CG2	1:C:88:VAL:N	2.51	0.73
1:C:144:ASN:ND2	1:C:149:MET:H	1.86	0.73
1:A:426:PRO:HG2	1:A:429:GLU:OE2	1.88	0.73
1:A:773:VAL:HG13	1:A:773:VAL:O	1.87	0.73
1:A:947:GLU:O	1:A:951:ASP:HB2	1.88	0.73
1:B:350:LEU:HB3	1:B:984:LEU:CD1	2.17	0.73
1:B:790:TYR:HE1	1:B:800:PRO:HB3	1.53	0.73
1:A:190:PRO:HG3	1:A:789:TRP:CD2	2.23	0.73
1:B:423:GLU:OE1	1:B:427:PRO:CD	2.37	0.73
1:C:922:THR:HG22	1:C:923:ASN:H	1.53	0.73
1:B:1018:ALA:O	1:B:1022:VAL:HG22	1.88	0.73
1:C:1:MET:HB2	1:C:2:PRO:CD	2.16	0.73
1:C:726:GLN:CD	1:C:812:GLY:HA3	2.08	0.73
1:A:428:LYS:HG3	1:A:429:GLU:H	1.52	0.73
1:C:45:ILE:CB	1:C:45:ILE:C	2.56	0.73
1:A:461:GLY:O	1:A:463:THR:O	2.06	0.73
1:A:540:ARG:HG3	1:A:541:TYR:H	1.53	0.73
1:A:919:ARG:CG	1:A:920:GLY:N	2.52	0.73
1:B:439:GLN:HA	1:B:442:LEU:HD12	1.71	0.73
1:B:759:VAL:HG12	1:B:760:ASN:HB2	1.70	0.73
1:B:7:ASP:O	1:B:8:ARG:HB2	1.89	0.73
1:C:144:ASN:HD21	1:C:149:MET:H	1.33	0.73
1:C:365:THR:O	1:C:368:PRO:HD2	1.88	0.73
1:A:102:ILE:HA	1:A:105:VAL:CG2	2.18	0.72
1:A:115:MET:C	1:A:117:LEU:H	1.92	0.72
1:A:801:PHE:HD2	1:A:805:SER:OG	1.70	0.72
1:B:42:ALA:HB2	1:B:93:THR:CG2	2.16	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ILE:HG22	1:A:90:ILE:O	1.85	0.72
1:A:822:LEU:HB3	1:A:823:PRO:HD2	1.69	0.72
1:B:136:PHE:HD2	1:B:290:GLY:O	1.72	0.72
1:B:412:VAL:HG13	1:B:435:MET:HE1	1.71	0.72
1:B:845:GLU:CG	1:B:857:TYR:OH	2.37	0.72
1:B:65:ILE:O	1:B:69:MET:HG2	1.89	0.72
1:B:750:LEU:C	1:B:750:LEU:HD13	2.10	0.72
1:A:10:ILE:HG12	1:B:893:GLU:O	1.90	0.72
1:B:740:GLY:O	1:B:794:ALA:N	2.22	0.72
1:C:108:GLN:C	2:C:1056:HOH:O	2.28	0.72
1:C:450:SER:O	1:C:451:ALA:CB	2.35	0.72
1:A:418:ARG:HG2	1:A:970:MET:CE	2.19	0.72
1:B:642:ASN:H	1:B:650:ARG:HH12	1.38	0.72
1:B:713:LEU:CD1	1:B:843:LEU:HD13	2.19	0.72
1:C:84:SER:C	1:C:86:GLY:H	1.92	0.72
1:C:729:ILE:CD1	1:C:786:ILE:HD13	2.18	0.72
1:B:412:VAL:HG13	1:B:435:MET:CE	2.20	0.72
1:B:489:THR:O	1:B:492:LEU:HB2	1.89	0.72
1:C:519:MET:HG3	1:C:520:PHE:N	2.03	0.72
1:C:592:ASN:ND2	1:C:592:ASN:H	1.87	0.72
1:C:946:VAL:O	1:C:946:VAL:HG12	1.90	0.72
1:A:225:VAL:HG22	1:B:778:LYS:NZ	2.04	0.72
1:A:415:ASN:HB3	1:A:434:SER:OG	1.90	0.72
1:B:30:LEU:HD23	1:B:390:ILE:HD11	1.72	0.72
1:B:48:SER:O	1:B:48:SER:OG	2.00	0.72
1:B:172:VAL:O	1:B:173:GLY:O	2.06	0.72
1:B:944:LEU:O	1:B:971:ARG:HD2	1.89	0.72
1:C:104:GLN:HG3	1:C:131:LYS:HG2	1.72	0.72
1:A:67:GLN:C	1:A:68:ASN:CA	2.57	0.72
1:A:69:MET:O	1:A:70:ASN:ND2	2.19	0.72
1:A:311:ALA:O	1:A:312:LYS:HB2	1.89	0.72
1:A:733:GLN:OE1	1:A:743:ILE:HG12	1.90	0.72
1:B:970:MET:HA	1:B:970:MET:HE2	1.72	0.72
2:B:1060:HOH:O	1:C:110:LYS:HD3	1.90	0.72
1:C:536:ARG:NH1	1:C:961:ILE:HD11	2.05	0.72
1:A:314:GLU:N	1:A:315:PRO:HD3	2.04	0.71
1:A:447:MET:HB3	1:A:887:CYS:SG	2.30	0.71
1:B:136:PHE:HE1	1:B:617:PHE:HZ	1.38	0.71
1:B:235:ILE:H	1:B:235:ILE:HD13	1.55	0.71
1:A:359:LEU:HD12	1:A:417:GLU:HG2	1.72	0.71
1:A:782:LEU:O	1:A:784:ASP:O	2.07	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:LEU:N	1:B:92:LEU:CD2	2.53	0.71
1:B:314:GLU:H	1:B:315:PRO:CD	2.03	0.71
1:A:406:VAL:CG1	1:A:407:ASP:H	2.02	0.71
1:A:436:GLY:HA2	1:A:439:GLN:HB2	1.73	0.71
1:A:729:ILE:CG2	1:A:730:ASP:H	1.99	0.71
1:B:714:THR:HG22	1:B:831:ALA:CA	2.20	0.71
1:B:892:TYR:HB3	1:B:897:ILE:HD11	1.71	0.71
1:C:108:GLN:HA	2:C:1056:HOH:O	1.89	0.71
1:C:327:TYR:HB3	1:C:628:PHE:HB3	1.70	0.71
1:C:764:ASP:OD2	1:C:765:ARG:HD2	1.90	0.71
1:A:896:SER:O	1:A:899:PHE:HB2	1.90	0.71
1:A:904:VAL:HG21	1:A:942:ALA:HB2	1.72	0.71
1:C:542:LEU:HD23	1:C:542:LEU:O	1.89	0.71
1:C:695:LEU:HD22	1:C:825:MET:HG3	1.73	0.71
1:C:713:LEU:CD1	1:C:834:GLY:HA3	2.16	0.71
1:A:11:PHE:CD1	1:B:890:ALA:HB1	2.26	0.71
1:A:644:VAL:O	1:A:648:THR:HG23	1.90	0.71
1:B:115:MET:O	1:B:123:GLN:NE2	2.23	0.71
1:B:116:PRO:HA	1:B:123:GLN:NE2	2.06	0.71
1:B:790:TYR:CE1	1:B:800:PRO:HB3	2.25	0.71
1:C:105:VAL:O	1:C:108:GLN:N	2.23	0.71
1:C:568:ASP:OD2	1:C:644:VAL:HG23	1.88	0.71
1:A:894:SER:OG	1:A:897:ILE:HB	1.90	0.71
1:A:1027:VAL:O	1:A:1029:VAL:O	2.07	0.71
1:B:219:LEU:HD12	1:B:234:ILE:HG12	1.71	0.71
1:B:623:ASN:HD22	1:B:624:THR:N	1.88	0.71
1:B:987:MET:HE2	1:B:987:MET:O	1.90	0.71
1:C:166:ILE:CG1	2:C:1075:HOH:O	2.38	0.71
1:C:169:THR:HG22	1:C:172:VAL:HG23	1.72	0.71
1:C:777:ALA:O	1:C:779:TYR:N	2.24	0.71
1:C:945:ILE:O	1:C:946:VAL:HG23	1.90	0.71
1:B:228:GLN:HG2	1:C:781:MET:HE1	1.73	0.71
1:B:231:ASN:C	1:B:231:ASN:ND2	2.43	0.71
1:B:518:ARG:HA	1:B:521:GLU:HB2	1.73	0.71
1:C:290:GLY:O	1:C:291:ILE:HG13	1.91	0.71
1:C:317:PHE:HB2	1:C:318:PRO:HD2	1.71	0.71
1:C:418:ARG:HG3	1:C:419:VAL:HG13	1.73	0.71
1:C:463:THR:HG22	1:C:464:GLY:N	2.05	0.71
1:A:65:ILE:O	1:A:68:ASN:HB2	1.91	0.71
1:C:350:LEU:HD13	1:C:984:LEU:HD23	1.73	0.71
1:C:552:MET:O	1:C:553:ALA:HB3	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ASN:HD21	1:A:192:GLU:CB	2.04	0.70
1:A:328:ASP:O	1:A:331:PRO:HD2	1.91	0.70
1:A:687:GLN:HG2	1:C:316:PHE:CD1	2.25	0.70
1:A:818:ARG:CB	1:A:818:ARG:NE	2.54	0.70
1:A:9:PRO:HB3	1:A:491:ALA:HB1	1.73	0.70
1:A:551:GLY:O	1:A:554:TYR:HB3	1.91	0.70
1:B:188:MET:SD	1:B:200:PRO:HB3	2.31	0.70
1:B:291:ILE:HG21	1:B:306:ILE:CD1	2.22	0.70
1:C:144:ASN:ND2	1:C:149:MET:HG3	2.07	0.70
1:C:158:VAL:CG2	1:C:158:VAL:CA	2.69	0.70
1:C:399:VAL:HA	1:C:402:ILE:CD1	2.21	0.70
1:C:959:GLY:H	1:C:962:GLU:HB2	1.56	0.70
1:B:556:PHE:N	1:B:913:LEU:HD21	2.06	0.70
1:A:228:GLN:HG2	1:B:781:MET:CG	2.22	0.70
1:B:279:ALA:HA	1:B:611:ALA:O	1.91	0.70
1:B:537:SER:HB2	1:B:540:ARG:CG	2.21	0.70
1:B:1005:THR:O	1:B:1005:THR:HG22	1.89	0.70
1:C:12:ALA:HB1	1:C:487:ILE:HG22	1.73	0.70
1:B:987:MET:O	1:B:990:VAL:HB	1.92	0.70
1:C:166:ILE:C	1:C:172:VAL:HG11	2.11	0.70
1:B:523:SER:HA	1:B:526:HIS:CD2	2.18	0.70
1:C:192:GLU:O	1:C:195:LYS:N	2.25	0.70
1:C:785:ASP:C	1:C:787:GLY:H	1.93	0.70
1:A:634:TRP:HE3	1:A:995:ALA:HB1	1.54	0.70
1:B:705:GLU:O	1:B:707:ALA:N	2.23	0.70
1:A:1013:THR:O	1:A:1017:LEU:HB3	1.91	0.70
1:A:73:ASP:CB	1:A:106:GLN:HE22	2.05	0.70
1:A:155:SER:HA	1:A:287:SER:OG	1.92	0.70
1:C:945:ILE:HB	1:C:971:ARG:HG3	1.72	0.70
1:C:1035:ARG:HA	1:C:1035:ARG:HE	1.57	0.70
1:A:68:ASN:O	1:A:70:ASN:N	2.25	0.69
1:A:936:GLY:O	1:A:940:LYS:HB2	1.91	0.69
1:B:542:LEU:HD11	1:B:1028:VAL:HG11	1.74	0.69
1:C:146:ASP:HB2	1:C:148:THR:OG1	1.92	0.69
1:C:166:ILE:CA	1:C:166:ILE:CG1	2.70	0.69
1:A:11:PHE:CE1	1:B:890:ALA:HB1	2.27	0.69
1:A:64:VAL:C	1:A:65:ILE:C	2.50	0.69
1:B:713:LEU:H	1:B:713:LEU:CD1	2.05	0.69
1:C:450:SER:O	1:C:451:ALA:HB2	1.92	0.69
1:C:915:ALA:HA	1:C:918:PHE:HB3	1.73	0.69
1:A:114:ALA:O	1:A:117:LEU:HB2	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:VAL:HA	1:A:534:ILE:CD1	2.14	0.69
1:B:118:LEU:HD23	1:B:122:VAL:HG11	1.74	0.69
1:B:13:TRP:O	1:B:17:ILE:HG12	1.92	0.69
1:B:225:VAL:HG22	1:C:781:MET:HE2	1.72	0.69
1:B:1024:VAL:HG12	1:B:1025:PHE:H	1.56	0.69
1:C:7:ASP:O	1:C:9:PRO:HD3	1.92	0.69
1:C:247:GLY:CA	1:C:268:ILE:HD13	2.23	0.69
1:A:901:VAL:HG11	1:A:943:ILE:HG12	1.74	0.69
1:B:49:TYR:CG	1:B:122:VAL:HG22	2.27	0.69
1:B:157:TYR:CA	1:B:161:ASN:HD22	2.05	0.69
1:B:851:LEU:N	1:B:852:PRO:HD3	2.08	0.69
1:B:986:VAL:O	1:B:990:VAL:HG23	1.92	0.69
1:A:340:VAL:HG13	1:A:399:VAL:CG2	2.23	0.69
1:C:131:LYS:C	1:C:295:THR:HG22	2.12	0.69
1:C:159:ALA:O	1:C:160:ALA:C	2.17	0.69
1:C:163:LYS:HG2	1:C:175:VAL:HG11	1.74	0.69
1:C:402:ILE:O	1:C:406:VAL:HG23	1.92	0.69
1:C:415:ASN:HD21	1:C:434:SER:HB2	1.57	0.69
1:C:556:PHE:HB2	1:C:913:LEU:CD1	2.22	0.69
1:A:115:MET:O	1:A:117:LEU:N	2.25	0.69
1:B:773:VAL:HG13	1:B:773:VAL:O	1.92	0.69
1:B:943:ILE:O	1:B:947:GLU:HB3	1.92	0.69
1:A:653:ARG:O	1:A:656:SER:N	2.24	0.69
1:A:731:ILE:HD12	1:A:731:ILE:N	2.07	0.69
1:A:822:LEU:HD22	1:A:822:LEU:N	2.08	0.69
1:B:572:PHE:CZ	1:B:629:VAL:HG21	2.27	0.69
1:B:845:GLU:HG3	1:B:857:TYR:OH	1.93	0.69
1:B:973:ARG:HG2	1:B:974:PRO:CD	2.22	0.69
1:C:184:MET:HA	1:C:184:MET:CE	2.23	0.69
1:A:108:GLN:CG	1:B:112:GLN:CD	2.62	0.69
1:B:211:ASN:ND2	1:B:246:PHE:HZ	1.91	0.69
1:B:929:VAL:O	1:B:933:THR:OG1	2.11	0.69
1:C:82:SER:OG	1:C:88:VAL:HG13	1.93	0.69
1:C:157:TYR:O	1:C:161:ASN:HB2	1.93	0.69
1:C:214:VAL:CG1	1:C:215:ALA:N	2.56	0.69
1:C:358:PHE:HB3	1:C:977:MET:CE	2.19	0.69
1:A:124:GLN:HG2	1:A:758:TYR:CE2	2.28	0.69
1:A:200:PRO:HG2	1:A:749:THR:HA	1.73	0.69
1:A:659:LYS:O	1:A:661:ALA:N	2.26	0.69
1:A:279:ALA:HA	1:A:612:VAL:HG12	1.74	0.68
1:B:151:GLN:HE22	1:B:279:ALA:H	1.39	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:LEU:HB3	1:B:498:LYS:O	1.93	0.68
1:B:1012:VAL:HG23	1:B:1013:THR:N	2.08	0.68
1:A:406:VAL:CG1	1:A:407:ASP:N	2.56	0.68
1:A:572:PHE:CE1	1:A:629:VAL:HG13	2.29	0.68
1:B:281:PHE:HE1	1:B:608:SER:HG	1.39	0.68
1:B:771:VAL:O	1:B:771:VAL:HG12	1.92	0.68
1:C:33:ALA:HB2	1:C:298:ASN:ND2	2.08	0.68
1:A:813:SER:HB3	1:A:816:LEU:HD21	1.73	0.68
1:A:950:LYS:O	1:A:951:ASP:HB3	1.93	0.68
1:B:207:ILE:CG2	1:B:759:VAL:HG11	2.22	0.68
1:B:214:VAL:HG21	1:C:747:ASN:HD21	1.58	0.68
1:C:590:VAL:O	1:C:594:VAL:HG23	1.92	0.68
1:C:592:ASN:O	1:C:593:GLU:CB	2.42	0.68
1:B:109:ASN:HD22	1:B:112:GLN:HE22	1.41	0.68
1:B:922:THR:OG1	1:B:923:ASN:N	2.26	0.68
1:C:939:ALA:O	1:C:943:ILE:CD1	2.42	0.68
1:A:73:ASP:HB3	2:C:1054:HOH:O	1.93	0.68
1:A:199:THR:HB	1:A:200:PRO:HD2	1.76	0.68
1:A:372:VAL:O	1:A:375:VAL:N	2.26	0.68
1:A:413:VAL:HG23	1:A:493:CYS:CB	2.23	0.68
1:A:596:HIS:C	1:A:598:TYR:H	1.95	0.68
1:B:584:GLN:HB2	1:B:622:GLN:HE21	1.58	0.68
1:A:106:GLN:O	1:A:107:VAL:C	2.26	0.68
1:A:521:GLU:HB3	1:A:522:LYS:NZ	2.08	0.68
1:B:327:TYR:CD2	1:B:628:PHE:HB3	2.28	0.68
1:C:713:LEU:HD12	1:C:833:PRO:O	1.91	0.68
1:B:659:LYS:HA	1:B:659:LYS:NZ	2.08	0.68
1:C:1016:VAL:O	1:C:1018:ALA:N	2.22	0.68
1:A:552:MET:HE1	1:A:906:PRO:CA	2.24	0.68
1:B:138:MET:HE3	1:B:306:ILE:HD13	1.76	0.68
1:B:356:TYR:C	1:B:358:PHE:H	1.95	0.68
1:B:420:MET:CE	1:B:425:LEU:HD23	2.23	0.68
1:B:739:LEU:O	1:B:793:ALA:HB1	1.94	0.68
1:B:919:ARG:HG3	1:B:1005:THR:HG21	1.76	0.68
1:A:773:VAL:O	1:A:773:VAL:CG1	2.42	0.68
1:B:129:VAL:O	1:B:129:VAL:HG12	1.94	0.68
1:C:420:MET:SD	1:C:498:LYS:CD	2.81	0.68
1:C:576:VAL:HG12	1:C:663:VAL:HG22	1.74	0.68
1:A:819:TYR:O	1:A:822:LEU:N	2.18	0.68
1:A:822:LEU:HB3	2:A:1059:HOH:O	1.94	0.68
1:A:855:VAL:HG23	1:A:855:VAL:O	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:ARG:HE	1:B:970:MET:HE3	1.58	0.68
1:B:591:LEU:O	1:B:595:THR:HG22	1.92	0.68
1:C:713:LEU:HD22	1:C:713:LEU:N	2.09	0.68
1:C:713:LEU:HB2	1:C:832:ALA:HB3	1.75	0.68
1:A:104:GLN:O	1:A:108:GLN:HB2	1.94	0.67
1:B:120:GLN:HG2	1:B:124:GLN:HG2	1.76	0.67
1:A:901:VAL:O	1:A:904:VAL:CG2	2.41	0.67
1:A:909:VAL:CG1	1:A:913:LEU:HD21	2.22	0.67
1:B:116:PRO:HA	1:B:123:GLN:HE22	1.59	0.67
1:B:119:PRO:HG2	1:B:122:VAL:CG2	2.24	0.67
1:B:358:PHE:CZ	1:B:976:LEU:HD12	2.27	0.67
1:B:404:LEU:HD13	1:B:449:LEU:HD13	1.75	0.67
1:C:110:LYS:O	1:C:112:GLN:N	2.27	0.67
1:C:658:ILE:H	1:C:658:ILE:HD12	1.60	0.67
1:C:727:PHE:CZ	1:C:783:PRO:HB3	2.29	0.67
1:A:342:LYS:HG3	1:A:343:THR:N	2.10	0.67
1:A:435:MET:HA	1:A:438:ILE:HD11	1.76	0.67
1:B:190:PRO:HG2	1:B:779:TYR:CG	2.30	0.67
1:B:525:HIS:HA	1:B:528:THR:CG2	2.25	0.67
1:C:58:GLN:OE1	1:C:82:SER:CA	2.43	0.67
1:C:58:GLN:OE1	1:C:82:SER:N	2.26	0.67
1:A:173:GLY:HA3	1:A:294:ALA:HA	1.76	0.67
1:A:815:ARG:CZ	2:A:1071:HOH:O	2.41	0.67
1:B:150:THR:H	1:B:153:ASP:CB	2.08	0.67
1:B:416:VAL:CG2	1:B:431:THR:HA	2.25	0.67
1:B:537:SER:O	1:B:540:ARG:HB2	1.94	0.67
1:C:159:ALA:C	1:C:161:ASN:H	1.98	0.67
1:C:778:LYS:O	1:C:779:TYR:HD2	1.77	0.67
1:C:905:VAL:HB	1:C:906:PRO:HD3	1.75	0.67
1:A:571:VAL:HG12	1:A:630:SER:CA	2.24	0.67
1:A:818:ARG:HA	1:A:824:SER:N	2.10	0.67
1:B:347:ALA:HB1	1:B:402:ILE:HG21	1.76	0.67
1:C:5:PHE:HE2	1:C:11:PHE:HD2	1.40	0.67
1:C:457:ALA:CB	1:C:468:ARG:HA	2.23	0.67
1:A:201:VAL:HG21	1:A:745:ASP:OD2	1.95	0.67
1:A:742:SER:HG	1:A:745:ASP:HB2	1.57	0.67
1:A:818:ARG:HE	1:A:818:ARG:HB2	1.57	0.67
1:C:426:PRO:HB2	1:C:429:GLU:HB2	1.77	0.67
1:B:94:PHE:HB2	1:B:98:THR:HG21	1.77	0.67
1:C:166:ILE:HA	1:C:166:ILE:CG1	2.24	0.67
1:C:613:ASN:C	1:C:613:ASN:OD1	2.32	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:ARG:H	1:A:536:ARG:HD2	1.60	0.67
1:B:6:ILE:HA	1:B:491:ALA:HA	1.77	0.67
1:B:175:VAL:HG12	1:B:175:VAL:O	1.94	0.67
1:B:178:PHE:HE1	1:B:615:PHE:CE2	2.13	0.67
1:B:298:ASN:O	1:B:302:THR:HG23	1.94	0.67
1:C:225:VAL:O	1:C:226:LYS:C	2.32	0.67
1:B:940:LYS:O	1:B:941:ASN:C	2.32	0.67
1:A:1018:ALA:HB1	1:A:1022:VAL:CG1	2.24	0.67
1:B:172:VAL:O	1:B:172:VAL:CG1	2.39	0.67
1:C:103:ALA:O	1:C:104:GLN:C	2.32	0.67
1:C:190:PRO:HG3	1:C:789:TRP:CH2	2.30	0.67
1:A:69:MET:C	1:A:70:ASN:ND2	2.48	0.66
1:A:583:THR:HG22	1:A:585:GLU:H	1.58	0.66
1:B:30:LEU:HD23	1:B:390:ILE:CG1	2.24	0.66
1:B:860:THR:HG22	1:B:861:GLY:N	2.10	0.66
1:C:389:SER:OG	1:C:391:ASN:ND2	2.28	0.66
1:C:953:MET:HE1	1:C:1030:ARG:HH22	1.61	0.66
1:A:376:LEU:O	1:A:377:LEU:C	2.34	0.66
1:A:521:GLU:HB3	1:A:522:LYS:HZ3	1.60	0.66
1:A:674:LEU:HD22	1:A:675:GLY:H	1.61	0.66
1:A:987:MET:N	1:A:988:PRO:HD2	2.10	0.66
1:B:74:ASN:O	1:B:94:PHE:HB3	1.95	0.66
1:B:124:GLN:O	1:B:125:GLN:HB2	1.95	0.66
1:B:125:GLN:O	1:B:125:GLN:HG2	1.94	0.66
1:B:330:THR:N	1:B:331:PRO:HD2	2.11	0.66
1:B:641:GLU:HA	1:B:650:ARG:NH1	2.11	0.66
1:C:457:ALA:N	1:C:459:PHE:CE2	2.61	0.66
1:C:713:LEU:O	1:C:831:ALA:HA	1.95	0.66
1:C:1024:VAL:O	1:C:1028:VAL:HG23	1.95	0.66
1:A:736:ALA:O	1:A:741:VAL:CG1	2.43	0.66
1:B:671:ILE:O	1:B:673:GLU:HB2	1.95	0.66
1:C:476:SER:C	1:C:478:MET:H	1.98	0.66
1:C:586:ARG:O	1:C:589:LYS:HB2	1.95	0.66
1:C:143:ILE:CD1	1:C:286:ALA:HB2	2.25	0.66
1:C:688:ALA:O	1:C:690:LEU:N	2.25	0.66
1:A:55:LYS:HD3	1:A:816:LEU:HD11	1.77	0.66
1:A:243:THR:HG22	1:A:268:ILE:HG22	1.78	0.66
1:B:990:VAL:CG1	1:B:1005:THR:OG1	2.38	0.66
1:C:317:PHE:HB2	1:C:318:PRO:CD	2.26	0.66
1:A:119:PRO:HG2	1:A:122:VAL:HG23	1.78	0.66
1:A:189:ASN:HD21	1:A:192:GLU:HB3	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:759:VAL:HG12	1:A:760:ASN:N	2.09	0.66
1:C:997:SER:O	1:C:998:GLY:C	2.31	0.66
1:A:693:GLU:O	1:A:696:THR:N	2.23	0.66
1:C:35:TYR:CD1	1:C:671:ILE:HG12	2.31	0.66
1:C:380:PHE:CE1	1:C:398:MET:SD	2.88	0.66
1:C:592:ASN:HD22	1:C:592:ASN:H	1.40	0.66
1:C:1026:PHE:O	1:C:1029:VAL:HB	1.96	0.66
1:A:540:ARG:HD2	1:A:541:TYR:CD2	2.30	0.66
1:C:189:ASN:CG	1:C:779:TYR:HE1	1.98	0.66
1:C:372:VAL:HG21	1:C:402:ILE:HG23	1.78	0.66
1:C:416:VAL:HG12	1:C:434:SER:OG	1.96	0.66
1:C:713:LEU:HG	1:C:832:ALA:C	2.17	0.66
1:C:714:THR:HG22	1:C:715:SER:H	1.60	0.66
1:C:801:PHE:HA	1:C:804:PHE:CZ	2.31	0.66
1:A:719:ASN:HB2	1:A:828:LEU:HD23	1.78	0.66
1:B:95:GLU:O	1:B:98:THR:HB	1.96	0.66
1:B:238:THR:OG1	1:B:239:ARG:N	2.29	0.66
1:B:940:LYS:NZ	1:B:978:THR:HG23	2.10	0.66
1:C:163:LYS:HD2	1:C:177:LEU:HB2	1.76	0.66
1:C:181:GLN:HG2	1:C:769:LYS:HE3	1.78	0.66
1:C:367:ILE:HG23	1:C:368:PRO:HD3	1.78	0.66
1:C:474:ILE:O	1:C:476:SER:O	2.14	0.66
1:C:843:LEU:O	1:C:846:GLN:HB2	1.96	0.66
1:A:111:LEU:O	1:A:113:LEU:N	2.29	0.66
1:A:344:LEU:CD2	1:A:402:ILE:CD1	2.68	0.66
1:B:1026:PHE:O	1:B:1030:ARG:HG3	1.95	0.66
1:C:901:VAL:HG11	1:C:943:ILE:HD13	1.76	0.66
1:B:199:THR:N	1:B:202:ASP:OD2	2.27	0.65
1:C:166:ILE:CA	1:C:166:ILE:HD13	2.12	0.65
1:C:423:GLU:O	1:C:426:PRO:HD3	1.97	0.65
1:A:44:THR:HA	1:A:91:THR:HA	1.79	0.65
1:A:706:ALA:HB3	1:A:716:VAL:HG21	1.77	0.65
1:B:30:LEU:HD23	1:B:390:ILE:CD1	2.26	0.65
1:C:102:ILE:O	1:C:103:ALA:C	2.31	0.65
1:C:633:ASP:O	1:C:634:TRP:HB2	1.95	0.65
1:A:330:THR:HG23	1:A:334:LYS:HE2	1.78	0.65
1:B:902:MET:O	1:B:905:VAL:HG12	1.97	0.65
1:C:939:ALA:O	1:C:943:ILE:HD11	1.95	0.65
1:B:644:VAL:HG23	1:B:645:GLU:H	1.61	0.65
1:C:188:MET:HA	1:C:266:ALA:HB1	1.78	0.65
1:B:495:THR:O	1:B:498:LYS:HE3	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:775:SER:HB3	1:B:780:ARG:CG	2.27	0.65
1:B:984:LEU:O	1:B:984:LEU:HD13	1.96	0.65
1:C:115:MET:HE1	1:C:118:LEU:CD2	2.27	0.65
1:A:83:ASP:HB3	2:A:1068:HOH:O	1.96	0.65
1:A:100:ALA:CB	1:A:131:LYS:HE3	2.27	0.65
1:A:108:GLN:CG	1:A:108:GLN:CA	2.74	0.65
1:A:128:SER:HB2	1:B:113:LEU:HD21	1.77	0.65
1:B:328:ASP:C	1:B:328:ASP:OD2	2.35	0.65
1:B:405:LEU:HD12	1:B:406:VAL:H	1.60	0.65
1:B:773:VAL:O	1:B:773:VAL:CG1	2.45	0.65
1:C:524:THR:O	1:C:527:TYR:HB3	1.97	0.65
1:C:713:LEU:CG	1:C:832:ALA:O	2.36	0.65
1:A:76:MET:CG	1:A:95:GLU:OE2	2.42	0.65
1:A:128:SER:CB	1:B:113:LEU:CD2	2.75	0.65
1:A:133:SER:HG	1:A:136:PHE:HE1	1.43	0.65
1:A:527:TYR:O	1:A:530:SER:OG	2.11	0.65
1:B:45:ILE:HG22	1:B:46:SER:N	2.12	0.65
1:B:293:LEU:HD22	1:B:294:ALA:O	1.97	0.65
1:B:330:THR:N	1:B:331:PRO:CD	2.59	0.65
1:B:655:PHE:HA	1:B:658:ILE:HG21	1.79	0.65
1:B:1024:VAL:CG1	1:B:1028:VAL:HG21	2.27	0.65
1:C:14:VAL:HG13	1:C:15:ILE:N	2.12	0.65
1:C:45:ILE:CA	1:C:45:ILE:CG2	2.71	0.65
1:C:74:ASN:HB3	1:C:95:GLU:HB2	1.78	0.65
1:C:197:GLN:HB3	1:C:798:MET:HE2	1.79	0.65
1:C:324:VAL:HG23	1:C:326:PRO:HD3	1.79	0.65
1:A:263:ARG:HB3	1:A:263:ARG:HH21	1.62	0.65
1:A:521:GLU:HG3	2:A:1075:HOH:O	1.97	0.65
1:B:6:ILE:CD1	1:B:490:PRO:HB2	2.26	0.65
1:B:601:LYS:O	1:B:603:LYS:N	2.30	0.65
1:C:169:THR:CB	1:C:169:THR:C	2.64	0.65
1:A:60:THR:CG2	1:A:119:PRO:HD3	2.26	0.65
1:A:100:ALA:HB1	1:A:131:LYS:HE3	1.79	0.65
1:A:222:THR:HG22	1:A:223:PRO:HD2	1.79	0.65
1:B:49:TYR:CE2	1:B:125:GLN:HB3	2.31	0.65
1:B:160:ALA:HB1	1:B:767:ARG:HD3	1.76	0.65
1:B:572:PHE:HB2	1:B:666:PHE:O	1.97	0.65
1:B:578:LEU:HB2	1:B:623:ASN:HB2	1.79	0.65
1:B:598:TYR:HB3	1:B:606:VAL:HG11	1.78	0.65
1:B:646:ALA:C	1:B:648:THR:N	2.46	0.65
1:C:54:ALA:N	1:C:57:VAL:HG23	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:431:THR:O	1:C:435:MET:HG2	1.96	0.65
1:C:592:ASN:O	1:C:593:GLU:HB3	1.97	0.65
1:C:728:LYS:HG3	1:C:729:ILE:H	1.60	0.65
1:A:56:THR:HG23	1:C:213:GLN:HG3	1.79	0.65
1:B:561:SER:HB2	1:B:838:GLY:HA3	1.78	0.65
1:B:699:ARG:HB3	1:B:699:ARG:HH11	1.62	0.65
1:B:835:LYS:HB2	1:B:839:GLU:OE2	1.96	0.65
1:C:60:THR:CG2	1:C:61:VAL:HG23	2.26	0.65
1:C:520:PHE:O	1:C:523:SER:N	2.29	0.65
1:C:786:ILE:HG22	1:C:786:ILE:O	1.97	0.65
1:C:1024:VAL:HG12	1:C:1028:VAL:HG21	1.78	0.65
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.78	0.64
1:B:1012:VAL:CG2	1:B:1013:THR:N	2.61	0.64
1:C:110:LYS:O	1:C:111:LEU:C	2.35	0.64
1:C:395:MET:O	1:C:398:MET:N	2.30	0.64
1:C:545:TYR:OH	1:C:1021:PHE:CG	2.49	0.64
1:C:657:GLN:O	1:C:659:LYS:N	2.30	0.64
1:C:844:MET:HA	1:C:847:LEU:HD21	1.78	0.64
1:A:95:GLU:O	1:A:98:THR:HG23	1.97	0.64
1:A:885:PHE:CD2	1:A:886:LEU:HD12	2.32	0.64
