



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 03:06 pm GMT

PDB ID : 2A6E  
Title : Crystal structure of the T. Thermophilus RNA polymerase holoenzyme  
Authors : Artsimovitch, I.; Vassilyeva, M.N.; Svetlov, D.; Svetlov, V.; Perederina, A.;  
Igarashi, N.; Matsugaki, N.; Wakatsuki, S.; Tahirov, T.H.; Vassilyev, D.G.;  
RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2005-07-02  
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.

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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	:	trunk31020
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk31020

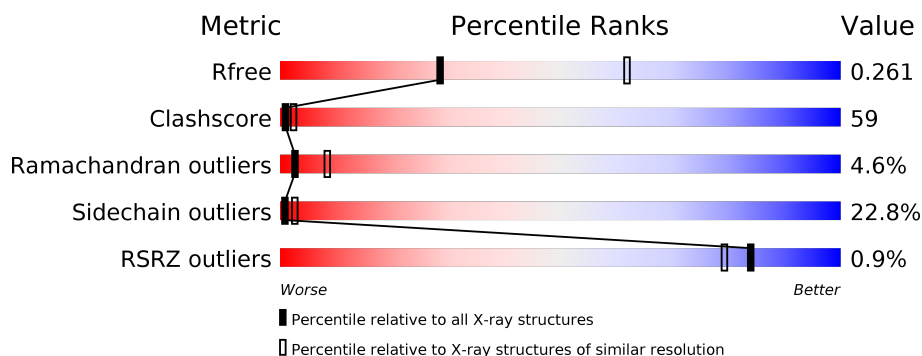
# 1 Overall quality at a glance

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))
$R_{free}$	111664	2792 (2.80-2.80)
Clashscore	122126	3209 (2.80-2.80)
Ramachandran outliers	120053	3158 (2.80-2.80)
Sidechain outliers	120020	3160 (2.80-2.80)
RSRZ outliers	108989	2726 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	315	
1	B	315	
1	K	315	
1	L	315	
2	C	1119	
2	M	1119	

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Mol	Chain	Length	Quality of chain
3	D	1524	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>23%51%17%•9%</div></div>
3	N	1524	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>24%51%15%•9%</div></div>
4	E	99	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>22%52%20%••</div></div>
4	O	99	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>28%48%19%•</div></div>
5	F	423	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>19%47%14%•18%</div></div>
5	P	423	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>22%49%10%18%</div></div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 58679 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 DNA-directed RNA polymerase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			
1	B	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			
1	K	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			
1	L	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			

- Molecule 2 is a protein called DNA-directed RNA polymerase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1119	Total	C	N	O	S	0	0	0
			8829	5581	1577	1647	24			
2	M	1119	Total	C	N	O	S	0	0	0
			8829	5581	1577	1647	24			

- Molecule 3 is a protein called DNA-directed RNA polymerase beta' chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1392	Total	C	N	O	S	0	0	0
			10797	6819	1925	2020	33			
3	N	1392	Total	C	N	O	S	0	0	0
			10797	6819	1925	2020	33			

- Molecule 4 is a protein called RNA polymerase omega chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	95	Total	C	N	O	S	0	0	0
			769	488	133	144	4			
4	O	95	Total	C	N	O	S	0	0	0
			769	488	133	144	4			

- Molecule 5 is a protein called RNA polymerase sigma factor rpoD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	345	Total	C	N	O	S	0	0	0
			2771	1744	504	519	4			
5	P	345	Total	C	N	O	S	0	0	0
			2771	1744	504	519	4			

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	2	Total	Zn	0	0
			2	2		
6	N	2	Total	Zn	0	0
			2	2		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total	Mg	0	0
			1	1		
7	N	1	Total	Mg	0	0
			1	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	191	Total	O	0	0
			191	191		
8	B	181	Total	O	0	0
			181	181		
8	C	767	Total	O	0	0
			767	767		
8	D	1100	Total	O	0	0
			1100	1100		
8	E	93	Total	O	0	0
			93	93		
8	F	333	Total	O	0	0
			333	333		
8	K	151	Total	O	0	0
			151	151		
8	L	179	Total	O	0	0
			179	179		
8	M	739	Total	O	0	0
			739	739		

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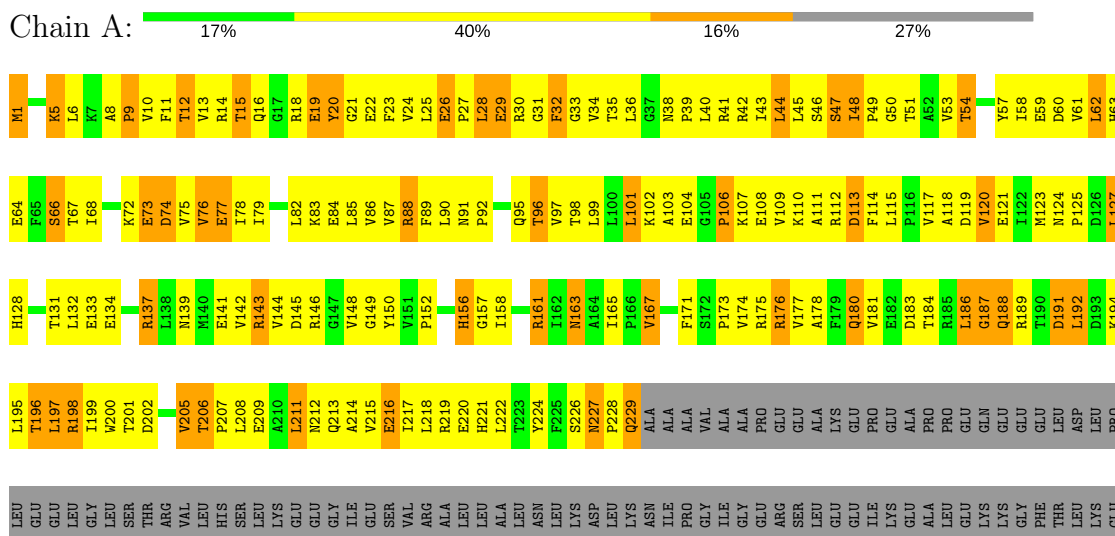
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	N	1038	Total 1038	O 1038	0	0
8	O	78	Total 78	O 78	0	0
8	P	267	Total 267	O 267	0	0

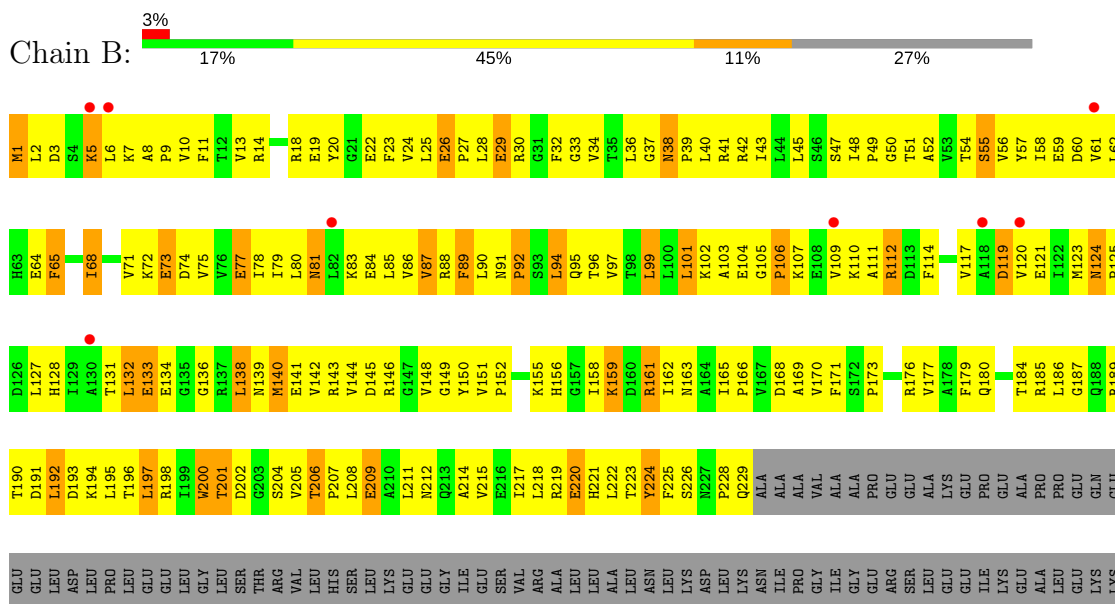
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: DNA-directed RNA polymerase alpha chain



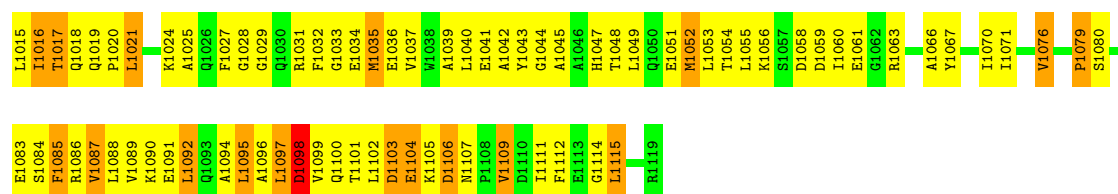
#### • Molecule 1: DNA-directed RNA polymerase alpha chain



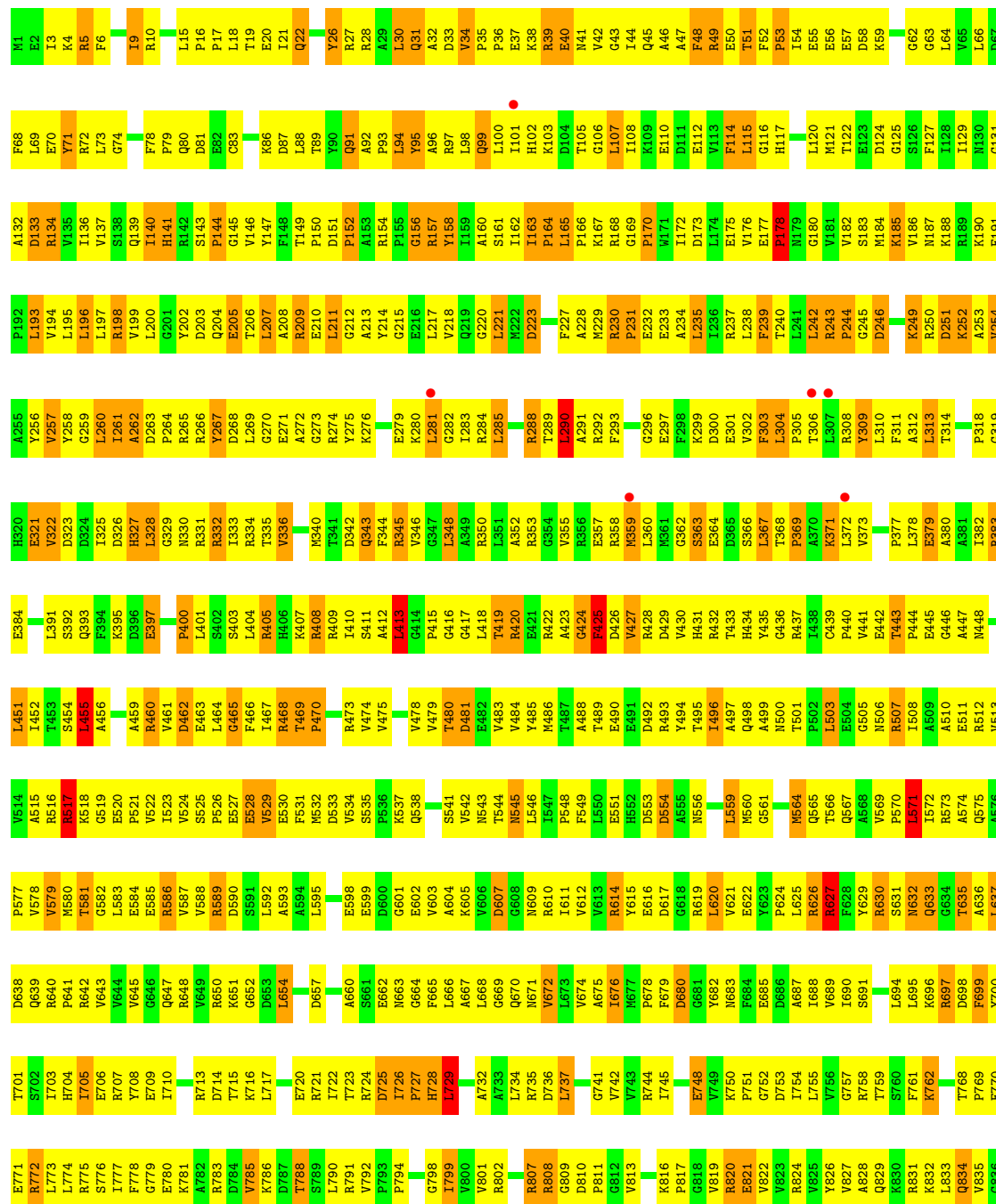


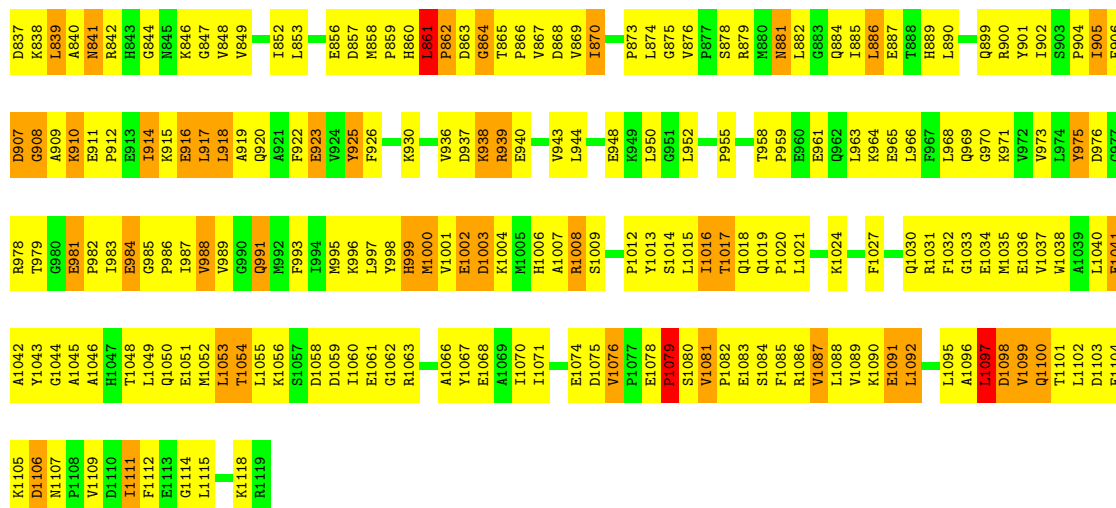




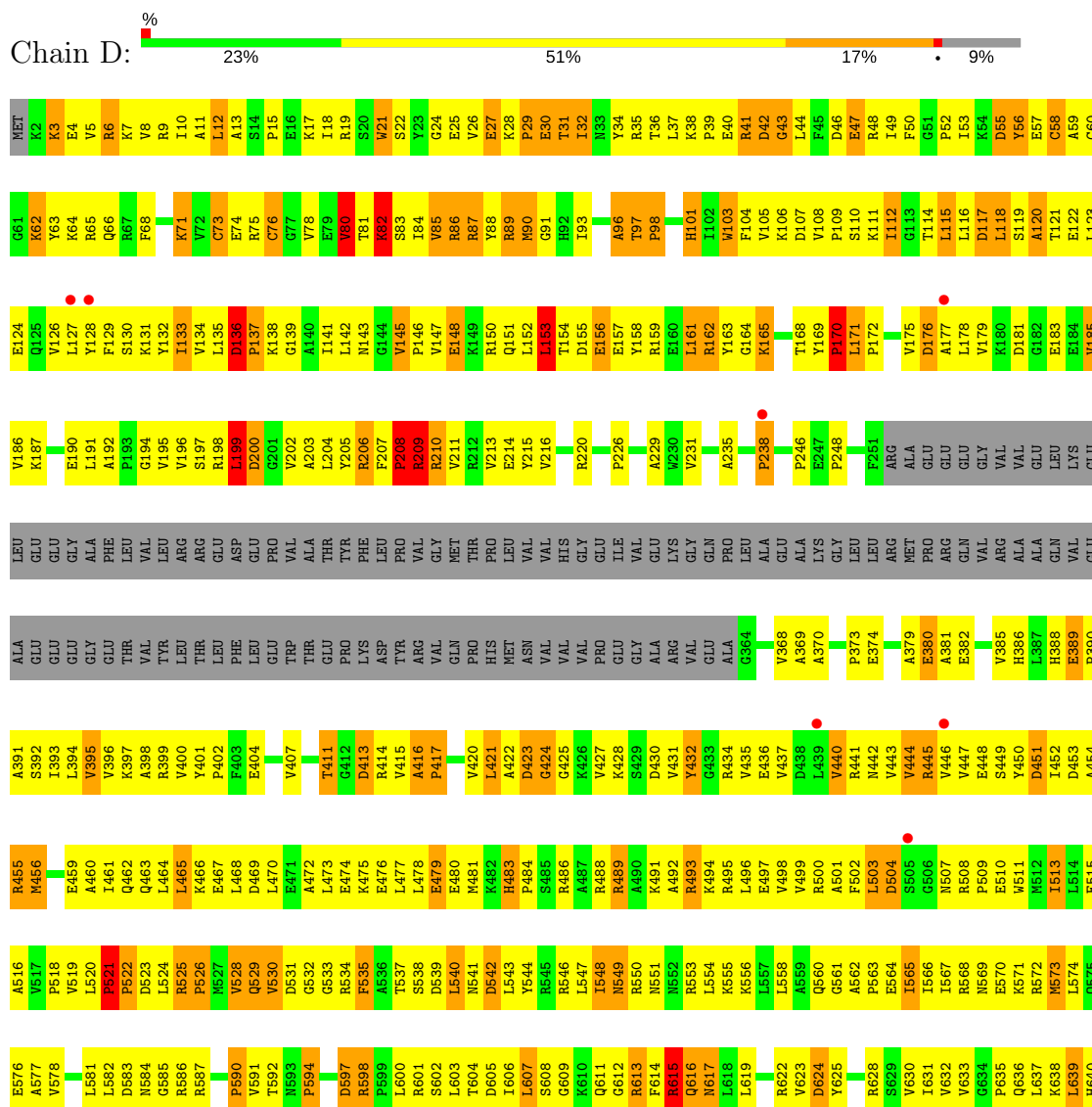


• Molecule 2: DNA-directed RNA polymerase beta chain





• Molecule 3: DNA-directed RNA polymerase beta' chain



Q1413	T1413	E1351	K1289	A1220	L1156	L1094	Q1033	L964	Y900	G831	N768	N703	Q641
P1414	P1414	I1352	K1290	I1221	G1157	L1095	Q1034	E965	Q901	R832	L769	R704	C642
V1415	V1415	Q1353	L1290	G1222	Y1158	R1096	I1035	E966	I902	E833	L770	A705	C643
A1416	A1416	S1291	I1223	I1224	Y1159	R1097	I1036	E967	D903	E834	S771	P706	L644
V1417	V1417	V1292	G1293	V1224	E1160	L1098	Q1037	D968	P905	S835	P772	L708	P645
K1418	K1418	F1293	G1294	G1225	E1161	L1099	L1038	R969	Q906	R836	A773	T707	K646
P1419	P1419	V1294	E1295	E1230	E1162	D1100	C1039	K970	G906	G837	S774	H709	R647
L1420	L1420	E1296	E1296	E1231	G1163	V1101	G1040	L971	E907	R838	G775	R710	H648
L1421	L1421	F1299	F1299	E1232	R1164	V1102	L1041	L972	K908	L839	G776	L711	A649
M1422	M1422	S1300	S1300	G1233	Y1165	H1103	Q1042	Q973	N909	R840	P777	G712	L650
G1423	G1423	K1361	K1361	T1234	L1166	E1104	G1043	Q974	S910	Y841	L778	I713	E651
V1424	V1424	K1301	K1301	Q1235	M1167	T1105	L1044	E975	L911	R842	A779	Q714	L652
T1425	T1425	H1364	H1364	L1236	M1168	V1106	M1045	Q976	K912	F843	K780	F715	F653
K1426	K1426	D1365	D1365	T1237	D1169	V1107	Q1046	A977	D913	A844		F716	K654
S1427	S1427	K1366	K1366	M1238	D1170	K1108	K1047	Y978	L914				P655
A1428	A1428	H1367	H1367	R1239	V1171	E1109	P1048	E979	V915	D847	P718	Q717	F656
L1429	L1429	P1306	P1306	T1240	L1174	A1110	S1049	N980	Y916	E848	L785	V719	L657
T1430	T1430	K1307	K1307	H1242	L1175	C1112	E1051	D985	Q917	A849	I786	L720	L658
V1371	V1371	R1310	R1310	F1241	K1176	G1113	T1052	D986	A918	L850	L787	V721	K659
L1372	L1372	L1311	L1311	G1244	A1177	T1114	F1053	R987	L920	L851	G788	E722	K660
K1373	K1373	V1312	V1312	G1245	A1178	N1115	E1054	R988	R921	A852	L789	G723	H661
V1374	V1374	L1313	L1313	G1246		T1116	V1055	L992	L922	V853	Y790	Q724	E662
M1375	M1375	K1314	K1314	G1248	E1182	Y1117	P1056	I993	G923	I857	I792	S725	E663
K1376	K1376	D1315	D1315	A1249	L1183	T1118	V1057	Q994	N924	V858	T793	Q727	L666
K1377	K1377	G1316	G1316	A1250	Q1184	S1119	R1058	Q995	E925	D859	Q794	L728	A667
N1442	N1442	D1317	D1317	D1251	E1185	P1120	S1059	L996	K926	L860	V795	H729	P669
T1443	T1443	V1379	V1379	T1252	L1186	F1121	S1060	K996	T927	Q861	R796	P730	N669
E1444	E1444	K1380	K1380	L1253	P1187	L1122	F1061	T997	A928	D862	K797	L731	V670
V1445	V1445	L1381	L1381	Q1254	L1188	F1123	R1062	E998	R929	V863	E798		K671
H1445	H1445	T1382	T1382	G1255	K1189	Q1124	E1063	T999	L930	R864	K799	E734	A672
L1446	L1446	D1383	D1383	L1256	S1190	P1125	G1064	T1000	L931	T865	K800		A673
K1447	K1447	G1322	G1322	L1257	P1191		L1065	E1001	Y936	V866		F736	A674
T1448	T1448	Q1323	Q1323	L1258	L1192	T1129	T1066	V1003	Y937	R867	L803	N737	R675
V1452	V1452	L1325	L1325	V1259		R1130	L1068	G938	G803	Y868	E805	D739	A676
L1453	L1453	K1326	K1326	I1260	Q1196	S1131	E1069	A1006	F939	M869	F806	F740	E678
G1454	G1454	R1327	R1327	E1261	R1197	L1132	F1071	V1007	T940	E874	A807	D741	R679
K1455	K1455	G1328	G1328	L1262	Y1198	R1133	L1072	F1008	S942	T875	P808	Q744	Q680
L1456	L1456	I1330	I1330	E1264	G1199	L1134	I1073	L1009	P909	S876	E810	M745	R681
D1457	D1457	D1331	D1331	A1265	V1200	R1135	S1073	N1010	T943	P877	E811	D682	D682
E1458	E1458	P1332	P1332	R1266	C1201	K1136	S1074	F1011	T944	G878	E812		L683
L1459	L1459	H1333	H1333	R1267	Q1202	R1137	G1075	E1012	S945	R879	A812	V749	K684
T1460	T1460	Q1334	Q1334	P1268	K1203	A1138	G1076	E1013	G946	I880	L813		D685
G1461	G1461	L1335	L1335	K1269	C1204	D1139	A1077	N1014	T947		A814	S752	E686
L1462	L1462	V1336	V1336	A1270	Y1205	E1140	T1078	Y1015	T948	A883	E817	S753	V687
K1463	K1463	E1337	E1337	K1271	G1206	E1141	K1079	P1019	T949	R884		F754	W688
V1464	V1464	K1339	K1339	A1272	Y1207	G1143		L1020	G950	E888	R818	A756	D689
N1465	N1465	G1340	G1340	I1274	L1209	L1144	D1083	Y1021	D952	A889	E820	A757	A690
L1467	L1467	P1341	P1341	T1277	S1210	Y1145	T1084	V1022	V955	V890	V821	E758	L691
P52	P52	E1342	E1342	D1278	M1211	G1146	L1085	I1023	P956	E891	A822	A759	E692
T53	T53	A1343	A1343	G1279	R1147	L1148	L1086	A1024	P957	D892	E821	R760	E693
K54	K54	L1406	L1406	T1213	R1213	V1148	R1087	Q1025	P957	E893	N824	I761	V694
L1471	L1471	L1407	L1407	V1280	P1214	T1088	S1074	S1026	E958	K894	A825	Q762	L695
V1472	V1472	R1346	R1346	V1281	V1215	A1089	G1076	G1027	E959	R895	P826	Q763	H696
P1473	P1473	Y1347	Y1347	R1282	S1216	E1151	D1090	A1028	K960	A896	I827	L764	K698
G58	G58	L1348	L1348	T1283	G1218	V1153	G1091	R1029	K961	W897	K828	A766	V699
L1474	L1474	E1284	E1284	E1284	G1218	V1153	G1092	P1032	Y963	E898	W829		
T1476	T1476	E1285	E1285	E1285	E1219	V1155	Y1093			L899	A830	H767	L702

• Molecule 3: DNA-directed RNA polymerase beta' chain



MET	K2	K3	K4	K5	K6	K7	K8	K9	K10	K11	K12	K13	K14	K15	K16	K17	K18	K19	K20	K21	K22	K23	K24	K25	K26	K27	K28	K29	K30	K31	K32	K33	K34	K35	K36	K37	K38	K39	K40	K41	K42	K43	K44	K45	K46	K47	K48	K49	K50	K51	K52	K53	K54	K55	K56	K57	K58	K59	K60
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M1023	I951	R884	W821	A755	A690	S629	I567	G506	R445	E382	GLN	GLU	G182	E122	G61
	D952	I885	A822	Q756	L691	V630	R568	N507	V446		VAL	GLY	E183	L123	K62
S1026	D953	R886	L823	Q756	E692	I631	N569	R508	V447	V385	ARG	VAL	E184	E124	Y63
G1027	A954	A887	N824	A759	E693	V632	E570	P509	E448	H388	ALA	GLU	V185	Q125	K64
A1028	V955	R888	A825	R760	V694	V633	K571	E510	S449	E389	ALA	GLU	V186	V126	R65
R1029	I956	A889	P826	I761	I695	G634	R572	N511	Y450	E389	GLN	LEU	K187	L127	Q66
G1030	P957	V890	L827	Q762	H696	P635	M573	M512	Y450	P390	VAL	LYS	G188	Y129	R67
P1031	E958	R891	K828	M763	G697	Q636	L574	E513	L452	A391	GLU	LEU	L191	F128	F68
Q1032	E959	R892	W829	L764	G698	L637	Q575	L514	D453	S392	ALA	LEU	S392	E69	E69
F1033	E960	R893	A830	S765	E699	K638	Q576	E515	A454	I393	GLU	GLU	A192	K130	G70
K1034	K961	R894	C831	A766	V700	L639	A577	A516	R455	L394	GLU	GLU	P193	Y132	K71
I1035	Q962	R895	R832	H767	L701	H640	W578	W517	M456	V395	GLU	GLY	G194	I133	V72
R1036	Q963	R896	E833	L770	L702	Q641	D579	P518		V396	GLY	ALA	V195	C73	C73
Q1037	L964	E897	T834		W703	C642	A580	V519	E459	K397	GLY	PHE	V196	E74	E74
E1038	E965	R898	S835		R704	G643	L581	L520	A460	A398	THR	LEU	S197	D136	R75
C1039		R899	W836	S774	A705	L644	L582	P521	T461	R399	VAL	VAL	R198	P137	R76
D1040	D968	I900	C837	G775	T707	K646	D583	P522	Q462	Y401	THR	LEU	L199	K138	G77
L1041	R969	Q901	R838	E776	L708	R647	G585	D523	Q463		ARG	ARG	D200	G139	V78
R1042	K970	L902	L839	P777	H709	H648	R586	R525	L464	F403	THR	ARG	G201	E79	E79
M1045	L972	Q906	K840	L778	L708	A649	R587	R526	L465	P402	LEU	LEU	V202	I141	V80
Q1046	Q973	E907	W841	A779	R710	A649	R587	P526	K466	E404	PHE	ASP	A203	L142	T81
K1047	K1047	K908	F843	K780	L711	L650	G588	M527	E467	D405	LEU	LEU	L204	N143	X82
E975	E975	N909	A844	S781	G712	E651	A589	V528	L468	D406	GLU	PRO	Y205	G144	S83
Q976		S910		S782			P590	Q529	D469	V407	THR	VAL	R206	V145	I84
I1049					A715	K654	V591	V530	L470	E408	THR	ALA	F207	P146	V85
G1050	E979	L911	P846	D784	F716	P655	T592	D531	E471		GLU	THR	P208	V147	R86
E1051		K912	D847	I785	Q717	F656	N593	G532	A472	T411	PRO	THR	R209	E148	R87
F1052	L913	D913	E848	L786	P718	L657	P594	G533	L473	G412	LYS	PHE	R210	Y88	R89
L1053	L914	A849	W719	L787	L718	L658	G595	R534	E474	D413	ASP	LEU	V211	K149	
E1054	T984	V915	L850	G788	L720	K659	S596	F535	K475	R414	THR	PRO	R212	Q151	M90
V1055		Y916	L851	L789	W721	K660	D597	A536	E476	V415	ARG	VAL	E213	L152	
P1056	E987	Q917	A852		E722	M661	R598	T537	L477	A416	VAL	VAL	E214	L153	I93
R1058	R988	F918	W853	L792	G723	E663	P599	S538	E478	P417	GLN	MET	Y215	T154	E94
S1059	Y989			T793	Q724	E663	L600	D539	E479	G418	PRO	THR	V216	D155	L95
F1060	I992	R921	T857	Q794	S725	K664	R601		E480	D419	HIS	PRO	K217	E156	A96
S1061	L993	R921	W858	W795	I726	G665	S802	D542	M481	V420	MET	LEU	R220	E157	T97
R1062	Q994	L922	R859	R796	Q727	L666	L603	L543	K482	L421	ASN	VAL	A221	P98	
E1063	L995	K926	L860	K797	L728	A667	T604	Y544	H483	A422	VAL	VAL	G222	R159	A99
G1064	W996	T927	D862	K799	H729	P668	D605	R545	P484	D423	VAL	HIS	E160	A100	
L1065	T997	A928	W863	K800	P730	N669	L606	R546	S485	G424	VAL	GLY	L223	H101	
T1066	E998	R929	T864	G801	W732	K671	S608	L548	R485	C425	PRO	GLU	V231	I102	
V1067	T999	L930	T865	A802	E733	A672	G609	N549	A487	K426	GLU	TLE	G231	Y163	Y103
L1068	T1000	L931	W866	G803	E734	K673	K610	R550	R488	V427	GLY	VAL	P238	G164	F104
E1069	E1001	D932	R867	L804	A735	R674	Q611	N551	R489	K428	ALA	GLU	G239	K165	V105
Y1070	K1002	A933	E868	E805	F736	R675	G612	N552	A490	S429	ARG	LYS	E240	Q166	K106
F1071	T1003	L934	K871	F806	N737	M676	R613	R553	K491	D430	VAL	GLY	E240	E167	D107
I1072	T1004	K335	T871	A807	A738	L677	F614	L554	A492	V431	GLU	GLN	I241	T168	V108
S1073	Q1005	Y936	R872	T808	D739	E678	R615	K555	R493	Y432	ALA	PRO	L242	Y169	P109
W1074	T1006	Y937	L873	P809	D739	R679	Q616	K556	R495	C433	LEU	LEU	A243	P170	S110
H1075	V1007	Y937	E874	R810	D743	Q680	M617	K556	R496	D365	ALA	ALA	E244	L171	K111
G1076	F1008	T940	T875	E811	Q744	R681	K621	L558	E497	V435	ALA	GLU	L245	P172	I112
A1077	K1009	T944	S876	A812	M745	D682	R622	A559	V498	V437	LYS	LYS	P246	P173	G113
R1078	N1010	T944	P877	L813	L683	L683	G623	Q560	V499	D438	GLY	GLY	G174	G174	T114
K1079	G945	S945	R878	A814	W749	K684	W623	G561	R500	L439	LEU	LEU	P248	V175	L115
G1080	M1018	G946	R879	R814	P750	D685	D624	A562	A501	L439	LEU	LEU	F251	D176	L116
P1019	P1019	I947	T880	E817	L751	E886	W624	E562	F502	V440	ARG	ARG	A177	D117	D117
L1020	T948	L881	L881	R818	S752	W687	Y625	P563	R441	R379	MET	PRO	ARG	L178	L118
A1085	F982	I949	F882	S752	S752	D689	G627	E564	N442	A379	ALA	ALA	ALA	V179	S119
Y1021	V1022	G950	A883	E820	F754	D689	R628	I566	D504	V443	ARG	ARG	E380	K180	A120
															T121





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	239.50Å 239.50Å 253.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.80 24.96 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.80) 92.0 (24.96-2.80)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.16 (at 2.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.231 , 0.268 0.227 , 0.261	Depositor DCC
$R_{free}$ test set	21166 reflections (5.78%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.9	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 79.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.499 for -h,-k,l 0.068 for h,-h-k,-l 0.068 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	58679	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.92% 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](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.80	1/1838 (0.1%)	0.88	1/2498 (0.0%)
1	B	0.75	0/1838	0.82	2/2498 (0.1%)
1	K	0.75	0/1838	0.86	2/2498 (0.1%)
1	L	0.72	0/1838	0.78	1/2498 (0.0%)
2	C	0.84	0/8997	0.90	8/12164 (0.1%)
2	M	0.82	0/8997	0.89	7/12164 (0.1%)
3	D	0.84	0/10975	0.94	20/14836 (0.1%)
3	N	0.83	0/10975	0.93	18/14836 (0.1%)
4	E	0.84	0/783	0.97	0/1054
4	O	0.88	0/783	1.00	1/1054 (0.1%)
5	F	0.75	0/2812	0.82	3/3781 (0.1%)
5	P	0.75	0/2812	0.80	1/3781 (0.0%)
All	All	0.82	1/54486 (0.0%)	0.90	64/73662 (0.1%)

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
3	N	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	48	ILE	C-N	5.57	1.44	1.34

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	199	LEU	CA-CB-CG	-8.69	95.30	115.30
1	B	138	LEU	CA-CB-CG	8.01	133.72	115.30
3	N	1389	LEU	CA-CB-CG	7.77	133.18	115.30
5	P	136	LEU	CA-CB-CG	7.49	132.51	115.30
3	N	76	CYS	CA-CB-SG	6.73	126.11	114.00
3	D	80	VAL	C-N-CA	6.66	138.36	121.70
3	N	199	LEU	CA-CB-CG	-6.61	100.09	115.30
1	K	211	LEU	CA-CB-CG	6.60	130.48	115.30
2	M	207	LEU	CA-CB-CG	6.53	130.32	115.30
3	D	73	CYS	CA-CB-SG	6.43	125.57	114.00
3	D	813	LEU	CA-CB-CG	6.40	130.02	115.30
3	D	708	LEU	CA-CB-CG	-6.38	100.62	115.30
1	A	192	LEU	CA-CB-CG	6.14	129.43	115.30
3	N	80	VAL	C-N-CA	6.05	136.82	121.70
2	C	98	LEU	CA-CB-CG	6.02	129.15	115.30
5	F	136	LEU	CA-CB-CG	5.96	129.01	115.30
5	F	354	LEU	CA-CB-CG	5.96	129.00	115.30
3	D	238	PRO	N-CA-CB	5.94	110.43	103.30
1	K	45	LEU	CA-CB-CG	-5.94	101.65	115.30
3	D	1209	LEU	N-CA-C	-5.90	95.06	111.00
3	N	380	GLU	N-CA-C	-5.90	95.07	111.00
3	D	1395	LEU	CA-CB-CG	5.89	128.84	115.30
3	N	1209	LEU	N-CA-C	-5.88	95.13	111.00
2	M	571	LEU	CA-CB-CG	5.86	128.78	115.30
3	N	705	ALA	C-N-CD	5.82	140.62	128.40
2	M	165	LEU	C-N-CD	-5.82	107.80	120.60
4	O	54	LEU	CA-CB-CG	5.74	128.51	115.30
3	N	238	PRO	N-CA-CB	5.74	110.19	103.30
3	D	208	PRO	CA-N-CD	-5.65	103.59	111.50
3	N	972	LEU	CA-CB-CG	5.59	128.16	115.30
2	C	243	ARG	C-N-CD	-5.53	108.43	120.60
2	C	858	MET	CA-CB-CG	5.53	122.70	113.30
3	D	380	GLU	N-CA-C	-5.51	96.11	111.00
2	C	1098	ASP	CB-CG-OD1	5.51	123.26	118.30
3	N	171	LEU	CA-CB-CG	5.51	127.97	115.30
2	C	882	LEU	CA-CB-CG	-5.50	102.65	115.30
3	D	1389	LEU	CA-CB-CG	5.46	127.87	115.30
3	D	839	LEU	CA-CB-CG	5.46	127.85	115.30
3	N	73	CYS	CA-CB-SG	5.46	123.82	114.00
3	D	248	PRO	N-CA-CB	5.45	109.84	103.30
3	N	1290	LEU	CA-CB-CG	5.45	127.84	115.30
3	D	80	VAL	CA-C-N	-5.45	105.22	117.20
2	C	620	LEU	CA-CB-CG	5.43	127.80	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	60	CYS	CA-CB-SG	5.39	123.71	114.00
1	B	132	LEU	CA-CB-CG	5.39	127.70	115.30
3	N	209	ARG	N-CA-C	5.36	125.48	111.00
3	N	554	LEU	CA-CB-CG	5.35	127.61	115.30
3	N	637	LEU	CA-CB-CG	5.34	127.58	115.30
3	N	248	PRO	N-CA-CB	5.30	109.66	103.30
3	N	208	PRO	CA-N-CD	-5.24	104.17	111.50
3	D	209	ARG	N-CA-C	5.21	125.06	111.00
2	M	729	LEU	N-CA-C	5.17	124.97	111.00
2	M	243	ARG	C-N-CD	-5.17	109.22	120.60
2	M	726	ILE	CG1-CB-CG2	-5.10	100.18	111.40
3	D	226	PRO	N-CA-CB	5.09	109.41	103.30
1	L	132	LEU	CA-CB-CG	5.09	127.00	115.30
2	C	58	ASP	C-N-CA	5.08	134.40	121.70
3	D	153	LEU	CA-CB-CG	5.07	126.95	115.30
3	N	434	ARG	NE-CZ-NH1	5.06	122.83	120.30
3	D	21	TRP	CA-CB-CG	5.05	123.29	113.70
5	F	361	LEU	CA-CB-CG	5.04	126.90	115.30
2	C	729	LEU	N-CA-C	5.03	124.58	111.00
3	D	423	ASP	N-CA-C	5.02	124.55	111.00
2	M	861	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	N	132	TYR	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1806	0	1861	216	0
1	B	1806	0	1861	199	0
1	K	1806	0	1861	208	0
1	L	1806	0	1861	206	0
2	C	8829	0	8933	1184	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	M	8829	0	8933	1106	0
3	D	10797	0	10873	1450	0
3	N	10797	0	10873	1345	0
4	E	769	0	775	97	0
4	O	769	0	775	108	0
5	F	2771	0	2844	336	0
5	P	2771	0	2844	342	0
6	D	2	0	0	0	0
6	N	2	0	0	0	0
7	D	1	0	0	0	0
7	N	1	0	0	0	0
8	A	191	0	0	37	0
8	B	181	0	0	34	0
8	C	767	0	0	174	0
8	D	1100	0	0	234	0
8	E	93	0	0	14	0
8	F	333	0	0	58	0
8	K	151	0	0	30	0
8	L	179	0	0	49	0
8	M	739	0	0	195	0
8	N	1038	0	0	225	0
8	O	78	0	0	24	0
8	P	267	0	0	61	0
All	All	58679	0	54294	6401	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 59.