1:B:468:ARG:O	1:B:469:GLN:C	2.34	0.64
1:B:537:SER:C	1:B:540:ARG:HE	2.00	0.64
1:B:544:LEU:CA	1:B:547:ILE:HD12	2.19	0.64
1:B:960:LEU:HD12	1:B:961:ILE:HG13	1.79	0.64
1:C:64:VAL:HG12	1:C:65:ILE:N	2.11	0.64
1:C:244:GLU:HA	1:C:263:ARG:HH22	1.61	0.64
1:A:355:MET:HE3	1:A:410:ILE:HG12	1.78	0.64
1:A:418:ARG:CD	1:A:970:MET:HG3	2.25	0.64
1:A:476:SER:O	1:A:480:LEU:HB2	1.96	0.64
1:B:139:VAL:O	1:B:139:VAL:HG12	1.96	0.64
1:B:972:LEU:CD1	1:B:976:LEU:HD23	2.28	0.64
1:C:222:THR:HB	1:C:223:PRO:CD	2.24	0.64
1:C:545:TYR:OH	1:C:1021:PHE:CB	2.45	0.64
1:A:298:ASN:HD22	1:A:300:LEU:N	1.95	0.64
1:A:534:ILE:HD12	1:A:540:ARG:NH2	2.13	0.64
1:A:574:THR:HG21	1:A:598:TYR:HE1	1.63	0.64
1:A:727:PHE:O	1:C:234:ILE:HA	1.97	0.64
1:B:654:ALA:O	1:B:656:SER:N	2.31	0.64
1:B:659:LYS:HA	1:B:659:LYS:HZ3	1.62	0.64
1:B:715:SER:HB2	1:B:830:GLN:NE2	2.12	0.64
1:C:62:THR:CB	2:C:1064:HOH:O	2.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:418:ARG:HG3	1:C:419:VAL:CG1	2.28	0.64
1:C:899:PHE:N	1:C:899:PHE:CD1	2.65	0.64
1:A:59:ASP:HB3	1:C:763:ILE:HD11	1.78	0.64
1:A:540:ARG:HG2	2:A:1064:HOH:O	1.96	0.64
1:A:785:ASP:O	1:A:788:ASP:N	2.30	0.64
1:B:314:GLU:N	1:B:315:PRO:HD2	2.12	0.64
1:C:1:MET:CE	1:C:439:GLN:HE22	2.11	0.64
1:C:710:PRO:O	1:C:712:MET:O	2.16	0.64
1:A:911:GLY:H	1:A:914:LEU:HD13	1.63	0.64
1:B:2:PRO:CD	1:B:486:LEU:HD12	2.28	0.64
1:B:1012:VAL:CG2	1:B:1013:THR:H	2.10	0.64
1:C:404:LEU:O	1:C:405:LEU:HD23	1.98	0.64
1:B:68:ASN:O	1:B:70:ASN:ND2	2.31	0.64
1:B:136:PHE:CE1	1:B:617:PHE:HZ	2.16	0.64
1:B:184:MET:O	1:B:184:MET:CG	2.46	0.64
1:C:26:ALA:O	1:C:30:LEU:HG	1.98	0.64
1:C:114:ALA:O	1:C:118:LEU:HD13	1.98	0.64
1:C:115:MET:SD	1:C:123:GLN:NE2	2.71	0.64
1:C:344:LEU:CD2	1:C:402:ILE:HD11	2.28	0.64
1:A:949:ALA:HB1	1:A:1026:PHE:CZ	2.33	0.64
1:B:328:ASP:OD2	1:B:330:THR:N	2.31	0.64
1:B:335:ILE:C	1:B:337:ILE:H	2.00	0.64
1:C:371:ALA:O	1:C:375:VAL:HG23	1.98	0.64
1:C:672:VAL:O	1:C:672:VAL:HG12	1.98	0.64
1:C:850:LYS:O	1:C:851:LEU:O	2.16	0.64
1:A:44:THR:HG22	1:A:89:GLN:HG3	1.80	0.64
1:A:255:GLN:O	1:A:256:ASP:OD1	2.16	0.64
1:A:601:LYS:HG3	1:A:601:LYS:O	1.98	0.64
1:A:692:HIS:O	1:A:696:THR:OG1	2.13	0.64
1:A:728:LYS:HZ3	1:C:235:ILE:HG22	1.60	0.64
1:B:9:PRO:O	1:B:12:ALA:HB3	1.97	0.64
1:B:187:TRP:HZ3	1:B:774:MET:HE3	1.61	0.64
1:B:356:TYR:C	1:B:358:PHE:N	2.50	0.64
1:B:437:GLN:HA	1:B:437:GLN:HE21	1.63	0.64
1:B:463:THR:HG21	1:B:869:SER:HB2	1.80	0.64
1:C:167:SER:N	1:C:167:SER:C	2.51	0.64
1:C:176:GLN:NE2	1:C:620:ARG:HH11	1.96	0.64
1:C:545:TYR:HA	1:C:548:ILE:HG13	1.80	0.64
1:C:894:SER:C	1:C:896:SER:H	2.01	0.64
1:A:46:SER:HA	1:A:88:VAL:O	1.99	0.63
1:A:225:VAL:HG12	1:A:226:LYS:N	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:935:ILE:HG22	1:A:935:ILE:O	1.97	0.63
1:B:410:ILE:HG23	1:B:414:GLU:OE2	1.98	0.63
1:B:750:LEU:HD13	1:B:750:LEU:O	1.98	0.63
1:C:687:GLN:HB2	1:C:854:GLY:O	1.97	0.63
1:A:367:ILE:HG12	1:A:413:VAL:HG21	1.80	0.63
1:A:649:MET:CB	1:A:653:ARG:HH21	2.04	0.63
1:B:371:ALA:O	1:B:375:VAL:HG23	1.98	0.63
1:B:953:MET:HG2	1:B:953:MET:O	1.98	0.63
1:C:60:THR:HG23	1:C:61:VAL:HG23	1.80	0.63
1:C:361:ASN:HB2	1:C:364:ALA:HB3	1.80	0.63
1:C:391:ASN:H	1:C:394:THR:HG23	1.63	0.63
1:A:298:ASN:HD22	1:A:300:LEU:H	1.44	0.63
1:A:818:ARG:CD	1:A:818:ARG:CB	2.76	0.63
1:B:314:GLU:N	1:B:315:PRO:CD	2.61	0.63
1:B:416:VAL:HG21	1:B:431:THR:HA	1.80	0.63
1:C:644:VAL:HG11	1:C:667:ASN:ND2	2.11	0.63
1:A:102:ILE:HA	1:A:105:VAL:HG23	1.80	0.63
1:A:348:ILE:HA	1:A:351:VAL:HG23	1.80	0.63
1:A:443:VAL:CG1	1:A:444:GLY:H	1.98	0.63
1:B:228:GLN:CG	1:C:781:MET:HE1	2.29	0.63
1:C:159:ALA:CA	2:C:1078:HOH:O	1.89	0.63
1:C:465:ALA:O	1:C:469:GLN:HG2	1.99	0.63
1:C:615:PHE:CD2	1:C:615:PHE:O	2.51	0.63
1:B:235:ILE:HD13	1:B:235:ILE:N	2.13	0.63
1:B:452:VAL:O	1:B:453:PHE:CB	2.46	0.63
1:C:598:TYR:CD2	1:C:606:VAL:HG21	2.33	0.63
1:C:924:ASP:C	1:C:925:VAL:O	2.31	0.63
1:A:516:PHE:C	1:A:518:ARG:H	2.00	0.63
1:A:688:ALA:O	1:A:689:GLY:C	2.36	0.63
1:A:968:VAL:HG21	1:A:1023:PRO:CB	2.29	0.63
1:A:983:ILE:HG13	1:A:984:LEU:N	2.14	0.63
1:A:989:LEU:HG	1:A:993:THR:HG23	1.81	0.63
1:B:674:LEU:HD13	1:B:860:THR:CG2	2.28	0.63
1:B:859:TRP:HB3	1:B:863:SER:CB	2.28	0.63
1:C:950:LYS:HZ3	1:C:1030:ARG:CD	2.06	0.63
1:A:255:GLN:CD	1:A:255:GLN:N	2.52	0.63
1:A:1024:VAL:HG12	1:A:1025:PHE:N	2.13	0.63
1:B:613:ASN:ND2	1:B:614:GLY:N	2.46	0.63
1:C:177:LEU:HD13	1:C:179:GLY:C	2.18	0.63
1:C:346:GLU:O	1:C:349:ILE:HB	1.99	0.63
1:B:10:ILE:HG13	1:C:893:GLU:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:GLN:O	1:B:361:ASN:HB2	1.99	0.63
1:C:391:ASN:N	1:C:394:THR:CG2	2.62	0.63
1:B:545:TYR:OH	1:B:906:PRO:HG3	1.99	0.63
1:B:713:LEU:HD12	1:B:713:LEU:N	2.14	0.63
1:C:114:ALA:O	1:C:115:MET:C	2.35	0.63
1:C:221:GLY:O	1:C:222:THR:C	2.37	0.63
1:A:54:ALA:O	1:A:58:GLN:N	2.29	0.62
1:A:73:ASP:CG	1:A:106:GLN:NE2	2.53	0.62
1:B:136:PHE:HA	1:B:292:LYS:HG3	1.81	0.62
1:A:154:ILE:O	1:A:158:VAL:HG23	1.99	0.62
1:A:574:THR:OG1	1:A:627:ALA:HB3	1.99	0.62
1:B:538:THR:HG23	1:B:540:ARG:NH2	2.14	0.62
1:B:775:SER:HB3	1:B:780:ARG:HG3	1.80	0.62
1:B:945:ILE:HD12	1:B:1026:PHE:CE2	2.31	0.62
1:C:204:ILE:HG12	1:C:759:VAL:CG1	2.29	0.62
1:C:274:ASN:CB	2:C:1060:HOH:O	2.20	0.62
1:A:5:PHE:CE1	1:A:12:ALA:HB2	2.33	0.62
1:A:64:VAL:O	1:A:65:ILE:O	2.17	0.62
1:A:756:GLY:CA	1:A:774:MET:HB2	2.29	0.62
1:C:457:ALA:H	1:C:459:PHE:HE2	1.42	0.62
1:A:106:GLN:O	1:A:110:LYS:HB2	1.98	0.62
1:A:298:ASN:C	1:A:298:ASN:ND2	2.52	0.62
1:B:252:LYS:HB3	1:B:260:VAL:CG1	2.30	0.62
1:B:831:ALA:HB3	1:B:840:ALA:HB2	1.80	0.62
1:C:190:PRO:HG3	1:C:789:TRP:CZ2	2.34	0.62
1:C:379:THR:HB	1:C:398:MET:HE3	1.81	0.62
1:B:148:THR:O	1:B:148:THR:HG22	2.00	0.62
1:B:589:LYS:O	1:B:592:ASN:HB2	2.00	0.62
1:B:723:ASP:HA	1:B:814:PRO:HD3	1.81	0.62
1:C:189:ASN:HD22	1:C:190:PRO:N	1.98	0.62
1:C:785:ASP:C	1:C:787:GLY:N	2.51	0.62
1:A:750:LEU:HD11	1:C:216:ALA:HB2	1.82	0.62
1:C:463:THR:HA	1:C:466:ILE:HD13	1.80	0.62
1:C:999:ALA:O	1:C:1003:VAL:HG23	1.99	0.62
1:A:184:MET:HB3	1:A:771:VAL:HG13	1.80	0.62
1:B:699:ARG:HG2	1:B:700:ASN:N	2.14	0.62
1:B:831:ALA:HB2	1:B:840:ALA:HB2	1.82	0.62
1:C:104:GLN:NE2	1:C:131:LYS:HE2	2.15	0.62
1:C:554:TYR:O	1:C:555:LEU:HB2	1.99	0.62
1:C:830:GLN:OE1	1:C:832:ALA:HA	2.00	0.62
1:C:925:VAL:C	1:C:927:PHE:H	2.03	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:H2	1:A:2:PRO:HD2	1.65	0.62
1:A:728:LYS:HG3	1:A:729:ILE:O	2.00	0.62
1:B:534:ILE:HG23	1:B:541:TYR:CZ	2.35	0.62
1:B:852:PRO:HA	1:B:855:VAL:HB	1.80	0.62
1:C:644:VAL:CG1	1:C:667:ASN:HB2	2.30	0.62
1:C:778:LYS:C	1:C:779:TYR:HD2	2.03	0.62
1:A:228:GLN:CG	1:B:781:MET:HG2	2.30	0.62
1:A:719:ASN:HB2	1:A:828:LEU:CD2	2.29	0.62
1:B:407:ASP:C	1:B:408:ASP:O	2.37	0.62
1:C:92:LEU:HD22	1:C:107:VAL:HG22	1.82	0.62
1:C:530:SER:O	1:C:534:ILE:HG23	1.99	0.62
1:C:657:GLN:HB3	1:C:658:ILE:HD12	1.82	0.62
1:C:899:PHE:N	1:C:899:PHE:HD1	1.96	0.62
1:A:113:LEU:CD2	1:C:128:SER:HA	2.27	0.62
1:A:513:PHE:CD1	1:A:517:ASN:ND2	2.63	0.62
1:A:713:LEU:HB3	1:A:831:ALA:O	1.99	0.62
1:B:921:LEU:CD2	1:B:1005:THR:HG22	2.30	0.62
1:C:143:ILE:CG2	1:C:284:GLN:HE22	2.08	0.62
1:C:259:ARG:HH11	1:C:259:ARG:CB	2.13	0.62
1:C:578:LEU:HD22	1:C:661:ALA:CB	2.30	0.62
1:C:703:LEU:O	1:C:706:ALA:HB3	2.00	0.62
1:A:709:HIS:N	1:A:710:PRO:HD3	2.14	0.61
1:C:167:SER:H	1:C:175:VAL:HG21	1.64	0.61
1:C:184:MET:HG2	1:C:246:PHE:CE1	2.35	0.61
1:C:417:GLU:HB3	1:C:973:ARG:HH12	1.64	0.61
1:C:693:GLU:O	1:C:694:LYS:C	2.38	0.61
1:B:49:TYR:HE2	1:B:125:GLN:HB3	1.65	0.61
1:B:978:THR:CG2	1:B:979:SER:N	2.62	0.61
1:C:164:ASP:O	1:C:168:ARG:HG3	1.99	0.61
1:C:345:VAL:O	1:C:348:ILE:HG12	2.00	0.61
1:C:418:ARG:NE	1:C:970:MET:HE2	2.15	0.61
1:A:61:VAL:HG13	1:A:118:LEU:HD13	1.81	0.61
1:A:340:VAL:HG13	1:A:399:VAL:HG21	1.83	0.61
1:A:950:LYS:O	1:A:951:ASP:CB	2.47	0.61
1:B:109:ASN:HD22	1:B:112:GLN:NE2	1.98	0.61
1:B:184:MET:HB3	1:B:771:VAL:HG22	1.82	0.61
1:B:280:GLU:CB	1:B:284:GLN:O	2.48	0.61
1:B:585:GLU:O	1:B:588:GLN:N	2.32	0.61
1:B:673:GLU:OE1	1:B:673:GLU:HA	2.00	0.61
1:C:54:ALA:HB2	1:C:84:SER:CB	2.20	0.61
1:C:344:LEU:HD22	1:C:402:ILE:HD11	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:410:ILE:HG22	1:C:411:VAL:H	1.65	0.61
1:C:607:GLU:HG3	1:C:607:GLU:O	2.00	0.61
1:C:62:THR:HG23	1:C:90:ILE:CD1	2.28	0.61
1:C:305:ALA:O	1:C:309:GLU:N	2.33	0.61
1:C:310:LEU:O	1:C:313:MET:N	2.31	0.61
1:A:44:THR:CG2	1:A:89:GLN:HG3	2.31	0.61
1:A:367:ILE:HG13	1:A:368:PRO:HD3	1.83	0.61
1:A:481:SER:O	1:A:484:VAL:N	2.32	0.61
1:A:909:VAL:HG12	1:A:913:LEU:HD23	1.81	0.61
1:A:950:LYS:HA	1:A:953:MET:HB3	1.80	0.61
1:B:280:GLU:HB2	1:B:284:GLN:O	2.01	0.61
1:B:697:GLN:O	1:B:699:ARG:O	2.18	0.61
1:B:703:LEU:HA	1:B:706:ALA:HB3	1.82	0.61
1:C:115:MET:HE2	1:C:115:MET:HA	1.83	0.61
1:C:600:THR:OG1	1:C:601:LYS:N	2.34	0.61
1:C:705:GLU:O	1:C:707:ALA:N	2.33	0.61
1:A:48:SER:HB2	1:A:125:GLN:HG3	1.83	0.61
1:A:554:TYR:CE1	1:A:558:ARG:HD3	2.36	0.61
1:A:563:PHE:O	1:A:564:LEU:HD12	2.00	0.61
1:B:115:MET:HA	1:B:115:MET:CE	2.30	0.61
1:C:57:VAL:CG1	1:C:88:VAL:CG2	2.79	0.61
1:C:131:LYS:HB2	1:C:295:THR:CG2	2.30	0.61
1:C:431:THR:HG21	1:C:494:ALA:CB	2.28	0.61
1:A:154:ILE:CG2	1:A:287:SER:HB3	2.27	0.61
1:A:544:LEU:O	1:A:547:ILE:HB	2.01	0.61
1:A:897:ILE:N	1:A:898:PRO:HD2	2.15	0.61
1:B:646:ALA:O	1:B:647:ILE:C	2.38	0.61
1:B:975:ILE:H	1:B:975:ILE:HD12	1.65	0.61
1:B:7:ASP:C	1:B:8:ARG:HD2	2.21	0.61
1:B:187:TRP:O	1:B:266:ALA:HA	2.01	0.61
1:C:161:ASN:N	1:C:164:ASP:OD2	2.34	0.61
1:C:911:GLY:CA	1:C:1013:THR:HG21	2.31	0.61
1:A:324:VAL:HG12	1:A:325:TYR:N	2.15	0.61
1:B:143:ILE:HD12	1:B:322:LYS:HB3	1.83	0.61
1:B:310:LEU:O	1:B:314:GLU:HG3	2.01	0.61
1:B:517:ASN:C	1:B:521:GLU:HG3	2.22	0.61
1:B:709:HIS:N	1:B:710:PRO:HD3	2.15	0.61
1:B:775:SER:HB3	1:B:780:ARG:CD	2.30	0.61
1:C:160:ALA:C	1:C:164:ASP:OD2	2.39	0.61
1:C:453:PHE:O	1:C:456:MET:HG2	2.00	0.61
1:A:171:GLY:O	1:A:172:VAL:C	2.39	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:ARG:HH12	1:A:973:ARG:HB3	1.65	0.60
1:B:235:ILE:N	1:B:235:ILE:CD1	2.64	0.60
1:C:254:ASN:OD1	1:C:258:SER:O	2.19	0.60
1:C:368:PRO:HG3	1:C:413:VAL:HG11	1.82	0.60
1:C:554:TYR:HD1	1:C:558:ARG:HH21	1.42	0.60
1:C:688:ALA:C	1:C:690:LEU:H	2.04	0.60
1:C:699:ARG:HG2	1:C:825:MET:HE1	1.82	0.60
1:C:851:LEU:HD12	1:C:851:LEU:N	2.16	0.60
1:C:908:GLY:HA2	1:C:1014:ALA:HB2	1.81	0.60
1:A:323:ILE:HG12	1:A:325:TYR:HE1	1.65	0.60
1:A:713:LEU:O	1:A:714:THR:CG2	2.44	0.60
1:B:143:ILE:HG23	1:B:286:ALA:HB2	1.84	0.60
1:B:157:TYR:C	1:B:161:ASN:HD22	2.04	0.60
1:B:219:LEU:CD2	1:C:783:PRO:HG3	2.31	0.60
1:B:314:GLU:HB2	1:B:315:PRO:HD3	1.82	0.60
1:B:543:VAL:O	1:B:547:ILE:CD1	2.49	0.60
1:C:2:PRO:O	1:C:6:ILE:HG13	2.00	0.60
1:A:58:GLN:HG3	1:A:63:GLN:HE22	1.66	0.60
1:A:391:ASN:H	1:A:394:THR:HG22	1.65	0.60
1:A:857:TYR:C	1:A:857:TYR:CD1	2.73	0.60
1:C:615:PHE:O	1:C:615:PHE:HD2	1.84	0.60
1:C:657:GLN:C	1:C:659:LYS:H	2.04	0.60
1:A:51:GLY:O	1:C:215:ALA:HB1	2.01	0.60
1:A:643:LYS:O	1:A:647:ILE:HG13	2.01	0.60
1:A:719:ASN:C	1:A:719:ASN:ND2	2.49	0.60
1:C:57:VAL:HG12	1:C:88:VAL:CG2	2.31	0.60
1:C:266:ALA:O	1:C:267:LYS:C	2.40	0.60
1:C:576:VAL:HG21	1:C:591:LEU:HD22	1.83	0.60
1:C:942:ALA:HA	1:C:945:ILE:HG22	1.84	0.60
1:A:108:GLN:CB	1:A:108:GLN:CD	2.66	0.60
1:B:591:LEU:CD1	1:B:611:ALA:HB1	2.31	0.60
1:C:552:MET:CE	1:C:909:VAL:HG21	2.31	0.60
1:A:246:PHE:O	1:A:249:ILE:CD1	2.49	0.60
1:A:905:VAL:O	1:A:909:VAL:HG23	2.00	0.60
1:C:10:ILE:HG22	1:C:10:ILE:O	2.00	0.60
1:C:291:ILE:O	1:C:291:ILE:HG22	1.99	0.60
1:C:560:PRO:O	1:C:922:THR:HG22	2.01	0.60
1:C:897:ILE:HG12	1:C:950:LYS:HE3	1.82	0.60
1:A:10:ILE:HD11	1:B:895:TRP:CB	2.29	0.60
1:A:425:LEU:HB3	1:A:426:PRO:HD2	1.82	0.60
1:C:663:VAL:O	1:C:664:PHE:HB3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1024:VAL:HG12	1:C:1028:VAL:CG2	2.32	0.60
1:A:758:TYR:O	1:A:758:TYR:CG	2.55	0.60
1:B:574:THR:HG23	1:B:665:ALA:CB	2.22	0.60
1:B:808:ARG:CB	1:B:808:ARG:HH21	2.15	0.60
1:C:485:ALA:O	1:C:490:PRO:HD3	2.02	0.60
1:C:933:THR:O	1:C:937:LEU:HB2	2.02	0.60
1:A:171:GLY:O	1:A:294:ALA:HB2	2.02	0.60
1:A:540:ARG:HD2	1:A:541:TYR:CE2	2.37	0.60
1:A:583:THR:HG22	1:A:585:GLU:N	2.17	0.60
1:A:728:LYS:HD2	1:C:235:ILE:HG22	1.84	0.60
1:A:827:ILE:N	1:A:827:ILE:HD12	2.16	0.60
1:A:952:LEU:HD12	1:A:953:MET:N	2.17	0.60
1:C:236:ALA:O	1:C:237:GLN:C	2.40	0.60
1:C:308:ALA:O	1:C:311:ALA:HB3	2.02	0.60
1:C:758:TYR:HB3	1:C:772:TYR:CE2	2.36	0.60
1:C:790:TYR:CD1	1:C:800:PRO:HB3	2.37	0.60
1:A:17:ILE:HG22	1:A:21:LEU:CD2	2.31	0.60
1:A:54:ALA:HB1	1:A:816:LEU:CG	2.24	0.60
1:A:699:ARG:NH2	1:A:722:GLU:OE1	2.35	0.60
1:B:3:ASN:N	1:B:6:ILE:HG12	2.13	0.60
1:B:207:ILE:HG21	1:B:759:VAL:HG11	1.82	0.60
1:B:418:ARG:HH21	1:B:970:MET:CG	2.14	0.60
1:C:684:LEU:HD11	1:C:855:VAL:CG1	2.32	0.60
1:A:196:PHE:O	1:A:197:GLN:HB2	2.03	0.59
1:A:528:THR:CG2	1:A:969:ARG:HE	2.10	0.59
1:B:214:VAL:HG21	1:C:747:ASN:ND2	2.16	0.59
1:B:623:ASN:C	1:B:623:ASN:ND2	2.53	0.59
1:C:166:ILE:O	1:C:172:VAL:HG11	2.02	0.59
1:C:590:VAL:O	1:C:592:ASN:O	2.20	0.59
1:A:68:ASN:N	1:A:68:ASN:CB	2.65	0.59
1:B:346:GLU:OE1	1:B:988:PRO:CB	2.48	0.59
1:B:431:THR:HG21	1:B:493:CYS:HB2	1.84	0.59
1:B:560:PRO:CB	1:B:836:SER:HB3	2.32	0.59
1:B:776:GLU:HG2	1:B:777:ALA:N	2.17	0.59
1:B:952:LEU:HA	1:B:956:GLU:OE2	2.02	0.59
1:C:140:VAL:O	1:C:288:GLY:HA3	2.02	0.59
1:C:200:PRO:HG2	1:C:749:THR:HA	1.83	0.59
1:C:211:ASN:C	1:C:211:ASN:HD22	2.05	0.59
1:C:540:ARG:HE	1:C:541:TYR:HE1	1.47	0.59
1:C:886:LEU:O	1:C:890:ALA:HB2	2.02	0.59
1:C:911:GLY:HA3	1:C:1013:THR:CG2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:912:ALA:C	1:C:914:LEU:H	2.04	0.59
1:A:26:ALA:O	1:A:30:LEU:HG	2.02	0.59
1:A:795:ASP:OD1	1:A:797:GLN:HG2	2.03	0.59
1:B:692:HIS:O	1:B:693:GLU:HG3	2.02	0.59
1:B:907:LEU:O	1:B:909:VAL:N	2.35	0.59
1:B:975:ILE:HD12	1:B:975:ILE:N	2.17	0.59
1:C:847:LEU:O	1:C:850:LYS:HG2	2.03	0.59
1:A:10:ILE:CD1	1:B:895:TRP:HB2	2.29	0.59
1:A:269:GLU:HG3	1:A:270:LEU:O	2.03	0.59
1:A:321:LEU:CD1	2:A:1061:HOH:O	2.49	0.59
1:A:548:ILE:CG2	1:A:910:ILE:HG12	2.32	0.59
1:A:571:VAL:CG1	1:A:630:SER:HA	2.30	0.59
1:B:281:PHE:CE2	1:B:324:VAL:HG11	2.37	0.59
1:B:330:THR:H	1:B:331:PRO:CD	2.14	0.59
1:C:84:SER:C	1:C:86:GLY:N	2.56	0.59
1:C:262:LEU:CD2	1:C:268:ILE:HD11	2.33	0.59
1:C:352:PHE:HA	1:C:369:THR:CG2	2.33	0.59
1:A:115:MET:C	1:A:117:LEU:N	2.56	0.59
1:A:166:ILE:O	1:A:168:ARG:N	2.36	0.59
1:A:223:PRO:HD3	1:B:275:TYR:HB2	1.84	0.59
1:A:435:MET:HA	1:A:438:ILE:CD1	2.32	0.59
1:B:568:ASP:O	1:B:634:TRP:CH2	2.55	0.59
1:B:754:TRP:CZ2	1:B:786:ILE:HG12	2.37	0.59
1:C:14:VAL:HG13	1:C:15:ILE:H	1.66	0.59
1:C:72:ILE:CG2	1:C:94:PHE:CE2	2.83	0.59
1:C:951:ASP:C	1:C:953:MET:N	2.48	0.59
1:A:576:VAL:HG11	1:A:591:LEU:HD23	1.84	0.59
1:A:644:VAL:C	1:A:646:ALA:H	2.06	0.59
1:A:687:GLN:HB3	1:A:854:GLY:O	2.03	0.59
1:B:99:ASP:C	1:B:99:ASP:OD2	2.39	0.59
1:B:371:ALA:HA	1:B:374:VAL:HG12	1.84	0.59
1:B:563:PHE:HB2	1:B:866:GLU:HG2	1.85	0.59
1:B:980:LEU:HD23	1:B:983:ILE:HD12	1.83	0.59
1:B:1024:VAL:HG12	1:B:1028:VAL:HG21	1.84	0.59
1:C:185:ARG:HD3	1:C:272:GLY:O	2.01	0.59
1:A:49:TYR:HE2	1:A:121:GLU:HG2	1.68	0.59
1:A:166:ILE:O	1:A:169:THR:HG23	2.03	0.59
1:A:282:ASN:ND2	1:A:609:VAL:H	2.00	0.59
1:A:534:ILE:HD12	1:A:540:ARG:HH22	1.68	0.59
1:A:886:LEU:HD21	1:C:17:ILE:CG2	2.31	0.59
1:B:196:PHE:O	1:B:197:GLN:HB2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1024:VAL:O	1:B:1025:PHE:HB2	2.03	0.59
1:C:94:PHE:O	1:C:95:GLU:O	2.20	0.59
1:C:414:GLU:OE2	1:C:977:MET:SD	2.61	0.59
1:A:30:LEU:HD21	1:A:384:ALA:HB2	1.85	0.59
1:A:90:ILE:O	1:A:90:ILE:CG2	2.50	0.59
1:A:467:TYR:HE1	1:A:925:VAL:CG2	2.15	0.59
1:A:857:TYR:CD1	1:A:857:TYR:O	2.55	0.59
1:B:6:ILE:HD12	1:B:491:ALA:N	2.17	0.59
1:B:606:VAL:HA	1:B:631:LEU:HD23	1.84	0.59
1:B:652:THR:O	1:B:656:SER:HB3	2.02	0.59
1:B:860:THR:CG2	1:B:861:GLY:N	2.66	0.59
1:C:60:THR:HG23	1:C:60:THR:O	2.00	0.59
1:C:459:PHE:O	1:C:460:GLY:O	2.19	0.59
1:C:547:ILE:O	1:C:550:VAL:HG12	2.03	0.59
1:C:925:VAL:O	1:C:927:PHE:N	2.35	0.59
1:C:972:LEU:N	1:C:974:PRO:HD2	2.17	0.59
1:A:193:LEU:HD12	1:A:265:VAL:CG1	2.32	0.59
1:A:709:HIS:H	1:A:710:PRO:HD3	1.68	0.59
1:B:231:ASN:C	1:B:231:ASN:HD22	2.06	0.59
1:A:5:PHE:HD1	1:A:12:ALA:HB2	1.64	0.58
1:A:702:LEU:HD11	1:A:844:MET:CE	2.32	0.58
1:A:855:VAL:O	1:A:855:VAL:CG2	2.51	0.58
1:A:961:ILE:O	1:A:965:LEU:HD23	2.02	0.58
1:B:876:LEU:CD1	1:B:932:LEU:HD11	2.27	0.58
1:B:986:VAL:HG12	1:B:990:VAL:HG23	1.85	0.58
1:C:545:TYR:HH	1:C:1021:PHE:CB	2.16	0.58
1:C:553:ALA:O	1:C:557:VAL:HG23	2.03	0.58
1:C:907:LEU:O	1:C:910:ILE:HG22	2.03	0.58
1:C:919:ARG:HB3	1:C:921:LEU:HD23	1.83	0.58
1:C:987:MET:HB3	1:C:988:PRO:CD	2.33	0.58
1:A:185:ARG:O	1:A:186:ILE:HG13	2.02	0.58
1:A:277:ILE:O	1:A:277:ILE:CG2	2.43	0.58
1:B:851:LEU:N	1:B:852:PRO:CD	2.65	0.58
1:B:921:LEU:HD23	1:B:1005:THR:O	2.03	0.58
1:A:375:VAL:O	1:A:379:THR:HG23	2.02	0.58
1:B:48:SER:N	1:B:49:TYR:CE1	2.62	0.58
1:B:80:SER:HB2	1:B:90:ILE:HG23	1.84	0.58
1:C:15:ILE:O	1:C:16:ALA:C	2.41	0.58
1:C:91:THR:CB	1:C:91:THR:C	2.68	0.58
1:C:162:MET:CG	1:C:313:MET:HE2	2.24	0.58
1:C:726:GLN:NE2	1:C:812:GLY:HA3	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:TRP:O	1:A:17:ILE:HG13	2.03	0.58
1:A:124:GLN:HG2	1:A:758:TYR:HE2	1.67	0.58
1:A:190:PRO:HG3	1:A:789:TRP:CZ2	2.38	0.58
1:B:13:TRP:HA	1:B:13:TRP:CE3	2.37	0.58
1:B:200:PRO:CD	1:B:749:THR:HG22	2.30	0.58
1:B:472:ILE:HG23	1:B:473:THR:H	1.68	0.58
1:C:181:GLN:OE1	1:C:767:ARG:NH2	2.37	0.58
1:A:685:ILE:HG22	1:A:687:GLN:N	2.18	0.58
1:B:456:MET:HA	1:B:876:LEU:HD21	1.86	0.58
1:B:842:GLU:O	1:B:846:GLN:HG3	2.04	0.58
1:C:327:TYR:CB	1:C:628:PHE:HB3	2.33	0.58
1:C:786:ILE:O	1:C:786:ILE:CG2	2.51	0.58
1:C:847:LEU:HD22	1:C:847:LEU:H	1.69	0.58
1:A:1:MET:N	1:A:2:PRO:CD	2.66	0.58
1:A:60:THR:HG22	1:A:119:PRO:CD	2.33	0.58
1:A:135:SER:O	1:A:136:PHE:CD2	2.56	0.58
1:B:328:ASP:CB	2:B:1059:HOH:O	2.48	0.58
1:B:646:ALA:C	1:B:648:THR:H	2.05	0.58
1:C:414:GLU:OE1	1:C:977:MET:HE1	2.03	0.58
1:A:69:MET:HA	1:A:69:MET:HE2	1.84	0.58
1:A:780:ARG:HG2	1:A:780:ARG:HH11	1.68	0.58
1:B:30:LEU:HD23	1:B:390:ILE:HG13	1.85	0.58
1:B:230:LEU:HD21	1:C:809:TRP:HH2	1.64	0.58
1:B:309:GLU:O	1:B:312:LYS:N	2.36	0.58
1:B:601:LYS:C	1:B:603:LYS:H	2.07	0.58
1:C:844:MET:HA	1:C:847:LEU:CD2	2.34	0.58
1:A:528:THR:O	1:A:532:GLY:N	2.35	0.58
1:A:588:GLN:HG2	1:A:613:ASN:ND2	2.19	0.58
1:B:602:GLU:C	1:B:604:ASN:H	2.06	0.58
1:C:762:PHE:H	1:C:771:VAL:CG2	2.17	0.58
1:A:463:THR:O	1:A:465:ALA:N	2.36	0.58
1:B:219:LEU:CD1	1:B:234:ILE:HG12	2.33	0.58
1:B:420:MET:HE2	1:B:425:LEU:HA	1.86	0.58
1:C:102:ILE:HG22	1:C:103:ALA:N	2.13	0.58
1:C:928:GLN:N	1:C:928:GLN:OE1	2.37	0.58
1:A:292:LYS:O	1:A:293:LEU:O	2.22	0.58
1:A:488:LEU:O	1:A:492:LEU:HB2	2.04	0.58
1:B:419:VAL:O	1:B:426:PRO:HG3	2.04	0.58
1:B:850:LYS:C	1:B:852:PRO:HD3	2.24	0.58
1:B:975:ILE:H	1:B:975:ILE:CD1	2.17	0.58
1:C:169:THR:O	1:C:170:SER:C	2.42	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:497:LEU:CD1	1:C:498:LYS:H	2.17	0.58
1:C:686:ASP:CG	1:C:690:LEU:HB2	2.23	0.58
1:C:1028:VAL:HG12	1:C:1032:ARG:NH1	2.18	0.58
1:B:369:THR:O	1:B:373:PRO:HD3	2.04	0.57
1:B:403:GLY:O	1:B:404:LEU:HD23	2.04	0.57
1:B:531:VAL:CG1	1:B:965:LEU:HD21	2.34	0.57
1:B:644:VAL:HG23	1:B:645:GLU:N	2.18	0.57
1:B:911:GLY:CA	1:B:1013:THR:HG21	2.30	0.57
1:C:185:ARG:HG3	1:C:271:GLY:CA	2.32	0.57
1:C:489:THR:N	1:C:490:PRO:HD2	2.18	0.57
1:A:164:ASP:OD1	1:A:164:ASP:N	2.35	0.57
1:A:401:ALA:HB2	1:A:474:ILE:HG12	1.86	0.57
1:A:1021:PHE:O	1:A:1024:VAL:HB	2.04	0.57
1:B:24:GLY:HA2	1:B:27:ILE:HG23	1.85	0.57
1:B:472:ILE:HG23	1:B:473:THR:N	2.20	0.57
1:C:220:GLY:CA	1:C:231:ASN:HD22	2.15	0.57
1:C:277:ILE:HD11	1:C:620:ARG:NH2	2.18	0.57
1:C:719:ASN:OD1	1:C:719:ASN:N	2.37	0.57
1:C:832:ALA:HB1	1:C:833:PRO:HD2	1.85	0.57
1:C:885:PHE:CD1	1:C:886:LEU:N	2.72	0.57
1:B:485:ALA:HA	1:B:489:THR:HB	1.86	0.57
1:C:314:GLU:O	1:C:317:PHE:CE2	2.57	0.57
1:C:399:VAL:HA	1:C:402:ILE:HD11	1.84	0.57
1:C:685:ILE:HD11	1:C:687:GLN:CA	2.33	0.57
1:C:721:LEU:HD12	1:C:815:ARG:O	2.04	0.57
1:A:139:VAL:O	1:A:139:VAL:HG22	2.04	0.57
1:A:600:THR:O	1:A:601:LYS:HB2	2.05	0.57
1:A:843:LEU:HA	1:A:846:GLN:HE21	1.66	0.57
1:B:115:MET:CE	1:B:127:VAL:HG21	2.32	0.57
1:C:66:GLU:OE2	1:C:818:ARG:HD3	2.05	0.57
1:A:182:TYR:HB3	1:A:270:LEU:HD12	1.85	0.57
1:A:194:ASN:ND2	1:A:790:TYR:CD2	2.72	0.57
1:B:65:ILE:HD11	1:B:118:LEU:HD21	1.87	0.57
1:B:211:ASN:ND2	1:B:246:PHE:CZ	2.71	0.57
1:B:531:VAL:HA	1:B:534:ILE:HG12	1.86	0.57
1:B:640:GLU:OE2	1:B:640:GLU:N	2.38	0.57
1:B:873:ALA:C	1:B:875:SER:H	2.08	0.57
1:B:873:ALA:O	1:B:875:SER:N	2.36	0.57
1:C:57:VAL:O	1:C:61:VAL:HB	2.03	0.57
1:C:831:ALA:HB2	1:C:840:ALA:HB2	1.85	0.57
1:A:318:PRO:O	1:A:319:SER:C	2.42	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:644:VAL:C	1:A:646:ALA:N	2.58	0.57
1:A:655:PHE:C	1:A:656:SER:O	2.41	0.57
1:B:49:TYR:CE2	1:B:122:VAL:HA	2.40	0.57
1:B:663:VAL:O	1:B:663:VAL:HG12	2.05	0.57
1:C:124:GLN:HB3	1:C:758:TYR:HE2	1.68	0.57
1:A:822:LEU:CB	1:A:823:PRO:HD2	2.22	0.57
1:A:911:GLY:N	1:A:914:LEU:HD13	2.19	0.57
1:B:940:LYS:HZ1	1:B:978:THR:HG23	1.69	0.57
1:C:105:VAL:HG12	1:C:106:GLN:N	2.18	0.57
1:A:345:VAL:O	1:A:349:ILE:HD13	2.05	0.57
1:B:622:GLN:CG	1:B:622:GLN:O	2.53	0.57
1:C:214:VAL:HG12	1:C:215:ALA:H	1.67	0.57
1:C:548:ILE:HD12	1:C:549:VAL:H	1.67	0.57
1:A:188:MET:HA	1:A:266:ALA:HB2	1.86	0.57
1:A:228:GLN:HG2	1:B:781:MET:SD	2.45	0.57
1:A:983:ILE:C	1:A:983:ILE:HD12	2.24	0.57
1:B:847:LEU:HD23	1:B:847:LEU:H	1.69	0.57
1:B:910:ILE:O	1:B:914:LEU:HG	2.05	0.57
1:B:1013:THR:HG23	1:B:1013:THR:O	2.05	0.57
1:C:50:PRO:HD3	1:C:125:GLN:HG3	1.86	0.57
1:C:92:LEU:N	1:C:92:LEU:HD12	2.19	0.57
1:A:45:ILE:HB	1:A:90:ILE:HB	1.86	0.57
1:A:583:THR:O	1:A:584:GLN:C	2.43	0.57
1:A:907:LEU:O	1:A:910:ILE:HG13	2.05	0.57
1:A:927:PHE:CE2	1:A:931:LEU:HD22	2.39	0.57
1:B:57:VAL:HG23	1:B:58:GLN:H	1.68	0.57
1:B:431:THR:CG2	1:B:493:CYS:CB	2.74	0.57
1:B:439:GLN:HA	1:B:442:LEU:CD1	2.34	0.57
1:B:945:ILE:HD11	1:B:1026:PHE:CE2	2.39	0.57
1:B:966:ASP:O	1:B:970:MET:HB2	2.04	0.57
1:B:1015:THR:O	1:B:1018:ALA:HB3	2.05	0.57
1:C:549:VAL:C	1:C:551:GLY:N	2.56	0.57
1:C:644:VAL:HG11	1:C:667:ASN:HB2	1.87	0.57
1:C:699:ARG:CD	1:C:703:LEU:HD11	2.32	0.57
1:A:170:SER:O	1:A:170:SER:OG	2.23	0.56
1:A:325:TYR:N	1:A:325:TYR:CD1	2.70	0.56
1:A:649:MET:O	1:A:653:ARG:NE	2.37	0.56
1:B:193:LEU:HD22	1:B:198:LEU:O	2.05	0.56
1:B:210:GLN:HG3	1:B:249:ILE:HG23	1.86	0.56
1:B:845:GLU:HG2	1:B:857:TYR:OH	2.03	0.56
1:C:189:ASN:HD22	1:C:189:ASN:C	2.08	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:GLN:O	1:C:230:LEU:HB3	2.05	0.56
1:C:699:ARG:CG	1:C:699:ARG:NH1	2.42	0.56
1:A:282:ASN:ND2	1:A:599:LEU:HD11	2.20	0.56
1:A:926:TYR:CE1	1:A:999:ALA:HB2	2.39	0.56
1:B:651:ALA:O	1:B:655:PHE:CE2	2.58	0.56
1:B:785:ASP:O	1:B:787:GLY:N	2.38	0.56
1:C:897:ILE:N	1:C:898:PRO:HD2	2.20	0.56
1:A:11:PHE:O	1:A:14:VAL:N	2.38	0.56
1:A:162:MET:CE	1:A:310:LEU:HD22	2.36	0.56
1:A:191:ASN:C	1:A:193:LEU:H	2.07	0.56
1:A:191:ASN:O	1:A:193:LEU:N	2.39	0.56
1:A:252:LYS:HB3	1:A:260:VAL:HG21	1.87	0.56
1:A:400:LEU:HG	1:A:929:VAL:HG12	1.87	0.56
1:A:516:PHE:CD1	1:A:517:ASN:N	2.73	0.56
1:B:221:GLY:HA3	1:C:780:ARG:HH11	1.71	0.56
1:B:585:GLU:O	1:B:586:ARG:C	2.42	0.56
1:B:913:LEU:O	1:B:917:THR:OG1	2.19	0.56
1:B:941:ASN:HD22	1:B:1015:THR:HA	1.70	0.56
1:C:58:GLN:OE1	1:C:82:SER:CB	2.54	0.56
1:C:123:GLN:O	1:C:125:GLN:N	2.37	0.56
1:C:311:ALA:O	1:C:313:MET:N	2.39	0.56
1:C:418:ARG:C	1:C:420:MET:N	2.50	0.56
1:C:527:TYR:OH	1:C:1019:ILE:HG13	2.05	0.56
1:C:988:PRO:O	1:C:989:LEU:C	2.43	0.56
1:A:298:ASN:HB3	1:A:301:ASP:OD1	2.05	0.56
1:A:394:THR:HG23	1:A:395:MET:HE2	1.88	0.56
1:A:726:GLN:N	1:A:810:GLU:O	2.38	0.56
1:B:639:GLY:HA2	1:B:643:LYS:NZ	2.20	0.56
1:C:274:ASN:ND2	2:C:1057:HOH:O	2.26	0.56
1:C:379:THR:CG2	1:C:477:ALA:HB2	2.36	0.56
1:C:601:LYS:O	1:C:603:LYS:N	2.37	0.56
1:C:912:ALA:C	1:C:914:LEU:N	2.59	0.56
1:A:60:THR:CG2	1:A:119:PRO:HG3	2.34	0.56
1:A:223:PRO:HD3	1:B:275:TYR:CG	2.39	0.56
1:A:400:LEU:HD11	1:A:1003:VAL:HG13	1.80	0.56
1:A:428:LYS:HG3	1:A:429:GLU:N	2.20	0.56
1:A:456:MET:O	1:A:457:ALA:HB3	2.05	0.56
1:A:911:GLY:HA2	1:A:914:LEU:HD13	1.86	0.56
1:B:571:VAL:O	1:B:572:PHE:HB3	2.05	0.56
1:C:391:ASN:O	1:C:392:THR:C	2.44	0.56
1:C:764:ASP:OD2	1:C:765:ARG:CD	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:953:MET:HE1	1:C:1030:ARG:NH2	2.21	0.56
1:A:263:ARG:NH2	1:A:263:ARG:HB3	2.20	0.56
1:A:268:ILE:N	1:A:268:ILE:HD12	2.20	0.56
1:A:530:SER:O	1:A:534:ILE:HG12	2.06	0.56
1:A:717:ARG:NH1	1:A:830:GLN:HE22	2.02	0.56
1:B:47:ALA:HB3	1:B:88:VAL:CB	2.31	0.56
1:C:5:PHE:CE2	1:C:11:PHE:HD2	2.22	0.56
1:C:5:PHE:CD2	1:C:12:ALA:HB2	2.41	0.56
1:C:56:THR:O	1:C:60:THR:HB	2.06	0.56
1:C:91:THR:CA	1:C:91:THR:CG2	2.76	0.56
1:C:306:ILE:O	1:C:309:GLU:N	2.38	0.56
1:C:697:GLN:O	1:C:698:ALA:C	2.41	0.56
1:C:764:ASP:CG	1:C:765:ARG:HD2	2.24	0.56
1:C:868:LEU:O	1:C:869:SER:HB3	2.06	0.56
1:A:102:ILE:O	1:A:102:ILE:HG23	2.01	0.56
1:A:169:THR:O	1:A:172:VAL:HG22	2.06	0.56
1:A:199:THR:HB	1:A:200:PRO:CD	2.35	0.56
1:A:897:ILE:O	1:A:900:SER:OG	2.20	0.56
1:B:48:SER:HA	1:B:87:THR:HA	1.86	0.56
1:B:370:ILE:HG22	1:B:370:ILE:O	2.05	0.56
1:C:62:THR:HG21	1:C:80:SER:HB3	1.88	0.56
1:C:409:ALA:O	1:C:413:VAL:HG12	2.04	0.56
1:C:427:PRO:O	1:C:431:THR:HG22	2.06	0.56
1:A:594:VAL:HA	1:A:655:PHE:CE2	2.41	0.56
1:A:687:GLN:HE22	1:A:856:GLY:HA3	1.70	0.56
1:A:690:LEU:HD11	1:A:854:GLY:C	2.26	0.56
1:A:901:VAL:HG13	1:A:942:ALA:HB3	1.87	0.56
1:A:911:GLY:HA3	1:A:1013:THR:CG2	2.32	0.56
1:B:25:LEU:C	1:B:27:ILE:H	2.09	0.56
1:B:104:GLN:CG	1:B:105:VAL:H	2.18	0.56
1:B:110:LYS:O	1:B:111:LEU:C	2.40	0.56
1:B:441:ALA:CB	1:B:947:GLU:HG2	2.13	0.56
1:B:591:LEU:HD12	1:B:611:ALA:HB1	1.87	0.56
1:B:681:ASP:O	1:B:859:TRP:HE3	1.88	0.56
1:B:701:GLN:HA	1:B:704:ALA:HB3	1.88	0.56
1:B:942:ALA:HA	1:B:1022:VAL:HG11	1.88	0.56
1:B:1026:PHE:HB3	1:B:1030:ARG:NH2	2.21	0.56
1:A:255:GLN:O	1:A:256:ASP:CG	2.43	0.56
1:A:731:ILE:N	1:A:731:ILE:CD1	2.69	0.56
1:B:186:ILE:HD13	1:B:262:LEU:HD13	1.88	0.56
1:B:905:VAL:N	1:B:906:PRO:HD2	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1024:VAL:HG12	1:B:1025:PHE:N	2.21	0.56
1:C:102:ILE:HG22	1:C:106:GLN:HG3	1.88	0.56
1:A:188:MET:HA	1:A:266:ALA:CB	2.36	0.56
1:A:418:ARG:HH12	1:A:973:ARG:CB	2.18	0.56
1:B:71:GLY:O	1:B:72:ILE:O	2.24	0.56
1:B:278:ILE:HD11	1:B:584:GLN:NE2	2.20	0.56
1:B:987:MET:CE	1:B:987:MET:CA	2.82	0.56
1:C:3:ASN:HD21	1:C:432:ARG:CD	2.15	0.56
1:C:169:THR:CA	1:C:169:THR:CG2	2.79	0.56
1:C:894:SER:O	1:C:896:SER:N	2.39	0.56
1:C:950:LYS:H	1:C:953:MET:CE	2.13	0.56
1:A:99:ASP:OD1	1:A:101:ASP:HB2	2.06	0.55
1:A:818:ARG:CG	2:A:1062:HOH:O	2.54	0.55
1:A:945:ILE:CG1	1:A:971:ARG:HG2	2.22	0.55
1:B:216:ALA:HB2	1:B:236:ALA:HB2	1.88	0.55
1:B:535:LEU:O	1:B:536:ARG:C	2.45	0.55
1:B:557:VAL:O	1:B:557:VAL:HG12	2.06	0.55
1:B:632:LYS:O	1:B:637:ARG:HD2	2.05	0.55
1:B:899:PHE:O	1:B:903:LEU:HG	2.06	0.55
1:C:615:PHE:CD2	1:C:615:PHE:C	2.79	0.55
1:C:847:LEU:CA	1:C:850:LYS:HD3	2.20	0.55
1:A:298:ASN:ND2	1:A:300:LEU:N	2.49	0.55
1:A:686:ASP:C	1:A:688:ALA:H	2.08	0.55
1:A:699:ARG:NH1	1:A:722:GLU:OE1	2.36	0.55
1:B:146:ASP:O	1:B:148:THR:N	2.39	0.55
1:B:419:VAL:O	1:B:419:VAL:HG12	2.06	0.55
1:B:699:ARG:O	1:B:701:GLN:N	2.38	0.55
1:B:737:GLN:O	1:B:737:GLN:HG2	2.06	0.55
1:B:1027:VAL:O	1:B:1030:ARG:O	2.24	0.55
1:C:415:ASN:HA	1:C:418:ARG:NH1	2.21	0.55
1:C:525:HIS:O	1:C:529:ASP:N	2.38	0.55
1:A:169:THR:O	1:A:170:SER:C	2.43	0.55
1:A:961:ILE:O	1:A:965:LEU:CD2	2.54	0.55
1:B:71:GLY:O	1:B:72:ILE:C	2.44	0.55
1:B:325:TYR:O	1:B:326:PRO:O	2.25	0.55
1:C:169:THR:CB	1:C:169:THR:N	2.62	0.55
1:C:192:GLU:O	1:C:194:ASN:N	2.39	0.55
1:C:457:ALA:HB1	1:C:468:ARG:CA	2.35	0.55
1:C:910:ILE:HG23	1:C:911:GLY:N	2.22	0.55
1:A:200:PRO:CD	1:A:749:THR:HG23	2.37	0.55
1:A:367:ILE:HG13	1:A:368:PRO:CD	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:485:ALA:HA	1:B:489:THR:CB	2.35	0.55
1:B:544:LEU:HD22	1:B:1021:PHE:HZ	1.72	0.55
1:B:743:ILE:HA	1:B:746:ILE:HD12	1.88	0.55
1:B:975:ILE:O	1:B:979:SER:HB2	2.07	0.55
1:A:29:LYS:HG2	1:A:29:LYS:O	2.07	0.55
1:A:325:TYR:N	1:A:325:TYR:HD1	2.04	0.55
1:A:400:LEU:HG	1:A:929:VAL:CG1	2.36	0.55
1:B:2:PRO:C	1:B:4:PHE:H	2.08	0.55
1:B:713:LEU:HD13	1:B:843:LEU:HD13	1.88	0.55
1:B:941:ASN:ND2	1:B:1015:THR:HA	2.21	0.55
1:A:47:ALA:HB2	1:A:127:VAL:HG22	1.88	0.55
1:A:548:ILE:HG23	1:A:910:ILE:HG12	1.87	0.55
1:A:901:VAL:HG13	1:A:942:ALA:CB	2.37	0.55
1:B:165:ALA:O	1:B:166:ILE:C	2.45	0.55
1:B:335:ILE:HG22	1:B:336:SER:N	2.20	0.55
1:B:356:TYR:O	1:B:358:PHE:N	2.39	0.55
1:B:545:TYR:O	1:B:547:ILE:N	2.40	0.55
1:B:785:ASP:O	1:B:786:ILE:C	2.44	0.55
1:B:807:SER:C	1:B:808:ARG:HG3	2.27	0.55
1:B:986:VAL:O	1:B:988:PRO:O	2.24	0.55
1:C:190:PRO:O	1:C:192:GLU:N	2.39	0.55
1:C:598:TYR:HB3	1:C:606:VAL:HG11	1.88	0.55
1:C:742:SER:O	1:C:746:ILE:HG13	2.07	0.55
1:C:819:TYR:O	1:C:820:ASN:HB2	2.05	0.55
1:C:824:SER:O	1:C:825:MET:HG2	2.06	0.55
1:A:513:PHE:HD1	1:A:517:ASN:HD21	1.55	0.55
1:A:717:ARG:NH2	1:A:828:LEU:HG	2.22	0.55
1:A:1009:GLY:C	1:A:1011:MET:H	2.07	0.55
1:B:493:CYS:O	1:B:494:ALA:CB	2.46	0.55
1:B:674:LEU:HD22	1:B:681:ASP:OD2	2.06	0.55
1:B:898:PRO:O	1:B:900:SER:N	2.40	0.55
1:C:767:ARG:O	1:C:769:LYS:HG2	2.07	0.55
1:A:68:ASN:N	1:A:69:MET:N	2.54	0.55
1:A:815:ARG:HD2	2:A:1068:HOH:O	2.06	0.55
1:B:707:ALA:O	1:B:708:LYS:CB	2.51	0.55
1:B:947:GLU:O	1:B:951:ASP:HB2	2.06	0.55
1:C:383:LEU:HD11	1:C:394:THR:OG1	2.07	0.55
1:C:533:GLY:O	1:C:536:ARG:HB2	2.07	0.55
1:C:570:GLY:O	1:C:571:VAL:HG13	2.07	0.55
1:C:1030:ARG:HA	1:C:1033:PHE:HD2	1.72	0.55
1:A:11:PHE:O	1:A:14:VAL:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:VAL:CG1	1:A:226:LYS:N	2.69	0.55
1:A:916:ALA:O	1:A:919:ARG:O	2.25	0.55
1:A:988:PRO:O	1:A:990:VAL:O	2.25	0.55
1:B:639:GLY:HA2	1:B:643:LYS:HZ3	1.70	0.55
1:B:960:LEU:C	1:B:960:LEU:CD1	2.76	0.55
1:C:136:PHE:CE2	1:C:292:LYS:HE2	2.41	0.55
1:C:156:ASP:O	1:C:159:ALA:HB3	2.07	0.55
1:C:328:ASP:OD1	1:C:330:THR:HB	2.06	0.55
1:C:456:MET:O	1:C:457:ALA:HB3	2.07	0.55
1:C:549:VAL:O	1:C:551:GLY:N	2.40	0.55
1:C:946:VAL:O	1:C:946:VAL:CG1	2.54	0.55
1:A:10:ILE:HG21	1:B:893:GLU:HB2	1.88	0.55
1:A:14:VAL:HG11	1:B:886:LEU:O	2.06	0.55
1:A:54:ALA:HB2	1:A:82:SER:O	2.07	0.55
1:A:354:VAL:O	1:A:355:MET:HB3	2.08	0.55
1:B:59:ASP:HA	1:B:63:GLN:HB2	1.89	0.55
1:B:570:GLY:N	1:B:634:TRP:CH2	2.75	0.55
1:C:87:THR:HG22	1:C:88:VAL:N	2.18	0.55
1:C:210:GLN:OE1	1:C:249:ILE:HG23	2.06	0.55
1:C:778:LYS:HD2	1:C:779:TYR:CE2	2.38	0.55
1:C:778:LYS:C	1:C:779:TYR:CD2	2.80	0.55
1:A:62:THR:O	1:A:63:GLN:O	2.24	0.54
1:A:689:GLY:O	1:A:690:LEU:O	2.25	0.54
1:A:987:MET:N	1:A:988:PRO:CD	2.69	0.54
1:B:228:GLN:HA	1:B:228:GLN:NE2	2.23	0.54
1:B:344:LEU:O	1:B:345:VAL:C	2.45	0.54
1:B:362:PHE:O	1:B:364:ALA:N	2.40	0.54
1:B:534:ILE:HA	1:B:541:TYR:CE1	2.42	0.54
1:B:641:GLU:HA	1:B:650:ARG:HH12	1.72	0.54
1:B:952:LEU:HD12	1:B:956:GLU:OE2	2.07	0.54
1:B:1001:ASN:O	1:B:1005:THR:HB	2.06	0.54
1:C:251:LEU:HB2	1:C:260:VAL:O	2.08	0.54
1:C:707:ALA:O	1:C:710:PRO:HD3	2.06	0.54
1:A:186:ILE:CB	1:A:773:VAL:HG23	2.34	0.54
1:A:310:LEU:HD12	1:A:325:TYR:OH	2.07	0.54
1:A:740:GLY:O	1:A:793:ALA:HB1	2.08	0.54
1:B:2:PRO:HG3	1:B:435:MET:HG2	1.87	0.54
1:B:372:VAL:HG22	1:B:373:PRO:CD	2.38	0.54
1:B:897:ILE:HG13	1:B:898:PRO:HD3	1.89	0.54
1:C:190:PRO:HD2	1:C:779:TYR:CD1	2.42	0.54
1:C:645:GLU:O	1:C:648:THR:HG22	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:847:LEU:O	1:C:851:LEU:HD11	2.07	0.54
1:C:860:THR:HG23	1:C:860:THR:O	2.07	0.54
1:A:329:THR:HG23	1:A:329:THR:O	2.06	0.54
1:B:7:ASP:O	1:B:8:ARG:CB	2.54	0.54
1:B:245:GLU:O	1:B:246:PHE:C	2.44	0.54
1:B:540:ARG:O	1:B:541:TYR:CD1	2.60	0.54
1:B:891:LEU:HD12	1:B:892:TYR:CE1	2.42	0.54
1:C:398:MET:O	1:C:402:ILE:HG13	2.07	0.54
1:C:475:VAL:CG1	1:C:476:SER:N	2.70	0.54
1:C:913:LEU:HD23	1:C:927:PHE:HZ	1.72	0.54
1:A:780:ARG:HG2	1:A:780:ARG:NH1	2.23	0.54
1:B:131:LYS:O	1:B:132:SER:HB3	2.06	0.54
1:B:156:ASP:OD2	1:B:182:TYR:HB2	2.07	0.54
1:B:399:VAL:HG11	1:B:989:LEU:HG	1.89	0.54
1:B:418:ARG:HE	1:B:970:MET:CE	2.21	0.54
1:B:448:VAL:O	1:B:452:VAL:CG2	2.53	0.54
1:B:945:ILE:HD11	1:B:1026:PHE:CZ	2.42	0.54
1:C:268:ILE:O	1:C:268:ILE:HG22	2.06	0.54
1:C:317:PHE:N	1:C:317:PHE:CD2	2.71	0.54
1:C:903:LEU:O	1:C:906:PRO:HD2	2.08	0.54
1:A:104:GLN:NE2	1:B:109:ASN:HB3	2.22	0.54
1:A:231:ASN:OD1	1:B:622:GLN:OE1	2.26	0.54
1:A:818:ARG:NE	1:A:818:ARG:HB2	2.19	0.54
1:B:49:TYR:CE2	1:B:122:VAL:O	2.61	0.54
1:B:136:PHE:CE1	1:B:617:PHE:CZ	2.90	0.54
1:B:706:ALA:HA	1:B:713:LEU:HD22	1.90	0.54
1:B:940:LYS:O	1:B:943:ILE:N	2.41	0.54
1:B:979:SER:CB	1:B:1011:MET:HE3	2.38	0.54
1:C:144:ASN:HD21	1:C:149:MET:N	2.05	0.54
1:C:144:ASN:OD1	1:C:320:GLY:O	2.25	0.54
1:C:477:ALA:H	1:C:480:LEU:HD23	1.72	0.54
1:C:633:ASP:O	1:C:633:ASP:CG	2.45	0.54
1:C:851:LEU:HD12	1:C:851:LEU:H	1.73	0.54
1:B:42:ALA:CB	1:B:93:THR:CG2	2.82	0.54
1:B:483:LEU:O	1:B:485:ALA:O	2.26	0.54
1:B:640:GLU:O	1:B:643:LYS:HB2	2.07	0.54
1:B:971:ARG:O	1:B:975:ILE:HD13	2.08	0.54
1:B:1010:GLY:HA2	1:B:1013:THR:CG2	2.38	0.54
1:C:731:ILE:HD13	1:C:805:SER:HB3	1.89	0.54
1:C:801:PHE:HA	1:C:804:PHE:CE1	2.42	0.54
1:C:951:ASP:O	1:C:953:MET:N	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:VAL:HG13	1:A:262:LEU:CD1	2.37	0.54
1:A:736:ALA:HA	1:A:741:VAL:CG1	2.38	0.54
1:A:843:LEU:O	1:A:846:GLN:N	2.40	0.54
1:B:130:GLU:OE1	1:C:110:LYS:HE2	2.08	0.54
1:B:431:THR:OG1	1:B:494:ALA:HB2	2.07	0.54
1:B:750:LEU:HB2	1:B:801:PHE:CE1	2.42	0.54
1:C:461:GLY:HA3	1:C:869:SER:OG	2.07	0.54
1:C:713:LEU:HD21	1:C:835:LYS:N	2.19	0.54
1:A:58:GLN:HG3	1:A:63:GLN:NE2	2.22	0.54
1:A:99:ASP:HB3	1:A:102:ILE:HG22	1.90	0.54
1:A:172:VAL:HG23	1:A:172:VAL:O	2.08	0.54
1:B:70:ASN:H	1:B:70:ASN:HD22	1.55	0.54
1:B:367:ILE:HG12	1:B:492:LEU:HD13	1.89	0.54
1:B:941:ASN:OD1	1:B:979:SER:OG	2.26	0.54
1:C:188:MET:CE	1:C:200:PRO:CB	2.82	0.54
1:C:241:THR:O	1:C:241:THR:OG1	2.25	0.54
1:C:578:LEU:HD21	1:C:590:VAL:HG21	1.90	0.54
1:C:778:LYS:HG3	1:C:779:TYR:CE2	2.43	0.54
1:C:861:GLY:H	1:C:864:TYR:HB2	1.73	0.54
1:A:1021:PHE:HB3	1:A:1025:PHE:CE1	2.43	0.54
1:B:372:VAL:HG22	1:B:373:PRO:HD3	1.90	0.54
1:B:740:GLY:HA3	1:B:794:ALA:HB2	1.90	0.54
1:B:885:PHE:CE2	1:B:898:PRO:HB2	2.42	0.54
1:C:87:THR:HG23	1:C:88:VAL:N	2.22	0.54
1:C:137:LEU:HG	1:C:293:LEU:HB2	1.90	0.54
1:A:38:ILE:O	1:A:462:SER:HA	2.08	0.54
1:A:65:ILE:O	1:A:68:ASN:OD1	2.26	0.54
1:A:210:GLN:HG3	1:A:249:ILE:CG2	2.34	0.54
1:A:966:ASP:O	1:A:969:ARG:HB2	2.08	0.54
1:B:143:ILE:CD1	1:B:322:LYS:HB3	2.37	0.54
1:C:115:MET:SD	1:C:127:VAL:HG11	2.48	0.54
1:C:666:PHE:CD2	1:C:666:PHE:O	2.61	0.54
1:C:682:PHE:HE2	1:C:702:LEU:HD11	1.73	0.54
1:C:924:ASP:O	1:C:925:VAL:O	2.25	0.54
1:C:966:ASP:HA	1:C:969:ARG:HB2	1.90	0.54
1:A:138:MET:HE3	1:A:306:ILE:HB	1.89	0.53
1:A:472:ILE:H	1:A:472:ILE:CD1	2.19	0.53
1:A:687:GLN:HA	2:A:1055:HOH:O	2.08	0.53
1:A:713:LEU:HB2	1:A:833:PRO:HD2	1.89	0.53
1:A:939:ALA:O	1:A:943:ILE:HG13	2.08	0.53
1:B:119:PRO:HG2	1:B:122:VAL:HG23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:PHE:HA	1:B:277:ILE:HG21	1.88	0.53
1:B:233:SER:OG	1:C:53:ASP:OD1	2.25	0.53
1:B:416:VAL:HG11	1:B:431:THR:CG2	2.36	0.53
1:B:537:SER:CA	1:B:540:ARG:HE	2.21	0.53
1:B:832:ALA:N	1:B:833:PRO:HD2	2.22	0.53
1:B:925:VAL:HA	1:B:928:GLN:OE1	2.08	0.53
1:C:484:VAL:HG12	1:C:489:THR:HG23	1.90	0.53
1:C:705:GLU:O	1:C:706:ALA:C	2.47	0.53
1:A:43:VAL:HG11	1:A:107:VAL:HG21	1.91	0.53
1:A:58:GLN:NE2	1:A:816:LEU:HD13	2.23	0.53
1:A:68:ASN:CB	1:A:68:ASN:C	2.72	0.53
1:A:575:MET:O	1:A:663:VAL:HA	2.08	0.53
1:A:764:ASP:HB3	1:A:769:LYS:HD2	1.90	0.53
1:B:146:ASP:O	1:B:147:GLY:C	2.44	0.53
1:B:184:MET:HB2	1:B:762:PHE:CE2	2.44	0.53
1:C:186:ILE:O	1:C:188:MET:N	2.41	0.53
1:C:410:ILE:O	1:C:412:VAL:N	2.40	0.53
1:C:476:SER:O	1:C:477:ALA:HB3	2.08	0.53
1:C:714:THR:HG22	1:C:715:SER:N	2.22	0.53
1:C:947:GLU:O	1:C:949:ALA:O	2.26	0.53
1:A:116:PRO:HB3	1:C:123:GLN:HG3	1.91	0.53
1:A:342:LYS:O	1:A:343:THR:C	2.46	0.53
1:A:344:LEU:HD22	1:A:376:LEU:HD11	1.89	0.53
1:A:568:ASP:O	1:A:634:TRP:HH2	1.91	0.53
1:A:638:PRO:HG2	1:A:639:GLY:H	1.73	0.53
1:A:694:LYS:O	1:A:698:ALA:HB2	2.08	0.53
1:B:525:HIS:CA	1:B:528:THR:HG22	2.38	0.53
1:C:35:TYR:CG	1:C:671:ILE:HG12	2.43	0.53
1:C:246:PHE:HZ	1:C:762:PHE:HB2	1.72	0.53
1:C:616:GLY:HA3	1:C:619:GLY:O	2.08	0.53
1:C:673:GLU:O	1:C:674:LEU:HB3	2.07	0.53
1:C:753:ALA:HB1	1:C:789:TRP:CZ2	2.43	0.53
1:C:776:GLU:O	1:C:777:ALA:C	2.46	0.53
1:C:778:LYS:CD	1:C:779:TYR:HE2	2.19	0.53
1:A:2:PRO:O	1:A:6:ILE:HG23	2.09	0.53
1:A:752:ALA:O	1:A:774:MET:HG3	2.08	0.53