All (6401) 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)
2:M:1054:THR:HG21	2:M:1079:PRO:HB3	1.28	1.11
1:A:95:GLN:HA	1:A:146:ARG:HH12	1.12	1.08
2:C:135:VAL:HG11	2:C:407:LYS:HA	1.36	1.04
1:A:42:ARG:HH12	2:C:857:ASP:HB3	1.14	1.04
3:N:1036:ARG:HH21	3:N:1042:ARG:HA	1.20	1.04
3:N:1481:VAL:HG13	4:O:18:ARG:HE	1.16	1.02
3:D:197:SER:HB3	3:D:203:ALA:HB3	1.42	1.02
3:N:197:SER:HB3	3:N:203:ALA:HB3	1.41	1.02
2:M:169:GLY:HA2	2:M:263:ASP:HB3	1.42	1.01
2:C:358:ARG:HH22	2:C:374:ASN:HB3	1.26	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:979:THR:HG23	2:C:981:GLU:H	1.26	1.00
2:C:328:LEU:HD13	2:C:433:THR:HB	1.41	0.99
3:N:1101:VAL:HG21	3:N:1424:VAL:HG22	1.40	0.99
3:D:1045:MET:HG2	3:D:1073:SER:HA	1.41	0.99
2:C:110:GLU:HG2	2:C:369:PRO:HB3	1.41	0.98
2:M:409:ARG:HA	2:M:454:SER:HA	1.44	0.98
3:N:1144:LEU:HD12	3:N:1171:VAL:HG13	1.44	0.98
3:N:52:PRO:HB2	3:N:80:VAL:HG13	1.45	0.98
2:M:157:ARG:HD2	2:M:314:THR:HG22	1.46	0.98
2:C:1114:GLY:H	2:C:1115:LEU:HD12	1.27	0.97
2:C:281:LEU:HD11	2:C:306:THR:HA	1.47	0.97
2:C:47:ALA:HB1	2:C:345:ARG:HB3	1.47	0.97
3:D:141:ILE:HG12	3:D:449:SER:HA	1.46	0.97
2:C:1008:ARG:HH21	2:C:1028:GLY:HA2	1.30	0.96
2:M:129:ILE:HD13	2:M:134:ARG:HB2	1.46	0.96
5:P:347:GLN:HA	5:P:350:LEU:HD22	1.47	0.96
3:D:422:ALA:HB3	3:D:427:VAL:HG22	1.45	0.96
2:M:110:GLU:HG2	2:M:369:PRO:HG3	1.46	0.96
1:K:89:PHE:HB2	1:K:94:LEU:HD13	1.48	0.96
2:C:630:ARG:HH21	2:C:705:ILE:HG22	1.27	0.95
3:N:1432:LYS:HD2	3:N:1433:SER:H	1.29	0.95
2:M:405:ARG:HG2	2:M:409:ARG:HH21	1.29	0.95
2:C:719:PRO:HB3	2:C:820:ARG:HE	1.29	0.95
2:C:773:LEU:HB2	5:F:373:LYS:HB3	1.47	0.95
2:C:332:ARG:HB3	2:C:332:ARG:HH11	1.32	0.95
5:P:88:ILE:HD13	5:P:193:ARG:HB2	1.45	0.95
5:P:164:LYS:HA	5:P:171:LYS:HE2	1.49	0.94
2:C:1090:LYS:HZ2	3:D:90:MET:HG3	1.31	0.93
3:N:55:ASP:HA	3:N:82:LYS:HG3	1.48	0.93
2:C:150:PRO:HA	2:C:158:TYR:HB3	1.50	0.93
1:A:95:GLN:HG2	1:A:146:ARG:HH22	1.33	0.93
2:C:1054:THR:HG21	2:C:1079:PRO:HB3	1.46	0.93
2:C:517:ARG:HH11	2:C:522:VAL:HG11	1.33	0.93
2:M:16:PRO:HB3	2:M:460:ARG:HH22	1.33	0.93
3:N:422:ALA:HB3	3:N:427:VAL:HG22	1.50	0.93
2:M:564:MET:HG3	2:M:997:LEU:HD21	1.50	0.93
4:E:67:GLU:HB2	4:E:73:LEU:HD11	1.51	0.93
3:D:493:ARG:HH21	3:D:1388:ARG:HB3	1.30	0.93
2:C:479:VAL:HG21	2:C:503:LEU:HD11	1.51	0.92
3:D:1101:VAL:HG21	3:D:1424:VAL:HG22	1.52	0.92
3:N:500:ARG:HH12	3:N:1388:ARG:HH11	1.13	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:698:LYS:HA	3:D:756:GLN:HE22	1.32	0.92
3:D:18:ILE:HG23	3:D:518:PRO:HG3	1.51	0.92
1:A:14:ARG:HH21	1:A:22:GLU:HB3	1.32	0.92
3:D:654:LYS:HB3	3:D:655:PRO:HD3	1.52	0.92
1:K:19:GLU:HB3	1:K:175:ARG:HH22	1.34	0.92
1:B:179:PHE:HB3	1:B:197:LEU:HD12	1.51	0.91
4:O:47:LYS:HA	8:O:4983:HOH:O	1.68	0.91
3:D:1066:THR:HG23	3:D:1069:GLU:H	1.34	0.91
3:D:630:VAL:HA	3:D:744:GLN:HG2	1.51	0.91
3:D:400:VAL:HG21	3:D:441:ARG:HH11	1.35	0.91
5:P:394:ARG:HA	5:P:397:ILE:HD12	1.51	0.91
3:D:908:LYS:HB3	3:D:1027:GLY:HA3	1.51	0.91
3:N:422:ALA:HB1	5:P:178:ARG:HH12	1.34	0.91
1:K:227:ASN:HD22	1:K:227:ASN:H	1.15	0.91
5:P:266:GLU:HA	5:P:269:ASN:HD22	1.35	0.91
1:B:152:PRO:HD2	1:B:155:LYS:HD3	1.51	0.91
2:C:282:GLY:HA2	2:C:308:ARG:HH22	1.32	0.90
3:D:143:ASN:HD21	3:D:145:VAL:HG12	1.35	0.90
2:M:92:ALA:HB2	2:M:120:LEU:HD11	1.53	0.90
2:C:724:ARG:HG3	2:C:741:GLY:H	1.36	0.90
3:D:118:LEU:HB3	3:D:123:LEU:HD22	1.54	0.90
5:F:268:ILE:HA	5:F:271:LEU:HD12	1.53	0.90
2:M:1111:ILE:HD12	2:M:1112:PHE:H	1.36	0.90
3:N:133:ILE:HG21	3:N:454:ALA:HB1	1.53	0.90
2:C:274:ARG:HD2	2:C:285:LEU:HB3	1.53	0.90
3:D:12:LEU:HD13	3:D:511:TRP:HB2	1.53	0.90
2:C:860:HIS:HB2	8:C:1175:HOH:O	1.72	0.89
5:F:392:VAL:HG11	5:F:396:ARG:HD2	1.55	0.89
3:N:9:ARG:HH12	3:N:506:GLY:HA2	1.37	0.89
3:N:131:LYS:HG3	3:N:568:ARG:HG2	1.53	0.89
3:N:928:ALA:HA	3:N:931:LEU:HD12	1.55	0.89
2:C:905:ILE:H	2:C:905:ILE:HD12	1.37	0.89
3:D:493:ARG:NH2	3:D:1388:ARG:HB3	1.87	0.89
3:N:787:LEU:HD11	3:N:947:ILE:HG12	1.53	0.89
2:M:150:PRO:HA	2:M:158:TYR:HB3	1.54	0.89
3:N:1290:LEU:HD23	3:N:1291:SER:H	1.37	0.89
3:D:119:SER:HB2	3:D:123:LEU:H	1.38	0.88
2:M:1054:THR:HG22	2:M:1059:ASP:HB2	1.55	0.88
2:M:176:VAL:HG12	2:M:182:VAL:HG13	1.53	0.88
2:M:979:THR:HG23	2:M:981:GLU:H	1.38	0.88
2:C:478:VAL:HG13	2:C:506:ASN:HB3	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:633:VAL:HG22	3:N:635:PRO:HD3	1.54	0.88
1:K:186:LEU:HB2	1:K:192:LEU:HD11	1.56	0.88
2:M:861:LEU:HD23	2:M:862:PRO:HD2	1.56	0.88
3:N:699:VAL:H	3:N:756:GLN:NE2	1.72	0.88
1:L:126:ASP:HA	8:L:4849:HOH:O	1.72	0.88
3:N:565:ILE:H	3:N:565:ILE:HD12	1.39	0.88
3:N:141:ILE:HG12	3:N:449:SER:HA	1.54	0.88
3:D:191:LEU:HD12	3:D:211:VAL:HG21	1.54	0.87
3:N:1476:THR:HG23	4:O:21:VAL:HG22	1.56	0.87
5:F:350:LEU:HD12	5:F:422:LEU:HD12	1.56	0.87
5:F:76:SER:O	5:F:80:PRO:HD2	1.73	0.87
1:B:24:VAL:HG13	1:B:196:THR:HG22	1.55	0.87
3:D:136:ASP:HB3	3:D:137:PRO:HD3	1.57	0.87
3:D:145:VAL:HG22	3:D:146:PRO:HD2	1.54	0.87
2:C:1095:LEU:HD11	3:D:607:LEU:HD11	1.54	0.87
2:M:704:HIS:HB2	2:M:831:ARG:HE	1.40	0.87
2:M:689:VAL:HB	2:M:870:ILE:HG13	1.56	0.87
2:M:904:PRO:HD2	2:M:908:GLY:HA2	1.57	0.86
2:C:689:VAL:HB	2:C:870:ILE:HG13	1.58	0.86
3:D:1087:ARG:HG2	3:D:1234:THR:HA	1.54	0.86
3:N:536:ALA:HA	5:P:315:VAL:H	1.40	0.86
3:N:535:PHE:HB3	5:P:314:PRO:HB3	1.55	0.86
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.57	0.86
2:C:1090:LYS:HE2	2:C:1112:PHE:HE1	1.39	0.86
2:M:614:ARG:HD2	2:M:620:LEU:HD12	1.54	0.86
1:B:87:VAL:HG21	1:B:144:VAL:HG11	1.58	0.86
1:B:41:ARG:HG3	1:B:177:VAL:HG21	1.57	0.85
2:C:376:ARG:HH22	5:F:285:GLU:HB3	1.40	0.85
3:D:148:GLU:HB3	3:D:151:GLN:HB2	1.58	0.85
3:N:1314:LYS:HZ3	3:N:1317:ASP:H	1.22	0.85
3:N:838:ARG:HA	8:N:9349:HOH:O	1.76	0.85
2:C:145:GLY:H	2:C:163:ILE:HG23	1.41	0.85
3:N:817:GLU:HG3	3:N:839:LEU:HD13	1.57	0.85
1:A:54:THR:HG23	1:A:158:ILE:HG13	1.59	0.85
3:D:1330:ILE:HA	8:D:9063:HOH:O	1.75	0.85
5:F:273:ARG:HA	5:F:276:ARG:HD2	1.59	0.85
3:D:1096:ARG:HH11	3:D:1096:ARG:HB2	1.39	0.85
3:D:667:ALA:HB2	3:D:676:MET:HE2	1.58	0.85
2:M:772:ARG:HD2	5:P:373:LYS:HD2	1.59	0.85
2:C:701:THR:HG23	2:C:832:LYS:HG3	1.59	0.85
2:M:139:GLN:HE21	2:M:334:ARG:HH11	1.22	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:597:ALA:HB2	2:C:655:LEU:HD21	1.55	0.85
8:C:1350:HOH:O	3:D:532:GLY:HA2	1.76	0.85
3:D:800:LYS:HE3	3:D:830:ALA:HB3	1.58	0.85
1:L:87:VAL:HG21	1:L:144:VAL:HG11	1.60	0.84
1:L:57:TYR:HB3	1:L:141:GLU:HG3	1.57	0.84
1:A:145:ASP:HB3	8:A:330:HOH:O	1.76	0.84
3:D:615:ARG:HH21	3:D:619:LEU:HD12	1.40	0.84
3:N:971:LEU:HA	3:N:974:ILE:HD12	1.59	0.84
3:N:1481:VAL:HG11	4:O:18:ARG:HA	1.58	0.84
1:B:103:ALA:HB1	1:B:107:LYS:HE3	1.57	0.84
2:M:512:ARG:HB3	2:M:523:ILE:HD11	1.59	0.84
2:C:768:THR:HB	2:C:771:GLU:HB3	1.60	0.84
2:M:274:ARG:HD2	2:M:285:LEU:HD22	1.58	0.84
1:A:206:THR:HG22	1:A:209:GLU:H	1.43	0.84
2:M:115:LEU:HD22	2:M:373:VAL:HG11	1.57	0.84
5:P:132:ARG:HH21	5:P:184:ARG:HH12	1.25	0.84
1:A:95:GLN:HA	1:A:146:ARG:NH1	1.92	0.84
3:D:1438:ALA:O	3:D:1443:THR:HG22	1.77	0.84
1:L:180:GLN:HB2	1:L:198:ARG:HH22	1.43	0.84
3:N:186:VAL:HG21	3:N:213:VAL:HB	1.59	0.84
2:C:129:ILE:HD13	2:C:134:ARG:HB2	1.60	0.83
2:C:579:VAL:HB	2:C:890:LEU:HD22	1.61	0.83
2:C:724:ARG:HH12	2:C:734:LEU:HD23	1.42	0.83
3:D:397:LYS:HE2	3:D:399:ARG:HE	1.44	0.83
5:P:358:LEU:HD13	5:P:370:LYS:HG3	1.59	0.83
2:C:126:SER:HB3	2:C:407:LYS:HE3	1.60	0.83
1:K:24:VAL:HG22	1:K:196:THR:HB	1.58	0.83
2:M:260:LEU:HG	2:M:261:ILE:HG13	1.60	0.83
2:M:710:ILE:HB	2:M:790:LEU:HD12	1.58	0.83
1:B:86:VAL:HG12	1:B:124:ASN:HD22	1.44	0.83
2:C:500:ASN:HD21	3:D:1067:VAL:HG23	1.42	0.83
3:D:1057:VAL:HG13	3:D:1069:GLU:HB3	1.60	0.83
3:D:520:LEU:HD12	3:D:521:PRO:HD2	1.60	0.83
1:K:78:ILE:HA	1:K:81:ASN:ND2	1.93	0.83
3:D:928:ALA:HA	3:D:931:LEU:HD12	1.59	0.83
1:A:87:VAL:HG21	1:A:144:VAL:HG11	1.61	0.83
1:K:89:PHE:HZ	1:K:146:ARG:HB2	1.43	0.83
3:N:212:ARG:HD3	3:N:445:ARG:HH12	1.43	0.83
3:D:658:LEU:HA	3:D:661:MET:HE3	1.60	0.83
3:D:1481:VAL:HG11	4:E:18:ARG:HA	1.61	0.83
5:F:394:ARG:HA	5:F:397:ILE:HD12	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:380:ALA:HA	2:M:383:ARG:HD2	1.61	0.83
3:N:704:ARG:HD2	3:N:705:ALA:H	1.43	0.83
2:C:578:VAL:HG11	2:C:991:GLN:HB3	1.60	0.82
1:K:87:VAL:HG21	1:K:144:VAL:HG11	1.61	0.82
2:C:1097:LEU:HD22	2:C:1097:LEU:H	1.44	0.82
3:D:1095:THR:O	3:D:1099:VAL:HG23	1.78	0.82
3:N:139:GLY:HA3	3:N:452:ILE:HD12	1.62	0.82
5:F:85:LEU:HA	5:F:88:ILE:HD12	1.59	0.82
1:L:56:VAL:HG13	1:L:142:VAL:HG12	1.62	0.82
2:M:534:VAL:H	2:M:538:GLN:HE22	1.27	0.82
3:N:422:ALA:H	3:N:427:VAL:HG11	1.44	0.82
5:P:166:LEU:HB3	5:P:170:HIS:HB2	1.61	0.82
2:C:232:GLU:HA	2:C:235:LEU:HD12	1.58	0.82
2:M:1009:SER:HB2	3:N:651:GLU:O	1.80	0.82
3:N:907:GLU:HA	8:N:9094:HOH:O	1.78	0.82
1:A:186:LEU:HB2	1:A:192:LEU:HD11	1.60	0.82
2:C:25:SER:HB2	2:C:335:THR:HB	1.62	0.82
3:D:187:LYS:HE2	3:D:213:VAL:HG12	1.62	0.82
2:M:1051:GLU:HG2	2:M:1056:LYS:HE3	1.61	0.82
5:F:125:ASP:HA	5:F:128:ARG:NH1	1.95	0.82
5:P:406:ARG:HA	5:P:409:LYS:HG2	1.60	0.82
2:C:176:VAL:HG12	2:C:182:VAL:HG13	1.62	0.81
1:L:65:PHE:HD1	3:N:813:LEU:HD22	1.45	0.81
2:M:905:ILE:HD12	2:M:905:ILE:H	1.43	0.81
3:D:785:ILE:HD12	3:D:785:ILE:H	1.44	0.81
1:A:8:ALA:HB1	1:B:224:TYR:HE1	1.44	0.81
2:C:802:ARG:HG2	2:C:826:TYR:HB2	1.62	0.81
3:N:628:ARG:HD3	3:N:744:GLN:HE22	1.45	0.81
2:C:675:ALA:HB2	2:C:867:VAL:HG11	1.61	0.81
3:N:420:VAL:HA	5:P:164:LYS:HD3	1.61	0.81
3:D:1209:LEU:HD13	3:D:1211:MET:HE1	1.60	0.81
3:N:187:LYS:HE2	3:N:213:VAL:HG12	1.62	0.81
2:C:710:ILE:HB	2:C:790:LEU:HD13	1.61	0.81
3:D:1310:ARG:HD3	3:D:1310:ARG:H	1.46	0.81
2:C:313:LEU:HA	2:C:321:GLU:HG3	1.63	0.81
1:A:42:ARG:NH1	2:C:857:ASP:HB3	1.94	0.81
3:D:1262:LEU:HD23	3:D:1352:ILE:HG13	1.61	0.81
3:D:179:VAL:HG13	3:D:389:GLU:HG3	1.62	0.81
2:M:1096:ALA:O	3:N:13:ALA:HB2	1.80	0.81
2:C:873:PRO:HG2	3:D:947:ILE:HD12	1.62	0.81
2:M:328:LEU:HD22	2:M:433:THR:HG22	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1045:MET:HG2	3:N:1073:SER:HA	1.62	0.81
3:N:658:LEU:HA	3:N:661:MET:HE3	1.63	0.81
3:N:906:GLN:HB3	3:N:911:LEU:HD11	1.61	0.81
4:O:12:MET:HB3	8:O:3864:HOH:O	1.81	0.80
2:C:367:LEU:HD22	2:C:371:LYS:HG2	1.63	0.80
3:D:611:GLN:HA	3:D:615:ARG:HD2	1.62	0.80
3:N:475:LYS:HA	3:N:478:LEU:HD12	1.64	0.80
3:N:865:THR:HG23	3:N:874:GLU:HG3	1.63	0.80
3:D:87:ARG:HA	8:D:9040:HOH:O	1.81	0.80
1:L:32:PHE:HB2	8:L:4886:HOH:O	1.81	0.80
5:P:120:THR:HG22	5:P:122:LEU:HD13	1.63	0.80
3:N:500:ARG:NH1	3:N:1388:ARG:HH11	1.79	0.80
2:C:281:LEU:HD12	2:C:309:TYR:HB2	1.63	0.80
3:N:850:LEU:H	3:N:850:LEU:HD12	1.46	0.80
2:M:537:LYS:HA	2:M:545:ASN:HD21	1.46	0.80
1:A:102:LYS:HG3	1:A:139:ASN:HB2	1.61	0.80
2:C:461:VAL:HG13	2:C:465:GLY:HA2	1.62	0.80
2:M:578:VAL:HG23	2:M:579:VAL:HG12	1.63	0.80
2:M:857:ASP:HB2	2:M:978:ARG:HG2	1.64	0.80
2:M:983:ILE:HG21	2:M:987:ILE:HD11	1.61	0.80
5:P:163:LEU:HD13	5:P:174:LEU:HD21	1.63	0.80
2:C:611:ILE:HD11	2:C:625:LEU:HD11	1.62	0.80
3:N:1352:ILE:O	3:N:1355:VAL:HG23	1.81	0.80
3:N:1393:GLN:HB2	3:N:1398:TRP:HE1	1.46	0.80
2:M:507:ARG:HB2	2:M:507:ARG:HH11	1.45	0.79
3:N:152:LEU:HD23	3:N:152:LEU:H	1.44	0.79
3:D:1350:GLU:HG3	3:D:1354:LYS:HE3	1.65	0.79
3:D:656:PHE:HB3	3:D:694:VAL:HG11	1.64	0.79
2:C:347:GLY:HA2	2:C:350:ARG:HD2	1.64	0.79
2:C:719:PRO:HB3	2:C:820:ARG:NE	1.96	0.79
3:D:1277:ILE:HD12	3:D:1301:LYS:HB2	1.65	0.79
2:M:146:VAL:HG22	2:M:162:ILE:HA	1.65	0.79
3:D:546:ARG:O	3:D:550:ARG:HG2	1.81	0.79
2:C:772:ARG:HG2	5:F:378:GLY:HA2	1.64	0.79
3:D:562:ALA:HB1	3:D:567:ILE:HD11	1.65	0.79
2:M:36:PRO:HG2	2:M:70:GLU:HB3	1.64	0.79
3:N:18:ILE:HG23	3:N:518:PRO:HG3	1.62	0.79
5:F:156:VAL:HA	5:F:159:ILE:HD12	1.63	0.79
2:M:182:VAL:HG12	2:M:193:LEU:HD13	1.65	0.79
2:M:244:PRO:HD2	2:M:245:GLY:H	1.48	0.79
3:N:1057:VAL:HG13	3:N:1069:GLU:HB3	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:470:LEU:H	3:N:470:LEU:HD23	1.46	0.79
3:N:53:ILE:HG23	3:N:54:LYS:H	1.48	0.79
1:L:219:ARG:HB3	1:L:219:ARG:HH11	1.48	0.79
1:A:24:VAL:HG13	1:A:196:THR:HG22	1.64	0.78
2:M:68:PHE:HE1	2:M:96:ALA:HB1	1.48	0.78
3:N:615:ARG:HB2	3:N:615:ARG:HH11	1.46	0.78
2:C:1090:LYS:NZ	3:D:90:MET:HG3	1.97	0.78
3:D:1383:ASP:HB2	3:D:1416:ALA:HB3	1.64	0.78
2:M:242:LEU:HB3	8:M:1549:HOH:O	1.83	0.78
3:N:806:PHE:CE1	3:N:813:LEU:HB3	2.18	0.78
1:B:13:VAL:HG23	8:B:493:HOH:O	1.82	0.78
3:D:1087:ARG:HA	3:D:1090:ASP:HB2	1.63	0.78
2:M:670:GLN:O	2:M:672:VAL:HG12	1.83	0.78
2:M:752:GLY:H	2:M:792:VAL:HB	1.45	0.78
2:C:1009:SER:HA	8:D:9195:HOH:O	1.82	0.78
2:M:397:GLU:H	2:M:633:GLN:NE2	1.81	0.78
2:C:71:TYR:HB2	8:C:1125:HOH:O	1.82	0.78
3:D:806:PHE:CE1	3:D:813:LEU:HB3	2.18	0.78
2:M:413:LEU:H	2:M:413:LEU:HD12	1.48	0.78
1:A:83:LYS:HE2	1:A:167:VAL:HG12	1.64	0.78
2:C:1111:ILE:HG13	2:C:1112:PHE:H	1.49	0.78
2:C:413:LEU:HD12	2:C:413:LEU:H	1.46	0.78
3:N:119:SER:HB2	3:N:123:LEU:HB2	1.66	0.78
3:D:152:LEU:HD23	3:D:152:LEU:H	1.48	0.78
3:D:422:ALA:H	3:D:427:VAL:HG11	1.48	0.78
3:D:86:ARG:O	3:D:522:PRO:HD2	1.83	0.78
5:F:130:VAL:HG21	5:F:159:ILE:HG21	1.64	0.78
2:M:710:ILE:HD12	2:M:790:LEU:HB2	1.64	0.78
2:M:966:LEU:HD11	2:M:986:PRO:HG2	1.66	0.78
1:A:63:HIS:HB3	2:C:746:GLY:HA2	1.66	0.78
2:C:876:VAL:HA	8:C:1494:HOH:O	1.84	0.78
3:N:1095:THR:O	3:N:1099:VAL:HG23	1.83	0.78
3:N:1112:CYS:HB2	3:N:1195:GLN:OE1	1.84	0.78
5:P:291:ILE:HG21	5:P:304:VAL:HG11	1.65	0.78
3:D:127:LEU:HD11	3:D:461:ILE:HD11	1.65	0.78
4:O:51:LEU:HG	4:O:53:GLY:H	1.49	0.78
1:A:175:ARG:HH11	1:A:202:ASP:HA	1.49	0.77
1:K:25:LEU:HD23	1:K:28:LEU:HD11	1.64	0.77
3:D:1272:ALA:HA	3:D:1326:THR:HB	1.66	0.77
3:N:631:ILE:HG21	3:N:745:MET:HG3	1.66	0.77
2:C:773:LEU:HB2	5:F:373:LYS:CB	2.15	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:205:ARG:HD2	5:F:251:ILE:HD13	1.66	0.77
2:M:1021:LEU:HD21	5:P:332:PHE:HA	1.66	0.77
2:C:137:VAL:HG23	2:C:391:LEU:HG	1.66	0.77
2:C:468:ARG:HG2	8:C:1431:HOH:O	1.82	0.77
5:P:260:ILE:HG23	5:P:264:MET:HB2	1.65	0.77
2:C:30:LEU:HB3	2:C:44:ILE:HD12	1.67	0.77
2:C:678:PRO:O	3:D:943:THR:HA	1.84	0.77
3:D:1166:LEU:HD12	3:D:1171:VAL:HG22	1.67	0.77
2:M:250:ARG:HG2	2:M:253:ALA:HB3	1.67	0.77
5:P:321:ILE:HD11	5:P:329:TYR:HB2	1.66	0.77
1:A:150:TYR:HE2	1:A:152:PRO:HG3	1.49	0.77
3:D:877:PRO:HA	8:D:9153:HOH:O	1.84	0.77
3:D:901:GLN:HB2	8:D:9514:HOH:O	1.84	0.77
3:N:119:SER:H	3:N:123:LEU:HD22	1.50	0.77
2:C:462:ASP:HB3	2:C:468:ARG:HD2	1.66	0.77
3:D:1312:LEU:HB2	8:D:9354:HOH:O	1.84	0.77
3:D:1468:LEU:HD13	3:D:1470:ARG:HD3	1.67	0.77
5:F:117:SER:HA	8:F:433:HOH:O	1.84	0.77
2:C:312:ALA:HB1	2:C:318:PRO:HG2	1.65	0.77
2:C:693:GLU:HA	2:C:696:LYS:HG3	1.65	0.77
2:C:846:LYS:HD3	3:D:741:ASP:HB2	1.67	0.77
5:F:412:GLU:HG3	5:F:418:LEU:HD22	1.67	0.77
3:D:131:LYS:HG2	3:D:568:ARG:HG2	1.66	0.76
3:D:1381:VAL:HB	3:D:1389:LEU:O	1.84	0.76
1:K:18:ARG:HD3	1:K:123:MET:HE3	1.67	0.76
3:D:41:ARG:HD3	3:D:42:ASP:H	1.47	0.76
3:D:876:SER:HA	8:D:9288:HOH:O	1.86	0.76
5:F:163:LEU:HB3	5:F:174:LEU:HG	1.67	0.76
2:M:1054:THR:HG21	2:M:1079:PRO:CB	2.11	0.76
2:M:263:ASP:HB2	2:M:264:PRO:HD3	1.67	0.76
3:N:107:ASP:HB2	8:N:9202:HOH:O	1.85	0.76
3:N:699:VAL:H	3:N:756:GLN:HE22	1.33	0.76
2:C:609:ASN:ND2	2:C:627:ARG:HH21	1.82	0.76
3:D:1223:ILE:HD12	3:D:1223:ILE:H	1.49	0.76
3:D:1209:LEU:HD21	4:E:16:LYS:NZ	1.99	0.76
2:M:816:LYS:HE2	2:M:819:VAL:HG21	1.66	0.76
3:N:1381:VAL:HB	3:N:1389:LEU:O	1.84	0.76
3:N:610:LYS:HG2	3:N:611:GLN:HE21	1.50	0.76
2:C:108:ILE:HB	2:C:368:THR:OG1	1.84	0.76
3:D:9:ARG:HE	3:D:11:ALA:HB2	1.51	0.76
2:M:709:GLU:HG3	2:M:824:ARG:HG3	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:890:VAL:HG11	3:N:922:LEU:HD13	1.65	0.76
1:A:109:VAL:HG23	8:A:356:HOH:O	1.85	0.76
2:C:1067:TYR:HA	2:C:1070:ILE:HD12	1.67	0.76
3:D:633:VAL:HG22	3:D:635:PRO:HD3	1.67	0.76
3:N:12:LEU:HD23	3:N:13:ALA:H	1.50	0.76
2:C:630:ARG:NH2	2:C:705:ILE:HG22	2.01	0.76
3:D:698:LYS:HA	3:D:756:GLN:NE2	2.01	0.76
2:M:943:VAL:HG23	2:M:985:GLY:H	1.51	0.76
3:N:639:LEU:HD12	3:N:639:LEU:H	1.51	0.76
2:C:41:ASN:HD22	2:C:41:ASN:H	1.30	0.76
2:C:944:LEU:HD21	2:C:963:LEU:HD22	1.67	0.76
3:D:1236:LEU:HD12	3:D:1256:LEU:HD12	1.67	0.76
2:M:199:VAL:HG13	2:M:235:LEU:HG	1.66	0.76
2:M:736:ASP:O	2:M:744:ARG:HG2	1.86	0.75
3:N:1040:GLY:O	3:N:1060:SER:HB3	1.86	0.75
3:N:1111:ASP:HB2	3:N:1203:LYS:HG3	1.67	0.75
2:C:534:VAL:H	2:C:538:GLN:HE22	1.34	0.75
2:M:154:ARG:HH21	2:M:156:GLY:HA3	1.50	0.75
2:M:186:VAL:HG23	2:M:187:ASN:H	1.51	0.75
3:N:1066:THR:HG23	3:N:1068:LEU:H	1.51	0.75
3:N:145:VAL:HG22	3:N:146:PRO:HD2	1.69	0.75
2:C:457:ALA:HB3	2:C:538:GLN:HA	1.67	0.75
3:D:842:VAL:HG23	8:D:9407:HOH:O	1.86	0.75
3:D:73:CYS:HB3	3:D:76:CYS:O	1.85	0.75
5:F:125:ASP:HA	5:F:128:ARG:HH12	1.51	0.75
2:M:22:GLN:NE2	2:M:336:VAL:HG21	2.01	0.75
2:M:490:GLU:HB3	8:M:1436:HOH:O	1.86	0.75
2:M:683:ASN:HA	2:M:687:ALA:HB3	1.68	0.75
5:P:358:LEU:HD11	5:P:370:LYS:HZ2	1.51	0.75
1:A:28:LEU:HD13	1:A:32:PHE:HB3	1.69	0.75
3:D:1412:LYS:O	3:D:1414:PRO:HD3	1.86	0.75
3:D:55:ASP:HA	3:D:82:LYS:HG3	1.69	0.75
2:C:987:ILE:HG23	3:D:948:THR:HG21	1.69	0.75
2:M:626:ARG:NH1	2:M:637:LEU:HD12	2.01	0.75
1:K:54:THR:HG22	1:K:158:ILE:HG13	1.68	0.75
1:L:206:THR:HG22	1:L:209:GLU:H	1.52	0.75
3:N:1223:ILE:H	3:N:1223:ILE:HD12	1.51	0.75
3:N:44:LEU:HB3	3:N:525:ARG:HH21	1.50	0.75
1:A:191:ASP:HB3	8:A:483:HOH:O	1.86	0.75
2:M:378:LEU:HG	2:M:382:ILE:HD11	1.69	0.75
2:M:447:ALA:HA	3:N:1085:ALA:HB1	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:558:LEU:HD13	5:P:145:PRO:HB3	1.67	0.75
3:N:58:CYS:HA	3:N:78:VAL:HG11	1.68	0.75
3:N:948:THR:HG22	3:N:949:ILE:H	1.51	0.75
5:P:76:SER:O	5:P:80:PRO:HD2	1.87	0.75
3:D:1109:GLU:HG2	3:D:1201:CYS:HA	1.67	0.75
3:N:1066:THR:HG22	3:N:1069:GLU:HG3	1.69	0.75
2:C:36:PRO:HG2	2:C:70:GLU:HB3	1.69	0.75
2:C:557:ARG:NH2	2:C:879:ARG:HD3	2.00	0.75
3:D:65:ARG:HG3	3:D:66:GLN:H	1.52	0.75
3:D:971:LEU:HA	3:D:974:ILE:HD12	1.69	0.75
1:A:8:ALA:HB1	1:B:224:TYR:CE1	2.22	0.74
3:D:493:ARG:NH1	3:D:1390:LEU:HB2	2.03	0.74
2:M:479:VAL:HG21	2:M:503:LEU:HD11	1.69	0.74
3:N:1393:GLN:HB2	3:N:1398:TRP:NE1	2.01	0.74
5:F:123:ASP:HB2	5:F:126:LEU:HD13	1.67	0.74
1:L:45:LEU:HD21	1:L:177:VAL:HG22	1.66	0.74
5:P:404:ALA:HB3	8:P:4587:HOH:O	1.87	0.74
1:A:189:ARG:HB3	8:A:366:HOH:O	1.86	0.74
1:B:85:LEU:HD12	1:B:124:ASN:HB3	1.68	0.74
3:D:194:GLY:H	3:D:206:ARG:HA	1.51	0.74
2:M:864:GLY:HA2	8:M:1164:HOH:O	1.87	0.74
3:N:470:LEU:HD12	3:N:503:LEU:HG	1.68	0.74
2:M:598:GLU:O	2:M:651:LYS:HG3	1.87	0.74
3:N:1271:LYS:HG2	3:N:1272:ALA:H	1.51	0.74
3:N:875:THR:HG21	3:N:902:LEU:HD13	1.67	0.74
3:D:1147:ARG:HB2	3:D:1166:LEU:HD21	1.69	0.74
3:D:1291:SER:HB2	3:D:1293:PHE:HE1	1.52	0.74
3:N:171:LEU:HB2	3:N:390:PRO:HA	1.68	0.74
3:D:1046:GLN:HG2	3:D:1052:THR:HG22	1.68	0.74
1:L:27:PRO:HB3	1:L:192:LEU:HD22	1.68	0.74
2:M:282:GLY:HA2	2:M:308:ARG:HH21	1.51	0.74
2:M:675:ALA:HA	2:M:989:VAL:HG12	1.70	0.74
3:N:135:LEU:HD13	3:N:147:VAL:HG23	1.68	0.74
2:C:603:VAL:HG21	2:C:643:VAL:HG11	1.67	0.74
2:M:197:LEU:HA	2:M:200:LEU:HD12	1.68	0.74
2:M:313:LEU:HD23	2:M:314:THR:HG23	1.68	0.74
2:C:115:LEU:HD13	2:C:351:LEU:HD21	1.70	0.74
3:D:1109:GLU:OE1	3:D:1201:CYS:HB2	1.88	0.74
5:F:247:ILE:HG22	5:F:251:ILE:HD11	1.69	0.74
5:F:88:ILE:HD13	5:F:193:ARG:HB2	1.67	0.74
2:M:282:GLY:HA2	2:M:308:ARG:NH2	2.01	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:605:LYS:HD3	2:M:610:ARG:CZ	2.18	0.74
2:M:671:ASN:HD21	2:M:993:PHE:HD2	1.32	0.74
3:N:486:ARG:HE	3:N:489:ARG:HD3	1.50	0.74
2:C:521:PRO:HB2	3:D:1055:VAL:HB	1.68	0.74
2:M:312:ALA:HB1	2:M:318:PRO:HG2	1.68	0.74
2:M:486:MET:HB3	8:M:1436:HOH:O	1.88	0.74
3:N:1259:VAL:HG22	3:N:1355:VAL:HG21	1.68	0.74
2:C:83:CYS:HA	2:C:88:LEU:HB3	1.70	0.74
3:D:715:ALA:HB3	3:D:764:LEU:HA	1.70	0.74
3:N:14:SER:H	3:N:17:LYS:HZ2	1.36	0.74
2:C:683:ASN:HA	2:C:687:ALA:HB3	1.69	0.73
2:C:124:ASP:HB3	2:C:592:LEU:HD12	1.69	0.73
3:D:1112:CYS:HB2	3:D:1195:GLN:OE1	1.88	0.73
1:L:133:GLU:HG3	1:L:134:GLU:HG2	1.70	0.73
2:M:436:GLY:HA2	2:M:538:GLN:O	1.88	0.73
2:C:269:LEU:HD23	2:C:285:LEU:HD21	1.69	0.73
3:D:795:VAL:HG11	3:D:863:VAL:HG13	1.70	0.73
2:M:89:THR:O	2:M:91:GLN:HG3	1.88	0.73
2:C:676:ILE:HG23	3:D:948:THR:HB	1.68	0.73
3:D:1289:LYS:HE3	3:D:1307:LYS:HE2	1.69	0.73
5:F:411:HIS:HA	5:F:414:ARG:HG3	1.70	0.73
2:M:362:GLY:HA3	2:M:367:LEU:HD23	1.68	0.73
3:N:661:MET:HG2	3:N:666:ILE:HD12	1.71	0.73
1:B:45:LEU:HA	8:B:343:HOH:O	1.88	0.73
1:B:58:ILE:HD13	1:B:140:MET:HB3	1.70	0.73
2:C:818:GLY:HA3	8:C:1350:HOH:O	1.88	0.73
3:D:459:GLU:HB3	8:D:9187:HOH:O	1.89	0.73
3:D:530:VAL:HB	3:D:534:ARG:HB2	1.70	0.73
1:L:63:HIS:HB2	8:L:3671:HOH:O	1.88	0.73
2:M:18:LEU:HD23	2:M:404:LEU:HD21	1.70	0.73
2:M:92:ALA:HB1	8:M:1276:HOH:O	1.89	0.73
2:M:1085:PHE:CD2	3:N:1468:LEU:HA	2.23	0.73
3:N:644:LEU:HD12	3:N:645:PRO:HD2	1.68	0.73
8:M:1349:HOH:O	3:N:651:GLU:HG3	1.88	0.73
5:P:358:LEU:HD21	5:P:370:LYS:HE3	1.70	0.73
1:B:206:THR:HG22	1:B:209:GLU:HB2	1.68	0.73
1:B:56:VAL:HG13	1:B:142:VAL:HG12	1.71	0.73
2:C:182:VAL:HG21	8:C:1366:HOH:O	1.89	0.73
5:P:247:ILE:HG22	5:P:251:ILE:HD11	1.70	0.73
1:B:131:THR:HG22	8:B:423:HOH:O	1.89	0.73
2:C:943:VAL:HG23	2:C:985:GLY:H	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1045:MET:CG	3:D:1073:SER:HA	2.17	0.73
3:D:637:LEU:HD21	3:D:642:CYS:HA	1.70	0.73
2:M:589:ARG:HB2	2:M:589:ARG:HH11	1.51	0.73
3:N:214:GLU:HB2	3:N:390:PRO:HD2	1.71	0.73
5:P:403:LYS:NZ	5:P:403:LYS:HA	2.03	0.73
1:A:98:THR:HG21	8:A:348:HOH:O	1.89	0.73
3:D:101:HIS:HD1	3:D:103:TRP:HB2	1.53	0.73
3:D:478:LEU:HD22	3:D:1388:ARG:CZ	2.18	0.73
3:D:186:VAL:HG21	3:D:213:VAL:HB	1.71	0.73
3:N:643:GLY:HA3	3:N:727:GLN:HB2	1.69	0.73
2:M:292:ARG:HB2	2:M:299:LYS:HE2	1.70	0.73
2:M:371:LYS:HA	8:M:1338:HOH:O	1.87	0.73
3:N:1194:CYS:HB3	3:N:1373:ARG:NH2	2.03	0.73
3:N:194:GLY:H	3:N:206:ARG:HA	1.53	0.73
2:C:366:SER:HA	8:C:1205:HOH:O	1.87	0.73
2:C:433:THR:HG21	2:C:488:ALA:HB1	1.70	0.73
2:C:874:LEU:HD21	3:D:787:LEU:HD22	1.71	0.73
2:M:1080:SER:HB2	8:M:1849:HOH:O	1.87	0.73
3:N:1481:VAL:HG13	4:O:18:ARG:NE	2.00	0.73
2:M:328:LEU:HD23	2:M:437:ARG:HD3	1.71	0.72
3:D:462:GLN:HA	3:D:513:ILE:HD13	1.71	0.72
1:K:150:TYR:HE2	1:K:152:PRO:HG3	1.51	0.72
3:N:1264:GLU:OE2	3:N:1424:VAL:HG12	1.88	0.72
1:A:14:ARG:NH2	1:A:22:GLU:HB3	2.03	0.72
2:C:704:HIS:HB2	2:C:831:ARG:HE	1.53	0.72
3:D:1209:LEU:HD22	3:D:1211:MET:HB3	1.71	0.72
2:C:1091:GLU:OE1	3:D:613:ARG:HG2	1.88	0.72
3:D:628:ARG:HD3	3:D:744:GLN:NE2	2.04	0.72
2:C:166:PRO:HA	8:C:1305:HOH:O	1.88	0.72
3:D:171:LEU:HB2	3:D:390:PRO:HA	1.70	0.72
2:M:54:ILE:HG21	8:M:1182:HOH:O	1.89	0.72
3:N:1210:SER:HA	8:N:9113:HOH:O	1.87	0.72
3:N:1429:LEU:HG	3:N:1441:GLN:HG3	1.70	0.72
2:C:54:ILE:HA	8:C:1491:HOH:O	1.89	0.72
3:N:669:ASN:HB3	8:N:9139:HOH:O	1.89	0.72
8:N:9109:HOH:O	5:P:319:THR:HA	1.88	0.72
2:M:573:ARG:HG3	2:M:698:ASP:O	1.90	0.72
3:N:656:PHE:CE2	3:N:698:LYS:HE3	2.23	0.72
3:N:715:ALA:HB3	3:N:764:LEU:HA	1.71	0.72
1:B:36:LEU:O	1:B:39:PRO:HD2	1.89	0.72
3:D:1267:ARG:HH22	3:D:1333:HIS:HD2	1.38	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1462:LEU:HD22	3:D:1472:ILE:HG23	1.70	0.72
1:K:133:GLU:HG2	1:K:134:GLU:N	2.05	0.72
3:N:1209:LEU:HD23	3:N:1210:SER:H	1.54	0.72
5:P:151:LEU:HB3	8:P:3247:HOH:O	1.89	0.72
5:F:93:LEU:HD22	5:F:98:GLU:HB3	1.69	0.72
1:K:89:PHE:CZ	1:K:146:ARG:HB2	2.25	0.72
3:N:207:PHE:HB3	3:N:208:PRO:HD2	1.70	0.72
2:C:473:ARG:HE	2:C:531:PHE:HE1	1.35	0.72
3:D:153:LEU:HD12	3:D:154:THR:N	2.05	0.72
3:D:699:VAL:HG21	3:D:760:ARG:HB3	1.72	0.72
1:L:23:PHE:HA	8:L:3037:HOH:O	1.90	0.72
2:M:1092:LEU:HD13	2:M:1099:VAL:HG21	1.72	0.72
3:N:1160:LEU:HD11	3:N:1174:LEU:HD21	1.70	0.72
2:C:244:PRO:HD2	2:C:245:GLY:H	1.53	0.72
2:C:64:LEU:HB2	2:C:359:MET:SD	2.30	0.72
3:D:1209:LEU:HD21	4:E:16:LYS:HZ2	1.54	0.72
3:D:671:LYS:HG3	5:F:422:LEU:HA	1.72	0.72
5:F:93:LEU:HG	5:F:190:ALA:CB	2.20	0.72
1:K:55:SER:OG	1:K:158:ILE:HB	1.90	0.72
4:O:51:LEU:HD12	4:O:52:GLU:H	1.55	0.72
5:P:132:ARG:NH2	5:P:184:ARG:HH12	1.86	0.72
2:C:29:ALA:HB2	2:C:337:GLY:CA	2.20	0.71
2:C:897:LEU:HB3	2:C:899:GLN:HE21	1.55	0.71
3:D:907:GLU:O	3:D:911:LEU:HD22	1.89	0.71
2:C:833:LEU:HD11	2:C:849:VAL:HG21	1.71	0.71
3:D:520:LEU:HD23	3:D:540:LEU:HD22	1.71	0.71
3:D:996:TRP:HA	3:D:999:THR:HG22	1.72	0.71
5:F:128:ARG:HG2	8:F:754:HOH:O	1.88	0.71
2:M:83:CYS:HA	2:M:88:LEU:HB3	1.73	0.71
3:N:1412:LYS:O	3:N:1414:PRO:HD3	1.89	0.71
5:P:404:ALA:HA	8:P:4644:HOH:O	1.90	0.71
1:A:14:ARG:NH2	1:A:24:VAL:HG23	2.05	0.71
2:C:157:ARG:HD2	2:C:314:THR:HG22	1.73	0.71
3:D:796:ARG:NH1	3:D:861:GLN:HB2	2.06	0.71
4:E:45:ARG:HA	8:E:180:HOH:O	1.88	0.71
3:N:171:LEU:HD22	3:N:390:PRO:HG3	1.72	0.71
3:D:153:LEU:CD1	3:D:157:GLU:HB2	2.20	0.71
3:D:374:GLU:HA	8:D:9065:HOH:O	1.90	0.71
3:D:737:ASN:HA	8:D:9006:HOH:O	1.89	0.71
2:M:31:GLN:HB3	2:M:71:TYR:OH	1.91	0.71
3:N:192:ALA:O	3:N:195:VAL:HG23	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:117:ASP:HB2	3:N:495:ARG:NH2	2.05	0.71
3:N:637:LEU:HD21	3:N:642:CYS:HA	1.71	0.71
3:N:1415:VAL:HG23	8:N:9265:HOH:O	1.89	0.71
3:N:808:THR:HB	3:N:809:PRO:HD3	1.72	0.71
1:A:175:ARG:NH1	1:A:202:ASP:HA	2.06	0.71
2:C:52:PHE:HA	8:C:1788:HOH:O	1.91	0.71
3:D:1087:ARG:CG	3:D:1234:THR:HA	2.21	0.71
3:D:513:ILE:HA	8:D:9491:HOH:O	1.91	0.71
3:N:215:TYR:O	3:N:389:GLU:HB3	1.89	0.71
2:M:1115:LEU:HD23	3:N:85:VAL:HG13	1.73	0.71
3:D:1046:GLN:HA	3:D:1052:THR:HA	1.72	0.71
3:D:1273:VAL:HG22	3:D:1326:THR:OG1	1.90	0.71
2:M:786:LYS:HA	8:M:1174:HOH:O	1.88	0.71
3:N:984:THR:HG22	3:N:987:GLU:HG3	1.72	0.71
5:P:361:LEU:HG	5:P:408:LEU:HD21	1.71	0.71
3:D:1251:ASP:O	3:D:1270:ALA:HB3	1.91	0.71
3:N:1109:GLU:HG2	3:N:1201:CYS:HA	1.73	0.71
3:N:139:GLY:O	3:N:147:VAL:HB	1.91	0.71
1:A:222:LEU:HD12	1:B:215:VAL:HB	1.71	0.71
2:C:113:VAL:HG13	8:C:1336:HOH:O	1.91	0.71
2:C:672:VAL:HG23	2:C:868:ASP:HB2	1.71	0.71
3:D:172:PRO:HD2	3:D:389:GLU:O	1.91	0.71
3:D:661:MET:HA	3:D:666:ILE:HD12	1.72	0.71
4:O:54:LEU:HG	4:O:58:PRO:HG2	1.73	0.71
5:P:160:ASP:HA	5:P:163:LEU:HD12	1.73	0.71
1:A:18:ARG:HH12	1:A:88:ARG:HH21	1.37	0.71
2:C:343:GLN:HG2	2:C:385:PHE:HB2	1.72	0.71
1:K:224:TYR:HB3	1:L:9:PRO:HB2	1.72	0.71
2:M:1051:GLU:HG3	2:M:1055:LEU:HD12	1.71	0.71
3:N:1173:LEU:HD23	3:N:1174:LEU:HD23	1.72	0.71
2:C:460:ARG:HH11	2:C:460:ARG:HB3	1.55	0.70
3:D:601:ARG:HD2	5:F:328:PHE:HE1	1.54	0.70
2:M:603:VAL:HG21	2:M:643:VAL:HG11	1.73	0.70
3:N:1488:ASP:HA	8:O:4394:HOH:O	1.91	0.70
3:N:26:VAL:HG11	3:N:44:LEU:HD23	1.73	0.70
2:C:264:PRO:HB3	2:C:289:THR:HG21	1.71	0.70
2:M:139:GLN:HG3	2:M:140:ILE:H	1.56	0.70
2:M:157:ARG:HE	2:M:158:TYR:H	1.36	0.70
2:M:535:SER:O	2:M:538:GLN:HG2	1.91	0.70
3:N:483:HIS:HB2	3:N:484:PRO:HD3	1.73	0.70
5:F:291:ILE:HG21	5:F:304:VAL:HG11	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:755:LEU:HB2	2:M:790:LEU:HD22	1.73	0.70
2:C:1067:TYR:O	2:C:1071:ILE:HG12	1.92	0.70
2:C:710:ILE:HD11	2:C:758:ARG:HH21	1.56	0.70
3:D:1077:ALA:HB2	8:D:2073:HOH:O	1.91	0.70
3:D:131:LYS:HD2	5:F:83:GLN:NE2	2.06	0.70
3:D:929:ARG:HB2	8:D:9499:HOH:O	1.90	0.70
5:F:260:ILE:HG23	5:F:264:MET:HB2	1.74	0.70
2:C:511:GLU:O	2:C:526:PRO:HD3	1.91	0.70
5:F:77:THR:O	5:F:81:VAL:HG23	1.91	0.70
2:M:884:GLN:HG3	2:M:885:ILE:HD13	1.72	0.70
2:C:108:ILE:HG21	8:C:1205:HOH:O	1.92	0.70
2:C:127:PHE:HA	8:C:1442:HOH:O	1.90	0.70
2:C:284:ARG:HG2	2:C:285:LEU:H	1.57	0.70
3:D:570:GLU:HB2	5:F:214:GLN:NE2	2.07	0.70
4:O:41:GLU:O	4:O:45:ARG:HG2	1.91	0.70
1:A:141:GLU:HG3	8:A:346:HOH:O	1.92	0.70
1:L:143:ARG:NH1	1:L:158:ILE:HD12	2.07	0.70
3:N:1220:ALA:HB1	3:N:1223:ILE:HD13	1.73	0.70
3:N:52:PRO:HG3	3:N:78:VAL:HG22	1.72	0.70
2:C:101:ILE:HG23	2:C:107:LEU:HD22	1.73	0.70
2:C:256:TYR:CE1	2:C:293:PHE:HB2	2.26	0.70
2:C:512:ARG:HB3	2:C:523:ILE:HD11	1.73	0.70
5:F:396:ARG:HG2	8:F:468:HOH:O	1.92	0.70
2:C:299:LYS:HB2	8:C:1374:HOH:O	1.90	0.70
3:D:1166:LEU:HD23	3:D:1166:LEU:H	1.56	0.70
3:D:1395:LEU:HB3	8:D:9369:HOH:O	1.91	0.70
1:L:97:VAL:HG11	1:L:120:VAL:HG21	1.74	0.70
1:L:58:ILE:HB	1:L:61:VAL:HB	1.73	0.70
2:M:1115:LEU:HD11	8:M:1678:HOH:O	1.90	0.70
2:M:218:VAL:HA	2:M:221:LEU:HD23	1.74	0.70
3:N:796:ARG:HD3	3:N:861:GLN:HB2	1.73	0.70
3:N:965:GLU:HG3	3:N:969:ARG:HH21	1.56	0.70
1:B:97:VAL:HG11	1:B:120:VAL:HG21	1.74	0.70
5:F:372:ARG:HB2	8:F:635:HOH:O	1.91	0.70
2:M:1098:ASP:HB2	3:N:21:TRP:HZ2	1.57	0.70
1:B:156:HIS:ND1	1:B:158:ILE:HG12	2.06	0.69
2:C:318:PRO:HB3	8:C:1564:HOH:O	1.90	0.69
2:C:455:LEU:HD12	2:C:459:ALA:HB3	1.72	0.69
2:C:49:ARG:HH11	2:C:49:ARG:HB2	1.57	0.69
2:C:517:ARG:NH1	2:C:522:VAL:HG11	2.05	0.69
2:C:958:THR:HG23	2:C:961:GLU:H	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:132:TYR:HA	8:D:9333:HOH:O	1.91	0.69
1:L:209:GLU:HB3	8:L:4878:HOH:O	1.92	0.69
2:M:343:GLN:HG3	8:M:1267:HOH:O	1.92	0.69
2:C:358:ARG:NH2	2:C:374:ASN:HB3	2.06	0.69
3:D:1352:ILE:HG21	3:D:1368:ILE:HG21	1.74	0.69
5:F:234:LYS:HD3	5:F:236:SER:HB3	1.72	0.69
2:C:1044:GLY:HA3	4:E:17:TYR:HE1	1.57	0.69
3:D:210:ARG:HH11	3:D:210:ARG:HB3	1.57	0.69
3:D:704:ARG:HD3	3:D:738:ALA:HB2	1.73	0.69
4:E:51:LEU:HD12	4:E:52:GLU:H	1.57	0.69
2:C:92:ALA:HB1	8:C:1294:HOH:O	1.92	0.69
3:D:793:THR:HB	3:D:879:ARG:HD3	1.74	0.69
1:L:161:ARG:HA	8:L:3450:HOH:O	1.92	0.69
2:M:511:GLU:O	2:M:526:PRO:HD3	1.92	0.69
3:N:15:PRO:HA	3:N:18:ILE:HG12	1.74	0.69
3:N:834:THR:HB	3:N:838:ARG:HB3	1.74	0.69
1:B:94:LEU:HD21	1:B:119:ASP:HB2	1.75	0.69
2:C:1056:LYS:HD3	3:D:623:VAL:HG13	1.73	0.69
2:C:405:ARG:NH2	2:C:566:THR:HG21	2.08	0.69
3:D:611:GLN:HG3	5:F:326:ASP:HB2	1.75	0.69
1:K:9:PRO:HB2	1:L:224:TYR:HB3	1.73	0.69
2:M:478:VAL:HA	2:M:506:ASN:O	1.92	0.69
3:N:468:LEU:HB3	8:N:9407:HOH:O	1.92	0.69
3:D:1462:LEU:HB3	3:D:1472:ILE:HD12	1.75	0.69
3:D:215:TYR:O	3:D:389:GLU:HB2	1.93	0.69
4:E:48:MET:HB2	4:E:54:LEU:HD12	1.73	0.69
5:F:120:THR:HB	8:F:433:HOH:O	1.91	0.69
5:F:335:ASP:OD2	5:F:338:LEU:HB2	1.92	0.69
3:N:119:SER:HB2	3:N:123:LEU:H	1.57	0.69
3:N:1389:LEU:HD12	3:N:1390:LEU:H	1.57	0.69
2:C:197:LEU:HA	2:C:200:LEU:HD12	1.75	0.69
2:C:670:GLN:O	2:C:672:VAL:HG12	1.93	0.69
3:D:811:GLU:HA	8:D:9196:HOH:O	1.93	0.69
3:D:929:ARG:HD3	8:D:9607:HOH:O	1.93	0.69
1:K:62:LEU:HD12	8:K:3844:HOH:O	1.91	0.69
2:M:516:ARG:HD2	2:M:521:PRO:HA	1.73	0.69
3:N:1033:GLN:HE21	3:N:1036:ARG:HD3	1.58	0.69
1:A:177:VAL:O	2:C:864:GLY:HA3	1.92	0.69
3:D:663:GLU:HA	8:D:9541:HOH:O	1.93	0.69
3:D:756:GLN:O	3:D:760:ARG:HG2	1.91	0.69
2:C:193:LEU:HD21	8:C:1760:HOH:O	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:971:LYS:HA	2:C:988:VAL:HA	1.74	0.69
3:D:996:TRP:CD2	3:D:1056:PRO:HG2	2.28	0.69
3:N:211:VAL:HG22	3:N:393:ILE:HG23	1.75	0.69
2:C:1067:TYR:CG	5:F:341:PRO:HB3	2.28	0.69
2:C:720:GLU:HG2	2:C:760:SER:HB3	1.75	0.69
2:C:958:THR:HG22	8:C:1364:HOH:O	1.92	0.69
3:D:964:LEU:HD13	3:D:1058:ARG:NH1	2.08	0.69
3:D:178:LEU:HG	3:D:200:ASP:H	1.58	0.69
2:M:1000:MET:SD	2:M:1001:VAL:HG22	2.32	0.69
2:M:136:ILE:HG21	2:M:336:VAL:HG13	1.75	0.69
1:B:57:TYR:HB3	1:B:141:GLU:CG	2.23	0.69
3:D:393:ILE:HD12	3:D:393:ILE:H	1.58	0.69
3:D:537:THR:C	5:F:317:LEU:HB2	2.12	0.69
3:D:62:LYS:HE2	3:D:75:ARG:HH12	1.58	0.69
3:N:761:ILE:HG21	8:O:3197:HOH:O	1.93	0.69
3:N:906:GLN:HB3	3:N:911:LEU:CD1	2.22	0.69
5:P:100:VAL:CG1	5:P:104:ARG:HH21	2.06	0.69
1:A:226:SER:O	1:A:228:PRO:HD3	1.93	0.68
1:A:218:LEU:HD23	1:B:222:LEU:HD21	1.74	0.68
1:K:100:LEU:HB2	1:K:115:LEU:HD11	1.75	0.68
2:M:526:PRO:HG2	8:M:1259:HOH:O	1.92	0.68
3:N:1205:TYR:CD2	3:N:1215:VAL:HG21	2.28	0.68
3:N:430:ASP:HB3	8:N:9241:HOH:O	1.93	0.68
3:N:542:ASP:O	3:N:546:ARG:HG2	1.94	0.68
2:C:1060:ILE:HD12	2:C:1063:ARG:NH1	2.08	0.68
2:C:282:GLY:HA2	2:C:308:ARG:NH2	2.07	0.68
2:C:437:ARG:HA	2:C:467:ILE:HG21	1.73	0.68
2:C:567:GLN:HA	8:C:1666:HOH:O	1.93	0.68
2:C:609:ASN:HD21	2:C:627:ARG:HH21	1.40	0.68
5:F:108:GLU:HG3	5:F:176:ILE:HG21	1.74	0.68
2:M:311:PHE:HB3	8:M:1560:HOH:O	1.93	0.68
2:M:704:HIS:CB	2:M:831:ARG:HE	2.05	0.68
2:M:672:VAL:HG23	2:M:868:ASP:HB2	1.74	0.68
2:C:1066:ALA:O	2:C:1070:ILE:HG13	1.93	0.68
2:C:479:VAL:CG2	2:C:503:LEU:HD11	2.21	0.68
3:D:808:THR:HB	3:D:809:PRO:HD3	1.73	0.68
3:D:1495:ILE:HG12	4:E:80:VAL:HG11	1.76	0.68
2:C:777:ILE:HG23	5:F:405:LEU:HD11	1.74	0.68
1:L:85:LEU:HD12	1:L:124:ASN:HB3	1.75	0.68
3:N:1205:TYR:HD2	3:N:1215:VAL:HG21	1.59	0.68
5:P:376:ILE:HG23	8:P:3758:HOH:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:244:PRO:HG2	2:C:246:ASP:OD2	1.93	0.68
3:D:478:LEU:HD21	3:D:500:ARG:NH2	2.08	0.68
3:D:572:ARG:HH12	5:F:79:ASP:CG	1.97	0.68
3:D:87:ARG:HB3	3:D:523:ASP:HB2	1.76	0.68
1:K:92:PRO:HD3	8:K:3642:HOH:O	1.92	0.68
1:L:156:HIS:ND1	1:L:158:ILE:HG12	2.08	0.68
1:L:58:ILE:HG23	8:L:4138:HOH:O	1.93	0.68
2:M:726:ILE:HG22	8:M:1255:HOH:O	1.92	0.68
3:N:760:ARG:HH21	4:O:3:GLU:CD	1.97	0.68
5:P:100:VAL:HG12	5:P:104:ARG:HH21	1.58	0.68
5:P:248:ASN:HA	5:P:251:ILE:HD12	1.76	0.68
1:B:132:LEU:HG	1:B:136:GLY:HA3	1.75	0.68
2:C:151:ASP:HB2	2:C:157:ARG:O	1.94	0.68
3:D:161:LEU:HD13	3:D:452:ILE:HD12	1.75	0.68
5:F:144:ILE:HB	5:F:145:PRO:HD3	1.76	0.68
2:M:368:THR:HB	2:M:369:PRO:HD3	1.74	0.68
2:M:675:ALA:HB2	2:M:867:VAL:HG11	1.75	0.68
2:M:983:ILE:HA	8:M:1335:HOH:O	1.92	0.68
5:P:403:LYS:NZ	5:P:406:ARG:HD2	2.08	0.68
1:A:206:THR:HG22	1:A:209:GLU:HG3	1.76	0.68
1:B:151:VAL:HG13	1:B:155:LYS:HE2	1.76	0.68
2:C:610:ARG:HB2	8:C:1501:HOH:O	1.93	0.68
2:C:1096:ALA:O	3:D:13:ALA:HB2	1.93	0.68
3:D:477:LEU:HD22	3:D:492:ALA:HB1	1.76	0.68
4:E:30:LEU:O	4:E:35:PHE:HA	1.94	0.68
1:A:198:ARG:HB2	1:A:200:TRP:CH2	2.29	0.68
1:A:9:PRO:HD2	1:B:224:TYR:CZ	2.28	0.68
2:C:1060:ILE:HD12	2:C:1063:ARG:HH12	1.58	0.68