1:A:818:ARG:HD3	1:A:822:LEU:N	2.23	0.53
1:B:261:LEU:HD13	1:B:261:LEU:N	2.23	0.53
1:B:562:SER:HB3	1:B:922:THR:HG21	1.90	0.53
1:B:989:LEU:HA	1:B:992:SER:HB2	1.90	0.53
1:C:103:ALA:O	1:C:105:VAL:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:ILE:HG12	1:C:759:VAL:HG13	1.90	0.53
1:C:915:ALA:O	1:C:919:ARG:N	2.40	0.53
1:C:949:ALA:C	1:C:951:ASP:H	2.11	0.53
1:A:399:VAL:C	1:A:401:ALA:H	2.12	0.53
1:A:402:ILE:O	1:A:405:LEU:HD13	2.08	0.53
1:A:575:MET:SD	1:A:626:ILE:HG13	2.49	0.53
1:B:25:LEU:O	1:B:27:ILE:N	2.41	0.53
1:B:291:ILE:CG2	1:B:306:ILE:HD11	2.38	0.53
1:B:395:MET:O	1:B:396:PHE:C	2.44	0.53
1:B:443:VAL:O	1:B:444:GLY:C	2.44	0.53
1:B:613:ASN:ND2	1:B:613:ASN:C	2.62	0.53
1:C:80:SER:O	1:C:81:ASN:HB3	2.08	0.53
1:C:743:ILE:H	1:C:743:ILE:CD1	2.04	0.53
1:C:901:VAL:HG12	1:C:942:ALA:HB1	1.90	0.53
1:C:965:LEU:O	1:C:969:ARG:HB2	2.09	0.53
1:A:393:LEU:HD11	1:A:466:ILE:HG12	1.91	0.53
1:A:897:ILE:HG21	1:A:950:LYS:HE2	1.89	0.53
1:B:58:GLN:HA	1:B:62:THR:HB	1.90	0.53
1:B:668:LEU:N	1:B:668:LEU:HD23	2.24	0.53
1:B:937:LEU:O	1:B:940:LYS:HB3	2.08	0.53
1:B:962:GLU:O	1:B:966:ASP:CB	2.48	0.53
1:C:157:TYR:CE1	1:C:318:PRO:HD3	2.43	0.53
1:C:175:VAL:O	1:C:175:VAL:HG12	2.08	0.53
1:A:443:VAL:CG1	1:A:444:GLY:N	2.65	0.53
1:A:472:ILE:N	1:A:472:ILE:CD1	2.72	0.53
1:A:780:ARG:NH2	1:C:223:PRO:HG2	2.24	0.53
1:A:901:VAL:HG11	1:A:943:ILE:CG1	2.38	0.53
1:A:1021:PHE:HB3	1:A:1025:PHE:CZ	2.44	0.53
1:B:6:ILE:HD13	1:B:6:ILE:N	2.24	0.53
1:B:525:HIS:O	1:B:529:ASP:OD2	2.27	0.53
1:B:944:LEU:CB	1:B:975:ILE:HD11	2.39	0.53
1:C:17:ILE:N	1:C:17:ILE:CD1	2.71	0.53
1:C:674:LEU:HD11	1:C:862:MET:CA	2.31	0.53
1:C:914:LEU:O	1:C:915:ALA:HB3	2.09	0.53
1:A:884:VAL:HG12	1:A:902:MET:HE3	1.91	0.53
1:A:911:GLY:H	1:A:914:LEU:CD1	2.20	0.53
1:B:987:MET:N	1:B:988:PRO:CD	2.70	0.53
1:C:389:SER:HG	1:C:391:ASN:HD22	1.52	0.53
1:A:141:GLY:N	1:A:324:VAL:O	2.38	0.53
1:A:774:MET:O	1:A:775:SER:O	2.26	0.53
1:C:4:PHE:O	1:C:8:ARG:HG2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:492:LEU:HA	1:C:495:THR:HB	1.91	0.53
1:A:143:ILE:HG21	1:A:281:PHE:CD2	2.44	0.53
1:A:444:GLY:O	1:A:448:VAL:HG23	2.09	0.53
1:B:586:ARG:HH22	1:B:660:ASP:HB2	1.74	0.53
1:C:155:SER:HB3	1:C:180:SER:H	1.74	0.53
1:C:564:LEU:CD2	1:C:671:ILE:HD12	2.39	0.53
1:C:868:LEU:O	1:C:869:SER:CB	2.57	0.53
1:A:64:VAL:O	1:A:68:ASN:OD1	2.27	0.52
1:A:600:THR:O	1:A:600:THR:HG22	2.10	0.52
1:A:649:MET:HE2	1:A:653:ARG:NH2	2.24	0.52
1:B:401:ALA:O	1:B:404:LEU:N	2.41	0.52
1:C:578:LEU:HB3	1:C:579:PRO:CD	2.35	0.52
1:C:699:ARG:HH11	1:C:699:ARG:HG3	1.67	0.52
1:A:739:LEU:HD22	1:A:739:LEU:H	1.74	0.52
1:B:541:TYR:C	1:B:543:VAL:H	2.12	0.52
1:B:613:ASN:HD22	1:B:614:GLY:CA	2.22	0.52
1:C:404:LEU:CD2	1:C:937:LEU:HD13	2.40	0.52
1:C:443:VAL:O	1:C:447:MET:HB2	2.09	0.52
1:C:997:SER:O	1:C:1000:GLN:N	2.42	0.52
1:A:61:VAL:HG22	1:A:118:LEU:HD22	1.90	0.52
1:A:986:VAL:O	1:A:991:ILE:HD12	2.09	0.52
1:A:1007:VAL:O	1:A:1011:MET:HB2	2.08	0.52
1:C:177:LEU:HD13	1:C:179:GLY:O	2.09	0.52
1:C:410:ILE:CG2	1:C:411:VAL:N	2.69	0.52
1:C:520:PHE:O	1:C:523:SER:OG	2.27	0.52
1:C:552:MET:O	1:C:553:ALA:CB	2.56	0.52
1:C:841:MET:O	1:C:845:GLU:HG3	2.10	0.52
1:A:189:ASN:HD21	1:A:192:GLU:HB2	1.72	0.52
1:A:902:MET:O	1:A:904:VAL:N	2.43	0.52
1:A:999:ALA:O	1:A:1002:ALA:HB3	2.10	0.52
1:B:777:ALA:O	1:B:780:ARG:HB2	2.09	0.52
1:B:952:LEU:O	1:B:963:ALA:HB2	2.09	0.52
1:B:961:ILE:O	1:B:965:LEU:HB2	2.09	0.52
1:C:6:ILE:HA	1:C:491:ALA:HB2	1.90	0.52
1:A:107:VAL:O	1:A:110:LYS:CB	2.58	0.52
1:A:399:VAL:O	1:A:401:ALA:N	2.43	0.52
1:A:406:VAL:O	1:A:407:ASP:C	2.45	0.52
1:A:572:PHE:N	1:A:572:PHE:CD1	2.78	0.52
1:A:616:GLY:HA3	1:A:624:THR:OG1	2.09	0.52
1:B:41:PRO:HG2	1:B:98:THR:HG22	1.90	0.52
1:B:162:MET:HB2	1:B:313:MET:SD	2.50	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:551:GLY:O	1:B:554:TYR:HB2	2.09	0.52
1:C:110:LYS:CA	1:C:113:LEU:HD12	2.20	0.52
1:C:161:ASN:N	1:C:161:ASN:CB	2.59	0.52
1:C:211:ASN:C	1:C:211:ASN:ND2	2.61	0.52
1:C:459:PHE:HD2	1:C:459:PHE:N	1.89	0.52
1:A:128:SER:HB2	1:B:113:LEU:HD22	1.90	0.52
1:A:133:SER:OG	1:A:136:PHE:HE1	1.91	0.52
1:A:407:ASP:O	1:A:408:ASP:C	2.48	0.52
1:A:644:VAL:O	1:A:646:ALA:N	2.43	0.52
1:B:87:THR:HG21	1:B:620:ARG:NH1	2.25	0.52
1:B:649:MET:O	1:B:653:ARG:HB2	2.10	0.52
1:C:324:VAL:CG2	1:C:326:PRO:HD3	2.39	0.52
1:C:419:VAL:HA	1:C:422:GLU:HB3	1.91	0.52
1:C:432:ARG:HH11	1:C:432:ARG:CG	2.02	0.52
1:A:246:PHE:O	1:A:249:ILE:HD12	2.09	0.52
1:B:34:GLN:HB2	1:B:333:VAL:HG22	1.92	0.52
1:B:365:THR:O	1:B:368:PRO:HD2	2.10	0.52
1:B:740:GLY:HA3	1:B:794:ALA:CB	2.39	0.52
1:B:960:LEU:HD11	1:B:1027:VAL:CG1	2.39	0.52
1:C:352:PHE:CA	1:C:369:THR:HG21	2.37	0.52
1:C:394:THR:O	1:C:395:MET:HE2	2.08	0.52
1:C:939:ALA:O	1:C:943:ILE:HG12	2.10	0.52
1:A:58:GLN:HG2	1:A:59:ASP:OD1	2.09	0.52
1:A:59:ASP:CB	1:C:763:ILE:HD11	2.38	0.52
1:A:67:GLN:NE2	2:A:1063:HOH:O	2.12	0.52
1:A:113:LEU:CD2	1:C:127:VAL:O	2.58	0.52
1:A:246:PHE:O	1:A:249:ILE:HD13	2.10	0.52
1:A:717:ARG:HH11	1:A:830:GLN:HE22	1.55	0.52
1:B:518:ARG:HA	1:B:521:GLU:CB	2.40	0.52
1:B:570:GLY:N	1:B:634:TRP:HH2	2.07	0.52
1:B:763:ILE:HD11	1:C:59:ASP:HB3	1.91	0.52
1:B:784:ASP:O	1:B:785:ASP:C	2.46	0.52
1:B:973:ARG:CG	1:B:974:PRO:HD3	2.37	0.52
1:C:752:ALA:O	1:C:774:MET:HA	2.10	0.52
1:C:877:TYR:O	1:C:880:SER:HB3	2.09	0.52
1:A:183:ALA:N	1:A:271:GLY:O	2.43	0.52
1:A:686:ASP:C	1:A:688:ALA:N	2.62	0.52
1:A:761:ASP:OD2	1:A:761:ASP:N	2.42	0.52
1:B:4:PHE:O	1:B:5:PHE:HB2	2.10	0.52
1:B:304:ALA:O	1:B:308:ALA:HB2	2.10	0.52
1:B:335:ILE:O	1:B:337:ILE:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:PHE:HB3	1:B:977:MET:CE	2.39	0.52
1:B:572:PHE:CE2	1:B:629:VAL:HG21	2.45	0.52
1:C:287:SER:OG	1:C:288:GLY:N	2.43	0.52
1:C:314:GLU:CB	1:C:315:PRO:CD	2.79	0.52
1:C:442:LEU:O	1:C:445:ILE:HG13	2.10	0.52
1:C:519:MET:O	1:C:523:SER:OG	2.24	0.52
1:C:572:PHE:CZ	1:C:629:VAL:HG11	2.45	0.52
1:C:599:LEU:O	1:C:603:LYS:HB2	2.10	0.52
1:C:1024:VAL:CG1	1:C:1028:VAL:CG2	2.88	0.52
1:B:168:ARG:HD3	1:C:69:MET:O	2.10	0.52
1:B:545:TYR:C	1:B:547:ILE:N	2.62	0.52
1:B:968:VAL:O	1:B:972:LEU:HB2	2.09	0.52
1:C:945:ILE:CB	1:C:971:ARG:HG3	2.40	0.52
1:A:102:ILE:HA	1:A:105:VAL:HG21	1.92	0.51
1:A:1004:GLY:O	1:A:1007:VAL:N	2.43	0.51
1:B:360:GLN:O	1:B:361:ASN:CB	2.58	0.51
1:B:399:VAL:O	1:B:400:LEU:C	2.47	0.51
1:C:159:ALA:C	2:C:1078:HOH:O	2.32	0.51
1:C:248:LYS:O	1:C:249:ILE:C	2.48	0.51
1:C:655:PHE:C	1:C:657:GLN:N	2.58	0.51
1:A:68:ASN:H	1:A:69:MET:N	2.08	0.51
1:A:100:ALA:HB1	1:A:131:LYS:CE	2.39	0.51
1:A:354:VAL:HG13	1:A:980:LEU:HD23	1.92	0.51
1:A:578:LEU:HD21	1:A:587:THR:CA	2.34	0.51
1:A:904:VAL:O	1:A:905:VAL:C	2.49	0.51
1:A:911:GLY:CA	1:A:914:LEU:HD13	2.38	0.51
1:B:6:ILE:HD12	1:B:490:PRO:CB	2.39	0.51
1:B:25:LEU:O	1:B:28:LEU:HG	2.10	0.51
1:B:55:LYS:O	1:B:57:VAL:N	2.43	0.51
1:B:659:LYS:HD3	1:B:660:ASP:H	1.72	0.51
1:C:1035:ARG:HA	1:C:1035:ARG:NE	2.25	0.51
1:A:65:ILE:C	1:A:65:ILE:N	2.61	0.51
1:A:783:PRO:C	1:A:784:ASP:O	2.48	0.51
1:A:819:TYR:O	1:A:820:ASN:C	2.48	0.51
1:B:358:PHE:HB3	1:B:977:MET:HE1	1.92	0.51
1:B:556:PHE:HA	1:B:913:LEU:HD11	1.92	0.51
1:B:712:MET:HB3	1:B:713:LEU:CD1	2.29	0.51
1:B:729:ILE:CG1	1:B:730:ASP:N	2.70	0.51
1:B:978:THR:HG22	1:B:979:SER:H	1.76	0.51
1:C:214:VAL:CG1	1:C:215:ALA:H	2.23	0.51
1:C:641:GLU:O	1:C:650:ARG:NH1	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:682:PHE:CE2	1:C:702:LEU:HD11	2.46	0.51
1:A:826:GLU:C	1:A:827:ILE:HD12	2.31	0.51
1:A:902:MET:C	1:A:904:VAL:H	2.13	0.51
1:B:594:VAL:HG22	1:B:663:VAL:HG11	1.91	0.51
1:C:121:GLU:O	1:C:758:TYR:OH	2.27	0.51
1:C:263:ARG:HG3	1:C:263:ARG:O	2.08	0.51
1:C:695:LEU:HD22	1:C:825:MET:HE2	1.92	0.51
1:A:116:PRO:HA	2:A:1072:HOH:O	2.10	0.51
1:A:148:THR:HG21	1:A:319:SER:OG	2.10	0.51
1:A:311:ALA:O	1:A:312:LYS:CB	2.53	0.51
1:A:314:GLU:H	1:A:315:PRO:HD3	1.74	0.51
1:B:105:VAL:O	1:B:109:ASN:N	2.35	0.51
1:B:736:ALA:C	1:B:738:ALA:H	2.12	0.51
1:B:1022:VAL:CG2	1:B:1023:PRO:CD	2.86	0.51
1:B:1026:PHE:HB3	1:B:1030:ARG:NE	2.25	0.51
1:C:341:VAL:O	1:C:345:VAL:HG23	2.11	0.51
1:A:11:PHE:CD1	1:B:890:ALA:CB	2.94	0.51
1:A:191:ASN:C	1:A:193:LEU:N	2.63	0.51
1:A:280:GLU:HB2	1:A:284:GLN:O	2.09	0.51
1:A:543:VAL:O	1:A:544:LEU:CB	2.55	0.51
1:A:621:GLY:O	1:A:623:ASN:N	2.43	0.51
1:B:104:GLN:HG2	1:B:105:VAL:H	1.74	0.51
1:B:330:THR:O	1:B:334:LYS:HG3	2.09	0.51
1:B:420:MET:HA	1:B:423:GLU:O	2.09	0.51
1:B:583:THR:HG22	1:B:586:ARG:HG3	1.93	0.51
1:B:1027:VAL:O	1:B:1031:ARG:HB3	2.10	0.51
1:C:760:ASN:C	1:C:760:ASN:OD1	2.49	0.51
1:C:978:THR:O	1:C:979:SER:C	2.46	0.51
1:A:63:GLN:O	1:A:65:ILE:C	2.49	0.51
1:A:158:VAL:HA	1:A:162:MET:HG2	1.92	0.51
1:A:651:ALA:O	1:A:655:PHE:HD1	1.93	0.51
1:A:687:GLN:O	1:A:688:ALA:HB2	2.09	0.51
1:A:831:ALA:HB2	1:A:837:THR:HA	1.93	0.51
1:C:115:MET:N	1:C:116:PRO:HD3	2.23	0.51
1:C:399:VAL:C	1:C:401:ALA:H	2.14	0.51
1:C:708:LYS:C	1:C:710:PRO:HD3	2.31	0.51
1:C:792:ARG:HG2	1:C:793:ALA:O	2.11	0.51
1:A:69:MET:CG	1:A:69:MET:CA	2.80	0.51
1:A:166:ILE:N	1:A:166:ILE:CD1	2.67	0.51
1:A:488:LEU:HG	1:A:492:LEU:HD22	1.93	0.51
1:A:1016:VAL:O	1:A:1016:VAL:HG12	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:ILE:HG23	1:B:266:ALA:HB1	1.91	0.51
1:B:476:SER:O	1:B:477:ALA:C	2.49	0.51
1:B:778:LYS:O	1:B:779:TYR:HB2	2.11	0.51
1:B:974:PRO:O	1:B:976:LEU:N	2.44	0.51
1:B:986:VAL:HG12	1:B:990:VAL:CG2	2.40	0.51
1:B:1024:VAL:HG13	1:B:1028:VAL:HG21	1.93	0.51
1:C:129:VAL:CG2	1:C:129:VAL:CA	2.84	0.51
1:A:14:VAL:CG1	1:B:886:LEU:HB3	2.41	0.51
1:B:552:MET:SD	1:B:909:VAL:CG2	2.96	0.51
1:B:863:SER:O	1:B:866:GLU:N	2.44	0.51
1:C:181:GLN:CD	1:C:769:LYS:HD2	2.31	0.51
1:C:326:PRO:O	1:C:327:TYR:C	2.50	0.51
1:C:392:THR:O	1:C:395:MET:N	2.42	0.51
1:C:482:VAL:O	1:C:486:LEU:HG	2.11	0.51
1:C:549:VAL:HG12	1:C:550:VAL:N	2.25	0.51
1:C:701:GLN:O	1:C:704:ALA:N	2.44	0.51
1:C:1016:VAL:O	1:C:1019:ILE:HG22	2.11	0.51
1:A:112:GLN:CA	1:A:112:GLN:NE2	2.65	0.51
1:A:579:PRO:O	1:A:580:ALA:C	2.49	0.51
1:A:584:GLN:N	1:A:622:GLN:HB3	2.23	0.51
1:A:691:GLY:O	1:A:692:HIS:C	2.50	0.51
1:A:750:LEU:HD11	1:C:216:ALA:CB	2.41	0.51
1:A:818:ARG:NH1	1:A:821:GLY:O	2.43	0.51
1:B:91:THR:C	1:B:92:LEU:HD22	2.31	0.51
1:B:168:ARG:HH11	1:C:69:MET:HB2	1.75	0.51
1:B:898:PRO:C	1:B:900:SER:N	2.63	0.51
1:C:16:ALA:O	1:C:20:MET:HG3	2.10	0.51
1:C:50:PRO:CD	1:C:125:GLN:HG3	2.41	0.51
1:C:280:GLU:HB3	1:C:284:GLN:O	2.11	0.51
1:C:713:LEU:CD1	1:C:833:PRO:O	2.59	0.51
1:C:734:GLU:O	1:C:738:ALA:N	2.44	0.51
1:C:754:TRP:CH2	1:C:780:ARG:HA	2.46	0.51
1:C:785:ASP:O	1:C:787:GLY:N	2.44	0.51
1:C:911:GLY:O	1:C:914:LEU:O	2.29	0.51
1:A:65:ILE:HG13	1:A:66:GLU:N	2.26	0.50
1:A:583:THR:HB	1:A:586:ARG:HG3	1.93	0.50
1:A:732:ASP:HB3	1:A:735:LYS:HB2	1.93	0.50
1:B:946:VAL:HG22	1:B:1026:PHE:CE1	2.45	0.50
1:C:418:ARG:CD	1:C:970:MET:HE2	2.40	0.50
1:C:425:LEU:N	1:C:426:PRO:HD3	2.26	0.50
1:C:655:PHE:O	1:C:657:GLN:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:907:LEU:HG	1:C:1017:LEU:HD23	1.93	0.50
1:A:107:VAL:O	1:A:110:LYS:HB3	2.11	0.50
1:A:533:GLY:O	1:A:534:ILE:C	2.49	0.50
1:A:658:ILE:O	1:A:659:LYS:O	2.27	0.50
1:B:149:MET:SD	1:B:154:ILE:HG22	2.51	0.50
1:B:316:PHE:CZ	1:C:687:GLN:HG3	2.46	0.50
1:B:595:THR:HB	1:B:609:VAL:HG11	1.93	0.50
1:B:987:MET:N	1:B:988:PRO:HD2	2.26	0.50
1:A:116:PRO:C	1:A:117:LEU:HD22	2.32	0.50
1:A:399:VAL:C	1:A:401:ALA:N	2.65	0.50
1:A:418:ARG:NH1	1:A:973:ARG:HB3	2.26	0.50
1:A:527:TYR:CD2	1:A:972:LEU:HG	2.47	0.50
1:A:599:LEU:O	1:A:600:THR:CB	2.59	0.50
1:B:462:SER:OG	1:B:865:GLN:NE2	2.44	0.50
1:C:188:MET:HA	1:C:266:ALA:CB	2.40	0.50
1:C:247:GLY:HA2	1:C:268:ILE:CD1	2.38	0.50
1:C:556:PHE:HB2	1:C:913:LEU:HD11	1.93	0.50
1:C:666:PHE:CD2	1:C:666:PHE:N	2.79	0.50
1:A:76:MET:SD	1:A:95:GLU:OE2	2.70	0.50
1:A:276:ASP:CB	1:C:222:THR:HG23	2.35	0.50
1:B:25:LEU:O	1:B:28:LEU:N	2.36	0.50
1:B:228:GLN:HA	1:B:228:GLN:HE21	1.76	0.50
1:B:679:GLY:HA2	1:B:830:GLN:HB3	1.94	0.50
1:B:960:LEU:C	1:B:960:LEU:HD13	2.31	0.50
1:C:102:ILE:O	1:C:105:VAL:HB	2.12	0.50
1:C:188:MET:HE2	1:C:200:PRO:HB3	1.92	0.50
1:C:490:PRO:C	1:C:491:ALA:O	2.47	0.50
1:A:73:ASP:CG	1:A:106:GLN:HE22	2.15	0.50
1:A:254:ASN:O	1:A:258:SER:OG	2.20	0.50
1:A:421:ALA:O	1:A:423:GLU:N	2.44	0.50
1:A:428:LYS:CG	1:A:429:GLU:H	2.22	0.50
1:A:635:ALA:C	1:A:637:ARG:H	2.14	0.50
1:A:952:LEU:HD12	1:A:952:LEU:C	2.32	0.50
1:B:578:LEU:HD12	1:B:586:ARG:NH2	2.26	0.50
1:C:226:LYS:HA	2:C:1072:HOH:O	2.11	0.50
1:C:467:TYR:C	1:C:469:GLN:H	2.15	0.50
1:C:726:GLN:N	1:C:810:GLU:O	2.38	0.50
1:A:552:MET:SD	1:A:909:VAL:HG11	2.52	0.50
1:B:49:TYR:CD1	1:B:122:VAL:HG13	2.46	0.50
1:B:317:PHE:CD1	1:B:321:LEU:HD23	2.47	0.50
1:B:728:LYS:HD3	1:B:810:GLU:OE1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:THR:CB	1:C:172:VAL:HG21	2.38	0.50
1:C:191:ASN:O	1:C:194:ASN:HB2	2.11	0.50
1:C:536:ARG:NH1	1:C:961:ILE:CD1	2.75	0.50
1:C:643:LYS:C	1:C:647:ILE:HG13	2.32	0.50
1:C:644:VAL:O	1:C:648:THR:HG22	2.12	0.50
1:C:674:LEU:HD12	1:C:865:GLN:OE1	2.12	0.50
1:C:695:LEU:CD2	1:C:825:MET:HG3	2.41	0.50
1:C:758:TYR:H	1:C:758:TYR:HD1	1.55	0.50
1:C:949:ALA:C	1:C:951:ASP:N	2.64	0.50
1:A:75:LEU:HD12	1:A:76:MET:N	2.26	0.50
1:A:193:LEU:HA	1:A:265:VAL:HG13	1.94	0.50
1:A:235:ILE:O	1:A:235:ILE:HG22	2.11	0.50
1:A:371:ALA:O	1:A:372:VAL:O	2.30	0.50
1:A:534:ILE:HD12	1:A:540:ARG:NH1	2.26	0.50
1:A:588:GLN:O	1:A:591:LEU:N	2.43	0.50
1:A:709:HIS:N	1:A:710:PRO:CD	2.74	0.50
1:B:10:ILE:O	1:B:11:PHE:C	2.48	0.50
1:B:324:VAL:C	1:B:326:PRO:HD2	2.32	0.50
1:B:833:PRO:HG2	1:B:834:GLY:H	1.77	0.50
1:C:243:THR:OG1	1:C:244:GLU:N	2.45	0.50
1:C:422:GLU:OE2	1:C:423:GLU:HG3	2.12	0.50
1:C:428:LYS:O	1:C:432:ARG:HB2	2.12	0.50
1:C:735:LYS:O	1:C:738:ALA:HB3	2.11	0.50
1:A:186:ILE:HD12	1:A:207:ILE:HD13	1.94	0.50
1:A:200:PRO:HG2	1:A:749:THR:HG23	1.93	0.50
1:A:578:LEU:H	1:A:578:LEU:HD22	1.76	0.50
1:B:8:ARG:H	1:B:9:PRO:HD3	1.76	0.50
1:B:572:PHE:HA	1:B:668:LEU:HD21	1.93	0.50
1:B:1019:ILE:O	1:B:1023:PRO:HG3	2.11	0.50
1:C:192:GLU:C	1:C:194:ASN:N	2.64	0.50
1:C:311:ALA:O	1:C:312:LYS:C	2.49	0.50
1:C:393:LEU:O	1:C:395:MET:N	2.45	0.50
1:C:463:THR:HG22	1:C:464:GLY:H	1.73	0.50
1:C:540:ARG:HG3	1:C:541:TYR:CD1	2.46	0.50
1:C:559:LEU:HD13	1:C:917:THR:HG23	1.94	0.50
1:C:997:SER:O	1:C:999:ALA:N	2.45	0.50
1:A:133:SER:HB3	1:A:136:PHE:CD1	2.46	0.50
1:A:689:GLY:O	1:A:690:LEU:C	2.51	0.50
1:B:129:VAL:H	1:C:109:ASN:HD21	1.58	0.50
1:B:693:GLU:C	1:B:695:LEU:H	2.15	0.50
1:B:703:LEU:O	1:B:704:ALA:C	2.50	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:830:GLN:H	1:B:830:GLN:NE2	2.04	0.50
1:C:127:VAL:CB	1:C:127:VAL:C	2.73	0.50
1:C:934:THR:O	1:C:936:GLY:N	2.45	0.50
1:A:218:GLN:HB3	1:A:231:ASN:HD21	1.77	0.49
1:A:395:MET:CE	1:A:395:MET:HA	2.41	0.49
1:B:25:LEU:C	1:B:27:ILE:N	2.64	0.49
1:B:115:MET:HA	1:B:118:LEU:HD13	1.94	0.49
1:B:401:ALA:HA	1:B:404:LEU:HB2	1.93	0.49
1:B:547:ILE:O	1:B:550:VAL:O	2.30	0.49
1:B:600:THR:OG1	1:B:601:LYS:HE2	2.13	0.49
1:B:712:MET:HA	1:B:712:MET:CE	2.42	0.49
1:B:1016:VAL:C	1:B:1018:ALA:H	2.16	0.49
1:B:1017:LEU:O	1:B:1021:PHE:HB2	2.12	0.49
1:B:1022:VAL:CG2	1:B:1023:PRO:HD3	2.33	0.49
1:C:260:VAL:O	1:C:260:VAL:HG13	2.11	0.49
1:C:376:LEU:HD22	1:C:398:MET:HE1	1.93	0.49
1:C:1010:GLY:C	1:C:1013:THR:HG22	2.32	0.49
1:C:1032:ARG:HG2	1:C:1032:ARG:O	2.11	0.49
1:B:542:LEU:HD11	1:B:1028:VAL:CG1	2.40	0.49
1:B:973:ARG:N	1:B:974:PRO:HD2	2.27	0.49
1:B:1012:VAL:C	1:B:1014:ALA:H	2.15	0.49
1:C:88:VAL:HG11	2:C:1064:HOH:O	2.12	0.49
1:C:519:MET:CG	1:C:520:PHE:N	2.75	0.49
1:C:966:ASP:HA	1:C:969:ARG:CB	2.42	0.49
1:A:455:PRO:HB2	1:A:877:TYR:CE1	2.48	0.49
1:A:728:LYS:HZ3	1:C:235:ILE:CG2	2.23	0.49
1:A:790:TYR:HE1	1:A:800:PRO:CG	2.14	0.49
1:B:100:ALA:HB1	1:B:131:LYS:HD2	1.94	0.49
1:B:413:VAL:HG13	1:B:414:GLU:N	2.27	0.49
1:C:100:ALA:O	1:C:101:ASP:C	2.50	0.49
1:C:847:LEU:HD22	1:C:847:LEU:N	2.28	0.49
1:C:847:LEU:HD23	1:C:847:LEU:C	2.33	0.49
1:A:38:ILE:HD11	1:A:671:ILE:HG21	1.94	0.49
1:A:359:LEU:CD1	1:A:417:GLU:HG2	2.41	0.49
1:A:516:PHE:C	1:A:518:ARG:N	2.66	0.49
1:A:568:ASP:HB3	1:A:634:TRP:CZ3	2.41	0.49
1:A:613:ASN:HA	1:A:625:GLY:HA3	1.95	0.49
1:A:682:PHE:CZ	1:A:857:TYR:HB2	2.48	0.49
1:B:119:PRO:HG2	1:B:122:VAL:HG21	1.95	0.49
1:B:690:LEU:HB2	1:B:694:LYS:HB3	1.94	0.49
1:C:184:MET:HB3	1:C:771:VAL:HG13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:LEU:O	1:C:220:GLY:O	2.30	0.49
1:C:333:VAL:O	1:C:337:ILE:HD12	2.12	0.49
1:C:561:SER:HA	1:C:923:ASN:CB	2.43	0.49
1:A:552:MET:C	1:A:554:TYR:H	2.16	0.49
1:A:719:ASN:N	1:A:826:GLU:O	2.46	0.49
1:A:843:LEU:HD23	1:A:846:GLN:NE2	2.27	0.49
1:A:1024:VAL:HG12	1:A:1028:VAL:HG23	1.94	0.49
1:B:158:VAL:HA	1:B:162:MET:CG	2.36	0.49
1:B:602:GLU:C	1:B:604:ASN:N	2.65	0.49
1:C:23:GLY:O	1:C:27:ILE:HG13	2.13	0.49
1:C:166:ILE:CA	1:C:166:ILE:CD1	2.75	0.49
1:C:389:SER:O	1:C:394:THR:HG21	2.12	0.49
1:C:454:VAL:O	1:C:456:MET:O	2.31	0.49
1:C:461:GLY:CA	1:C:869:SER:OG	2.61	0.49
1:C:1022:VAL:N	1:C:1023:PRO:CD	2.75	0.49
1:C:1025:PHE:C	1:C:1029:VAL:HG23	2.33	0.49
1:A:330:THR:H	1:A:331:PRO:HD2	1.78	0.49
1:A:533:GLY:O	1:A:535:LEU:HB2	2.12	0.49
1:A:574:THR:HG21	1:A:598:TYR:CE1	2.44	0.49
1:A:693:GLU:C	1:A:695:LEU:N	2.65	0.49
1:A:754:TRP:CZ2	1:A:786:ILE:HG12	2.48	0.49
1:B:343:THR:O	1:B:347:ALA:N	2.39	0.49
1:B:410:ILE:C	1:B:412:VAL:H	2.15	0.49
1:B:701:GLN:HB3	1:B:851:LEU:HD13	1.95	0.49
1:B:1026:PHE:HB3	1:B:1030:ARG:CZ	2.42	0.49
1:C:8:ARG:HG2	1:C:8:ARG:HH21	1.78	0.49
1:C:166:ILE:CA	1:C:166:ILE:CG2	2.85	0.49
1:C:314:GLU:HA	1:C:317:PHE:CZ	2.47	0.49
1:C:399:VAL:HA	1:C:402:ILE:HD12	1.92	0.49
1:C:492:LEU:O	1:C:496:MET:HG2	2.13	0.49
1:C:545:TYR:CZ	1:C:1021:PHE:CD2	3.01	0.49
1:C:781:MET:O	1:C:782:LEU:HD23	2.13	0.49
1:A:68:ASN:H	1:A:69:MET:H	1.61	0.49
1:A:219:LEU:HD23	1:B:754:TRP:HZ3	1.78	0.49
1:A:372:VAL:HB	1:A:373:PRO:CD	2.37	0.49
1:A:999:ALA:HA	1:A:1002:ALA:CB	2.43	0.49
1:B:380:PHE:CZ	1:B:398:MET:HE2	2.48	0.49
1:B:619:GLY:H	1:B:721:LEU:CD1	2.26	0.49
1:C:513:PHE:CA	1:C:516:PHE:HB3	2.33	0.49
1:C:562:SER:OG	1:C:922:THR:HG21	2.12	0.49
1:C:912:ALA:O	1:C:914:LEU:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:631:LEU:HD11	1:A:644:VAL:HG22	1.94	0.49
1:A:818:ARG:HG3	2:A:1062:HOH:O	2.11	0.49
1:A:963:ALA:O	1:A:965:LEU:N	2.46	0.49
1:B:20:MET:HG3	1:B:374:VAL:HG23	1.94	0.49
1:B:404:LEU:HD13	1:B:449:LEU:CD1	2.42	0.49
1:B:471:SER:O	1:B:475:VAL:HB	2.13	0.49
1:C:80:SER:O	1:C:89:GLN:O	2.31	0.49
1:C:476:SER:C	1:C:478:MET:N	2.66	0.49
1:C:568:ASP:OD1	1:C:634:TRP:CD1	2.65	0.49
1:C:650:ARG:O	1:C:653:ARG:HG2	2.12	0.49
1:C:685:ILE:HD12	1:C:686:ASP:N	2.28	0.49
1:C:705:GLU:O	1:C:708:LYS:N	2.45	0.49
1:A:521:GLU:CG	2:A:1075:HOH:O	2.57	0.49
1:B:125:GLN:O	1:B:125:GLN:CG	2.59	0.49
1:B:183:ALA:H	1:B:272:GLY:HA2	1.78	0.49
1:B:490:PRO:O	1:B:493:CYS:O	2.30	0.49
1:B:642:ASN:N	1:B:650:ARG:HH12	2.05	0.49
1:C:102:ILE:O	1:C:105:VAL:N	2.46	0.49
1:C:188:MET:HE2	1:C:200:PRO:HA	1.95	0.49
1:C:192:GLU:O	1:C:193:LEU:C	2.51	0.49
1:C:987:MET:HB3	1:C:988:PRO:HD3	1.94	0.49
1:A:171:GLY:O	1:A:173:GLY:N	2.45	0.49
1:A:736:ALA:CA	1:A:741:VAL:HG13	2.42	0.49
1:A:832:ALA:CB	1:A:835:LYS:HB2	2.40	0.49
1:B:362:PHE:HA	1:B:365:THR:HG22	1.95	0.49
1:B:453:PHE:HA	1:B:456:MET:SD	2.52	0.49
1:B:485:ALA:HA	1:B:489:THR:OG1	2.13	0.49
1:B:583:THR:HG23	1:B:585:GLU:H	1.78	0.49
1:B:905:VAL:N	1:B:906:PRO:CD	2.76	0.49
1:C:4:PHE:HB3	1:C:8:ARG:NH2	2.16	0.49
1:C:396:PHE:HA	1:C:399:VAL:HB	1.94	0.49
1:C:574:THR:O	1:C:626:ILE:HD13	2.12	0.49
1:A:63:GLN:O	1:A:64:VAL:C	2.50	0.48
1:A:67:GLN:CB	2:A:1057:HOH:O	2.60	0.48
1:A:193:LEU:HB2	1:A:265:VAL:HG13	1.95	0.48
1:B:7:ASP:CG	1:B:8:ARG:HH21	2.16	0.48
1:B:355:MET:O	1:B:365:THR:OG1	2.30	0.48
1:B:369:THR:O	1:B:372:VAL:HG13	2.13	0.48
1:B:578:LEU:HD12	1:B:586:ARG:CZ	2.42	0.48
1:B:586:ARG:NH2	1:B:660:ASP:HB2	2.26	0.48
1:B:638:PRO:HG2	1:B:639:GLY:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:900:SER:O	1:B:903:LEU:N	2.39	0.48
1:B:942:ALA:O	1:B:945:ILE:HG12	2.13	0.48
1:B:969:ARG:HG2	1:B:969:ARG:HH11	1.78	0.48
1:A:64:VAL:HG12	1:A:65:ILE:N	2.27	0.48
1:A:449:LEU:O	1:A:453:PHE:HD1	1.96	0.48
1:A:534:ILE:HD12	1:A:540:ARG:CZ	2.43	0.48
1:A:554:TYR:HE1	1:A:558:ARG:HD3	1.76	0.48
1:B:218:GLN:HA	1:B:234:ILE:HG13	1.95	0.48
1:B:261:LEU:HD13	1:B:261:LEU:H	1.78	0.48
1:B:261:LEU:CD2	1:B:263:ARG:HB2	2.43	0.48
1:B:743:ILE:HD12	1:B:743:ILE:H	1.78	0.48
1:B:956:GLU:H	1:B:956:GLU:CD	2.17	0.48
1:C:65:ILE:O	1:C:66:GLU:C	2.48	0.48
1:C:324:VAL:HG23	1:C:325:TYR:N	2.27	0.48
1:C:449:LEU:O	1:C:452:VAL:N	2.26	0.48
1:C:576:VAL:HG21	1:C:591:LEU:CD2	2.43	0.48
1:C:753:ALA:HB1	1:C:775:SER:HB2	1.95	0.48
1:C:893:GLU:O	1:C:893:GLU:HG3	2.13	0.48
1:A:72:ILE:O	1:A:72:ILE:HG22	2.13	0.48
1:A:671:ILE:O	1:A:672:VAL:C	2.51	0.48
1:B:4:PHE:O	1:B:6:ILE:N	2.44	0.48
1:B:341:VAL:CG1	1:B:342:LYS:N	2.76	0.48
1:C:110:LYS:HA	1:C:113:LEU:CD1	2.20	0.48
1:C:127:VAL:CA	1:C:127:VAL:CG1	2.83	0.48
1:C:252:LYS:O	1:C:260:VAL:CG1	2.57	0.48
1:C:435:MET:HA	1:C:438:ILE:HG22	1.95	0.48
1:C:545:TYR:OH	1:C:1021:PHE:HB3	2.13	0.48
1:A:190:PRO:HG2	1:A:788:ASP:HB3	1.95	0.48
1:A:281:PHE:O	1:A:282:ASN:C	2.51	0.48
1:A:819:TYR:N	1:A:822:LEU:O	2.45	0.48
1:B:174:ASP:CG	1:B:175:VAL:H	2.16	0.48
1:B:197:GLN:O	1:B:792:ARG:NH2	2.45	0.48
1:B:220:GLY:O	1:B:221:GLY:O	2.30	0.48
1:B:418:ARG:HG3	1:B:970:MET:HE3	1.92	0.48
1:B:423:GLU:OE1	1:B:427:PRO:HD3	2.10	0.48
1:B:610:PHE:O	1:B:627:ALA:CB	2.59	0.48
1:C:4:PHE:CB	1:C:8:ARG:NH2	2.68	0.48
1:C:163:LYS:O	1:C:165:ALA:N	2.46	0.48
1:A:60:THR:CG2	1:A:119:PRO:CD	2.90	0.48
1:A:189:ASN:ND2	1:A:192:GLU:HB3	2.27	0.48
1:A:289:LEU:HD23	1:A:289:LEU:C	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:GLU:O	1:A:311:ALA:O	2.32	0.48
1:A:531:VAL:CA	1:A:534:ILE:HD11	2.17	0.48
1:A:600:THR:O	1:A:601:LYS:CB	2.61	0.48
1:A:686:ASP:O	1:A:687:GLN:C	2.50	0.48
1:A:924:ASP:O	1:A:925:VAL:C	2.50	0.48
1:B:26:ALA:O	1:B:30:LEU:HB2	2.14	0.48
1:B:709:HIS:N	1:B:710:PRO:CD	2.76	0.48
1:B:912:ALA:HB1	1:B:1006:GLY:O	2.13	0.48
1:C:386:PHE:O	1:C:388:PHE:HD1	1.96	0.48
1:C:417:GLU:HB3	1:C:973:ARG:NH1	2.28	0.48
1:C:466:ILE:N	1:C:466:ILE:HD12	2.28	0.48
1:C:925:VAL:O	1:C:926:TYR:HB2	2.14	0.48
1:C:964:THR:O	1:C:967:ALA:HB3	2.13	0.48
1:A:56:THR:HG22	1:A:56:THR:O	2.12	0.48
1:A:105:VAL:HA	1:B:109:ASN:HD21	1.79	0.48
1:A:255:GLN:N	1:A:255:GLN:OE1	2.46	0.48
1:A:818:ARG:CD	1:A:821:GLY:O	2.51	0.48
1:B:327:TYR:HD2	1:B:628:PHE:HB3	1.75	0.48
1:B:335:ILE:C	1:B:337:ILE:N	2.66	0.48
1:B:648:THR:HG21	1:B:666:PHE:HA	1.95	0.48
1:B:742:SER:CB	1:B:745:ASP:OD2	2.52	0.48
1:B:892:TYR:C	1:B:894:SER:H	2.16	0.48
1:C:997:SER:HA	1:C:1000:GLN:OE1	2.12	0.48
1:C:1018:ALA:HA	1:C:1021:PHE:HB2	1.94	0.48
1:A:189:ASN:O	1:A:189:ASN:CG	2.52	0.48
1:B:407:ASP:O	1:B:410:ILE:HG22	2.13	0.48
1:B:416:VAL:HG22	1:B:431:THR:HA	1.94	0.48
1:B:932:LEU:HA	1:B:935:ILE:HD12	1.95	0.48
1:C:1:MET:HE3	1:C:439:GLN:HE22	1.75	0.48
1:C:528:THR:O	1:C:531:VAL:HG22	2.14	0.48
1:C:758:TYR:CD2	1:C:770:LYS:HE2	2.49	0.48
1:C:846:GLN:O	1:C:849:SER:OG	2.29	0.48
1:C:910:ILE:CG2	1:C:911:GLY:N	2.77	0.48
1:C:958:LYS:HD2	1:C:958:LYS:N	2.29	0.48
1:A:99:ASP:O	1:A:102:ILE:HG22	2.13	0.48
1:A:158:VAL:O	1:A:158:VAL:HG12	2.13	0.48
1:A:578:LEU:HD21	1:A:587:THR:CG2	2.42	0.48
1:A:702:LEU:HA	1:A:705:GLU:HB2	1.96	0.48
1:B:20:MET:HE2	1:B:373:PRO:O	2.13	0.48
1:B:252:LYS:HB3	1:B:260:VAL:HG11	1.95	0.48
1:B:485:ALA:O	1:B:486:LEU:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:ALA:C	2:C:1075:HOH:O	2.52	0.48
1:C:350:LEU:HD12	1:C:985:GLY:CA	2.39	0.48
1:C:545:TYR:OH	1:C:1021:PHE:CD2	2.51	0.48
1:C:913:LEU:HD23	1:C:927:PHE:CZ	2.49	0.48
1:A:218:GLN:OE1	1:A:221:GLY:HA3	2.14	0.48
1:A:307:ARG:NH1	1:A:325:TYR:CD2	2.82	0.48
1:A:391:ASN:O	1:A:392:THR:C	2.51	0.48
1:A:498:LYS:HA	1:A:498:LYS:HE2	1.95	0.48
1:A:841:MET:O	1:A:844:MET:HB3	2.14	0.48
1:B:101:ASP:O	1:B:105:VAL:HG23	2.14	0.48
1:B:298:ASN:HB2	1:B:301:ASP:OD1	2.14	0.48
1:B:362:PHE:C	1:B:364:ALA:H	2.16	0.48
1:B:409:ALA:HB2	1:B:485:ALA:HB2	1.94	0.48
1:C:644:VAL:HG12	1:C:667:ASN:HB2	1.95	0.48
1:C:950:LYS:HZ3	1:C:1030:ARG:NH1	2.11	0.48
1:C:974:PRO:O	1:C:975:ILE:C	2.52	0.48
1:A:108:GLN:CD	1:B:112:GLN:CD	2.72	0.48
1:B:219:LEU:HD12	1:B:219:LEU:H	1.79	0.48
1:B:324:VAL:O	1:B:326:PRO:HD2	2.13	0.48
1:B:341:VAL:HG13	1:B:342:LYS:N	2.29	0.48
1:B:423:GLU:OE1	1:B:427:PRO:CG	2.60	0.48
1:B:438:ILE:CD1	1:B:971:ARG:NH1	2.77	0.48
1:B:830:GLN:HE21	1:B:830:GLN:N	2.06	0.48
1:B:833:PRO:O	1:B:834:GLY:O	2.31	0.48
1:C:104:GLN:HG3	1:C:131:LYS:CG	2.42	0.48
1:C:115:MET:HE1	1:C:118:LEU:HD23	1.96	0.48
1:C:121:GLU:N	1:C:121:GLU:OE2	2.44	0.48
1:C:246:PHE:HZ	1:C:762:PHE:CB	2.27	0.48
1:C:262:LEU:HD23	1:C:268:ILE:HD11	1.95	0.48
1:C:420:MET:SD	1:C:498:LYS:HD3	2.53	0.48
1:C:536:ARG:HH21	1:C:536:ARG:HG2	1.79	0.48
1:A:251:LEU:CD1	1:A:262:LEU:HA	2.29	0.47
1:A:978:THR:C	1:A:980:LEU:H	2.16	0.47
1:A:1004:GLY:O	1:A:1005:THR:C	2.52	0.47
1:B:366:LEU:O	1:B:369:THR:N	2.41	0.47
1:B:391:ASN:H	1:B:394:THR:HG1	1.57	0.47
1:B:525:HIS:O	1:B:529:ASP:HB2	2.14	0.47
1:B:562:SER:HA	1:B:837:THR:OG1	2.14	0.47
1:B:626:ILE:HD11	1:B:628:PHE:CZ	2.49	0.47
1:B:665:ALA:O	1:B:666:PHE:CG	2.67	0.47
1:C:115:MET:HB2	1:C:116:PRO:HD3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:GLN:OE1	1:C:767:ARG:CZ	2.62	0.47
1:C:244:GLU:O	1:C:263:ARG:NH2	2.47	0.47
1:C:653:ARG:O	1:C:655:PHE:O	2.32	0.47
1:C:945:ILE:C	1:C:945:ILE:HD12	2.34	0.47
1:A:54:ALA:O	1:A:55:LYS:C	2.50	0.47
1:A:418:ARG:HH21	1:A:970:MET:HA	1.78	0.47
1:A:574:THR:HG22	1:A:665:ALA:HB2	1.96	0.47
1:A:639:GLY:O	1:A:642:ASN:N	2.37	0.47
1:A:729:ILE:O	1:A:730:ASP:HB2	2.13	0.47
1:A:964:THR:HG22	1:A:964:THR:O	2.12	0.47
1:B:58:GLN:HB2	1:B:82:SER:CB	2.44	0.47
1:B:247:GLY:HA2	1:B:268:ILE:HD11	1.78	0.47
1:B:249:ILE:O	1:B:261:LEU:HB2	2.14	0.47
1:B:280:GLU:CA	1:B:284:GLN:O	2.62	0.47
1:B:339:GLU:HB3	1:B:1000:GLN:HE22	1.79	0.47
1:B:573:MET:HE2	1:B:626:ILE:HD12	1.96	0.47
1:B:575:MET:O	1:B:663:VAL:HA	2.14	0.47
1:B:984:LEU:CD1	1:B:984:LEU:O	2.60	0.47
1:C:131:LYS:HB2	1:C:295:THR:HG21	1.96	0.47
1:C:950:LYS:HE2	1:C:1030:ARG:CZ	2.45	0.47
1:C:1024:VAL:CG1	1:C:1028:VAL:HG21	2.44	0.47
1:A:102:ILE:CA	1:A:105:VAL:HG23	2.44	0.47
1:A:111:LEU:O	1:A:112:GLN:C	2.47	0.47
1:A:538:THR:C	1:A:540:ARG:H	2.17	0.47
1:A:568:ASP:CG	1:A:637:ARG:HH12	2.16	0.47
1:A:592:ASN:O	1:A:595:THR:HB	2.14	0.47
1:A:779:TYR:N	1:A:779:TYR:CD1	2.82	0.47
1:A:920:GLY:O	1:A:921:LEU:HD23	2.14	0.47
1:A:999:ALA:HA	1:A:1002:ALA:HB3	1.97	0.47
1:B:330:THR:H	1:B:331:PRO:HD2	1.74	0.47
1:B:415:ASN:ND2	1:B:438:ILE:HD13	2.29	0.47
1:B:489:THR:N	1:B:490:PRO:HD2	2.29	0.47
1:B:560:PRO:O	1:B:922:THR:OG1	2.32	0.47
1:B:889:ALA:O	1:B:892:TYR:O	2.33	0.47
1:B:988:PRO:O	1:B:989:LEU:CB	2.45	0.47
1:B:1024:VAL:O	1:B:1025:PHE:CB	2.62	0.47
1:C:13:TRP:O	1:C:17:ILE:HD13	2.14	0.47
1:C:57:VAL:CG1	1:C:88:VAL:HG23	2.45	0.47
1:C:300:LEU:O	1:C:303:ALA:N	2.48	0.47
1:A:113:LEU:HD23	1:C:127:VAL:O	2.14	0.47
1:A:455:PRO:HB2	1:A:877:TYR:HE1	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:SER:OG	1:A:482:VAL:N	2.46	0.47
1:A:1019:ILE:O	1:A:1023:PRO:HG3	2.14	0.47
1:B:20:MET:O	1:B:23:GLY:O	2.32	0.47
1:B:281:PHE:O	1:B:284:GLN:HB3	2.15	0.47
1:B:418:ARG:NE	1:B:970:MET:SD	2.87	0.47
1:B:548:ILE:HD13	1:B:1017:LEU:HD23	1.95	0.47
1:B:953:MET:HA	1:B:958:LYS:HA	1.96	0.47
1:B:972:LEU:CD1	1:B:976:LEU:CD2	2.92	0.47
1:C:71:GLY:C	1:C:72:ILE:HG13	2.33	0.47
1:C:358:PHE:CB	1:C:977:MET:HE2	2.25	0.47
1:C:978:THR:O	1:C:981:ALA:N	2.47	0.47
1:A:96:SER:OG	1:A:97:GLY:N	2.44	0.47
1:A:277:ILE:HA	1:A:613:ASN:O	2.13	0.47
1:A:438:ILE:HD13	1:A:438:ILE:H	1.79	0.47
1:A:736:ALA:HA	1:A:741:VAL:HG13	1.95	0.47
1:A:877:TYR:OH	1:A:932:LEU:HD11	2.15	0.47
1:B:185:ARG:NH2	2:B:1054:HOH:O	2.47	0.47
1:B:450:SER:O	1:B:451:ALA:C	2.50	0.47
1:B:600:THR:O	1:B:603:LYS:HG2	2.15	0.47
1:C:66:GLU:HB3	1:C:78:MET:CE	2.45	0.47
1:C:438:ILE:O	1:C:441:ALA:HB3	2.14	0.47
1:B:158:VAL:CA	1:B:162:MET:HG2	2.36	0.47
1:B:355:MET:SD	1:B:368:PRO:HB2	2.54	0.47
1:B:568:ASP:HA	1:B:644:VAL:HG21	1.96	0.47
1:B:729:ILE:CG1	1:B:730:ASP:H	2.24	0.47
1:B:750:LEU:C	1:B:750:LEU:CD1	2.82	0.47
1:B:864:TYR:O	1:B:868:LEU:HB2	2.14	0.47
1:B:892:TYR:HB2	1:B:897:ILE:HD11	1.95	0.47
1:B:944:LEU:HB2	1:B:975:ILE:HD11	1.96	0.47
1:C:1:MET:HE1	1:C:439:GLN:HE22	1.80	0.47
1:C:140:VAL:O	1:C:140:VAL:HG12	2.13	0.47
1:C:474:ILE:O	1:C:478:MET:HB2	2.15	0.47
1:C:767:ARG:HG2	1:C:769:LYS:HD3	1.96	0.47
1:A:65:ILE:CA	1:A:66:GLU:N	2.66	0.47
1:A:65:ILE:C	1:A:65:ILE:HD12	2.34	0.47
1:A:69:MET:HA	1:A:69:MET:CE	2.44	0.47
1:A:95:GLU:O	1:A:98:THR:CG2	2.62	0.47
1:A:114:ALA:O	1:A:115:MET:C	2.53	0.47
1:A:130:GLU:HG2	1:B:113:LEU:HD11	1.97	0.47
1:A:185:ARG:NH2	1:A:774:MET:HE2	2.29	0.47
1:A:200:PRO:CG	1:A:749:THR:HG23	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:LEU:HD22	1:A:402:ILE:CD1	2.45	0.47
1:A:674:LEU:HD13	1:A:675:GLY:N	2.30	0.47
1:A:1015:THR:C	1:A:1017:LEU:H	2.18	0.47
1:A:1026:PHE:O	1:A:1030:ARG:HB2	2.14	0.47
1:B:85:THR:HG23	1:B:87:THR:HB	1.95	0.47
1:B:144:ASN:OD1	1:B:149:MET:HG3	2.15	0.47
1:B:166:ILE:HG22	1:B:167:SER:N	2.30	0.47
1:B:314:GLU:HA	1:B:317:PHE:CD2	2.50	0.47
1:B:467:TYR:O	1:B:470:PHE:HB2	2.14	0.47
1:B:612:VAL:HG23	1:B:626:ILE:O	2.15	0.47
1:B:908:GLY:C	1:B:910:ILE:H	2.17	0.47
1:B:978:THR:HG23	1:B:979:SER:N	2.30	0.47
1:C:1:MET:CB	1:C:2:PRO:HD2	2.21	0.47
1:C:62:THR:O	1:C:66:GLU:HG3	2.15	0.47
1:C:66:GLU:HB3	1:C:78:MET:HE1	1.97	0.47
1:C:300:LEU:O	1:C:301:ASP:C	2.53	0.47
1:C:327:TYR:HD1	1:C:571:VAL:HB	1.80	0.47
1:C:415:ASN:HD21	1:C:434:SER:CB	2.27	0.47
1:C:417:GLU:OE2	1:C:417:GLU:CA	2.55	0.47
1:C:607:GLU:HB2	1:C:632:LYS:HD3	1.97	0.47
1:C:925:VAL:C	1:C:927:PHE:N	2.68	0.47
1:C:934:THR:O	1:C:935:ILE:C	2.52	0.47
1:A:221:GLY:C	1:A:222:THR:O	2.50	0.47
1:A:711:ASP:C	1:A:713:LEU:H	2.18	0.47
1:B:17:ILE:HG21	1:C:886:LEU:HD21	1.97	0.47
1:B:314:GLU:O	1:B:316:PHE:N	2.47	0.47
1:B:354:VAL:HG21	1:B:981:ALA:HA	1.96	0.47
1:B:418:ARG:HH21	1:B:970:MET:HG2	1.80	0.47
1:B:425:LEU:HA	1:B:426:PRO:HD3	1.70	0.47
1:B:904:VAL:HG13	1:B:907:LEU:CD1	2.25	0.47
1:B:945:ILE:HG13	1:B:946:VAL:N	2.30	0.47
1:A:8:ARG:O	1:A:8:ARG:HG3	2.15	0.47
1:A:150:THR:O	1:A:151:GLN:C	2.54	0.47
1:A:223:PRO:HD3	1:B:275:TYR:CB	2.45	0.47
1:A:298:ASN:HB3	1:A:301:ASP:HB2	1.97	0.47
1:A:426:PRO:CB	1:A:427:PRO:HD2	2.45	0.47
1:A:695:LEU:HG	1:A:695:LEU:O	2.14	0.47
1:A:831:ALA:HA	1:A:840:ALA:CB	2.45	0.47
1:B:343:THR:HG21	1:B:1000:GLN:OE1	2.15	0.47
1:B:588:GLN:OE1	1:B:588:GLN:HA	2.14	0.47
1:B:692:HIS:CE1	1:B:723:ASP:OD1	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:VAL:O	1:C:32:VAL:CG1	2.56	0.47
1:C:355:MET:HA	1:C:355:MET:CE	2.45	0.47
1:C:688:ALA:C	1:C:690:LEU:N	2.66	0.47
1:C:695:LEU:O	1:C:696:THR:C	2.54	0.47
1:A:118:LEU:HA	1:A:118:LEU:HD23	1.50	0.47
1:B:57:VAL:HG11	1:B:86:GLY:HA2	1.97	0.47
1:B:262:LEU:HD22	1:B:266:ALA:HB3	1.96	0.47
1:B:428:LYS:O	1:B:432:ARG:HB2	2.15	0.47
1:B:790:TYR:HD1	1:B:800:PRO:N	2.13	0.47
1:B:792:ARG:HB2	1:B:798:MET:HE1	1.97	0.47
1:C:184:MET:HE3	1:C:270:LEU:HA	1.97	0.47
1:C:393:LEU:C	1:C:395:MET:H	2.18	0.47
1:C:705:GLU:C	1:C:707:ALA:N	2.67	0.47
1:C:721:LEU:HD23	1:C:721:LEU:O	2.15	0.47
1:A:58:GLN:HE21	1:A:816:LEU:CD1	2.28	0.46
1:A:713:LEU:HB2	1:A:833:PRO:CD	2.45	0.46
1:A:922:THR:C	1:A:924:ASP:H	2.18	0.46
1:B:115:MET:HE1	1:B:127:VAL:CG2	2.36	0.46
1:B:538:THR:H	1:B:540:ARG:HH21	1.61	0.46
1:B:556:PHE:CA	1:B:913:LEU:HD21	2.46	0.46
1:B:979:SER:HB3	1:B:1011:MET:HE3	1.97	0.46
1:C:315:PRO:HB2	1:C:316:PHE:CD1	2.50	0.46
1:C:332:PHE:CE1	1:C:569:GLN:HG2	2.50	0.46
1:C:578:LEU:CD2	1:C:590:VAL:HG21	2.45	0.46
1:C:713:LEU:CD2	1:C:835:LYS:H	2.24	0.46
1:C:729:ILE:HD11	1:C:786:ILE:CD1	2.33	0.46
1:C:872:GLN:HB2	1:C:875:SER:CB	2.37	0.46
1:A:335:ILE:HD12	1:A:335:ILE:C	2.36	0.46
1:B:174:ASP:CG	1:B:175:VAL:N	2.69	0.46
1:B:217:GLY:HA3	1:C:754:TRP:O	2.16	0.46
1:B:375:VAL:HG22	1:B:484:VAL:HG21	1.97	0.46
1:B:538:THR:HG23	1:B:540:ARG:HH22	1.77	0.46
1:B:546:LEU:O	1:B:550:VAL:HB	2.15	0.46
1:B:690:LEU:HD22	1:B:694:LYS:HB2	1.97	0.46
1:B:743:ILE:O	1:B:747:ASN:ND2	2.48	0.46
1:C:52:ALA:O	1:C:53:ASP:CG	2.53	0.46
1:C:169:THR:CG2	1:C:172:VAL:CG2	2.93	0.46
1:C:228:GLN:O	1:C:228:GLN:HG3	2.15	0.46
1:C:259:ARG:CB	1:C:259:ARG:NH1	2.77	0.46
1:C:279:ALA:HA	1:C:611:ALA:O	2.16	0.46
1:C:399:VAL:O	1:C:401:ALA:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:445:ILE:HD13	1:C:940:LYS:HE3	1.97	0.46
1:C:719:ASN:N	2:C:1063:HOH:O	2.26	0.46
1:A:113:LEU:HD13	1:C:108:GLN:HE22	1.80	0.46
1:A:572:PHE:CD1	1:A:629:VAL:HG13	2.50	0.46
1:A:728:LYS:HZ2	1:C:235:ILE:HG22	1.78	0.46
1:A:822:LEU:O	1:A:823:PRO:C	2.52	0.46
1:A:909:VAL:O	1:A:912:ALA:CB	2.59	0.46
1:B:42:ALA:HA	1:B:93:THR:HA	1.97	0.46
1:B:189:ASN:HB3	1:B:192:GLU:HB3	1.98	0.46
1:B:345:VAL:HG12	1:B:349:ILE:CD1	2.45	0.46
1:B:355:MET:CE	1:B:369:THR:HG22	2.46	0.46
1:B:366:LEU:O	1:B:370:ILE:HG13	2.15	0.46
1:B:804:PHE:O	1:B:805:SER:CB	2.63	0.46
1:B:898:PRO:O	1:B:899:PHE:C	2.53	0.46
1:C:16:ALA:HB2	1:C:488:LEU:HD22	1.97	0.46
1:C:26:ALA:O	1:C:30:LEU:CG	2.64	0.46
1:C:559:LEU:HD13	1:C:917:THR:CG2	2.45	0.46
1:C:674:LEU:HD21	1:C:862:MET:N	2.29	0.46
1:C:989:LEU:HD12	1:C:1000:GLN:HA	1.96	0.46
1:A:135:SER:O	1:A:136:PHE:CG	2.69	0.46
1:A:316:PHE:O	1:A:321:LEU:HD11	2.15	0.46
1:A:741:VAL:HG22	1:A:746:ILE:HD11	1.97	0.46
1:A:822:LEU:HG	2:A:1055:HOH:O	2.15	0.46
1:B:11:PHE:O	1:B:14:VAL:N	2.48	0.46
1:B:316:PHE:CE2	1:C:687:GLN:HG3	2.50	0.46
1:B:693:GLU:C	1:B:695:LEU:N	2.68	0.46
1:C:169:THR:HG22	1:C:172:VAL:CG2	2.41	0.46
1:C:470:PHE:CD2	1:C:929:VAL:HG11	2.50	0.46
1:C:897:ILE:HD13	1:C:950:LYS:HG3	1.98	0.46
1:C:1022:VAL:O	1:C:1023:PRO:C	2.50	0.46
1:A:203:VAL:HG13	1:A:262:LEU:HD11	1.97	0.46
1:A:713:LEU:CG	1:A:832:ALA:HA	2.46	0.46
1:A:729:ILE:HD13	1:C:234:ILE:HG23	1.97	0.46
1:A:1015:THR:OG1	1:A:1016:VAL:N	2.48	0.46
1:B:41:PRO:HG2	1:B:98:THR:CG2	2.46	0.46
1:B:104:GLN:HG2	1:B:105:VAL:N	2.27	0.46
1:B:287:SER:OG	1:B:288:GLY:N	2.49	0.46
1:B:518:ARG:HA	1:B:521:GLU:CG	2.46	0.46
1:B:518:ARG:O	1:B:520:PHE:N	2.48	0.46
1:B:1020:PHE:O	1:B:1023:PRO:HG2	2.15	0.46
2:B:1060:HOH:O	1:C:110:LYS:CD	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:THR:HG22	1:C:61:VAL:HG23	1.97	0.46
1:C:321:LEU:C	1:C:321:LEU:HD13	2.36	0.46
1:C:696:THR:O	1:C:697:GLN:C	2.52	0.46
1:A:109:ASN:CG	1:C:108:GLN:OE1	2.53	0.46
1:A:166:ILE:HG22	1:A:172:VAL:HG11	1.98	0.46
1:A:252:LYS:HB3	1:A:260:VAL:CG2	2.45	0.46
1:A:552:MET:HB2	1:A:910:ILE:HG23	1.96	0.46
1:A:572:PHE:CE1	1:A:629:VAL:CG1	2.99	0.46
1:A:820:ASN:HB3	1:C:168:ARG:NH2	2.31	0.46
1:B:174:ASP:OD1	1:B:175:VAL:N	2.49	0.46
1:B:613:ASN:O	1:B:625:GLY:HA2	2.16	0.46
1:B:693:GLU:O	1:B:695:LEU:N	2.49	0.46
1:C:58:GLN:C	2:C:1079:HOH:O	2.54	0.46
1:C:355:MET:CE	1:C:977:MET:HG2	2.45	0.46
1:C:418:ARG:NH2	1:C:948:PHE:HZ	2.14	0.46
1:C:666:PHE:N	1:C:666:PHE:HD2	2.13	0.46
1:C:895:TRP:HA	1:C:895:TRP:CE3	2.51	0.46
1:A:58:GLN:NE2	1:A:816:LEU:CD1	2.78	0.46
1:A:349:ILE:N	1:A:349:ILE:CD1	2.79	0.46
1:A:639:GLY:O	1:A:640:GLU:C	2.54	0.46
1:B:213:GLN:CG	1:C:56:THR:HG23	2.45	0.46
1:B:252:LYS:HG2	1:B:253:VAL:H	1.80	0.46
1:B:470:PHE:O	1:B:471:SER:C	2.52	0.46
1:B:819:TYR:O	1:B:820:ASN:C	2.54	0.46
1:B:920:GLY:O	1:B:921:LEU:O	2.34	0.46
1:C:400:LEU:HD12	1:C:930:GLY:HA2	1.98	0.46
1:C:663:VAL:HG12	1:C:664:PHE:N	2.30	0.46
1:A:187:TRP:HH2	1:C:223:PRO:HG3	1.79	0.46
1:A:443:VAL:O	1:A:444:GLY:C	2.54	0.46
1:A:572:PHE:N	1:A:572:PHE:HD1	2.13	0.46
1:A:576:VAL:HG11	1:A:591:LEU:CD2	2.45	0.46
1:B:219:LEU:HD21	1:C:783:PRO:HG3	1.97	0.46
1:B:231:ASN:O	1:B:231:ASN:CG	2.52	0.46
1:B:344:LEU:O	1:B:347:ALA:HB3	2.16	0.46
1:B:671:ILE:HB	1:B:672:VAL:H	1.50	0.46
1:B:716:VAL:HA	1:B:828:LEU:O	2.16	0.46
1:B:897:ILE:HG13	1:B:898:PRO:CD	2.46	0.46
1:B:973:ARG:CG	1:B:974:PRO:CD	2.92	0.46
1:C:356:TYR:C	1:C:358:PHE:H	2.18	0.46
1:A:23:GLY:O	1:A:27:ILE:HG12	2.16	0.46
1:A:44:THR:C	1:A:45:ILE:HG13	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:GLU:OE2	1:A:818:ARG:HD2	2.16	0.46
1:A:988:PRO:O	1:A:989:LEU:C	2.54	0.46
1:B:20:MET:HE2	1:B:377:LEU:HD12	1.98	0.46
1:B:396:PHE:CD2	1:B:1003:VAL:HG21	2.50	0.46
1:B:429:GLU:HA	1:B:432:ARG:HB3	1.97	0.46
1:B:575:MET:HA	1:B:626:ILE:HG22	1.96	0.46
1:B:778:LYS:O	1:B:779:TYR:CB	2.64	0.46
1:C:49:TYR:HB3	1:C:52:ALA:HB3	1.98	0.46
1:C:66:GLU:O	1:C:69:MET:N	2.49	0.46
1:C:165:ALA:O	1:C:166:ILE:O	2.34	0.46
1:C:307:ARG:HA	1:C:310:LEU:HD12	1.98	0.46
1:C:514:GLY:O	1:C:518:ARG:HG3	2.16	0.46
1:C:545:TYR:CZ	1:C:1025:PHE:CZ	3.04	0.46
1:A:171:GLY:O	1:A:294:ALA:CB	2.64	0.46
1:A:371:ALA:O	1:A:372:VAL:C	2.54	0.46