2:C:428:ARG:HG2	2:C:449:ILE:O	1.94	0.68
3:D:1406:ARG:NH2	3:D:1407:LEU:HG	2.09	0.68
1:L:208:LEU:HD23	8:L:3127:HOH:O	1.94	0.68
2:M:300:ASP:HB2	8:M:1252:HOH:O	1.93	0.68
3:N:108:VAL:HG23	3:N:109:PRO:HD3	1.76	0.68
1:A:74:ASP:OD1	1:A:77:GLU:HB2	1.93	0.68
3:D:539:ASP:OD2	5:F:318:GLU:HB2	1.93	0.68
3:N:1273:VAL:HG22	3:N:1326:THR:OG1	1.93	0.68
2:C:64:LEU:HD13	2:C:359:MET:HG3	1.74	0.68
2:C:1109:VAL:HG23	3:D:3:LYS:HG2	1.75	0.68
5:F:119:ILE:HD13	5:F:170:HIS:ND1	2.09	0.68
2:C:516:ARG:HD3	2:C:521:PRO:HA	1.75	0.68
3:D:133:ILE:HG21	3:D:454:ALA:HB1	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:46:ASP:HB3	3:D:49:ILE:HG13	1.75	0.68
1:L:184:THR:HG23	1:L:192:LEU:HB3	1.76	0.68
3:N:1058:ARG:HH11	3:N:1058:ARG:HG3	1.59	0.68
3:N:535:PHE:O	5:P:315:VAL:N	2.26	0.68
2:C:605:LYS:HD3	2:C:610:ARG:NH1	2.09	0.67
3:D:1459:LEU:HD22	3:D:1465:ASN:ND2	2.09	0.67
3:D:401:TYR:HB2	8:D:9802:HOH:O	1.93	0.67
3:D:422:ALA:HB3	3:D:427:VAL:CG2	2.21	0.67
1:L:112:ARG:HD2	8:L:4849:HOH:O	1.93	0.67
1:L:100:LEU:HB2	1:L:115:LEU:HD21	1.77	0.67
3:N:86:ARG:O	3:N:522:PRO:HD2	1.93	0.67
3:N:543:LEU:HD22	3:N:580:ALA:HB1	1.74	0.67
3:N:961:LYS:HG2	8:N:9231:HOH:O	1.93	0.67
2:C:186:VAL:HG23	2:C:187:ASN:H	1.58	0.67
2:C:36:PRO:HB3	8:C:1554:HOH:O	1.94	0.67
2:C:478:VAL:HA	2:C:506:ASN:O	1.94	0.67
3:D:1082:ALA:O	3:D:1086:LEU:HD13	1.94	0.67
3:D:1235:GLN:C	3:D:1359:GLN:HE22	1.98	0.67
3:D:1318:TYR:HB3	8:D:9569:HOH:O	1.94	0.67
2:M:144:PRO:HA	2:M:163:ILE:HG12	1.76	0.67
2:M:952:LEU:HD12	2:M:969:GLN:NE2	2.09	0.67
3:N:1046:GLN:HA	3:N:1052:THR:HA	1.76	0.67
5:P:87:GLU:O	5:P:91:VAL:HG23	1.94	0.67
2:C:227:PHE:HD2	2:C:230:ARG:HH21	1.42	0.67
2:C:598:GLU:O	2:C:651:LYS:HG3	1.94	0.67
3:D:547:LEU:HD11	3:D:578:VAL:HG22	1.74	0.67
4:E:60:ALA:O	4:E:63:TRP:HB2	1.94	0.67
4:E:86:GLN:HB2	8:E:158:HOH:O	1.94	0.67
1:K:43:ILE:HD11	1:L:35:THR:HG21	1.76	0.67
2:M:165:LEU:O	2:M:265:ARG:HB2	1.93	0.67
3:N:75:ARG:HB3	8:N:9208:HOH:O	1.94	0.67
5:P:234:LYS:HG3	8:P:4168:HOH:O	1.94	0.67
1:A:24:VAL:HG22	1:A:196:THR:HB	1.75	0.67
3:D:1336:LEU:HA	3:D:1344:VAL:HG22	1.75	0.67
3:D:175:VAL:HG12	3:D:176:ASP:OD1	1.94	0.67
3:D:707:THR:HA	8:D:9216:HOH:O	1.93	0.67
5:F:351:SER:O	5:F:355:GLU:HB2	1.93	0.67
2:M:260:LEU:HB2	2:M:291:ALA:HB1	1.77	0.67
3:N:400:VAL:HG12	3:N:401:TYR:HD1	1.59	0.67
1:B:38:ASN:OD1	2:C:979:THR:HA	1.95	0.67
3:D:1095:THR:HG23	3:D:1230:GLY:HA3	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:523:ASP:N	8:D:9040:HOH:O	2.27	0.67
3:D:93:ILE:HD11	3:D:548:ILE:HD13	1.76	0.67
3:D:834:THR:HG22	3:D:838:ARG:HD2	1.76	0.67
2:M:205:GLU:O	2:M:209:ARG:HD2	1.94	0.67
2:M:546:LEU:HA	2:M:581:THR:HG21	1.76	0.67
2:M:736:ASP:HA	2:M:744:ARG:HD3	1.75	0.67
3:N:1420:LEU:HD12	3:N:1421:LEU:N	2.09	0.67
3:N:153:LEU:HD11	3:N:158:TYR:N	2.08	0.67
2:C:100:LEU:HB2	8:C:1196:HOH:O	1.93	0.67
2:M:1040:LEU:HG	2:M:1045:ALA:HB3	1.77	0.67
3:N:1127:GLU:HG3	3:N:1133:ARG:HH12	1.60	0.67
3:N:105:VAL:HG21	3:N:128:TYR:HE2	1.60	0.67
3:N:1383:ASP:HB2	3:N:1416:ALA:HB3	1.77	0.67
3:N:730:PRO:HA	3:N:733:CYS:SG	2.35	0.67
3:D:1087:ARG:HB3	3:D:1234:THR:HG23	1.75	0.67
3:D:1389:LEU:HD13	8:D:9579:HOH:O	1.94	0.67
1:L:65:PHE:HB2	8:L:3211:HOH:O	1.94	0.67
2:M:630:ARG:HH21	2:M:707:ARG:N	1.93	0.67
3:N:1397:LYS:HG2	8:N:9561:HOH:O	1.93	0.67
3:N:1485:GLN:HE21	4:O:80:VAL:H	1.43	0.67
1:A:20:TYR:HD2	1:A:21:GLY:N	1.93	0.67
2:C:777:ILE:HG22	2:C:778:PHE:HD1	1.59	0.67
3:D:793:THR:HG22	3:D:879:ARG:HA	1.77	0.67
1:K:99:LEU:HB3	1:K:114:PHE:HD2	1.57	0.67
3:N:654:LYS:HD3	3:N:674:ARG:HH22	1.59	0.67
5:F:112:ALA:HA	5:F:173:TYR:HD2	1.59	0.67
1:K:99:LEU:HB3	1:K:114:PHE:CD2	2.30	0.67
1:L:62:LEU:HD13	1:L:63:HIS:ND1	2.10	0.67
3:N:124:GLU:HB2	8:N:9808:HOH:O	1.94	0.67
3:N:1314:LYS:HD3	3:N:1314:LYS:H	1.60	0.67
4:O:60:ALA:O	4:O:63:TRP:HB2	1.95	0.67
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.76	0.66
3:D:1144:LEU:HB3	3:D:1166:LEU:HD11	1.77	0.66
3:D:1271:LYS:HG2	3:D:1272:ALA:H	1.60	0.66
3:D:156:GLU:HB3	8:D:9191:HOH:O	1.95	0.66
3:D:210:ARG:CZ	3:D:398:ALA:HB3	2.25	0.66
3:D:821:VAL:HG21	8:D:9498:HOH:O	1.96	0.66
5:F:282:LEU:HD11	5:F:286:PRO:HG3	1.76	0.66
2:M:140:ILE:HA	2:M:332:ARG:O	1.94	0.66
2:M:911:GLU:O	2:M:915:LYS:HG2	1.94	0.66
2:C:328:LEU:HB2	2:C:433:THR:HG21	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:498:GLN:NE2	3:D:1068:LEU:HD12	2.10	0.66
1:K:227:ASN:N	1:K:227:ASN:HD22	1.91	0.66
2:M:1085:PHE:O	2:M:1089:VAL:HG23	1.95	0.66
2:M:367:LEU:HB3	2:M:371:LYS:HG2	1.78	0.66
3:N:120:ALA:HB1	8:N:9749:HOH:O	1.94	0.66
3:N:423:ASP:OD1	5:P:174:LEU:HD13	1.95	0.66
3:N:807:ALA:HB2	3:N:833:GLU:OE1	1.94	0.66
5:P:148:LYS:HG2	8:P:3932:HOH:O	1.95	0.66
5:P:208:SER:HB3	8:P:3885:HOH:O	1.95	0.66
1:A:161:ARG:HB2	1:A:161:ARG:NH1	2.10	0.66
1:B:52:ALA:HB1	8:B:430:HOH:O	1.94	0.66
2:C:290:LEU:HA	8:C:1381:HOH:O	1.96	0.66
2:M:660:ALA:HB1	2:M:667:ALA:O	1.96	0.66
2:M:52:PHE:CE1	2:M:66:LEU:HG	2.31	0.66
3:N:1342:GLU:CD	3:N:1342:GLU:H	1.99	0.66
3:N:1376:MET:SD	3:N:1421:LEU:HD12	2.36	0.66
2:C:750:LYS:HB3	8:C:1606:HOH:O	1.93	0.66
2:C:930:LYS:HA	8:C:1252:HOH:O	1.96	0.66
3:D:1169:ASP:HB3	8:D:9030:HOH:O	1.95	0.66
1:L:131:THR:HA	8:L:2956:HOH:O	1.95	0.66
3:N:1080:GLY:HA3	8:N:9701:HOH:O	1.95	0.66
3:N:1434:TRP:CZ3	3:N:1457:ASP:HB2	2.29	0.66
3:N:209:ARG:NH2	3:N:397:LYS:HG3	2.11	0.66
3:N:863:VAL:HG23	8:N:9129:HOH:O	1.94	0.66
2:C:480:THR:HG22	2:C:482:GLU:H	1.61	0.66
3:D:1349:VAL:HG11	8:D:9752:HOH:O	1.94	0.66
3:D:1468:LEU:HD22	3:D:1470:ARG:HB2	1.77	0.66
3:D:528:VAL:O	3:D:535:PHE:HA	1.95	0.66
4:E:26:ARG:O	4:E:29:GLN:HG3	1.95	0.66
1:L:95:GLN:H	1:L:95:GLN:HE21	1.43	0.66
3:N:191:LEU:HD12	3:N:211:VAL:HG21	1.77	0.66
3:N:209:ARG:HH22	3:N:397:LYS:HG3	1.60	0.66
1:A:198:ARG:NH2	2:C:932:GLU:HG2	2.11	0.66
2:C:155:PRO:HB2	8:C:1225:HOH:O	1.95	0.66
3:D:1413:THR:HG21	8:D:9279:HOH:O	1.94	0.66
3:D:783:ARG:HE	3:D:1029:ARG:NE	1.91	0.66
3:D:89:ARG:O	3:D:521:PRO:HG3	1.96	0.66
1:L:74:ASP:HA	8:L:3261:HOH:O	1.94	0.66
2:M:513:VAL:HB	8:M:1319:HOH:O	1.95	0.66
3:N:1004:THR:HG21	8:N:9281:HOH:O	1.93	0.66
3:N:1459:LEU:HA	3:N:1464:GLU:OE1	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:325:LYS:HE2	8:P:2932:HOH:O	1.94	0.66
5:P:371:LEU:HD22	5:P:375:LEU:HD22	1.77	0.66
2:C:95:TYR:CD2	2:C:114:PHE:HB3	2.30	0.66
2:C:41:ASN:H	2:C:41:ASN:ND2	1.92	0.66
2:C:455:LEU:H	2:C:455:LEU:HD23	1.60	0.66
2:C:504:GLU:OE2	2:C:509:ALA:HB2	1.94	0.66
2:M:516:ARG:HE	3:N:1068:LEU:HD13	1.61	0.66
1:A:161:ARG:HB2	1:A:161:ARG:HH11	1.59	0.66
1:A:20:TYR:HD2	1:A:21:GLY:H	1.44	0.66
1:A:219:ARG:CZ	1:B:219:ARG:HG2	2.26	0.66
2:C:722:ILE:HG23	2:C:805:ARG:HH21	1.60	0.66
3:D:652:LEU:HA	8:D:9195:HOH:O	1.95	0.66
3:N:1105:ILE:HD11	3:N:1374:GLN:NE2	2.10	0.66
3:D:148:GLU:HG2	3:D:151:GLN:NE2	2.11	0.66
3:D:964:LEU:HD13	3:D:1058:ARG:HH11	1.61	0.66
5:F:171:LYS:HE3	5:F:175:HIS:NE2	2.11	0.66
1:K:86:VAL:HG23	8:K:3038:HOH:O	1.95	0.66
2:M:197:LEU:HD13	2:M:207:LEU:HD11	1.78	0.66
2:C:325:ILE:HG22	8:C:1411:HOH:O	1.96	0.66
2:C:42:VAL:HG12	2:C:43:GLY:H	1.61	0.66
2:C:328:LEU:HD22	2:C:433:THR:HG22	1.77	0.66
2:C:710:ILE:HD11	2:C:758:ARG:NH2	2.11	0.66
3:D:424:GLY:HA2	3:D:436:GLU:HA	1.78	0.66
3:D:562:ALA:HB1	3:D:567:ILE:CD1	2.25	0.66
5:F:160:ASP:HA	5:F:163:LEU:HD12	1.78	0.66
1:L:19:GLU:HG3	1:L:201:THR:O	1.96	0.66
2:M:151:ASP:HB2	2:M:157:ARG:O	1.96	0.66
3:N:1094:LEU:HD23	3:N:1230:GLY:HA2	1.78	0.66
3:N:1281:VAL:HG21	3:N:1313:VAL:HG21	1.77	0.66
3:N:642:CYS:SG	3:N:716:PHE:HB2	2.36	0.66
1:B:99:LEU:HD12	1:B:114:PHE:HB3	1.77	0.65
3:D:1087:ARG:HD2	3:D:1256:LEU:HD22	1.78	0.65
1:L:152:PRO:HD2	1:L:155:LYS:HD2	1.76	0.65
2:M:1040:LEU:HD21	2:M:1048:THR:HG22	1.78	0.65
2:M:137:VAL:HG23	2:M:391:LEU:HG	1.78	0.65
3:N:656:PHE:HE2	3:N:698:LYS:HE3	1.59	0.65
3:N:877:PRO:O	3:N:880:ILE:HG22	1.95	0.65
5:P:323:ASP:HB3	8:P:3957:HOH:O	1.94	0.65
2:C:197:LEU:HD12	2:C:207:LEU:HD11	1.78	0.65
3:D:955:VAL:HB	3:D:1011:PHE:HE1	1.61	0.65
3:D:908:LYS:CB	3:D:1027:GLY:HA3	2.24	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:850:LEU:HD12	3:D:850:LEU:H	1.60	0.65
5:F:248:ASN:HA	5:F:251:ILE:HD12	1.78	0.65
2:M:211:LEU:HD12	2:M:308:ARG:HG3	1.76	0.65
3:N:1272:ALA:HA	3:N:1326:THR:HB	1.76	0.65
3:N:141:ILE:HD11	8:N:9550:HOH:O	1.95	0.65
3:N:35:ARG:HG3	3:N:36:THR:N	2.10	0.65
3:N:656:PHE:HB3	3:N:694:VAL:HG11	1.77	0.65
3:N:844:ALA:O	3:N:867:ARG:HB3	1.95	0.65
1:B:38:ASN:HB3	1:B:39:PRO:HD3	1.78	0.65
3:D:396:VAL:HA	8:D:9468:HOH:O	1.96	0.65
5:F:113:ILE:HA	5:F:116:LEU:HD12	1.78	0.65
1:L:106:PRO:HD3	8:L:3583:HOH:O	1.97	0.65
2:M:3:ILE:HG23	8:M:1340:HOH:O	1.94	0.65
2:M:773:LEU:O	2:M:777:ILE:HG13	1.95	0.65
2:M:859:PRO:O	2:M:867:VAL:HG22	1.96	0.65
2:M:73:LEU:HB3	2:M:94:LEU:HB2	1.79	0.65
3:N:161:LEU:HD22	3:N:452:ILE:HG21	1.78	0.65
2:C:265:ARG:HG2	2:C:267:TYR:H	1.61	0.65
3:D:1455:LYS:HD3	3:D:1456:LYS:N	2.11	0.65
3:D:1492:LEU:HA	8:D:2041:HOH:O	1.96	0.65
3:N:1087:ARG:HA	3:N:1090:ASP:HB2	1.79	0.65
3:N:1294:VAL:HB	8:N:9539:HOH:O	1.95	0.65
3:N:576:GLU:HB2	8:N:9391:HOH:O	1.95	0.65
5:P:104:ARG:HB3	8:P:3870:HOH:O	1.97	0.65
5:P:175:HIS:O	5:P:179:GLU:HG3	1.97	0.65
5:P:352:GLU:O	5:P:356:LYS:HG3	1.96	0.65
5:P:85:LEU:HA	5:P:88:ILE:HD12	1.79	0.65
2:C:185:LYS:HG2	2:C:190:LYS:HG2	1.79	0.65
2:C:838:LYS:HG3	2:C:997:LEU:HB2	1.78	0.65
3:D:1120:VAL:HB	3:D:1144:LEU:HD21	1.77	0.65
3:D:434:ARG:HB2	3:D:447:VAL:HG13	1.77	0.65
3:D:704:ARG:NE	3:D:705:ALA:H	1.94	0.65
1:K:54:THR:HG21	8:K:3561:HOH:O	1.96	0.65
2:M:274:ARG:HB2	2:M:285:LEU:HD13	1.77	0.65
3:N:520:LEU:HD12	3:N:521:PRO:HD2	1.78	0.65
3:N:655:PRO:HA	3:N:658:LEU:HD12	1.78	0.65
1:B:90:LEU:HD23	8:B:356:HOH:O	1.97	0.65
2:C:186:VAL:HG23	8:C:1357:HOH:O	1.95	0.65
2:C:926:PHE:O	2:C:930:LYS:HG3	1.96	0.65
3:D:111:LYS:HE2	3:D:1452:ILE:HG12	1.78	0.65
3:D:1160:LEU:HD11	3:D:1174:LEU:HD21	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:166:LEU:O	5:F:171:LYS:HB2	1.96	0.65
2:M:45:GLN:HA	8:M:1223:HOH:O	1.95	0.65
8:N:9970:HOH:O	5:P:135:ILE:HD11	1.97	0.65
5:P:163:LEU:HB3	5:P:174:LEU:HG	1.78	0.65
2:C:678:PRO:HB2	3:D:942:SER:OG	1.97	0.65
2:C:798:GLY:H	2:C:827:VAL:CG1	2.09	0.65
3:D:1154:GLU:HG3	3:D:1159:ARG:HG3	1.78	0.65
3:D:427:VAL:CG2	3:D:435:VAL:HB	2.26	0.65
1:K:117:VAL:HB	1:K:120:VAL:HG12	1.78	0.65
2:M:816:LYS:HB2	2:M:819:VAL:HG21	1.79	0.65
3:N:119:SER:H	3:N:123:LEU:HB2	1.61	0.65
3:N:14:SER:H	3:N:17:LYS:NZ	1.94	0.65
1:A:27:PRO:HD2	8:A:350:HOH:O	1.97	0.65
3:D:570:GLU:HB2	5:F:214:GLN:HE21	1.62	0.65
3:D:537:THR:HA	5:F:317:LEU:HD12	1.77	0.65
3:N:187:LYS:HA	8:N:9174:HOH:O	1.97	0.65
3:N:434:ARG:HB2	3:N:447:VAL:HG22	1.78	0.65
5:P:154:LYS:O	5:P:158:GLU:HG3	1.97	0.65
1:B:47:SER:O	1:B:49:PRO:N	2.29	0.65
2:C:29:ALA:HB2	2:C:337:GLY:HA3	1.78	0.65
2:C:405:ARG:HH12	2:C:563:ASN:ND2	1.94	0.65
2:C:580:MET:HB3	2:C:584:GLU:CD	2.16	0.65
3:D:1036:ARG:HH21	3:D:1042:ARG:HA	1.61	0.65
3:D:1264:GLU:OE1	3:D:1424:VAL:HG12	1.97	0.65
3:D:398:ALA:HB2	3:D:445:ARG:HE	1.61	0.65
3:D:817:GLU:HG3	3:D:840:LYS:NZ	2.12	0.65
4:E:59:ASN:HB3	4:E:62:THR:OG1	1.97	0.65
2:M:416:GLY:HA3	8:M:1698:HOH:O	1.96	0.65
2:M:690:ILE:HG23	2:M:852:ILE:HA	1.78	0.65
3:N:783:ARG:HH21	3:N:1029:ARG:CG	2.09	0.65
3:N:654:LYS:HB3	3:N:655:PRO:HD3	1.79	0.65
2:M:918:LEU:HD23	2:M:968:LEU:HA	1.78	0.65
5:P:260:ILE:HD11	5:P:310:ILE:HG22	1.79	0.65
5:P:275:ALA:HA	5:P:278:LEU:HD12	1.79	0.65
3:D:116:LEU:HB3	3:D:118:LEU:HD21	1.79	0.64
3:D:26:VAL:HG11	3:D:44:LEU:HD23	1.79	0.64
3:D:483:HIS:HB2	3:D:484:PRO:HD3	1.79	0.64
2:M:304:LEU:HD21	8:M:1371:HOH:O	1.96	0.64
2:M:157:ARG:HD2	2:M:314:THR:CG2	2.23	0.64
3:N:147:VAL:HG21	8:N:9806:HOH:O	1.96	0.64
3:N:708:LEU:HA	8:N:9285:HOH:O	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:THR:HB	1:B:194:LYS:NZ	2.12	0.64
1:B:73:GLU:HB3	1:B:77:GLU:CG	2.27	0.64
2:C:1090:LYS:HE2	2:C:1112:PHE:CE1	2.27	0.64
2:C:771:GLU:O	2:C:775:ARG:HG2	1.98	0.64
3:D:550:ARG:NH1	3:D:573:MET:HB3	2.11	0.64
2:M:1018:GLN:HG3	2:M:1060:ILE:HD11	1.79	0.64
3:N:487:ALA:HB3	8:N:9323:HOH:O	1.97	0.64
3:N:890:VAL:HG13	3:N:926:LYS:HD3	1.79	0.64
1:B:58:ILE:HB	1:B:61:VAL:HB	1.77	0.64
2:C:12:VAL:HG13	2:C:13:ILE:HG23	1.78	0.64
3:D:1243:THR:HB	3:D:1253:THR:HG22	1.78	0.64
3:D:1274:ILE:HD11	3:D:1334:GLN:HB3	1.79	0.64
3:D:699:VAL:HG12	3:D:717:GLN:HA	1.79	0.64
4:E:33:HIS:CD2	4:E:89:MET:HG2	2.33	0.64
2:M:1037:VAL:HG13	2:M:1049:LEU:HD11	1.79	0.64
2:M:35:PRO:HD2	2:M:38:LYS:HG2	1.77	0.64
2:M:498:GLN:O	2:M:501:THR:HG23	1.97	0.64
2:M:669:GLY:O	2:M:670:GLN:HG3	1.97	0.64
3:N:1310:ARG:O	3:N:1327:ARG:HG3	1.97	0.64
3:N:911:LEU:O	3:N:915:VAL:HG23	1.98	0.64
4:O:25:LYS:HA	4:O:28:GLN:NE2	2.12	0.64
2:C:342:ASP:O	2:C:346:VAL:HG23	1.96	0.64
2:C:660:ALA:HB1	2:C:667:ALA:O	1.98	0.64
3:D:1075:HIS:HB3	8:D:9589:HOH:O	1.98	0.64
2:C:685:GLU:HG3	3:D:783:ARG:HD2	1.78	0.64
3:D:85:VAL:HG21	8:D:9019:HOH:O	1.96	0.64
2:M:1082:PRO:HG2	3:N:1469:GLY:HA3	1.78	0.64
2:M:1084:SER:O	2:M:1087:VAL:HG12	1.97	0.64
1:A:101:LEU:HG	1:A:114:PHE:HA	1.79	0.64
2:C:881:ASN:HD22	2:C:881:ASN:H	1.42	0.64
3:D:135:LEU:HD13	3:D:147:VAL:HG23	1.77	0.64
3:D:810:GLU:O	3:D:813:LEU:HG	1.98	0.64
2:M:678:PRO:HD2	8:N:9142:HOH:O	1.96	0.64
2:M:565:GLN:OE1	2:M:842:ARG:HG2	1.98	0.64
3:D:1306:PRO:HB3	3:D:1307:LYS:HE3	1.79	0.64
3:D:448:GLU:HG3	8:D:9492:HOH:O	1.98	0.64
2:M:627:ARG:HA	8:M:1225:HOH:O	1.96	0.64
2:M:636:ALA:HB2	2:M:703:ILE:HG22	1.80	0.64
3:N:448:GLU:HG2	8:N:9338:HOH:O	1.98	0.64
3:N:560:GLN:NE2	5:P:221:ILE:HB	2.13	0.64
1:A:18:ARG:HH12	1:A:88:ARG:NH2	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:ARG:NH1	1:A:191:ASP:HB2	2.13	0.64
1:B:156:HIS:CE1	1:B:166:PRO:HB3	2.33	0.64
1:B:37:GLY:HA2	1:B:40:LEU:HD12	1.79	0.64
3:D:1129:THR:O	3:D:1130:ARG:HD2	1.98	0.64
3:D:1501:GLU:HA	8:D:9088:HOH:O	1.95	0.64
3:D:544:TYR:O	3:D:548:ILE:HG12	1.97	0.64
3:D:996:TRP:CE3	3:D:999:THR:HG21	2.32	0.64
1:K:35:THR:HG21	1:L:43:ILE:HD11	1.79	0.64
3:N:1137:ARG:HA	3:N:1140:ILE:HD12	1.79	0.64
3:N:400:VAL:HG21	3:N:441:ARG:HH11	1.61	0.64
3:N:443:VAL:HG11	3:N:445:ARG:HE	1.63	0.64
3:N:615:ARG:NH1	3:N:615:ARG:HB2	2.13	0.64
3:N:698:LYS:HA	8:N:9643:HOH:O	1.98	0.64
1:A:30:ARG:HH11	1:A:191:ASP:HB2	1.62	0.64
2:C:172:ILE:H	2:C:172:ILE:HD12	1.62	0.64
2:C:56:GLU:HG3	2:C:64:LEU:HD23	1.80	0.64
2:C:675:ALA:HA	2:C:989:VAL:HG12	1.80	0.64
3:D:1261:GLU:OE1	3:D:1268:PRO:HA	1.97	0.64
3:D:1384:PRO:HD3	8:D:9043:HOH:O	1.98	0.64
3:D:1466:VAL:HG23	3:D:1472:ILE:HD11	1.79	0.64
3:D:139:GLY:H	3:D:147:VAL:HG21	1.62	0.64
3:D:208:PRO:HB2	3:D:395:VAL:HG22	1.80	0.64
3:D:836:VAL:HG12	8:D:9602:HOH:O	1.96	0.64
5:F:273:ARG:HB3	8:F:555:HOH:O	1.97	0.64
2:M:95:TYR:CD2	2:M:114:PHE:HB3	2.32	0.64
2:M:16:PRO:HG2	2:M:460:ARG:HH12	1.61	0.64
2:M:612:VAL:HG22	2:M:622:GLU:HA	1.80	0.64
2:M:93:PRO:HA	8:M:1237:HOH:O	1.97	0.64
3:N:907:GLU:O	3:N:911:LEU:HD13	1.98	0.64
1:B:103:ALA:O	1:B:138:LEU:HD23	1.98	0.64
2:C:838:LYS:HD2	2:C:846:LYS:NZ	2.13	0.64
3:D:804:LEU:HB2	3:D:830:ALA:O	1.98	0.64
1:K:100:LEU:HG	8:K:3093:HOH:O	1.97	0.64
1:K:36:LEU:O	1:K:39:PRO:HD2	1.98	0.64
2:M:1114:GLY:H	2:M:1115:LEU:HD12	1.62	0.64
2:M:367:LEU:O	2:M:372:LEU:HD13	1.97	0.64
3:N:1031:ASN:HB3	3:N:1034:GLN:CD	2.19	0.64
3:N:396:VAL:HG21	3:N:447:VAL:HB	1.80	0.64
3:N:422:ALA:HB3	3:N:427:VAL:CG2	2.26	0.64
3:N:899:LEU:HD12	3:N:900:ILE:HG23	1.79	0.64
3:N:917:GLN:HA	8:N:9246:HOH:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:317:LEU:HD23	5:P:330:GLY:HA3	1.79	0.64
5:P:403:LYS:HZ1	5:P:406:ARG:HD2	1.61	0.64
1:B:59:GLU:HG2	1:B:139:ASN:O	1.98	0.64
2:C:886:LEU:HD23	3:D:951:ILE:HG13	1.79	0.64
2:C:904:PRO:HD2	2:C:908:GLY:HA2	1.80	0.64
3:D:1215:VAL:HG23	8:D:9465:HOH:O	1.97	0.64
3:D:136:ASP:CB	3:D:137:PRO:HD3	2.27	0.64
3:D:1459:LEU:HB2	3:D:1470:ARG:HH12	1.63	0.64
3:D:501:ALA:HB1	3:D:1453:ALA:HA	1.80	0.64
3:D:590:PRO:HA	8:D:2066:HOH:O	1.98	0.64
5:F:225:GLU:HB3	8:F:496:HOH:O	1.96	0.64
2:M:1000:MET:O	2:M:1003:ASP:HB3	1.97	0.64
2:M:188:LYS:HD3	8:M:1768:HOH:O	1.96	0.64
2:M:860:HIS:CE1	2:M:975:TYR:HB2	2.33	0.64
3:N:1018:ASN:O	3:N:1022:VAL:HG23	1.98	0.64
3:N:1243:THR:OG1	3:N:1253:THR:HB	1.98	0.64
3:N:1279:GLY:O	3:N:1318:TYR:HA	1.98	0.64
3:N:188:GLY:HA3	8:N:9237:HOH:O	1.97	0.64
3:N:422:ALA:H	3:N:427:VAL:CG1	2.11	0.64
3:N:6:ARG:NH1	3:N:6:ARG:HB3	2.13	0.64
3:N:87:ARG:CB	3:N:523:ASP:HB2	2.27	0.64
3:N:693:GLU:HG3	4:O:48:MET:SD	2.38	0.64
5:P:95:THR:HB	5:P:96:LEU:HD23	1.78	0.64
1:A:27:PRO:HG2	1:A:186:LEU:HD22	1.80	0.63
1:B:123:MET:C	1:B:125:PRO:HD3	2.19	0.63
2:M:1013:TYR:HE1	2:M:1020:PRO:HG3	1.62	0.63
4:O:30:LEU:O	4:O:35:PHE:HA	1.97	0.63
5:P:416:ARG:NH1	5:P:419:ARG:HB2	2.13	0.63
1:A:58:ILE:HG21	1:A:68:ILE:HD11	1.79	0.63
2:C:704:HIS:CB	2:C:831:ARG:HE	2.10	0.63
2:C:716:LYS:HE2	8:F:558:HOH:O	1.98	0.63
3:D:97:THR:HG21	3:D:571:LYS:HD3	1.80	0.63
3:D:804:LEU:HD23	3:D:804:LEU:H	1.63	0.63
2:M:1115:LEU:HD12	2:M:1115:LEU:N	2.14	0.63
2:M:290:LEU:HB3	2:M:302:VAL:CG1	2.28	0.63
2:M:34:VAL:HB	2:M:38:LYS:HG3	1.80	0.63
3:N:1147:ARG:HB3	3:N:1188:VAL:HG21	1.79	0.63
3:N:1422:MET:HE2	3:N:1427:SER:HA	1.81	0.63
3:N:65:ARG:HG3	3:N:66:GLN:H	1.61	0.63
5:P:351:SER:O	5:P:355:GLU:HB2	1.97	0.63
1:B:206:THR:HG22	1:B:209:GLU:H	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:PRO:O	1:B:28:LEU:HD23	1.99	0.63
2:C:470:PRO:HB3	2:C:485:TYR:CZ	2.33	0.63
2:C:663:ASN:HB2	8:C:1359:HOH:O	1.97	0.63
2:C:859:PRO:O	2:C:867:VAL:HG22	1.97	0.63
3:D:510:GLU:O	3:D:513:ILE:HD12	1.99	0.63
3:D:1481:VAL:HG13	4:E:18:ARG:HE	1.62	0.63
1:L:108:GLU:HG2	8:L:2956:HOH:O	1.98	0.63
2:M:431:HIS:CD2	2:M:433:THR:H	2.16	0.63
2:M:461:VAL:HG13	2:M:465:GLY:HA2	1.81	0.63
3:N:424:GLY:HA2	3:N:436:GLU:HA	1.80	0.63
4:O:16:LYS:HD3	4:O:17:TYR:HE2	1.62	0.63
1:A:128:HIS:HB2	8:A:408:HOH:O	1.96	0.63
1:A:97:VAL:HG23	8:A:316:HOH:O	1.99	0.63
3:D:1399:ASP:O	3:D:1403:LEU:HB2	1.99	0.63
3:D:178:LEU:HD21	8:D:9071:HOH:O	1.97	0.63
3:D:64:LYS:HD3	5:F:376:ILE:O	1.99	0.63
5:F:321:ILE:HD11	5:F:329:TYR:HB2	1.78	0.63
1:L:89:PHE:HB2	1:L:94:LEU:HD13	1.79	0.63
2:M:1050:GLN:HG2	2:M:1079:PRO:HG2	1.80	0.63
2:M:571:LEU:HD21	2:M:700:TYR:HD2	1.62	0.63
3:N:11:ALA:HB1	3:N:507:ASN:OD1	1.98	0.63
3:N:496:LEU:HD23	3:N:1388:ARG:HG2	1.80	0.63
3:D:1311:LEU:HA	8:D:9045:HOH:O	1.99	0.63
3:D:1350:GLU:O	3:D:1354:LYS:HG2	1.98	0.63
3:D:177:ALA:HB1	3:D:199:LEU:HD22	1.79	0.63
1:K:157:GLY:HA3	8:K:5051:HOH:O	1.99	0.63
1:K:197:LEU:H	1:K:197:LEU:HD23	1.62	0.63
2:M:1101:THR:HB	3:N:5:VAL:CG1	2.29	0.63
2:M:432:ARG:HD2	2:M:519:GLY:HA3	1.80	0.63
2:M:833:LEU:HD11	2:M:849:VAL:HG21	1.79	0.63
3:N:1123:PHE:HE2	3:N:1184:GLN:HA	1.62	0.63
3:N:178:LEU:HD21	8:N:9082:HOH:O	1.97	0.63
3:N:240:GLU:HA	8:N:9487:HOH:O	1.97	0.63
3:N:25:GLU:HB2	8:N:9156:HOH:O	1.98	0.63
1:A:36:LEU:O	1:A:39:PRO:HD2	1.98	0.63
1:B:80:LEU:HD21	8:D:9557:HOH:O	1.99	0.63
2:C:579:VAL:HB	2:C:890:LEU:CD2	2.28	0.63
3:D:1047:LYS:HD2	3:D:1051:GLU:OE1	1.99	0.63
3:D:9:ARG:HA	3:D:1434:TRP:HH2	1.63	0.63
2:M:157:ARG:NE	2:M:158:TYR:H	1.95	0.63
2:M:841:ASN:HD22	2:M:841:ASN:C	2.02	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:899:GLN:HA	8:M:1664:HOH:O	1.97	0.63
3:N:116:LEU:O	3:N:118:LEU:HG	1.98	0.63
3:N:699:VAL:HG12	3:N:717:GLN:HG3	1.80	0.63
3:N:417:PRO:HA	5:P:168:LYS:NZ	2.13	0.63
2:C:220:GLY:HA3	8:C:1329:HOH:O	1.98	0.63
2:C:777:ILE:HG22	2:C:778:PHE:CD1	2.34	0.63
1:L:13:VAL:HA	8:L:3037:HOH:O	1.98	0.63
2:M:958:THR:OG1	2:M:961:GLU:HG2	1.98	0.63
2:M:983:ILE:CG2	2:M:987:ILE:HD11	2.29	0.63
1:A:35:THR:HG21	1:B:43:ILE:HD11	1.81	0.63
3:D:1096:ARG:CB	3:D:1096:ARG:HH11	2.11	0.63
3:D:139:GLY:O	3:D:147:VAL:HB	1.99	0.63
3:D:208:PRO:HB2	3:D:395:VAL:HG13	1.79	0.63
3:D:616:GLN:OE1	3:D:619:LEU:HB3	1.98	0.63
5:F:317:LEU:O	5:F:329:TYR:HB3	1.99	0.63
2:M:1081:VAL:HG11	2:M:1111:ILE:HG22	1.81	0.63
2:M:397:GLU:H	2:M:633:GLN:HE22	1.47	0.63
3:N:1310:ARG:HD2	3:N:1327:ARG:NH2	2.12	0.63
4:O:93:TYR:HB2	8:O:3948:HOH:O	1.99	0.63
1:B:170:VAL:HG22	8:B:430:HOH:O	1.97	0.63
2:C:1004:LYS:HE3	2:C:1027:PHE:HE1	1.62	0.63
2:C:113:VAL:HG22	8:C:1632:HOH:O	1.97	0.63
2:C:462:ASP:HA	8:C:1164:HOH:O	1.97	0.63
3:D:165:LYS:HB3	3:D:395:VAL:HG11	1.81	0.63
2:M:329:GLY:HA3	2:M:489:THR:HG23	1.81	0.63
2:M:601:GLY:HA2	2:M:616:GLU:HG2	1.79	0.63
3:N:197:SER:HB2	3:N:205:TYR:CZ	2.34	0.63
4:O:5:GLY:O	4:O:9:LEU:HG	1.99	0.63
5:P:278:LEU:HD22	5:P:290:GLU:HB3	1.79	0.63
1:A:184:THR:HG23	1:A:192:LEU:HD12	1.79	0.62
5:F:283:GLY:HA3	8:F:696:HOH:O	1.98	0.62
2:M:31:GLN:HA	8:M:1127:HOH:O	1.98	0.62
2:M:71:TYR:HD2	2:M:71:TYR:H	1.47	0.62
3:N:536:ALA:HA	5:P:315:VAL:O	1.99	0.62
3:N:810:GLU:O	3:N:813:LEU:HG	1.98	0.62
3:N:975:GLU:O	3:N:979:GLU:HG3	1.99	0.62
5:P:112:ALA:HA	5:P:173:TYR:HD2	1.64	0.62
1:A:14:ARG:HH22	1:A:24:VAL:HG23	1.63	0.62
1:A:91:ASN:HB2	8:A:426:HOH:O	1.98	0.62
2:C:162:ILE:O	2:C:164:PRO:HD3	1.99	0.62
2:C:910:LYS:HB2	2:C:913:GLU:OE1	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1406:ARG:HA	8:D:2023:HOH:O	1.98	0.62
3:D:817:GLU:O	3:D:821:VAL:HG23	1.99	0.62
2:M:379:GLU:O	2:M:383:ARG:HB3	1.99	0.62
3:N:1026:SER:HA	8:N:9094:HOH:O	1.99	0.62
3:N:610:LYS:HG2	3:N:611:GLN:NE2	2.14	0.62
3:N:928:ALA:CA	3:N:931:LEU:HD12	2.29	0.62
3:D:1209:LEU:HD23	3:D:1210:SER:N	2.13	0.62
3:D:156:GLU:CD	3:D:156:GLU:H	2.00	0.62
1:L:78:ILE:HA	8:L:2800:HOH:O	1.99	0.62
2:M:846:LYS:HE3	8:M:1413:HOH:O	1.99	0.62
1:K:42:ARG:HH12	2:M:857:ASP:HB3	1.65	0.62
2:M:890:LEU:HA	2:M:914:ILE:HD13	1.81	0.62
3:N:102:ILE:HD11	8:N:9432:HOH:O	1.99	0.62
3:N:423:ASP:HB2	5:P:178:ARG:HD2	1.80	0.62
1:B:212:ASN:O	1:B:215:VAL:HG22	2.00	0.62
2:C:150:PRO:CA	2:C:158:TYR:HB3	2.28	0.62
2:C:650:ARG:HG3	2:C:653:ASP:HB2	1.80	0.62
2:C:937:ASP:HB2	2:C:940:GLU:HG3	1.80	0.62
3:D:142:LEU:HA	8:D:9173:HOH:O	1.97	0.62
5:F:196:VAL:HG22	5:F:213:ILE:HD13	1.81	0.62
1:L:30:ARG:HH11	1:L:30:ARG:HB2	1.64	0.62
2:M:809:GLY:HA2	8:M:1515:HOH:O	1.98	0.62
3:N:1123:PHE:CE2	3:N:1184:GLN:HA	2.34	0.62
3:N:1277:ILE:HD12	3:N:1301:LYS:HB2	1.81	0.62
1:A:41:ARG:O	1:A:45:LEU:HD12	1.98	0.62
3:D:119:SER:HB2	3:D:123:LEU:N	2.11	0.62
3:D:1337:GLU:HA	8:D:2052:HOH:O	1.98	0.62
3:D:1372:VAL:HA	3:D:1375:MET:SD	2.39	0.62
5:F:196:VAL:HG13	5:F:213:ILE:HD11	1.81	0.62
2:M:584:GLU:CD	2:M:584:GLU:H	2.02	0.62
2:M:971:LYS:HA	2:M:988:VAL:HA	1.80	0.62
3:N:1166:LEU:HD23	3:N:1166:LEU:H	1.63	0.62
3:N:1435:LEU:HD23	3:N:1464:GLU:HB2	1.80	0.62
3:N:728:LEU:HA	8:N:9469:HOH:O	1.99	0.62
2:C:254:VAL:HG13	2:C:258:TYR:HE1	1.64	0.62
2:C:338:GLU:HA	2:C:341:THR:HG22	1.81	0.62
2:C:328:LEU:HD11	2:C:434:HIS:HD2	1.64	0.62
2:C:640:ARG:NH1	2:C:642:ARG:HH22	1.96	0.62
3:D:9:ARG:HA	3:D:1434:TRP:CH2	2.35	0.62
1:K:91:ASN:O	1:K:94:LEU:HD12	1.98	0.62
1:L:57:TYR:HE1	1:L:163:ASN:HB2	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:185:ARG:HG3	1:L:190:THR:HG22	1.80	0.62
2:M:48:PHE:HD2	8:M:1223:HOH:O	1.82	0.62
2:M:676:ILE:HG23	2:M:676:ILE:O	1.98	0.62
3:N:1122:LEU:HD11	3:N:1186:VAL:HG23	1.81	0.62
3:N:62:LYS:HE2	3:N:75:ARG:NH1	2.15	0.62
3:N:783:ARG:HH21	3:N:1029:ARG:HG2	1.64	0.62
1:A:42:ARG:NH1	2:C:978:ARG:HA	2.14	0.62
2:C:162:ILE:HB	2:C:172:ILE:HD13	1.82	0.62
2:C:72:ARG:NH1	2:C:72:ARG:HB2	2.15	0.62
3:D:1214:PRO:HB2	8:D:2011:HOH:O	1.98	0.62
3:D:207:PHE:HB3	3:D:208:PRO:HD2	1.81	0.62
3:N:41:ARG:HD3	3:N:42:ASP:H	1.65	0.62
3:N:478:LEU:HD21	3:N:500:ARG:HH21	1.65	0.62
3:N:488:ARG:HB3	3:N:488:ARG:NH1	2.15	0.62
5:P:396:ARG:HB2	8:P:2872:HOH:O	2.00	0.62
2:C:3:ILE:HG22	8:C:1178:HOH:O	1.99	0.62
2:C:516:ARG:CZ	3:D:1068:LEU:HD22	2.30	0.62
2:C:704:HIS:CD2	2:C:831:ARG:HH21	2.18	0.62
3:D:1279:GLY:O	3:D:1318:TYR:HA	1.99	0.62
3:D:537:THR:O	5:F:317:LEU:HB2	1.99	0.62
3:D:723:GLY:HA3	8:D:9008:HOH:O	1.99	0.62
1:K:94:LEU:HD21	1:K:119:ASP:HB3	1.81	0.62
2:M:777:ILE:HG22	8:M:1241:HOH:O	2.00	0.62
3:N:421:LEU:HD12	3:N:435:VAL:HG11	1.80	0.62
3:N:704:ARG:HG3	3:N:736:PHE:HB3	1.82	0.62
3:N:95:LEU:CD2	3:N:574:LEU:HD11	2.30	0.62
2:C:706:GLU:HB3	2:C:708:TYR:CE1	2.34	0.62
3:D:28:LYS:HD3	3:D:41:ARG:CZ	2.29	0.62
3:D:570:GLU:OE2	5:F:214:GLN:HG3	1.98	0.62
4:E:26:ARG:HA	4:E:29:GLN:OE1	2.00	0.62
1:L:212:ASN:O	1:L:215:VAL:HG22	2.00	0.62
2:M:254:VAL:HG11	8:M:1850:HOH:O	1.99	0.62
3:N:1129:THR:HG23	3:N:1130:ARG:H	1.65	0.62
3:N:178:LEU:HB2	8:N:9874:HOH:O	1.99	0.62
3:N:441:ARG:O	3:N:443:VAL:HG23	1.99	0.62
3:D:1280:VAL:HG23	3:D:1295:GLU:O	2.00	0.62
3:D:1389:LEU:HD12	3:D:1390:LEU:N	2.15	0.62
3:D:161:LEU:HD22	3:D:452:ILE:HG21	1.81	0.62
3:D:625:TYR:O	3:D:749:VAL:HG23	1.98	0.62
3:D:696:HIS:CD2	4:E:59:ASN:HB2	2.35	0.62
3:D:844:ALA:O	3:D:867:ARG:HB3	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:361:LEU:CD2	5:F:362:SER:H	2.13	0.62
1:K:20:TYR:HD2	1:K:21:GLY:H	1.47	0.62
2:M:232:GLU:HA	2:M:235:LEU:HD12	1.82	0.62
2:M:495:THR:HB	2:M:530:GLU:HG3	1.82	0.62
2:M:768:THR:HB	2:M:771:GLU:HB3	1.82	0.62
3:N:136:ASP:CB	3:N:137:PRO:HD3	2.30	0.62
3:N:705:ALA:HB3	3:N:706:PRO:HD3	1.81	0.62
5:P:277:GLN:O	5:P:280:GLN:HB3	1.99	0.62
5:P:361:LEU:HD23	5:P:362:SER:H	1.65	0.62
1:B:184:THR:HB	1:B:194:LYS:HZ3	1.63	0.61
2:C:71:TYR:H	2:C:71:TYR:HD2	1.48	0.61
2:C:816:LYS:HB2	2:C:819:VAL:HG21	1.81	0.61
3:D:605:ASP:HB3	8:D:2071:HOH:O	2.00	0.61
2:C:686:ASP:H	3:D:740:PHE:HD1	1.48	0.61
2:M:197:LEU:HB3	2:M:202:TYR:HB2	1.82	0.61
2:M:775:ARG:HD3	8:M:1274:HOH:O	1.99	0.61
2:M:910:LYS:HB3	2:M:912:PRO:HD2	1.81	0.61
2:M:976:ASP:CB	2:M:979:THR:HG22	2.29	0.61
3:N:12:LEU:HD11	3:N:512:MET:HG2	1.81	0.61
3:N:529:GLN:HG2	3:N:535:PHE:HE2	1.65	0.61
3:N:561:GLY:HA3	5:P:184:ARG:NH2	2.14	0.61
5:P:142:ARG:HD2	8:P:2896:HOH:O	1.99	0.61
5:P:347:GLN:HA	5:P:350:LEU:CD2	2.27	0.61
8:M:1274:HOH:O	5:P:421:PHE:HE2	1.83	0.61
1:B:206:THR:CG2	1:B:209:GLU:H	2.13	0.61
2:C:243:ARG:HB3	8:C:1850:HOH:O	1.99	0.61
2:C:89:THR:HG21	2:C:383:ARG:HH21	1.65	0.61
3:D:1169:ASP:HB2	8:D:9180:HOH:O	1.99	0.61
3:D:117:ASP:HA	8:D:9025:HOH:O	2.00	0.61
3:D:1197:ARG:HG3	3:D:1198:TYR:H	1.64	0.61
3:D:85:VAL:O	3:D:89:ARG:HD3	1.99	0.61
1:K:41:ARG:HH11	1:K:177:VAL:HB	1.64	0.61
2:M:101:ILE:HG23	2:M:107:LEU:HD22	1.82	0.61
2:M:261:ILE:HD13	8:M:1497:HOH:O	2.00	0.61
2:M:16:PRO:CG	2:M:460:ARG:HH12	2.13	0.61
8:M:1241:HOH:O	5:P:409:LYS:HB2	1.99	0.61
3:D:153:LEU:HD11	3:D:158:TYR:N	2.15	0.61
3:D:127:LEU:HD21	3:D:461:ILE:HD11	1.82	0.61
2:M:158:TYR:HD1	2:M:313:LEU:HD21	1.65	0.61
2:M:839:LEU:HD21	2:M:849:VAL:HG23	1.81	0.61
3:N:543:LEU:HA	3:N:546:ARG:HG3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:80:LEU:HD23	3:N:867:ARG:HH12	1.65	0.61
1:B:97:VAL:HG13	8:B:346:HOH:O	2.00	0.61
2:C:1018:GLN:HE21	2:C:1063:ARG:HH22	1.48	0.61
2:C:409:ARG:HA	2:C:454:SER:HA	1.80	0.61
2:C:49:ARG:NH1	2:C:49:ARG:HB2	2.14	0.61
2:C:78:PHE:HB2	2:C:88:LEU:HD21	1.81	0.61
2:C:94:LEU:HD21	8:C:1125:HOH:O	1.99	0.61
3:D:15:PRO:HA	3:D:18:ILE:HG12	1.82	0.61
3:D:675:ARG:HH21	5:F:421:PHE:N	1.97	0.61
2:M:244:PRO:HB2	8:M:1637:HOH:O	2.00	0.61
2:M:492:ASP:HB3	2:M:518:LYS:HD2	1.81	0.61
2:M:545:ASN:O	2:M:581:THR:HG21	2.00	0.61
2:M:549:PHE:CD2	2:M:886:LEU:HB3	2.35	0.61
2:M:625:LEU:HB3	2:M:639:GLN:HB2	1.82	0.61
3:N:1000:THR:O	3:N:1003:VAL:HG22	2.00	0.61
3:N:400:VAL:HG21	3:N:441:ARG:NH1	2.15	0.61
5:P:262:VAL:HG12	5:P:266:GLU:OE1	2.00	0.61
1:A:123:MET:O	1:A:125:PRO:HD3	2.01	0.61
2:C:208:ALA:O	2:C:218:VAL:HG21	2.01	0.61
2:C:651:LYS:HA	8:C:1288:HOH:O	2.01	0.61
3:D:1021:TYR:CE1	3:D:1025:GLN:HG3	2.35	0.61
3:D:1236:LEU:HD23	3:D:1359:GLN:NE2	2.16	0.61
3:D:1302:GLU:HB3	8:D:2003:HOH:O	1.99	0.61
3:D:4:GLU:HA	8:D:9462:HOH:O	2.01	0.61
3:D:778:LEU:O	3:D:778:LEU:HD23	2.00	0.61
3:D:998:GLU:HA	8:D:9447:HOH:O	1.99	0.61
2:M:332:ARG:HG2	2:M:332:ARG:NH1	2.15	0.61
2:M:350:ARG:HD3	2:M:353:ARG:NH2	2.16	0.61
2:M:605:LYS:HD3	2:M:610:ARG:NH1	2.15	0.61
3:N:427:VAL:CG2	3:N:435:VAL:HB	2.30	0.61
3:N:9:ARG:HG3	3:N:1455:LYS:O	2.01	0.61
5:P:400:ILE:HA	8:P:3326:HOH:O	1.99	0.61
1:A:86:VAL:HG21	1:A:202:ASP:O	2.00	0.61
1:A:54:THR:CG2	1:A:158:ILE:HG13	2.30	0.61
2:C:532:MET:HG3	2:C:533:ASP:N	2.16	0.61
3:D:1147:ARG:O	3:D:1165:TYR:HA	2.01	0.61
3:D:7:LYS:HD3	3:D:1456:LYS:HZ2	1.66	0.61
3:D:965:GLU:O	3:D:968:ASP:HB2	2.00	0.61
5:F:361:LEU:HD22	5:F:362:SER:H	1.65	0.61
2:M:1007:ALA:HB2	3:N:648:MET:HG3	1.83	0.61
3:N:130:SER:HB3	3:N:132:TYR:CE1	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:144:ILE:HB	5:P:145:PRO:HD3	1.81	0.61
3:D:1487:VAL:HG11	3:D:1492:LEU:HD23	1.81	0.61
3:D:705:ALA:HB3	3:D:706:PRO:HD3	1.83	0.61
1:L:100:LEU:O	1:L:115:LEU:HG	2.01	0.61
2:M:110:GLU:CG	2:M:369:PRO:HG3	2.28	0.61
3:N:100:ALA:HA	8:N:9084:HOH:O	1.99	0.61
3:N:116:LEU:HB3	3:N:118:LEU:HD21	1.82	0.61
3:N:208:PRO:HB2	3:N:395:VAL:HG13	1.82	0.61
3:N:99:ALA:HA	3:N:575:GLN:HE22	1.65	0.61
5:P:337:HIS:H	5:P:337:HIS:CD2	2.19	0.61
2:C:140:ILE:HD11	2:C:412:ALA:HA	1.82	0.61
3:D:1033:GLN:HE22	3:D:1036:ARG:NH1	1.97	0.61
3:D:652:LEU:HB3	3:D:653:PHE:HD1	1.65	0.61
4:E:25:LYS:O	4:E:29:GLN:HG2	2.01	0.61
5:F:220:LEU:HB2	5:F:243:ILE:HD11	1.83	0.61
3:D:598:ARG:HH22	5:F:318:GLU:C	2.04	0.61
1:L:188:GLN:HG3	8:N:9878:HOH:O	2.01	0.61
2:M:251:ASP:HB3	2:M:252:LYS:HD2	1.81	0.61
3:N:123:LEU:HD11	3:N:152:LEU:HD21	1.82	0.61
3:N:172:PRO:HD2	3:N:389:GLU:O	2.01	0.61
5:P:156:VAL:HA	5:P:159:ILE:HD12	1.81	0.61
2:C:64:LEU:HD22	2:C:359:MET:HG3	1.81	0.61
2:C:431:HIS:H	2:C:434:HIS:CE1	2.18	0.61
2:C:56:GLU:CG	2:C:64:LEU:HD23	2.31	0.61
2:C:575:GLN:N	2:C:667:ALA:HB1	2.15	0.61
2:C:976:ASP:CB	2:C:979:THR:HG22	2.31	0.61
3:D:133:ILE:HG22	3:D:455:ARG:N	2.15	0.61
3:D:1394:VAL:HB	3:D:1397:LYS:HD2	1.83	0.61
2:M:63:GLY:HA3	2:M:103:LYS:HE2	1.82	0.61
2:M:807:ARG:HB2	2:M:807:ARG:CZ	2.30	0.61
3:N:1147:ARG:O	3:N:1165:TYR:HA	2.00	0.61
3:N:164:GLY:HA2	8:N:9338:HOH:O	2.00	0.61
3:N:817:GLU:O	3:N:821:VAL:HG23	2.00	0.61
3:N:984:THR:HG22	3:N:987:GLU:H	1.65	0.61
2:C:605:LYS:HG3	2:C:612:VAL:HB	1.81	0.61
2:C:861:LEU:HG	2:C:862:PRO:HD2	1.83	0.61
1:K:216:GLU:O	1:K:220:GLU:HG3	2.00	0.61
1:L:84:GLU:HB2	8:N:9025:HOH:O	2.01	0.61
3:N:1324:PRO:HA	8:N:9087:HOH:O	2.00	0.61
3:N:842:VAL:HG23	8:N:9576:HOH:O	2.01	0.61
1:A:150:TYR:CE1	2:C:696:LYS:HA	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1018:GLN:HG3	2:C:1060:ILE:HD13	1.82	0.60
2:C:1044:GLY:HA3	4:E:17:TYR:CE1	2.36	0.60
2:C:537:LYS:HD2	2:C:537:LYS:H	1.65	0.60
3:D:1299:PHE:HB2	8:D:9130:HOH:O	2.01	0.60
3:N:1493:LYS:HA	3:N:1493:LYS:NZ	2.16	0.60
3:N:661:MET:CE	3:N:677:LEU:HD11	2.31	0.60
1:A:11:PHE:CD1	1:B:225:PHE:HA	2.36	0.60
2:C:682:TYR:HE2	8:D:9907:HOH:O	1.85	0.60
2:C:724:ARG:CD	2:C:740:GLU:HA	2.31	0.60
2:C:724:ARG:HD2	2:C:740:GLU:HA	1.81	0.60
2:C:833:LEU:HD12	2:C:834:GLN:N	2.17	0.60
2:C:837:ASP:OD1	2:C:996:LYS:HE3	2.01	0.60
3:D:1107:VAL:HG12	3:D:1217:ILE:HA	1.82	0.60
3:D:190:GLU:HB3	8:D:9257:HOH:O	2.01	0.60
1:K:102:LYS:HE2	1:K:139:ASN:ND2	2.15	0.60
1:L:86:VAL:HG12	1:L:124:ASN:HD22	1.66	0.60
2:M:567:GLN:HB2	2:M:997:LEU:HD23	1.83	0.60
3:N:119:SER:N	3:N:123:LEU:HB2	2.16	0.60
3:N:1468:LEU:HD13	3:N:1470:ARG:HB2	1.83	0.60
3:N:130:SER:O	3:N:568:ARG:NH2	2.34	0.60
4:O:70:THR:HG21	4:O:72:ARG:NH2	2.16	0.60
5:P:403:LYS:HA	5:P:403:LYS:HZ2	1.65	0.60
1:A:5:LYS:O	1:A:8:ALA:HB2	2.01	0.60
1:B:5:LYS:O	1:B:8:ALA:HB2	2.02	0.60
2:C:91:GLN:HG2	2:C:119:PRO:HG3	1.83	0.60
3:D:119:SER:HB2	3:D:123:LEU:HB2	1.81	0.60
3:D:1320:GLU:HB2	3:D:1323:GLN:HE21	1.65	0.60
3:D:1393:GLN:HB2	3:D:1398:TRP:CZ2	2.36	0.60
3:D:658:LEU:HD11	3:D:674:ARG:NH1	2.16	0.60
3:D:966:GLU:HA	3:D:969:ARG:HD2	1.83	0.60
4:E:48:MET:N	4:E:54:LEU:HB2	2.15	0.60
1:K:58:ILE:HB	1:K:61:VAL:HB	1.83	0.60
1:K:5:LYS:O	1:K:8:ALA:HB2	2.01	0.60
1:L:2:LEU:HD12	1:L:3:ASP:H	1.66	0.60
2:M:39:ARG:NE	2:M:39:ARG:HA	2.16	0.60
2:M:52:PHE:CD2	2:M:68:PHE:HB2	2.37	0.60
3:N:1314:LYS:HD3	3:N:1314:LYS:N	2.17	0.60
3:N:35:ARG:HG3	3:N:36:THR:H	1.66	0.60
3:N:767:HIS:CD2	4:O:6:ILE:HG12	2.35	0.60
1:B:132:LEU:HD21	1:B:136:GLY:O	2.01	0.60
1:B:158:ILE:HD13	8:B:396:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:327:HIS:CE1	2:C:489:THR:HA	2.35	0.60
3:D:1307:LYS:CD	3:D:1307:LYS:H	2.14	0.60
3:D:162:ARG:HB2	3:D:162:ARG:CZ	2.31	0.60
3:D:561:GLY:HA3	5:F:184:ARG:HH12	1.65	0.60
3:D:608:SER:HB3	3:D:1443:THR:OG1	2.01	0.60
5:F:112:ALA:O	5:F:116:LEU:HG	2.01	0.60
2:M:395:LYS:HE3	2:M:403:SER:OG	2.01	0.60
2:M:515:ALA:O	2:M:516:ARG:HD3	2.01	0.60
2:M:564:MET:HG2	2:M:840:ALA:HB3	1.83	0.60
3:N:1146:GLY:HA3	3:N:1207:TYR:HB2	1.83	0.60
3:N:9:ARG:NH1	3:N:506:GLY:HA2	2.14	0.60
3:N:566:ILE:HD11	5:P:192:LEU:HD21	1.84	0.60
3:N:658:LEU:HD11	3:N:674:ARG:NH1	2.16	0.60
3:N:831:GLY:HA3	8:N:9080:HOH:O	2.01	0.60
3:N:950:GLY:H	3:N:953:ASP:HB2	1.66	0.60
4:O:31:LEU:HD23	4:O:35:PHE:CE1	2.36	0.60
5:P:82:ARG:HG2	5:P:86:HIS:CD2	2.36	0.60
2:C:162:ILE:HD12	2:C:172:ILE:HB	1.83	0.60
2:C:193:LEU:HB2	8:C:1179:HOH:O	2.01	0.60
2:C:625:LEU:HD22	2:C:639:GLN:HB2	1.84	0.60
3:D:1267:ARG:HH22	3:D:1333:HIS:CD2	2.17	0.60
3:D:1406:ARG:HH21	3:D:1407:LEU:HG	1.67	0.60
3:D:3:LYS:HE2	8:D:9538:HOH:O	2.01	0.60
5:F:278:LEU:HB3	5:F:286:PRO:HG2	1.83	0.60
5:F:287:THR:HG23	5:F:289:GLU:HB2	1.83	0.60
5:F:363:GLU:HA	5:F:367:MET:CE	2.31	0.60
1:K:227:ASN:ND2	1:K:227:ASN:H	1.94	0.60
1:L:36:LEU:O	1:L:39:PRO:HD2	2.02	0.60
2:M:902:ILE:HG13	8:M:1340:HOH:O	2.00	0.60
3:N:1124:GLN:N	3:N:1133:ARG:O	2.34	0.60
1:A:43:ILE:HG13	8:A:322:HOH:O	2.01	0.60
2:C:433:THR:HG21	2:C:488:ALA:CB	2.32	0.60
3:D:1341:PRO:HA	3:D:1344:VAL:HG23	1.83	0.60
3:D:58:CYS:HA	3:D:78:VAL:HG11	1.84	0.60
4:E:45:ARG:O	4:E:47:LYS:HE3	2.02	0.60
3:D:566:ILE:HG23	5:F:214:GLN:OE1	2.02	0.60