1:A:428:LYS:HE3	1:A:429:GLU:OE2	2.15	0.46
1:A:521:GLU:N	1:A:522:LYS:HE2	2.31	0.46
1:A:543:VAL:HG22	1:A:544:LEU:H	1.80	0.46
1:B:686:ASP:CB	1:B:823:PRO:O	2.62	0.46
1:C:228:GLN:NE2	1:C:230:LEU:O	2.49	0.46
1:C:367:ILE:HG13	1:C:368:PRO:N	2.30	0.46
1:C:446:ALA:C	1:C:448:VAL:H	2.20	0.46
1:C:549:VAL:C	1:C:551:GLY:H	2.18	0.46
1:C:711:ASP:CG	1:C:712:MET:N	2.70	0.46
1:C:759:VAL:O	1:C:760:ASN:CB	2.47	0.46
1:C:818:ARG:NH2	1:C:821:GLY:O	2.47	0.46
1:C:945:ILE:CG2	1:C:1022:VAL:HG11	2.46	0.46
1:A:427:PRO:HG3	1:A:497:LEU:O	2.16	0.45
1:B:45:ILE:CG2	1:B:46:SER:N	2.79	0.45
1:B:74:ASN:O	1:B:94:PHE:CB	2.62	0.45
1:B:112:GLN:HB2	2:B:1055:HOH:O	2.16	0.45
1:B:157:TYR:O	1:B:161:ASN:ND2	2.45	0.45
1:B:162:MET:CB	1:B:313:MET:SD	3.04	0.45
1:B:170:SER:C	1:B:172:VAL:H	2.19	0.45
1:B:189:ASN:HD22	1:B:190:PRO:HD2	1.81	0.45
1:B:193:LEU:HD23	1:B:265:VAL:HG21	1.98	0.45
1:B:579:PRO:HD3	1:B:660:ASP:O	2.16	0.45
1:B:597:TYR:CE1	1:B:654:ALA:CB	2.99	0.45
1:B:602:GLU:CD	1:B:650:ARG:HH21	2.19	0.45
1:B:714:THR:HG22	1:B:831:ALA:N	2.30	0.45
1:B:907:LEU:O	1:B:910:ILE:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:939:ALA:O	1:B:943:ILE:HB	2.15	0.45
1:B:975:ILE:N	1:B:975:ILE:CD1	2.78	0.45
1:B:987:MET:HE2	1:B:991:ILE:HG23	1.98	0.45
1:B:1005:THR:CG2	1:B:1005:THR:O	2.60	0.45
1:C:44:THR:O	1:C:45:ILE:C	2.54	0.45
1:C:88:VAL:HG12	1:C:89:GLN:N	2.32	0.45
1:C:114:ALA:HA	1:C:117:LEU:HD12	1.97	0.45
1:C:143:ILE:CG2	1:C:284:GLN:NE2	2.64	0.45
1:C:246:PHE:O	1:C:249:ILE:HG13	2.17	0.45
1:C:350:LEU:HD13	1:C:984:LEU:HD22	1.93	0.45
1:C:491:ALA:O	1:C:493:CYS:N	2.38	0.45
1:C:695:LEU:HD22	1:C:825:MET:CE	2.46	0.45
1:C:939:ALA:O	1:C:943:ILE:CG1	2.64	0.45
1:A:189:ASN:HB2	1:A:779:TYR:CZ	2.51	0.45
1:A:243:THR:HG22	1:A:268:ILE:CG2	2.46	0.45
1:A:552:MET:C	1:A:554:TYR:N	2.69	0.45
1:A:569:GLN:O	1:A:570:GLY:C	2.55	0.45
1:A:1018:ALA:HB1	1:A:1022:VAL:HG13	1.95	0.45
1:B:513:PHE:N	1:B:513:PHE:CD1	2.83	0.45
1:B:539:GLY:C	1:B:541:TYR:H	2.20	0.45
1:B:545:TYR:C	1:B:547:ILE:H	2.20	0.45
1:B:633:ASP:CG	1:B:634:TRP:N	2.68	0.45
1:C:111:LEU:C	1:C:111:LEU:HD13	2.35	0.45
1:C:162:MET:O	1:C:166:ILE:HG12	2.16	0.45
1:C:343:THR:O	1:C:344:LEU:C	2.55	0.45
1:C:399:VAL:C	1:C:401:ALA:N	2.70	0.45
1:C:547:ILE:HA	1:C:550:VAL:HG12	1.98	0.45
1:C:626:ILE:HD13	1:C:627:ALA:H	1.80	0.45
1:C:907:LEU:HD23	1:C:1018:ALA:HA	1.99	0.45
1:C:1017:LEU:O	1:C:1017:LEU:CD2	2.56	0.45
1:A:696:THR:O	1:A:699:ARG:N	2.49	0.45
1:A:913:LEU:C	1:A:915:ALA:H	2.20	0.45
1:B:970:MET:HE2	1:B:970:MET:CA	2.45	0.45
1:C:159:ALA:HB1	1:C:181:GLN:HG3	1.98	0.45
1:C:363:ARG:O	1:C:367:ILE:HG22	2.15	0.45
1:C:535:LEU:HG	1:C:535:LEU:O	2.16	0.45
1:A:552:MET:O	1:A:554:TYR:N	2.50	0.45
1:A:1022:VAL:N	1:A:1023:PRO:HD2	2.31	0.45
1:B:97:GLY:O	1:B:98:THR:O	2.34	0.45
1:B:602:GLU:O	1:B:604:ASN:N	2.50	0.45
1:B:693:GLU:O	1:B:696:THR:OG1	2.26	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:705:GLU:C	1:B:707:ALA:N	2.70	0.45
1:B:972:LEU:HD13	1:B:976:LEU:CD2	2.41	0.45
1:C:108:GLN:HG3	1:C:129:VAL:HG21	1.97	0.45
1:C:160:ALA:HA	1:C:767:ARG:CZ	2.47	0.45
1:C:614:GLY:HA2	1:C:621:GLY:O	2.17	0.45
1:C:858:ASP:OD1	1:C:859:TRP:N	2.50	0.45
1:A:294:ALA:HB3	1:A:297:ALA:HB3	1.97	0.45
1:A:740:GLY:O	1:A:794:ALA:N	2.43	0.45
1:B:659:LYS:HD3	1:B:659:LYS:C	2.36	0.45
1:B:776:GLU:CG	1:B:777:ALA:N	2.79	0.45
1:C:140:VAL:HB	1:C:289:LEU:HB2	1.99	0.45
1:C:218:GLN:HG2	1:C:232:ALA:O	2.17	0.45
1:C:685:ILE:CG1	1:C:687:GLN:OE1	2.61	0.45
1:C:897:ILE:HG12	1:C:950:LYS:CE	2.47	0.45
1:A:11:PHE:C	1:A:13:TRP:H	2.18	0.45
1:A:281:PHE:CZ	1:A:324:VAL:HG11	2.52	0.45
1:A:583:THR:HG22	1:A:584:GLN:N	2.31	0.45
1:A:607:GLU:HB2	1:A:631:LEU:O	2.17	0.45
1:B:26:ALA:HB1	1:B:384:ALA:HB2	1.98	0.45
1:B:65:ILE:HG23	1:B:111:LEU:HD13	1.98	0.45
1:B:188:MET:HE1	1:B:203:VAL:HG11	1.97	0.45
1:B:569:GLN:OE1	1:B:569:GLN:HA	2.16	0.45
1:B:680:PHE:CD1	1:B:680:PHE:C	2.90	0.45
1:B:709:HIS:O	1:B:711:ASP:N	2.50	0.45
1:B:725:PRO:HB2	1:B:809:TRP:CZ3	2.51	0.45
1:B:847:LEU:HD23	1:B:847:LEU:N	2.29	0.45
1:C:114:ALA:O	1:C:115:MET:O	2.34	0.45
1:C:577:GLN:HB3	1:C:624:THR:CG2	2.42	0.45
1:C:714:THR:CG2	1:C:716:VAL:HG23	2.46	0.45
1:C:721:LEU:CD1	1:C:815:ARG:O	2.64	0.45
1:C:758:TYR:CG	1:C:758:TYR:O	2.70	0.45
1:C:937:LEU:O	1:C:940:LYS:HB3	2.16	0.45
1:C:940:LYS:HA	1:C:943:ILE:HG12	1.99	0.45
1:C:1016:VAL:C	1:C:1018:ALA:H	2.16	0.45
1:A:1:MET:H3	1:A:2:PRO:HD2	1.75	0.45
1:A:492:LEU:HD12	1:A:492:LEU:HA	1.64	0.45
1:A:684:LEU:HD11	1:A:851:LEU:HD13	1.98	0.45
1:A:822:LEU:HA	1:A:823:PRO:HD3	1.32	0.45
1:B:376:LEU:O	1:B:379:THR:N	2.49	0.45
1:B:418:ARG:NH2	1:B:970:MET:CG	2.79	0.45
1:B:863:SER:O	1:B:864:TYR:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:868:LEU:O	1:B:869:SER:C	2.55	0.45
1:B:974:PRO:C	1:B:976:LEU:N	2.70	0.45
1:B:987:MET:CE	1:B:990:VAL:HB	2.47	0.45
1:B:1018:ALA:O	1:B:1020:PHE:N	2.50	0.45
1:C:162:MET:CB	1:C:313:MET:HE3	2.35	0.45
1:C:950:LYS:NZ	1:C:1030:ARG:NE	2.65	0.45
1:C:987:MET:HA	1:C:1008:MET:HE1	1.99	0.45
1:A:65:ILE:O	1:A:68:ASN:CB	2.63	0.45
1:B:174:ASP:C	1:B:175:VAL:HG23	2.37	0.45
1:B:187:TRP:CZ3	1:B:774:MET:CE	2.94	0.45
1:B:269:GLU:HB3	1:B:270:LEU:H	1.61	0.45
1:B:687:GLN:CD	1:B:856:GLY:HA3	2.34	0.45
1:B:987:MET:CE	1:B:987:MET:O	2.62	0.45
1:C:14:VAL:CG1	1:C:15:ILE:N	2.79	0.45
1:C:34:GLN:HA	1:C:333:VAL:CG1	2.47	0.45
1:C:176:GLN:HE21	1:C:620:ARG:HH11	1.64	0.45
1:C:242:SER:O	1:C:243:THR:C	2.55	0.45
1:C:249:ILE:HD13	1:C:249:ILE:HG21	1.61	0.45
1:C:310:LEU:HD22	1:C:323:ILE:HD13	1.99	0.45
1:C:758:TYR:HA	1:C:772:TYR:HA	1.98	0.45
1:C:774:MET:HG2	1:C:775:SER:N	2.31	0.45
1:C:779:TYR:N	1:C:779:TYR:CD2	2.83	0.45
1:A:73:ASP:O	1:A:75:LEU:N	2.42	0.45
1:A:82:SER:HB2	1:A:816:LEU:HB2	1.99	0.45
1:A:372:VAL:O	1:A:373:PRO:C	2.55	0.45
1:A:400:LEU:HD21	1:A:1003:VAL:HG22	1.98	0.45
1:A:418:ARG:NH2	1:A:970:MET:HA	2.32	0.45
1:A:713:LEU:CG	1:A:714:THR:H	2.30	0.45
1:B:271:GLY:HA3	1:B:275:TYR:OH	2.17	0.45
1:B:345:VAL:HG12	1:B:349:ILE:HD13	1.98	0.45
1:B:690:LEU:CB	1:B:694:LYS:HB2	2.38	0.45
1:B:775:SER:CB	1:B:780:ARG:HG3	2.46	0.45
1:C:104:GLN:CD	1:C:131:LYS:HE2	2.38	0.45
1:C:163:LYS:HG2	1:C:175:VAL:CG1	2.45	0.45
1:C:355:MET:HE1	1:C:977:MET:HG2	1.98	0.45
1:C:395:MET:C	1:C:397:GLY:N	2.69	0.45
1:C:439:GLN:HG3	1:C:440:GLY:N	2.32	0.45
1:C:463:THR:CG2	1:C:464:GLY:H	2.28	0.45
1:C:680:PHE:HB2	1:C:859:TRP:HZ3	1.82	0.45
1:C:753:ALA:O	1:C:775:SER:CB	2.65	0.45
1:A:102:ILE:O	1:A:106:GLN:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:LYS:HA	1:A:760:ASN:HD21	1.82	0.45
1:A:219:LEU:HD12	1:A:232:ALA:HB3	1.99	0.45
1:A:298:ASN:O	1:A:299:ALA:C	2.55	0.45
1:A:407:ASP:OD2	1:A:978:THR:HG21	2.17	0.45
1:A:418:ARG:HH11	1:A:973:ARG:NE	2.14	0.45
1:A:820:ASN:HB3	1:C:168:ARG:CZ	2.46	0.45
1:A:836:SER:OG	1:A:839:GLU:CG	2.62	0.45
1:A:897:ILE:HG21	1:A:950:LYS:CE	2.47	0.45
1:B:438:ILE:HD12	1:B:971:ARG:NH1	2.32	0.45
1:B:640:GLU:H	1:B:643:LYS:HG3	1.82	0.45
1:B:762:PHE:HE1	1:B:764:ASP:HB2	1.82	0.45
1:B:819:TYR:CE1	1:B:860:THR:OG1	2.70	0.45
1:C:497:LEU:HD13	1:C:498:LYS:H	1.81	0.45
1:C:682:PHE:HE2	1:C:702:LEU:CD1	2.29	0.45
1:A:102:ILE:C	1:A:105:VAL:HG23	2.37	0.44
1:A:115:MET:N	1:A:116:PRO:CD	2.80	0.44
1:A:330:THR:N	1:A:331:PRO:HD2	2.32	0.44
1:A:843:LEU:O	1:A:844:MET:C	2.56	0.44
1:A:846:GLN:HE21	1:A:846:GLN:HB2	1.60	0.44
1:B:341:VAL:HG23	1:B:395:MET:CE	2.47	0.44
1:B:371:ALA:O	1:B:372:VAL:C	2.55	0.44
1:B:592:ASN:HA	1:B:595:THR:HG23	2.00	0.44
1:B:640:GLU:N	1:B:643:LYS:HG3	2.32	0.44
1:B:643:LYS:C	1:B:647:ILE:HG13	2.38	0.44
1:B:762:PHE:CE1	1:B:764:ASP:HB2	2.52	0.44
1:C:72:ILE:CG2	1:C:94:PHE:CZ	3.00	0.44
1:C:130:GLU:OE1	1:C:174:ASP:HB2	2.17	0.44
1:C:166:ILE:HD11	2:C:1075:HOH:O	2.05	0.44
1:C:188:MET:HE1	1:C:200:PRO:CB	2.38	0.44
1:C:934:THR:HG22	1:C:1011:MET:SD	2.57	0.44
1:A:94:PHE:HZ	1:A:107:VAL:HG22	1.82	0.44
1:A:356:TYR:C	1:A:358:PHE:H	2.21	0.44
1:A:393:LEU:HD13	1:A:466:ILE:HG23	1.98	0.44
1:A:537:SER:O	1:A:538:THR:C	2.55	0.44
1:A:562:SER:HB3	1:A:924:ASP:HB3	1.99	0.44
1:A:713:LEU:HB2	1:A:832:ALA:HA	1.90	0.44
1:A:790:TYR:CE1	1:A:800:PRO:CG	2.96	0.44
1:B:115:MET:HA	1:B:115:MET:HE2	1.98	0.44
1:B:139:VAL:O	1:B:140:VAL:C	2.55	0.44
1:B:155:SER:O	1:B:156:ASP:C	2.55	0.44
1:B:314:GLU:C	1:B:316:PHE:H	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:778:LYS:HZ2	1:B:778:LYS:HB3	1.82	0.44
1:B:891:LEU:HD12	1:B:892:TYR:CD1	2.52	0.44
1:C:58:GLN:NE2	1:C:82:SER:O	2.50	0.44
1:C:335:ILE:HD13	1:C:634:TRP:CZ3	2.51	0.44
1:C:354:VAL:C	1:C:356:TYR:H	2.20	0.44
1:C:418:ARG:NH2	1:C:948:PHE:CZ	2.85	0.44
1:C:657:GLN:C	1:C:659:LYS:N	2.71	0.44
1:C:873:ALA:O	1:C:876:LEU:N	2.50	0.44
1:A:207:ILE:HG22	1:A:207:ILE:O	2.17	0.44
1:A:545:TYR:HE1	1:A:907:LEU:HD11	1.82	0.44
1:A:678:THR:O	1:A:679:GLY:O	2.35	0.44
1:A:702:LEU:HD11	1:A:844:MET:HE2	1.99	0.44
1:A:1029:VAL:HG12	1:A:1030:ARG:N	2.21	0.44
1:B:115:MET:HE1	1:B:127:VAL:HG11	2.00	0.44
1:B:696:THR:O	1:B:699:ARG:HB3	2.17	0.44
1:B:703:LEU:O	1:B:705:GLU:HB2	2.17	0.44
1:B:740:GLY:O	1:B:794:ALA:HB2	2.17	0.44
1:C:323:ILE:HG22	1:C:324:VAL:O	2.17	0.44
1:C:527:TYR:O	1:C:531:VAL:HG13	2.17	0.44
1:C:758:TYR:CD1	1:C:758:TYR:N	2.83	0.44
1:C:801:PHE:CD1	1:C:804:PHE:HE1	2.36	0.44
1:C:912:ALA:O	1:C:914:LEU:O	2.34	0.44
1:C:931:LEU:O	1:C:935:ILE:HB	2.17	0.44
1:C:948:PHE:O	1:C:952:LEU:HB2	2.16	0.44
1:A:94:PHE:CZ	1:A:103:ALA:HB1	2.52	0.44
1:A:178:PHE:N	1:A:178:PHE:HD1	2.15	0.44
1:A:340:VAL:HG13	1:A:399:VAL:HG23	1.96	0.44
1:A:540:ARG:O	1:A:543:VAL:HG12	2.18	0.44
1:A:978:THR:C	1:A:980:LEU:N	2.70	0.44
1:A:1018:ALA:HB1	1:A:1022:VAL:HG11	1.98	0.44
1:B:44:THR:HG22	1:B:45:ILE:O	2.17	0.44
1:B:79:SER:O	1:B:79:SER:OG	2.26	0.44
1:B:150:THR:O	1:B:151:GLN:C	2.55	0.44
1:B:188:MET:HB2	1:B:775:SER:HA	1.99	0.44
1:B:362:PHE:O	1:B:365:THR:N	2.43	0.44
1:B:520:PHE:O	1:B:523:SER:N	2.43	0.44
1:B:682:PHE:HD1	1:B:859:TRP:CZ3	2.36	0.44
1:B:785:ASP:O	1:B:788:ASP:N	2.47	0.44
1:B:804:PHE:O	1:B:805:SER:HB3	2.17	0.44
1:B:835:LYS:HD2	1:B:839:GLU:OE1	2.18	0.44
1:B:945:ILE:O	1:B:949:ALA:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:286:ALA:HB1	1:C:287:SER:H	1.48	0.44
1:C:395:MET:O	1:C:397:GLY:N	2.50	0.44
1:C:685:ILE:HD11	1:C:687:GLN:CD	2.38	0.44
1:A:130:GLU:HB3	2:A:1074:HOH:O	2.17	0.44
1:A:307:ARG:NH1	1:A:325:TYR:CE2	2.86	0.44
1:A:407:ASP:OD1	1:A:940:LYS:NZ	2.40	0.44
1:A:437:GLN:HG2	1:A:948:PHE:CE2	2.52	0.44
1:A:687:GLN:HG2	1:C:316:PHE:CD2	2.49	0.44
1:A:746:ILE:HD13	1:A:804:PHE:CE1	2.52	0.44
1:A:820:ASN:HB3	1:C:168:ARG:NH1	2.33	0.44
1:B:26:ALA:O	1:B:30:LEU:CB	2.65	0.44
1:B:702:LEU:HD22	1:B:702:LEU:HA	1.78	0.44
1:B:1021:PHE:HB3	1:B:1025:PHE:CE1	2.53	0.44
1:C:181:GLN:HG2	1:C:769:LYS:CE	2.46	0.44
1:C:197:GLN:HB3	1:C:197:GLN:HE21	1.57	0.44
1:C:434:SER:O	1:C:438:ILE:HB	2.17	0.44
1:A:83:ASP:OD1	1:A:83:ASP:C	2.56	0.44
1:A:87:THR:HG21	1:A:620:ARG:NH2	2.33	0.44
1:A:254:ASN:O	1:A:256:ASP:N	2.50	0.44
1:A:323:ILE:HG12	1:A:325:TYR:CE1	2.49	0.44
1:A:362:PHE:C	1:A:364:ALA:H	2.21	0.44
1:A:521:GLU:O	1:A:521:GLU:HG2	2.18	0.44
1:A:621:GLY:C	1:A:623:ASN:H	2.21	0.44
1:A:687:GLN:HE21	1:A:687:GLN:HB2	1.18	0.44
1:A:729:ILE:N	1:A:729:ILE:CD1	2.78	0.44
1:A:946:VAL:O	1:A:946:VAL:HG12	2.18	0.44
1:A:971:ARG:C	1:A:974:PRO:HD2	2.38	0.44
1:A:1020:PHE:C	1:A:1023:PRO:HD2	2.38	0.44
1:B:53:ASP:HB2	1:B:56:THR:HB	1.99	0.44
1:B:58:GLN:NE2	1:B:818:ARG:HH11	2.15	0.44
1:C:35:TYR:HB3	1:C:36:PRO:HD2	2.00	0.44
1:C:163:LYS:C	1:C:165:ALA:N	2.71	0.44
1:C:262:LEU:HG	1:C:268:ILE:HD11	2.00	0.44
1:C:686:ASP:HB2	1:C:695:LEU:HD12	1.98	0.44
1:C:901:VAL:HG12	1:C:942:ALA:CB	2.47	0.44
1:A:3:ASN:O	1:A:6:ILE:HD13	2.18	0.44
1:A:979:SER:O	1:A:983:ILE:HG22	2.17	0.44
1:B:118:LEU:O	1:B:119:PRO:C	2.56	0.44
1:B:338:HIS:O	1:B:341:VAL:HG12	2.18	0.44
1:B:378:GLY:O	1:B:381:ALA:HB3	2.18	0.44
1:B:682:PHE:HD1	1:B:859:TRP:CH2	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:712:MET:SD	1:B:839:GLU:HB3	2.57	0.44
1:B:767:ARG:HG2	1:B:769:LYS:HE3	2.00	0.44
1:C:169:THR:O	1:C:172:VAL:HG23	2.18	0.44
1:C:182:TYR:HA	1:C:271:GLY:O	2.18	0.44
1:C:198:LEU:HA	1:C:792:ARG:NH2	2.33	0.44
1:C:467:TYR:C	1:C:469:GLN:N	2.71	0.44
1:C:538:THR:O	1:C:540:ARG:HG2	2.18	0.44
1:C:696:THR:O	1:C:699:ARG:N	2.50	0.44
1:C:888:LEU:O	1:C:891:LEU:HB3	2.17	0.44
1:C:894:SER:C	1:C:896:SER:N	2.66	0.44
1:A:3:ASN:HA	1:A:6:ILE:HD12	1.99	0.44
1:A:313:MET:C	1:A:315:PRO:CD	2.85	0.44
1:A:594:VAL:HA	1:A:655:PHE:CZ	2.53	0.44
1:A:649:MET:CE	1:A:653:ARG:NH2	2.80	0.44
1:A:1024:VAL:CG1	1:A:1025:PHE:H	2.09	0.44
1:B:38:ILE:O	1:B:462:SER:HB2	2.18	0.44
1:B:58:GLN:NE2	1:B:818:ARG:NH1	2.66	0.44
1:C:87:THR:HG23	1:C:88:VAL:H	1.82	0.44
1:C:124:GLN:HB3	1:C:758:TYR:CE2	2.50	0.44
1:C:432:ARG:NH1	1:C:432:ARG:CG	2.62	0.44
1:C:470:PHE:O	1:C:471:SER:C	2.55	0.44
1:C:892:TYR:OH	1:C:943:ILE:HG23	2.17	0.44
1:C:1010:GLY:HA2	1:C:1013:THR:CG2	2.48	0.44
1:A:256:ASP:HB2	1:A:258:SER:HB3	1.99	0.44
1:A:339:GLU:HA	1:A:342:LYS:HG2	1.99	0.44
1:A:520:PHE:O	1:A:522:LYS:N	2.51	0.44
1:A:525:HIS:O	1:A:526:HIS:C	2.53	0.44
1:A:540:ARG:NH1	1:A:541:TYR:CZ	2.86	0.44
1:A:722:GLU:HA	2:A:1060:HOH:O	2.17	0.44
1:A:935:ILE:O	1:A:935:ILE:CG2	2.64	0.44
1:B:13:TRP:HA	1:B:13:TRP:HE3	1.80	0.44
1:B:534:ILE:HG23	1:B:541:TYR:CE2	2.53	0.44
1:C:163:LYS:O	1:C:166:ILE:CA	2.61	0.44
1:C:832:ALA:HB1	1:C:833:PRO:CD	2.48	0.44
1:C:928:GLN:O	1:C:932:LEU:HG	2.18	0.44
1:C:941:ASN:O	1:C:945:ILE:HG22	2.18	0.44
1:A:216:ALA:O	1:A:217:GLY:O	2.36	0.43
1:A:541:TYR:O	1:A:543:VAL:O	2.36	0.43
1:B:699:ARG:NH2	1:B:722:GLU:OE1	2.51	0.43
1:B:881:LEU:HD21	1:B:905:VAL:HG21	1.99	0.43
1:B:921:LEU:CD2	1:B:1005:THR:CG2	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:LYS:HE3	1:C:267:LYS:HB2	1.71	0.43
1:C:692:HIS:HE1	1:C:721:LEU:HD21	1.83	0.43
1:A:116:PRO:CA	1:A:117:LEU:HD22	2.48	0.43
1:A:455:PRO:O	1:A:876:LEU:HD13	2.18	0.43
1:A:583:THR:CG2	1:A:584:GLN:N	2.80	0.43
1:A:958:LYS:HB3	1:A:959:GLY:H	1.64	0.43
1:B:612:VAL:HG23	1:B:626:ILE:HG13	2.00	0.43
1:B:732:ASP:HB2	1:B:735:LYS:HG3	2.00	0.43
1:B:818:ARG:HH11	1:B:818:ARG:HG3	1.82	0.43
1:B:885:PHE:HE2	1:B:898:PRO:HB2	1.83	0.43
1:B:1031:ARG:O	1:B:1035:ARG:HB2	2.17	0.43
1:C:34:GLN:C	1:C:35:TYR:CG	2.91	0.43
1:C:72:ILE:CG2	1:C:94:PHE:HE2	2.23	0.43
1:C:191:ASN:HA	1:C:194:ASN:OD1	2.18	0.43
1:C:226:LYS:HG2	2:C:1072:HOH:O	2.17	0.43
1:C:262:LEU:O	1:C:264:ASP:N	2.51	0.43
1:C:379:THR:HG23	1:C:477:ALA:HB2	1.99	0.43
1:C:403:GLY:C	1:C:405:LEU:H	2.21	0.43
1:C:711:ASP:CG	1:C:712:MET:H	2.22	0.43
1:C:713:LEU:HD11	1:C:835:LYS:H	1.82	0.43
1:A:72:ILE:O	1:A:73:ASP:O	2.37	0.43
1:A:178:PHE:N	1:A:178:PHE:CD1	2.86	0.43
1:A:943:ILE:O	1:A:947:GLU:HB2	2.17	0.43
1:B:145:THR:O	1:B:146:ASP:CG	2.56	0.43
1:B:185:ARG:NH1	1:B:772:TYR:HB3	2.33	0.43
1:B:362:PHE:C	1:B:364:ALA:N	2.72	0.43
1:B:408:ASP:C	1:B:410:ILE:H	2.20	0.43
1:B:453:PHE:CZ	1:B:474:ILE:HD13	2.53	0.43
1:B:538:THR:C	1:B:540:ARG:H	2.20	0.43
1:B:538:THR:O	1:B:540:ARG:N	2.51	0.43
1:B:699:ARG:O	1:B:700:ASN:HB2	2.18	0.43
1:B:801:PHE:HA	1:B:804:PHE:CE1	2.54	0.43
1:B:922:THR:HG1	1:B:923:ASN:H	1.62	0.43
1:B:987:MET:HB3	1:B:988:PRO:HD3	1.99	0.43
1:B:999:ALA:O	1:B:1003:VAL:HG23	2.19	0.43
1:C:51:GLY:O	1:C:53:ASP:OD2	2.36	0.43
1:C:532:GLY:O	1:C:534:ILE:HD12	2.19	0.43
1:C:681:ASP:OD2	1:C:828:LEU:HD11	2.18	0.43
1:C:686:ASP:OD1	1:C:686:ASP:C	2.55	0.43
1:C:719:ASN:O	1:C:721:LEU:N	2.52	0.43
1:C:764:ASP:OD2	1:C:765:ARG:NE	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:790:TYR:CE1	1:C:800:PRO:HB3	2.52	0.43
1:A:778:LYS:HB2	1:A:778:LYS:HE2	1.48	0.43
1:B:110:LYS:HD3	1:B:110:LYS:HA	1.62	0.43
1:B:183:ALA:N	1:B:271:GLY:O	2.52	0.43
1:B:225:VAL:CG2	1:C:781:MET:HE3	2.37	0.43
1:C:35:TYR:HD2	1:C:392:THR:HG1	1.65	0.43
1:C:591:LEU:HA	1:C:591:LEU:HD13	1.67	0.43
1:C:841:MET:O	1:C:842:GLU:C	2.56	0.43
1:C:881:LEU:O	1:C:882:ILE:C	2.57	0.43
1:A:649:MET:HE3	1:A:653:ARG:CZ	2.46	0.43
1:A:818:ARG:NH2	1:A:823:PRO:HG3	2.33	0.43
1:A:857:TYR:O	1:A:857:TYR:CG	2.71	0.43
1:A:988:PRO:C	1:A:990:VAL:N	2.67	0.43
1:B:9:PRO:O	1:B:13:TRP:N	2.42	0.43
1:B:18:ILE:HG22	1:B:19:ILE:N	2.34	0.43
1:B:58:GLN:HA	1:B:62:THR:CB	2.48	0.43
1:B:234:ILE:O	1:B:234:ILE:CG2	2.50	0.43
1:B:326:PRO:HB2	1:B:327:TYR:H	1.55	0.43
1:B:831:ALA:C	1:B:833:PRO:HD2	2.39	0.43
1:C:238:THR:CG2	1:C:239:ARG:N	2.82	0.43
1:C:356:TYR:C	1:C:358:PHE:N	2.72	0.43
1:C:764:ASP:CB	1:C:765:ARG:HD2	2.49	0.43
1:C:850:LYS:O	1:C:851:LEU:C	2.57	0.43
1:C:896:SER:C	1:C:898:PRO:HD2	2.39	0.43
1:A:222:THR:HG22	1:A:223:PRO:CD	2.48	0.43
1:A:454:VAL:N	1:A:455:PRO:HD2	2.33	0.43
1:A:904:VAL:HG21	1:A:942:ALA:CB	2.45	0.43
1:B:109:ASN:ND2	1:B:112:GLN:HE22	2.14	0.43
1:B:115:MET:HA	1:B:115:MET:HE3	2.00	0.43
1:B:207:ILE:HG22	1:B:759:VAL:HG11	1.97	0.43
1:B:396:PHE:HE2	1:B:999:ALA:HB1	1.82	0.43
1:B:776:GLU:HG2	1:B:777:ALA:H	1.83	0.43
1:B:819:TYR:O	1:B:822:LEU:N	2.51	0.43
1:B:873:ALA:C	1:B:875:SER:N	2.71	0.43
1:B:904:VAL:C	1:B:906:PRO:HD2	2.39	0.43
1:B:1030:ARG:C	1:B:1032:ARG:H	2.22	0.43
1:C:4:PHE:CG	1:C:8:ARG:NH2	2.87	0.43
1:C:44:THR:HG22	1:C:91:THR:CA	2.47	0.43
1:C:82:SER:CB	1:C:88:VAL:HA	2.19	0.43
1:C:91:THR:CA	1:C:91:THR:HB	2.20	0.43
1:C:695:LEU:O	1:C:696:THR:O	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:768:VAL:O	1:C:768:VAL:CG1	2.66	0.43
1:A:11:PHE:O	1:A:13:TRP:N	2.52	0.43
1:A:65:ILE:HG13	1:A:66:GLU:H	1.83	0.43
1:A:113:LEU:C	1:A:116:PRO:HD2	2.39	0.43
1:A:418:ARG:O	1:A:421:ALA:HB3	2.19	0.43
1:A:574:THR:HA	1:A:665:ALA:HA	2.01	0.43
1:A:809:TRP:O	1:A:810:GLU:CB	2.51	0.43
1:A:818:ARG:HG2	2:A:1062:HOH:O	2.16	0.43
1:B:245:GLU:O	1:B:248:LYS:N	2.51	0.43
1:B:415:ASN:O	1:B:434:SER:OG	2.28	0.43
1:B:639:GLY:O	1:B:641:GLU:O	2.37	0.43
1:C:17:ILE:N	1:C:17:ILE:HD12	2.34	0.43
1:C:118:LEU:N	1:C:118:LEU:CD1	2.82	0.43
1:C:534:ILE:H	1:C:534:ILE:HG13	1.55	0.43
1:C:544:LEU:HD12	1:C:1021:PHE:HZ	1.83	0.43
1:C:578:LEU:HA	1:C:661:ALA:HB1	2.00	0.43
1:C:685:ILE:O	1:C:685:ILE:HG13	2.08	0.43
1:C:878:ALA:C	1:C:880:SER:N	2.70	0.43
1:A:2:PRO:O	1:A:6:ILE:N	2.51	0.43
1:A:13:TRP:CZ2	1:A:492:LEU:HD11	2.54	0.43
1:A:43:VAL:HA	1:A:130:GLU:O	2.19	0.43
1:A:66:GLU:CD	2:A:1054:HOH:O	2.56	0.43
1:A:359:LEU:HD13	1:A:359:LEU:HA	1.81	0.43
1:A:822:LEU:N	1:A:822:LEU:CD2	2.81	0.43
1:B:228:GLN:HE21	1:B:228:GLN:CA	2.32	0.43
1:B:231:ASN:HD22	1:B:232:ALA:N	2.17	0.43