2:M:154:ARG:NH2	2:M:156:GLY:HA3	2.15	0.60
2:M:31:GLN:HB2	8:M:1418:HOH:O	2.00	0.60
2:M:775:ARG:HA	8:M:1274:HOH:O	2.01	0.60
2:M:914:ILE:HD11	2:M:918:LEU:HD13	1.84	0.60
3:N:1301:LYS:HB3	8:N:9539:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1034:GLU:HA	2:C:1037:VAL:HG23	1.84	0.60
2:C:146:VAL:HG22	2:C:162:ILE:HA	1.84	0.60
3:D:1428:ALA:O	3:D:1431:THR:HG23	2.02	0.60
3:D:65:ARG:HG2	8:D:9136:HOH:O	2.00	0.60
8:D:2041:HOH:O	4:E:80:VAL:HG21	2.00	0.60
1:L:57:TYR:CE1	1:L:163:ASN:HB2	2.37	0.60
3:N:699:VAL:HG21	3:N:760:ARG:HB3	1.83	0.60
1:B:29:GLU:HG3	8:B:446:HOH:O	2.00	0.60
2:C:1115:LEU:H	2:C:1115:LEU:HD12	1.67	0.60
2:C:542:VAL:HG23	2:C:543:ASN:H	1.65	0.60
2:C:698:ASP:HA	8:C:1248:HOH:O	2.00	0.60
3:D:402:PRO:HG2	3:D:444:VAL:HG11	1.83	0.60
3:D:491:LYS:HD3	3:D:492:ALA:N	2.17	0.60
3:D:891:GLU:HG3	8:D:2090:HOH:O	2.01	0.60
1:L:123:MET:C	1:L:125:PRO:HD3	2.22	0.60
2:M:455:LEU:HD12	2:M:456:ALA:O	2.01	0.60
3:N:1271:LYS:HG2	3:N:1272:ALA:N	2.16	0.60
3:N:584:ASN:ND2	3:N:590:PRO:HD2	2.15	0.60
3:N:865:THR:CG2	3:N:874:GLU:HG3	2.32	0.60
5:P:416:ARG:CZ	5:P:419:ARG:HB2	2.31	0.60
2:C:1014:SER:OG	5:F:331:ASP:HA	2.01	0.60
2:C:19:THR:O	2:C:23:VAL:HG23	2.02	0.60
2:C:241:LEU:HB2	8:C:1346:HOH:O	2.02	0.60
2:C:493:ARG:HD2	8:C:1692:HOH:O	2.02	0.60
2:C:569:VAL:HG12	2:C:996:LYS:O	2.01	0.60
2:C:583:LEU:O	2:C:587:VAL:HG23	2.02	0.60
3:D:1144:LEU:HA	3:D:1147:ARG:HG3	1.84	0.60
3:D:1262:LEU:HD23	3:D:1352:ILE:CG1	2.32	0.60
3:D:660:LYS:HA	3:D:660:LYS:HE3	1.84	0.60
1:L:98:THR:HB	8:L:4416:HOH:O	2.02	0.60
2:M:1080:SER:HA	8:M:1763:HOH:O	2.02	0.60
2:M:367:LEU:HD11	8:M:1686:HOH:O	2.01	0.60
2:M:64:LEU:HA	8:M:1327:HOH:O	2.00	0.60
2:M:774:LEU:HA	2:M:777:ILE:HD12	1.83	0.60
3:N:1262:LEU:HD21	3:N:1351:GLU:HG3	1.83	0.60
3:N:1389:LEU:HD12	3:N:1390:LEU:N	2.16	0.60
3:N:127:LEU:HD21	3:N:461:ILE:HD11	1.83	0.60
3:N:630:VAL:HA	3:N:744:GLN:HG2	1.82	0.60
5:P:226:LYS:HB2	5:P:238:TYR:OH	2.02	0.60
1:A:198:ARG:HH21	2:C:932:GLU:HG2	1.66	0.60
2:C:408:ARG:NH1	2:C:455:LEU:HG	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1310:ARG:NE	3:D:1327:ARG:HB3	2.17	0.60
3:D:1459:LEU:HD13	3:D:1470:ARG:NH1	2.16	0.60
3:D:560:GLN:HG3	5:F:221:ILE:HG21	1.81	0.60
3:D:796:ARG:HH11	3:D:861:GLN:HB2	1.67	0.60
5:F:356:LYS:O	5:F:360:LYS:HG2	2.02	0.60
5:F:85:LEU:HD12	8:F:574:HOH:O	2.01	0.60
1:L:219:ARG:HB3	1:L:219:ARG:NH1	2.14	0.60
2:M:208:ALA:O	2:M:218:VAL:HG21	2.02	0.60
5:P:261:PRO:O	5:P:265:VAL:HG23	2.02	0.60
5:P:359:SER:HA	8:P:4306:HOH:O	2.02	0.60
2:C:211:LEU:HD11	2:C:308:ARG:HA	1.83	0.59
2:C:516:ARG:HH11	2:C:521:PRO:HB3	1.66	0.59
2:C:585:GLU:O	2:C:588:VAL:HG22	2.01	0.59
2:C:68:PHE:HE1	2:C:96:ALA:HB1	1.67	0.59
3:D:1243:THR:OG1	3:D:1253:THR:HB	2.02	0.59
3:D:1412:LYS:HG2	3:D:1414:PRO:HG3	1.84	0.59
3:D:1463:LYS:O	3:D:1467:ILE:HD12	2.01	0.59
3:D:540:LEU:HA	3:D:543:LEU:HD12	1.84	0.59
3:D:584:ASN:ND2	3:D:590:PRO:HD2	2.17	0.59
3:D:820:GLU:HB2	3:D:836:VAL:HG11	1.84	0.59
5:F:126:LEU:O	5:F:130:VAL:HG23	2.02	0.59
5:F:278:LEU:CB	5:F:286:PRO:HG2	2.32	0.59
2:M:1054:THR:CG2	2:M:1079:PRO:HB3	2.18	0.59
2:M:1097:LEU:HD22	2:M:1097:LEU:H	1.67	0.59
2:M:769:PRO:HB2	8:N:9172:HOH:O	2.02	0.59
2:M:1043:TYR:HE1	3:N:710:ARG:O	1.85	0.59
2:C:398:THR:OG1	2:C:633:GLN:HG3	2.02	0.59
3:D:601:ARG:NH2	3:D:612:GLY:HA2	2.17	0.59
3:D:734:GLU:HB3	8:D:9079:HOH:O	2.03	0.59
2:M:89:THR:HA	2:M:129:ILE:O	2.03	0.59
2:M:367:LEU:HD23	2:M:371:LYS:HZ2	1.66	0.59
2:M:41:ASN:O	2:M:46:ALA:HB2	2.02	0.59
2:M:626:ARG:H	2:M:639:GLN:NE2	2.00	0.59
3:N:1462:LEU:HD22	3:N:1472:ILE:HG23	1.84	0.59
3:N:471:GLU:O	3:N:475:LYS:HD2	2.02	0.59
5:P:404:ALA:O	5:P:408:LEU:HD23	2.02	0.59
2:C:116:GLY:HA3	2:C:378:LEU:HD23	1.84	0.59
2:C:181:VAL:HB	8:C:1316:HOH:O	2.02	0.59
2:C:317:VAL:HG12	8:C:1247:HOH:O	2.02	0.59
2:C:530:GLU:HA	8:C:1268:HOH:O	2.03	0.59
2:C:755:LEU:HD21	2:C:792:VAL:HG22	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1213:ARG:HB2	3:D:1214:PRO:CD	2.32	0.59
3:D:168:THR:HA	8:D:9120:HOH:O	2.02	0.59
3:D:775:GLY:HA3	3:D:1145:TYR:HE1	1.67	0.59
1:K:156:HIS:HD2	1:K:157:GLY:H	1.49	0.59
2:M:1002:GLU:HG2	8:P:3095:HOH:O	2.02	0.59
2:M:455:LEU:CD1	2:M:459:ALA:HB3	2.32	0.59
3:N:397:LYS:HD3	8:N:9216:HOH:O	2.01	0.59
1:L:175:ARG:O	3:N:851:LEU:HD21	2.03	0.59
2:C:263:ASP:HB2	2:C:264:PRO:HD3	1.84	0.59
2:C:602:GLU:HA	2:C:647:GLN:O	2.03	0.59
3:D:1385:GLY:HA2	8:D:9279:HOH:O	2.01	0.59
2:C:1052:MET:HG3	3:D:623:VAL:CG2	2.32	0.59
1:L:180:GLN:HG2	8:N:9258:HOH:O	2.02	0.59
2:M:1095:LEU:HD23	3:N:582:LEU:HD22	1.84	0.59
2:M:342:ASP:O	2:M:346:VAL:HG23	2.02	0.59
2:M:69:LEU:HB2	2:M:97:ARG:HB2	1.84	0.59
2:M:904:PRO:HA	8:M:1161:HOH:O	2.01	0.59
3:N:1147:ARG:HB3	3:N:1188:VAL:CG2	2.32	0.59
3:N:572:ARG:HH22	5:P:83:GLN:HG3	1.68	0.59
3:N:847:ASP:HA	3:N:850:LEU:HD13	1.84	0.59
3:N:907:GLU:HG2	3:N:908:LYS:N	2.18	0.59
2:C:22:GLN:O	2:C:121:MET:HE1	2.02	0.59
2:C:25:SER:CB	2:C:335:THR:HB	2.32	0.59
2:C:895:TYR:HD1	2:C:991:GLN:HE21	1.51	0.59
3:D:1061:PHE:HA	8:D:9283:HOH:O	2.01	0.59
3:D:1157:GLY:HA2	8:D:9700:HOH:O	2.02	0.59
3:D:1272:ALA:CA	3:D:1326:THR:HB	2.31	0.59
1:K:141:GLU:HA	8:K:3093:HOH:O	2.00	0.59
1:L:180:GLN:HA	8:N:9258:HOH:O	2.02	0.59
3:N:1267:ARG:HH11	3:N:1267:ARG:HB2	1.67	0.59
3:N:152:LEU:HD23	3:N:152:LEU:N	2.15	0.59
3:N:462:GLN:HG3	3:N:513:ILE:HD13	1.83	0.59
3:N:661:MET:HE2	3:N:677:LEU:HD11	1.84	0.59
3:N:983:LEU:HA	3:N:987:GLU:OE2	2.02	0.59
2:C:709:GLU:CD	2:C:824:ARG:HH12	2.05	0.59
2:C:720:GLU:HA	2:C:759:THR:O	2.03	0.59
3:D:1354:LYS:HD2	8:D:9706:HOH:O	2.03	0.59
3:D:491:LYS:HB2	8:D:9725:HOH:O	2.02	0.59
3:D:764:LEU:HB3	8:D:9083:HOH:O	2.02	0.59
3:D:860:LEU:HA	3:D:877:PRO:HB2	1.83	0.59
2:C:983:ILE:HG23	3:D:944:THR:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:10:VAL:HG12	1:K:12:THR:HG22	1.85	0.59
1:K:14:ARG:HG3	1:K:22:GLU:HB2	1.85	0.59
1:L:5:LYS:O	1:L:8:ALA:HB2	2.02	0.59
2:M:1014:SER:HB3	2:M:1017:THR:O	2.02	0.59
2:M:212:GLY:HA3	2:M:218:VAL:HG23	1.83	0.59
2:M:332:ARG:HG2	2:M:332:ARG:HH11	1.67	0.59
2:M:603:VAL:HG21	2:M:643:VAL:CG1	2.33	0.59
2:M:798:GLY:H	2:M:827:VAL:CG1	2.15	0.59
3:N:705:ALA:HB2	8:N:9482:HOH:O	2.02	0.59
3:N:843:PHE:HE1	3:N:864:VAL:HG11	1.67	0.59
2:C:135:VAL:O	2:C:392:SER:HA	2.03	0.59
2:C:51:THR:HB	2:C:348:LEU:HD23	1.85	0.59
3:D:1304:LYS:HA	8:D:9240:HOH:O	2.02	0.59
3:D:126:VAL:HG12	3:D:132:TYR:HB2	1.85	0.59
1:K:222:LEU:HD11	1:L:218:LEU:HD23	1.85	0.59
2:M:938:LYS:HB3	2:M:939:ARG:HH21	1.67	0.59
3:N:149:LYS:HD3	8:N:9307:HOH:O	2.02	0.59
5:P:166:LEU:O	5:P:171:LYS:HB2	2.02	0.59
1:A:133:GLU:HG2	1:A:134:GLU:N	2.16	0.59
2:C:290:LEU:HB3	2:C:302:VAL:CG1	2.33	0.59
2:C:905:ILE:H	2:C:905:ILE:CD1	2.07	0.59
3:D:1050:GLY:HA2	8:D:9344:HOH:O	2.02	0.59
1:L:117:VAL:HG13	8:L:3779:HOH:O	2.02	0.59
8:K:3080:HOH:O	1:L:36:LEU:HD12	2.02	0.59
1:L:64:GLU:HG3	8:L:3767:HOH:O	2.01	0.59
1:L:80:LEU:HD23	3:N:867:ARG:NH1	2.18	0.59
2:M:173:ASP:O	2:M:184:MET:HA	2.03	0.59
2:M:274:ARG:NH2	2:M:284:ARG:HG2	2.17	0.59
3:N:133:ILE:HG21	3:N:454:ALA:CB	2.31	0.59
3:N:169:TYR:HD1	3:N:169:TYR:H	1.49	0.59
3:N:588:GLY:HA2	8:N:9699:HOH:O	2.03	0.59
3:N:679:ARG:HB2	3:N:682:ASP:OD1	2.02	0.59
2:M:685:GLU:HG2	3:N:739:ASP:HB2	1.85	0.59
3:N:920:LEU:HB2	8:N:9246:HOH:O	2.01	0.59
2:M:1015:LEU:HB2	5:P:334:PRO:O	2.02	0.59
2:C:328:LEU:HB2	2:C:488:ALA:HB2	1.84	0.59
2:C:470:PRO:HB2	2:C:534:VAL:HG21	1.83	0.59
2:C:682:TYR:HB3	2:C:689:VAL:HG22	1.85	0.59
2:C:70:GLU:HA	8:C:1554:HOH:O	2.03	0.59
3:D:128:TYR:CE1	3:D:461:ILE:HG13	2.37	0.59
3:D:1320:GLU:H	3:D:1323:GLN:NE2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:380:GLU:O	3:D:382:GLU:N	2.35	0.59
3:D:477:LEU:HD11	3:D:495:ARG:HD3	1.84	0.59
3:D:817:GLU:HG3	3:D:840:LYS:HZ2	1.68	0.59
4:E:31:LEU:HD12	4:E:32:ARG:HD3	1.84	0.59
5:F:102:LEU:O	5:F:106:VAL:HG23	2.03	0.59
2:C:778:PHE:CZ	5:F:409:LYS:HB2	2.38	0.59
3:N:1036:ARG:HH21	3:N:1042:ARG:CA	2.07	0.59
3:N:1091:SER:HA	8:N:9056:HOH:O	2.02	0.59
3:N:984:THR:HB	3:N:987:GLU:OE1	2.01	0.59
5:P:245:GLN:HB3	8:P:4764:HOH:O	2.02	0.59
1:B:101:LEU:HG	1:B:114:PHE:HA	1.84	0.59
1:B:73:GLU:HB3	1:B:77:GLU:HG3	1.85	0.59
2:C:1115:LEU:HD23	3:D:85:VAL:HG13	1.85	0.59
2:C:313:LEU:HD13	2:C:321:GLU:O	2.02	0.59
2:C:798:GLY:HA3	2:C:828:ALA:O	2.03	0.59
3:D:500:ARG:HH11	3:D:500:ARG:HG3	1.68	0.59
4:E:88:GLU:OE1	4:E:91:ARG:HD2	2.03	0.59
5:F:416:ARG:HB3	8:F:511:HOH:O	2.02	0.59
5:F:420:ASP:O	5:F:422:LEU:HD23	2.03	0.59
2:M:691:SER:HB2	2:M:858:MET:SD	2.42	0.59
2:M:714:ASP:HB2	8:M:1654:HOH:O	2.03	0.59
3:N:434:ARG:HB2	3:N:447:VAL:CG2	2.33	0.59
3:N:125:GLN:HE22	3:N:587:ARG:HH21	1.51	0.59
2:C:549:PHE:CE2	2:C:886:LEU:HB3	2.38	0.58
3:D:130:SER:HB3	3:D:132:TYR:CE1	2.38	0.58
3:D:424:GLY:HA2	3:D:435:VAL:O	2.02	0.58
1:L:62:LEU:H	1:L:62:LEU:HD12	1.67	0.58
2:M:1090:LYS:HE3	3:N:88:TYR:O	2.03	0.58
3:N:629:SER:O	3:N:744:GLN:HG2	2.03	0.58
3:N:984:THR:H	3:N:987:GLU:CD	2.07	0.58
5:P:85:LEU:HD22	5:P:193:ARG:HD3	1.84	0.58
1:A:216:GLU:HG2	8:A:475:HOH:O	2.02	0.58
2:C:49:ARG:HG3	2:C:266:ARG:HH22	1.68	0.58
5:F:403:LYS:HA	5:F:403:LYS:NZ	2.18	0.58
1:K:126:ASP:HB3	8:K:4974:HOH:O	2.03	0.58
2:M:604:ALA:HB3	2:M:612:VAL:O	2.03	0.58
3:N:1104:GLU:O	3:N:1106:VAL:HG23	2.04	0.58
2:C:113:VAL:HG11	2:C:373:VAL:HB	1.84	0.58
2:C:578:VAL:HG13	2:C:671:ASN:HB3	1.86	0.58
3:D:1412:LYS:HG3	8:D:9515:HOH:O	2.03	0.58
3:D:150:ARG:HH11	3:D:150:ARG:HG3	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:420:VAL:HG23	8:D:9627:HOH:O	2.02	0.58
3:D:637:LEU:HD11	3:D:641:GLN:HB2	1.84	0.58
5:F:168:LYS:HG3	8:F:516:HOH:O	2.03	0.58
5:F:366:ALA:HB3	5:F:367:MET:HE2	1.83	0.58
1:L:132:LEU:HG	1:L:136:GLY:HA3	1.84	0.58
2:M:203:ASP:OD1	2:M:205:GLU:HG3	2.02	0.58
2:M:580:MET:HB3	2:M:584:GLU:CD	2.23	0.58
2:M:54:ILE:HG22	2:M:66:LEU:HB3	1.84	0.58
3:N:1124:GLN:HG2	3:N:1133:ARG:HG2	1.85	0.58
1:B:102:LYS:HE2	1:B:104:GLU:OE1	2.02	0.58
3:D:907:GLU:HG2	3:D:1027:GLY:N	2.17	0.58
3:D:1146:GLY:HA3	3:D:1207:TYR:HB2	1.85	0.58
3:D:1209:LEU:HD23	3:D:1211:MET:H	1.68	0.58
4:E:26:ARG:HD2	4:E:29:GLN:OE1	2.02	0.58
2:M:162:ILE:O	2:M:164:PRO:HD3	2.02	0.58
2:M:357:GLU:O	2:M:360:LEU:HG	2.04	0.58
2:M:579:VAL:HG11	2:M:887:GLU:HG3	1.84	0.58
2:M:575:GLN:H	2:M:667:ALA:HB1	1.68	0.58
2:M:722:ILE:HG13	2:M:757:GLY:O	2.02	0.58
2:M:862:PRO:HG3	2:M:975:TYR:HE1	1.67	0.58
3:N:1304:LYS:HA	8:N:2011:HOH:O	2.03	0.58
3:N:947:ILE:HD12	3:N:947:ILE:O	2.03	0.58
5:P:152:ASP:HA	8:P:2840:HOH:O	2.03	0.58
5:P:152:ASP:HB2	5:P:153:PRO:HD3	1.84	0.58
5:P:163:LEU:HB3	5:P:174:LEU:CG	2.33	0.58
5:P:393:THR:HG22	5:P:394:ARG:H	1.66	0.58
2:C:139:GLN:HE22	2:C:415:PRO:CD	2.17	0.58
2:C:139:GLN:HA	2:C:411:SER:O	2.03	0.58
2:C:487:THR:HA	8:C:1431:HOH:O	2.02	0.58
3:D:810:GLU:HA	3:D:813:LEU:HD23	1.83	0.58
5:F:129:GLU:HB3	5:F:142:ARG:HH21	1.67	0.58
5:F:166:LEU:HB3	5:F:170:HIS:HB2	1.85	0.58
3:N:52:PRO:CG	3:N:78:VAL:HG13	2.32	0.58
5:P:358:LEU:HD11	5:P:370:LYS:NZ	2.19	0.58
1:B:57:TYR:HE1	1:B:163:ASN:HB2	1.68	0.58
2:C:1032:PHE:CE1	2:C:1052:MET:HG2	2.37	0.58
2:C:1054:THR:HG22	2:C:1059:ASP:HB2	1.86	0.58
2:C:166:PRO:HD3	2:C:265:ARG:HE	1.68	0.58
2:C:115:LEU:HD22	2:C:373:VAL:HG11	1.86	0.58
2:C:437:ARG:O	2:C:467:ILE:HD13	2.04	0.58
2:C:690:ILE:HD13	2:C:833:LEU:HD21	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:881:ASN:HD22	2:C:881:ASN:N	1.99	0.58
3:D:1104:GLU:HA	3:D:1461:GLY:HA2	1.86	0.58
3:D:28:LYS:HB2	8:D:9050:HOH:O	2.03	0.58
3:D:523:ASP:O	3:D:526:PRO:HG3	2.04	0.58
3:D:704:ARG:HE	3:D:705:ALA:H	1.50	0.58
3:D:877:PRO:O	3:D:880:ILE:HG22	2.03	0.58
5:F:278:LEU:O	5:F:282:LEU:HG	2.03	0.58
5:F:282:LEU:HD12	5:F:284:ARG:O	2.03	0.58
5:F:79:ASP:HB3	5:F:80:PRO:CD	2.33	0.58
3:N:1122:LEU:O	3:N:1134:LEU:HD23	2.04	0.58
3:N:1478:SER:O	3:N:1482:ARG:HG3	2.04	0.58
3:N:134:VAL:HG12	3:N:152:LEU:HB3	1.86	0.58
3:N:208:PRO:HB2	3:N:395:VAL:HG22	1.84	0.58
4:O:47:LYS:HE2	4:O:47:LYS:N	2.19	0.58
1:B:41:ARG:HG3	1:B:177:VAL:CG2	2.33	0.58
2:C:110:GLU:HB2	2:C:368:THR:HB	1.86	0.58
3:D:41:ARG:HD2	8:D:9050:HOH:O	2.03	0.58
2:M:210:GLU:HA	8:M:1749:HOH:O	2.03	0.58
3:N:756:GLN:O	3:N:760:ARG:HG2	2.04	0.58
4:O:70:THR:HG21	4:O:72:ARG:CZ	2.34	0.58
1:B:10:VAL:HA	8:B:381:HOH:O	2.02	0.58
1:B:80:LEU:HD11	8:D:9557:HOH:O	2.04	0.58
2:C:44:ILE:HB	8:C:1185:HOH:O	2.04	0.58
2:C:897:LEU:HG	2:C:920:GLN:NE2	2.19	0.58
3:D:1129:THR:HG23	3:D:1130:ARG:H	1.68	0.58
3:D:865:THR:HG23	3:D:874:GLU:HG2	1.84	0.58
2:M:460:ARG:HD2	2:M:485:TYR:CE2	2.38	0.58
3:N:131:LYS:HA	3:N:456:MET:HG3	1.86	0.58
5:P:392:VAL:HG12	8:P:2872:HOH:O	2.04	0.58
1:A:91:ASN:OD1	1:A:92:PRO:HD2	2.04	0.58
2:C:159:ILE:HG22	8:C:1786:HOH:O	2.03	0.58
2:C:758:ARG:HB3	2:C:788:THR:O	2.04	0.58
2:C:946:ARG:HB2	8:C:1715:HOH:O	2.03	0.58
3:D:1277:ILE:CD1	3:D:1301:LYS:HB2	2.33	0.58
3:D:207:PHE:CB	3:D:208:PRO:HD2	2.33	0.58
5:F:291:ILE:O	5:F:295:MET:HB2	2.03	0.58
5:F:82:ARG:HG2	5:F:86:HIS:CD2	2.39	0.58
1:L:23:PHE:HD1	8:L:3037:HOH:O	1.86	0.58
2:M:342:ASP:O	2:M:345:ARG:HG3	2.04	0.58
2:M:807:ARG:HB2	2:M:807:ARG:NH1	2.18	0.58
3:N:104:PHE:CD2	3:N:1448:THR:HG23	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:998:GLU:HG3	8:N:9582:HOH:O	2.04	0.58
5:P:93:LEU:HD12	5:P:191:ASN:HD21	1.68	0.58
5:P:232:ARG:HB3	8:P:3790:HOH:O	2.03	0.58
1:A:36:LEU:O	1:A:40:LEU:HG	2.03	0.58
1:A:57:TYR:CE2	1:A:59:GLU:HA	2.39	0.58
2:C:1040:LEU:HD21	2:C:1048:THR:HG22	1.84	0.58
2:C:1085:PHE:O	2:C:1089:VAL:HG23	2.04	0.58
2:C:276:LYS:O	2:C:280:LYS:HB2	2.04	0.58
2:C:678:PRO:HG3	3:D:947:ILE:HD11	1.84	0.58
2:C:695:LEU:HD22	2:C:832:LYS:HG2	1.86	0.58
3:D:1341:PRO:O	3:D:1344:VAL:HG23	2.04	0.58
3:D:1491:THR:O	3:D:1495:ILE:HD13	2.04	0.58
3:D:178:LEU:HD21	3:D:199:LEU:H	1.69	0.58
3:D:28:LYS:HG2	8:D:9642:HOH:O	2.04	0.58
3:D:470:LEU:HD11	3:D:509:PRO:HG3	1.86	0.58
3:D:619:LEU:HB2	8:D:9069:HOH:O	2.04	0.58
5:F:218:GLN:HE21	5:F:221:ILE:HD12	1.67	0.58
5:F:220:LEU:O	5:F:224:VAL:HG23	2.03	0.58
1:K:152:PRO:HD2	1:K:155:LYS:HG3	1.85	0.58
1:K:39:PRO:O	1:K:43:ILE:HG12	2.04	0.58
2:M:1111:ILE:CD1	2:M:1112:PHE:H	2.14	0.58
2:M:166:PRO:HD3	2:M:265:ARG:HG3	1.85	0.58
2:M:276:LYS:O	2:M:280:LYS:HB2	2.02	0.58
3:N:1356:TYR:CD2	3:N:1363:LEU:HD23	2.39	0.58
3:N:184:GLU:HA	8:N:9224:HOH:O	2.04	0.58
5:P:154:LYS:HB3	8:P:3247:HOH:O	2.03	0.58
5:P:220:LEU:O	5:P:224:VAL:HG23	2.04	0.58
1:A:103:ALA:HB2	8:A:343:HOH:O	2.03	0.57
1:A:211:LEU:O	1:A:215:VAL:HG13	2.04	0.57
2:C:29:ALA:HB2	2:C:337:GLY:HA2	1.86	0.57
2:C:66:LEU:HD22	2:C:372:LEU:HD23	1.86	0.57
2:C:433:THR:HA	8:C:1154:HOH:O	2.02	0.57
2:C:847:GLY:HA3	8:C:1126:HOH:O	2.04	0.57
3:D:1047:LYS:HA	3:D:1053:PHE:CE1	2.38	0.57
3:D:1164:ARG:HG3	3:D:1164:ARG:HH11	1.68	0.57
3:D:1205:TYR:HE1	3:D:1221:VAL:HG13	1.67	0.57
3:D:675:ARG:O	3:D:678:GLU:HG2	2.04	0.57
3:D:920:LEU:HD21	8:D:9121:HOH:O	2.03	0.57
3:D:957:PRO:HB3	3:D:959:GLU:OE1	2.04	0.57
5:F:93:LEU:HG	5:F:190:ALA:HB1	1.86	0.57
2:M:611:ILE:HD11	2:M:641:PRO:HG3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:119:SER:OG	3:N:123:LEU:HD13	2.03	0.57
3:N:810:GLU:HA	3:N:813:LEU:HD23	1.84	0.57
5:P:187:LEU:HD23	5:P:191:ASN:ND2	2.18	0.57
1:A:191:ASP:O	1:A:192:LEU:HD23	2.04	0.57
1:B:150:TYR:CD2	3:D:857:ILE:HG13	2.38	0.57
2:C:200:LEU:HB2	8:C:1211:HOH:O	2.04	0.57
2:C:383:ARG:HB2	2:C:383:ARG:NH1	2.19	0.57
2:C:752:GLY:H	2:C:792:VAL:HB	1.70	0.57
1:A:178:ALA:CB	2:C:864:GLY:H	2.18	0.57
3:D:1472:ILE:HG22	3:D:1474:ALA:H	1.68	0.57
1:L:38:ASN:HB3	1:L:39:PRO:HD3	1.86	0.57
2:M:503:LEU:HB3	8:M:1190:HOH:O	2.04	0.57
2:M:678:PRO:HG2	3:N:947:ILE:HD11	1.85	0.57
2:M:759:THR:HB	2:M:785:VAL:HG21	1.87	0.57
1:L:65:PHE:CD1	3:N:813:LEU:HD22	2.33	0.57
5:P:362:SER:O	5:P:367:MET:HE2	2.04	0.57
2:C:320:HIS:HB2	8:C:1663:HOH:O	2.04	0.57
3:D:1232:PRO:HA	3:D:1235:GLN:OE1	2.04	0.57
3:D:153:LEU:HD12	3:D:154:THR:H	1.69	0.57
5:F:113:ILE:HG23	5:F:127:ILE:CG2	2.34	0.57
5:F:152:ASP:HB2	5:F:153:PRO:HD3	1.85	0.57
2:M:328:LEU:H	2:M:433:THR:HG21	1.69	0.57
3:N:957:PRO:CG	3:N:1007:VAL:HA	2.35	0.57
2:M:1101:THR:HB	3:N:5:VAL:HG13	1.87	0.57
5:P:81:VAL:HG12	5:P:85:LEU:HG	1.86	0.57
1:A:46:SER:HB3	2:C:856:GLU:HG3	1.86	0.57
2:C:1051:GLU:HG2	2:C:1056:LYS:HD2	1.86	0.57
2:C:110:GLU:HG2	2:C:369:PRO:CB	2.26	0.57
2:C:57:GLU:OE1	2:C:63:GLY:HA2	2.05	0.57
3:D:1285:GLU:H	3:D:1285:GLU:CD	2.08	0.57
3:D:1209:LEU:HD11	4:E:16:LYS:HD3	1.87	0.57
1:L:143:ARG:HH12	1:L:158:ILE:HD12	1.68	0.57
2:M:27:ARG:HD2	8:M:1403:HOH:O	2.04	0.57
2:M:874:LEU:CD1	3:N:783:ARG:HB2	2.35	0.57
3:N:1127:GLU:HG3	3:N:1133:ARG:NH1	2.18	0.57
3:N:1379:VAL:HG11	3:N:1395:LEU:HD23	1.85	0.57
3:N:1433:SER:HB2	3:N:1457:ASP:OD1	2.04	0.57
3:N:823:LEU:HD11	8:N:9446:HOH:O	2.03	0.57
5:P:93:LEU:HG	5:P:190:ALA:CB	2.34	0.57
1:B:89:PHE:HB3	1:B:94:LEU:HD13	1.86	0.57
2:C:157:ARG:HA	8:C:1144:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:177:GLU:HB3	8:C:1316:HOH:O	2.02	0.57
2:C:954:THR:OG1	2:C:957:LYS:HG3	2.03	0.57
3:D:955:VAL:HG21	3:D:1015:TYR:CE2	2.39	0.57
3:D:105:VAL:HG13	3:D:124:GLU:OE1	2.05	0.57
3:D:159:ARG:HB2	3:D:159:ARG:HH11	1.69	0.57
2:C:750:LYS:HB2	3:D:681:ARG:NH2	2.19	0.57
5:F:120:THR:HA	8:F:562:HOH:O	2.04	0.57
1:K:162:ILE:HG13	1:K:163:ASN:OD1	2.04	0.57
2:M:318:PRO:HD3	8:M:1200:HOH:O	2.05	0.57
3:N:1143:GLY:HA2	3:N:1365:ASP:OD1	2.05	0.57
3:N:399:ARG:HG2	8:N:9313:HOH:O	2.04	0.57
2:C:1092:LEU:HD13	2:C:1099:VAL:HG21	1.86	0.57
2:C:157:ARG:CZ	2:C:314:THR:HA	2.34	0.57
2:C:575:GLN:H	2:C:667:ALA:HB1	1.68	0.57
2:C:626:ARG:H	2:C:639:GLN:HE21	1.51	0.57
2:C:769:PRO:O	2:C:772:ARG:HB3	2.05	0.57
2:C:885:ILE:HG23	3:D:949:ILE:O	2.05	0.57
3:D:159:ARG:HB2	3:D:159:ARG:NH1	2.20	0.57
3:D:42:ASP:O	3:D:46:ASP:HB2	2.04	0.57
3:D:478:LEU:HD23	3:D:496:LEU:HD21	1.86	0.57
3:D:840:LYS:HD2	8:D:9835:HOH:O	2.05	0.57
2:M:473:ARG:HD2	2:M:475:VAL:HG22	1.85	0.57
2:M:534:VAL:N	2:M:538:GLN:HE22	2.01	0.57
3:N:421:LEU:HD11	3:N:437:VAL:HG22	1.86	0.57
3:N:524:LEU:HD23	8:N:9282:HOH:O	2.04	0.57
3:N:899:LEU:HB3	3:N:921:ARG:NH1	2.19	0.57
4:O:54:LEU:O	4:O:54:LEU:HD23	2.04	0.57
5:P:385:GLU:O	5:P:397:ILE:HD13	2.04	0.57
1:A:127:LEU:HD12	1:A:128:HIS:N	2.18	0.57
1:B:112:ARG:NH1	1:B:112:ARG:HB3	2.20	0.57
2:C:724:ARG:NE	2:C:737:LEU:O	2.38	0.57
3:D:1389:LEU:HD12	3:D:1390:LEU:H	1.68	0.57
3:D:1377:LYS:HE2	3:D:1394:VAL:HG22	1.87	0.57
3:D:30:GLU:HA	8:D:9510:HOH:O	2.05	0.57
3:D:56:TYR:CE2	3:D:66:GLN:HA	2.39	0.57
3:D:601:ARG:HD2	5:F:328:PHE:CE1	2.38	0.57
8:D:2049:HOH:O	5:F:168:LYS:HE3	2.03	0.57
1:L:143:ARG:HH11	1:L:158:ILE:CG2	2.17	0.57
2:M:10:ARG:HA	2:M:10:ARG:CZ	2.34	0.57
2:M:182:VAL:CG1	2:M:193:LEU:HD13	2.33	0.57
2:M:139:GLN:NE2	2:M:418:LEU:HD22	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:78:PHE:HB2	2:M:88:LEU:HD21	1.86	0.57
2:M:516:ARG:NE	3:N:1068:LEU:HD22	2.20	0.57
3:N:1128:VAL:HB	8:N:9347:HOH:O	2.05	0.57
3:N:477:LEU:HD21	3:N:495:ARG:HD3	1.86	0.57
3:N:843:PHE:CE1	3:N:864:VAL:HG11	2.39	0.57
1:A:101:LEU:HD21	1:A:113:ASP:HB3	1.85	0.57
2:C:300:ASP:HB2	8:C:1289:HOH:O	2.04	0.57
3:D:1220:ALA:HB1	3:D:1223:ILE:HD13	1.87	0.57
3:D:1266:ARG:O	3:D:1268:PRO:HD3	2.04	0.57
3:D:235:ALA:HB3	8:D:2026:HOH:O	2.04	0.57
3:D:397:LYS:HG3	8:D:9912:HOH:O	2.05	0.57
3:D:637:LEU:CD1	3:D:641:GLN:HB2	2.33	0.57
4:E:54:LEU:O	4:E:54:LEU:HD23	2.05	0.57
5:F:385:GLU:O	5:F:397:ILE:HD13	2.05	0.57
2:M:1006:HIS:O	3:N:648:MET:HE2	2.04	0.57
2:M:145:GLY:O	2:M:163:ILE:HG23	2.04	0.57
2:M:150:PRO:CA	2:M:158:TYR:HB3	2.31	0.57
2:M:252:LYS:NZ	2:M:296:GLY:HA3	2.20	0.57
2:M:820:ARG:HD3	2:M:821:GLU:HB3	1.86	0.57
3:N:1231:GLU:OE1	3:N:1232:PRO:HG3	2.04	0.57
3:N:380:GLU:O	3:N:382:GLU:N	2.37	0.57
2:M:1106:ASP:OD1	3:N:7:LYS:HD2	2.05	0.57
4:O:17:TYR:CD2	4:O:17:TYR:N	2.72	0.57
5:P:207:LEU:HB3	5:P:212:LEU:HG	1.87	0.57
1:A:137:ARG:H	1:A:137:ARG:HD2	1.68	0.57
1:B:196:THR:HG23	8:B:382:HOH:O	2.05	0.57
2:C:41:ASN:O	2:C:46:ALA:HB2	2.05	0.57
3:D:1491:THR:HG23	8:D:9315:HOH:O	2.03	0.57
3:D:519:VAL:HA	3:D:544:TYR:OH	2.05	0.57
2:C:882:LEU:HD22	3:D:951:ILE:HD13	1.85	0.57
5:F:260:ILE:HD11	5:F:310:ILE:HG22	1.86	0.57
1:K:68:ILE:HD13	1:K:138:LEU:HD11	1.86	0.57
1:K:198:ARG:HB2	1:K:200:TRP:CZ3	2.40	0.57
3:N:119:SER:N	3:N:123:LEU:HD22	2.18	0.57
3:N:1379:VAL:HA	3:N:1420:LEU:HB3	1.85	0.57
3:N:191:LEU:HB3	3:N:195:VAL:HG21	1.86	0.57
2:C:945:ARG:NH1	2:C:945:ARG:HB3	2.20	0.57
2:C:498:GLN:OE1	3:D:1067:VAL:HB	2.05	0.57
3:D:1364:HIS:CE1	3:D:1366:LYS:HG3	2.39	0.57
3:D:210:ARG:NH1	3:D:210:ARG:HB3	2.20	0.57
3:D:427:VAL:HB	3:D:435:VAL:HB	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:43:GLU:HG2	4:E:44:GLU:H	1.69	0.57
5:F:139:ALA:HB2	8:F:644:HOH:O	2.04	0.57
1:K:198:ARG:HB2	1:K:200:TRP:CH2	2.40	0.57
1:L:27:PRO:O	1:L:28:LEU:HD23	2.03	0.57
2:M:680:ASP:HB2	2:M:682:TYR:CD2	2.40	0.57
3:N:1406:ARG:HD2	3:N:1412:LYS:HD2	1.86	0.57
3:N:53:ILE:HG23	3:N:54:LYS:N	2.19	0.57
3:N:679:ARG:HD2	8:N:9182:HOH:O	2.03	0.57
3:N:899:LEU:HB3	3:N:921:ARG:HH12	1.70	0.57
3:N:988:ARG:HD2	3:N:989:TYR:N	2.20	0.57
1:B:228:PRO:O	1:B:229:GLN:HG3	2.05	0.56
2:C:352:ALA:HA	2:C:355:VAL:HG12	1.87	0.56
2:C:604:ALA:HB3	2:C:612:VAL:O	2.04	0.56
2:C:674:VAL:HG23	2:C:869:VAL:O	2.05	0.56
3:D:1147:ARG:HB3	3:D:1188:VAL:CG2	2.35	0.56
3:D:525:ARG:HB2	3:D:541:ASN:HD21	1.69	0.56
2:C:1042:ALA:CB	3:D:710:ARG:HB3	2.35	0.56
2:M:206:THR:HA	8:M:1787:HOH:O	2.05	0.56
2:M:26:TYR:HD2	2:M:121:MET:HB2	1.70	0.56
3:N:799:LYS:H	3:N:826:PRO:HG2	1.70	0.56
4:O:31:LEU:HD21	4:O:60:ALA:HB2	1.86	0.56
2:C:630:ARG:NH1	2:C:630:ARG:HG2	2.20	0.56
2:C:728:HIS:HB3	2:C:729:LEU:HD12	1.87	0.56
3:D:1198:TYR:OH	3:D:1432:LYS:HG2	2.05	0.56
3:D:133:ILE:HG23	3:D:456:MET:SD	2.46	0.56
3:D:952:ASP:HA	3:D:1062:ARG:HH21	1.70	0.56
1:L:14:ARG:HG2	8:L:3275:HOH:O	2.04	0.56
2:M:1040:LEU:HG	2:M:1045:ALA:CB	2.35	0.56
2:M:569:VAL:HG12	2:M:996:LYS:O	2.05	0.56
2:M:674:VAL:HG23	2:M:869:VAL:O	2.05	0.56
3:N:197:SER:CB	3:N:203:ALA:HB3	2.27	0.56
3:N:486:ARG:HB3	8:N:9366:HOH:O	2.05	0.56
5:P:350:LEU:HG	5:P:354:LEU:HD12	1.87	0.56
1:A:150:TYR:HE1	2:C:696:LYS:HA	1.71	0.56
3:D:1200:VAL:HG22	3:D:1373:ARG:NH1	2.20	0.56
3:D:44:LEU:HB3	3:D:525:ARG:NH2	2.21	0.56
3:D:996:TRP:HE3	3:D:999:THR:HG21	1.68	0.56
1:K:123:MET:O	1:K:125:PRO:HD3	2.05	0.56
2:M:460:ARG:HB3	2:M:460:ARG:NH1	2.20	0.56
4:O:48:MET:HG2	4:O:49:GLN:H	1.70	0.56
1:B:57:TYR:HB3	1:B:141:GLU:HG2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:231:PRO:HB3	8:C:1721:HOH:O	2.04	0.56
2:C:672:VAL:CG2	2:C:868:ASP:HB2	2.34	0.56
2:C:874:LEU:HD23	3:D:1023:MET:SD	2.45	0.56
2:C:97:ARG:HD2	8:C:1601:HOH:O	2.06	0.56
3:D:1324:PRO:HG3	3:D:1330:ILE:HD11	1.86	0.56
3:D:1379:VAL:HG12	3:D:1419:PRO:HA	1.87	0.56
3:D:386:HIS:HA	8:D:9065:HOH:O	2.04	0.56
3:N:835:SER:HA	8:N:9080:HOH:O	2.05	0.56
3:N:860:LEU:HD22	3:N:878:GLY:HA2	1.86	0.56
5:P:134:LYS:HG3	5:P:178:ARG:NH2	2.20	0.56
5:P:131:VAL:HG12	5:P:181:GLU:HG3	1.86	0.56
5:P:88:ILE:CD1	5:P:193:ARG:HB2	2.30	0.56
5:P:361:LEU:HD22	5:P:366:ALA:HB2	1.87	0.56
1:A:40:LEU:O	1:A:44:LEU:HD12	2.05	0.56
3:D:214:GLU:HB2	3:D:390:PRO:HD2	1.88	0.56
3:D:703:ASN:ND2	3:D:704:ARG:H	2.03	0.56
3:D:93:ILE:CD1	3:D:548:ILE:HD13	2.36	0.56
4:E:54:LEU:HG	4:E:58:PRO:HG2	1.88	0.56
1:K:102:LYS:HE2	1:K:139:ASN:CG	2.26	0.56
2:M:139:GLN:HE22	2:M:415:PRO:HG2	1.69	0.56
2:M:139:GLN:O	2:M:333:ILE:HA	2.05	0.56
2:M:580:MET:SD	2:M:584:GLU:HG3	2.46	0.56
3:N:1341:PRO:O	3:N:1344:VAL:HG23	2.04	0.56
3:N:42:ASP:O	3:N:46:ASP:HB2	2.06	0.56
3:N:633:VAL:HG22	3:N:635:PRO:CD	2.30	0.56
2:M:1042:ALA:HB3	3:N:710:ARG:HB3	1.87	0.56
3:N:953:ASP:HA	8:N:9114:HOH:O	2.05	0.56
1:A:62:LEU:HD12	8:A:375:HOH:O	2.04	0.56
2:C:736:ASP:HA	2:C:744:ARG:NH1	2.21	0.56
2:C:987:ILE:HG23	3:D:948:THR:CG2	2.36	0.56
3:D:1307:LYS:HD3	3:D:1307:LYS:H	1.71	0.56
3:D:422:ALA:H	3:D:427:VAL:CG1	2.18	0.56
3:D:639:LEU:HD22	3:D:766:ALA:HA	1.87	0.56
3:D:916:TYR:HE2	3:D:920:LEU:HD13	1.69	0.56
5:F:120:THR:HG22	5:F:122:LEU:HD13	1.87	0.56
1:K:20:TYR:CD2	1:K:21:GLY:N	2.74	0.56
2:M:479:VAL:CG2	2:M:503:LEU:HD11	2.35	0.56
3:N:1036:ARG:NH2	3:N:1042:ARG:HA	2.05	0.56
3:N:1038:LEU:O	3:N:1060:SER:HB2	2.05	0.56
3:N:1066:THR:HG22	3:N:1069:GLU:CG	2.33	0.56
3:N:1136:LYS:O	3:N:1139:ASP:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:459:GLU:HG3	3:N:460:ALA:N	2.20	0.56
3:N:695:ILE:HG21	3:N:720:LEU:HD11	1.88	0.56
3:N:628:ARG:HD3	3:N:744:GLN:NE2	2.17	0.56
4:O:21:VAL:O	4:O:25:LYS:HG3	2.06	0.56
5:P:358:LEU:CD2	5:P:370:LYS:HE3	2.34	0.56
2:C:129:ILE:HG12	2:C:386:PHE:O	2.05	0.56
2:C:173:ASP:O	2:C:184:MET:HA	2.06	0.56
2:C:979:THR:HG23	2:C:981:GLU:N	2.09	0.56
3:D:1003:VAL:O	3:D:1006:ALA:HB3	2.06	0.56
3:D:1376:MET:HE2	3:D:1421:LEU:HB2	1.86	0.56
5:F:226:LYS:HD2	5:F:242:TRP:CZ2	2.40	0.56
1:K:150:TYR:HE1	2:M:696:LYS:HA	1.70	0.56
1:K:44:LEU:O	1:K:174:VAL:HG21	2.06	0.56
1:K:8:ALA:HB1	1:L:224:TYR:CE1	2.41	0.56
2:M:208:ALA:HB1	2:M:218:VAL:HG13	1.87	0.56
2:M:26:TYR:O	2:M:30:LEU:HD12	2.06	0.56
2:M:630:ARG:HD3	2:M:705:ILE:HG13	1.87	0.56
2:M:798:GLY:H	2:M:827:VAL:HG11	1.70	0.56
2:M:948:GLU:HB3	8:M:1188:HOH:O	2.04	0.56
2:M:577:PRO:HG3	2:M:993:PHE:CE2	2.40	0.56
3:N:953:ASP:OD1	3:N:1019:PRO:HG2	2.06	0.56
3:N:1031:ASN:HB3	3:N:1034:GLN:NE2	2.21	0.56
3:N:116:LEU:HD23	3:N:468:LEU:HD11	1.87	0.56
2:M:1046:ALA:HB1	3:N:1471:LEU:HD11	1.87	0.56
3:N:706:PRO:HA	8:N:9170:HOH:O	2.06	0.56
3:N:84:ILE:HG12	8:N:9092:HOH:O	2.06	0.56
3:N:87:ARG:HD2	3:N:88:TYR:HE2	1.71	0.56
3:N:989:TYR:CZ	3:N:993:LEU:HD11	2.40	0.56
5:P:407:LYS:HB2	8:P:4644:HOH:O	2.05	0.56
3:D:1087:ARG:O	3:D:1091:SER:HB2	2.06	0.56
3:D:1478:SER:O	3:D:1482:ARG:HG3	2.06	0.56
3:D:423:ASP:HB2	5:F:178:ARG:HD2	1.87	0.56
3:D:475:LYS:HA	3:D:478:LEU:HG	1.87	0.56
3:D:829:VAL:HG21	8:D:9103:HOH:O	2.05	0.56
4:E:91:ARG:HB3	8:E:105:HOH:O	2.05	0.56
2:M:269:LEU:HG	2:M:288:ARG:N	2.19	0.56
2:M:63:GLY:CA	2:M:103:LYS:HE2	2.36	0.56
2:M:602:GLU:HA	2:M:647:GLN:O	2.06	0.56
3:N:1490:LYS:HB3	8:O:4026:HOH:O	2.05	0.56
3:N:423:ASP:OD2	5:P:174:LEU:HD22	2.05	0.56
3:N:434:ARG:HB2	3:N:447:VAL:HG13	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:176:VAL:C	2:C:178:PRO:HD3	2.25	0.56
2:C:189:ARG:HB3	8:C:1497:HOH:O	2.06	0.56
2:C:633:GLN:NE2	2:C:633:GLN:H	2.04	0.56
2:C:724:ARG:HG3	2:C:741:GLY:N	2.14	0.56
2:C:918:LEU:HB3	2:C:968:LEU:HD23	1.88	0.56
3:D:1217:ILE:HD13	3:D:1480:PHE:CE2	2.41	0.56
3:D:214:GLU:CD	3:D:390:PRO:HB2	2.26	0.56
3:D:607:LEU:HB3	3:D:614:PHE:HE2	1.70	0.56
2:M:1015:LEU:HA	5:P:335:ASP:HB3	1.88	0.56
2:M:21:ILE:HD12	2:M:21:ILE:H	1.70	0.56
2:M:49:ARG:HH11	2:M:49:ARG:HB2	1.71	0.56
3:N:1404:ASN:ND2	3:N:1408:ILE:HD12	2.21	0.56
3:N:552:ASN:HA	3:N:555:LYS:HD2	1.87	0.56
3:N:928:ALA:O	3:N:931:LEU:HB2	2.06	0.56
4:O:33:HIS:HB2	4:O:37:ASN:ND2	2.20	0.56
4:O:73:LEU:HD23	8:O:4394:HOH:O	2.06	0.56
1:B:2:LEU:HD12	1:B:3:ASP:N	2.21	0.56
1:B:86:VAL:HG12	1:B:124:ASN:ND2	2.19	0.56
2:C:1042:ALA:HB3	3:D:710:ARG:HB3	1.88	0.56
2:C:289:THR:HG22	2:C:290:LEU:HD22	1.86	0.56
2:C:352:ALA:O	2:C:356:ARG:HG3	2.05	0.56
2:C:987:ILE:HD11	3:D:946:GLY:HA3	1.86	0.56
3:D:153:LEU:HD13	3:D:157:GLU:HB2	1.87	0.56
5:F:166:LEU:HD13	5:F:170:HIS:HB2	1.88	0.56
1:L:41:ARG:CZ	1:L:177:VAL:HG23	2.36	0.56
3:N:1087:ARG:NE	3:N:1238:MET:HB2	2.21	0.56
3:N:1478:SER:OG	3:N:1480:PHE:HB3	2.05	0.56
3:N:493:ARG:O	3:N:497:GLU:HG3	2.06	0.56
3:N:560:GLN:HE21	5:P:218:GLN:NE2	2.04	0.56
5:P:135:ILE:O	5:P:135:ILE:HD13	2.06	0.56
5:P:144:ILE:HA	8:P:4865:HOH:O	2.05	0.56
5:P:401:GLU:O	5:P:405:LEU:HB2	2.05	0.56
5:P:82:ARG:HG2	5:P:86:HIS:NE2	2.21	0.56
2:C:212:GLY:HA3	2:C:218:VAL:HG23	1.88	0.56
2:C:281:LEU:CD1	2:C:306:THR:HA	2.28	0.56
2:C:39:ARG:HE	2:C:39:ARG:HA	1.71	0.56
2:C:445:GLU:HB2	8:C:1296:HOH:O	2.06	0.56
2:C:724:ARG:CG	2:C:740:GLU:HA	2.36	0.56
3:D:654:LYS:HB3	3:D:655:PRO:CD	2.32	0.56
3:D:969:ARG:O	3:D:972:LEU:HB3	2.06	0.56
5:F:328:PHE:HB3	8:F:674:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:417:LYS:HG3	8:F:684:HOH:O	2.06	0.56
1:L:143:ARG:HH11	1:L:158:ILE:HG23	1.70	0.56
2:M:1067:TYR:CE1	2:M:1071:ILE:HD11	2.40	0.56
2:M:404:LEU:O	2:M:407:LYS:HB2	2.06	0.56
2:M:493:ARG:HD2	8:M:1824:HOH:O	2.06	0.56
3:N:1310:ARG:HG3	3:N:1327:ARG:HB2	1.86	0.56
3:N:28:LYS:HB2	3:N:41:ARG:HD2	1.87	0.56
3:N:82:LYS:HE2	8:N:9124:HOH:O	2.05	0.56
3:N:875:THR:HG23	3:N:879:ARG:HE	1.71	0.56
5:P:153:PRO:HG2	5:P:154:LYS:H	1.71	0.56
1:A:178:ALA:HB2	2:C:864:GLY:H	1.69	0.55
2:C:290:LEU:HB3	2:C:302:VAL:HG11	1.88	0.55
2:C:313:LEU:CA	2:C:321:GLU:HG3	2.33	0.55
3:D:434:ARG:HB2	3:D:447:VAL:CG1	2.35	0.55
3:D:116:LEU:HD23	3:D:468:LEU:HD11	1.88	0.55
3:D:728:LEU:HD22	3:D:745:MET:SD	2.46	0.55
4:E:54:LEU:HG	4:E:58:PRO:CG	2.36	0.55
1:K:101:LEU:HD21	1:K:113:ASP:HB3	1.87	0.55
1:K:224:TYR:CD2	1:L:9:PRO:HG2	2.41	0.55
2:M:773:LEU:HG	2:M:777:ILE:HD11	1.88	0.55
2:M:5:ARG:HB3	2:M:902:ILE:HB	1.88	0.55
3:N:1047:LYS:HB3	3:N:1048:PRO:CD	2.36	0.55
3:N:1262:LEU:HD11	3:N:1351:GLU:HG2	1.88	0.55
3:N:245:LEU:HA	8:N:9639:HOH:O	2.06	0.55
3:N:530:VAL:HG23	3:N:534:ARG:O	2.06	0.55
3:N:894:LYS:HG3	8:N:9120:HOH:O	2.06	0.55
5:P:201:LYS:HG2	8:P:3872:HOH:O	2.04	0.55
5:P:264:MET:O	5:P:268:ILE:HG13	2.06	0.55
1:B:150:TYR:CE2	3:D:857:ILE:HG13	2.40	0.55
2:C:902:ILE:O	2:C:904:PRO:HD3	2.06	0.55
2:C:956:GLY:HA2	8:C:1408:HOH:O	2.05	0.55
3:D:1290:LEU:HD22	3:D:1291:SER:H	1.71	0.55
3:D:29:PRO:HG3	3:D:549:ASN:HD21	1.71	0.55
2:C:1029:GLY:O	3:D:622:ARG:HD3	2.07	0.55
5:F:132:ARG:O	5:F:136:LEU:HG	2.06	0.55
2:M:410:ILE:HD11	2:M:455:LEU:HB3	1.88	0.55
2:M:575:GLN:OE1	2:M:670:GLN:HB3	2.06	0.55
2:M:5:ARG:HG3	8:M:1295:HOH:O	2.05	0.55
3:N:1102:THR:HG22	3:N:1222:GLY:HA2	1.87	0.55
3:N:183:GLU:HA	3:N:186:VAL:HG12	1.87	0.55
3:N:80:VAL:HG12	3:N:81:THR:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:112:ILE:HG13	3:D:124:GLU:OE2	2.06	0.55
3:D:604:THR:HA	3:D:607:LEU:HD12	1.88	0.55
3:D:890:VAL:HA	8:D:9150:HOH:O	2.06	0.55
3:D:980:MET:HG3	8:D:9110:HOH:O	2.06	0.55
1:K:37:GLY:HA3	1:K:179:PHE:CD1	2.41	0.55
1:L:18:ARG:HG3	8:L:3742:HOH:O	2.06	0.55
2:M:549:PHE:CE2	2:M:886:LEU:HB3	2.41	0.55
2:M:97:ARG:HG3	8:M:1631:HOH:O	2.06	0.55
3:N:1020:LEU:HA	3:N:1023:MET:HE2	1.89	0.55
3:N:1042:ARG:O	3:N:1057:VAL:HB	2.05	0.55
3:N:1428:ALA:O	3:N:1431:THR:HG23	2.05	0.55
3:N:488:ARG:HH22	3:N:491:LYS:NZ	2.04	0.55
3:N:659:LYS:HE3	3:N:663:GLU:CD	2.27	0.55
3:N:834:THR:HG22	3:N:838:ARG:HD2	1.86	0.55
5:P:351:SER:HA	8:P:3059:HOH:O	2.06	0.55
5:P:355:GLU:HA	8:P:2808:HOH:O	2.06	0.55
1:B:184:THR:O	1:B:192:LEU:HB2	2.07	0.55
1:A:222:LEU:HD12	1:B:215:VAL:CB	2.37	0.55
2:C:1033:GLY:HA3	8:C:1885:HOH:O	2.07	0.55
2:C:197:LEU:HB3	2:C:202:TYR:HB2	1.88	0.55
2:C:802:ARG:HD2	8:C:1186:HOH:O	2.06	0.55
3:D:211:VAL:HG11	8:D:9373:HOH:O	2.06	0.55
3:D:584:ASN:OD1	3:D:590:PRO:HD2	2.06	0.55
5:F:398:ARG:HG2	5:F:402:ASN:HD22	1.72	0.55
1:K:104:GLU:HG2	1:K:105:GLY:N	2.21	0.55
1:K:38:ASN:HB3	1:K:39:PRO:HD3	1.87	0.55
1:L:206:THR:CG2	1:L:209:GLU:H	2.18	0.55
2:M:140:ILE:HD11	2:M:412:ALA:HA	1.88	0.55
2:M:583:LEU:O	2:M:587:VAL:HG23	2.06	0.55
2:M:979:THR:HG23	2:M:981:GLU:HB2	1.88	0.55
3:N:1109:GLU:OE1	3:N:1201:CYS:HB2	2.06	0.55
3:N:1462:LEU:HD22	3:N:1472:ILE:CG2	2.36	0.55
3:N:414:ARG:HG2	8:N:9890:HOH:O	2.06	0.55
5:P:218:GLN:NE2	5:P:221:ILE:HD12	2.21	0.55
5:P:264:MET:O	5:P:267:THR:HB	2.07	0.55
5:P:327:SER:HG	5:P:332:PHE:HZ	1.54	0.55
5:P:403:LYS:HD3	8:P:4835:HOH:O	2.07	0.55
1:B:148:VAL:HA	8:B:322:HOH:O	2.05	0.55
1:A:219:ARG:NH2	1:B:223:THR:HG23	2.22	0.55
1:B:27:PRO:HD2	8:B:363:HOH:O	2.06	0.55
2:C:113:VAL:HG21	2:C:373:VAL:HG21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:666:LEU:CD2	2:C:668:LEU:HD11	2.36	0.55
3:D:1109:GLU:CD	3:D:1202:GLN:H	2.09	0.55
3:D:183:GLU:HA	3:D:186:VAL:HG12	1.88	0.55
3:D:210:ARG:HG3	3:D:398:ALA:H	1.72	0.55
3:D:29:PRO:HG3	3:D:549:ASN:ND2	2.21	0.55
3:D:592:THR:N	3:D:600:LEU:HD21	2.22	0.55
4:E:4:PRO:HB3	8:E:138:HOH:O	2.07	0.55
1:K:150:TYR:CE2	1:K:152:PRO:HG3	2.38	0.55
2:M:114:PHE:H	2:M:114:PHE:HD1	1.52	0.55
2:M:207:LEU:HD22	2:M:221:LEU:HD13	1.86	0.55
2:M:140:ILE:CG2	2:M:333:ILE:HG13	2.35	0.55
2:M:585:GLU:HG2	2:M:665:PHE:HD2	1.70	0.55
2:M:697:ARG:HG3	2:M:699:PHE:CD1	2.41	0.55
3:N:1200:VAL:HG22	3:N:1373:ARG:NH1	2.22	0.55
1:A:180:GLN:HB3	8:A:328:HOH:O	2.06	0.55
2:C:203:ASP:HB3	8:C:1639:HOH:O	2.05	0.55
2:C:478:VAL:HG11	8:C:1719:HOH:O	2.06	0.55
2:C:51:THR:HG22	8:C:1597:HOH:O	2.06	0.55
2:C:534:VAL:H	2:C:538:GLN:NE2	2.02	0.55
2:C:64:LEU:HD11	8:C:1196:HOH:O	2.05	0.55
2:C:595:LEU:O	2:C:655:LEU:HG	2.07	0.55
2:C:716:LYS:HG2	8:C:1417:HOH:O	2.06	0.55
2:C:918:LEU:HD23	2:C:967:PHE:O	2.07	0.55
2:C:976:ASP:HB2	2:C:979:THR:HG22	1.89	0.55
3:D:108:VAL:HB	3:D:109:PRO:HD3	1.88	0.55
3:D:1278:ASP:HA	3:D:1319:VAL:O	2.05	0.55
4:E:37:ASN:HD22	4:E:89:MET:HE3	1.72	0.55
5:F:370:LYS:HZ3	5:F:371:LEU:HG	1.71	0.55
1:K:9:PRO:HD2	1:L:224:TYR:CE1	2.41	0.55
2:M:397:GLU:HG3	2:M:633:GLN:NE2	2.22	0.55
2:M:517:ARG:HB2	8:M:1758:HOH:O	2.07	0.55
2:M:601:GLY:O	2:M:648:ARG:HA	2.06	0.55
2:M:770:GLU:HA	8:M:1825:HOH:O	2.06	0.55
3:N:1047:LYS:HE2	8:N:9823:HOH:O	2.06	0.55
3:N:1278:ASP:HB2	3:N:1318:TYR:OH	2.07	0.55
3:N:1290:LEU:HD11	3:N:1311:LEU:HD22	1.89	0.55
3:N:1357:ARG:HD3	8:N:9210:HOH:O	2.06	0.55
1:A:219:ARG:NH1	1:B:223:THR:HG23	2.22	0.55
1:B:110:LYS:HZ3	1:B:112:ARG:HD2	1.70	0.55
2:C:732:ALA:HB2	8:C:1371:HOH:O	2.07	0.55
3:D:134:VAL:HG12	3:D:152:LEU:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1397:LYS:O	3:D:1400:VAL:HB	2.07	0.55
3:D:551:ASN:O	3:D:555:LYS:HG3	2.06	0.55
3:D:695:ILE:HG21	3:D:720:LEU:HD11	1.88	0.55
3:D:704:ARG:HG2	3:D:736:PHE:HB3	1.89	0.55
3:D:842:VAL:HG12	8:D:9557:HOH:O	2.07	0.55
3:D:899:LEU:HD12	3:D:900:ILE:HG23	1.89	0.55
2:M:196:LEU:HB2	8:M:1510:HOH:O	2.05	0.55
2:M:520:GLU:HB2	8:M:1758:HOH:O	2.07	0.55
2:M:585:GLU:HG2	2:M:665:PHE:CD2	2.42	0.55
2:M:878:SER:HB3	3:N:1029:ARG:HD3	1.89	0.55
3:N:1097:LYS:HA	8:N:9081:HOH:O	2.05	0.55
3:N:402:PRO:HG2	3:N:444:VAL:HG11	1.87	0.55
4:O:33:HIS:HB3	8:O:3948:HOH:O	2.06	0.55
4:O:43:GLU:H	4:O:43:GLU:CD	2.10	0.55
5:P:218:GLN:HA	5:P:221:ILE:CD1	2.37	0.55
2:C:160:ALA:O	2:C:173:ASP:HA	2.07	0.55
2:C:195:LEU:HD23	2:C:238:LEU:HG	1.89	0.55
2:C:251:ASP:HB3	2:C:252:LYS:HD2	1.89	0.55
3:D:809:PRO:HB2	3:D:812:ALA:HB2	1.88	0.55
5:F:222:ARG:HA	8:F:496:HOH:O	2.07	0.55
5:F:82:ARG:HA	8:F:574:HOH:O	2.06	0.55
2:M:643:VAL:HG13	2:M:647:GLN:CD	2.27	0.55
2:M:722:ILE:HG21	2:M:821:GLU:OE2	2.07	0.55
3:N:1220:ALA:O	3:N:1224:VAL:HG23	2.07	0.55
3:N:178:LEU:HG	3:N:200:ASP:H	1.71	0.55
3:N:131:LYS:CG	3:N:568:ARG:HG2	2.31	0.55
3:N:838:ARG:HH11	3:N:874:GLU:HG2	1.71	0.55
4:O:69:LEU:HB3	8:O:3383:HOH:O	2.05	0.55
1:A:218:LEU:O	1:A:222:LEU:HD23	2.06	0.55
2:C:436:GLY:HA3	2:C:469:THR:OG1	2.06	0.55
3:D:10:ILE:HG13	3:D:1434:TRP:CZ2	2.42	0.55
3:D:631:ILE:HG21	3:D:745:MET:HG3	1.89	0.55
3:D:722:GLU:HB3	8:D:9352:HOH:O	2.07	0.55
3:D:764:LEU:HD12	3:D:765:SER:N	2.22	0.55
4:E:47:LYS:HA	4:E:54:LEU:HB3	1.88	0.55
2:M:132:ALA:HB1	2:M:632:ASN:HD21	1.71	0.55
2:M:209:ARG:O	2:M:213:ALA:HB2	2.07	0.55
2:M:244:PRO:HD3	8:M:1549:HOH:O	2.06	0.55
2:M:51:THR:OG1	2:M:348:LEU:HD23	2.07	0.55
2:M:902:ILE:O	2:M:904:PRO:HD3	2.07	0.55
3:N:154:THR:HA	8:N:9161:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:181:ASP:OD2	3:N:199:LEU:HB2	2.07	0.55
3:N:795:VAL:HG11	3:N:863:VAL:HG13	1.88	0.55
1:B:60:ASP:HB2	8:B:383:HOH:O	2.07	0.55
2:C:139:GLN:HB3	2:C:334:ARG:HD2	1.89	0.55
2:C:290:LEU:HD12	8:C:1289:HOH:O	2.06	0.55
2:C:355:VAL:CG2	2:C:372:LEU:HG	2.37	0.55
2:C:52:PHE:O	2:C:54:ILE:HG13	2.05	0.55
3:D:460:ALA:O	3:D:464:LEU:HG	2.07	0.55
3:D:644:LEU:HD12	3:D:645:PRO:HD2	1.89	0.55
5:F:369:LEU:HD11	5:F:401:GLU:HB2	1.88	0.55
1:L:180:GLN:CB	1:L:198:ARG:HH22	2.16	0.55
2:M:1115:LEU:HB3	3:N:85:VAL:HG13	1.88	0.55
2:M:49:ARG:HB3	2:M:266:ARG:HH12	1.71	0.55
3:N:1278:ASP:HA	3:N:1319:VAL:O	2.07	0.55
3:N:1346:ARG:CZ	3:N:1346:ARG:HA	2.37	0.55
3:N:421:LEU:HD12	3:N:435:VAL:CG1	2.37	0.55
3:N:573:MET:SD	5:P:210:LEU:HD13	2.47	0.55
3:N:933:ALA:O	3:N:937:TYR:HD1	1.90	0.55
5:P:268:ILE:HA	5:P:271:LEU:HD12	1.89	0.55
1:A:176:ARG:O	1:A:200:TRP:HE3	1.90	0.54
2:C:1115:LEU:HD12	2:C:1115:LEU:N	2.22	0.54
3:D:1066:THR:HG22	3:D:1069:GLU:HB2	1.88	0.54
3:D:1376:MET:CE	3:D:1421:LEU:HB2	2.36	0.54
3:D:192:ALA:O	3:D:195:VAL:HG23	2.07	0.54
3:D:49:ILE:HB	3:D:50:PHE:CD1	2.41	0.54
3:D:565:ILE:HD11	5:F:189:GLU:OE1	2.07	0.54
3:D:790:TYR:CD2	3:D:1026:SER:HB3	2.42	0.54
8:C:1147:HOH:O	3:D:943:THR:HG21	2.07	0.54
4:E:33:HIS:HB2	4:E:37:ASN:ND2	2.22	0.54
3:D:553:ARG:HD3	5:F:214:GLN:HB3	1.89	0.54
1:L:102:LYS:HG3	1:L:139:ASN:HB2	1.89	0.54
2:M:496:ILE:HD12	2:M:496:ILE:H	1.72	0.54
3:N:1369:GLU:O	3:N:1372:VAL:HG12	2.07	0.54
5:P:323:ASP:HB2	8:P:2932:HOH:O	2.07	0.54
2:C:1014:SER:HB3	2:C:1017:THR:O	2.07	0.54
3:D:126:VAL:O	3:D:132:TYR:HD1	1.91	0.54
3:D:213:VAL:HG22	3:D:214:GLU:H	1.71	0.54
3:D:36:THR:C	3:D:38:LYS:H	2.11	0.54
3:D:842:VAL:HG12	8:D:9009:HOH:O	2.07	0.54
4:E:40:LEU:HD22	8:E:184:HOH:O	2.05	0.54
5:F:218:GLN:NE2	5:F:221:ILE:HD12	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:101:LEU:HG	1:K:114:PHE:HA	1.88	0.54
1:K:58:ILE:HG21	1:K:68:ILE:HD11	1.87	0.54
1:K:91:ASN:H	1:K:94:LEU:HD12	1.73	0.54
2:M:1015:LEU:HB3	2:M:1016:ILE:HD13	1.90	0.54
2:M:1049:LEU:HG	2:M:1053:LEU:HD12	1.88	0.54
2:M:160:ALA:O	2:M:173:ASP:HA	2.08	0.54
2:M:254:VAL:O	2:M:257:VAL:HG23	2.08	0.54
2:M:431:HIS:H	2:M:434:HIS:CE1	2.25	0.54
2:M:54:ILE:HG23	2:M:54:ILE:O	2.07	0.54
3:N:637:LEU:HD11	3:N:642:CYS:N	2.22	0.54
3:N:73:CYS:HB3	3:N:76:CYS:O	2.07	0.54
3:N:863:VAL:HG21	8:N:9257:HOH:O	2.06	0.54
3:N:970:LYS:HB2	3:N:970:LYS:NZ	2.22	0.54
5:P:162:LYS:HA	8:P:1319:HOH:O	2.06	0.54
3:N:419:ASP:OD2	5:P:171:LYS:HE3	2.08	0.54
1:A:53:VAL:HG21	1:A:82:LEU:HD22	1.88	0.54
1:B:159:LYS:N	1:B:159:LYS:HD3	2.23	0.54
1:B:78:ILE:HA	8:B:366:HOH:O	2.05	0.54
2:C:196:LEU:HD11	2:C:303:PHE:CE1	2.43	0.54
2:C:486:MET:SD	2:C:491:GLU:HA	2.48	0.54
3:D:1406:ARG:HE	3:D:1406:ARG:C	2.11	0.54
3:D:1404:ASN:ND2	3:D:1408:ILE:HD12	2.22	0.54
3:D:462:GLN:HG2	8:D:9662:HOH:O	2.07	0.54
3:D:794:GLN:HG2	3:D:905:PRO:HB3	1.90	0.54
3:D:787:LEU:HD21	3:D:947:ILE:HD13	1.88	0.54
3:D:974:ILE:HG22	8:D:9303:HOH:O	2.06	0.54
1:L:108:GLU:HB3	8:L:3562:HOH:O	2.07	0.54
2:M:1082:PRO:HA	8:M:1607:HOH:O	2.06	0.54
2:M:688:ILE:HD11	2:M:847:GLY:HA3	1.89	0.54
2:M:9:ILE:HG12	2:M:907:ASP:OD2	2.07	0.54
3:N:28:LYS:HG3	3:N:29:PRO:HD2	1.90	0.54
3:N:36:THR:C	3:N:38:LYS:H	2.10	0.54
3:N:614:PHE:O	3:N:617:ASN:HB2	2.07	0.54
3:N:56:TYR:HE2	3:N:69:GLU:HB3	1.72	0.54
3:N:68:PHE:O	3:N:71:LYS:HG2	2.08	0.54
3:N:809:PRO:HB2	3:N:812:ALA:HB2	1.89	0.54
3:N:838:ARG:NH1	3:N:874:GLU:HG2	2.22	0.54
5:P:161:GLN:HA	5:P:164:LYS:NZ	2.22	0.54
2:C:196:LEU:HD21	2:C:303:PHE:CD1	2.41	0.54
2:C:724:ARG:HB2	2:C:740:GLU:HG3	1.89	0.54
3:D:957:PRO:HG2	3:D:1007:VAL:HG12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1068:LEU:HD23	3:D:1072:ILE:HG12	1.89	0.54
3:D:529:GLN:OE1	3:D:533:GLY:HA2	2.08	0.54
3:D:584:ASN:HB2	3:D:602:SER:HB3	1.90	0.54
3:D:615:ARG:HD3	3:D:616:GLN:N	2.22	0.54
5:F:108:GLU:HG3	5:F:176:ILE:CG2	2.38	0.54
5:F:369:LEU:HD23	8:F:443:HOH:O	2.07	0.54
1:K:133:GLU:HG2	1:K:134:GLU:H	1.71	0.54
1:K:209:GLU:C	1:K:213:GLN:HE21	2.10	0.54
2:M:1034:GLU:HA	2:M:1037:VAL:HG23	1.89	0.54
2:M:710:ILE:CD1	2:M:790:LEU:HB2	2.37	0.54
2:M:838:LYS:HB3	2:M:848:VAL:HG22	1.88	0.54
3:N:1110:ALA:HB2	8:N:9805:HOH:O	2.07	0.54
3:N:1380:GLU:HG3	3:N:1381:VAL:N	2.23	0.54
3:N:629:SER:C	3:N:744:GLN:HG2	2.28	0.54
3:N:804:LEU:HB2	3:N:830:ALA:O	2.06	0.54
1:A:47:SER:HG	1:B:32:PHE:HZ	1.56	0.54
2:C:1012:PRO:HD2	2:C:1021:LEU:O	2.07	0.54
2:C:146:VAL:HG22	2:C:162:ILE:HG23	1.90	0.54
2:C:732:ALA:HA	2:C:735:ARG:CZ	2.37	0.54
2:C:89:THR:HA	2:C:129:ILE:O	2.08	0.54
2:C:945:ARG:HD3	2:C:949:LYS:NZ	2.23	0.54
3:D:116:LEU:CD2	3:D:468:LEU:HD11	2.38	0.54
3:D:1333:HIS:CE1	3:D:1421:LEU:HD23	2.43	0.54
3:D:1367:HIS:O	3:D:1371:VAL:HG23	2.07	0.54
3:D:628:ARG:HD3	3:D:744:GLN:HE21	1.71	0.54
3:D:795:VAL:HG23	3:D:879:ARG:HH12	1.73	0.54
3:D:868:TYR:CG	3:D:869:MET:N	2.75	0.54
3:D:754:PHE:HZ	4:E:21:VAL:HG13	1.72	0.54
3:D:553:ARG:HH22	5:F:211:ASP:CG	2.11	0.54
1:L:186:LEU:O	1:L:186:LEU:HD23	2.07	0.54
1:L:81:ASN:O	1:L:84:GLU:HB3	2.07	0.54
2:M:227:PHE:HA	2:M:230:ARG:HE	1.71	0.54
3:N:1290:LEU:HD23	3:N:1291:SER:N	2.17	0.54
3:N:167:GLU:HG3	8:N:9466:HOH:O	2.06	0.54
3:N:601:ARG:NH2	3:N:606:ILE:HA	2.23	0.54
2:C:749:VAL:HG11	2:C:755:LEU:HD23	1.88	0.54
2:C:820:ARG:HG2	8:C:1605:HOH:O	2.08	0.54
3:D:1232:PRO:HB3	3:D:1361:VAL:HG21	1.90	0.54
3:D:1468:LEU:HD22	3:D:1470:ARG:CB	2.38	0.54
5:F:245:GLN:HA	8:F:572:HOH:O	2.06	0.54
1:K:20:TYR:HD2	1:K:21:GLY:N	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:185:LYS:HB3	2:M:188:LYS:O	2.07	0.54
2:M:358:ARG:HB3	2:M:371:LYS:O	2.08	0.54
2:M:408:ARG:NH1	2:M:542:VAL:HG23	2.23	0.54
2:M:424:GLY:O	2:M:427:VAL:HG23	2.08	0.54
2:M:455:LEU:HD12	2:M:459:ALA:HB3	1.89	0.54
2:M:607:ASP:HB3	2:M:609:ASN:H	1.72	0.54
3:N:1104:GLU:HA	3:N:1461:GLY:HA2	1.89	0.54
3:N:702:LEU:HD13	3:N:716:PHE:CD1	2.43	0.54
5:P:167:PRO:HB2	5:P:169:GLU:OE2	2.08	0.54
1:A:90:LEU:HD12	1:A:119:ASP:O	2.07	0.54
2:C:194:VAL:HG23	8:C:1179:HOH:O	2.06	0.54
2:C:242:LEU:HD23	8:C:1853:HOH:O	2.08	0.54
2:C:333:ILE:CD1	2:C:467:ILE:HG13	2.37	0.54
2:C:341:THR:CG2	2:C:345:ARG:HH21	2.20	0.54
2:C:631:SER:HB3	2:C:637:LEU:HD21	1.89	0.54
3:D:1047:LYS:HG2	3:D:1053:PHE:CE2	2.42	0.54
2:C:555:ALA:HA	3:D:1070:TYR:OH	2.06	0.54
3:D:1314:LYS:HB2	8:D:9676:HOH:O	2.06	0.54
3:D:1465:ASN:HD21	3:D:1470:ARG:HD3	1.73	0.54
3:D:154:THR:HG22	3:D:157:GLU:CD	2.28	0.54
3:D:948:THR:O	3:D:949:ILE:HD13	2.08	0.54
2:C:886:LEU:CD2	3:D:951:ILE:HG13	2.38	0.54
1:K:30:ARG:HD3	8:K:3174:HOH:O	2.07	0.54
1:K:43:ILE:HD12	1:L:32:PHE:CZ	2.43	0.54
2:M:202:TYR:HA	8:M:1314:HOH:O	2.07	0.54
2:M:204:GLN:HG3	8:M:1527:HOH:O	2.08	0.54
2:M:210:GLU:HB3	8:M:1386:HOH:O	2.07	0.54
2:M:672:VAL:CG2	2:M:868:ASP:HB2	2.37	0.54
3:N:1277:ILE:HA	8:N:9618:HOH:O	2.07	0.54
3:N:211:VAL:HG13	3:N:393:ILE:HA	1.90	0.54
3:N:523:ASP:O	3:N:526:PRO:HG3	2.08	0.54
3:N:828:LYS:HB3	8:N:9129:HOH:O	2.08	0.54
3:N:860:LEU:HA	3:N:877:PRO:HB2	1.89	0.54
1:A:212:ASN:O	1:A:215:VAL:HG22	2.07	0.54
2:C:535:SER:H	2:C:538:GLN:NE2	2.06	0.54
2:C:580:MET:HB3	2:C:584:GLU:OE2	2.08	0.54
2:C:83:CYS:HA	2:C:88:LEU:HD23	1.90	0.54
2:C:73:LEU:HB3	2:C:94:LEU:HB2	1.90	0.54
3:D:1205:TYR:CD2	3:D:1215:VAL:HG21	2.42	0.54
3:D:135:LEU:CD1	3:D:147:VAL:HG23	2.38	0.54
3:D:530:VAL:HG12	3:D:531:ASP:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:929:ARG:HH11	3:D:929:ARG:HG3	1.73	0.54
8:C:1147:HOH:O	3:D:940:THR:HA	2.07	0.54
4:E:9:LEU:HD22	4:E:19:LEU:HD11	1.90	0.54
1:K:218:LEU:O	1:K:222:LEU:HD23	2.07	0.54
1:L:67:THR:HA	8:L:3261:HOH:O	2.07	0.54
2:M:1013:TYR:HD1	2:M:1020:PRO:HA	1.73	0.54
2:M:103:LYS:HD2	8:M:1331:HOH:O	2.06	0.54
2:M:1090:LYS:HE2	2:M:1112:PHE:CE1	2.43	0.54
2:M:328:LEU:CD2	2:M:437:ARG:HD3	2.37	0.54
2:M:42:VAL:HG12	2:M:43:GLY:H	1.72	0.54
2:M:630:ARG:HH21	2:M:707:ARG:H	1.54	0.54
2:M:397:GLU:OE2	2:M:632:ASN:HB2	2.08	0.54
3:N:1280:VAL:O	3:N:1294:VAL:HA	2.08	0.54
3:N:478:LEU:HD21	3:N:500:ARG:NH2	2.22	0.54
3:N:584:ASN:CG	3:N:590:PRO:HD2	2.28	0.54
2:M:1109:VAL:HG11	3:N:5:VAL:HG22	1.90	0.54
3:N:834:THR:CG2	3:N:838:ARG:HD2	2.38	0.54
2:C:214:TYR:HB3	8:C:1697:HOH:O	2.08	0.54
2:C:691:SER:HB3	2:C:868:ASP:O	2.07	0.54
2:C:715:THR:HG22	2:C:717:LEU:HG	1.89	0.54
2:C:722:ILE:HG22	8:C:1846:HOH:O	2.06	0.54
2:C:3:ILE:HD13	2:C:900:ARG:O	2.07	0.54
3:D:1102:THR:HG22	3:D:1222:GLY:HA2	1.90	0.54
3:D:1114:THR:O	3:D:1114:THR:HG23	2.08	0.54
3:D:1382:THR:HG21	3:D:1418:LYS:NZ	2.23	0.54
3:D:379:ALA:HB3	8:D:9652:HOH:O	2.08	0.54
3:D:503:LEU:HA	3:D:508:ARG:HH22	1.73	0.54
5:F:99:GLU:HB2	8:F:540:HOH:O	2.08	0.54
2:M:37:GLU:HG2	8:M:1585:HOH:O	2.08	0.54
3:N:1156:LEU:CD1	3:N:1176:LYS:HD2	2.38	0.54
3:N:1382:THR:HG22	8:N:9076:HOH:O	2.08	0.54
3:N:1425:THR:HG23	3:N:1426:LYS:N	2.23	0.54
3:N:217:LYS:HA	8:N:9812:HOH:O	2.08	0.54
3:N:852:ALA:O	3:N:857:ILE:HG12	2.08	0.54
3:N:864:VAL:HA	8:N:9349:HOH:O	2.07	0.54
3:N:892:ASP:HB3	3:N:895:VAL:CG2	2.38	0.54
1:A:128:HIS:CE1	1:A:131:THR:HG23	2.43	0.54
1:B:65:PHE:CD1	3:D:813:LEU:HD22	2.43	0.54
3:D:1271:LYS:HG2	8:D:9063:HOH:O	2.07	0.54
3:D:391:ALA:HB3	8:D:9451:HOH:O	2.08	0.54
3:D:28:LYS:HB2	3:D:41:ARG:HD2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:860:LEU:HD23	3:D:877:PRO:HB2	1.91	0.54
2:C:1090:LYS:HE3	3:D:88:TYR:O	2.08	0.54
3:D:992:ILE:O	3:D:995:LEU:HB3	2.08	0.54
4:E:63:TRP:O	4:E:67:GLU:HG3	2.08	0.54
3:D:767:HIS:CD2	4:E:6:ILE:HG12	2.43	0.54
1:K:159:LYS:HE2	8:K:3739:HOH:O	2.07	0.54
1:K:19:GLU:HB3	1:K:175:ARG:NH2	2.15	0.54
2:M:1012:PRO:HD2	2:M:1021:LEU:O	2.08	0.54
2:M:1067:TYR:O	2:M:1071:ILE:HG12	2.08	0.54
2:M:158:TYR:CD1	2:M:313:LEU:HD21	2.42	0.54
2:M:176:VAL:C	2:M:178:PRO:HD3	2.28	0.54
2:M:290:LEU:HB3	2:M:302:VAL:HG11	1.89	0.54
2:M:578:VAL:HG13	2:M:671:ASN:OD1	2.08	0.54
3:N:1066:THR:CG2	3:N:1069:GLU:HG3	2.36	0.54
3:N:1220:ALA:HB1	3:N:1223:ILE:CD1	2.37	0.54
3:N:1321:ALA:HB3	3:N:1339:LYS:HE2	1.90	0.54
3:N:1472:ILE:HG22	3:N:1474:ALA:H	1.72	0.54
3:N:424:GLY:HA2	3:N:435:VAL:O	2.08	0.54
4:O:48:MET:HB2	4:O:54:LEU:HB2	1.90	0.54
2:M:1015:LEU:HD13	5:P:335:ASP:HA	1.89	0.54
5:P:376:ILE:HG22	5:P:377:ASP:OD1	2.08	0.54
5:P:74:LYS:HE3	8:P:2868:HOH:O	2.07	0.54
1:A:18:ARG:O	1:A:207:PRO:HD3	2.08	0.53
1:B:214:ALA:HA	1:B:217:ILE:HD12	1.89	0.53
2:C:487:THR:HG23	8:C:1431:HOH:O	2.08	0.53
2:C:405:ARG:HD3	2:C:543:ASN:OD1	2.08	0.53
2:C:798:GLY:H	2:C:827:VAL:HG11	1.70	0.53
3:D:1236:LEU:HA	3:D:1359:GLN:OE1	2.08	0.53
3:D:1463:LYS:HG2	8:D:9761:HOH:O	2.08	0.53
3:D:154:THR:CG2	3:D:156:GLU:HG2	2.37	0.53
2:C:848:VAL:HG23	3:D:740:PHE:O	2.08	0.53
1:L:86:VAL:HG12	1:L:124:ASN:ND2	2.22	0.53
1:L:24:VAL:HG12	1:L:26:GLU:OE2	2.08	0.53
1:L:29:GLU:C	8:L:4886:HOH:O	2.46	0.53
2:M:431:HIS:HD2	2:M:433:THR:H	1.56	0.53
2:M:473:ARG:HA	2:M:531:PHE:HD1	1.73	0.53
2:M:499:ALA:HA	8:M:1410:HOH:O	2.08	0.53
2:M:549:PHE:CZ	2:M:886:LEU:HD12	2.43	0.53
2:M:697:ARG:HB2	8:M:1159:HOH:O	2.07	0.53
2:M:876:VAL:O	2:M:879:ARG:O	2.26	0.53
3:N:1420:LEU:HD12	3:N:1421:LEU:H	1.70	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:165:LYS:HE2	3:N:165:LYS:HA	1.89	0.53
3:N:396:VAL:HG13	3:N:447:VAL:HA	1.90	0.53
1:A:108:GLU:HB3	8:A:384:HOH:O	2.07	0.53
1:B:146:ARG:HG3	1:B:146:ARG:O	2.08	0.53
2:C:1060:ILE:CG2	2:C:1061:GLU:N	2.71	0.53
2:C:1100:GLN:HG3	2:C:1101:THR:O	2.08	0.53
2:C:138:SER:HB2	2:C:410:ILE:HG13	1.90	0.53
2:C:193:LEU:HD11	8:C:1760:HOH:O	2.08	0.53
2:C:216:GLU:HA	8:C:1237:HOH:O	2.07	0.53
2:C:586:ARG:HG2	8:C:1243:HOH:O	2.08	0.53
2:C:812:GLY:HA3	8:C:1432:HOH:O	2.07	0.53
2:C:554:ASP:HB2	2:C:880:MET:HB2	1.89	0.53
3:D:1095:THR:N	8:D:9051:HOH:O	2.41	0.53
3:D:1264:GLU:OE2	3:D:1425:THR:HG22	2.08	0.53
3:D:400:VAL:HG21	3:D:441:ARG:NH1	2.14	0.53
3:D:674:ARG:HD2	8:F:469:HOH:O	2.09	0.53
3:D:650:LEU:HD22	3:D:688:TRP:CZ3	2.43	0.53
3:D:704:ARG:HH11	3:D:738:ALA:HB2	1.73	0.53
3:D:903:ASP:HB2	8:D:9514:HOH:O	2.07	0.53
4:E:28:GLN:O	4:E:31:LEU:HG	2.07	0.53
1:K:2:LEU:HB2	8:K:5032:HOH:O	2.08	0.53
1:L:153:ALA:HA	1:L:156:HIS:NE2	2.23	0.53
1:L:185:ARG:HA	8:L:4811:HOH:O	2.08	0.53
2:M:572:ILE:O	2:M:573:ARG:HG2	2.08	0.53
3:N:127:LEU:HD12	3:N:128:TYR:N	2.23	0.53
3:N:1273:VAL:O	3:N:1325:LEU:HB2	2.08	0.53
3:N:690:ALA:O	3:N:694:VAL:HG23	2.08	0.53
5:P:201:LYS:HD2	8:P:3919:HOH:O	2.08	0.53
1:B:109:VAL:HG21	1:B:138:LEU:HD21	1.89	0.53
2:C:145:GLY:N	2:C:163:ILE:HG23	2.18	0.53
2:C:195:LEU:HD12	2:C:234:ALA:HB1	1.89	0.53
2:C:332:ARG:HD3	2:C:465:GLY:HA3	1.91	0.53
2:C:839:LEU:HD21	2:C:849:VAL:HG22	1.89	0.53
2:C:69:LEU:HB2	2:C:97:ARG:HB2	1.91	0.53
3:D:847:ASP:O	3:D:851:LEU:HG	2.09	0.53
2:M:1013:TYR:CE1	2:M:1020:PRO:HG3	2.43	0.53
2:M:571:LEU:HG	2:M:700:TYR:HA	1.91	0.53
3:N:105:VAL:HG21	3:N:128:TYR:CE2	2.43	0.53
3:N:1502:ALA:HA	8:N:9322:HOH:O	2.09	0.53
3:N:18:ILE:HG23	3:N:518:PRO:CG	2.37	0.53
3:N:514:LEU:HD23	8:N:9079:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:534:ARG:HH11	3:N:534:ARG:HG3	1.74	0.53
3:N:656:PHE:HB3	3:N:694:VAL:CG1	2.38	0.53
4:O:66:LYS:HE3	8:O:3745:HOH:O	2.08	0.53
5:P:138:SER:O	5:P:141:VAL:HG12	2.08	0.53
1:A:59:GLU:HG3	1:A:139:ASN:CG	2.29	0.53
2:C:102:HIS:HB2	2:C:106:GLY:O	2.09	0.53
2:C:52:PHE:CG	2:C:68:PHE:HB2	2.44	0.53
2:C:944:LEU:HD21	2:C:963:LEU:CD2	2.37	0.53
3:D:1041:LEU:HD12	3:D:1058:ARG:HA	1.90	0.53
3:D:430:ASP:CG	3:D:431:VAL:H	2.12	0.53
3:D:584:ASN:CG	3:D:590:PRO:HD2	2.28	0.53
5:F:306:GLU:O	5:F:310:ILE:HG13	2.08	0.53
5:F:365:GLU:CD	5:F:397:ILE:HA	2.29	0.53
5:F:79:ASP:HB3	5:F:80:PRO:HD3	1.90	0.53
1:K:222:LEU:HD12	1:L:215:VAL:HB	1.91	0.53
2:M:1054:THR:HG22	2:M:1059:ASP:CB	2.34	0.53
2:M:198:ARG:HB3	8:M:1370:HOH:O	2.09	0.53
2:M:380:ALA:HA	2:M:383:ARG:CD	2.35	0.53
3:N:951:ILE:HG23	3:N:1062:ARG:HE	1.74	0.53
3:N:1498:ALA:HB3	8:N:9099:HOH:O	2.09	0.53
3:N:165:LYS:HB3	3:N:395:VAL:HG11	1.89	0.53
4:O:86:GLN:O	4:O:90:GLU:HG3	2.07	0.53
1:B:226:SER:O	1:B:228:PRO:HD3	2.07	0.53
2:C:1009:SER:HB2	3:D:651:GLU:OE1	2.08	0.53
2:C:1063:ARG:O	2:C:1066:ALA:HB3	2.09	0.53
2:C:601:GLY:O	2:C:648:ARG:HA	2.09	0.53
3:D:1000:THR:O	3:D:1003:VAL:HG22	2.07	0.53
3:D:1295:GLU:HB3	3:D:1300:SER:OG	2.09	0.53
3:D:652:LEU:HB3	3:D:653:PHE:CD1	2.44	0.53
3:D:786:ILE:HD13	3:D:908:LYS:HB3	1.89	0.53
4:E:61:GLU:O	4:E:65:MET:HG3	2.08	0.53
5:F:305:GLU:O	5:F:309:LYS:HG3	2.08	0.53
5:F:402:ASN:O	5:F:406:ARG:HG3	2.08	0.53
1:L:115:LEU:O	1:L:115:LEU:HD12	2.08	0.53
1:L:42:ARG:HB3	8:L:3652:HOH:O	2.08	0.53
2:M:565:GLN:HG2	2:M:995:MET:HE1	1.88	0.53
8:M:1680:HOH:O	3:N:1088:THR:HG21	2.09	0.53
3:N:1423:GLY:HA3	8:N:9011:HOH:O	2.08	0.53
3:N:196:VAL:HG13	3:N:202:VAL:CG1	2.38	0.53
5:P:393:THR:O	5:P:397:ILE:HG13	2.09	0.53
1:A:66:SER:O	1:A:75:VAL:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:384:GLU:HG3	2:C:388:ARG:HE	1.74	0.53
3:D:1192:LEU:HD22	3:D:1345:GLU:OE2	2.08	0.53
3:D:1351:GLU:OE1	3:D:1354:LYS:HG3	2.07	0.53
3:D:168:THR:OG1	3:D:393:ILE:HB	2.09	0.53
3:D:63:TYR:HB3	3:D:68:PHE:CE1	2.44	0.53
2:M:411:SER:HA	2:M:452:ILE:HA	1.90	0.53
2:M:139:GLN:HE22	2:M:415:PRO:CG	2.21	0.53
3:N:1197:ARG:HG3	3:N:1198:TYR:H	1.73	0.53
3:N:554:LEU:HD12	3:N:558:LEU:HD11	1.89	0.53
3:N:738:ALA:HB3	8:N:9159:HOH:O	2.08	0.53
4:O:51:LEU:HD12	4:O:52:GLU:N	2.24	0.53
5:P:270:LYS:HA	5:P:273:ARG:HD2	1.89	0.53
1:A:117:VAL:HG12	8:A:360:HOH:O	2.07	0.53
1:A:150:TYR:CE2	1:A:152:PRO:HG3	2.37	0.53
2:C:1003:ASP:O	2:C:1005:MET:N	2.41	0.53
2:C:1025:ALA:HA	8:C:1228:HOH:O	2.07	0.53
2:C:141:HIS:HB3	2:C:418:LEU:HB3	1.90	0.53
2:C:577:PRO:HB2	2:C:580:MET:HG3	1.91	0.53
2:C:673:LEU:CD2	2:C:867:VAL:HA	2.38	0.53
1:A:31:GLY:HA2	2:C:939:ARG:HH22	1.73	0.53
2:C:945:ARG:HH11	2:C:945:ARG:HB3	1.74	0.53
3:D:1242:HIS:CE1	3:D:1266:ARG:HD3	2.43	0.53
3:D:1349:VAL:HG21	8:D:9752:HOH:O	2.07	0.53
3:D:420:VAL:HA	5:F:164:LYS:HE3	1.91	0.53
3:D:531:ASP:C	3:D:533:GLY:H	2.11	0.53
3:D:714:GLN:OE1	3:D:765:SER:HB2	2.08	0.53
1:L:110:LYS:HZ3	1:L:110:LYS:HB2	1.73	0.53
2:M:139:GLN:HG2	2:M:418:LEU:HD22	1.90	0.53
2:M:271:GLU:OE1	2:M:275:TYR:HB2	2.09	0.53
2:M:630:ARG:HA	2:M:705:ILE:HD11	1.89	0.53
2:M:752:GLY:N	2:M:792:VAL:HB	2.21	0.53
3:N:104:PHE:CE2	3:N:1448:THR:HG23	2.44	0.53
3:N:1253:THR:OG1	3:N:1258:ARG:HD3	2.07	0.53
3:N:197:SER:HA	8:N:9553:HOH:O	2.09	0.53
3:N:137:PRO:HD2	3:N:453:ASP:CB	2.39	0.53
5:P:155:THR:HA	5:P:158:GLU:OE2	2.09	0.53
5:P:163:LEU:HB3	5:P:174:LEU:CD1	2.39	0.53
5:P:209:PHE:O	5:P:213:ILE:HG13	2.08	0.53
1:B:27:PRO:HG2	1:B:186:LEU:HD12	1.90	0.53
2:C:1058:ASP:OD2	2:C:1083:GLU:HB2	2.09	0.53
2:C:274:ARG:HG2	8:C:1235:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:444:PRO:HD2	2:C:452:ILE:HG13	1.91	0.53
2:C:496:ILE:HD12	2:C:496:ILE:H	1.74	0.53
2:C:964:LYS:HD2	8:C:1456:HOH:O	2.09	0.53
3:D:1097:LYS:O	3:D:1101:VAL:HG23	2.09	0.53
3:D:191:LEU:HB3	3:D:195:VAL:HG21	1.91	0.53
3:D:477:LEU:HD13	3:D:492:ALA:O	2.08	0.53
2:C:874:LEU:HD13	3:D:783:ARG:HB2	1.90	0.53
1:K:182:GLU:O	1:K:194:LYS:HB3	2.09	0.53
2:M:129:ILE:HD13	2:M:134:ARG:CB	2.29	0.53
2:M:489:THR:HG21	8:M:1667:HOH:O	2.07	0.53
2:M:564:MET:HE1	8:M:1413:HOH:O	2.09	0.53
2:M:571:LEU:HD12	2:M:701:THR:O	2.08	0.53
2:M:758:ARG:NH1	2:M:788:THR:HB	2.24	0.53
2:M:905:ILE:HG22	2:M:906:PHE:CD1	2.44	0.53
2:M:500:ASN:HD21	3:N:1067:VAL:CG2	2.22	0.53
3:N:1101:VAL:HG22	3:N:1428:ALA:HB2	1.90	0.53
3:N:1459:LEU:HD13	3:N:1465:ASN:ND2	2.24	0.53
3:N:480:GLU:O	3:N:484:PRO:HD2	2.09	0.53
5:P:205:ARG:HH11	5:P:251:ILE:HG21	1.74	0.53
5:P:253:ASP:HA	5:P:259:ARG:NH1	2.24	0.53
5:P:269:ASN:O	5:P:273:ARG:HG3	2.09	0.53
1:B:143:ARG:HD2	1:B:158:ILE:HG21	1.91	0.53
2:C:329:GLY:HA3	2:C:489:THR:HG23	1.91	0.53
2:C:358:ARG:HB3	2:C:371:LYS:O	2.09	0.53
2:C:115:LEU:HA	2:C:375:SER:HB3	1.90	0.53
2:C:380:ALA:O	2:C:384:GLU:HB2	2.09	0.53
2:C:578:VAL:HG11	2:C:991:GLN:CB	2.35	0.53
3:D:119:SER:CB	3:D:123:LEU:HB2	2.39	0.53
3:D:1281:VAL:HG23	3:D:1317:ASP:O	2.09	0.53
3:D:1381:VAL:HG23	3:D:1391:GLU:O	2.09	0.53
2:C:1043:TYR:HE1	3:D:710:ARG:O	1.91	0.53
3:D:86:ARG:HH11	3:D:86:ARG:HG2	1.72	0.53
3:D:880:ILE:O	3:D:883:ALA:HB3	2.09	0.53
3:D:957:PRO:CG	3:D:1007:VAL:HA	2.39	0.53
5:F:203:THR:HG22	8:F:514:HOH:O	2.07	0.53
5:F:398:ARG:HG2	5:F:402:ASN:ND2	2.24	0.53
1:L:101:LEU:HG	1:L:114:PHE:HA	1.90	0.53
1:L:94:LEU:HD11	1:L:119:ASP:HB3	1.89	0.53
2:M:167:LYS:HD3	2:M:168:ARG:HD2	1.90	0.53
2:M:217:LEU:HD12	2:M:311:PHE:CD2	2.44	0.53
2:M:326:ASP:HB2	2:M:431:HIS:ND1	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:639:GLN:HG3	8:M:1290:HOH:O	2.09	0.53
3:N:1087:ARG:HG2	3:N:1087:ARG:HH11	1.73	0.53
3:N:1432:LYS:HD2	3:N:1433:SER:N	2.12	0.53
3:N:774:SER:C	3:N:776:GLU:H	2.13	0.53
4:O:8:LYS:HG3	8:O:3467:HOH:O	2.09	0.53
5:P:337:HIS:H	5:P:337:HIS:HD2	1.56	0.53
5:P:420:ASP:HB2	8:P:2629:HOH:O	2.08	0.53
1:A:176:ARG:HG3	1:A:200:TRP:HB2	1.91	0.53
1:A:221:HIS:HA	1:A:224:TYR:CD2	2.44	0.53
2:C:1054:THR:HG22	2:C:1059:ASP:OD2	2.09	0.53
2:C:431:HIS:CD2	2:C:433:THR:H	2.27	0.53
2:C:525:SER:OG	2:C:528:GLU:HG3	2.08	0.53
2:C:690:ILE:HD12	2:C:849:VAL:HG13	1.91	0.53
3:D:122:GLU:O	3:D:126:VAL:HG23	2.09	0.53
3:D:478:LEU:HD22	3:D:1388:ARG:NH1	2.23	0.53
3:D:774:SER:C	3:D:776:GLU:H	2.12	0.53
3:D:890:VAL:HG13	3:D:926:LYS:HE2	1.91	0.53
4:E:26:ARG:HE	4:E:30:LEU:HD13	1.73	0.53
4:E:33:HIS:HB2	4:E:37:ASN:HD21	1.73	0.53
2:M:16:PRO:HA	8:M:1782:HOH:O	2.08	0.53
2:M:296:GLY:HA2	8:M:1743:HOH:O	2.09	0.53
2:M:520:GLU:O	2:M:522:VAL:HG23	2.08	0.53
3:N:1278:ASP:OD1	3:N:1321:ALA:HB2	2.08	0.53
3:N:462:GLN:CG	3:N:513:ILE:HD13	2.38	0.53
3:N:699:VAL:CG1	3:N:717:GLN:HE21	2.20	0.53
5:P:191:ASN:HA	8:P:2854:HOH:O	2.09	0.53
1:A:123:MET:C	1:A:125:PRO:HD3	2.29	0.52
1:A:197:LEU:HD23	1:A:197:LEU:N	2.25	0.52
2:C:1054:THR:CG2	2:C:1079:PRO:HB3	2.30	0.52
2:C:140:ILE:CD1	2:C:412:ALA:HA	2.38	0.52
2:C:985:GLY:O	2:C:987:ILE:HD12	2.09	0.52
3:D:1230:GLY:CA	8:D:9051:HOH:O	2.57	0.52
3:D:669:ASN:HD21	5:F:417:LYS:HA	1.74	0.52
3:D:684:LYS:HD3	3:D:686:GLU:OE1	2.09	0.52
3:D:720:LEU:HD12	3:D:720:LEU:H	1.75	0.52
3:D:52:PRO:HG3	3:D:78:VAL:HG13	1.91	0.52
4:E:95:GLY:HA3	8:E:104:HOH:O	2.08	0.52
5:F:388:ALA:HB1	8:F:443:HOH:O	2.08	0.52
1:L:9:PRO:HB3	1:L:25:LEU:HG	1.91	0.52
1:L:74:ASP:O	1:L:78:ILE:HG13	2.09	0.52
2:M:172:ILE:HD12	2:M:172:ILE:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:380:ALA:O	2:M:384:GLU:HB2	2.09	0.52
2:M:510:ALA:HB1	8:M:1203:HOH:O	2.09	0.52
2:M:627:ARG:O	2:M:638:ASP:HB3	2.09	0.52
2:M:720:GLU:HA	2:M:759:THR:O	2.08	0.52
2:M:710:ILE:HD11	2:M:758:ARG:HH21	1.73	0.52
3:N:1106:VAL:HG22	8:N:9413:HOH:O	2.10	0.52
8:M:1245:HOH:O	3:N:603:LEU:HD11	2.09	0.52
3:N:799:LYS:O	3:N:799:LYS:HD3	2.09	0.52
3:N:950:GLY:O	3:N:953:ASP:N	2.38	0.52
4:O:45:ARG:HB2	4:O:46:PRO:CD	2.39	0.52
1:A:53:VAL:HG12	1:A:167:VAL:HG21	1.91	0.52
2:C:1039:ALA:O	2:C:1043:TYR:HD1	1.92	0.52
2:C:1049:LEU:O	2:C:1053:LEU:HG	2.08	0.52
2:C:1056:LYS:HB3	3:D:624:ASP:H	1.74	0.52
2:C:19:THR:HG21	2:C:124:ASP:O	2.09	0.52
2:C:260:LEU:HB2	2:C:291:ALA:HB1	1.90	0.52
2:C:292:ARG:HD2	2:C:299:LYS:HE2	1.91	0.52
2:C:685:GLU:H	3:D:740:PHE:HE1	1.57	0.52
3:D:911:LEU:O	3:D:915:VAL:HG23	2.09	0.52
3:D:955:VAL:HG21	3:D:1015:TYR:HE2	1.74	0.52
1:L:184:THR:O	1:L:192:LEU:HB2	2.08	0.52
2:M:102:HIS:HB2	2:M:106:GLY:O	2.09	0.52
2:M:170:PRO:HG2	2:M:258:TYR:CD2	2.44	0.52
3:N:1087:ARG:HE	3:N:1238:MET:HB2	1.74	0.52
3:N:507:ASN:HA	8:N:9017:HOH:O	2.08	0.52
3:N:702:LEU:HD13	3:N:716:PHE:HD1	1.74	0.52
1:A:10:VAL:HG12	1:A:12:THR:HG22	1.91	0.52
1:A:20:TYR:CD2	1:A:21:GLY:N	2.76	0.52
1:A:58:ILE:HB	1:A:61:VAL:HB	1.91	0.52
1:B:22:GLU:HG2	1:B:198:ARG:HG2	1.91	0.52
2:C:1111:ILE:HG13	2:C:1112:PHE:N	2.19	0.52
2:C:559:LEU:HD23	2:C:560:MET:HG3	1.90	0.52
2:C:671:ASN:ND2	2:C:671:ASN:H	2.06	0.52
2:C:732:ALA:O	2:C:735:ARG:HG3	2.10	0.52
2:C:861:LEU:HD23	2:C:862:PRO:N	2.24	0.52
3:D:956:ILE:HG12	3:D:1039:CYS:O	2.08	0.52
3:D:131:LYS:CG	3:D:568:ARG:HG2	2.36	0.52
3:D:564:GLU:HA	3:D:567:ILE:HD12	1.91	0.52
3:D:607:LEU:HB3	3:D:614:PHE:CE2	2.44	0.52
3:D:895:VAL:O	3:D:899:LEU:HG	2.10	0.52
3:D:98:PRO:HG3	3:D:515:GLU:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:191:ASN:HB3	5:F:220:LEU:HD11	1.91	0.52
5:F:263:HIS:HB2	8:F:604:HOH:O	2.08	0.52
5:F:340:SER:OG	5:F:342:VAL:HG23	2.09	0.52
2:M:19:THR:HG21	2:M:125:GLY:HA3	1.92	0.52
2:M:352:ALA:HA	2:M:355:VAL:HG12	1.90	0.52
2:M:411:SER:HB2	2:M:452:ILE:HG23	1.91	0.52
2:M:629:TYR:HB2	2:M:637:LEU:HG	1.92	0.52
2:M:798:GLY:HA3	2:M:828:ALA:O	2.09	0.52
3:N:1033:GLN:HB3	8:N:9763:HOH:O	2.09	0.52
3:N:1366:LYS:O	3:N:1370:ILE:HG12	2.10	0.52
3:N:1103:HIS:CD2	3:N:1463:LYS:H	2.28	0.52
3:N:697:GLY:HA3	8:O:2665:HOH:O	2.08	0.52
5:P:278:LEU:CB	5:P:286:PRO:HG2	2.39	0.52
1:A:23:PHE:HE1	1:A:208:LEU:HD13	1.73	0.52
2:C:1092:LEU:HA	2:C:1095:LEU:HD12	1.90	0.52
2:C:468:ARG:HD3	2:C:485:TYR:HB3	1.90	0.52
2:C:625:LEU:HD13	2:C:639:GLN:O	2.10	0.52
3:D:116:LEU:O	3:D:118:LEU:HG	2.08	0.52
3:D:1448:THR:O	3:D:1452:ILE:HD13	2.09	0.52
2:C:1095:LEU:CD1	3:D:607:LEU:HD11	2.32	0.52
3:D:799:LYS:H	3:D:826:PRO:HG2	1.74	0.52
3:D:858:VAL:HG11	3:D:864:VAL:HG21	1.92	0.52
3:D:884:ARG:HG2	8:D:9790:HOH:O	2.10	0.52
3:D:996:TRP:O	3:D:999:THR:HG22	2.08	0.52
8:D:9510:HOH:O	5:F:259:ARG:HB2	2.07	0.52
3:D:537:THR:CA	5:F:317:LEU:HD12	2.39	0.52
2:C:777:ILE:HG23	5:F:405:LEU:CD1	2.39	0.52
5:F:401:GLU:O	5:F:405:LEU:HB2	2.10	0.52
1:K:219:ARG:HH11	1:K:219:ARG:HG3	1.74	0.52
1:K:91:ASN:HA	8:K:3642:HOH:O	2.09	0.52
1:L:123:MET:O	1:L:125:PRO:HD3	2.10	0.52
1:L:156:HIS:CE1	1:L:166:PRO:HB3	2.44	0.52
2:M:165:LEU:HB2	8:M:1197:HOH:O	2.09	0.52
2:M:378:LEU:HG	2:M:382:ILE:CD1	2.40	0.52
2:M:56:GLU:CG	2:M:64:LEU:HD23	2.39	0.52
2:M:15:LEU:HD11	2:M:583:LEU:HD11	1.90	0.52
2:M:842:ARG:HB2	8:M:1165:HOH:O	2.07	0.52
2:M:694:LEU:HD11	2:M:868:ASP:HB3	1.91	0.52
3:N:420:VAL:HG23	8:N:9890:HOH:O	2.07	0.52
3:N:631:ILE:HD13	3:N:745:MET:HG3	1.91	0.52
5:P:185:GLN:O	5:P:189:GLU:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:772:ARG:CD	5:P:373:LYS:HD2	2.37	0.52
1:B:5:LYS:HA	1:B:5:LYS:HE3	1.90	0.52
2:C:1005:MET:CE	3:D:648:MET:HB2	2.39	0.52
2:C:630:ARG:HH22	2:C:707:ARG:HB2	1.73	0.52
2:C:778:PHE:HB2	8:C:1741:HOH:O	2.09	0.52
2:C:673:LEU:HD22	2:C:867:VAL:HA	1.90	0.52
3:D:399:ARG:HB2	3:D:444:VAL:HG13	1.92	0.52
3:D:584:ASN:HB3	8:D:9062:HOH:O	2.08	0.52
3:D:659:LYS:C	3:D:659:LYS:HD3	2.29	0.52
2:C:1104:GLU:HA	3:D:6:ARG:HH12	1.75	0.52
3:D:643:GLY:CA	3:D:727:GLN:HB2	2.35	0.52
5:F:234:LYS:CD	5:F:236:SER:HB3	2.37	0.52
1:K:94:LEU:HD11	1:K:119:ASP:OD1	2.09	0.52
1:K:97:VAL:HG23	8:K:3015:HOH:O	2.07	0.52
2:M:162:ILE:HB	2:M:172:ILE:HB	1.90	0.52
2:M:428:ARG:HE	2:M:451:LEU:HD21	1.75	0.52
3:N:1381:VAL:HG23	3:N:1391:GLU:O	2.10	0.52
3:N:712:GLY:HA2	8:N:9111:HOH:O	2.09	0.52
3:N:853:VAL:HG13	3:N:858:VAL:O	2.10	0.52
5:P:93:LEU:HG	5:P:190:ALA:HB1	1.90	0.52
2:C:1024:LYS:HB2	8:C:1173:HOH:O	2.08	0.52
2:C:1047:HIS:CD2	3:D:1471:LEU:HD11	2.45	0.52
2:C:1109:VAL:HG22	8:D:9538:HOH:O	2.10	0.52
2:C:332:ARG:HA	2:C:465:GLY:O	2.10	0.52
2:C:567:GLN:HB2	2:C:997:LEU:HD22	1.91	0.52
2:C:627:ARG:HG3	2:C:628:PHE:H	1.75	0.52
2:C:777:ILE:HG12	5:F:405:LEU:HD11	1.91	0.52
2:C:899:GLN:HG3	2:C:901:TYR:CZ	2.45	0.52
2:C:911:GLU:HG2	2:C:915:LYS:HZ2	1.74	0.52
3:D:996:TRP:HB2	3:D:1044:LEU:HD11	1.92	0.52
3:D:1147:ARG:HB3	3:D:1188:VAL:HG21	1.90	0.52
2:M:269:LEU:HD23	2:M:285:LEU:HD21	1.90	0.52
2:M:139:GLN:HE22	2:M:415:PRO:HD2	1.73	0.52
2:M:52:PHE:CG	2:M:68:PHE:HB2	2.45	0.52
3:N:1047:LYS:HG2	3:N:1053:PHE:CE1	2.45	0.52
3:N:87:ARG:HG3	3:N:88:TYR:CD2	2.44	0.52
1:A:205:VAL:HG23	1:A:206:THR:N	2.23	0.52
2:C:118:ILE:HG22	2:C:382:ILE:HD13	1.92	0.52
2:C:200:LEU:HD13	2:C:300:ASP:CG	2.30	0.52
2:C:480:THR:HG22	2:C:481:ASP:N	2.24	0.52
2:C:510:ALA:HB3	2:C:513:VAL:HG23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:730:SER:O	2:C:734:LEU:HD13	2.10	0.52
2:C:862:PRO:HG3	2:C:975:TYR:HE1	1.73	0.52
3:D:1033:GLN:HE21	3:D:1033:GLN:HA	1.74	0.52
3:D:38:LYS:HD3	8:D:9533:HOH:O	2.09	0.52
3:D:679:ARG:HD3	3:D:682:ASP:OD2	2.10	0.52
1:K:18:ARG:O	1:K:207:PRO:HD3	2.08	0.52
1:K:68:ILE:HA	8:K:4050:HOH:O	2.09	0.52
2:M:645:VAL:HG22	8:M:1487:HOH:O	2.09	0.52
3:N:1330:ILE:N	3:N:1330:ILE:HD12	2.25	0.52
3:N:180:LYS:O	3:N:184:GLU:HG3	2.09	0.52
3:N:490:ALA:HB2	8:N:9895:HOH:O	2.10	0.52
4:O:74:VAL:HG12	4:O:79:LEU:HD21	1.90	0.52
5:P:102:LEU:HD22	5:P:183:ALA:O	2.09	0.52
5:P:365:GLU:OE1	5:P:400:ILE:HD12	2.09	0.52
5:P:367:MET:HA	5:P:370:LYS:NZ	2.24	0.52
2:C:208:ALA:HA	2:C:218:VAL:HG22	1.92	0.52
2:C:22:GLN:NE2	2:C:336:VAL:HG21	2.24	0.52
2:C:32:ALA:HB2	2:C:73:LEU:HD21	1.91	0.52
2:C:532:MET:HE3	8:C:1857:HOH:O	2.10	0.52
2:C:402:SER:OG	2:C:566:THR:HG22	2.10	0.52
2:C:884:GLN:HG3	2:C:885:ILE:N	2.22	0.52
2:C:551:GLU:OE1	2:C:906:PHE:HA	2.09	0.52
2:C:897:LEU:HG	2:C:920:GLN:HE21	1.75	0.52
3:D:148:GLU:CB	3:D:151:GLN:HB2	2.34	0.52
3:D:819:GLY:HA3	8:D:9099:HOH:O	2.08	0.52
5:F:247:ILE:O	5:F:251:ILE:HG13	2.10	0.52
1:K:80:LEU:HB3	8:K:3096:HOH:O	2.10	0.52
1:L:226:SER:O	1:L:228:PRO:HD3	2.09	0.52
2:M:1101:THR:O	2:M:1102:LEU:HD23	2.10	0.52
2:M:412:ALA:CB	2:M:451:LEU:HB3	2.40	0.52
2:M:473:ARG:HA	2:M:531:PHE:CD1	2.45	0.52
2:M:97:ARG:HD2	8:M:1366:HOH:O	2.10	0.52
3:N:1041:LEU:HD12	3:N:1057:VAL:O	2.08	0.52
3:N:1047:LYS:HA	3:N:1053:PHE:CE1	2.44	0.52
3:N:951:ILE:HG23	3:N:1062:ARG:HH21	1.75	0.52
3:N:1109:GLU:HG2	3:N:1202:GLN:H	1.75	0.52
3:N:1102:THR:HG22	3:N:1222:GLY:CA	2.40	0.52
3:N:1240:THR:O	3:N:1257:PRO:HB3	2.10	0.52
3:N:1344:VAL:HG12	3:N:1348:LEU:CD2	2.40	0.52
3:N:500:ARG:HH12	3:N:1388:ARG:HD2	1.75	0.52
3:N:434:ARG:HB2	3:N:447:VAL:CG1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:167:PRO:HG2	8:P:3728:HOH:O	2.10	0.52
1:B:204:SER:HB2	8:B:371:HOH:O	2.09	0.52
2:C:1060:ILE:HG23	2:C:1061:GLU:N	2.24	0.52
2:C:114:PHE:HB2	8:C:1287:HOH:O	2.10	0.52
2:C:232:GLU:O	2:C:235:LEU:HB2	2.09	0.52
2:C:305:PRO:HG3	2:C:308:ARG:HH21	1.75	0.52
2:C:333:ILE:HD12	2:C:333:ILE:N	2.25	0.52
2:C:139:GLN:OE1	2:C:415:PRO:HD2	2.09	0.52
2:C:612:VAL:HG22	2:C:622:GLU:HA	1.91	0.52
2:C:724:ARG:HG3	2:C:740:GLU:HA	1.91	0.52
2:C:722:ILE:HD12	2:C:805:ARG:HH21	1.74	0.52
2:C:841:ASN:HD21	2:C:845:ASN:H	1.58	0.52
3:D:1318:TYR:HD1	3:D:1319:VAL:H	1.56	0.52
3:D:136:ASP:HB3	3:D:137:PRO:CD	2.35	0.52
3:D:191:LEU:HD13	3:D:195:VAL:HG11	1.91	0.52
3:D:211:VAL:HG13	3:D:393:ILE:HA	1.91	0.52
3:D:879:ARG:HH21	3:D:903:ASP:C	2.14	0.52
3:D:918:ALA:O	3:D:922:LEU:HG	2.10	0.52
3:D:972:LEU:HD23	3:D:973:GLN:N	2.24	0.52
5:F:274:THR:O	5:F:278:LEU:HG	2.10	0.52
1:K:123:MET:C	1:K:125:PRO:HD3	2.31	0.52
1:K:219:ARG:NH1	1:K:219:ARG:HG3	2.25	0.52
1:K:226:SER:O	1:K:228:PRO:HD3	2.10	0.52
2:M:1034:GLU:HB2	8:M:1373:HOH:O	2.09	0.52
2:M:244:PRO:CD	2:M:245:GLY:H	2.17	0.52
2:M:322:VAL:HA	8:M:1189:HOH:O	2.09	0.52
2:M:442:GLU:HG2	2:M:454:SER:OG	2.10	0.52
2:M:571:LEU:HD23	2:M:670:GLN:NE2	2.25	0.52
1:K:46:SER:HB3	2:M:856:GLU:CD	2.30	0.52
3:N:963:TYR:CD2	3:N:1002:LYS:HB3	2.45	0.52
3:N:1112:CYS:HA	3:N:1195:GLN:HE22	1.74	0.52
5:P:363:GLU:HA	5:P:367:MET:HG2	1.92	0.52
1:B:151:VAL:HB	1:B:169:ALA:HB3	1.92	0.52
2:C:1084:SER:O	2:C:1087:VAL:HG12	2.10	0.52
2:C:399:ASN:N	2:C:399:ASN:HD22	2.08	0.52
2:C:41:ASN:N	2:C:41:ASN:HD22	1.97	0.52
2:C:470:PRO:HD3	2:C:485:TYR:CE2	2.45	0.52
2:C:625:LEU:CD1	2:C:641:PRO:HG3	2.40	0.52
2:C:597:ALA:CB	2:C:655:LEU:HD21	2.35	0.52
2:C:724:ARG:HH11	2:C:724:ARG:HB3	1.73	0.52
3:D:445:ARG:HG2	3:D:445:ARG:HH11	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:58:CYS:SG	3:D:59:ALA:N	2.83	0.52
4:E:19:LEU:O	4:E:23:VAL:HG23	2.10	0.52
5:F:408:LEU:HA	5:F:411:HIS:CE1	2.44	0.52
1:K:143:ARG:HG3	1:K:144:VAL:N	2.25	0.52
1:L:46:SER:HB2	8:L:3700:HOH:O	2.09	0.52
1:L:85:LEU:HD13	1:L:127:LEU:HD23	1.92	0.52
2:M:451:LEU:HD12	2:M:451:LEU:H	1.75	0.52
3:N:1194:CYS:HB3	3:N:1373:ARG:CZ	2.40	0.52
3:N:1194:CYS:HB3	3:N:1373:ARG:HH22	1.74	0.52
3:N:126:VAL:O	3:N:132:TYR:HD1	1.92	0.52
3:N:15:PRO:HG3	8:N:9079:HOH:O	2.10	0.52
3:N:411:THR:HB	8:N:9297:HOH:O	2.10	0.52
3:N:750:PRO:HB2	3:N:756:GLN:OE1	2.09	0.52
3:N:81:THR:HG22	8:N:9092:HOH:O	2.10	0.52
3:N:97:THR:HG21	3:N:571:LYS:HD3	1.92	0.52
5:P:253:ASP:HA	5:P:259:ARG:HH12	1.75	0.52
5:P:323:ASP:O	5:P:325:LYS:N	2.43	0.52
5:P:321:ILE:HB	5:P:327:SER:OG	2.10	0.52
2:C:554:ASP:HA	3:D:1061:PHE:CZ	2.45	0.51
3:D:1076:GLY:O	3:D:1079:LYS:HG2	2.10	0.51
3:D:1277:ILE:HG21	8:D:9249:HOH:O	2.10	0.51
3:D:1403:LEU:HG	8:D:9163:HOH:O	2.10	0.51
3:D:1333:HIS:ND1	3:D:1421:LEU:HD23	2.26	0.51
3:D:213:VAL:HG21	8:D:9600:HOH:O	2.09	0.51
3:D:529:GLN:HG2	3:D:535:PHE:CE1	2.45	0.51
3:D:543:LEU:HD21	3:D:600:LEU:HD12	1.92	0.51
3:D:542:ASP:O	3:D:546:ARG:HG2	2.10	0.51
3:D:819:GLY:O	3:D:822:ALA:HB3	2.10	0.51
3:D:777:PRO:HG2	3:D:915:VAL:HB	1.92	0.51
3:D:573:MET:CE	5:F:210:LEU:HB3	2.39	0.51
5:F:87:GLU:O	5:F:91:VAL:HG23	2.10	0.51
1:K:62:LEU:H	1:K:62:LEU:HD12	1.75	0.51
2:M:200:LEU:HD13	2:M:300:ASP:CG	2.30	0.51
2:M:290:LEU:HD13	8:M:1252:HOH:O	2.10	0.51
2:M:52:PHE:HB3	2:M:53:PRO:HD3	1.92	0.51
2:M:626:ARG:HB2	8:M:1290:HOH:O	2.11	0.51
3:N:1210:SER:HB2	8:O:3546:HOH:O	2.10	0.51
3:N:119:SER:HB2	3:N:123:LEU:N	2.24	0.51
3:N:30:GLU:HG3	3:N:41:ARG:HG2	1.91	0.51
1:A:117:VAL:HB	1:A:120:VAL:HG12	1.91	0.51
1:B:83:LYS:HE2	1:B:168:ASP:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1097:LEU:HD21	3:D:103:TRP:CZ3	2.45	0.51
2:C:269:LEU:HG	2:C:288:ARG:N	2.24	0.51
3:D:1045:MET:HG2	3:D:1073:SER:CA	2.27	0.51
3:D:1242:HIS:HE1	3:D:1266:ARG:HB3	1.75	0.51
1:K:58:ILE:HG21	1:K:68:ILE:CD1	2.40	0.51
1:L:170:VAL:HG23	8:L:3287:HOH:O	2.10	0.51
2:M:103:LYS:HB2	8:M:1613:HOH:O	2.10	0.51
2:M:309:TYR:HA	2:M:312:ALA:HB3	1.92	0.51
2:M:405:ARG:HE	2:M:543:ASN:ND2	2.08	0.51
2:M:958:THR:HA	8:M:1596:HOH:O	2.09	0.51
3:N:1033:GLN:HE21	3:N:1036:ARG:HH11	1.57	0.51
3:N:1133:ARG:HB2	8:N:9380:HOH:O	2.09	0.51
3:N:171:LEU:HD13	3:N:389:GLU:C	2.30	0.51