1:B:345:VAL:CA	1:B:348:ILE:HD12	2.43	0.43
1:A:166:ILE:HD13	1:A:166:ILE:H	1.78	0.43
1:A:367:ILE:HD13	1:A:489:THR:HG23	2.00	0.43
1:A:845:GLU:CD	1:A:859:TRP:HE1	2.22	0.43
1:B:144:ASN:O	1:B:144:ASN:ND2	2.52	0.43
1:B:327:TYR:HB2	1:B:628:PHE:HB3	1.99	0.43
1:B:492:LEU:O	1:B:496:MET:HB2	2.18	0.43
1:B:556:PHE:C	1:B:558:ARG:H	2.22	0.43
1:B:892:TYR:CG	1:B:897:ILE:HD11	2.54	0.43
1:B:1022:VAL:HB	1:B:1026:PHE:CZ	2.54	0.43
1:C:14:VAL:CG1	1:C:15:ILE:H	2.31	0.43
1:C:184:MET:HE1	1:C:270:LEU:N	2.34	0.43
1:C:529:ASP:O	1:C:531:VAL:O	2.36	0.43
1:C:591:LEU:HD23	1:C:613:ASN:HB2	1.99	0.43
1:C:653:ARG:HG3	1:C:654:ALA:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:728:LYS:CG	1:C:729:ILE:N	2.76	0.43
1:A:182:TYR:CB	1:A:270:LEU:HD12	2.49	0.43
1:A:197:GLN:HA	1:A:798:MET:HE2	2.00	0.43
1:A:394:THR:CG2	1:A:395:MET:HE2	2.48	0.43
1:A:531:VAL:O	1:A:534:ILE:HG13	2.19	0.43
1:A:1023:PRO:C	1:A:1024:VAL:O	2.58	0.43
1:B:173:GLY:H	1:B:294:ALA:H	1.65	0.43
1:B:328:ASP:OD2	1:B:330:THR:HB	2.19	0.43
1:B:411:VAL:HG12	1:B:974:PRO:HB3	2.00	0.43
1:B:489:THR:HB	1:B:490:PRO:CD	2.49	0.43
1:B:819:TYR:CZ	1:B:860:THR:OG1	2.72	0.43
1:C:47:ALA:HB1	1:C:122:VAL:CG1	2.49	0.43
1:C:158:VAL:HG12	1:C:159:ALA:N	2.29	0.43
1:C:163:LYS:HB2	2:C:1078:HOH:O	2.18	0.43
1:C:166:ILE:HG21	1:C:291:ILE:HD11	2.01	0.43
1:C:194:ASN:HB3	2:C:1059:HOH:O	2.19	0.43
1:C:247:GLY:O	1:C:263:ARG:HB2	2.19	0.43
1:C:778:LYS:CD	1:C:779:TYR:CE2	3.01	0.43
1:A:59:ASP:HB3	1:C:763:ILE:CD1	2.47	0.42
1:A:66:GLU:O	1:A:68:ASN:N	2.52	0.42
1:A:83:ASP:OD1	1:A:84:SER:N	2.52	0.42
1:A:108:GLN:HG3	1:B:112:GLN:NE2	2.30	0.42
1:A:308:ALA:O	1:A:311:ALA:HB3	2.19	0.42
1:A:449:LEU:O	1:A:451:ALA:O	2.37	0.42
1:B:48:SER:C	1:B:49:TYR:CG	2.93	0.42
1:B:330:THR:O	1:B:330:THR:CG2	2.67	0.42
1:B:709:HIS:C	1:B:711:ASP:N	2.72	0.42
1:B:760:ASN:O	1:B:771:VAL:HB	2.19	0.42
1:B:858:ASP:OD1	1:B:859:TRP:N	2.52	0.42
1:C:92:LEU:HD22	1:C:107:VAL:CG2	2.47	0.42
1:C:169:THR:C	1:C:169:THR:CG2	2.87	0.42
1:C:354:VAL:HG13	1:C:980:LEU:HD23	2.01	0.42
1:C:532:GLY:O	1:C:534:ILE:N	2.52	0.42
1:C:701:GLN:O	1:C:702:LEU:C	2.58	0.42
1:A:57:VAL:HG12	1:A:58:GLN:CA	2.49	0.42
1:A:156:ASP:O	1:A:157:TYR:C	2.55	0.42
1:A:208:LYS:HA	1:A:760:ASN:ND2	2.34	0.42
1:A:219:LEU:HD22	1:B:781:MET:O	2.18	0.42
1:A:337:ILE:O	1:A:339:GLU:O	2.38	0.42
1:A:351:VAL:HG13	1:A:410:ILE:HD11	2.00	0.42
1:A:453:PHE:CZ	1:A:474:ILE:HG21	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:TYR:HB2	1:A:1021:PHE:CZ	2.53	0.42
1:A:947:GLU:O	1:A:951:ASP:CB	2.63	0.42
1:A:978:THR:HG23	1:A:979:SER:N	2.33	0.42
1:B:45:ILE:HD13	1:B:65:ILE:CG2	2.50	0.42
1:B:318:PRO:HD2	1:B:321:LEU:HD22	2.00	0.42
1:B:418:ARG:NH2	1:B:970:MET:HG3	2.35	0.42
1:C:54:ALA:CB	1:C:84:SER:HB2	2.22	0.42
1:C:159:ALA:CB	1:C:181:GLN:HG3	2.49	0.42
1:C:409:ALA:O	1:C:410:ILE:O	2.37	0.42
1:C:484:VAL:HG13	1:C:488:LEU:HB3	2.00	0.42
1:C:532:GLY:C	1:C:534:ILE:N	2.71	0.42
1:A:25:LEU:HD13	1:A:25:LEU:C	2.40	0.42
1:A:108:GLN:OE1	1:B:112:GLN:NE2	2.53	0.42
1:A:276:ASP:HB3	1:C:222:THR:CG2	2.42	0.42
1:A:471:SER:O	1:A:472:ILE:C	2.57	0.42
1:A:532:GLY:HA2	1:A:965:LEU:HD11	2.01	0.42
1:A:593:GLU:O	1:A:594:VAL:C	2.55	0.42
1:A:702:LEU:HD11	1:A:844:MET:HE3	2.01	0.42
1:A:937:LEU:HD12	1:A:1011:MET:SD	2.59	0.42
1:A:948:PHE:CD2	1:A:948:PHE:N	2.86	0.42
1:B:404:LEU:O	1:B:406:VAL:N	2.53	0.42
1:B:715:SER:O	1:B:716:VAL:C	2.57	0.42
1:B:863:SER:C	1:B:865:GLN:N	2.71	0.42
1:B:1004:GLY:O	1:B:1007:VAL:HG12	2.18	0.42
1:C:21:LEU:O	1:C:24:GLY:N	2.50	0.42
1:C:123:GLN:HB3	1:C:124:GLN:H	1.68	0.42
1:C:344:LEU:O	1:C:348:ILE:HG23	2.19	0.42
1:C:524:THR:O	1:C:527:TYR:N	2.50	0.42
1:C:547:ILE:O	1:C:551:GLY:N	2.52	0.42
1:C:750:LEU:HD23	1:C:750:LEU:HA	1.53	0.42
1:C:983:ILE:HG23	1:C:1008:MET:HG3	2.01	0.42
1:A:455:PRO:HG3	1:A:880:SER:HB2	2.02	0.42
1:A:562:SER:OG	1:A:563:PHE:N	2.51	0.42
1:B:114:ALA:O	1:B:115:MET:C	2.58	0.42
1:B:671:ILE:H	1:B:671:ILE:HG12	1.71	0.42
1:B:778:LYS:HZ2	1:B:778:LYS:H	1.66	0.42
1:B:870:GLY:O	1:B:872:GLN:N	2.52	0.42
1:B:885:PHE:CD2	1:B:898:PRO:HB2	2.55	0.42
1:C:18:ILE:O	1:C:19:ILE:C	2.56	0.42
1:C:144:ASN:HA	1:C:320:GLY:O	2.20	0.42
1:C:417:GLU:OE2	1:C:420:MET:CE	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:491:ALA:C	1:C:493:CYS:H	2.22	0.42
1:C:894:SER:OG	1:C:897:ILE:N	2.33	0.42
1:A:116:PRO:HB2	1:A:117:LEU:HD22	2.02	0.42
1:A:225:VAL:CG2	1:B:778:LYS:NZ	2.80	0.42
1:A:407:ASP:O	1:A:411:VAL:HG23	2.20	0.42
1:A:995:ALA:O	1:A:996:GLY:C	2.57	0.42
1:B:396:PHE:O	1:B:399:VAL:N	2.44	0.42
1:C:281:PHE:O	1:C:282:ASN:C	2.57	0.42
1:C:775:SER:HG	1:C:789:TRP:HZ2	1.66	0.42
1:C:1021:PHE:N	1:C:1023:PRO:HD2	2.35	0.42
1:A:47:ALA:HB3	1:A:88:VAL:CG2	2.50	0.42
1:A:197:GLN:HA	1:A:798:MET:CE	2.49	0.42
1:A:515:TRP:HD1	1:A:516:PHE:HB2	1.84	0.42
1:B:12:ALA:O	1:B:13:TRP:C	2.58	0.42
1:B:126:GLY:C	1:B:127:VAL:HG23	2.39	0.42
1:B:182:TYR:HD1	1:B:271:GLY:O	2.02	0.42
1:B:314:GLU:C	1:B:316:PHE:N	2.72	0.42
1:B:413:VAL:C	1:B:415:ASN:H	2.23	0.42
1:B:472:ILE:O	1:B:473:THR:C	2.55	0.42
1:B:578:LEU:HD13	1:B:661:ALA:HB2	2.00	0.42
1:B:712:MET:HA	1:B:712:MET:HE3	2.01	0.42
1:B:915:ALA:C	1:B:917:THR:H	2.23	0.42
1:B:970:MET:CE	1:B:970:MET:HA	2.47	0.42
1:C:44:THR:HA	1:C:91:THR:HA	2.01	0.42
1:C:55:LYS:CE	1:C:59:ASP:OD1	2.60	0.42
1:C:305:ALA:O	1:C:306:ILE:C	2.55	0.42
1:C:417:GLU:CB	1:C:973:ARG:HH12	2.32	0.42
1:C:457:ALA:CB	1:C:468:ARG:CA	2.93	0.42
1:C:545:TYR:CZ	1:C:1021:PHE:CG	3.08	0.42
1:A:534:ILE:HD12	1:A:540:ARG:HH12	1.85	0.42
1:A:547:ILE:O	1:A:551:GLY:N	2.47	0.42
1:A:596:HIS:C	1:A:598:TYR:N	2.65	0.42
1:A:924:ASP:O	1:A:927:PHE:HB3	2.20	0.42
1:B:578:LEU:HB3	1:B:579:PRO:HD2	2.00	0.42
1:B:683:GLU:O	1:B:857:TYR:HA	2.18	0.42
1:C:12:ALA:C	1:C:14:VAL:H	2.23	0.42
1:C:331:PRO:O	1:C:332:PHE:C	2.56	0.42
1:C:685:ILE:HD12	1:C:686:ASP:C	2.39	0.42
1:C:702:LEU:HD12	1:C:851:LEU:HD21	2.02	0.42
1:C:910:ILE:HG23	1:C:1013:THR:OG1	2.18	0.42
1:A:105:VAL:HB	1:A:106:GLN:H	1.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:SER:O	1:A:181:GLN:HB2	2.20	0.42
1:A:187:TRP:CH2	1:C:223:PRO:HG3	2.55	0.42
1:A:370:ILE:O	1:A:370:ILE:HG22	2.19	0.42
1:A:635:ALA:C	1:A:637:ARG:N	2.73	0.42
1:A:820:ASN:O	1:A:822:LEU:CD2	2.68	0.42
1:B:407:ASP:O	1:B:408:ASP:O	2.38	0.42
1:B:455:PRO:C	1:B:457:ALA:N	2.72	0.42
1:B:463:THR:HA	1:B:466:ILE:HG13	2.00	0.42
1:B:543:VAL:O	1:B:543:VAL:HG12	2.20	0.42
1:B:873:ALA:HB3	1:B:874:PRO:CD	2.50	0.42
1:B:898:PRO:C	1:B:900:SER:H	2.23	0.42
1:C:123:GLN:C	1:C:125:GLN:N	2.73	0.42
1:C:352:PHE:CD1	1:C:369:THR:HG21	2.55	0.42
1:C:379:THR:HB	1:C:398:MET:CE	2.47	0.42
1:C:489:THR:N	1:C:490:PRO:CD	2.81	0.42
1:C:666:PHE:CD2	1:C:666:PHE:C	2.92	0.42
1:C:696:THR:HG22	1:C:699:ARG:HH12	1.85	0.42
1:C:777:ALA:HA	1:C:780:ARG:CZ	2.50	0.42
1:C:857:TYR:CD1	1:C:857:TYR:C	2.92	0.42
1:A:104:GLN:HB2	1:A:131:LYS:NZ	2.35	0.42
1:A:186:ILE:HD13	1:A:262:LEU:HD21	2.02	0.42
1:A:469:GLN:O	1:A:473:THR:OG1	2.31	0.42
1:A:728:LYS:HD2	1:C:235:ILE:CG2	2.49	0.42
1:A:983:ILE:HD13	1:A:1008:MET:SD	2.60	0.42
1:A:983:ILE:CG1	1:A:984:LEU:N	2.81	0.42
1:B:653:ARG:C	1:B:654:ALA:O	2.55	0.42
1:B:674:LEU:CD1	1:B:860:THR:HG21	2.43	0.42
1:C:17:ILE:O	1:C:20:MET:HB2	2.20	0.42
1:C:478:MET:O	1:C:481:SER:HB3	2.19	0.42
1:C:536:ARG:C	1:C:538:THR:H	2.22	0.42
1:C:549:VAL:O	1:C:550:VAL:C	2.57	0.42
1:C:775:SER:HB3	1:C:780:ARG:HD3	2.02	0.42
1:C:816:LEU:HD23	1:C:816:LEU:HA	1.83	0.42
1:C:986:VAL:O	1:C:986:VAL:HG12	2.20	0.42
1:A:348:ILE:O	1:A:351:VAL:N	2.53	0.42
1:A:515:TRP:C	1:A:515:TRP:CD1	2.93	0.42
1:A:571:VAL:HG12	1:A:629:VAL:O	2.19	0.42
1:A:653:ARG:O	1:A:655:PHE:N	2.52	0.42
1:A:753:ALA:HB3	1:A:754:TRP:H	1.61	0.42
1:A:754:TRP:CZ3	1:A:780:ARG:HA	2.54	0.42
1:A:760:ASN:O	1:A:771:VAL:HB	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:ASN:HD22	1:B:114:ALA:HB2	1.85	0.42
1:B:336:SER:O	1:B:392:THR:HG22	2.20	0.42
1:B:470:PHE:CD2	1:B:929:VAL:HG11	2.55	0.42
1:B:808:ARG:HH21	1:B:808:ARG:HB3	1.85	0.42
1:B:841:MET:O	1:B:845:GLU:HB2	2.20	0.42
1:B:1021:PHE:O	1:B:1024:VAL:HB	2.20	0.42
1:C:50:PRO:O	1:C:52:ALA:N	2.49	0.42
1:C:246:PHE:O	1:C:249:ILE:N	2.33	0.42
1:C:415:ASN:OD1	1:C:418:ARG:CZ	2.67	0.42
1:C:865:GLN:O	1:C:868:LEU:O	2.38	0.42
1:C:880:SER:O	1:C:884:VAL:HG23	2.20	0.42
1:C:922:THR:HG22	1:C:923:ASN:N	2.26	0.42
1:A:104:GLN:O	1:A:105:VAL:C	2.57	0.41
1:A:198:LEU:HD22	1:A:202:ASP:HB3	2.00	0.41
1:A:466:ILE:O	1:A:469:GLN:N	2.50	0.41
1:A:605:ASN:O	1:A:632:LYS:N	2.52	0.41
1:A:753:ALA:O	1:A:774:MET:CG	2.68	0.41
1:A:1015:THR:O	1:A:1017:LEU:N	2.53	0.41
1:B:462:SER:OG	1:B:865:GLN:CD	2.58	0.41
1:B:474:ILE:O	1:B:475:VAL:C	2.59	0.41
1:B:544:LEU:O	1:B:547:ILE:HB	2.19	0.41
1:B:644:VAL:O	1:B:645:GLU:C	2.58	0.41
1:B:941:ASN:O	1:B:942:ALA:C	2.58	0.41
1:B:972:LEU:HD21	1:B:1019:ILE:HG12	2.02	0.41
1:B:1021:PHE:HB3	1:B:1025:PHE:HE1	1.84	0.41
1:C:353:LEU:O	1:C:356:TYR:HB3	2.19	0.41
1:C:904:VAL:O	1:C:905:VAL:C	2.58	0.41
1:C:1015:THR:O	1:C:1019:ILE:HB	2.20	0.41
1:A:114:ALA:C	1:A:116:PRO:HD2	2.41	0.41
1:A:144:ASN:ND2	1:A:320:GLY:O	2.53	0.41
1:A:211:ASN:ND2	1:A:760:ASN:OD1	2.53	0.41
1:A:330:THR:CG2	1:A:334:LYS:HE2	2.47	0.41
1:A:355:MET:HE1	1:A:410:ILE:HA	2.02	0.41
1:A:545:TYR:HB2	1:A:1021:PHE:HE1	1.76	0.41
1:A:578:LEU:CD2	1:A:587:THR:HA	2.37	0.41
1:A:621:GLY:C	1:A:623:ASN:N	2.73	0.41
1:A:894:SER:CB	1:A:897:ILE:HD13	2.50	0.41
1:B:47:ALA:HB3	1:B:88:VAL:CG2	2.50	0.41
1:B:47:ALA:CB	1:B:61:VAL:HG21	2.50	0.41
1:B:352:PHE:HE1	1:B:365:THR:HG23	1.84	0.41
1:B:354:VAL:O	1:B:358:PHE:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:544:LEU:HD22	1:B:1021:PHE:CZ	2.54	0.41
1:B:648:THR:O	1:B:652:THR:N	2.40	0.41
1:C:77:TYR:CE1	1:C:860:THR:OG1	2.68	0.41
1:C:375:VAL:HG23	1:C:375:VAL:H	1.64	0.41
1:C:375:VAL:HB	1:C:405:LEU:HD13	2.02	0.41
1:C:417:GLU:O	1:C:420:MET:HB3	2.20	0.41
1:C:527:TYR:O	1:C:529:ASP:N	2.53	0.41
1:C:699:ARG:HB3	1:C:825:MET:HE3	2.01	0.41
1:A:61:VAL:HG13	1:A:118:LEU:CD1	2.46	0.41
1:A:185:ARG:HD3	1:A:272:GLY:O	2.20	0.41
1:A:594:VAL:HA	1:A:655:PHE:HE2	1.85	0.41
1:A:596:HIS:O	1:A:599:LEU:O	2.37	0.41
1:A:831:ALA:HA	1:A:840:ALA:HB1	2.01	0.41
1:A:879:ILE:H	1:A:879:ILE:HG13	1.64	0.41
1:A:988:PRO:HB2	1:A:989:LEU:H	1.57	0.41
1:B:84:SER:O	1:B:86:GLY:N	2.54	0.41
1:B:144:ASN:HD22	1:B:144:ASN:H	1.68	0.41
1:B:410:ILE:O	1:B:413:VAL:HG12	2.20	0.41
1:C:485:ALA:HA	1:C:489:THR:OG1	2.21	0.41
1:C:673:GLU:O	1:C:674:LEU:CB	2.67	0.41
1:C:973:ARG:N	1:C:974:PRO:CD	2.83	0.41
1:A:583:THR:O	1:A:586:ARG:N	2.54	0.41
1:A:683:GLU:OE1	1:A:826:GLU:HB2	2.20	0.41
1:A:686:ASP:HB2	1:A:823:PRO:HB2	2.02	0.41
1:A:690:LEU:CD1	1:A:854:GLY:HA3	2.20	0.41
1:A:978:THR:O	1:A:980:LEU:N	2.53	0.41
1:B:468:ARG:HA	1:B:471:SER:HB2	2.01	0.41
1:B:669:PRO:HB2	1:B:670:ALA:H	1.65	0.41
1:B:730:ASP:O	1:B:805:SER:HA	2.20	0.41
1:B:732:ASP:O	1:B:734:GLU:N	2.53	0.41
1:B:750:LEU:HB2	1:B:801:PHE:HE1	1.82	0.41
1:B:961:ILE:O	1:B:965:LEU:CB	2.68	0.41
1:C:144:ASN:CG	1:C:149:MET:HG3	2.40	0.41
1:C:533:GLY:HA3	2:C:1068:HOH:O	2.20	0.41
1:C:680:PHE:HB2	1:C:859:TRP:CZ3	2.55	0.41
1:C:914:LEU:HA	1:C:917:THR:OG1	2.20	0.41
1:A:44:THR:C	1:A:45:ILE:CG1	2.89	0.41
1:A:72:ILE:CG1	1:A:107:VAL:HA	2.51	0.41
1:A:72:ILE:HG13	1:A:106:GLN:HB2	2.02	0.41
1:A:294:ALA:HB3	1:A:297:ALA:CB	2.51	0.41
1:A:307:ARG:NH2	1:A:328:ASP:OD2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:LEU:HD13	1:A:405:LEU:H	1.85	0.41
1:A:493:CYS:O	1:A:497:LEU:HB2	2.21	0.41
1:B:43:VAL:O	1:B:92:LEU:N	2.42	0.41
1:B:404:LEU:HD21	1:B:937:LEU:HD21	2.02	0.41
1:B:788:ASP:N	1:B:788:ASP:OD1	2.52	0.41
1:B:986:VAL:C	1:B:988:PRO:HD2	2.39	0.41
1:C:253:VAL:HG12	1:C:259:ARG:HG3	2.03	0.41
1:C:395:MET:O	1:C:396:PHE:C	2.58	0.41
1:C:544:LEU:HD12	1:C:1021:PHE:CZ	2.56	0.41
1:C:681:ASP:OD2	1:C:828:LEU:CD1	2.68	0.41
1:C:775:SER:OG	1:C:789:TRP:HZ2	2.03	0.41
1:A:116:PRO:N	2:A:1072:HOH:O	2.54	0.41
1:A:126:GLY:HA3	1:B:116:PRO:HB3	2.01	0.41
1:A:206:ALA:C	1:A:208:LYS:N	2.74	0.41
1:A:298:ASN:O	1:A:302:THR:HG23	2.20	0.41
1:A:589:LYS:HA	1:A:592:ASN:ND2	2.36	0.41
1:B:482:VAL:HG13	1:B:483:LEU:HD23	2.02	0.41
1:B:498:LYS:HE2	1:B:498:LYS:HB3	1.66	0.41
1:B:763:ILE:HD11	1:C:59:ASP:CB	2.50	0.41
1:B:988:PRO:C	1:B:990:VAL:H	2.24	0.41
1:B:989:LEU:CA	1:B:992:SER:HB2	2.50	0.41
1:C:40:PRO:CB	1:C:76:MET:HE1	2.51	0.41
1:C:143:ILE:HA	1:C:143:ILE:HD13	1.26	0.41
1:C:193:LEU:HA	1:C:193:LEU:HD23	1.86	0.41
1:C:303:ALA:O	1:C:304:ALA:C	2.58	0.41
1:C:425:LEU:H	1:C:426:PRO:HD3	1.84	0.41
1:C:528:THR:O	1:C:528:THR:HG22	2.20	0.41
1:C:894:SER:OG	1:C:897:ILE:HG13	2.20	0.41
1:A:324:VAL:CG1	1:A:325:TYR:N	2.81	0.41
1:A:370:ILE:O	1:A:370:ILE:CG2	2.68	0.41
1:A:426:PRO:HB2	1:A:427:PRO:HD2	2.03	0.41
1:A:661:ALA:O	1:A:662:MET:C	2.58	0.41
1:A:902:MET:C	1:A:904:VAL:N	2.74	0.41
1:B:836:SER:OG	1:B:838:GLY:N	2.54	0.41
1:B:1014:ALA:O	1:B:1018:ALA:HB2	2.20	0.41
1:B:1026:PHE:HB3	1:B:1030:ARG:HE	1.85	0.41
1:C:4:PHE:HD2	1:C:8:ARG:HH12	1.69	0.41
1:C:115:MET:CB	1:C:116:PRO:HD3	2.48	0.41
1:C:187:TRP:HZ3	1:C:774:MET:CE	2.34	0.41
1:C:372:VAL:HG23	1:C:376:LEU:HG	2.02	0.41
1:C:901:VAL:O	1:C:902:MET:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:989:LEU:HB3	1:C:1004:GLY:HA3	2.02	0.41
1:A:193:LEU:HD12	1:A:265:VAL:HG11	2.02	0.41
1:A:453:PHE:O	1:A:454:VAL:C	2.59	0.41
1:A:1022:VAL:N	1:A:1023:PRO:CD	2.83	0.41
1:B:213:GLN:HG3	1:C:56:THR:HG23	2.03	0.41
1:B:470:PHE:CE2	1:B:929:VAL:HG11	2.55	0.41
1:B:741:VAL:HG22	1:B:793:ALA:HA	2.03	0.41
1:B:850:LYS:CA	1:B:852:PRO:HD3	2.51	0.41
1:B:896:SER:O	1:B:899:PHE:HB2	2.20	0.41
1:B:901:VAL:HG21	1:B:943:ILE:HD13	2.02	0.41
1:B:1026:PHE:HB3	1:B:1030:ARG:HH21	1.82	0.41
1:C:196:PHE:O	1:C:252:LYS:NZ	2.36	0.41
1:C:552:MET:HE1	1:C:909:VAL:HG21	2.02	0.41
1:C:894:SER:HB3	1:C:897:ILE:HD12	2.03	0.41
1:C:1030:ARG:HE	1:C:1030:ARG:HB3	1.21	0.41
1:A:24:GLY:O	1:A:27:ILE:HB	2.20	0.41
1:A:49:TYR:O	1:A:50:PRO:C	2.59	0.41
1:A:137:LEU:O	1:A:329:THR:HG22	2.21	0.41
1:A:223:PRO:HA	1:A:224:PRO:HD3	1.92	0.41
1:A:360:GLN:HE21	1:A:360:GLN:HB3	1.58	0.41
1:A:472:ILE:HA	1:A:475:VAL:HG12	2.01	0.41
1:A:493:CYS:C	1:A:494:ALA:O	2.59	0.41
1:A:539:GLY:CA	1:A:542:LEU:HB2	2.45	0.41
1:A:655:PHE:O	1:A:658:ILE:HG12	2.20	0.41
1:A:685:ILE:CG2	1:A:687:GLN:H	2.27	0.41
1:A:736:ALA:O	1:A:741:VAL:HG12	2.20	0.41
1:A:975:ILE:O	1:A:976:LEU:C	2.59	0.41
1:A:991:ILE:HG13	1:A:1004:GLY:HA3	2.03	0.41
1:B:33:ALA:O	1:B:337:ILE:HD11	2.20	0.41
1:B:64:VAL:O	1:B:66:GLU:N	2.54	0.41
1:B:66:GLU:OE2	1:B:818:ARG:HD3	2.21	0.41
1:B:121:GLU:H	1:B:121:GLU:HG2	1.41	0.41
1:B:216:ALA:CB	1:B:236:ALA:HB2	2.50	0.41
1:B:340:VAL:O	1:B:341:VAL:C	2.59	0.41
1:B:578:LEU:H	1:B:578:LEU:CD2	2.33	0.41
1:B:702:LEU:C	1:B:703:LEU:O	2.58	0.41
1:B:743:ILE:H	1:B:743:ILE:CD1	2.32	0.41
1:B:935:ILE:O	1:B:935:ILE:HG22	2.20	0.41
1:B:945:ILE:HG13	1:B:946:VAL:H	1.86	0.41
1:C:9:PRO:C	1:C:11:PHE:H	2.24	0.41
1:C:66:GLU:OE1	1:C:821:GLY:HA2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:LEU:N	1:C:291:ILE:O	2.53	0.41
1:C:166:ILE:HG22	1:C:172:VAL:CG1	2.51	0.41
1:C:218:GLN:HG3	1:C:233:SER:HA	2.03	0.41
1:C:322:LYS:HG2	1:C:323:ILE:N	2.34	0.41
1:C:344:LEU:O	1:C:345:VAL:C	2.59	0.41
1:C:392:THR:O	1:C:393:LEU:C	2.59	0.41
1:C:418:ARG:HD2	1:C:970:MET:CE	2.51	0.41
1:C:764:ASP:O	1:C:765:ARG:C	2.59	0.41
1:C:826:GLU:O	2:C:1063:HOH:O	2.22	0.41
1:C:844:MET:O	1:C:847:LEU:CD2	2.69	0.41
1:C:1014:ALA:O	1:C:1018:ALA:HB3	2.21	0.41
1:A:183:ALA:O	1:A:185:ARG:N	2.54	0.41
1:A:428:LYS:CG	1:A:429:GLU:N	2.83	0.41
1:A:456:MET:HG2	1:A:459:PHE:HE1	1.86	0.41
1:A:541:TYR:C	1:A:543:VAL:O	2.59	0.41
1:A:542:LEU:HD23	1:A:1028:VAL:HG21	2.02	0.41
1:A:729:ILE:CG2	1:A:730:ASP:N	2.62	0.41
1:B:38:ILE:HD12	1:B:466:ILE:CD1	2.52	0.41
1:B:139:VAL:O	1:B:326:PRO:HG2	2.21	0.41
1:B:775:SER:OG	1:B:776:GLU:N	2.54	0.41
1:C:75:LEU:HD22	1:C:77:TYR:O	2.21	0.41
1:C:188:MET:CE	1:C:200:PRO:HA	2.51	0.41
1:C:202:ASP:O	1:C:205:THR:N	2.54	0.41
1:C:593:GLU:O	1:C:597:TYR:N	2.32	0.41
1:C:790:TYR:C	1:C:791:VAL:HG23	2.40	0.41
1:A:44:THR:O	1:A:45:ILE:HG12	2.17	0.40
1:A:143:ILE:HG12	1:A:144:ASN:N	2.37	0.40
1:A:198:LEU:HD11	1:A:252:LYS:HB2	2.03	0.40
1:A:333:VAL:O	1:A:337:ILE:HD13	2.21	0.40
1:A:380:PHE:CZ	1:A:398:MET:HE1	2.56	0.40
1:A:696:THR:O	1:A:697:GLN:C	2.58	0.40
1:A:815:ARG:NH2	2:A:1071:HOH:O	2.54	0.40
1:A:897:ILE:HG21	1:A:950:LYS:NZ	2.36	0.40
1:B:592:ASN:O	1:B:595:THR:HG23	2.21	0.40
1:C:178:PHE:CD1	1:C:610:PHE:HE2	2.38	0.40
1:C:317:PHE:CB	1:C:318:PRO:CD	2.92	0.40
1:C:663:VAL:CG1	1:C:664:PHE:N	2.84	0.40
1:C:889:ALA:O	1:C:890:ALA:C	2.59	0.40
1:C:900:SER:HA	1:C:1029:VAL:HG21	2.03	0.40
1:C:919:ARG:HD2	1:C:919:ARG:HA	1.92	0.40
1:C:949:ALA:O	1:C:951:ASP:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:PHE:HD2	1:A:4:PHE:HA	1.80	0.40
1:A:193:LEU:CB	1:A:265:VAL:HG13	2.50	0.40
1:A:240:LEU:HD12	1:A:240:LEU:N	2.37	0.40
1:A:461:GLY:O	1:A:462:SER:C	2.58	0.40
1:A:545:TYR:HA	1:A:548:ILE:HG12	2.03	0.40
1:A:753:ALA:O	1:A:774:MET:HG3	2.21	0.40
1:A:952:LEU:HD11	1:A:963:ALA:HB1	2.03	0.40
1:B:58:GLN:C	1:B:60:THR:H	2.25	0.40
1:B:418:ARG:HH21	1:B:970:MET:HG3	1.85	0.40
1:B:756:GLY:HA2	1:B:773:VAL:O	2.20	0.40
1:B:974:PRO:O	1:B:978:THR:HG22	2.21	0.40
1:C:30:LEU:HA	1:C:31:PRO:HD3	1.95	0.40
1:C:315:PRO:HB2	1:C:316:PHE:CE1	2.56	0.40
1:C:337:ILE:N	1:C:337:ILE:HD13	2.36	0.40
1:C:410:ILE:O	1:C:411:VAL:C	2.59	0.40
1:C:568:ASP:OD1	1:C:568:ASP:O	2.39	0.40
1:C:760:ASN:O	1:C:771:VAL:HG23	2.21	0.40
1:C:885:PHE:O	1:C:888:LEU:N	2.53	0.40
1:A:405:LEU:O	1:A:406:VAL:C	2.57	0.40
1:A:462:SER:HB2	1:A:674:LEU:CD2	2.52	0.40
1:A:693:GLU:O	1:A:694:LYS:C	2.59	0.40
1:A:790:TYR:CE1	1:A:800:PRO:HB3	2.56	0.40
1:A:971:ARG:O	1:A:974:PRO:HD2	2.20	0.40
1:B:223:PRO:HA	1:B:224:PRO:HD3	1.98	0.40
1:B:460:GLY:HA2	1:B:872:GLN:OE1	2.21	0.40
1:B:670:ALA:H	1:B:862:MET:HE1	1.85	0.40
1:C:203:VAL:O	1:C:204:ILE:C	2.58	0.40
1:C:400:LEU:O	1:C:933:THR:HG21	2.21	0.40
1:C:551:GLY:O	1:C:554:TYR:HB2	2.21	0.40
1:C:754:TRP:CE3	1:C:780:ARG:HB2	2.56	0.40
1:C:817:GLU:O	1:C:818:ARG:HG2	2.21	0.40
1:A:243:THR:CG2	1:A:268:ILE:HG22	2.49	0.40
1:A:418:ARG:CG	1:A:970:MET:CE	2.96	0.40
1:A:489:THR:HB	1:A:490:PRO:HD3	2.03	0.40
1:A:520:PHE:C	1:A:522:LYS:H	2.25	0.40
1:A:713:LEU:HG	1:A:833:PRO:CD	2.25	0.40
1:A:959:GLY:HA3	1:A:962:GLU:CB	2.30	0.40