3:N:610:LYS:HG2	3:N:611:GLN:HG2	1.92	0.51
3:N:637:LEU:HD21	8:N:9469:HOH:O	2.10	0.51
2:M:1071:ILE:O	3:N:659:LYS:HB2	2.10	0.51
3:N:87:ARG:HB3	3:N:523:ASP:HB2	1.91	0.51
3:N:963:TYR:CE2	3:N:1002:LYS:HB3	2.45	0.51
5:P:303:ARG:O	5:P:307:THR:HG23	2.10	0.51
1:A:106:PRO:HG3	1:A:133:GLU:O	2.11	0.51
2:C:1015:LEU:HA	8:C:1202:HOH:O	2.09	0.51
2:C:198:ARG:HD2	8:C:1571:HOH:O	2.09	0.51
2:C:208:ALA:HB1	2:C:218:VAL:HG13	1.92	0.51
2:C:264:PRO:HB2	8:C:1418:HOH:O	2.10	0.51
2:C:265:ARG:HG2	2:C:267:TYR:CG	2.45	0.51
2:C:329:GLY:N	2:C:488:ALA:HB3	2.24	0.51
2:C:920:GLN:HG3	8:C:1216:HOH:O	2.11	0.51
3:D:1008:PHE:HZ	3:D:1032:PRO:HA	1.73	0.51
2:C:1098:ASP:HB2	3:D:21:TRP:HZ2	1.75	0.51
5:F:153:PRO:HG2	5:F:154:LYS:H	1.75	0.51
2:M:244:PRO:HG2	2:M:246:ASP:OD2	2.09	0.51
2:M:137:VAL:O	2:M:391:LEU:HD21	2.10	0.51
3:N:996:TRP:CE2	3:N:1056:PRO:HG3	2.45	0.51
3:N:1123:PHE:HA	3:N:1135:ARG:H	1.75	0.51
3:N:1310:ARG:HB2	3:N:1327:ARG:HE	1.75	0.51
3:N:1396:GLU:O	3:N:1400:VAL:HG23	2.10	0.51
3:N:168:THR:HG21	8:N:9101:HOH:O	2.10	0.51
3:N:213:VAL:HG22	3:N:214:GLU:H	1.75	0.51
4:O:88:GLU:HA	4:O:91:ARG:HD2	1.93	0.51
5:P:119:ILE:HD13	5:P:170:HIS:CG	2.44	0.51
5:P:299:TRP:CZ3	5:P:303:ARG:HG2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:ASN:OD1	1:B:127:LEU:HB2	2.11	0.51
1:B:42:ARG:HH11	1:B:42:ARG:HG2	1.75	0.51
2:C:1004:LYS:O	2:C:1006:HIS:ND1	2.42	0.51
2:C:199:VAL:HG13	2:C:235:LEU:HG	1.92	0.51
2:C:574:ALA:HB1	2:C:667:ALA:HB3	1.92	0.51
2:C:72:ARG:HB2	2:C:72:ARG:HH11	1.75	0.51
2:C:701:THR:CG2	2:C:832:LYS:HG3	2.37	0.51
2:C:876:VAL:HB	2:C:877:PRO:HD3	1.92	0.51
3:D:1135:ARG:HB2	3:D:1140:ILE:HD11	1.92	0.51
3:D:1138:ALA:O	3:D:1141:GLU:HB2	2.10	0.51
3:D:1254:GLN:OE1	3:D:1254:GLN:HA	2.09	0.51
3:D:1382:THR:HG22	8:D:9873:HOH:O	2.09	0.51
3:D:181:ASP:O	3:D:185:VAL:HG23	2.11	0.51
3:D:507:ASN:HA	8:D:9186:HOH:O	2.11	0.51
3:D:889:ALA:O	3:D:929:ARG:HD2	2.11	0.51
4:E:81:PRO:HG3	8:E:183:HOH:O	2.09	0.51
1:K:115:LEU:HD13	8:K:3936:HOH:O	2.09	0.51
1:K:127:LEU:HD12	1:K:128:HIS:N	2.23	0.51
1:K:181:VAL:O	2:M:938:LYS:HD3	2.10	0.51
1:K:184:THR:O	1:K:192:LEU:HD12	2.10	0.51
1:K:72:LYS:HD2	1:K:73:GLU:OE2	2.09	0.51
2:M:191:PHE:CE2	2:M:195:LEU:HB3	2.46	0.51
2:M:22:GLN:HE22	2:M:336:VAL:HG21	1.74	0.51
2:M:254:VAL:HG13	2:M:258:TYR:HE1	1.76	0.51
2:M:274:ARG:HD2	2:M:285:LEU:HB3	1.91	0.51
2:M:4:LYS:HD3	8:M:1624:HOH:O	2.10	0.51
2:M:546:LEU:CA	2:M:581:THR:HG21	2.41	0.51
2:M:741:GLY:HA3	8:M:1430:HOH:O	2.09	0.51
3:N:127:LEU:HD11	3:N:461:ILE:HD11	1.92	0.51
3:N:1311:LEU:H	3:N:1311:LEU:HD23	1.74	0.51
3:N:491:LYS:HD3	3:N:492:ALA:N	2.25	0.51
3:N:550:ARG:HH12	3:N:577:ALA:HB2	1.76	0.51
2:M:1076:VAL:CG2	3:N:752:SER:HB3	2.40	0.51
1:A:132:LEU:HD13	8:A:356:HOH:O	2.09	0.51
2:C:183:SER:HB2	2:C:190:LYS:HD3	1.91	0.51
2:C:410:ILE:HD12	2:C:410:ILE:N	2.26	0.51
3:D:1088:THR:HA	8:D:9405:HOH:O	2.10	0.51
3:D:1393:GLN:HB2	3:D:1398:TRP:HZ2	1.75	0.51
3:D:1478:SER:OG	3:D:1481:VAL:HG23	2.11	0.51
3:D:178:LEU:HD12	3:D:200:ASP:HB2	1.93	0.51
3:D:483:HIS:ND1	3:D:483:HIS:N	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1104:GLU:HA	3:D:6:ARG:NH1	2.26	0.51
3:D:764:LEU:HD12	3:D:765:SER:H	1.75	0.51
1:L:57:TYR:CE1	1:L:161:ARG:HB3	2.46	0.51
2:M:37:GLU:HA	8:M:1458:HOH:O	2.11	0.51
2:M:420:ARG:HG2	2:M:422:ARG:HG2	1.91	0.51
3:N:957:PRO:HG2	3:N:1007:VAL:HA	1.92	0.51
3:N:1390:LEU:HD13	8:N:9614:HOH:O	2.11	0.51
3:N:498:VAL:HG12	8:N:9641:HOH:O	2.10	0.51
3:N:729:HIS:HE1	3:N:731:LEU:HG	1.75	0.51
4:O:24:ALA:O	4:O:28:GLN:HG3	2.10	0.51
4:O:47:LYS:HA	4:O:54:LEU:HB3	1.93	0.51
5:P:113:ILE:O	5:P:116:LEU:HB2	2.11	0.51
5:P:214:GLN:HA	5:P:214:GLN:OE1	2.10	0.51
5:P:412:GLU:OE1	5:P:418:LEU:HD13	2.10	0.51
1:B:105:GLY:O	1:B:132:LEU:HD23	2.09	0.51
1:B:217:ILE:O	1:B:221:HIS:ND1	2.44	0.51
1:B:91:ASN:O	1:B:94:LEU:HD12	2.11	0.51
2:C:209:ARG:O	2:C:213:ALA:HB2	2.11	0.51
2:C:958:THR:CG2	2:C:961:GLU:HB2	2.40	0.51
3:D:1320:GLU:HB2	3:D:1323:GLN:NE2	2.25	0.51
3:D:486:ARG:HA	3:D:489:ARG:HG2	1.91	0.51
3:D:543:LEU:O	3:D:546:ARG:HB2	2.11	0.51
2:C:1071:ILE:HD13	3:D:655:PRO:HB3	1.92	0.51
4:E:48:MET:CB	4:E:54:LEU:HB2	2.41	0.51
5:F:213:ILE:HG22	5:F:217:ASN:ND2	2.26	0.51
3:D:669:ASN:HB3	5:F:349:LEU:HD11	1.92	0.51
5:F:371:LEU:HD22	5:F:375:LEU:HD22	1.91	0.51
5:F:393:THR:HG22	5:F:394:ARG:H	1.76	0.51
1:L:173:PRO:HA	1:L:202:ASP:OD2	2.10	0.51
1:L:216:GLU:HG3	1:L:219:ARG:HH12	1.76	0.51
2:M:154:ARG:HH21	2:M:157:ARG:H	1.58	0.51
2:M:319:GLY:HA2	8:M:1247:HOH:O	2.11	0.51
2:M:36:PRO:HD3	8:M:1244:HOH:O	2.09	0.51
3:N:1065:LEU:CD1	3:N:1069:GLU:HB2	2.41	0.51
3:N:513:ILE:HA	8:N:9084:HOH:O	2.10	0.51
3:N:720:LEU:H	3:N:720:LEU:HD12	1.75	0.51
4:O:48:MET:HG2	4:O:49:GLN:N	2.24	0.51
4:O:86:GLN:HG2	8:O:2986:HOH:O	2.09	0.51
5:P:153:PRO:HG3	8:P:3659:HOH:O	2.10	0.51
2:C:1018:GLN:NE2	2:C:1063:ARG:HH22	2.08	0.51
2:C:15:LEU:HD12	2:C:15:LEU:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:218:VAL:HA	2:C:221:LEU:HD23	1.93	0.51
2:C:693:GLU:HG3	8:C:1199:HOH:O	2.11	0.51
2:C:6:PHE:CE2	2:C:913:GLU:HB3	2.46	0.51
2:C:701:THR:HG23	2:C:832:LYS:HA	1.92	0.51
3:D:1231:GLU:HB3	3:D:1232:PRO:HD3	1.93	0.51
3:D:1420:LEU:HD12	3:D:1421:LEU:N	2.26	0.51
3:D:550:ARG:HH11	3:D:573:MET:HB3	1.76	0.51
3:D:671:LYS:O	3:D:671:LYS:HD3	2.11	0.51
3:D:702:LEU:HG	3:D:745:MET:HE2	1.92	0.51
1:K:13:VAL:HG12	1:K:15:THR:HG22	1.93	0.51
1:L:101:LEU:HB2	1:L:114:PHE:CD2	2.46	0.51
2:M:147:TYR:HB3	2:M:323:ASP:OD2	2.11	0.51
2:M:252:LYS:HZ2	2:M:296:GLY:HA3	1.74	0.51
2:M:584:GLU:O	2:M:588:VAL:HG13	2.11	0.51
2:M:944:LEU:O	2:M:948:GLU:HG2	2.10	0.51
3:N:1176:LYS:HA	3:N:1179:GLU:CD	2.30	0.51
3:N:1183:ILE:HG22	8:N:2022:HOH:O	2.10	0.51
3:N:1363:LEU:HD12	3:N:1364:HIS:O	2.11	0.51
3:N:550:ARG:HG3	3:N:550:ARG:NH1	2.26	0.51
3:N:6:ARG:CZ	3:N:6:ARG:HB3	2.41	0.51
4:O:17:TYR:HD2	4:O:17:TYR:N	2.08	0.51
5:P:291:ILE:HG23	5:P:304:VAL:HG21	1.91	0.51
1:B:101:LEU:HB2	1:B:114:PHE:CD2	2.45	0.51
2:C:157:ARG:NH2	2:C:314:THR:HA	2.24	0.51
2:C:42:VAL:HG12	2:C:43:GLY:N	2.26	0.51
3:D:1139:ASP:O	3:D:1142:ALA:HB3	2.11	0.51
3:D:1223:ILE:HD12	3:D:1223:ILE:N	2.23	0.51
3:D:1389:LEU:HD12	3:D:1390:LEU:HG	1.93	0.51
3:D:775:GLY:HA3	3:D:1145:TYR:CE1	2.46	0.51
3:D:81:THR:O	3:D:82:LYS:O	2.28	0.51
3:D:84:ILE:O	3:D:87:ARG:HG3	2.11	0.51
3:D:561:GLY:HA3	5:F:184:ARG:HH22	1.76	0.51
3:D:563:PRO:HG3	5:F:188:ILE:HG21	1.93	0.51
5:F:264:MET:O	5:F:267:THR:HB	2.10	0.51
5:F:316:SER:HB2	5:F:319:THR:OG1	2.11	0.51
3:N:1156:LEU:HD11	3:N:1176:LYS:HD2	1.92	0.51
3:N:1372:VAL:O	3:N:1375:MET:HB2	2.10	0.51
3:N:191:LEU:HD22	3:N:195:VAL:HG21	1.92	0.51
3:N:524:LEU:C	3:N:526:PRO:HD3	2.31	0.51
3:N:550:ARG:NH1	3:N:577:ALA:HB2	2.26	0.51
3:N:554:LEU:O	3:N:558:LEU:HG	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:54:LEU:HG	4:O:58:PRO:CG	2.40	0.51
5:P:203:THR:HG22	5:P:204:GLY:N	2.26	0.51
1:B:220:GLU:HG2	8:B:449:HOH:O	2.10	0.51
2:C:113:VAL:N	8:C:1822:HOH:O	2.41	0.51
2:C:64:LEU:HD22	2:C:359:MET:CG	2.41	0.51
2:C:34:VAL:CG1	2:C:38:LYS:HG3	2.41	0.51
2:C:897:LEU:HD23	2:C:899:GLN:NE2	2.26	0.51
3:D:524:LEU:C	3:D:526:PRO:HD3	2.31	0.51
3:D:705:ALA:CB	3:D:706:PRO:HD3	2.41	0.51
3:D:790:TYR:CD1	3:D:1022:VAL:HG13	2.46	0.51
5:F:170:HIS:H	5:F:170:HIS:CD2	2.28	0.51
5:F:259:ARG:N	8:F:509:HOH:O	2.43	0.51
1:K:149:GLY:O	1:K:171:PHE:HB2	2.11	0.51
2:M:256:TYR:CE1	2:M:293:PHE:HB2	2.46	0.51
2:M:321:GLU:HG2	8:M:1221:HOH:O	2.10	0.51
2:M:571:LEU:HD12	2:M:701:THR:C	2.31	0.51
2:M:885:ILE:HD12	8:N:9188:HOH:O	2.11	0.51
3:N:1059:SER:HA	8:N:9131:HOH:O	2.11	0.51
3:N:1487:VAL:HG11	3:N:1492:LEU:HD23	1.92	0.51
3:N:1500:LYS:HD3	8:N:9564:HOH:O	2.11	0.51
5:P:256:ARG:NH2	5:P:258:ILE:HB	2.26	0.51
1:A:14:ARG:CZ	1:A:24:VAL:HG23	2.41	0.51
1:A:83:LYS:HE2	1:A:167:VAL:CG1	2.40	0.51
1:B:19:GLU:HG3	1:B:201:THR:O	2.10	0.51
2:C:21:ILE:HD12	2:C:21:ILE:H	1.74	0.51
2:C:362:GLY:HA3	2:C:367:LEU:HD22	1.92	0.51
2:C:394:PHE:H	2:C:394:PHE:HD2	1.59	0.51
2:C:577:PRO:HG3	2:C:993:PHE:CE2	2.46	0.51
3:D:1295:GLU:HB3	3:D:1300:SER:CB	2.41	0.51
3:D:152:LEU:HD23	3:D:152:LEU:N	2.23	0.51
5:F:268:ILE:HG22	8:F:510:HOH:O	2.11	0.51
5:F:336:GLU:HG2	8:F:426:HOH:O	2.11	0.51
2:M:303:PHE:HD1	8:M:1252:HOH:O	1.93	0.51
2:M:626:ARG:HB2	2:M:639:GLN:HE21	1.74	0.51
2:M:704:HIS:O	2:M:705:ILE:HG23	2.11	0.51
3:N:1144:LEU:HA	3:N:1147:ARG:HG3	1.91	0.51
3:N:1288:GLU:HA	8:N:9629:HOH:O	2.11	0.51
3:N:170:PRO:HA	8:N:9445:HOH:O	2.11	0.51
3:N:178:LEU:HA	3:N:181:ASP:OD2	2.11	0.51
3:N:195:VAL:HG22	8:N:9187:HOH:O	2.11	0.51
3:N:58:CYS:SG	3:N:59:ALA:N	2.84	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:47:LYS:N	4:O:54:LEU:HD13	2.26	0.51
4:O:83:ASP:O	4:O:86:GLN:HG3	2.11	0.51
5:P:208:SER:HB2	5:P:211:ASP:CG	2.31	0.51
5:P:287:THR:C	5:P:289:GLU:H	2.15	0.51
2:C:358:ARG:HH22	2:C:374:ASN:CB	2.11	0.50
2:C:724:ARG:NH1	2:C:734:LEU:HD23	2.20	0.50
2:C:549:PHE:CD2	2:C:886:LEU:HB3	2.47	0.50
3:D:1271:LYS:HG2	3:D:1272:ALA:N	2.25	0.50
3:D:805:GLU:OE1	3:D:809:PRO:HD2	2.11	0.50
5:F:407:LYS:HD3	8:F:437:HOH:O	2.10	0.50
1:K:227:ASN:ND2	8:K:3074:HOH:O	2.43	0.50
1:K:32:PHE:HB2	8:K:3631:HOH:O	2.11	0.50
1:K:91:ASN:H	1:K:94:LEU:CD1	2.24	0.50
1:L:176:ARG:HB2	8:N:9402:HOH:O	2.12	0.50
1:L:23:PHE:O	1:L:196:THR:HA	2.12	0.50
1:K:9:PRO:HD2	1:L:224:TYR:CZ	2.46	0.50
2:M:1107:ASN:HA	8:M:1421:HOH:O	2.11	0.50
2:M:72:ARG:HH21	2:M:112:GLU:HG3	1.76	0.50
3:N:1003:VAL:O	3:N:1006:ALA:HB3	2.10	0.50
3:N:1436:SER:HB3	8:N:9153:HOH:O	2.11	0.50
3:N:564:GLU:HA	3:N:567:ILE:HD12	1.93	0.50
3:N:576:GLU:HA	3:N:579:ASP:OD2	2.11	0.50
3:N:647:ARG:HG2	8:N:9316:HOH:O	2.11	0.50
1:A:96:THR:HB	8:A:441:HOH:O	2.09	0.50
2:C:128:ILE:HG22	8:C:1224:HOH:O	2.10	0.50
2:C:175:GLU:HB3	2:C:183:SER:OG	2.11	0.50
2:C:838:LYS:HD2	2:C:846:LYS:HZ1	1.76	0.50
3:D:1164:ARG:HG3	3:D:1164:ARG:NH1	2.25	0.50
3:D:1314:LYS:HB3	8:D:9482:HOH:O	2.10	0.50
3:D:1493:LYS:O	3:D:1497:GLU:HG2	2.10	0.50
3:D:420:VAL:HA	5:F:164:LYS:CE	2.41	0.50
3:D:642:CYS:SG	3:D:716:PHE:HB2	2.51	0.50
3:D:653:PHE:CD1	3:D:653:PHE:N	2.80	0.50
2:M:208:ALA:HA	2:M:218:VAL:HG22	1.92	0.50
2:M:208:ALA:HA	2:M:221:LEU:HD21	1.93	0.50
2:M:290:LEU:HD22	2:M:302:VAL:HG11	1.92	0.50
2:M:575:GLN:HA	2:M:662:GLU:OE2	2.11	0.50
1:K:46:SER:HB3	2:M:856:GLU:HG2	1.93	0.50
3:N:999:THR:O	3:N:1002:LYS:HB2	2.11	0.50
3:N:1119:SER:HA	3:N:1186:VAL:O	2.10	0.50
3:N:27:GLU:N	8:N:9386:HOH:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:399:ARG:HH21	3:N:432:TYR:HE2	1.59	0.50
3:N:422:ALA:O	3:N:427:VAL:HG21	2.11	0.50
5:P:278:LEU:HB3	5:P:286:PRO:HG2	1.94	0.50
1:A:115:LEU:O	1:A:115:LEU:HD12	2.12	0.50
1:B:173:PRO:HB2	1:B:205:VAL:HG22	1.92	0.50
2:C:1097:LEU:CD2	2:C:1097:LEU:H	2.19	0.50
2:C:157:ARG:HD3	2:C:158:TYR:H	1.76	0.50
2:C:288:ARG:HH11	2:C:288:ARG:HB2	1.76	0.50
2:C:256:TYR:HE1	2:C:293:PHE:HB2	1.73	0.50
2:C:405:ARG:HH12	2:C:563:ASN:HD21	1.57	0.50
2:C:497:ALA:HA	2:C:515:ALA:HA	1.93	0.50
2:C:625:LEU:HB3	2:C:639:GLN:HG3	1.93	0.50
2:C:679:PHE:C	3:D:943:THR:HG22	2.31	0.50
2:C:712:ALA:HB1	2:C:820:ARG:HH11	1.76	0.50
2:C:969:GLN:HA	8:D:9594:HOH:O	2.11	0.50
3:D:1152:GLU:CD	3:D:1159:ARG:HH12	2.15	0.50
3:D:1271:LYS:HE3	3:D:1334:GLN:HE22	1.75	0.50
3:D:195:VAL:HG13	8:D:9005:HOH:O	2.11	0.50
3:D:428:LYS:HB3	3:D:450:TYR:CE1	2.46	0.50
3:D:480:GLU:O	3:D:484:PRO:HD2	2.11	0.50
3:D:633:VAL:HG22	3:D:635:PRO:CD	2.40	0.50
1:K:54:THR:HG23	1:K:156:HIS:CE1	2.46	0.50
2:M:350:ARG:HD3	2:M:353:ARG:HH22	1.76	0.50
3:N:183:GLU:HA	3:N:186:VAL:CG1	2.42	0.50
4:O:84:ARG:CZ	4:O:84:ARG:HB2	2.42	0.50
1:A:97:VAL:HG12	1:A:99:LEU:HD12	1.93	0.50
1:B:84:GLU:HB3	1:B:127:LEU:HD21	1.92	0.50
2:C:1088:LEU:HB2	8:D:9002:HOH:O	2.10	0.50
2:C:175:GLU:HA	8:C:1786:HOH:O	2.11	0.50
2:C:404:LEU:O	2:C:407:LYS:HB2	2.11	0.50
2:C:66:LEU:HB2	8:C:1196:HOH:O	2.11	0.50
3:D:1047:LYS:HB2	3:D:1051:GLU:OE2	2.10	0.50
3:D:1117:TYR:HE2	3:D:1151:ARG:HH21	1.59	0.50
3:D:111:LYS:CE	3:D:1452:ILE:HG12	2.40	0.50
3:D:1200:VAL:HG22	3:D:1373:ARG:HH12	1.76	0.50
3:D:960:LYS:HZ2	3:D:1041:LEU:HB3	1.77	0.50
4:E:17:TYR:O	4:E:21:VAL:HG23	2.11	0.50
5:F:142:ARG:HB3	5:F:142:ARG:HH11	1.77	0.50
1:K:86:VAL:HG12	1:K:124:ASN:HD22	1.76	0.50
1:L:33:GLY:O	1:L:195:LEU:HD22	2.11	0.50
2:M:1067:TYR:HA	2:M:1070:ILE:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:333:ILE:O	2:M:465:GLY:HA3	2.11	0.50
2:M:706:GLU:HB3	2:M:708:TYR:CE1	2.47	0.50
3:N:1097:LYS:HD2	8:N:9081:HOH:O	2.10	0.50
3:N:1258:ARG:HG3	3:N:1262:LEU:HD22	1.92	0.50
3:N:1422:MET:HE2	8:N:9147:HOH:O	2.11	0.50
3:N:554:LEU:HD21	3:N:571:LYS:HG3	1.93	0.50
3:N:639:LEU:HD12	3:N:639:LEU:N	2.25	0.50
5:P:164:LYS:HD2	8:P:4625:HOH:O	2.10	0.50
5:P:132:ARG:HE	5:P:184:ARG:NH1	2.07	0.50
1:A:44:LEU:O	1:A:174:VAL:HG21	2.12	0.50
2:C:254:VAL:HG13	2:C:258:TYR:CE1	2.44	0.50
2:C:572:ILE:CG2	2:C:703:ILE:HD13	2.41	0.50
2:C:722:ILE:HD13	2:C:722:ILE:O	2.12	0.50
2:C:876:VAL:O	2:C:879:ARG:O	2.29	0.50
2:C:432:ARG:HD3	3:D:1048:PRO:HG2	1.92	0.50
3:D:1119:SER:HA	3:D:1186:VAL:O	2.11	0.50
3:D:1429:LEU:HG	3:D:1441:GLN:OE1	2.11	0.50
3:D:526:PRO:O	3:D:537:THR:HA	2.12	0.50
3:D:762:GLN:NE2	4:E:20:THR:HG21	2.27	0.50
3:D:904:VAL:HG22	8:D:9514:HOH:O	2.09	0.50
5:F:149:GLU:OE1	5:F:149:GLU:HA	2.11	0.50
1:K:173:PRO:HB3	1:K:204:SER:HB3	1.93	0.50
1:L:132:LEU:HD21	1:L:136:GLY:O	2.12	0.50
2:M:1016:ILE:HD13	2:M:1016:ILE:N	2.27	0.50
2:M:199:VAL:HG13	2:M:235:LEU:CG	2.39	0.50
2:M:680:ASP:HB2	2:M:682:TYR:CE2	2.46	0.50
2:M:755:LEU:HB2	2:M:790:LEU:CD2	2.40	0.50
2:M:707:ARG:HG3	2:M:826:TYR:CE2	2.46	0.50
3:N:1090:ASP:O	3:N:1093:TYR:HB3	2.12	0.50
3:N:1263:PHE:CD2	3:N:1371:VAL:HG11	2.47	0.50
3:N:175:VAL:HG11	8:N:9190:HOH:O	2.11	0.50
3:N:699:VAL:N	3:N:756:GLN:NE2	2.53	0.50
5:P:102:LEU:O	5:P:106:VAL:HG23	2.12	0.50
5:P:113:ILE:HG23	5:P:127:ILE:CG2	2.41	0.50
8:N:9535:HOH:O	5:P:140:ARG:HB2	2.10	0.50
1:A:213:GLN:O	1:A:217:ILE:HG13	2.11	0.50
1:B:11:PHE:CD1	1:B:25:LEU:HD13	2.47	0.50
1:B:158:ILE:HA	8:B:396:HOH:O	2.11	0.50
2:C:72:ARG:HD3	8:C:1601:HOH:O	2.12	0.50
3:D:1205:TYR:HE1	3:D:1221:VAL:CG1	2.23	0.50
3:D:1105:ILE:HD11	3:D:1374:GLN:NE2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1396:GLU:O	3:D:1400:VAL:HG23	2.12	0.50
3:D:178:LEU:CD2	3:D:199:LEU:H	2.24	0.50
3:D:470:LEU:HD12	3:D:508:ARG:HH21	1.77	0.50
3:D:902:LEU:HD12	3:D:902:LEU:H	1.76	0.50
1:K:173:PRO:HB2	1:K:205:VAL:HG22	1.93	0.50
1:K:56:VAL:HG21	1:K:82:LEU:HD12	1.93	0.50
1:L:81:ASN:HB2	8:L:2800:HOH:O	2.12	0.50
2:M:139:GLN:O	2:M:334:ARG:N	2.43	0.50
2:M:165:LEU:HD12	2:M:166:PRO:C	2.32	0.50
2:M:191:PHE:CD2	2:M:238:LEU:HD21	2.47	0.50
2:M:377:PRO:HA	8:M:1544:HOH:O	2.11	0.50
2:M:589:ARG:HD2	8:M:1552:HOH:O	2.12	0.50
2:M:852:ILE:N	2:M:852:ILE:HD12	2.27	0.50
2:M:853:LEU:HD23	2:M:858:MET:HB3	1.94	0.50
3:N:951:ILE:CG2	3:N:1062:ARG:HH21	2.24	0.50
3:N:1335:LEU:HD23	3:N:1344:VAL:HG22	1.94	0.50
3:N:21:TRP:HZ3	3:N:518:PRO:HG2	1.77	0.50
5:P:287:THR:N	5:P:290:GLU:OE1	2.44	0.50
5:P:412:GLU:HG3	5:P:418:LEU:HD22	1.92	0.50
1:A:13:VAL:HG12	1:A:15:THR:HG22	1.94	0.50
1:A:156:HIS:CD2	1:A:157:GLY:H	2.29	0.50
1:A:206:THR:CG2	1:A:209:GLU:HG3	2.39	0.50
1:A:26:GLU:HG2	1:A:27:PRO:HA	1.94	0.50
2:C:103:LYS:HG3	8:C:1421:HOH:O	2.12	0.50
2:C:1101:THR:HB	3:D:5:VAL:HG13	1.92	0.50
2:C:18:LEU:HB2	2:C:590:ASP:HB3	1.93	0.50
2:C:195:LEU:CD2	2:C:238:LEU:HG	2.42	0.50
2:C:136:ILE:HG21	2:C:336:VAL:HG13	1.93	0.50
2:C:437:ARG:HA	2:C:467:ILE:CG2	2.40	0.50
2:C:534:VAL:HB	2:C:538:GLN:NE2	2.27	0.50
2:C:572:ILE:HG21	2:C:703:ILE:HD13	1.92	0.50
3:D:1009:LYS:O	3:D:1012:GLU:HG2	2.11	0.50
3:D:1147:ARG:O	3:D:1166:LEU:HD23	2.11	0.50
3:D:7:LYS:HD3	3:D:1456:LYS:NZ	2.26	0.50
3:D:396:VAL:HG13	3:D:446:VAL:O	2.12	0.50
3:D:399:ARG:NH2	3:D:432:TYR:HE2	2.09	0.50
3:D:661:MET:CE	3:D:673:ALA:HB1	2.40	0.50
5:F:289:GLU:O	5:F:293:GLU:HG3	2.11	0.50
8:C:1739:HOH:O	5:F:370:LYS:HG2	2.12	0.50
1:K:42:ARG:HG2	1:K:42:ARG:HH11	1.76	0.50
2:M:1027:PHE:HA	8:M:1757:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:214:TYR:HB2	8:M:1457:HOH:O	2.12	0.50
2:M:428:ARG:HG2	2:M:451:LEU:HG	1.93	0.50
2:M:704:HIS:CG	2:M:831:ARG:HH21	2.30	0.50
2:M:837:ASP:O	2:M:848:VAL:HG13	2.12	0.50
2:M:889:HIS:CD2	2:M:970:GLY:HA3	2.46	0.50
3:N:186:VAL:HG13	3:N:187:LYS:N	2.27	0.50
3:N:207:PHE:CB	3:N:208:PRO:HD2	2.35	0.50
3:N:30:GLU:HB3	3:N:40:GLU:HB3	1.93	0.50
3:N:574:LEU:O	3:N:578:VAL:HG23	2.11	0.50
5:P:108:GLU:OE1	5:P:108:GLU:HA	2.12	0.50
2:C:197:LEU:HD22	2:C:202:TYR:HD2	1.76	0.50
2:C:404:LEU:HD22	2:C:591:SER:HB3	1.93	0.50
2:C:627:ARG:O	2:C:638:ASP:HB3	2.12	0.50
3:D:1192:LEU:HG	3:D:1369:GLU:HG2	1.92	0.50
3:D:404:GLU:HB3	3:D:414:ARG:HD3	1.94	0.50
3:D:690:ALA:O	3:D:694:VAL:HG23	2.12	0.50
3:D:834:THR:HB	3:D:838:ARG:HB3	1.92	0.50
3:D:916:TYR:CE2	3:D:920:LEU:HD13	2.46	0.50
8:D:9410:HOH:O	5:F:147:LEU:HD11	2.11	0.50
5:F:404:ALA:O	5:F:408:LEU:HD23	2.12	0.50
2:M:228:ALA:HB2	8:M:1214:HOH:O	2.11	0.50
2:M:955:PRO:HA	8:M:1188:HOH:O	2.11	0.50
3:N:1114:THR:CG2	3:N:1195:GLN:HB3	2.41	0.50
3:N:148:GLU:HB3	3:N:151:GLN:HB3	1.93	0.50
3:N:421:LEU:HD11	3:N:437:VAL:CG2	2.42	0.50
3:N:462:GLN:HA	3:N:513:ILE:HD13	1.94	0.50
3:N:898:GLU:HB3	3:N:921:ARG:HH22	1.76	0.50
1:A:42:ARG:NH2	1:B:34:VAL:HB	2.27	0.50
2:C:1045:ALA:HB1	2:C:1048:THR:HB	1.94	0.50
2:C:157:ARG:CD	2:C:314:THR:HG22	2.40	0.50
2:C:464:LEU:O	2:C:466:PHE:N	2.45	0.50
2:C:437:ARG:CZ	2:C:469:THR:HG22	2.42	0.50
3:D:1230:GLY:HA3	8:D:9051:HOH:O	2.11	0.50
3:D:15:PRO:HA	3:D:18:ILE:CG1	2.41	0.50
3:D:42:ASP:O	3:D:43:GLY:O	2.29	0.50
3:D:462:GLN:HA	3:D:513:ILE:CD1	2.41	0.50
3:D:658:LEU:HD11	3:D:674:ARG:HH11	1.77	0.50
3:D:864:VAL:HG12	3:D:865:THR:H	1.77	0.50
3:D:965:GLU:HA	3:D:968:ASP:HB2	1.94	0.50
5:F:255:ALA:HB3	8:F:561:HOH:O	2.11	0.50
2:M:136:ILE:CG2	2:M:336:VAL:HG13	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:751:PRO:HA	2:M:792:VAL:CG1	2.42	0.50
3:N:16:GLU:HB2	8:N:9939:HOH:O	2.11	0.50
3:N:428:LYS:HB3	3:N:450:TYR:CE1	2.46	0.50
3:N:9:ARG:HH22	3:N:507:ASN:HD21	1.60	0.50
3:N:813:LEU:HD12	3:N:817:GLU:OE1	2.12	0.50
3:N:846:PRO:HD3	8:N:9226:HOH:O	2.10	0.50
5:P:419:ARG:HG3	5:P:420:ASP:N	2.26	0.50
1:B:145:ASP:O	1:B:171:PHE:HE1	1.94	0.49
2:C:137:VAL:HG22	2:C:391:LEU:O	2.12	0.49
2:C:218:VAL:HG22	2:C:221:LEU:HD23	1.93	0.49
2:C:437:ARG:HB3	2:C:467:ILE:HB	1.93	0.49
2:C:630:ARG:HH11	2:C:630:ARG:HG2	1.76	0.49
3:D:1003:VAL:O	3:D:1007:VAL:HG13	2.12	0.49
3:D:1102:THR:HG22	3:D:1222:GLY:CA	2.41	0.49
3:D:400:VAL:HG12	3:D:401:TYR:HD1	1.75	0.49
2:C:1044:GLY:CA	4:E:17:TYR:HE1	2.25	0.49
4:E:66:LYS:HB2	4:E:66:LYS:NZ	2.26	0.49
1:K:49:PRO:HB3	1:K:148:VAL:HG22	1.94	0.49
1:K:64:GLU:HB2	8:K:3487:HOH:O	2.10	0.49
2:M:723:THR:HG21	2:M:783:ARG:HH22	1.77	0.49
2:M:86:LYS:CG	2:M:813:VAL:HG12	2.41	0.49
3:N:1397:LYS:O	3:N:1400:VAL:HB	2.12	0.49
3:N:1481:VAL:HA	4:O:18:ARG:HH21	1.77	0.49
3:N:183:GLU:O	3:N:186:VAL:HG12	2.12	0.49
3:N:427:VAL:HG21	3:N:435:VAL:HB	1.93	0.49
3:N:543:LEU:O	3:N:546:ARG:HB2	2.11	0.49
3:N:733:CYS:HA	8:N:9159:HOH:O	2.12	0.49
3:N:836:VAL:HA	3:N:839:LEU:HB2	1.94	0.49
1:A:219:ARG:CZ	1:B:223:THR:HG23	2.42	0.49
2:C:1004:LYS:HE3	2:C:1027:PHE:CE1	2.45	0.49
2:C:217:LEU:HA	8:C:1241:HOH:O	2.10	0.49
2:C:551:GLU:HB3	2:C:906:PHE:HD2	1.77	0.49
2:C:761:PHE:CD1	2:C:761:PHE:N	2.80	0.49
3:D:1197:ARG:HG3	8:D:9036:HOH:O	2.10	0.49
3:D:1310:ARG:HG2	3:D:1327:ARG:HB3	1.94	0.49
3:D:1363:LEU:HD12	3:D:1364:HIS:O	2.12	0.49
3:D:191:LEU:HD22	3:D:195:VAL:HG21	1.94	0.49
3:D:549:ASN:HB3	8:F:611:HOH:O	2.12	0.49
3:D:630:VAL:HG23	3:D:744:GLN:OE1	2.12	0.49
4:E:86:GLN:O	4:E:90:GLU:HG3	2.12	0.49
5:F:167:PRO:HD2	5:F:170:HIS:CD2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:211:LEU:O	1:K:215:VAL:HG22	2.12	0.49
1:K:66:SER:O	1:K:75:VAL:HG23	2.12	0.49
2:M:157:ARG:HA	2:M:157:ARG:NE	2.27	0.49
2:M:259:GLY:HA3	8:M:1296:HOH:O	2.11	0.49
2:M:49:ARG:NH1	2:M:49:ARG:HB2	2.27	0.49
2:M:508:ILE:HG21	8:M:1319:HOH:O	2.12	0.49
2:M:745:ILE:HD11	8:M:1269:HOH:O	2.11	0.49
2:M:826:TYR:N	2:M:826:TYR:CD1	2.80	0.49
3:N:1496:GLU:O	3:N:1500:LYS:HG3	2.12	0.49
3:N:583:ASP:HA	3:N:602:SER:HB2	1.93	0.49
3:N:60:CYS:SG	3:N:62:LYS:HG2	2.52	0.49
4:O:39:VAL:HB	4:O:72:ARG:HD2	1.94	0.49
5:P:142:ARG:HH11	5:P:142:ARG:HB3	1.76	0.49
1:A:61:VAL:HG12	8:A:482:HOH:O	2.12	0.49
2:C:141:HIS:ND1	2:C:418:LEU:HG	2.27	0.49
2:C:710:ILE:CB	2:C:790:LEU:HD13	2.39	0.49
3:D:1205:TYR:HD2	8:D:9465:HOH:O	1.95	0.49
3:D:1213:ARG:HB2	3:D:1214:PRO:HD3	1.92	0.49
3:D:197:SER:CB	3:D:203:ALA:HB3	2.28	0.49
3:D:525:ARG:HB2	3:D:541:ASN:ND2	2.26	0.49
3:D:850:LEU:O	3:D:853:VAL:HB	2.12	0.49
1:L:62:LEU:HD12	8:L:2996:HOH:O	2.12	0.49
2:M:170:PRO:HG2	2:M:258:TYR:HD2	1.76	0.49
2:M:708:TYR:N	2:M:708:TYR:CD1	2.79	0.49
3:N:1168:MET:HE2	3:N:1168:MET:O	2.11	0.49
3:N:1225:ALA:HA	3:N:1367:HIS:ND1	2.27	0.49
3:N:1263:PHE:CE2	3:N:1371:VAL:HG11	2.48	0.49
3:N:1281:VAL:HG21	3:N:1313:VAL:CG2	2.43	0.49
3:N:9:ARG:HG3	3:N:1455:LYS:C	2.33	0.49
3:N:379:ALA:HB2	8:N:9176:HOH:O	2.12	0.49
3:N:462:GLN:HB3	8:N:9127:HOH:O	2.12	0.49
3:N:474:GLU:O	3:N:478:LEU:HG	2.12	0.49
3:N:645:PRO:HG3	3:N:725:SER:O	2.13	0.49
3:N:844:ALA:HA	3:N:867:ARG:NH1	2.27	0.49
1:B:27:PRO:HB3	1:B:192:LEU:HD22	1.93	0.49
2:C:146:VAL:HG13	2:C:161:SER:O	2.12	0.49
2:C:443:THR:HG23	2:C:449:ILE:HD12	1.92	0.49
2:C:503:LEU:HD13	2:C:507:ARG:O	2.12	0.49
2:C:15:LEU:HD13	2:C:586:ARG:HG3	1.94	0.49
3:D:1105:ILE:HA	8:D:9253:HOH:O	2.12	0.49
3:D:1283:ILE:N	3:D:1315:ASP:OD1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:111:LYS:HE2	3:D:1452:ILE:HG21	1.95	0.49
3:D:395:VAL:HG12	8:D:2022:HOH:O	2.11	0.49
3:D:809:PRO:O	3:D:812:ALA:HB3	2.12	0.49
3:D:87:ARG:CB	3:D:523:ASP:HB2	2.41	0.49
3:D:85:VAL:HG12	3:D:89:ARG:NE	2.28	0.49
4:E:55:PHE:HB3	8:E:116:HOH:O	2.12	0.49
2:C:777:ILE:HA	5:F:405:LEU:HD21	1.93	0.49
1:K:57:TYR:CE2	1:K:161:ARG:HD2	2.47	0.49
1:K:68:ILE:HG21	1:K:138:LEU:CD1	2.42	0.49
1:L:101:LEU:HD11	1:L:113:ASP:HB2	1.95	0.49
1:L:57:TYR:CE2	1:L:161:ARG:HG2	2.47	0.49
2:M:490:GLU:HG2	2:M:494:TYR:CE1	2.47	0.49
2:M:92:ALA:HB2	2:M:120:LEU:CD1	2.34	0.49
3:N:203:ALA:HA	8:N:9962:HOH:O	2.13	0.49
2:M:1118:LYS:HG2	3:N:23:TYR:HE1	1.78	0.49
3:N:781:PRO:HB3	3:N:785:ILE:CG2	2.42	0.49
3:N:7:LYS:HD3	3:N:1456:LYS:NZ	2.28	0.49
3:N:868:TYR:HE2	3:N:880:ILE:HD11	1.78	0.49
5:P:107:GLU:HG3	8:P:4460:HOH:O	2.11	0.49
5:P:218:GLN:HE21	5:P:221:ILE:HD12	1.78	0.49
5:P:247:ILE:O	5:P:251:ILE:HG13	2.13	0.49
5:P:363:GLU:HA	5:P:367:MET:CE	2.42	0.49
5:P:358:LEU:CD1	5:P:370:LYS:HG3	2.38	0.49
1:B:101:LEU:HD12	1:B:114:PHE:CE1	2.47	0.49
2:C:147:TYR:HE2	2:C:280:LYS:HZ3	1.59	0.49
2:C:327:HIS:HD2	2:C:433:THR:OG1	1.96	0.49
2:C:461:VAL:HG22	8:C:1321:HOH:O	2.12	0.49
2:C:551:GLU:HG3	2:C:552:HIS:CD2	2.48	0.49
2:C:577:PRO:HA	2:C:671:ASN:OD1	2.13	0.49
2:C:710:ILE:HB	2:C:790:LEU:HD22	1.94	0.49
3:D:1107:VAL:CG1	3:D:1217:ILE:HA	2.43	0.49
3:D:1240:THR:O	3:D:1257:PRO:HB3	2.11	0.49
3:D:473:LEU:HD21	3:D:495:ARG:CZ	2.42	0.49
3:D:44:LEU:HB3	3:D:525:ARG:HH21	1.77	0.49
3:D:543:LEU:HA	3:D:546:ARG:HG3	1.93	0.49
4:E:26:ARG:HE	4:E:30:LEU:CD1	2.25	0.49
5:F:203:THR:HB	8:F:436:HOH:O	2.11	0.49
5:F:287:THR:C	5:F:289:GLU:H	2.15	0.49
5:F:299:TRP:CE3	5:F:303:ARG:HD3	2.47	0.49
1:K:65:PHE:CE1	2:M:799:ILE:HD11	2.46	0.49
2:M:937:ASP:HB2	2:M:940:GLU:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1197:ARG:HD2	3:N:1198:TYR:CE1	2.48	0.49
3:N:119:SER:HB2	3:N:123:LEU:CB	2.38	0.49
3:N:720:LEU:HD12	8:N:9443:HOH:O	2.12	0.49
3:N:970:LYS:HE3	8:N:9931:HOH:O	2.13	0.49
3:N:570:GLU:OE2	5:P:214:GLN:HG3	2.12	0.49
5:P:260:ILE:CG2	5:P:264:MET:HB2	2.41	0.49
5:P:291:ILE:HB	8:P:4032:HOH:O	2.13	0.49
5:P:323:ASP:C	5:P:325:LYS:H	2.15	0.49
1:A:187:GLY:HA3	8:A:335:HOH:O	2.11	0.49
2:C:328:LEU:HB2	2:C:433:THR:CG2	2.42	0.49
2:C:422:ARG:HG2	8:C:1141:HOH:O	2.12	0.49
2:C:332:ARG:NE	2:C:464:LEU:HD11	2.28	0.49
2:C:479:VAL:HG22	2:C:508:ILE:HD13	1.95	0.49
2:C:609:ASN:ND2	2:C:627:ARG:NH2	2.58	0.49
8:A:501:HOH:O	2:C:644:VAL:HG13	2.13	0.49
2:C:726:ILE:O	2:C:726:ILE:HG22	2.11	0.49
2:C:896:PHE:O	2:C:924:VAL:HG11	2.12	0.49
3:D:1141:GLU:HG2	3:D:1168:MET:CE	2.43	0.49
3:D:1289:LYS:HE3	3:D:1307:LYS:CE	2.41	0.49
3:D:785:ILE:HG22	3:D:789:LEU:HD12	1.94	0.49
3:D:862:ASP:O	3:D:877:PRO:HD3	2.12	0.49
3:D:96:ALA:CB	3:D:554:LEU:HD12	2.42	0.49
5:F:277:GLN:O	5:F:280:GLN:HB3	2.12	0.49
5:F:419:ARG:O	5:F:421:PHE:N	2.46	0.49
1:L:102:LYS:HG3	1:L:139:ASN:CB	2.42	0.49
1:L:196:THR:HB	8:L:4937:HOH:O	2.11	0.49
1:L:84:GLU:HG3	1:L:127:LEU:HD22	1.94	0.49
2:M:1060:ILE:HG22	2:M:1061:GLU:N	2.28	0.49
2:M:139:GLN:HE22	2:M:415:PRO:CD	2.25	0.49
2:M:420:ARG:HD2	2:M:420:ARG:H	1.76	0.49
2:M:802:ARG:HD2	8:M:1213:HOH:O	2.12	0.49
2:M:882:LEU:HD12	3:N:1061:PHE:HB3	1.95	0.49
2:M:861:LEU:HD21	2:M:925:TYR:CE2	2.48	0.49
2:M:965:GLU:HA	2:M:968:LEU:HD12	1.94	0.49
3:N:1139:ASP:O	3:N:1142:ALA:HB3	2.13	0.49
3:N:121:THR:C	8:N:9808:HOH:O	2.51	0.49
3:N:133:ILE:HG23	3:N:455:ARG:N	2.28	0.49
3:N:135:LEU:CD1	3:N:147:VAL:HG23	2.41	0.49
3:N:169:TYR:N	3:N:170:PRO:CD	2.76	0.49
3:N:28:LYS:CB	3:N:41:ARG:HD2	2.43	0.49
3:N:567:ILE:C	3:N:571:LYS:HZ2	2.16	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:728:LEU:HD12	8:N:9339:HOH:O	2.12	0.49
3:N:890:VAL:CG1	3:N:926:LYS:HD3	2.42	0.49
3:N:906:GLN:HA	3:N:906:GLN:OE1	2.11	0.49
1:A:72:LYS:HB3	1:A:73:GLU:OE2	2.13	0.49
2:C:274:ARG:HG3	2:C:274:ARG:O	2.13	0.49
2:C:366:SER:O	2:C:367:LEU:HD23	2.12	0.49
2:C:433:THR:O	2:C:433:THR:HG22	2.13	0.49
2:C:589:ARG:HG2	8:C:1213:HOH:O	2.12	0.49
3:D:916:TYR:HH	3:D:1145:TYR:HH	1.60	0.49
3:D:124:GLU:HG2	3:D:128:TYR:CZ	2.47	0.49
3:D:1403:LEU:O	3:D:1407:LEU:HB2	2.11	0.49
3:D:156:GLU:N	3:D:156:GLU:CD	2.66	0.49
3:D:131:LYS:HB3	3:D:456:MET:CE	2.43	0.49
4:E:51:LEU:CD1	4:E:52:GLU:H	2.26	0.49
1:L:20:TYR:HE2	1:L:198:ARG:HB3	1.78	0.49
2:M:332:ARG:NE	2:M:464:LEU:HG	2.28	0.49
2:M:333:ILE:HD13	2:M:467:ILE:HG13	1.93	0.49
2:M:580:MET:HB3	2:M:584:GLU:OE2	2.13	0.49
2:M:768:THR:O	2:M:772:ARG:HB3	2.12	0.49
3:N:957:PRO:HG2	3:N:1007:VAL:HG12	1.94	0.49
3:N:27:GLU:O	3:N:28:LYS:HD2	2.13	0.49
3:N:574:LEU:O	3:N:577:ALA:HB3	2.11	0.49
3:N:602:SER:O	3:N:606:ILE:HG12	2.13	0.49
3:N:1476:THR:CG2	4:O:21:VAL:HG22	2.36	0.49
4:O:54:LEU:HB3	8:O:4983:HOH:O	2.12	0.49
5:P:142:ARG:NH1	5:P:142:ARG:HB3	2.26	0.49
5:P:184:ARG:O	5:P:188:ILE:HG13	2.12	0.49
1:B:65:PHE:HD1	3:D:813:LEU:HD22	1.76	0.49
2:C:84:ARG:HH21	2:C:128:ILE:HD11	1.78	0.49
2:C:172:ILE:HD12	2:C:172:ILE:N	2.27	0.49
2:C:412:ALA:CB	2:C:451:LEU:HB3	2.42	0.49
2:C:717:LEU:HB3	8:C:1140:HOH:O	2.13	0.49
2:C:751:PRO:HA	2:C:792:VAL:CG1	2.42	0.49
3:D:1157:GLY:HA3	8:D:9057:HOH:O	2.11	0.49
3:D:1206:GLY:HA3	3:D:1366:LYS:NZ	2.27	0.49
3:D:229:ALA:HA	8:D:2026:HOH:O	2.12	0.49
3:D:436:GLU:HB2	3:D:445:ARG:HB3	1.93	0.49
3:D:493:ARG:HD2	8:D:9698:HOH:O	2.13	0.49
3:D:696:HIS:HD2	4:E:59:ASN:HB2	1.74	0.49
3:D:790:TYR:CG	3:D:1026:SER:HB3	2.48	0.49
3:D:939:PHE:O	3:D:943:THR:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:404:ALA:HA	8:F:429:HOH:O	2.12	0.49
2:M:345:ARG:HH11	2:M:345:ARG:HB3	1.77	0.49
2:M:492:ASP:HB3	2:M:518:LYS:CD	2.42	0.49
2:M:62:GLY:O	2:M:103:LYS:HG3	2.13	0.49
2:M:571:LEU:HD23	2:M:670:GLN:HE21	1.77	0.49
2:M:770:GLU:HB2	8:N:9595:HOH:O	2.12	0.49
3:N:1007:VAL:HG23	3:N:1008:PHE:N	2.28	0.49
3:N:1314:LYS:HE2	3:N:1317:ASP:OD2	2.12	0.49
3:N:1442:ASN:HA	8:N:9244:HOH:O	2.11	0.49
3:N:687:VAL:O	3:N:690:ALA:HB3	2.12	0.49
5:P:128:ARG:O	5:P:132:ARG:HG2	2.13	0.49
5:P:181:GLU:O	5:P:184:ARG:HB3	2.13	0.49
1:A:95:GLN:HG2	1:A:146:ARG:NH2	2.14	0.49
1:B:57:TYR:CE1	1:B:163:ASN:HB2	2.46	0.49
2:C:100:LEU:HD12	2:C:101:ILE:O	2.12	0.49
2:C:397:GLU:HA	2:C:403:SER:HB3	1.94	0.49
2:C:637:LEU:HD13	8:C:1532:HOH:O	2.12	0.49
2:C:536:PRO:HB3	2:C:906:PHE:HD1	1.77	0.49
3:D:1148:VAL:HG11	3:D:1203:LYS:HD2	1.95	0.49
3:D:1290:LEU:CD2	3:D:1291:SER:H	2.25	0.49
3:D:1431:THR:HB	8:D:9481:HOH:O	2.13	0.49
3:D:440:VAL:HG22	8:D:9349:HOH:O	2.13	0.49
5:F:395:GLU:O	5:F:399:GLN:HB2	2.13	0.49
2:M:139:GLN:HG3	2:M:140:ILE:N	2.26	0.49
2:M:326:ASP:HB2	2:M:431:HIS:CE1	2.48	0.49
2:M:525:SER:H	2:M:528:GLU:HG3	1.77	0.49
2:M:758:ARG:HB3	2:M:788:THR:O	2.13	0.49
2:M:841:ASN:ND2	2:M:844:GLY:H	2.11	0.49
3:N:1147:ARG:O	3:N:1166:LEU:HD23	2.13	0.49
3:N:674:ARG:HG2	3:N:674:ARG:HH11	1.76	0.49
3:N:704:ARG:HG3	3:N:736:PHE:CB	2.43	0.49
3:N:68:PHE:HA	3:N:71:LYS:HZ1	1.78	0.49
1:A:62:LEU:HB3	1:A:163:ASN:HD21	1.78	0.49
2:C:207:LEU:HD22	2:C:221:LEU:HD22	1.95	0.49
2:C:603:VAL:HG12	8:C:1221:HOH:O	2.13	0.49
3:D:1101:VAL:HG22	3:D:1428:ALA:HB2	1.95	0.49
3:D:959:GLU:CD	3:D:959:GLU:H	2.16	0.49
4:E:84:ARG:NH1	4:E:84:ARG:HB2	2.26	0.49
5:F:142:ARG:HG3	8:F:482:HOH:O	2.12	0.49
5:F:362:SER:C	5:F:364:ARG:H	2.15	0.49
1:K:96:THR:HG21	8:K:3321:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:285:LEU:O	2:M:285:LEU:HD23	2.13	0.49
2:M:497:ALA:HA	2:M:515:ALA:HA	1.94	0.49
2:M:614:ARG:CD	2:M:620:LEU:HD12	2.36	0.49
2:M:722:ILE:O	2:M:722:ILE:HG23	2.13	0.49
3:N:466:LYS:HB2	8:N:9423:HOH:O	2.12	0.49
3:N:558:LEU:HD13	5:P:145:PRO:CB	2.40	0.49
3:N:99:ALA:HA	3:N:575:GLN:NE2	2.28	0.49
3:N:948:THR:O	3:N:949:ILE:HD13	2.13	0.49
4:O:48:MET:N	4:O:54:LEU:HB2	2.28	0.49
4:O:54:LEU:HD23	4:O:58:PRO:HD2	1.94	0.49
5:P:176:ILE:HD12	8:P:3516:HOH:O	2.13	0.49
1:B:89:PHE:CD1	1:B:120:VAL:HG13	2.48	0.48
2:C:137:VAL:O	2:C:391:LEU:HD21	2.13	0.48
2:C:166:PRO:HD2	8:C:1392:HOH:O	2.13	0.48
2:C:286:SER:HB3	8:C:1755:HOH:O	2.12	0.48
2:C:292:ARG:HB2	2:C:299:LYS:HE2	1.95	0.48
2:C:352:ALA:HA	2:C:355:VAL:CG1	2.42	0.48
3:D:1109:GLU:HG2	3:D:1201:CYS:CA	2.39	0.48
3:D:32:ILE:HG12	3:D:38:LYS:O	2.13	0.48
1:K:100:LEU:HD11	8:K:4816:HOH:O	2.13	0.48
1:L:32:PHE:O	1:L:36:LEU:HD23	2.12	0.48
2:M:998:TYR:CZ	2:M:1000:MET:HA	2.48	0.48
2:M:200:LEU:HD13	2:M:300:ASP:OD2	2.13	0.48
2:M:510:ALA:HA	8:M:1122:HOH:O	2.13	0.48
2:M:537:LYS:CA	2:M:545:ASN:HD21	2.22	0.48
2:M:589:ARG:CB	2:M:589:ARG:HH11	2.23	0.48
2:M:721:ARG:O	2:M:758:ARG:HA	2.13	0.48
2:M:778:PHE:HD2	8:M:1700:HOH:O	1.95	0.48
2:M:810:ASP:HB3	2:M:813:VAL:HG22	1.95	0.48
3:N:1108:ARG:HH21	3:N:1198:TYR:C	2.16	0.48
3:N:433:GLY:HA3	3:N:450:TYR:HD1	1.78	0.48
3:N:550:ARG:CZ	3:N:573:MET:HB3	2.43	0.48
3:N:890:VAL:HG12	8:N:9462:HOH:O	2.12	0.48
1:A:198:ARG:C	1:A:199:ILE:HD12	2.34	0.48
1:B:18:ARG:O	1:B:207:PRO:HD3	2.13	0.48
2:C:1013:TYR:CE1	2:C:1020:PRO:HG3	2.48	0.48
2:C:470:PRO:HB3	2:C:485:TYR:CE1	2.48	0.48
2:C:498:GLN:O	2:C:501:THR:HG23	2.12	0.48
2:C:583:LEU:HG	2:C:583:LEU:O	2.13	0.48
3:D:1310:ARG:NH1	3:D:1327:ARG:HD3	2.28	0.48
3:D:1330:ILE:HB	3:D:1347:TYR:CZ	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:679:ARG:HB2	3:D:682:ASP:OD2	2.13	0.48
3:D:843:PHE:CD1	3:D:849:ALA:HA	2.48	0.48
3:D:971:LEU:O	3:D:975:GLU:HG3	2.12	0.48
2:M:283:ILE:HG23	8:M:1216:HOH:O	2.13	0.48
2:M:605:LYS:HB3	8:M:1452:HOH:O	2.11	0.48
2:M:637:LEU:N	2:M:637:LEU:HD23	2.28	0.48
3:N:1046:GLN:OE1	3:N:1046:GLN:N	2.46	0.48
2:M:516:ARG:CZ	3:N:1068:LEU:HD22	2.43	0.48
3:N:119:SER:H	3:N:123:LEU:CD2	2.23	0.48
3:N:12:LEU:HD22	3:N:511:TRP:CB	2.44	0.48
3:N:785:ILE:HG12	3:N:935:LYS:HA	1.96	0.48
4:O:48:MET:CB	4:O:54:LEU:HB2	2.43	0.48
5:P:193:ARG:HG2	8:P:3920:HOH:O	2.13	0.48
5:P:208:SER:HB2	5:P:211:ASP:OD1	2.13	0.48
1:B:103:ALA:HB1	1:B:107:LYS:CE	2.37	0.48
2:C:1008:ARG:NH2	2:C:1028:GLY:HA2	2.13	0.48
2:C:1034:GLU:HA	2:C:1037:VAL:CG2	2.42	0.48
2:C:367:LEU:CD2	2:C:371:LYS:HG2	2.41	0.48
2:C:742:VAL:HG12	2:C:743:VAL:N	2.28	0.48
2:C:759:THR:HB	2:C:785:VAL:HG21	1.95	0.48
2:C:802:ARG:HB3	8:C:1186:HOH:O	2.11	0.48
2:C:552:HIS:CD2	2:C:886:LEU:HD12	2.47	0.48
3:D:104:PHE:CD2	3:D:1448:THR:HG23	2.48	0.48
3:D:63:TYR:HE2	8:D:9643:HOH:O	1.96	0.48
3:D:768:ASN:N	3:D:768:ASN:ND2	2.61	0.48
3:D:829:VAL:HA	8:D:2081:HOH:O	2.13	0.48
4:E:85:LEU:HD23	4:E:86:GLN:N	2.28	0.48
5:F:142:ARG:HA	8:F:755:HOH:O	2.13	0.48
5:F:231:ARG:HB3	5:F:233:PHE:CZ	2.49	0.48
1:K:109:VAL:HG23	1:K:132:LEU:HD13	1.95	0.48
1:K:140:MET:HG3	1:K:142:VAL:HG12	1.94	0.48
1:L:143:ARG:NH1	1:L:158:ILE:HG23	2.28	0.48
2:M:1063:ARG:O	2:M:1066:ALA:HB3	2.12	0.48
2:M:407:LYS:HD2	8:M:1363:HOH:O	2.12	0.48
2:M:707:ARG:HD2	2:M:824:ARG:HG2	1.93	0.48
2:M:790:LEU:C	2:M:790:LEU:HD23	2.34	0.48
2:M:882:LEU:HD11	3:N:1038:LEU:HD23	1.94	0.48
3:N:126:VAL:HG12	3:N:132:TYR:HB2	1.95	0.48
3:N:1493:LYS:O	3:N:1497:GLU:HG2	2.13	0.48
3:N:15:PRO:HA	3:N:18:ILE:CG1	2.42	0.48
3:N:179:VAL:HG23	8:N:9425:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:668:PRO:HD2	3:N:672:ALA:CB	2.43	0.48
3:N:756:GLN:HG2	8:N:9643:HOH:O	2.12	0.48
3:N:844:ALA:HB1	8:N:9025:HOH:O	2.11	0.48
3:N:860:LEU:HB2	3:N:861:GLN:NE2	2.28	0.48
1:A:118:ALA:HB3	8:A:444:HOH:O	2.14	0.48
2:C:379:GLU:O	2:C:383:ARG:HB3	2.12	0.48
2:C:872:ASN:HB3	8:C:1870:HOH:O	2.13	0.48
2:C:839:LEU:HD12	2:C:994:ILE:HG21	1.95	0.48
2:C:500:ASN:ND2	3:D:1067:VAL:HG23	2.20	0.48
3:D:1291:SER:HB2	3:D:1293:PHE:CE1	2.42	0.48
3:D:139:GLY:N	3:D:147:VAL:HG21	2.27	0.48
3:D:586:ARG:NH1	3:D:1444:THR:HG21	2.28	0.48
3:D:396:VAL:HG21	3:D:447:VAL:HB	1.96	0.48
3:D:608:SER:O	3:D:612:GLY:HA3	2.14	0.48
5:F:134:LYS:HB3	5:F:178:ARG:NH1	2.28	0.48
5:F:226:LYS:HE3	8:F:741:HOH:O	2.12	0.48
5:F:310:ILE:HB	8:F:438:HOH:O	2.12	0.48
1:L:13:VAL:HG22	8:L:3037:HOH:O	2.13	0.48
1:L:2:LEU:HD12	1:L:3:ASP:N	2.27	0.48
2:M:1060:ILE:HG12	2:M:1063:ARG:HH21	1.78	0.48
2:M:141:HIS:HB3	2:M:418:LEU:HD23	1.94	0.48
2:M:195:LEU:CD2	2:M:238:LEU:HG	2.43	0.48
2:M:281:LEU:CD1	2:M:306:THR:HA	2.44	0.48
2:M:748:GLU:HA	2:M:799:ILE:HG22	1.95	0.48
2:M:939:ARG:HD3	2:M:982:PRO:HD3	1.95	0.48
3:N:1004:THR:O	3:N:1007:VAL:HG22	2.13	0.48
3:N:1045:MET:HG2	3:N:1073:SER:CA	2.39	0.48
3:N:1176:LYS:HA	3:N:1179:GLU:OE2	2.14	0.48
3:N:566:ILE:HB	8:N:9165:HOH:O	2.13	0.48
4:O:35:PHE:HB3	8:O:3746:HOH:O	2.14	0.48
2:C:892:LEU:HD21	2:C:967:PHE:CE1	2.49	0.48
3:D:65:ARG:HG3	3:D:66:GLN:N	2.25	0.48
3:D:768:ASN:H	3:D:768:ASN:HD22	1.61	0.48
5:F:138:SER:HB2	5:F:140:ARG:HG2	1.96	0.48
5:F:194:LEU:HB2	8:F:523:HOH:O	2.12	0.48
5:F:278:LEU:HB3	5:F:286:PRO:CG	2.43	0.48
8:D:9332:HOH:O	5:F:80:PRO:HA	2.13	0.48
1:K:18:ARG:NH1	1:K:123:MET:HE1	2.28	0.48
1:L:103:ALA:HB1	1:L:107:LYS:CE	2.43	0.48
1:L:173:PRO:HB3	1:L:204:SER:HB3	1.94	0.48
2:M:264:PRO:HB2	2:M:289:THR:OG1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:474:VAL:HG23	2:M:478:VAL:O	2.13	0.48
2:M:607:ASP:HB2	2:M:610:ARG:HG3	1.95	0.48
3:N:565:ILE:CD1	3:N:565:ILE:H	2.10	0.48
5:P:223:ALA:HB2	5:P:242:TRP:HB2	1.95	0.48
1:B:110:LYS:HZ3	1:B:110:LYS:HB2	1.78	0.48
1:B:162:ILE:HG22	8:B:463:HOH:O	2.12	0.48
2:C:115:LEU:HD22	2:C:373:VAL:CG1	2.43	0.48
2:C:127:PHE:O	2:C:133:ASP:HA	2.13	0.48
2:C:41:ASN:HB3	8:C:1231:HOH:O	2.13	0.48
2:C:669:GLY:C	2:C:670:GLN:HG3	2.33	0.48
2:C:630:ARG:HH22	2:C:707:ARG:N	2.11	0.48
2:C:708:TYR:N	2:C:708:TYR:CD1	2.81	0.48
3:D:1009:LYS:HA	3:D:1012:GLU:CD	2.34	0.48
3:D:101:HIS:ND1	3:D:103:TRP:HB2	2.26	0.48
3:D:1209:LEU:HD21	4:E:16:LYS:HZ3	1.76	0.48
3:D:1264:GLU:HB3	3:D:1266:ARG:NE	2.29	0.48
3:D:576:GLU:C	3:D:576:GLU:CD	2.72	0.48
3:D:827:ILE:O	3:D:837:GLY:HA3	2.14	0.48
4:E:87:LYS:O	4:E:91:ARG:HG3	2.14	0.48
1:K:215:VAL:HG11	1:L:225:PHE:CD1	2.48	0.48
2:M:19:THR:HG21	2:M:124:ASP:O	2.14	0.48
2:M:239:PHE:HE2	8:M:1222:HOH:O	1.97	0.48
2:M:301:GLU:O	2:M:305:PRO:HG2	2.13	0.48
2:M:688:ILE:N	2:M:688:ILE:HD12	2.29	0.48
2:M:759:THR:HB	2:M:785:VAL:CG2	2.43	0.48
2:M:833:LEU:HD12	2:M:834:GLN:N	2.29	0.48
2:M:879:ARG:NH1	3:N:1029:ARG:NH2	2.62	0.48
3:N:42:ASP:O	3:N:43:GLY:O	2.31	0.48
3:N:973:GLN:HG2	8:N:9252:HOH:O	2.13	0.48
4:O:45:ARG:O	4:O:47:LYS:HD3	2.13	0.48
5:P:350:LEU:HG	5:P:354:LEU:CD1	2.43	0.48
1:A:58:ILE:HG21	1:A:68:ILE:CD1	2.43	0.48
2:C:44:ILE:HG23	2:C:344:PHE:CE1	2.48	0.48
2:C:471:TYR:HA	2:C:534:VAL:HG23	1.96	0.48
2:C:603:VAL:H	2:C:647:GLN:H	1.61	0.48
2:C:810:ASP:HA	2:C:811:PRO:HD3	1.76	0.48
2:C:91:GLN:HE22	2:C:383:ARG:NH2	2.11	0.48
3:D:1129:THR:HA	8:D:9218:HOH:O	2.14	0.48
3:D:1130:ARG:HG3	8:D:2021:HOH:O	2.13	0.48
3:D:389:GLU:O	3:D:389:GLU:HG2	2.13	0.48
3:D:428:LYS:HB3	3:D:450:TYR:HE1	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:666:ILE:H	3:D:666:ILE:HG13	1.33	0.48
3:D:704:ARG:NH1	3:D:738:ALA:HA	2.28	0.48
3:D:813:LEU:O	3:D:839:LEU:HD11	2.13	0.48
3:D:860:LEU:O	3:D:877:PRO:HD2	2.13	0.48
3:D:899:LEU:HD21	3:D:922:LEU:HD21	1.96	0.48
4:E:17:TYR:N	4:E:17:TYR:CD2	2.82	0.48
4:E:43:GLU:HG2	4:E:44:GLU:N	2.28	0.48
1:K:178:ALA:HB3	1:K:198:ARG:HD3	1.94	0.48
1:K:209:GLU:O	1:K:213:GLN:HG3	2.13	0.48
2:M:1045:ALA:HB1	2:M:1048:THR:HB	1.96	0.48
2:M:57:GLU:HG3	2:M:58:ASP:OD2	2.13	0.48
2:M:599:GLU:OE1	2:M:651:LYS:HD2	2.14	0.48
2:M:80:GLN:O	2:M:83:CYS:HB2	2.13	0.48
3:N:1243:THR:HB	3:N:1253:THR:HG22	1.95	0.48
3:N:880:ILE:O	3:N:883:ALA:HB3	2.14	0.48
3:N:907:GLU:CD	3:N:909:ASN:HD22	2.17	0.48
1:A:110:LYS:HB2	8:A:442:HOH:O	2.14	0.48
1:A:86:VAL:HG12	1:A:124:ASN:HB2	1.96	0.48
1:A:161:ARG:NH2	8:A:348:HOH:O	2.46	0.48
1:A:85:LEU:HD12	1:A:86:VAL:N	2.29	0.48
1:A:9:PRO:HD2	1:B:224:TYR:CE1	2.49	0.48
2:C:289:THR:HB	8:C:1418:HOH:O	2.12	0.48
2:C:302:VAL:C	2:C:305:PRO:HD2	2.34	0.48
2:C:309:TYR:HA	2:C:312:ALA:HB3	1.95	0.48
2:C:773:LEU:HG	2:C:777:ILE:HD11	1.96	0.48
2:C:937:ASP:HB3	2:C:939:ARG:HG2	1.96	0.48
3:D:1164:ARG:HH21	3:D:1170:ASP:CG	2.16	0.48
3:D:1114:THR:CG2	3:D:1195:GLN:HB3	2.43	0.48
3:D:18:ILE:HG23	3:D:518:PRO:CG	2.33	0.48
3:D:494:LYS:HD3	8:D:9340:HOH:O	2.14	0.48
3:D:550:ARG:HA	8:D:9108:HOH:O	2.14	0.48
3:D:598:ARG:CZ	5:F:320:PRO:HD3	2.44	0.48
3:D:633:VAL:HB	3:D:740:PHE:CZ	2.48	0.48
4:E:54:LEU:HA	4:E:58:PRO:HG2	1.96	0.48
4:E:6:ILE:HA	4:E:9:LEU:HD12	1.95	0.48
5:F:171:LYS:HG3	5:F:175:HIS:CD2	2.49	0.48
3:D:32:ILE:O	5:F:258:ILE:HG23	2.14	0.48
2:M:852:ILE:HD12	2:M:852:ILE:H	1.79	0.48
2:M:863:ASP:O	2:M:865:THR:N	2.46	0.48
2:M:925:TYR:C	2:M:925:TYR:CD1	2.87	0.48
2:M:975:TYR:HA	2:M:982:PRO:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1117:TYR:CD2	3:N:1117:TYR:N	2.82	0.48
3:N:1173:LEU:CD2	3:N:1174:LEU:HD23	2.43	0.48
3:N:1310:ARG:HD2	3:N:1327:ARG:HH21	1.76	0.48
3:N:208:PRO:CB	3:N:395:VAL:HG13	2.44	0.48
3:N:470:LEU:HD21	3:N:508:ARG:HH21	1.77	0.48
3:N:93:ILE:HD13	3:N:548:ILE:HD11	1.95	0.48
3:N:631:ILE:O	3:N:632:VAL:HG23	2.13	0.48
3:N:676:MET:HE2	3:N:684:LYS:HD2	1.96	0.48
3:N:799:LYS:HE2	3:N:824:ASN:O	2.13	0.48
5:P:125:ASP:OD2	5:P:126:LEU:HD13	2.14	0.48
5:P:169:GLU:H	5:P:169:GLU:CD	2.17	0.48
1:A:137:ARG:N	1:A:137:ARG:HD2	2.29	0.48
2:C:536:PRO:HG2	8:C:1330:HOH:O	2.14	0.48
2:C:715:THR:CG2	2:C:717:LEU:HG	2.44	0.48
2:C:721:ARG:O	2:C:758:ARG:HA	2.14	0.48
2:C:694:LEU:HD11	2:C:868:ASP:HB3	1.96	0.48
2:C:669:GLY:HA3	2:C:995:MET:HA	1.96	0.48
3:D:1137:ARG:O	3:D:1141:GLU:HG3	2.13	0.48
3:D:1339:LYS:HB3	3:D:1343:ALA:CB	2.44	0.48
3:D:183:GLU:O	3:D:186:VAL:HG12	2.14	0.48
3:D:161:LEU:CD1	3:D:452:ILE:HD12	2.44	0.48
3:D:645:PRO:HG3	3:D:725:SER:O	2.12	0.48
5:F:323:ASP:O	5:F:325:LYS:N	2.46	0.48
1:K:50:GLY:HA3	1:K:173:PRO:HG3	1.95	0.48
1:L:218:LEU:O	1:L:222:LEU:HG	2.14	0.48
2:M:1104:GLU:HG2	8:M:1597:HOH:O	2.13	0.48
2:M:208:ALA:HB1	2:M:218:VAL:CG1	2.43	0.48
2:M:305:PRO:HA	2:M:308:ARG:HB2	1.96	0.48
2:M:310:LEU:O	2:M:314:THR:HG23	2.14	0.48
2:M:31:GLN:HG2	2:M:34:VAL:HG23	1.96	0.48
2:M:586:ARG:HD2	2:M:590:ASP:OD2	2.14	0.48
2:M:952:LEU:HB3	2:M:969:GLN:HE22	1.78	0.48
3:N:1020:LEU:HA	3:N:1023:MET:CE	2.44	0.48
3:N:1149:LEU:HD12	3:N:1161:GLU:O	2.13	0.48
3:N:1272:ALA:CA	3:N:1326:THR:HB	2.41	0.48
3:N:393:ILE:H	3:N:393:ILE:HD12	1.79	0.48
3:N:661:MET:CE	3:N:673:ALA:HB1	2.43	0.48
3:N:754:PHE:CG	4:O:24:ALA:HB1	2.49	0.48
3:N:788:GLY:O	3:N:792:ILE:HG22	2.13	0.48
3:N:804:LEU:HB3	8:N:9574:HOH:O	2.13	0.48
3:N:879:ARG:NE	3:N:902:LEU:O	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:47:LYS:HE2	4:O:47:LYS:H	1.78	0.48
8:N:9310:HOH:O	4:O:89:MET:HA	2.14	0.48
5:P:267:THR:HG21	8:P:3894:HOH:O	2.14	0.48
2:M:114:PHE:CZ	5:P:283:GLY:HA3	2.49	0.48
5:P:291:ILE:O	5:P:295:MET:HB2	2.13	0.48
2:C:378:LEU:HG	2:C:382:ILE:CD1	2.44	0.48
2:C:395:LYS:HE2	2:C:403:SER:HB2	1.94	0.48
2:C:704:HIS:O	2:C:705:ILE:HG13	2.14	0.48
3:D:1107:VAL:HG21	3:D:1215:VAL:HG11	1.94	0.48
3:D:1262:LEU:HD21	3:D:1351:GLU:HG3	1.96	0.48
3:D:1250:ALA:O	3:D:1269:LYS:HE2	2.14	0.48
3:D:1280:VAL:O	3:D:1294:VAL:HA	2.14	0.48
3:D:137:PRO:HD2	3:D:453:ASP:CB	2.44	0.48
3:D:516:ALA:O	3:D:518:PRO:HD3	2.14	0.48
4:E:13:VAL:HG12	4:E:75:PHE:CE1	2.49	0.48
4:E:64:ALA:HA	4:E:67:GLU:CD	2.34	0.48
5:F:323:ASP:C	5:F:325:LYS:H	2.17	0.48
2:M:207:LEU:O	2:M:211:LEU:HB3	2.13	0.48
2:M:415:PRO:HB2	2:M:418:LEU:HD13	1.96	0.48
2:M:835:VAL:HG13	3:N:725:SER:OG	2.14	0.48
3:N:1003:VAL:O	3:N:1007:VAL:HG13	2.14	0.48
3:N:1242:HIS:NE2	3:N:1266:ARG:HD3	2.29	0.48
3:N:1333:HIS:O	3:N:1336:LEU:HB3	2.14	0.48
3:N:1475:GLY:O	3:N:1478:SER:HB3	2.14	0.48
3:N:759:ALA:HA	3:N:763:MET:HE2	1.96	0.48
3:N:761:ILE:HD13	8:O:3197:HOH:O	2.13	0.48
3:N:787:LEU:O	3:N:787:LEU:HD12	2.14	0.48
5:P:396:ARG:HH11	5:P:399:GLN:HE21	1.62	0.48
5:P:396:ARG:NH1	5:P:399:GLN:HE21	2.12	0.48
1:A:184:THR:HG23	1:A:192:LEU:CD1	2.44	0.47
1:A:9:PRO:HB3	1:A:25:LEU:CG	2.44	0.47
1:B:102:LYS:HG3	1:B:139:ASN:HB2	1.96	0.47
2:C:1090:LYS:HG2	2:C:1112:PHE:CZ	2.48	0.47
2:C:335:THR:CG2	2:C:461:VAL:HG11	2.44	0.47
2:C:694:LEU:O	2:C:699:PHE:HB2	2.14	0.47
2:C:776:SER:HA	2:C:780:GLU:HB3	1.96	0.47
2:C:926:PHE:CD2	2:C:930:LYS:HE2	2.49	0.47
2:C:958:THR:HG23	2:C:961:GLU:HB2	1.96	0.47
3:D:1128:VAL:O	3:D:1129:THR:C	2.52	0.47
3:D:209:ARG:NH2	3:D:397:LYS:HG3	2.29	0.47
3:D:924:MET:O	3:D:927:THR:HB	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:115:LYS:HE2	5:F:115:LYS:HA	1.96	0.47
5:F:200:LYS:HE2	8:F:705:HOH:O	2.14	0.47
5:F:295:MET:HB3	5:F:299:TRP:CD1	2.48	0.47
1:L:143:ARG:HG3	8:L:3482:HOH:O	2.13	0.47
1:L:190:THR:HA	8:L:4811:HOH:O	2.14	0.47
2:M:178:PRO:HA	8:M:1432:HOH:O	2.11	0.47
2:M:367:LEU:HD23	2:M:371:LYS:NZ	2.29	0.47
2:M:611:ILE:N	2:M:611:ILE:HD12	2.29	0.47
2:M:575:GLN:N	2:M:667:ALA:HB1	2.29	0.47
2:M:728:HIS:HB3	2:M:729:LEU:HD12	1.96	0.47
2:M:735:ARG:HG2	2:M:735:ARG:HH11	1.79	0.47
2:M:810:ASP:HB3	8:M:1642:HOH:O	2.13	0.47
2:M:808:ARG:HH21	2:M:820:ARG:HG2	1.78	0.47
2:M:857:ASP:HB2	2:M:978:ARG:CG	2.42	0.47
3:N:1197:ARG:HB3	3:N:1396:GLU:OE1	2.13	0.47
3:N:443:VAL:CG1	3:N:445:ARG:HE	2.26	0.47
3:N:658:LEU:O	3:N:661:MET:HB2	2.14	0.47
5:P:370:LYS:HB3	5:P:370:LYS:NZ	2.29	0.47
5:P:80:PRO:HA	5:P:83:GLN:HB2	1.96	0.47
1:A:54:THR:HG22	1:A:143:ARG:HG2	1.95	0.47
1:B:159:LYS:HE2	8:B:396:HOH:O	2.12	0.47
1:B:11:PHE:HD1	1:B:25:LEU:HD13	1.79	0.47
2:C:103:LYS:HB2	8:C:1576:HOH:O	2.13	0.47
2:C:260:LEU:HA	2:C:291:ALA:CB	2.43	0.47
2:C:625:LEU:HD11	2:C:641:PRO:HG3	1.96	0.47
3:D:1342:GLU:H	3:D:1342:GLU:CD	2.18	0.47
3:D:1432:LYS:CG	3:D:1433:SER:H	2.27	0.47
3:D:42:ASP:HA	3:D:46:ASP:OD1	2.14	0.47
3:D:43:GLY:N	8:D:9050:HOH:O	2.47	0.47
3:D:585:GLY:N	8:D:9822:HOH:O	2.47	0.47
3:D:699:VAL:HG12	3:D:717:GLN:CA	2.43	0.47
3:D:829:VAL:HG11	8:D:9103:HOH:O	2.12	0.47
3:D:787:LEU:HD21	3:D:947:ILE:CD1	2.44	0.47
5:F:306:GLU:HG2	8:F:517:HOH:O	2.14	0.47
2:M:19:THR:HG22	2:M:22:GLN:HB2	1.94	0.47
2:M:776:SER:HB3	8:M:1776:HOH:O	2.12	0.47
2:M:916:GLU:HG3	2:M:917:LEU:N	2.29	0.47
3:N:185:VAL:CG1	3:N:191:LEU:HD21	2.43	0.47
3:N:169:TYR:HA	3:N:392:SER:HA	1.96	0.47
3:N:427:VAL:HB	3:N:435:VAL:CG2	2.45	0.47
3:N:471:GLU:OE2	3:N:503:LEU:HD21	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:583:ASP:OD2	3:N:586:ARG:HD2	2.14	0.47
3:N:761:ILE:HG23	4:O:6:ILE:HD11	1.95	0.47
3:N:792:ILE:O	3:N:878:GLY:HA3	2.14	0.47
2:M:984:GLU:HG3	3:N:944:THR:O	2.14	0.47
1:A:59:GLU:HG3	1:A:139:ASN:ND2	2.30	0.47
2:C:584:GLU:H	2:C:584:GLU:CD	2.16	0.47
2:C:80:GLN:O	2:C:83:CYS:HB2	2.14	0.47
2:C:553:ASP:HA	2:C:881:ASN:HA	1.97	0.47
2:C:959:PRO:O	2:C:963:LEU:HD23	2.14	0.47
3:D:1155:VAL:HG11	3:D:1183:ILE:HD11	1.95	0.47
3:D:1318:TYR:HD1	3:D:1319:VAL:N	2.12	0.47
3:D:1366:LYS:O	3:D:1369:GLU:HB2	2.14	0.47
3:D:169:TYR:N	3:D:170:PRO:CD	2.77	0.47
3:D:477:LEU:HD22	3:D:492:ALA:CB	2.43	0.47
4:E:37:ASN:HD22	4:E:89:MET:CE	2.27	0.47
5:F:138:SER:O	5:F:141:VAL:HG12	2.14	0.47
5:F:198:ILE:HA	8:F:618:HOH:O	2.14	0.47
5:F:216:GLY:O	5:F:243:ILE:HG12	2.14	0.47
5:F:80:PRO:HA	5:F:83:GLN:HB2	1.96	0.47
1:L:13:VAL:HG11	1:L:208:LEU:HD11	1.96	0.47
1:L:32:PHE:N	8:L:4886:HOH:O	2.47	0.47
2:M:534:VAL:H	2:M:538:GLN:NE2	2.03	0.47
2:M:603:VAL:H	2:M:647:GLN:H	1.63	0.47
2:M:687:ALA:C	2:M:688:ILE:HD12	2.35	0.47
3:N:957:PRO:CD	3:N:1007:VAL:HG12	2.44	0.47
1:A:157:GLY:HA3	8:A:320:HOH:O	2.14	0.47
1:B:211:LEU:O	1:B:215:VAL:HG13	2.14	0.47
2:C:157:ARG:HD3	2:C:158:TYR:N	2.29	0.47
2:C:557:ARG:CZ	2:C:879:ARG:HD3	2.44	0.47
3:D:119:SER:H	3:D:123:LEU:HD13	1.79	0.47
3:D:1207:TYR:N	8:D:9465:HOH:O	2.46	0.47
3:D:1250:ALA:HB3	8:D:9181:HOH:O	2.14	0.47
3:D:1317:ASP:N	8:D:9664:HOH:O	2.47	0.47
3:D:214:GLU:OE2	3:D:390:PRO:HB2	2.15	0.47
3:D:573:MET:HE3	5:F:210:LEU:HB3	1.95	0.47
3:D:639:LEU:HD12	3:D:640:HIS:H	1.80	0.47
3:D:711:LEU:CD1	3:D:778:LEU:HD13	2.44	0.47
5:F:223:ALA:HB2	5:F:242:TRP:HB2	1.96	0.47
5:F:267:THR:O	5:F:271:LEU:HG	2.14	0.47
5:F:282:LEU:HB2	5:F:284:ARG:H	1.79	0.47
5:F:303:ARG:HG3	8:F:507:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:368:VAL:HG12	8:F:443:HOH:O	2.14	0.47
1:K:150:TYR:CE1	2:M:696:LYS:HA	2.48	0.47
1:K:95:GLN:HG3	8:K:3203:HOH:O	2.14	0.47
2:M:172:ILE:HD12	2:M:172:ILE:N	2.30	0.47
2:M:198:ARG:NH1	2:M:231:PRO:HG3	2.30	0.47
2:M:405:ARG:HG2	2:M:409:ARG:NH2	2.11	0.47
2:M:460:ARG:HD2	2:M:485:TYR:CD2	2.49	0.47
2:M:716:LYS:HB2	8:M:1298:HOH:O	2.13	0.47
3:N:1475:GLY:HA2	4:O:17:TYR:CD1	2.49	0.47
3:N:147:VAL:HG11	8:N:9806:HOH:O	2.13	0.47
3:N:1485:GLN:HE21	4:O:80:VAL:N	2.09	0.47
3:N:827:ILE:HG23	3:N:837:GLY:CA	2.45	0.47
4:O:54:LEU:HA	4:O:58:PRO:HG2	1.95	0.47
5:P:128:ARG:HB2	5:P:128:ARG:NH1	2.30	0.47
5:P:336:GLU:HG2	5:P:337:HIS:HD2	1.80	0.47
5:P:409:LYS:HG3	5:P:410:TYR:N	2.29	0.47
2:C:1055:LEU:HG	2:C:1079:PRO:HG3	1.97	0.47
2:C:232:GLU:HG3	2:C:235:LEU:CD1	2.44	0.47
2:C:384:GLU:CD	2:C:388:ARG:HH21	2.18	0.47
2:C:473:ARG:HD2	2:C:475:VAL:HG23	1.95	0.47
2:C:510:ALA:HB2	8:C:1220:HOH:O	2.14	0.47
2:C:526:PRO:HB2	8:C:1311:HOH:O	2.13	0.47
2:C:398:THR:HG22	2:C:568:ALA:O	2.13	0.47
2:C:773:LEU:O	2:C:777:ILE:HG13	2.14	0.47
2:C:567:GLN:CB	2:C:997:LEU:HD22	2.45	0.47
3:D:104:PHE:CE2	3:D:1448:THR:HG23	2.50	0.47
3:D:1153:VAL:O	3:D:1160:LEU:HG	2.14	0.47
3:D:1250:ALA:HB2	8:D:9571:HOH:O	2.13	0.47
3:D:186:VAL:HG13	3:D:187:LYS:N	2.28	0.47
3:D:432:TYR:HB3	3:D:448:GLU:HA	1.96	0.47
3:D:465:LEU:CD1	3:D:513:ILE:HD11	2.44	0.47
3:D:912:LYS:O	3:D:915:VAL:HG23	2.15	0.47
3:D:420:VAL:HA	5:F:164:LYS:NZ	2.29	0.47
5:F:209:PHE:CE2	5:F:213:ILE:HD11	2.49	0.47
5:F:411:HIS:HB2	8:F:598:HOH:O	2.13	0.47
2:M:1059:ASP:O	2:M:1063:ARG:HG2	2.13	0.47
2:M:1090:LYS:HG2	2:M:1112:PHE:CZ	2.49	0.47
2:M:197:LEU:CD1	2:M:207:LEU:HD11	2.44	0.47
2:M:260:LEU:HA	2:M:291:ALA:CB	2.45	0.47
2:M:625:LEU:O	2:M:627:ARG:N	2.47	0.47
2:M:645:VAL:HG13	8:M:1487:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:862:PRO:HA	2:M:975:TYR:CE1	2.49	0.47
3:N:1138:ALA:HA	3:N:1141:GLU:HG3	1.96	0.47
3:N:1310:ARG:HB2	8:N:9400:HOH:O	2.14	0.47
3:N:132:TYR:HA	8:N:9161:HOH:O	2.14	0.47
3:N:493:ARG:NH1	3:N:1390:LEU:H	2.12	0.47
3:N:417:PRO:HA	5:P:168:LYS:HZ2	1.77	0.47
3:N:459:GLU:HG2	8:N:9337:HOH:O	2.14	0.47
3:N:561:GLY:HA2	8:N:9133:HOH:O	2.14	0.47
3:N:568:ARG:HA	3:N:571:LYS:NZ	2.29	0.47
3:N:864:VAL:HG12	3:N:865:THR:H	1.79	0.47
3:N:871:LYS:HB3	3:N:873:LEU:HD11	1.97	0.47
3:N:886:VAL:HG13	3:N:930:LEU:HD11	1.96	0.47
4:O:84:ARG:HG3	4:O:84:ARG:O	2.15	0.47
5:P:112:ALA:HA	5:P:173:TYR:CD2	2.48	0.47
5:P:302:LYS:HA	8:P:3021:HOH:O	2.14	0.47
5:P:392:VAL:HG21	8:P:3999:HOH:O	2.14	0.47
1:A:149:GLY:O	1:A:171:PHE:HB2	2.14	0.47
1:B:68:ILE:HD12	1:B:71:VAL:HG21	1.95	0.47
2:C:139:GLN:HG2	2:C:140:ILE:H	1.79	0.47
3:D:1071:PHE:HB3	8:D:9526:HOH:O	2.14	0.47
3:D:416:ALA:H	3:D:417:PRO:CD	2.26	0.47
3:D:640:HIS:HE1	4:E:3:GLU:HG2	1.79	0.47
3:D:852:ALA:O	3:D:857:ILE:HG12	2.14	0.47
5:F:117:SER:OG	5:F:124:PRO:HG3	2.15	0.47
5:F:371:LEU:O	5:F:375:LEU:HB3	2.15	0.47
3:D:675:ARG:HH21	5:F:421:PHE:H	1.61	0.47
1:K:228:PRO:HG3	8:K:4456:HOH:O	2.13	0.47
1:K:69:PRO:O	1:K:71:VAL:HG23	2.13	0.47
2:M:1030:GLN:HB3	3:N:626:SER:HB2	1.97	0.47
2:M:32:ALA:HA	8:M:1342:HOH:O	2.15	0.47
2:M:820:ARG:HB2	8:M:1654:HOH:O	2.14	0.47
2:M:839:LEU:HD21	2:M:849:VAL:CG2	2.44	0.47
2:M:916:GLU:O	2:M:919:ALA:HB3	2.15	0.47
3:N:1054:GLU:HB2	8:N:9488:HOH:O	2.15	0.47
3:N:1184:GLN:HG2	8:N:9892:HOH:O	2.15	0.47
3:N:1123:PHE:CE2	3:N:1184:GLN:HG3	2.50	0.47
3:N:1320:GLU:HG2	3:N:1339:LYS:HE3	1.96	0.47
3:N:396:VAL:CG2	3:N:447:VAL:HB	2.45	0.47
3:N:572:ARG:NH1	5:P:80:PRO:HD3	2.29	0.47
3:N:607:LEU:HA	3:N:613:ARG:HB3	1.96	0.47
3:N:80:VAL:HG12	3:N:81:THR:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:829:VAL:HA	8:N:9426:HOH:O	2.15	0.47
3:N:902:LEU:O	3:N:902:LEU:HD12	2.15	0.47
2:M:987:ILE:HG23	3:N:948:THR:HG21	1.96	0.47
3:N:1485:GLN:NE2	4:O:80:VAL:H	2.12	0.47
5:P:396:ARG:HA	5:P:399:GLN:HB2	1.95	0.47
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.97	0.47
2:C:52:PHE:O	2:C:54:ILE:N	2.47	0.47
2:C:878:SER:HB2	8:C:1420:HOH:O	2.14	0.47
3:D:1009:LYS:HE2	3:D:1013:GLU:OE1	2.14	0.47
3:D:1314:LYS:HZ1	3:D:1317:ASP:HB2	1.80	0.47
3:D:1393:GLN:CB	3:D:1398:TRP:HE1	2.28	0.47
3:D:488:ARG:NH1	3:D:488:ARG:HB3	2.29	0.47
3:D:502:PHE:CE2	3:D:1452:ILE:HG23	2.50	0.47
3:D:729:HIS:HE1	3:D:731:LEU:HG	1.79	0.47
3:D:780:LYS:HE2	8:D:9604:HOH:O	2.13	0.47
3:D:848:GLU:HB2	8:D:9179:HOH:O	2.13	0.47
3:D:890:VAL:HG11	3:D:922:LEU:HD13	1.96	0.47
1:K:9:PRO:HB3	1:K:25:LEU:HG	1.96	0.47
2:M:1090:LYS:HZ1	3:N:90:MET:CG	2.27	0.47
2:M:207:LEU:HD22	2:M:221:LEU:HD22	1.97	0.47
2:M:470:PRO:HB2	2:M:534:VAL:HG21	1.96	0.47
2:M:724:ARG:HE	2:M:734:LEU:HG	1.78	0.47
2:M:770:GLU:HG2	8:N:9172:HOH:O	2.15	0.47
2:M:578:VAL:HG11	2:M:991:GLN:HB3	1.96	0.47
3:N:1068:LEU:C	3:N:1070:TYR:N	2.67	0.47
3:N:153:LEU:CD1	3:N:157:GLU:HB2	2.45	0.47
3:N:442:ASN:HB3	8:N:9376:HOH:O	2.14	0.47
3:N:598:ARG:NE	8:N:9109:HOH:O	2.47	0.47
3:N:960:LYS:HB3	8:N:9231:HOH:O	2.13	0.47
5:P:155:THR:O	5:P:159:ILE:HG13	2.14	0.47
2:C:1067:TYR:CE2	5:F:345:ALA:HB2	2.50	0.47
2:C:301:GLU:O	2:C:305:PRO:HG2	2.15	0.47
2:C:193:LEU:HD23	2:C:307:LEU:CD1	2.45	0.47
2:C:372:LEU:HD21	8:C:1196:HOH:O	2.14	0.47
2:C:403:SER:O	2:C:407:LYS:HD2	2.14	0.47
2:C:739:GLU:HB2	8:C:1284:HOH:O	2.14	0.47
2:C:798:GLY:HA2	8:C:1158:HOH:O	2.15	0.47
3:D:1047:LYS:HB3	3:D:1048:PRO:CD	2.45	0.47
3:D:519:VAL:HG13	3:D:544:TYR:CZ	2.50	0.47
3:D:543:LEU:CD2	3:D:600:LEU:HD12	2.45	0.47
3:D:601:ARG:CD	3:D:606:ILE:HD13	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:647:ARG:HG2	8:D:9811:HOH:O	2.14	0.47
3:D:83:SER:O	3:D:86:ARG:HB3	2.14	0.47
3:D:96:ALA:HB1	3:D:554:LEU:HD12	1.97	0.47
4:E:69:LEU:HD11	8:E:181:HOH:O	2.15	0.47
5:F:273:ARG:HG2	8:F:571:HOH:O	2.15	0.47
2:M:1038:TRP:HA	2:M:1041:GLU:HB2	1.96	0.47
2:M:1076:VAL:HG22	3:N:752:SER:HB3	1.96	0.47
2:M:112:GLU:HB2	8:M:1448:HOH:O	2.15	0.47
2:M:470:PRO:HB2	2:M:483:VAL:HG11	1.97	0.47
2:M:52:PHE:O	2:M:54:ILE:N	2.48	0.47
2:M:762:LYS:HB2	2:M:762:LYS:NZ	2.30	0.47
2:M:824:ARG:HB3	2:M:826:TYR:CE1	2.50	0.47
3:N:1166:LEU:HD23	3:N:1166:LEU:N	2.29	0.47
3:N:1281:VAL:HG23	3:N:1317:ASP:O	2.15	0.47
3:N:1379:VAL:CG1	3:N:1395:LEU:HD23	2.45	0.47
3:N:1462:LEU:HD22	3:N:1473:PRO:HD2	1.95	0.47
3:N:470:LEU:HD21	3:N:508:ARG:NH2	2.30	0.47
3:N:47:GLU:OE1	3:N:52:PRO:HA	2.15	0.47
3:N:666:ILE:HG23	3:N:686:GLU:OE2	2.15	0.47
2:M:1115:LEU:CD2	3:N:85:VAL:HG13	2.43	0.47
3:N:89:ARG:O	3:N:521:PRO:HG3	2.14	0.47
5:P:159:ILE:O	5:P:163:LEU:HG	2.14	0.47
1:B:57:TYR:HB3	1:B:141:GLU:HG3	1.95	0.47
2:C:1054:THR:HG22	2:C:1059:ASP:CB	2.45	0.47
2:C:285:LEU:HD12	2:C:288:ARG:O	2.15	0.47
2:C:946:ARG:NH2	3:D:859:ASP:HA	2.30	0.47
3:D:1033:GLN:HE22	3:D:1036:ARG:HH11	1.63	0.47
3:D:1066:THR:HG23	3:D:1069:GLU:N	2.16	0.47
3:D:115:LEU:HD23	3:D:116:LEU:N	2.30	0.47
3:D:1312:LEU:N	8:D:9045:HOH:O	2.42	0.47
3:D:1354:LYS:HD3	8:D:9078:HOH:O	2.15	0.47
3:D:414:ARG:HG2	8:D:9627:HOH:O	2.13	0.47
3:D:421:LEU:HD11	3:D:437:VAL:HG22	1.95	0.47
3:D:528:VAL:HG12	8:D:9096:HOH:O	2.15	0.47
3:D:591:VAL:HG12	3:D:592:THR:O	2.15	0.47
3:D:645:PRO:HB3	3:D:723:GLY:O	2.14	0.47
3:D:996:TRP:HA	3:D:999:THR:CG2	2.43	0.47
5:F:316:SER:HB3	5:F:318:GLU:O	2.15	0.47
1:L:50:GLY:O	1:L:146:ARG:HA	2.15	0.47
1:L:149:GLY:O	1:L:171:PHE:HB2	2.14	0.47
1:L:212:ASN:N	1:L:212:ASN:HD22	2.11	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:61:VAL:HA	8:L:2996:HOH:O	2.15	0.47
2:M:206:THR:HG21	8:M:1314:HOH:O	2.15	0.47
2:M:290:LEU:HB3	2:M:302:VAL:HG12	1.97	0.47
2:M:332:ARG:HB2	2:M:466:PHE:HE1	1.78	0.47
2:M:409:ARG:HA	2:M:454:SER:CA	2.32	0.47
2:M:53:PRO:HD3	8:M:1173:HOH:O	2.14	0.47
2:M:572:ILE:CG2	2:M:703:ILE:HD13	2.45	0.47
2:M:624:PRO:O	2:M:625:LEU:HD23	2.15	0.47
2:M:723:THR:HG23	2:M:725:ASP:HB2	1.97	0.47
3:N:1123:PHE:HB3	3:N:1133:ARG:O	2.15	0.47
3:N:1465:ASN:ND2	3:N:1470:ARG:HD3	2.30	0.47
3:N:486:ARG:HH21	3:N:489:ARG:CD	2.28	0.47
3:N:536:ALA:HA	5:P:315:VAL:N	2.19	0.47
3:N:587:ARG:HD3	8:N:9432:HOH:O	2.14	0.47
4:O:10:PHE:HE2	4:O:16:LYS:HG3	1.80	0.47
5:P:110:MET:HA	5:P:113:ILE:HD12	1.97	0.47
5:P:195:VAL:HG11	5:P:217:ASN:OD1	2.15	0.47
2:C:207:LEU:HD22	2:C:221:LEU:CD2	2.45	0.47
2:C:244:PRO:CD	2:C:245:GLY:H	2.20	0.47
3:D:1148:VAL:HG13	3:D:1163:GLY:O	2.15	0.47
3:D:129:PHE:CE2	3:D:587:ARG:HD3	2.50	0.47
3:D:1341:PRO:HD2	3:D:1342:GLU:OE2	2.14	0.47
3:D:1382:THR:HG21	3:D:1418:LYS:HE3	1.95	0.47
3:D:171:LEU:HD22	3:D:390:PRO:HG3	1.97	0.47
3:D:169:TYR:HA	3:D:392:SER:HA	1.97	0.47
3:D:434:ARG:HB2	3:D:447:VAL:HG22	1.97	0.47
3:D:476:GLU:HG2	8:D:9254:HOH:O	2.14	0.47
3:D:645:PRO:HA	3:D:721:VAL:O	2.14	0.47
3:D:843:PHE:HA	3:D:848:GLU:OE1	2.14	0.47
4:E:13:VAL:HG21	4:E:19:LEU:HB2	1.96	0.47
1:K:86:VAL:HG12	1:K:124:ASN:ND2	2.29	0.47
2:M:1105:LYS:HB2	2:M:1107:ASN:HD22	1.80	0.47
2:M:671:ASN:ND2	2:M:993:PHE:CD2	2.81	0.47
2:M:551:GLU:HA	2:M:906:PHE:CE2	2.49	0.47
3:N:1267:ARG:HH11	3:N:1267:ARG:CB	2.27	0.47
3:N:181:ASP:O	3:N:185:VAL:HG23	2.14	0.47
3:N:188:GLY:HA2	3:N:210:ARG:NH1	2.30	0.47
3:N:204:LEU:HG	8:N:9317:HOH:O	2.14	0.47
3:N:209:ARG:HB2	3:N:395:VAL:O	2.15	0.47
3:N:463:GLN:O	3:N:467:GLU:HG3	2.15	0.47
3:N:882:PHE:CE1	3:N:906:GLN:HG3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:1335:HOH:O	3:N:944:THR:HA	2.14	0.47
3:N:950:GLY:H	3:N:953:ASP:CB	2.27	0.47
4:O:54:LEU:CD2	4:O:63:TRP:HE1	2.27	0.47
5:P:109:GLY:O	5:P:113:ILE:HG13	2.14	0.47
5:P:335:ASP:CG	5:P:338:LEU:HD12	2.35	0.47
5:P:421:PHE:C	5:P:423:ASP:H	2.17	0.47
1:B:180:GLN:HB3	8:D:9039:HOH:O	2.15	0.47
1:B:20:TYR:OH	1:B:198:ARG:HD3	2.14	0.47
2:C:269:LEU:HD22	8:C:1709:HOH:O	2.14	0.47
2:C:302:VAL:O	2:C:306:THR:HG23	2.15	0.47
2:C:625:LEU:O	2:C:627:ARG:N	2.48	0.47
2:C:645:VAL:HA	8:C:1221:HOH:O	2.15	0.47
2:C:722:ILE:CG2	2:C:805:ARG:HH21	2.27	0.47
2:C:690:ILE:CD1	2:C:833:LEU:HD21	2.45	0.47
3:D:1183:ILE:N	3:D:1183:ILE:HD12	2.29	0.47
3:D:1336:LEU:HA	3:D:1344:VAL:CG2	2.45	0.47
3:D:422:ALA:O	3:D:427:VAL:HG21	2.15	0.47
3:D:474:GLU:O	3:D:478:LEU:HG	2.15	0.47
3:D:80:VAL:HG12	8:D:9019:HOH:O	2.14	0.47
3:D:928:ALA:O	3:D:931:LEU:HB2	2.14	0.47
5:F:261:PRO:O	5:F:265:VAL:HG23	2.15	0.47
5:F:388:ALA:HA	8:F:635:HOH:O	2.15	0.47
1:L:54:THR:HG22	1:L:158:ILE:HG13	1.97	0.47
2:M:215:GLY:HA3	8:M:1560:HOH:O	2.15	0.47
2:M:44:ILE:HD13	2:M:344:PHE:CE1	2.50	0.47
2:M:405:ARG:HD3	2:M:543:ASN:HB2	1.97	0.47
2:M:412:ALA:HB3	2:M:451:LEU:HB3	1.97	0.47
2:M:462:ASP:HB3	2:M:468:ARG:HD2	1.97	0.47
2:M:605:LYS:HA	8:M:1487:HOH:O	2.15	0.47
2:M:926:PHE:O	2:M:930:LYS:HG3	2.15	0.47
3:N:1023:MET:O	3:N:1028:ALA:HB3	2.15	0.47
3:N:1462:LEU:CD2	3:N:1473:PRO:HD2	2.45	0.47
3:N:397:LYS:HE2	3:N:399:ARG:HE	1.80	0.47
3:N:90:MET:SD	3:N:521:PRO:HD3	2.54	0.47
3:N:566:ILE:HG12	5:P:217:ASN:HD22	1.80	0.47
3:N:678:GLU:HG3	3:N:679:ARG:HG3	1.97	0.47
3:N:916:TYR:O	3:N:919:PHE:HB3	2.15	0.47
4:O:74:VAL:CG1	4:O:79:LEU:HD21	2.45	0.47
2:C:1100:GLN:O	2:C:1102:LEU:HD12	2.15	0.46
2:C:195:LEU:CD1	2:C:234:ALA:HB1	2.46	0.46
2:C:281:LEU:HB2	2:C:309:TYR:CG	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:285:LEU:HD23	2:C:285:LEU:O	2.15	0.46
2:C:687:ALA:C	2:C:688:ILE:HD12	2.35	0.46
2:C:805:ARG:HG3	2:C:823:VAL:HG22	1.97	0.46
2:C:941:VAL:O	2:C:944:LEU:HB2	2.14	0.46
3:D:1124:GLN:HA	3:D:1125:PRO:HD3	1.76	0.46
3:D:1459:LEU:HD22	3:D:1465:ASN:HD22	1.79	0.46
3:D:797:LYS:HD2	3:D:797:LYS:N	2.30	0.46
5:F:282:LEU:N	5:F:282:LEU:HD23	2.30	0.46
5:F:363:GLU:HA	5:F:367:MET:SD	2.55	0.46
1:K:115:LEU:HB3	8:K:4097:HOH:O	2.14	0.46
1:K:68:ILE:CD1	1:K:138:LEU:HD11	2.45	0.46
1:K:88:ARG:HD2	1:K:123:MET:HE1	1.97	0.46
2:M:345:ARG:CB	2:M:345:ARG:HH11	2.27	0.46
2:M:422:ARG:HG3	8:M:1745:HOH:O	2.13	0.46
2:M:464:LEU:O	2:M:466:PHE:N	2.48	0.46
2:M:918:LEU:HD23	2:M:968:LEU:CA	2.43	0.46
3:N:1275:SER:HB3	3:N:1325:LEU:CD1	2.45	0.46
3:N:196:VAL:HG13	3:N:202:VAL:HG11	1.97	0.46
3:N:44:LEU:HG	8:N:9867:HOH:O	2.16	0.46
3:N:645:PRO:HA	3:N:721:VAL:O	2.15	0.46
3:N:827:ILE:O	3:N:837:GLY:HA3	2.15	0.46
1:A:101:LEU:HG	1:A:113:ASP:O	2.15	0.46
1:A:50:GLY:O	1:A:146:ARG:HA	2.15	0.46
2:C:521:PRO:HB2	3:D:1055:VAL:CB	2.43	0.46
2:C:534:VAL:N	2:C:538:GLN:NE2	2.63	0.46
1:A:67:THR:HG21	2:C:609:ASN:HD21	1.80	0.46
2:C:798:GLY:C	2:C:799:ILE:HD13	2.36	0.46
2:C:9:ILE:HD12	2:C:9:ILE:O	2.15	0.46
3:D:495:ARG:O	3:D:495:ARG:HG2	2.16	0.46
3:D:962:GLN:N	3:D:962:GLN:OE1	2.47	0.46
5:F:282:LEU:H	5:F:282:LEU:HD23	1.79	0.46
5:F:416:ARG:NH1	5:F:419:ARG:HB2	2.30	0.46
1:K:117:VAL:HB	1:K:120:VAL:CG1	2.42	0.46
1:K:78:ILE:O	1:K:82:LEU:HG	2.15	0.46
2:M:1101:THR:HB	3:N:5:VAL:HG11	1.98	0.46
2:M:1118:LYS:HD3	3:N:20:SER:O	2.14	0.46
2:M:195:LEU:HD12	2:M:234:ALA:HB1	1.97	0.46
2:M:325:ILE:HG23	8:M:1502:HOH:O	2.16	0.46
2:M:44:ILE:HG22	8:M:1223:HOH:O	2.14	0.46
2:M:621:VAL:HG22	8:M:1199:HOH:O	2.16	0.46
2:M:817:PRO:C	2:M:819:VAL:H	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1056:PRO:HD2	8:N:9483:HOH:O	2.14	0.46
3:N:1243:THR:HG22	3:N:1244:GLY:H	1.79	0.46
3:N:400:VAL:HA	3:N:442:ASN:O	2.15	0.46
3:N:484:PRO:O	3:N:489:ARG:HD2	2.14	0.46
3:N:551:ASN:O	3:N:555:LYS:HG3	2.15	0.46
3:N:759:ALA:HA	3:N:763:MET:HB3	1.96	0.46
4:O:40:LEU:CD2	4:O:67:GLU:HA	2.46	0.46
5:P:365:GLU:CD	5:P:397:ILE:HA	2.35	0.46
1:A:19:GLU:O	1:A:200:TRP:HA	2.16	0.46
1:B:26:GLU:HG2	1:B:27:PRO:HA	1.97	0.46
2:C:208:ALA:HB1	2:C:218:VAL:CG1	2.45	0.46
2:C:780:GLU:CD	2:C:781:LYS:H	2.18	0.46
2:C:863:ASP:O	2:C:865:THR:N	2.48	0.46
2:C:987:ILE:HG22	2:C:988:VAL:O	2.15	0.46
3:D:783:ARG:HH21	3:D:1029:ARG:CZ	2.28	0.46
3:D:1085:ALA:HA	8:D:9707:HOH:O	2.14	0.46
3:D:907:GLU:OE1	3:D:908:LYS:HG2	2.14	0.46
5:F:141:VAL:O	5:F:145:PRO:HD2	2.16	0.46
5:F:218:GLN:HA	5:F:221:ILE:HD12	1.96	0.46
1:K:115:LEU:HD12	1:K:115:LEU:O	2.15	0.46
2:M:1050:GLN:CG	2:M:1079:PRO:HG2	2.44	0.46
2:M:1111:ILE:HD11	8:M:1318:HOH:O	2.14	0.46
2:M:428:ARG:HE	2:M:451:LEU:HD11	1.80	0.46
2:M:93:PRO:HG3	2:M:117:HIS:HE1	1.80	0.46
3:N:93:ILE:CD1	3:N:548:ILE:HD11	2.46	0.46
3:N:828:LYS:HD2	8:N:9129:HOH:O	2.15	0.46
4:O:59:ASN:HD22	4:O:59:ASN:HA	1.59	0.46
1:A:218:LEU:HB2	8:A:322:HOH:O	2.14	0.46
1:B:92:PRO:HA	1:B:146:ARG:NH2	2.31	0.46
1:B:19:GLU:O	1:B:200:TRP:HA	2.15	0.46
1:B:73:GLU:HB2	1:B:78:ILE:HD11	1.96	0.46
1:B:86:VAL:HG22	8:B:371:HOH:O	2.15	0.46
2:C:265:ARG:HG2	2:C:267:TYR:N	2.30	0.46
2:C:441:VAL:HG12	2:C:559:LEU:HA	1.96	0.46
2:C:442:GLU:HG2	2:C:454:SER:HB2	1.98	0.46
2:C:835:VAL:HG11	8:D:9008:HOH:O	2.16	0.46
3:D:1093:TYR:HA	8:D:9017:HOH:O	2.16	0.46
3:D:110:SER:HB3	8:D:9091:HOH:O	2.15	0.46
3:D:1380:GLU:HB3	3:D:1418:LYS:HB2	1.98	0.46
3:D:396:VAL:HG13	3:D:447:VAL:HA	1.98	0.46
3:D:574:LEU:O	3:D:578:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:68:PHE:O	3:D:71:LYS:HG2	2.15	0.46
3:D:704:ARG:HD2	3:D:704:ARG:HA	1.76	0.46
4:E:41:GLU:O	4:E:45:ARG:HG2	2.15	0.46
5:F:276:ARG:HA	8:F:735:HOH:O	2.14	0.46
5:F:256:ARG:NH2	5:F:310:ILE:O	2.48	0.46
1:K:210:ALA:HA	1:K:213:GLN:NE2	2.31	0.46
2:M:101:ILE:HG22	2:M:102:HIS:N	2.30	0.46
2:M:191:PHE:CE2	2:M:238:LEU:HD21	2.51	0.46
2:M:710:ILE:HB	2:M:790:LEU:CD1	2.38	0.46
2:M:801:VAL:HG23	8:M:1213:HOH:O	2.15	0.46
3:N:957:PRO:HA	3:N:1010:ASN:ND2	2.30	0.46
3:N:1109:GLU:CD	3:N:1202:GLN:H	2.18	0.46
3:N:1114:THR:O	3:N:1114:THR:HG23	2.15	0.46
3:N:1156:LEU:HD12	8:N:9485:HOH:O	2.16	0.46
3:N:416:ALA:H	3:N:417:PRO:CD	2.28	0.46
2:C:218:VAL:HG22	2:C:221:LEU:CD2	2.46	0.46
2:C:310:LEU:O	2:C:314:THR:HG23	2.15	0.46
2:C:490:GLU:HG2	2:C:494:TYR:OH	2.15	0.46
2:C:647:GLN:HA	8:C:1176:HOH:O	2.16	0.46
2:C:979:THR:CG2	2:C:981:GLU:HB2	2.45	0.46
3:D:190:GLU:HG3	3:D:210:ARG:CD	2.46	0.46
3:D:208:PRO:CB	3:D:395:VAL:HG13	2.43	0.46
3:D:501:ALA:HA	3:D:504:ASP:HB2	1.97	0.46
3:D:84:ILE:HA	3:D:87:ARG:HG2	1.97	0.46
3:D:952:ASP:HA	3:D:1062:ARG:NH2	2.30	0.46
4:E:18:ARG:HD3	8:E:126:HOH:O	2.15	0.46
5:F:336:GLU:HB2	8:F:726:HOH:O	2.15	0.46
1:L:69:PRO:O	1:L:71:VAL:HG23	2.16	0.46
2:M:143:SER:HB3	2:M:332:ARG:HB2	1.97	0.46
2:M:52:PHE:HE1	2:M:66:LEU:HG	1.75	0.46
2:M:810:ASP:HA	2:M:811:PRO:HD3	1.79	0.46
2:M:842:ARG:HD3	8:M:1636:HOH:O	2.16	0.46
2:M:875:GLY:O	2:M:879:ARG:HD3	2.15	0.46
2:M:976:ASP:HB3	2:M:979:THR:HG22	1.96	0.46
3:N:1434:TRP:HZ3	3:N:1457:ASP:H	1.62	0.46
3:N:28:LYS:HD3	3:N:41:ARG:NH1	2.30	0.46
3:N:404:GLU:OE1	3:N:414:ARG:HD3	2.16	0.46
3:N:891:GLU:HG2	8:N:9646:HOH:O	2.15	0.46
3:N:926:LYS:HE2	8:N:9736:HOH:O	2.16	0.46
4:O:29:GLN:HB2	4:O:33:HIS:CD2	2.51	0.46
5:P:104:ARG:HG2	8:P:3629:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:215:GLU:HA	5:P:215:GLU:OE1	2.15	0.46
3:N:560:GLN:HE21	5:P:218:GLN:HE22	1.63	0.46
2:C:113:VAL:HG11	2:C:373:VAL:CB	2.46	0.46
2:C:73:LEU:HD22	2:C:94:LEU:HD22	1.97	0.46
3:D:1114:THR:HG22	3:D:1195:GLN:HB3	1.97	0.46
3:D:1272:ALA:HB2	8:D:9364:HOH:O	2.16	0.46
3:D:1382:THR:HG22	8:D:9579:HOH:O	2.16	0.46
3:D:1476:THR:CG2	4:E:21:VAL:HG22	2.46	0.46
1:K:23:PHE:O	1:K:196:THR:HA	2.15	0.46
2:M:478:VAL:HG13	2:M:506:ASN:HB3	1.97	0.46
2:M:688:ILE:CD1	2:M:847:GLY:HA3	2.45	0.46
3:N:1342:GLU:HG2	8:N:9105:HOH:O	2.15	0.46
3:N:1353:GLN:HG2	3:N:1368:ILE:HD12	1.98	0.46
3:N:508:ARG:HB3	3:N:510:GLU:OE2	2.16	0.46
3:N:516:ALA:O	3:N:518:PRO:HD3	2.16	0.46
3:N:550:ARG:HH11	3:N:550:ARG:HG3	1.79	0.46
3:N:608:SER:O	3:N:612:GLY:HA3	2.16	0.46
2:M:1091:GLU:OE2	3:N:613:ARG:HD2	2.15	0.46
3:N:646:LYS:HA	3:N:720:LEU:HD23	1.97	0.46
3:N:809:PRO:O	3:N:812:ALA:HB3	2.16	0.46
3:N:820:GLU:HA	3:N:825:ALA:O	2.16	0.46
2:M:1090:LYS:HZ1	3:N:90:MET:HG2	1.79	0.46
2:C:1005:MET:HE1	3:D:648:MET:HB2	1.96	0.46
2:C:1054:THR:HG22	2:C:1059:ASP:CG	2.36	0.46
2:C:144:PRO:HA	2:C:163:ILE:HG12	1.98	0.46
2:C:328:LEU:CD2	2:C:437:ARG:HD3	2.46	0.46
3:D:1042:ARG:O	3:D:1057:VAL:HB	2.15	0.46
3:D:1274:ILE:HB	3:D:1322:GLY:HA2	1.98	0.46
3:D:829:VAL:H	3:D:835:SER:HB2	1.81	0.46
4:E:69:LEU:HD21	8:E:181:HOH:O	2.15	0.46
2:C:376:ARG:NH2	5:F:285:GLU:HB3	2.21	0.46
5:F:375:LEU:HG	5:F:376:ILE:HG13	1.97	0.46
1:K:175:ARG:HH21	1:K:201:THR:H	1.62	0.46
1:K:27:PRO:HG2	1:K:186:LEU:HD22	1.98	0.46
1:L:138:LEU:O	1:L:138:LEU:HD23	2.16	0.46
1:L:26:GLU:HB2	1:L:27:PRO:HA	1.98	0.46
2:M:1033:GLY:O	2:M:1036:GLU:HB2	2.15	0.46
2:M:1040:LEU:HD23	2:M:1049:LEU:HA	1.98	0.46
2:M:127:PHE:O	2:M:133:ASP:HA	2.16	0.46
2:M:218:VAL:HG22	2:M:221:LEU:CD2	2.45	0.46
2:M:253:ALA:HB3	8:M:1251:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1378:TYR:CD1	3:N:1378:TYR:N	2.84	0.46
3:N:136:ASP:HB3	3:N:137:PRO:HD3	1.98	0.46
3:N:470:LEU:HD12	3:N:503:LEU:CG	2.43	0.46
3:N:530:VAL:HB	3:N:531:ASP:H	1.56	0.46
3:N:586:ARG:HA	8:N:2001:HOH:O	2.15	0.46
3:N:671:LYS:N	8:N:9139:HOH:O	2.48	0.46
3:N:819:GLY:O	3:N:822:ALA:HB3	2.16	0.46
3:N:81:THR:O	3:N:82:LYS:C	2.54	0.46
5:P:292:ALA:HB1	5:P:299:TRP:O	2.16	0.46
5:P:319:THR:HB	5:P:321:ILE:HD11	1.96	0.46
1:A:181:VAL:O	2:C:937:ASP:HA	2.16	0.46
1:B:81:ASN:HB2	8:B:366:HOH:O	2.16	0.46
2:C:194:VAL:HG21	2:C:221:LEU:HA	1.98	0.46
2:C:129:ILE:CG1	2:C:386:PHE:HB3	2.46	0.46
2:C:744:ARG:HG3	2:C:747:ALA:HB2	1.97	0.46
3:D:116:LEU:HB3	3:D:118:LEU:CD2	2.46	0.46
3:D:126:VAL:O	3:D:132:TYR:CD1	2.68	0.46
3:D:1293:PHE:CE2	3:D:1302:GLU:HB2	2.51	0.46
3:D:1432:LYS:HD2	3:D:1433:SER:N	2.29	0.46
3:D:684:LYS:HD3	3:D:686:GLU:CD	2.35	0.46
2:C:1039:ALA:HB2	3:D:707:THR:HG21	1.98	0.46
5:F:273:ARG:O	5:F:276:ARG:HB2	2.16	0.46
2:M:157:ARG:HH11	2:M:157:ARG:HG2	1.80	0.46
2:M:146:VAL:HG13	2:M:161:SER:O	2.16	0.46
2:M:145:GLY:C	2:M:163:ILE:HG23	2.36	0.46
3:N:957:PRO:HG3	3:N:1007:VAL:HA	1.97	0.46
3:N:1115:THR:HB	8:N:9719:HOH:O	2.15	0.46
3:N:1137:ARG:O	3:N:1140:ILE:N	2.49	0.46
3:N:1209:LEU:HD22	3:N:1211:MET:SD	2.55	0.46
3:N:1269:LYS:HE3	8:N:9213:HOH:O	2.16	0.46
3:N:1441:GLN:NE2	3:N:1442:ASN:H	2.14	0.46
3:N:159:ARG:HB2	3:N:159:ARG:CZ	2.46	0.46
3:N:521:PRO:O	3:N:525:ARG:HG2	2.14	0.46
3:N:805:GLU:HB2	8:N:9612:HOH:O	2.16	0.46
3:N:813:LEU:HA	3:N:839:LEU:HD11	1.97	0.46
3:N:850:LEU:O	3:N:853:VAL:HB	2.15	0.46
4:O:11:GLY:HA3	8:O:3878:HOH:O	2.15	0.46
5:P:274:THR:O	5:P:278:LEU:HG	2.15	0.46
2:C:1076:VAL:HG23	3:D:752:SER:HA	1.98	0.46
2:C:47:ALA:CB	2:C:345:ARG:HB3	2.33	0.46
2:C:495:THR:HG21	2:C:524:VAL:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:643:VAL:HG13	2:C:647:GLN:CD	2.36	0.46
2:C:702:SER:OG	2:C:996:LYS:NZ	2.49	0.46
2:C:873:PRO:O	2:C:876:VAL:HG23	2.16	0.46
2:C:975:TYR:HA	2:C:982:PRO:HA	1.98	0.46
3:D:1337:GLU:HB3	8:D:9228:HOH:O	2.16	0.46
3:D:569:ASN:HD21	5:F:210:LEU:HD22	1.80	0.46
3:D:97:THR:CG2	3:D:571:LYS:HD3	2.46	0.46
3:D:592:THR:HA	8:D:9540:HOH:O	2.16	0.46
2:C:1109:VAL:HG11	3:D:5:VAL:HG13	1.98	0.46
3:D:863:VAL:HA	8:D:2082:HOH:O	2.16	0.46
2:M:408:ARG:CZ	2:M:542:VAL:HG23	2.46	0.46
2:M:423:ALA:HB1	8:M:1764:HOH:O	2.16	0.46
2:M:473:ARG:HG2	2:M:473:ARG:HH11	1.80	0.46
2:M:602:GLU:HG2	2:M:603:VAL:N	2.31	0.46
2:M:685:GLU:CG	3:N:739:ASP:HB2	2.46	0.46
2:M:861:LEU:HD23	2:M:862:PRO:CD	2.37	0.46
3:N:1109:GLU:HG2	3:N:1201:CYS:CA	2.43	0.46
3:N:1114:THR:HA	8:N:9054:HOH:O	2.14	0.46
3:N:1342:GLU:CD	3:N:1342:GLU:N	2.67	0.46
3:N:600:LEU:HD12	3:N:600:LEU:H	1.81	0.46
3:N:860:LEU:HD22	3:N:878:GLY:CA	2.46	0.46
5:P:163:LEU:HB3	5:P:174:LEU:HD11	1.96	0.46
5:P:302:LYS:HG3	5:P:303:ARG:N	2.31	0.46
1:A:219:ARG:HH12	1:B:223:THR:HG23	1.81	0.46
1:B:85:LEU:CD1	1:B:124:ASN:HB3	2.42	0.46
1:A:219:ARG:HH22	1:B:223:THR:HG23	1.80	0.46
1:B:74:ASP:O	1:B:78:ILE:HG13	2.16	0.46
2:C:1103:ASP:N	2:C:1107:ASN:O	2.49	0.46
2:C:216:GLU:OE1	2:C:217:LEU:HG	2.15	0.46
2:C:352:ALA:O	2:C:355:VAL:HG12	2.16	0.46
2:C:473:ARG:NE	2:C:531:PHE:HE1	2.09	0.46
2:C:546:LEU:HD21	2:C:587:VAL:HG21	1.97	0.46
2:C:751:PRO:HB2	3:D:680:GLN:HG3	1.98	0.46
2:C:904:PRO:HB2	2:C:907:ASP:OD2	2.16	0.46
3:D:1135:ARG:NH2	8:D:9592:HOH:O	2.49	0.46
3:D:1164:ARG:HA	8:D:9221:HOH:O	2.15	0.46
3:D:1122:LEU:HD23	3:D:1178:ALA:HB2	1.97	0.46