1:A:1036:LYS:C	1:A:1036:LYS:HD2	2.42	0.40
1:B:317:PHE:CE2	1:B:323:ILE:HD11	2.56	0.40
1:B:598:TYR:HD1	1:B:606:VAL:HG21	1.85	0.40
1:B:641:GLU:CA	1:B:650:ARG:HH12	2.33	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:921:LEU:HD22	1:B:1005:THR:HG22	2.02	0.40
1:C:4:PHE:CD2	1:C:8:ARG:NH1	2.89	0.40
1:C:360:GLN:OE1	1:C:516:PHE:HE2	2.04	0.40
1:C:475:VAL:HG12	1:C:476:SER:N	2.35	0.40
1:C:713:LEU:HD11	1:C:835:LYS:N	2.36	0.40
1:C:844:MET:O	1:C:848:ALA:N	2.53	0.40
1:C:957:GLY:C	1:C:958:LYS:HD2	2.42	0.40
1:A:65:ILE:HD13	1:A:111:LEU:HD23	2.02	0.40
1:A:114:ALA:O	1:A:117:LEU:CD2	2.70	0.40
1:A:151:GLN:NE2	1:A:279:ALA:H	2.19	0.40
1:A:541:TYR:CD2	1:A:541:TYR:N	2.89	0.40
1:A:607:GLU:O	1:A:607:GLU:OE2	2.40	0.40
1:B:194:ASN:O	1:B:194:ASN:ND2	2.55	0.40
1:B:345:VAL:O	1:B:348:ILE:HB	2.21	0.40
1:B:490:PRO:C	1:B:492:LEU:N	2.75	0.40
1:B:552:MET:HA	1:B:910:ILE:HD12	2.04	0.40
1:B:776:GLU:CG	1:B:777:ALA:H	2.35	0.40
1:B:945:ILE:CD1	1:B:1022:VAL:CG2	3.00	0.40
1:C:5:PHE:HA	1:C:8:ARG:O	2.22	0.40
1:C:714:THR:HG22	1:C:716:VAL:H	1.85	0.40
1:C:746:ILE:O	1:C:747:ASN:C	2.59	0.40
1:C:950:LYS:N	1:C:953:MET:HE2	2.18	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	1018/1053 (97%)	621 (61%)	243 (24%)	154 (15%)	<b>0</b> <b>0</b>
1	B	1018/1053 (97%)	611 (60%)	259 (25%)	148 (14%)	<b>0</b> <b>0</b>
1	C	1018/1053 (97%)	642 (63%)	225 (22%)	151 (15%)	<b>0</b> <b>0</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3054/3159 (97%)	1874 (61%)	727 (24%)	453 (15%)	<b>0</b> <b>0</b>

All (453) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	ASP
1	A	63	GLN
1	A	64	VAL
1	A	65	ILE
1	A	67	GLN
1	A	69	MET
1	A	73	ASP
1	A	74	ASN
1	A	76	MET
1	A	96	SER
1	A	105	VAL
1	A	112	GLN
1	A	137	LEU
1	A	146	ASP
1	A	167	SER
1	A	172	VAL
1	A	181	GLN
1	A	255	GLN
1	A	277	ILE
1	A	293	LEU
1	A	294	ALA
1	A	318	PRO
1	A	330	THR
1	A	376	LEU
1	A	422	GLU
1	A	439	GLN
1	A	443	VAL
1	A	444	GLY
1	A	521	GLU
1	A	538	THR
1	A	597	TYR
1	A	601	LYS
1	A	638	PRO
1	A	659	LYS
1	A	660	ASP
1	A	672	VAL
1	A	676	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	677	ALA
1	A	687	GLN
1	A	690	LEU
1	A	713	LEU
1	A	715	SER
1	A	730	ASP
1	A	759	VAL
1	A	775	SER
1	A	820	ASN
1	A	868	LEU
1	A	925	VAL
1	A	988	PRO
1	A	991	ILE
1	A	1016	VAL
1	A	1024	VAL
1	B	8	ARG
1	B	50	PRO
1	B	51	GLY
1	B	54	ALA
1	B	56	THR
1	B	72	ILE
1	B	85	THR
1	B	98	THR
1	B	104	GLN
1	B	147	GLY
1	B	173	GLY
1	B	175	VAL
1	B	228	GLN
1	B	258	SER
1	B	268	ILE
1	B	270	LEU
1	B	326	PRO
1	B	361	ASN
1	B	363	ARG
1	B	517	ASN
1	B	519	MET
1	B	535	LEU
1	B	536	ARG
1	B	538	THR
1	B	549	VAL
1	B	602	GLU
1	B	606	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	647	ILE
1	B	654	ALA
1	B	655	PHE
1	B	671	ILE
1	B	688	ALA
1	B	689	GLY
1	B	693	GLU
1	B	703	LEU
1	B	705	GLU
1	B	712	MET
1	B	733	GLN
1	B	820	ASN
1	B	831	ALA
1	B	871	ASN
1	B	891	LEU
1	B	907	LEU
1	B	908	GLY
1	B	921	LEU
1	B	1012	VAL
1	B	1019	ILE
1	B	1034	SER
1	C	52	ALA
1	C	61	VAL
1	C	68	ASN
1	C	95	GLU
1	C	110	LYS
1	C	111	LEU
1	C	157	TYR
1	C	160	ALA
1	C	167	SER
1	C	187	TRP
1	C	226	LYS
1	C	311	ALA
1	C	312	LYS
1	C	314	GLU
1	C	319	SER
1	C	394	THR
1	C	410	ILE
1	C	411	VAL
1	C	419	VAL
1	C	464	GLY
1	C	540	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	601	LYS
1	C	658	ILE
1	C	720	GLY
1	C	778	LYS
1	C	851	LEU
1	C	869	SER
1	C	871	ASN
1	C	895	TRP
1	C	925	VAL
1	C	946	VAL
1	C	960	LEU
1	C	965	LEU
1	C	975	ILE
1	C	989	LEU
1	C	993	THR
1	C	1035	ARG
1	A	12	ALA
1	A	54	ALA
1	A	66	GLU
1	A	90	ILE
1	A	135	SER
1	A	147	GLY
1	A	170	SER
1	A	218	GLN
1	A	221	GLY
1	A	256	ASP
1	A	265	VAL
1	A	400	LEU
1	A	435	MET
1	A	446	ALA
1	A	453	PHE
1	A	455	PRO
1	A	459	PHE
1	A	496	MET
1	A	548	ILE
1	A	553	ALA
1	A	580	ALA
1	A	582	ALA
1	A	600	THR
1	A	622	GLN
1	A	654	ALA
1	A	679	GLY

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	688	ALA
1	A	689	GLY
1	A	784	ASP
1	A	866	GLU
1	A	869	SER
1	A	903	LEU
1	A	926	TYR
1	A	951	ASP
1	A	958	LYS
1	A	964	THR
1	A	971	ARG
1	A	1010	GLY
1	A	1012	VAL
1	A	1025	PHE
1	B	22	ALA
1	B	103	ALA
1	B	125	GLN
1	B	221	GLY
1	B	254	ASN
1	B	265	VAL
1	B	291	ILE
1	B	424	GLY
1	B	453	PHE
1	B	471	SER
1	B	539	GLY
1	B	557	VAL
1	B	567	GLU
1	B	603	LYS
1	B	638	PRO
1	B	659	LYS
1	B	669	PRO
1	B	715	SER
1	B	723	ASP
1	B	794	ALA
1	B	805	SER
1	B	834	GLY
1	B	852	PRO
1	B	899	PHE
1	B	901	VAL
1	B	918	PHE
1	B	966	ASP
1	B	975	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	1013	THR
1	C	10	ILE
1	C	34	GLN
1	C	51	GLY
1	C	74	ASN
1	C	164	ASP
1	C	182	TYR
1	C	217	GLY
1	C	220	GLY
1	C	243	THR
1	C	258	SER
1	C	263	ARG
1	C	396	PHE
1	C	404	LEU
1	C	418	ARG
1	C	451	ALA
1	C	460	GLY
1	C	468	ARG
1	C	536	ARG
1	C	576	VAL
1	C	656	SER
1	C	678	THR
1	C	690	LEU
1	C	696	THR
1	C	706	ALA
1	C	715	SER
1	C	803	ALA
1	C	872	GLN
1	C	935	ILE
1	C	998	GLY
1	C	1017	LEU
1	C	1029	VAL
1	A	192	GLU
1	A	206	ALA
1	A	301	ASP
1	A	317	PHE
1	A	319	SER
1	A	320	GLY
1	A	353	LEU
1	A	357	LEU
1	A	372	VAL
1	A	428	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	447	MET
1	A	458	PHE
1	A	515	TRP
1	A	535	LEU
1	A	656	SER
1	A	694	LYS
1	A	753	ALA
1	A	831	ALA
1	A	881	LEU
1	B	2	PRO
1	B	48	SER
1	B	171	GLY
1	B	319	SER
1	B	336	SER
1	B	357	LEU
1	B	405	LEU
1	B	408	ASP
1	B	422	GLU
1	B	491	ALA
1	B	495	THR
1	B	601	LYS
1	B	640	GLU
1	B	675	GLY
1	B	788	ASP
1	B	804	PHE
1	B	1011	MET
1	C	190	PRO
1	C	191	ASN
1	C	193	LEU
1	C	327	TYR
1	C	336	SER
1	C	386	PHE
1	C	422	GLU
1	C	427	PRO
1	C	463	THR
1	C	491	ALA
1	C	497	LEU
1	C	530	SER
1	C	593	GLU
1	C	600	THR
1	C	639	GLY
1	C	671	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	675	GLY
1	C	747	ASN
1	C	760	ASN
1	C	801	PHE
1	C	950	LYS
1	C	952	LEU
1	C	983	ILE
1	C	994	GLY
1	C	1010	GLY
1	A	68	ASN
1	A	116	PRO
1	A	184	MET
1	A	217	GLY
1	A	362	PHE
1	A	384	ALA
1	A	434	SER
1	A	436	GLY
1	A	577	GLN
1	A	712	MET
1	A	810	GLU
1	A	907	LEU
1	A	923	ASN
1	A	960	LEU
1	A	1004	GLY
1	A	1005	THR
1	B	12	ALA
1	B	36	PRO
1	B	59	ASP
1	B	131	LYS
1	B	327	TYR
1	B	407	ASP
1	B	414	GLU
1	B	427	PRO
1	B	461	GLY
1	B	485	ALA
1	B	656	SER
1	B	694	LYS
1	B	870	GLY
1	B	941	ASN
1	B	950	LYS
1	B	959	GLY
1	B	960	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	1014	ALA
1	B	1026	PHE
1	C	54	ALA
1	C	81	ASN
1	C	124	GLN
1	C	159	ALA
1	C	343	THR
1	C	490	PRO
1	C	520	PHE
1	C	620	ARG
1	C	664	PHE
1	C	674	LEU
1	C	777	ALA
1	C	967	ALA
1	C	974	PRO
1	C	976	LEU
1	C	988	PRO
1	A	19	ILE
1	A	174	ASP
1	A	216	ALA
1	A	224	PRO
1	A	392	THR
1	A	417	GLU
1	A	549	VAL
1	A	692	HIS
1	A	714	THR
1	A	818	ARG
1	A	1002	ALA
1	B	10	ILE
1	B	409	ALA
1	B	542	LEU
1	B	618	ALA
1	B	716	VAL
1	B	777	ALA
1	B	849	SER
1	B	851	LEU
1	B	909	VAL
1	B	954	ASP
1	B	1006	GLY
1	B	1017	LEU
1	C	192	GLU
1	C	237	GLN

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Mol	Chain	Res	Type
1	C	332	PHE
1	C	392	THR
1	C	425	LEU
1	C	438	ILE
1	C	458	PHE
1	C	519	MET
1	C	528	THR
1	C	546	LEU
1	C	640	GLU
1	C	716	VAL
1	C	837	THR
1	C	850	LYS
1	C	852	PRO
1	C	963	ALA
1	A	18	ILE
1	A	109	ASN
1	A	191	ASN
1	A	397	GLY
1	A	471	SER
1	A	794	ALA
1	A	892	TYR
1	B	23	GLY
1	B	65	ILE
1	B	105	VAL
1	B	127	VAL
1	B	474	ILE
1	B	477	ALA
1	B	674	LEU
1	B	786	ILE
1	B	942	ALA
1	B	1016	VAL
1	C	80	SER
1	C	106	GLN
1	C	207	ILE
1	C	315	PRO
1	C	333	VAL
1	C	399	VAL
1	C	447	MET
1	C	537	SER
1	C	796	GLY
1	C	926	TYR
1	C	1007	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	709	HIS
1	B	315	PRO
1	B	444	GLY
1	B	484	VAL
1	B	710	PRO
1	B	821	GLY
1	C	19	ILE
1	C	32	VAL
1	C	223	PRO
1	C	426	PRO
1	C	550	VAL
1	A	51	GLY
1	A	539	GLY
1	B	19	ILE
1	B	31	PRO
1	B	190	PRO
1	B	771	VAL
1	C	709	HIS
1	A	729	ILE
1	A	874	PRO
1	B	224	PRO
1	B	974	PRO
1	C	9	PRO
1	C	50	PRO
1	C	291	ILE
1	C	533	GLY
1	A	15	ILE
1	A	716	VAL
1	A	905	VAL
1	B	464	GLY
1	C	15	ILE
1	C	424	GLY
1	C	448	VAL
1	C	571	VAL
1	C	786	ILE
1	C	800	PRO
1	A	326	PRO
1	B	783	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	833/859 (97%)	678 (81%)	155 (19%)	1	5
1	B	833/859 (97%)	688 (83%)	145 (17%)	2	6
1	C	833/859 (97%)	679 (82%)	154 (18%)	1	5
All	All	2499/2577 (97%)	2045 (82%)	454 (18%)	1	5

All (454) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	PHE
1	A	5	PHE
1	A	6	ILE
1	A	14	VAL
1	A	21	LEU
1	A	25	LEU
1	A	38	ILE
1	A	46	SER
1	A	49	TYR
1	A	55	LYS
1	A	58	GLN
1	A	62	THR
1	A	63	GLN
1	A	65	ILE
1	A	66	GLU
1	A	69	MET
1	A	74	ASN
1	A	79	SER
1	A	80	SER
1	A	83	ASP
1	A	84	SER
1	A	88	VAL
1	A	91	THR
1	A	93	THR
1	A	98	THR
1	A	102	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	105	VAL
1	A	109	ASN
1	A	112	GLN
1	A	115	MET
1	A	120	GLN
1	A	130	GLU
1	A	137	LEU
1	A	139	VAL
1	A	143	ILE
1	A	150	THR
1	A	164	ASP
1	A	166	ILE
1	A	170	SER
1	A	193	LEU
1	A	202	ASP
1	A	213	GLN
1	A	222	THR
1	A	226	LYS
1	A	230	LEU
1	A	243	THR
1	A	277	ILE
1	A	284	GLN
1	A	298	ASN
1	A	302	THR
1	A	319	SER
1	A	323	ILE
1	A	325	TYR
1	A	330	THR
1	A	335	ILE
1	A	337	ILE
1	A	349	ILE
1	A	356	TYR
1	A	357	LEU
1	A	359	LEU
1	A	361	ASN
1	A	367	ILE
1	A	376	LEU
1	A	379	THR
1	A	394	THR
1	A	405	LEU
1	A	414	GLU
1	A	417	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	433	LYS
1	A	438	ILE
1	A	447	MET
1	A	453	PHE
1	A	480	LEU
1	A	481	SER
1	A	498	LYS
1	A	513	PHE
1	A	515	TRP
1	A	518	ARG
1	A	522	LYS
1	A	523	SER
1	A	536	ARG
1	A	544	LEU
1	A	546	LEU
1	A	556	PHE
1	A	557	VAL
1	A	558	ARG
1	A	561	SER
1	A	572	PHE
1	A	576	VAL
1	A	577	GLN
1	A	578	LEU
1	A	586	ARG
1	A	607	GLU
1	A	610	PHE
1	A	612	VAL
1	A	617	PHE
1	A	620	ARG
1	A	623	ASN
1	A	626	ILE
1	A	630	SER
1	A	641	GLU
1	A	648	THR
1	A	653	ARG
1	A	659	LYS
1	A	668	LEU
1	A	671	ILE
1	A	687	GLN
1	A	690	LEU
1	A	702	LEU
1	A	705	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	711	ASP
1	A	713	LEU
1	A	717	ARG
1	A	719	ASN
1	A	721	LEU
1	A	722	GLU
1	A	729	ILE
1	A	750	LEU
1	A	758	TYR
1	A	763	ILE
1	A	768	VAL
1	A	774	MET
1	A	775	SER
1	A	778	LYS
1	A	779	TYR
1	A	780	ARG
1	A	782	LEU
1	A	786	ILE
1	A	801	PHE
1	A	805	SER
1	A	807	SER
1	A	815	ARG
1	A	818	ARG
1	A	822	LEU
1	A	824	SER
1	A	828	LEU
1	A	843	LEU
1	A	855	VAL
1	A	867	ARG
1	A	887	CYS
1	A	899	PHE
1	A	917	THR
1	A	954	ASP
1	A	955	LYS
1	A	960	LEU
1	A	976	LEU
1	A	982	PHE
1	A	983	ILE
1	A	986	VAL
1	A	992	SER
1	A	993	THR
1	A	1013	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1022	VAL
1	A	1030	ARG
1	A	1036	LYS
1	B	6	ILE
1	B	8	ARG
1	B	11	PHE
1	B	13	TRP
1	B	21	LEU
1	B	27	ILE
1	B	34	GLN
1	B	48	SER
1	B	50	PRO
1	B	53	ASP
1	B	57	VAL
1	B	59	ASP
1	B	61	VAL
1	B	67	GLN
1	B	70	ASN
1	B	72	ILE
1	B	74	ASN
1	B	79	SER
1	B	81	ASN
1	B	91	THR
1	B	92	LEU
1	B	93	THR
1	B	96	SER
1	B	102	ILE
1	B	104	GLN
1	B	121	GLU
1	B	131	LYS
1	B	144	ASN
1	B	145	THR
1	B	150	THR
1	B	153	ASP
1	B	170	SER
1	B	174	ASP
1	B	176	GLN
1	B	180	SER
1	B	182	TYR
1	B	185	ARG
1	B	188	MET
1	B	189	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	191	ASN
1	B	193	LEU
1	B	194	ASN
1	B	210	GLN
1	B	223	PRO
1	B	226	LYS
1	B	228	GLN
1	B	231	ASN
1	B	235	ILE
1	B	237	GLN
1	B	243	THR
1	B	253	VAL
1	B	254	ASN
1	B	256	ASP
1	B	261	LEU
1	B	270	LEU
1	B	289	LEU
1	B	293	LEU
1	B	298	ASN
1	B	319	SER
1	B	335	ILE
1	B	336	SER
1	B	342	LYS
1	B	343	THR
1	B	349	ILE
1	B	356	TYR
1	B	365	THR
1	B	372	VAL
1	B	373	PRO
1	B	379	THR
1	B	394	THR
1	B	405	LEU
1	B	410	ILE
1	B	428	LYS
1	B	435	MET
1	B	437	GLN
1	B	452	VAL
1	B	456	MET
1	B	473	THR
1	B	482	VAL
1	B	483	LEU
1	B	488	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	496	MET
1	B	497	LEU
1	B	513	PHE
1	B	516	PHE
1	B	538	THR
1	B	540	ARG
1	B	549	VAL
1	B	554	TYR
1	B	562	SER
1	B	574	THR
1	B	591	LEU
1	B	595	THR
1	B	601	LYS
1	B	607	GLU
1	B	612	VAL
1	B	623	ASN
1	B	629	VAL
1	B	641	GLU
1	B	653	ARG
1	B	655	PHE
1	B	659	LYS
1	B	668	LEU
1	B	673	GLU
1	B	680	PHE
1	B	681	ASP
1	B	696	THR
1	B	712	MET
1	B	743	ILE
1	B	757	SER
1	B	758	TYR
1	B	760	ASN
1	B	764	ASP
1	B	770	LYS
1	B	778	LYS
1	B	781	MET
1	B	782	LEU
1	B	788	ASP
1	B	799	VAL
1	B	808	ARG
1	B	830	GLN
1	B	836	SER
1	B	847	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	864	TYR
1	B	868	LEU
1	B	871	ASN
1	B	876	LEU
1	B	879	ILE
1	B	895	TRP
1	B	900	SER
1	B	933	THR
1	B	943	ILE
1	B	946	VAL
1	B	951	ASP
1	B	956	GLU
1	B	960	LEU
1	B	965	LEU
1	B	966	ASP
1	B	970	MET
1	B	978	THR
1	B	984	LEU
1	B	987	MET
1	B	993	THR
1	B	1027	VAL
1	B	1036	LYS
1	C	4	PHE
1	C	13	TRP
1	C	17	ILE
1	C	19	ILE
1	C	37	THR
1	C	45	ILE
1	C	48	SER
1	C	49	TYR
1	C	58	GLN
1	C	60	THR
1	C	63	GLN
1	C	65	ILE
1	C	70	ASN
1	C	74	ASN
1	C	75	LEU
1	C	82	SER
1	C	83	ASP
1	C	89	GLN
1	C	91	THR
1	C	102	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	104	GLN
1	C	107	VAL
1	C	108	GLN
1	C	110	LYS
1	C	111	LEU
1	C	117	LEU
1	C	118	LEU
1	C	134	SER
1	C	137	LEU
1	C	143	ILE
1	C	148	THR
1	C	149	MET
1	C	151	GLN
1	C	152	GLU
1	C	153	ASP
1	C	168	ARG
1	C	169	THR
1	C	170	SER
1	C	177	LEU
1	C	184	MET
1	C	185	ARG
1	C	189	ASN
1	C	194	ASN
1	C	207	ILE
1	C	210	GLN
1	C	211	ASN
1	C	228	GLN
1	C	231	ASN
1	C	233	SER
1	C	239	ARG
1	C	253	VAL
1	C	258	SER
1	C	259	ARG
1	C	265	VAL
1	C	268	ILE
1	C	269	GLU
1	C	274	ASN
1	C	295	THR
1	C	301	ASP
1	C	313	MET
1	C	316	PHE
1	C	317	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	337	ILE
1	C	339	GLU
1	C	341	VAL
1	C	355	MET
1	C	367	ILE
1	C	372	VAL
1	C	377	LEU
1	C	400	LEU
1	C	417	GLU
1	C	419	VAL
1	C	420	MET
1	C	425	LEU
1	C	432	ARG
1	C	437	GLN
1	C	438	ILE
1	C	458	PHE
1	C	459	PHE
1	C	475	VAL
1	C	492	LEU
1	C	493	CYS
1	C	497	LEU
1	C	521	GLU
1	C	535	LEU
1	C	536	ARG
1	C	538	THR
1	C	544	LEU
1	C	546	LEU
1	C	568	ASP
1	C	576	VAL
1	C	577	GLN
1	C	588	GLN
1	C	591	LEU
1	C	592	ASN
1	C	608	SER
1	C	613	ASN
1	C	617	PHE
1	C	622	GLN
1	C	624	THR
1	C	626	ILE
1	C	650	ARG
1	C	662	MET
1	C	666	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	668	LEU
1	C	674	LEU
1	C	685	ILE
1	C	696	THR
1	C	699	ARG
1	C	713	LEU
1	C	719	ASN
1	C	721	LEU
1	C	722	GLU
1	C	724	THR
1	C	733	GLN
1	C	743	ILE
1	C	745	ASP
1	C	750	LEU
1	C	759	VAL
1	C	762	PHE
1	C	764	ASP
1	C	765	ARG
1	C	768	VAL
1	C	770	LYS
1	C	778	LYS
1	C	782	LEU
1	C	799	VAL
1	C	808	ARG
1	C	813	SER
1	C	847	LEU
1	C	850	LYS
1	C	867	ARG
1	C	868	LEU
1	C	872	GLN
1	C	876	LEU
1	C	885	PHE
1	C	899	PHE
1	C	904	VAL
1	C	907	LEU
1	C	922	THR
1	C	935	ILE
1	C	941	ASN
1	C	945	ILE
1	C	952	LEU
1	C	954	ASP
1	C	958	LYS

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Mol	Chain	Res	Type
1	C	960	LEU
1	C	982	PHE
1	C	984	LEU
1	C	993	THR
1	C	1021	PHE
1	C	1030	ARG
1	C	1035	ARG
1	C	1036	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	63	GLN
1	A	68	ASN
1	A	70	ASN
1	A	89	GLN
1	A	106	GLN
1	A	108	GLN
1	A	109	ASN
1	A	123	GLN
1	A	124	GLN
1	A	181	GLN
1	A	191	ASN
1	A	210	GLN
1	A	231	ASN
1	A	274	ASN
1	A	282	ASN
1	A	284	GLN
1	A	298	ASN
1	A	360	GLN
1	A	361	ASN
1	A	577	GLN
1	A	622	GLN
1	A	623	ASN
1	A	687	GLN
1	A	719	ASN
1	A	830	GLN
1	A	846	GLN
1	A	865	GLN
1	A	871	ASN
1	B	34	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	58	GLN
1	B	68	ASN
1	B	70	ASN
1	B	108	GLN
1	B	109	ASN
1	B	112	GLN
1	B	120	GLN
1	B	125	GLN
1	B	151	GLN
1	B	161	ASN
1	B	189	ASN
1	B	210	GLN
1	B	213	GLN
1	B	218	GLN
1	B	228	GLN
1	B	231	ASN
1	B	237	GLN
1	B	254	ASN
1	B	415	ASN
1	B	437	GLN
1	B	439	GLN
1	B	469	GLN
1	B	517	ASN
1	B	526	HIS
1	B	577	GLN
1	B	584	GLN
1	B	613	ASN
1	B	623	ASN
1	B	642	ASN
1	B	726	GLN
1	B	744	ASN
1	B	760	ASN
1	B	830	GLN
1	B	846	GLN
1	B	865	GLN
1	B	871	ASN
1	C	3	ASN
1	C	63	GLN
1	C	104	GLN
1	C	106	GLN
1	C	120	GLN
1	C	123	GLN

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Mol	Chain	Res	Type
1	C	125	GLN
1	C	144	ASN
1	C	176	GLN
1	C	189	ASN
1	C	197	GLN
1	C	211	ASN
1	C	231	ASN
1	C	237	GLN
1	C	284	GLN
1	C	391	ASN
1	C	439	GLN
1	C	577	GLN
1	C	588	GLN
1	C	592	ASN
1	C	605	ASN
1	C	667	ASN
1	C	747	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1022/1053 (97%)	-0.06	38 (3%) 41 31	5, 97, 116, 127	0
1	B	1022/1053 (97%)	0.05	44 (4%) 35 25	49, 102, 116, 127	0
1	C	1022/1053 (97%)	-0.06	44 (4%) 35 25	5, 94, 118, 127	0
All	All	3066/3159 (97%)	-0.02	126 (4%) 37 27	5, 99, 117, 127	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1034	SER	11.4
1	C	870	GLY	8.3
1	C	513	PHE	6.5
1	C	538	THR	6.4
1	C	536	ARG	5.7
1	B	529	ASP	5.6
1	A	526	HIS	5.3
1	C	514	GLY	5.2
1	C	515	TRP	5.0
1	C	539	GLY	4.8
1	C	656	SER	4.7
1	C	869	SER	4.7
1	B	526	HIS	4.4
1	B	957	GLY	4.4
1	C	525	HIS	4.3
1	B	554	TYR	4.2
1	C	920	GLY	4.1
1	A	253	VAL	4.0
1	A	318	PRO	4.0
1	B	811	TYR	3.9
1	B	958	LYS	3.9
1	A	801	PHE	3.9
1	B	424	GLY	3.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	596	HIS	3.8
1	A	145	THR	3.7
1	C	1034	SER	3.7
1	B	192	GLU	3.6
1	A	515	TRP	3.6
1	A	871	ASN	3.6
1	B	832	ALA	3.5
1	C	521	GLU	3.3
1	B	563	PHE	3.3
1	C	670	ALA	3.3
1	A	135	SER	3.3
1	C	554	TYR	3.2
1	C	526	HIS	3.2
1	A	536	ARG	3.2
1	C	649	MET	3.2
1	B	420	MET	3.2
1	A	519	MET	3.1
1	C	957	GLY	3.1
1	B	1036	LYS	3.1
1	B	1035	ARG	3.0
1	A	962	GLU	3.0
1	B	711	ASP	3.0
1	C	425	LEU	3.0
1	A	1035	ARG	2.9
1	B	515	TRP	2.9
1	C	520	PHE	2.9
1	C	436	GLY	2.9
1	C	671	ILE	2.9
1	B	652	THR	2.9
1	C	597	TYR	2.9
1	A	955	LYS	2.8
1	A	918	PHE	2.8
1	B	546	LEU	2.8
1	A	957	GLY	2.8
1	B	320	GLY	2.8
1	A	257	GLY	2.8
1	B	338	HIS	2.8
1	B	304	ALA	2.8
1	A	951	ASP	2.8
1	A	537	SER	2.7
1	A	557	VAL	2.7
1	C	951	ASP	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	437	GLN	2.7
1	B	52	ALA	2.7
1	A	1034	SER	2.7
1	A	597	TYR	2.7
1	B	145	THR	2.7
1	A	254	ASN	2.6
1	A	250	LEU	2.6
1	C	993	THR	2.6
1	C	658	ILE	2.6
1	C	424	GLY	2.6
1	C	833	PRO	2.6
1	C	4	PHE	2.6
1	B	951	ASP	2.6
1	C	537	SER	2.6
1	C	34	GLN	2.6
1	A	521	GLU	2.6
1	C	872	GLN	2.5
1	C	522	LYS	2.5
1	B	657	GLN	2.5
1	C	1035	ARG	2.5
1	B	521	GLU	2.5
1	B	1033	PHE	2.5
1	A	954	ASP	2.5
1	A	167	SER	2.5
1	A	192	GLU	2.5
1	B	708	LYS	2.4
1	A	134	SER	2.4
1	B	604	ASN	2.4
1	C	546	LEU	2.4
1	A	969	ARG	2.4
1	B	918	PHE	2.4
1	B	319	SER	2.4
1	A	546	LEU	2.4
1	B	253	VAL	2.4
1	C	194	ASN	2.3
1	A	615	PHE	2.3
1	A	538	THR	2.3
1	B	697	GLN	2.3
1	B	981	ALA	2.3
1	A	518	ARG	2.3
1	A	1033	PHE	2.3
1	B	651	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	342	LYS	2.3
1	B	675	GLY	2.2
1	C	544	LEU	2.2
1	B	20	MET	2.2
1	B	1032	ARG	2.2
1	B	346	GLU	2.1
1	B	495	THR	2.1
1	C	868	LEU	2.1
1	A	554	TYR	2.1
1	A	555	LEU	2.1
1	C	540	ARG	2.1
1	C	498	LYS	2.0
1	A	923	ASN	2.0
1	B	3	ASN	2.0
1	B	520	PHE	2.0
1	B	976	LEU	2.0
1	B	314	GLU	2.0
1	C	257	GLY	2.0
1	A	589	LYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.