3:D:1327:ARG:HG2	8:D:9891:HOH:O	2.16	0.46
3:D:1481:VAL:HG11	4:E:18:ARG:CA	2.40	0.46
3:D:186:VAL:HG11	3:D:213:VAL:HB	1.98	0.46
3:D:210:ARG:NE	3:D:398:ALA:HB3	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:400:VAL:HG23	8:D:9178:HOH:O	2.15	0.46
3:D:421:LEU:HD23	3:D:421:LEU:O	2.15	0.46
3:D:543:LEU:HD21	3:D:600:LEU:HB2	1.97	0.46
1:L:43:ILE:HD13	8:L:3139:HOH:O	2.16	0.46
2:M:1100:GLN:HG3	2:M:1101:THR:O	2.16	0.46
2:M:121:MET:HE3	2:M:127:PHE:CE2	2.51	0.46
2:M:260:LEU:HA	2:M:291:ALA:HB2	1.98	0.46
2:M:420:ARG:CD	2:M:420:ARG:H	2.29	0.46
2:M:455:LEU:HD13	2:M:459:ALA:HB3	1.97	0.46
3:N:1341:PRO:O	3:N:1344:VAL:N	2.48	0.46
3:N:500:ARG:HD2	8:N:9705:HOH:O	2.15	0.46
3:N:529:GLN:HG2	3:N:535:PHE:CE2	2.48	0.46
3:N:52:PRO:CB	3:N:80:VAL:HG13	2.31	0.46
3:N:844:ALA:HB3	3:N:848:GLU:OE2	2.16	0.46
3:N:976:GLN:HA	3:N:979:GLU:OE1	2.15	0.46
5:P:342:VAL:HG23	5:P:343:ASP:OD1	2.15	0.46
5:P:361:LEU:HD21	5:P:404:ALA:HB1	1.98	0.46
1:B:149:GLY:O	1:B:171:PHE:HB2	2.16	0.45
2:C:101:ILE:HG22	2:C:102:HIS:N	2.31	0.45
2:C:338:GLU:O	2:C:341:THR:HG22	2.16	0.45
2:C:694:LEU:HD21	2:C:868:ASP:HB3	1.98	0.45
2:C:979:THR:HG23	2:C:981:GLU:HB2	1.98	0.45
3:D:1104:GLU:O	3:D:1106:VAL:HG23	2.16	0.45
3:D:1397:LYS:HB3	8:D:9838:HOH:O	2.15	0.45
3:D:183:GLU:HA	3:D:186:VAL:CG1	2.46	0.45
3:D:441:ARG:O	3:D:443:VAL:N	2.49	0.45
3:D:585:GLY:HA3	8:D:9104:HOH:O	2.16	0.45
3:D:838:ARG:HD3	3:D:874:GLU:HB3	1.97	0.45
3:D:875:THR:HG22	3:D:879:ARG:HB2	1.98	0.45
5:F:117:SER:N	5:F:127:ILE:HD12	2.31	0.45
5:F:202:TYR:OH	5:F:244:ARG:HD2	2.16	0.45
5:F:340:SER:O	5:F:342:VAL:N	2.49	0.45
1:K:224:TYR:HB3	1:L:9:PRO:CB	2.42	0.45
2:M:1050:GLN:NE2	8:M:1526:HOH:O	2.48	0.45
2:M:1059:ASP:CG	2:M:1062:GLY:HA3	2.37	0.45
2:M:114:PHE:HE1	8:P:4072:HOH:O	1.99	0.45
2:M:157:ARG:HG2	2:M:157:ARG:NH1	2.32	0.45
2:M:169:GLY:HA2	2:M:263:ASP:CB	2.30	0.45
2:M:194:VAL:HA	2:M:197:LEU:HD12	1.97	0.45
2:M:232:GLU:O	2:M:235:LEU:HB2	2.16	0.45
2:M:473:ARG:HG2	2:M:473:ARG:NH1	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:704:HIS:CD2	2:M:705:ILE:H	2.33	0.45
3:N:411:THR:HG23	3:N:429:SER:OG	2.16	0.45
3:N:527:MET:CE	3:N:537:THR:HB	2.45	0.45
3:N:567:ILE:HG13	3:N:567:ILE:H	1.51	0.45
3:N:130:SER:C	3:N:568:ARG:HH21	2.20	0.45
3:N:729:HIS:HB3	3:N:732:VAL:HG22	1.98	0.45
4:O:5:GLY:HA3	4:O:8:LYS:HD2	1.98	0.45
2:M:770:GLU:OE1	5:P:354:LEU:HD13	2.17	0.45
5:P:89:GLY:HA2	8:P:4492:HOH:O	2.15	0.45
1:A:9:PRO:HB3	1:A:25:LEU:HG	1.98	0.45
2:C:1016:ILE:CD1	3:D:526:PRO:HG2	2.46	0.45
2:C:142:ARG:NH1	2:C:325:ILE:HG12	2.30	0.45
2:C:203:ASP:OD1	2:C:206:THR:HG22	2.16	0.45
2:C:502:PRO:HB2	2:C:509:ALA:HB3	1.98	0.45
2:C:598:GLU:HG3	8:C:1515:HOH:O	2.15	0.45
2:C:794:PRO:HD3	8:C:1635:HOH:O	2.15	0.45
3:D:1211:MET:SD	3:D:1213:ARG:HD2	2.57	0.45
3:D:1377:LYS:O	3:D:1395:LEU:N	2.47	0.45
3:D:1494:ALA:HB3	8:D:9315:HOH:O	2.16	0.45
3:D:455:ARG:HH11	3:D:455:ARG:HG2	1.81	0.45
3:D:806:PHE:CZ	3:D:813:LEU:HB3	2.51	0.45
3:D:890:VAL:HG13	3:D:926:LYS:HD3	1.98	0.45
5:F:196:VAL:HG13	5:F:213:ILE:CD1	2.45	0.45
5:F:302:LYS:HG3	5:F:303:ARG:N	2.31	0.45
5:F:373:LYS:HD3	5:F:378:GLY:C	2.36	0.45
1:L:188:GLN:HA	8:N:9218:HOH:O	2.17	0.45
2:M:1078:GLU:HA	2:M:1078:GLU:OE1	2.17	0.45
2:M:56:GLU:HG2	2:M:64:LEU:HD23	1.97	0.45
2:M:778:PHE:HA	8:M:1278:HOH:O	2.16	0.45
2:M:998:TYR:OH	2:M:1000:MET:HA	2.16	0.45
2:M:435:TYR:HA	3:N:1071:PHE:HE2	1.81	0.45
3:N:1151:ARG:HA	3:N:1162:GLU:HG3	1.99	0.45
3:N:814:ALA:HA	8:N:9843:HOH:O	2.15	0.45
1:A:20:TYR:HB3	8:A:358:HOH:O	2.16	0.45
1:A:26:GLU:HG2	1:A:27:PRO:CA	2.46	0.45
1:B:50:GLY:O	1:B:146:ARG:HA	2.16	0.45
2:C:1015:LEU:HD12	8:C:1202:HOH:O	2.17	0.45
2:C:1105:LYS:O	2:C:1107:ASN:N	2.49	0.45
2:C:144:PRO:O	2:C:276:LYS:HD3	2.16	0.45
2:C:148:PHE:HD2	2:C:160:ALA:HA	1.80	0.45
2:C:207:LEU:O	2:C:211:LEU:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:218:VAL:HB	8:C:1237:HOH:O	2.17	0.45
2:C:254:VAL:HA	2:C:257:VAL:HG23	1.96	0.45
2:C:289:THR:HG22	2:C:290:LEU:H	1.81	0.45
2:C:471:TYR:CE2	2:C:496:ILE:HG21	2.51	0.45
2:C:479:VAL:HG23	2:C:506:ASN:C	2.37	0.45
2:C:456:ALA:HB1	2:C:538:GLN:O	2.16	0.45
2:C:643:VAL:HG13	2:C:647:GLN:OE1	2.17	0.45
2:C:683:ASN:N	2:C:683:ASN:OD1	2.49	0.45
2:C:837:ASP:O	2:C:849:VAL:HG23	2.16	0.45
2:C:881:ASN:N	2:C:881:ASN:ND2	2.64	0.45
2:C:897:LEU:CD1	2:C:921:ALA:HA	2.46	0.45
3:D:1331:ASP:OD1	3:D:1334:GLN:HG3	2.16	0.45
3:D:1333:HIS:O	3:D:1336:LEU:HB3	2.15	0.45
3:D:170:PRO:HG3	8:D:9430:HOH:O	2.16	0.45
3:D:400:VAL:HA	3:D:442:ASN:O	2.17	0.45
3:D:770:LEU:HB2	3:D:1210:SER:O	2.17	0.45
3:D:757:ALA:CB	4:E:24:ALA:HB2	2.46	0.45
5:F:253:ASP:O	5:F:259:ARG:HD2	2.17	0.45
1:K:2:LEU:O	1:K:6:LEU:HB3	2.16	0.45
1:L:62:LEU:HD22	1:L:63:HIS:CE1	2.52	0.45
2:M:17:PRO:O	2:M:20:GLU:HB3	2.16	0.45
2:M:254:VAL:HA	2:M:257:VAL:HG23	1.98	0.45
2:M:69:LEU:HD21	2:M:99:GLN:NE2	2.31	0.45
2:M:737:LEU:HD21	2:M:741:GLY:O	2.16	0.45
2:M:838:LYS:HG2	8:M:1507:HOH:O	2.16	0.45
3:N:1112:CYS:HB3	3:N:1201:CYS:SG	2.56	0.45
3:N:1290:LEU:CD2	3:N:1291:SER:H	2.20	0.45
3:N:177:ALA:HB1	3:N:199:LEU:HD22	1.97	0.45
3:N:416:ALA:HB3	3:N:417:PRO:HD3	1.98	0.45
3:N:396:VAL:HG13	3:N:446:VAL:O	2.16	0.45
3:N:480:GLU:OE2	3:N:484:PRO:HG2	2.17	0.45
3:N:486:ARG:HA	3:N:489:ARG:HD3	1.96	0.45
2:M:1009:SER:OG	3:N:655:PRO:HD3	2.15	0.45
3:N:820:GLU:HG2	3:N:825:ALA:O	2.17	0.45
3:N:875:THR:HG23	3:N:879:ARG:NE	2.32	0.45
3:N:950:GLY:O	3:N:951:ILE:C	2.54	0.45
5:P:148:LYS:HB2	8:P:4930:HOH:O	2.16	0.45
5:P:308:LEU:O	5:P:312:GLN:HG3	2.15	0.45
5:P:336:GLU:HA	8:P:2842:HOH:O	2.16	0.45
1:A:26:GLU:HG3	1:A:184:THR:HG21	1.99	0.45
1:A:33:GLY:HA2	1:A:195:LEU:HD22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:ARG:HB2	8:B:337:HOH:O	2.16	0.45
1:B:14:ARG:HA	8:B:324:HOH:O	2.14	0.45
1:B:64:GLU:HG3	1:B:79:ILE:HD13	1.97	0.45
2:C:1096:ALA:HB2	3:D:101:HIS:CD2	2.51	0.45
2:C:16:PRO:O	2:C:18:LEU:HD12	2.16	0.45
2:C:19:THR:HG22	2:C:19:THR:O	2.16	0.45
2:C:399:ASN:ND2	2:C:402:SER:HB2	2.31	0.45
2:C:535:SER:H	2:C:538:GLN:HE21	1.64	0.45
2:C:603:VAL:HG22	2:C:613:VAL:HG12	1.99	0.45
2:C:668:LEU:HD12	2:C:668:LEU:N	2.32	0.45
2:C:826:TYR:HB3	8:C:1718:HOH:O	2.15	0.45
2:C:911:GLU:O	2:C:915:LYS:HG2	2.17	0.45
3:D:1094:LEU:O	3:D:1098:LEU:HD13	2.17	0.45
3:D:1339:LYS:HE3	8:D:2030:HOH:O	2.14	0.45
3:D:1192:LEU:HD21	3:D:1372:VAL:CG1	2.46	0.45
3:D:1264:GLU:CD	3:D:1425:THR:H	2.20	0.45
3:D:1440:PHE:HD1	3:D:1441:GLN:H	1.64	0.45
3:D:473:LEU:HD21	3:D:495:ARG:NE	2.30	0.45
3:D:581:LEU:CD1	3:D:603:LEU:HD12	2.46	0.45
3:D:704:ARG:NH1	3:D:737:ASN:O	2.50	0.45
3:D:792:ILE:O	3:D:878:GLY:HA3	2.16	0.45
3:D:827:ILE:HG23	3:D:837:GLY:HA2	1.99	0.45
3:D:900:ILE:CD1	3:D:902:LEU:HG	2.47	0.45
4:E:61:GLU:OE2	4:E:62:THR:N	2.50	0.45
5:F:358:LEU:HD12	5:F:367:MET:HE1	1.98	0.45
1:K:54:THR:CG2	1:K:158:ILE:HG13	2.40	0.45
1:L:110:LYS:HE3	8:L:3562:HOH:O	2.15	0.45
2:M:217:LEU:HD12	2:M:311:PHE:HD2	1.81	0.45
2:M:437:ARG:CZ	2:M:488:ALA:HA	2.47	0.45
3:N:1075:HIS:HB3	8:N:9012:HOH:O	2.16	0.45
3:N:1171:VAL:HG12	3:N:1171:VAL:O	2.17	0.45
3:N:119:SER:CB	3:N:123:LEU:HB2	2.39	0.45
2:M:874:LEU:HD12	3:N:783:ARG:HB2	1.97	0.45
3:N:950:GLY:C	3:N:953:ASP:H	2.20	0.45
3:N:992:ILE:O	3:N:995:LEU:HB3	2.15	0.45
4:O:78:ASN:HB2	8:O:4376:HOH:O	2.16	0.45
5:P:403:LYS:HA	5:P:403:LYS:HZ3	1.81	0.45
1:A:18:ARG:NH1	1:A:88:ARG:HE	2.14	0.45
1:B:194:LYS:HZ2	1:B:194:LYS:HB2	1.82	0.45
2:C:352:ALA:C	2:C:355:VAL:HG12	2.37	0.45
2:C:460:ARG:HG2	8:C:1486:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:657:ASP:HB3	8:C:1152:HOH:O	2.17	0.45
2:C:670:GLN:HE22	2:C:699:PHE:C	2.20	0.45
2:C:94:LEU:HD12	2:C:95:TYR:N	2.32	0.45
2:C:957:LYS:HE2	2:C:965:GLU:OE2	2.16	0.45
3:D:1035:ILE:HA	3:D:1038:LEU:HD12	1.97	0.45
3:D:1281:VAL:HG21	3:D:1313:VAL:HG21	1.99	0.45
3:D:1337:GLU:HG3	8:D:2052:HOH:O	2.16	0.45
3:D:502:PHE:CE2	3:D:1452:ILE:HG13	2.52	0.45
3:D:1455:LYS:C	3:D:1455:LYS:HD3	2.36	0.45
3:D:145:VAL:HG21	8:D:9724:HOH:O	2.16	0.45
3:D:178:LEU:CG	3:D:200:ASP:H	2.26	0.45
3:D:41:ARG:CD	3:D:42:ASP:H	2.23	0.45
3:D:584:ASN:HD21	3:D:590:PRO:HD2	1.80	0.45
3:D:583:ASP:HA	3:D:602:SER:OG	2.16	0.45
3:D:6:ARG:HH11	3:D:6:ARG:CB	2.30	0.45
3:D:717:GLN:HB2	3:D:717:GLN:HE21	1.51	0.45
3:D:850:LEU:HB2	8:D:9338:HOH:O	2.16	0.45
3:D:890:VAL:HG21	3:D:922:LEU:CD1	2.47	0.45
3:D:972:LEU:O	3:D:976:GLN:HG3	2.17	0.45
5:F:105:LYS:NZ	5:F:179:GLU:HB3	2.31	0.45
5:F:197:SER:HA	8:F:484:HOH:O	2.14	0.45
1:L:101:LEU:HD12	1:L:114:PHE:CD1	2.52	0.45
1:L:123:MET:HG2	8:L:3100:HOH:O	2.15	0.45
1:L:206:THR:HG22	1:L:209:GLU:HG3	1.99	0.45
2:M:157:ARG:CD	2:M:158:TYR:H	2.28	0.45
2:M:244:PRO:HD2	2:M:245:GLY:N	2.25	0.45
2:M:669:GLY:HA3	2:M:995:MET:HA	1.98	0.45
3:N:123:LEU:HA	8:N:9192:HOH:O	2.16	0.45
3:N:1433:SER:HB2	3:N:1457:ASP:CG	2.37	0.45
3:N:1465:ASN:HD22	3:N:1465:ASN:HA	1.53	0.45
3:N:569:ASN:HA	3:N:572:ARG:HD2	1.98	0.45
3:N:800:LYS:HD3	3:N:804:LEU:HD22	1.98	0.45
2:M:987:ILE:HG23	3:N:948:THR:CG2	2.47	0.45
1:B:156:HIS:CE1	1:B:158:ILE:H	2.35	0.45
2:C:549:PHE:HE2	2:C:887:GLU:N	2.15	0.45
2:C:622:GLU:OE1	2:C:624:PRO:HG3	2.17	0.45
8:A:413:HOH:O	2:C:642:ARG:HA	2.17	0.45
2:C:817:PRO:C	2:C:819:VAL:H	2.20	0.45
2:C:941:VAL:HA	2:C:944:LEU:HD12	1.98	0.45
2:C:948:GLU:HG3	2:C:949:LYS:N	2.31	0.45
2:C:521:PRO:CB	3:D:1055:VAL:HB	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1233:GLY:O	3:D:1256:LEU:HD13	2.16	0.45
3:D:1291:SER:HB3	8:D:9240:HOH:O	2.15	0.45
3:D:36:THR:O	3:D:38:LYS:N	2.50	0.45
3:D:396:VAL:CG2	3:D:447:VAL:HB	2.46	0.45
3:D:859:ASP:N	3:D:859:ASP:OD2	2.48	0.45
3:D:86:ARG:NH1	3:D:86:ARG:HG2	2.31	0.45
3:D:87:ARG:HB3	3:D:523:ASP:CB	2.45	0.45
1:K:57:TYR:CZ	1:K:161:ARG:HD2	2.52	0.45
1:K:183:ASP:HB2	8:K:4658:HOH:O	2.16	0.45
1:K:176:ARG:HG3	1:K:200:TRP:CE3	2.52	0.45
1:L:81:ASN:ND2	1:L:127:LEU:HD11	2.30	0.45
2:M:207:LEU:HD22	2:M:221:LEU:CD1	2.46	0.45
2:M:571:LEU:HD12	2:M:701:THR:N	2.32	0.45
2:M:863:ASP:OD1	2:M:865:THR:HG22	2.16	0.45
3:N:1128:VAL:O	3:N:1129:THR:C	2.55	0.45
3:N:1213:ARG:HB2	3:N:1214:PRO:CD	2.46	0.45
3:N:115:LEU:CD1	3:N:499:VAL:HG22	2.47	0.45
3:N:728:LEU:HD22	3:N:745:MET:CE	2.47	0.45
5:P:102:LEU:HD13	5:P:187:LEU:HG	1.97	0.45
5:P:272:SER:O	5:P:276:ARG:HG2	2.16	0.45
1:A:103:ALA:HB1	1:A:107:LYS:NZ	2.32	0.45
1:B:24:VAL:HG13	1:B:196:THR:CG2	2.37	0.45
2:C:794:PRO:HD2	8:C:1228:HOH:O	2.16	0.45
3:D:1155:VAL:CG1	3:D:1183:ILE:HD11	2.47	0.45
3:D:1504:GLU:HB3	8:D:9773:HOH:O	2.15	0.45
3:D:27:GLU:HG3	3:D:28:LYS:HD2	1.98	0.45
3:D:396:VAL:HG22	8:D:9882:HOH:O	2.17	0.45
3:D:503:LEU:HG	3:D:508:ARG:NH2	2.32	0.45
3:D:957:PRO:HG2	3:D:1007:VAL:HA	1.98	0.45
4:E:41:GLU:HG3	8:E:170:HOH:O	2.15	0.45
5:F:217:ASN:O	5:F:221:ILE:HG13	2.17	0.45
2:M:144:PRO:HB3	8:M:1235:HOH:O	2.16	0.45
2:M:290:LEU:HD12	8:M:1503:HOH:O	2.17	0.45
2:M:73:LEU:HD12	2:M:73:LEU:O	2.17	0.45
2:M:86:LYS:HG2	2:M:813:VAL:HG12	1.99	0.45
2:M:943:VAL:HG11	2:M:973:VAL:HG22	1.99	0.45
3:N:1127:GLU:HB2	8:N:9303:HOH:O	2.17	0.45
3:N:1129:THR:O	3:N:1130:ARG:HD2	2.17	0.45
3:N:1175:ILE:HG22	3:N:1179:GLU:OE1	2.16	0.45
3:N:1262:LEU:HD11	3:N:1351:GLU:CG	2.46	0.45
3:N:13:ALA:HA	3:N:17:LYS:NZ	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:399:ARG:HB3	3:N:402:PRO:HG3	1.98	0.45
3:N:491:LYS:HG3	8:N:9735:HOH:O	2.17	0.45
3:N:866:VAL:HG12	3:N:867:ARG:N	2.32	0.45
3:N:892:ASP:HB3	3:N:895:VAL:HG23	1.99	0.45
5:P:153:PRO:O	5:P:157:GLU:HG2	2.16	0.45
1:A:184:THR:HB	1:A:194:LYS:HD2	1.98	0.45
1:A:20:TYR:CE2	1:A:22:GLU:HG3	2.51	0.45
1:A:227:ASN:H	1:A:227:ASN:ND2	2.14	0.45
1:B:20:TYR:HB3	8:B:319:HOH:O	2.15	0.45
2:C:265:ARG:HD2	8:C:1452:HOH:O	2.17	0.45
2:C:304:LEU:HG	2:C:305:PRO:N	2.31	0.45
2:C:39:ARG:HA	2:C:39:ARG:NE	2.30	0.45
2:C:874:LEU:HB3	3:D:1029:ARG:HD2	1.98	0.45
3:D:1314:LYS:NZ	3:D:1317:ASP:HB2	2.31	0.45
3:D:1342:GLU:O	3:D:1346:ARG:HB2	2.17	0.45
3:D:164:GLY:HA2	8:D:9127:HOH:O	2.16	0.45
3:D:462:GLN:NE2	3:D:513:ILE:HB	2.32	0.45
2:C:1056:LYS:HE2	3:D:625:TYR:HB2	1.98	0.45
2:C:1043:TYR:CE1	3:D:710:ARG:O	2.70	0.45
3:D:957:PRO:HG3	3:D:1007:VAL:HA	1.99	0.45
3:D:985:ASP:O	3:D:988:ARG:HD2	2.16	0.45
1:K:40:LEU:O	1:K:44:LEU:HD12	2.17	0.45
1:K:74:ASP:O	1:K:78:ILE:HG13	2.17	0.45
1:L:128:HIS:CE1	1:L:131:THR:HG23	2.52	0.45
1:L:194:LYS:HG2	8:L:4937:HOH:O	2.17	0.45
2:M:503:LEU:HD12	2:M:505:GLY:O	2.17	0.45
2:M:762:LYS:HD3	2:M:771:GLU:OE2	2.16	0.45
2:M:922:PHE:HD2	2:M:964:LYS:HD3	1.82	0.45
3:N:1136:LYS:HE3	3:N:1139:ASP:OD2	2.16	0.45
3:N:1200:VAL:HG22	3:N:1373:ARG:HH12	1.81	0.45
3:N:119:SER:CB	3:N:123:LEU:HD13	2.46	0.45
3:N:1238:MET:HG2	3:N:1256:LEU:HD23	1.98	0.45
3:N:141:ILE:HD13	3:N:450:TYR:HB2	1.98	0.45
3:N:703:ASN:ND2	3:N:704:ARG:H	2.15	0.45
4:O:9:LEU:CD2	4:O:69:LEU:HG	2.47	0.45
1:A:102:LYS:HE2	1:A:139:ASN:CG	2.37	0.45
1:A:48:ILE:HG22	1:A:173:PRO:CD	2.47	0.45
1:B:28:LEU:HB2	1:B:193:ASP:HB2	1.99	0.45
2:C:1006:HIS:N	2:C:1006:HIS:HD1	2.14	0.45
2:C:1033:GLY:O	2:C:1037:VAL:HG23	2.17	0.45
2:C:112:GLU:HA	8:C:1822:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:203:ASP:OD1	2:C:205:GLU:HG3	2.16	0.45
2:C:217:LEU:HD23	8:C:1241:HOH:O	2.17	0.45
2:C:333:ILE:O	2:C:465:GLY:HA3	2.17	0.45
2:C:433:THR:CG2	2:C:488:ALA:HB1	2.42	0.45
2:C:405:ARG:CZ	2:C:566:THR:HG21	2.47	0.45
2:C:5:ARG:HG2	2:C:5:ARG:HH11	1.82	0.45
2:C:98:LEU:HD11	8:C:1822:HOH:O	2.17	0.45
3:D:1086:LEU:HD22	8:D:9242:HOH:O	2.16	0.45
3:D:198:ARG:HG3	8:D:9736:HOH:O	2.16	0.45
3:D:22:SER:OG	3:D:91:GLY:HA2	2.17	0.45
3:D:639:LEU:N	3:D:729:HIS:CD2	2.84	0.45
3:D:704:ARG:HB2	3:D:736:PHE:CD2	2.52	0.45
3:D:848:GLU:HA	3:D:851:LEU:CD1	2.46	0.45
5:F:364:ARG:O	5:F:368:VAL:HG23	2.17	0.45
1:K:161:ARG:HB2	1:K:161:ARG:NH1	2.32	0.45
2:M:164:PRO:HA	8:M:1235:HOH:O	2.17	0.45
2:M:210:GLU:HG3	8:M:1787:HOH:O	2.17	0.45
2:M:620:LEU:N	2:M:620:LEU:HD13	2.32	0.45
3:N:1320:GLU:HG3	8:N:9381:HOH:O	2.16	0.45
3:N:9:ARG:HA	3:N:1455:LYS:O	2.16	0.45
3:N:1459:LEU:HD13	3:N:1465:ASN:HD21	1.81	0.45
3:N:399:ARG:HB2	3:N:444:VAL:HG13	1.99	0.45
3:N:456:MET:HG2	3:N:456:MET:O	2.16	0.45
3:N:52:PRO:HD2	3:N:79:GLU:O	2.16	0.45
3:N:640:HIS:NE2	3:N:717:GLN:OE1	2.48	0.45
3:N:645:PRO:HB3	3:N:723:GLY:O	2.17	0.45
3:N:704:ARG:CZ	3:N:737:ASN:O	2.65	0.45
3:N:872:ARG:NH2	8:N:9086:HOH:O	2.50	0.45
1:B:23:PHE:O	1:B:196:THR:HA	2.17	0.45
2:C:1083:GLU:OE1	2:C:1083:GLU:HA	2.17	0.45
2:C:374:ASN:ND2	2:C:377:PRO:HD3	2.32	0.45
2:C:115:LEU:HD12	2:C:378:LEU:HD22	1.99	0.45
2:C:535:SER:O	2:C:538:GLN:HG2	2.16	0.45
2:C:718:GLY:HA3	2:C:761:PHE:CZ	2.52	0.45
2:C:774:LEU:HA	2:C:777:ILE:HD12	1.99	0.45
2:C:579:VAL:HG11	2:C:887:GLU:HG3	1.99	0.45
2:C:911:GLU:HB3	2:C:912:PRO:HD3	1.99	0.45
2:C:952:LEU:HB3	2:C:966:LEU:CD1	2.47	0.45
3:D:1495:ILE:HG12	4:E:80:VAL:CG1	2.46	0.45
3:D:495:ARG:O	3:D:499:VAL:HG23	2.17	0.45
3:D:90:MET:HE3	3:D:519:VAL:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:768:ASN:N	3:D:768:ASN:HD22	2.13	0.45
8:D:9004:HOH:O	5:F:132:ARG:NH1	2.49	0.45
5:F:209:PHE:HE2	5:F:213:ILE:HD11	1.81	0.45
2:C:729:LEU:HD21	5:F:421:PHE:HD1	1.82	0.45
1:L:22:GLU:OE2	1:L:198:ARG:HG2	2.17	0.45
2:M:139:GLN:NE2	2:M:418:LEU:HD13	2.32	0.45
2:M:366:SER:HB2	8:M:1234:HOH:O	2.17	0.45
2:M:437:ARG:HG2	2:M:467:ILE:HG22	1.98	0.45
2:M:498:GLN:O	2:M:532:MET:SD	2.75	0.45
2:M:15:LEU:CD2	2:M:583:LEU:HD21	2.47	0.45
2:M:679:PHE:HD2	2:M:682:TYR:HD2	1.65	0.45
3:N:1087:ARG:NH1	3:N:1234:THR:O	2.50	0.45
3:N:130:SER:HB3	3:N:132:TYR:HE1	1.80	0.45
3:N:1372:VAL:HA	3:N:1375:MET:CE	2.47	0.45
3:N:1455:LYS:HE3	8:N:9604:HOH:O	2.17	0.45
3:N:402:PRO:HG2	3:N:444:VAL:CG1	2.47	0.45
3:N:634:GLY:O	3:N:637:LEU:HB3	2.17	0.45
3:N:778:LEU:HD12	3:N:778:LEU:HA	1.78	0.45
3:N:806:PHE:CG	3:N:806:PHE:O	2.70	0.45
4:O:7:ASP:HB2	8:O:3467:HOH:O	2.16	0.45
4:O:85:LEU:HD23	4:O:86:GLN:N	2.32	0.45
5:P:132:ARG:HD3	5:P:181:GLU:CD	2.37	0.45
5:P:131:VAL:HG13	5:P:178:ARG:HG2	1.98	0.45
5:P:366:ALA:HB3	5:P:367:MET:HE2	1.98	0.45
1:B:106:PRO:HB2	8:B:403:HOH:O	2.17	0.44
2:C:260:LEU:HA	2:C:291:ALA:HB2	1.98	0.44
2:C:405:ARG:HD2	2:C:442:GLU:OE1	2.17	0.44
2:C:499:ALA:HB1	8:C:1368:HOH:O	2.18	0.44
2:C:603:VAL:HG21	2:C:643:VAL:CG1	2.41	0.44
2:C:693:GLU:OE2	2:C:855:VAL:HG21	2.16	0.44
2:C:737:LEU:HD12	2:C:754:ILE:HB	1.98	0.44
2:C:884:GLN:HG3	2:C:885:ILE:HD13	1.98	0.44
3:D:1258:ARG:HH21	3:D:1351:GLU:HG2	1.82	0.44
3:D:1320:GLU:CB	3:D:1323:GLN:HE21	2.30	0.44
3:D:1192:LEU:HD21	3:D:1372:VAL:HG13	1.99	0.44
3:D:10:ILE:HD13	3:D:1447:LEU:HG	1.99	0.44
3:D:630:VAL:O	3:D:726:ILE:HG13	2.16	0.44
3:D:756:GLN:NE2	3:D:760:ARG:HD2	2.32	0.44
3:D:795:VAL:CG1	3:D:863:VAL:HG13	2.44	0.44
1:K:19:GLU:O	1:K:200:TRP:HA	2.16	0.44
1:L:76:VAL:HA	1:L:79:ILE:HG12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:1013:TYR:CD1	2:M:1020:PRO:HA	2.52	0.44
2:M:1037:VAL:HG12	2:M:1041:GLU:OE1	2.17	0.44
2:M:1040:LEU:HD23	2:M:1049:LEU:CA	2.47	0.44
2:M:1066:ALA:O	2:M:1070:ILE:HG13	2.16	0.44
2:M:333:ILE:N	2:M:333:ILE:HD12	2.32	0.44
2:M:332:ARG:HG3	2:M:333:ILE:N	2.33	0.44
2:M:139:GLN:HB3	2:M:334:ARG:HD3	1.99	0.44
2:M:34:VAL:CB	2:M:38:LYS:HG3	2.47	0.44
2:M:134:ARG:HD3	2:M:393:GLN:O	2.17	0.44
2:M:429:ASP:HB3	8:M:1324:HOH:O	2.17	0.44
2:M:559:LEU:HD23	2:M:560:MET:N	2.33	0.44
3:N:1197:ARG:HD2	3:N:1198:TYR:CD1	2.52	0.44
3:N:1249:ALA:HB2	8:N:9831:HOH:O	2.16	0.44
3:N:1280:VAL:HG12	3:N:1281:VAL:N	2.32	0.44
3:N:1403:LEU:O	3:N:1407:LEU:HB2	2.16	0.44
3:N:400:VAL:C	3:N:402:PRO:HD3	2.38	0.44
2:M:1043:TYR:CE1	3:N:710:ARG:HB2	2.52	0.44
3:N:799:LYS:N	3:N:826:PRO:HG2	2.31	0.44
5:P:144:ILE:HG23	8:P:4865:HOH:O	2.17	0.44
5:P:141:VAL:O	5:P:145:PRO:HD2	2.15	0.44
5:P:217:ASN:O	5:P:221:ILE:HG13	2.18	0.44
1:B:173:PRO:HA	1:B:202:ASP:OD2	2.17	0.44
2:C:162:ILE:HB	2:C:172:ILE:CD1	2.47	0.44
2:C:304:LEU:HD23	2:C:305:PRO:HD3	1.99	0.44
2:C:515:ALA:C	2:C:516:ARG:HG2	2.38	0.44
2:C:71:TYR:HD2	8:C:1554:HOH:O	1.99	0.44
3:D:112:ILE:O	3:D:112:ILE:HD12	2.18	0.44
3:D:1155:VAL:CG1	3:D:1177:ALA:HB1	2.47	0.44
3:D:1211:MET:CG	3:D:1213:ARG:HG2	2.47	0.44
3:D:1211:MET:HG2	3:D:1213:ARG:HG2	1.99	0.44
3:D:574:LEU:O	3:D:577:ALA:HB3	2.16	0.44
3:D:637:LEU:HD12	3:D:641:GLN:OE1	2.18	0.44
3:D:806:PHE:O	3:D:807:ALA:C	2.55	0.44
5:F:302:LYS:O	5:F:306:GLU:HB2	2.17	0.44
2:M:139:GLN:CG	2:M:140:ILE:N	2.80	0.44
2:M:329:GLY:N	2:M:488:ALA:HB3	2.33	0.44
2:M:873:PRO:HB3	3:N:949:ILE:HG12	1.98	0.44
3:N:1000:THR:HG23	3:N:1001:GLU:N	2.32	0.44
3:N:951:ILE:HG23	3:N:1062:ARG:NH2	2.32	0.44
3:N:423:ASP:HB3	5:P:175:HIS:HA	1.99	0.44
3:N:500:ARG:HH12	3:N:1388:ARG:NH1	1.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:63:TYR:HB3	3:N:68:PHE:CE1	2.53	0.44
3:N:891:GLU:HA	3:N:891:GLU:OE1	2.17	0.44
5:P:369:LEU:O	5:P:373:LYS:HB2	2.17	0.44
2:C:1067:TYR:HE2	5:F:345:ALA:HB2	1.82	0.44
2:C:305:PRO:HG2	8:C:1135:HOH:O	2.16	0.44
2:C:338:GLU:CA	2:C:341:THR:HG22	2.46	0.44
2:C:436:GLY:O	2:C:459:ALA:HB2	2.18	0.44
2:C:630:ARG:NH2	2:C:706:GLU:C	2.71	0.44
2:C:79:PRO:HG2	2:C:82:GLU:HB2	2.00	0.44
2:C:841:ASN:ND2	2:C:844:GLY:H	2.15	0.44
2:C:842:ARG:HH21	2:C:887:GLU:CD	2.21	0.44
3:D:1328:GLY:HA2	8:D:9891:HOH:O	2.16	0.44
3:D:1369:GLU:O	3:D:1372:VAL:HG12	2.17	0.44
3:D:209:ARG:HB2	3:D:395:VAL:O	2.17	0.44
3:D:658:LEU:O	3:D:661:MET:HB2	2.17	0.44
3:D:62:LYS:HB2	3:D:73:CYS:SG	2.57	0.44
3:D:978:TYR:HE1	3:D:985:ASP:HA	1.82	0.44
5:F:93:LEU:HD11	5:F:187:LEU:HG	2.00	0.44
5:F:335:ASP:CG	5:F:338:LEU:HB2	2.37	0.44
1:L:55:SER:OG	1:L:158:ILE:HB	2.18	0.44
2:M:469:THR:HG23	2:M:470:PRO:HD2	1.99	0.44
2:M:713:ARG:HG3	2:M:713:ARG:HH11	1.82	0.44
2:M:561:GLY:HA3	2:M:842:ARG:O	2.18	0.44
3:N:1031:ASN:OD1	3:N:1033:GLN:N	2.50	0.44
3:N:1393:GLN:CB	3:N:1398:TRP:HE1	2.25	0.44
3:N:1498:ALA:HA	3:N:1501:GLU:OE2	2.18	0.44
3:N:436:GLU:HB2	3:N:445:ARG:HB2	1.98	0.44
3:N:465:LEU:HD22	3:N:509:PRO:O	2.17	0.44
3:N:893:GLU:O	3:N:896:ALA:HB3	2.17	0.44
3:N:899:LEU:CD1	3:N:900:ILE:HG23	2.45	0.44
4:O:16:LYS:HD3	4:O:17:TYR:CE2	2.46	0.44
5:P:256:ARG:HD2	8:P:3047:HOH:O	2.17	0.44
5:P:317:LEU:O	5:P:329:TYR:HB3	2.16	0.44
1:A:112:ARG:HD3	8:A:442:HOH:O	2.16	0.44
1:A:195:LEU:HD11	1:A:197:LEU:HD22	1.98	0.44
2:C:1002:GLU:HB2	3:D:628:ARG:HH12	1.82	0.44
2:C:1060:ILE:CG2	2:C:1061:GLU:H	2.29	0.44
2:C:884:GLN:CG	2:C:885:ILE:N	2.80	0.44
3:D:1109:GLU:HG2	3:D:1202:GLN:H	1.83	0.44
3:D:1350:GLU:HG3	3:D:1354:LYS:CE	2.43	0.44
3:D:477:LEU:HD23	8:D:9254:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:581:LEU:HD12	3:D:603:LEU:HD12	2.00	0.44
3:D:970:LYS:HD2	3:D:995:LEU:HD13	1.99	0.44
2:M:1114:GLY:N	2:M:1115:LEU:HD12	2.31	0.44
2:M:534:VAL:N	2:M:538:GLN:NE2	2.63	0.44
2:M:816:LYS:HB2	2:M:819:VAL:CG2	2.47	0.44
2:M:832:LYS:O	2:M:833:LEU:C	2.55	0.44
2:M:975:TYR:HE2	8:M:1126:HOH:O	2.01	0.44
2:M:674:VAL:O	2:M:989:VAL:HA	2.17	0.44
3:N:472:ALA:HB3	8:N:9566:HOH:O	2.17	0.44
3:N:486:ARG:CZ	8:N:9895:HOH:O	2.65	0.44
3:N:584:ASN:H	3:N:602:SER:CB	2.30	0.44
3:N:650:LEU:HD12	3:N:691:LEU:HD22	2.00	0.44
3:N:699:VAL:HG12	3:N:717:GLN:HA	1.98	0.44
5:P:123:ASP:HB2	5:P:126:LEU:HD22	1.98	0.44
5:P:276:ARG:HB2	8:P:3917:HOH:O	2.16	0.44
1:A:184:THR:O	1:A:192:LEU:HD12	2.17	0.44
1:B:71:VAL:HG22	1:B:132:LEU:HD12	1.99	0.44
1:B:14:ARG:HH21	1:B:24:VAL:HG21	1.82	0.44
2:C:1033:GLY:O	2:C:1036:GLU:HB2	2.18	0.44
2:C:129:ILE:HG13	2:C:386:PHE:HB3	1.99	0.44
2:C:212:GLY:C	2:C:215:GLY:H	2.21	0.44
2:C:447:ALA:O	2:C:449:ILE:HG22	2.18	0.44
2:C:917:LEU:HD23	2:C:917:LEU:HA	1.89	0.44
3:D:1278:ASP:HB2	3:D:1318:TYR:HE1	1.82	0.44
3:D:1394:VAL:HG21	3:D:1397:LYS:NZ	2.32	0.44
3:D:1462:LEU:N	3:D:1462:LEU:HD23	2.32	0.44
3:D:548:ILE:HG12	3:D:548:ILE:H	1.47	0.44
3:D:554:LEU:O	3:D:558:LEU:HG	2.16	0.44
3:D:583:ASP:OD2	3:D:586:ARG:HD2	2.18	0.44
3:D:661:MET:HE3	3:D:673:ALA:HB1	2.00	0.44
2:C:1035:MET:HG2	3:D:707:THR:O	2.17	0.44
3:D:879:ARG:HG3	3:D:879:ARG:NH1	2.33	0.44
3:D:925:GLU:HG2	4:E:7:ASP:OD1	2.18	0.44
4:E:40:LEU:HD13	8:E:180:HOH:O	2.18	0.44
1:K:156:HIS:HD2	1:K:157:GLY:N	2.15	0.44
1:K:64:GLU:OE2	1:K:76:VAL:HG13	2.18	0.44
2:M:1068:GLU:OE1	5:P:345:ALA:HA	2.17	0.44
2:M:239:PHE:HD1	8:M:1629:HOH:O	2.00	0.44
2:M:979:THR:CG2	2:M:981:GLU:HB2	2.46	0.44
3:N:128:TYR:HB3	3:N:129:PHE:CD1	2.53	0.44
3:N:1399:ASP:O	3:N:1403:LEU:HD12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1441:GLN:CD	3:N:1442:ASN:HB2	2.38	0.44
3:N:206:ARG:HH11	3:N:206:ARG:HG2	1.82	0.44
3:N:591:VAL:CG1	3:N:597:ASP:HA	2.48	0.44
5:P:128:ARG:CZ	5:P:128:ARG:HB2	2.48	0.44
5:P:287:THR:O	5:P:289:GLU:N	2.50	0.44
5:P:395:GLU:O	5:P:399:GLN:HB2	2.18	0.44
5:P:416:ARG:HD2	5:P:419:ARG:HB3	1.99	0.44
1:A:107:LYS:HG3	8:A:494:HOH:O	2.17	0.44
1:A:27:PRO:HG3	1:A:186:LEU:HD13	2.00	0.44
1:B:54:THR:HG22	1:B:158:ILE:HG13	1.99	0.44
1:B:73:GLU:HB2	1:B:78:ILE:CG1	2.48	0.44
2:C:383:ARG:HB2	2:C:383:ARG:CZ	2.46	0.44
2:C:470:PRO:HB2	2:C:483:VAL:HG11	1.99	0.44
2:C:666:LEU:HD21	2:C:668:LEU:HD11	1.99	0.44
2:C:690:ILE:HD12	2:C:849:VAL:CG1	2.47	0.44
2:C:789:SER:O	2:C:791:ARG:HG2	2.17	0.44
2:C:78:PHE:CB	2:C:88:LEU:HD21	2.48	0.44
3:D:1447:LEU:O	3:D:1448:THR:C	2.56	0.44
4:E:49:GLN:HA	4:E:51:LEU:O	2.18	0.44
5:F:136:LEU:HD12	5:F:137:GLY:N	2.32	0.44
5:F:81:VAL:O	5:F:85:LEU:HG	2.17	0.44
1:K:58:ILE:HD13	1:K:140:MET:CB	2.47	0.44
1:L:107:LYS:HB2	8:L:4739:HOH:O	2.16	0.44
2:M:1061:GLU:HB3	8:M:1529:HOH:O	2.17	0.44
2:M:428:ARG:O	3:N:1078:ARG:NH1	2.50	0.44
3:N:1416:ALA:HA	8:N:9145:HOH:O	2.16	0.44
3:N:631:ILE:HG12	3:N:743:ASP:O	2.18	0.44
3:N:759:ALA:O	3:N:763:MET:HB3	2.17	0.44
3:N:955:VAL:HA	8:N:9249:HOH:O	2.17	0.44
3:N:968:ASP:O	3:N:971:LEU:HB3	2.17	0.44
1:A:156:HIS:CD2	1:A:157:GLY:N	2.86	0.44
1:A:49:PRO:O	1:A:173:PRO:HG3	2.18	0.44
1:A:191:ASP:O	1:A:191:ASP:CG	2.55	0.44
2:C:141:HIS:NE2	2:C:332:ARG:NH1	2.65	0.44
2:C:281:LEU:HD11	2:C:306:THR:CA	2.34	0.44
2:C:41:ASN:HB2	8:C:1831:HOH:O	2.17	0.44
2:C:953:VAL:HG22	2:C:966:LEU:HD13	2.00	0.44
3:D:9:ARG:HH21	3:D:11:ALA:CB	2.31	0.44
3:D:1236:LEU:HA	3:D:1359:GLN:CD	2.38	0.44
3:D:1371:VAL:HG12	3:D:1375:MET:HE3	1.99	0.44
3:D:369:ALA:HB3	8:D:9717:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:400:VAL:CG1	3:D:441:ARG:HD3	2.48	0.44
3:D:90:MET:CE	3:D:518:PRO:HB3	2.47	0.44
3:D:57:GLU:HG2	3:D:58:CYS:N	2.33	0.44
3:D:999:THR:O	3:D:1002:LYS:HB2	2.17	0.44
1:L:13:VAL:HG13	1:L:23:PHE:CD1	2.53	0.44
2:M:129:ILE:N	2:M:129:ILE:HD12	2.31	0.44
2:M:164:PRO:HD2	2:M:170:PRO:O	2.18	0.44
2:M:211:LEU:CD1	2:M:308:ARG:HG3	2.44	0.44
2:M:445:GLU:HA	2:M:445:GLU:OE2	2.17	0.44
2:M:95:TYR:N	2:M:95:TYR:CD1	2.86	0.44
3:N:1470:ARG:HG2	3:N:1471:LEU:N	2.32	0.44
3:N:18:ILE:HG21	3:N:516:ALA:HB1	1.99	0.44
3:N:464:LEU:HD11	8:N:9491:HOH:O	2.18	0.44
3:N:563:PRO:HA	5:P:185:GLN:OE1	2.18	0.44
3:N:82:LYS:HB2	3:N:82:LYS:HE3	1.85	0.44
3:N:884:ARG:NH1	8:N:9403:HOH:O	2.49	0.44
3:N:950:GLY:C	3:N:952:ASP:N	2.64	0.44
4:O:45:ARG:HB2	4:O:46:PRO:HD2	1.99	0.44
3:N:566:ILE:HG23	5:P:214:GLN:HE22	1.82	0.44
5:P:290:GLU:CD	5:P:290:GLU:H	2.20	0.44
1:A:73:GLU:N	1:A:73:GLU:OE2	2.51	0.44
1:B:1:MET:O	1:B:6:LEU:HD13	2.18	0.44
2:C:1086:ARG:HG2	2:C:1112:PHE:CE2	2.52	0.44
2:C:1101:THR:HB	3:D:5:VAL:CG1	2.48	0.44
2:C:176:VAL:HG13	8:C:1607:HOH:O	2.17	0.44
2:C:185:LYS:HB3	2:C:188:LYS:O	2.17	0.44
2:C:27:ARG:HG2	2:C:27:ARG:HH11	1.82	0.44
2:C:51:THR:CB	2:C:348:LEU:HD23	2.48	0.44
2:C:470:PRO:HG2	2:C:538:GLN:OE1	2.18	0.44
2:C:597:ALA:HB2	2:C:655:LEU:CD2	2.37	0.44
2:C:820:ARG:HB3	8:C:1508:HOH:O	2.18	0.44
2:C:93:PRO:HG3	2:C:117:HIS:HE1	1.82	0.44
3:D:1106:VAL:O	3:D:1108:ARG:HG2	2.18	0.44
3:D:1207:TYR:C	8:D:9465:HOH:O	2.56	0.44
3:D:1369:GLU:HA	3:D:1372:VAL:HG12	1.99	0.44
3:D:1472:ILE:HA	3:D:1473:PRO:HD3	1.86	0.44
3:D:168:THR:O	3:D:393:ILE:N	2.49	0.44
3:D:196:VAL:HG13	3:D:202:VAL:CG1	2.48	0.44
3:D:472:ALA:HB3	8:D:9440:HOH:O	2.17	0.44
3:D:653:PHE:HD1	3:D:653:PHE:N	2.16	0.44
3:D:6:ARG:HH11	3:D:6:ARG:HB3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:175:ARG:HH21	1:K:201:THR:N	2.16	0.44
1:K:50:GLY:O	1:K:146:ARG:HA	2.18	0.44
2:M:1032:PHE:CE2	2:M:1052:MET:HG2	2.52	0.44
2:M:146:VAL:HG11	2:M:306:THR:HG22	2.00	0.44
2:M:218:VAL:O	2:M:221:LEU:HG	2.18	0.44
2:M:250:ARG:HG2	8:M:1251:HOH:O	2.18	0.44
2:M:364:GLU:HG2	8:M:1471:HOH:O	2.17	0.44
2:M:397:GLU:N	2:M:633:GLN:CD	2.71	0.44
2:M:619:ARG:C	2:M:620:LEU:HD13	2.37	0.44
2:M:625:LEU:HD13	2:M:639:GLN:O	2.18	0.44
2:M:752:GLY:O	3:N:679:ARG:HG2	2.18	0.44
2:M:80:GLN:HE22	2:M:122:THR:HG23	1.83	0.44
2:M:695:LEU:HD22	2:M:832:LYS:HB3	2.00	0.44
3:N:1123:PHE:HA	3:N:1135:ARG:N	2.32	0.44
3:N:119:SER:CB	3:N:123:LEU:H	2.27	0.44
3:N:12:LEU:HD23	3:N:13:ALA:N	2.26	0.44
3:N:459:GLU:HA	8:N:9127:HOH:O	2.17	0.44
3:N:85:VAL:HG12	3:N:89:ARG:NE	2.33	0.44
3:N:907:GLU:HG2	3:N:908:LYS:H	1.81	0.44
4:O:10:PHE:CE2	4:O:16:LYS:HG3	2.53	0.44
4:O:33:HIS:HB2	4:O:37:ASN:HD21	1.80	0.44
5:P:133:ALA:HB2	5:P:142:ARG:CZ	2.48	0.44
1:A:107:LYS:HB3	8:A:463:HOH:O	2.18	0.44
1:B:57:TYR:CE1	1:B:161:ARG:HB3	2.53	0.44
1:B:170:VAL:HG23	1:B:170:VAL:O	2.17	0.44
2:C:1049:LEU:HG	2:C:1053:LEU:HD11	1.99	0.44
2:C:108:ILE:HG12	8:C:1205:HOH:O	2.18	0.44
2:C:208:ALA:HA	2:C:221:LEU:HD21	1.99	0.44
2:C:577:PRO:HG3	2:C:993:PHE:CD2	2.53	0.44
2:C:601:GLY:HA3	2:C:615:TYR:HA	1.99	0.44
2:C:31:GLN:HB3	2:C:71:TYR:OH	2.16	0.44
2:C:722:ILE:HG23	2:C:805:ARG:NH2	2.30	0.44
2:C:778:PHE:HB3	8:C:1664:HOH:O	2.18	0.44
2:C:902:ILE:HD13	8:C:1742:HOH:O	2.18	0.44
2:C:916:GLU:O	2:C:919:ALA:HB3	2.18	0.44
2:C:971:LYS:HB3	2:C:987:ILE:C	2.38	0.44
3:D:783:ARG:NH2	3:D:1029:ARG:CZ	2.81	0.44
3:D:1122:LEU:HD11	3:D:1186:VAL:HG23	1.99	0.44
3:D:1379:VAL:HA	3:D:1420:LEU:HB3	1.99	0.44
3:D:135:LEU:HA	3:D:453:ASP:O	2.18	0.44
3:D:780:LYS:NZ	8:D:9079:HOH:O	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:799:LYS:N	3:D:826:PRO:HG2	2.32	0.44
3:D:910:SER:O	3:D:913:ASP:HB2	2.18	0.44
3:D:955:VAL:HB	3:D:1011:PHE:CE1	2.46	0.44
5:F:287:THR:O	5:F:289:GLU:N	2.51	0.44
5:F:295:MET:HB3	5:F:299:TRP:CG	2.52	0.44
3:D:611:GLN:CG	5:F:326:ASP:HB2	2.46	0.44
5:F:361:LEU:HD13	5:F:366:ALA:HB2	1.99	0.44
1:K:69:PRO:HA	2:M:607:ASP:OD2	2.17	0.44
2:M:1049:LEU:O	2:M:1053:LEU:HD12	2.17	0.44
2:M:1105:LYS:O	2:M:1107:ASN:N	2.50	0.44
2:M:577:PRO:HD3	8:M:1226:HOH:O	2.17	0.44
2:M:943:VAL:HG11	2:M:973:VAL:CG2	2.48	0.44
3:N:119:SER:H	3:N:123:LEU:CB	2.28	0.44
3:N:1109:GLU:CG	3:N:1202:GLN:H	2.31	0.44
3:N:1231:GLU:HB3	3:N:1232:PRO:HD3	2.00	0.44
3:N:1302:GLU:OE2	3:N:1304:LYS:HG3	2.17	0.44
3:N:664:LYS:HE3	3:N:693:GLU:OE1	2.18	0.44
2:M:1042:ALA:HB1	3:N:710:ARG:CD	2.48	0.44
4:O:50:THR:HB	8:O:4472:HOH:O	2.18	0.44
5:P:376:ILE:HB	8:P:4564:HOH:O	2.18	0.44
1:A:150:TYR:HD1	2:C:696:LYS:HD3	1.83	0.43
1:A:218:LEU:HD23	1:B:222:LEU:CD2	2.44	0.43
2:C:162:ILE:HD12	2:C:172:ILE:CB	2.46	0.43
2:C:305:PRO:HB3	2:C:308:ARG:NH2	2.33	0.43
2:C:435:TYR:C	2:C:437:ARG:H	2.21	0.43
2:C:786:LYS:HA	8:C:1481:HOH:O	2.17	0.43
2:C:861:LEU:HD23	2:C:863:ASP:H	1.83	0.43
2:C:873:PRO:HG2	3:D:947:ILE:CD1	2.43	0.43
2:C:927:GLY:HA2	2:C:930:LYS:HE3	1.99	0.43
2:C:961:GLU:HG3	8:C:1364:HOH:O	2.18	0.43
3:D:1098:LEU:N	3:D:1098:LEU:HD12	2.33	0.43
3:D:1223:ILE:CD1	3:D:1223:ILE:H	2.25	0.43
3:D:1135:ARG:NH1	3:D:1357:ARG:HH12	2.16	0.43
3:D:34:TYR:OH	5:F:261:PRO:HD2	2.18	0.43
3:D:639:LEU:HD22	3:D:766:ALA:CB	2.48	0.43
4:E:14:ASP:N	4:E:14:ASP:OD1	2.46	0.43
5:F:132:ARG:HD3	5:F:181:GLU:CD	2.39	0.43
1:K:58:ILE:HD13	1:K:140:MET:HB2	2.00	0.43
1:L:176:ARG:HG3	1:L:200:TRP:CE3	2.52	0.43
1:L:75:VAL:O	1:L:79:ILE:HG23	2.17	0.43
2:M:176:VAL:O	2:M:178:PRO:HD3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:47:ALA:HB3	2:M:344:PHE:CE1	2.53	0.43
2:M:566:THR:HG22	2:M:566:THR:O	2.18	0.43
2:M:761:PHE:HB3	8:M:1358:HOH:O	2.17	0.43
1:K:42:ARG:NH1	2:M:857:ASP:HB3	2.30	0.43
2:M:91:GLN:CD	2:M:117:HIS:HB3	2.37	0.43
3:N:1350:GLU:O	3:N:1354:LYS:HG2	2.18	0.43
3:N:136:ASP:HB2	3:N:137:PRO:HD3	1.98	0.43
3:N:177:ALA:HB1	3:N:199:LEU:HB3	2.00	0.43
2:M:1087:VAL:HG23	3:N:524:LEU:CD2	2.48	0.43
3:N:637:LEU:HD12	3:N:641:GLN:OE1	2.18	0.43
3:N:783:ARG:HE	3:N:1029:ARG:HG3	1.83	0.43
5:P:101:GLU:O	5:P:105:LYS:HG3	2.18	0.43
5:P:133:ALA:O	5:P:137:GLY:O	2.36	0.43
5:P:320:PRO:C	5:P:321:ILE:HD13	2.38	0.43
1:A:51:THR:HA	1:A:145:ASP:O	2.18	0.43
1:A:99:LEU:HB3	1:A:114:PHE:CD2	2.53	0.43
1:A:219:ARG:NE	1:B:219:ARG:HG2	2.33	0.43
2:C:65:VAL:HB	2:C:101:ILE:HB	2.00	0.43
2:C:338:GLU:HA	2:C:341:THR:CG2	2.46	0.43
2:C:677:MET:HE1	2:C:983:ILE:HD13	1.99	0.43
2:C:754:ILE:HD13	2:C:791:ARG:CD	2.48	0.43
3:D:1198:TYR:HE1	8:D:9137:HOH:O	2.00	0.43
3:D:178:LEU:CD1	3:D:200:ASP:H	2.32	0.43
3:D:131:LYS:HA	3:D:456:MET:HG3	2.00	0.43
3:D:530:VAL:HG12	3:D:531:ASP:N	2.32	0.43
3:D:631:ILE:O	3:D:632:VAL:HG23	2.18	0.43
3:D:814:ALA:HB3	8:D:9196:HOH:O	2.17	0.43
3:D:817:GLU:O	3:D:840:LYS:NZ	2.51	0.43
3:D:890:VAL:HG13	3:D:926:LYS:CE	2.48	0.43
5:F:155:THR:O	5:F:159:ILE:HG13	2.17	0.43
5:F:416:ARG:HD2	5:F:419:ARG:HB3	1.98	0.43
1:K:169:ALA:HB1	1:K:171:PHE:CE1	2.53	0.43
1:L:94:LEU:HD21	1:L:119:ASP:HB2	2.01	0.43
2:M:357:GLU:HB2	8:M:1297:HOH:O	2.17	0.43
2:M:462:ASP:CG	2:M:463:GLU:H	2.21	0.43
2:M:484:VAL:HG21	8:M:1124:HOH:O	2.18	0.43
2:M:50:GLU:OE2	2:M:345:ARG:NH1	2.52	0.43
2:M:603:VAL:HG23	2:M:647:GLN:O	2.17	0.43
2:M:916:GLU:HA	8:M:1178:HOH:O	2.16	0.43
3:N:1004:THR:OG1	3:N:1036:ARG:HG3	2.18	0.43
3:N:1314:LYS:HZ3	3:N:1317:ASP:N	2.03	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1353:GLN:O	3:N:1357:ARG:HD2	2.18	0.43
3:N:163:TYR:O	3:N:447:VAL:HG21	2.18	0.43
3:N:530:VAL:HA	8:N:9503:HOH:O	2.17	0.43
3:N:560:GLN:NE2	5:P:218:GLN:NE2	2.65	0.43
3:N:644:LEU:HD12	3:N:645:PRO:CD	2.42	0.43
3:N:754:PHE:HZ	4:O:21:VAL:HG13	1.83	0.43
3:N:996:TRP:HA	3:N:996:TRP:CE3	2.53	0.43
4:O:46:PRO:CB	4:O:54:LEU:HD22	2.48	0.43
5:P:130:VAL:HG21	5:P:159:ILE:HG21	2.01	0.43
8:N:9109:HOH:O	5:P:319:THR:HG23	2.17	0.43
1:A:107:LYS:CG	8:A:494:HOH:O	2.66	0.43
1:B:189:ARG:H	1:B:189:ARG:HG2	1.61	0.43
2:C:108:ILE:H	2:C:108:ILE:HG13	1.55	0.43
2:C:54:ILE:HG12	8:C:1597:HOH:O	2.19	0.43
2:C:688:ILE:N	2:C:688:ILE:HD12	2.33	0.43
2:C:746:GLY:C	2:C:799:ILE:HG22	2.38	0.43
2:C:876:VAL:HG21	3:D:949:ILE:HG13	2.00	0.43
3:D:1141:GLU:HG2	3:D:1168:MET:HE1	1.99	0.43
3:D:185:VAL:CG1	3:D:191:LEU:HD21	2.48	0.43
3:D:34:TYR:CE1	3:D:35:ARG:HG3	2.53	0.43
3:D:179:VAL:HG22	3:D:389:GLU:CD	2.38	0.43
3:D:521:PRO:O	3:D:525:ARG:HD3	2.19	0.43
4:E:57:ASP:H	4:E:58:PRO:HD3	1.83	0.43
5:F:323:ASP:HB3	5:F:325:LYS:HG3	2.00	0.43
5:F:408:LEU:HD13	5:F:411:HIS:HE1	1.83	0.43
1:K:1:MET:O	1:K:6:LEU:HB2	2.18	0.43
2:M:1002:GLU:HG3	2:M:1002:GLU:H	1.42	0.43
2:M:1075:ASP:HB2	4:O:31:LEU:HD12	1.99	0.43
2:M:378:LEU:N	8:M:1288:HOH:O	2.51	0.43
2:M:435:TYR:C	2:M:437:ARG:H	2.20	0.43
2:M:333:ILE:CD1	2:M:467:ILE:HG13	2.48	0.43
2:M:523:ILE:O	2:M:523:ILE:HG23	2.18	0.43
2:M:710:ILE:HD11	2:M:758:ARG:HE	1.83	0.43
2:M:999:HIS:HE1	8:M:1359:HOH:O	2.00	0.43
3:N:1051:GLU:HG3	3:N:1051:GLU:H	1.50	0.43
3:N:1197:ARG:HB3	3:N:1396:GLU:HG3	2.00	0.43
2:M:1052:MET:HG3	3:N:623:VAL:CG2	2.48	0.43
3:N:660:LYS:HD2	3:N:663:GLU:OE2	2.18	0.43
5:P:134:LYS:HE3	5:P:160:ASP:OD2	2.18	0.43
2:M:1018:GLN:NE2	5:P:338:LEU:HD13	2.33	0.43
1:A:49:PRO:HB3	1:A:148:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:VAL:HA	1:A:78:ILE:HD12	1.99	0.43
1:B:101:LEU:HD12	1:B:114:PHE:CD1	2.54	0.43
2:C:127:PHE:CE1	2:C:386:PHE:HE2	2.36	0.43
2:C:289:THR:O	2:C:291:ALA:N	2.52	0.43
2:C:396:ASP:HA	2:C:633:GLN:OE1	2.18	0.43
2:C:401:LEU:HD13	2:C:587:VAL:HG11	1.99	0.43
3:D:119:SER:H	3:D:123:LEU:CB	2.31	0.43
3:D:1382:THR:HG21	3:D:1418:LYS:CE	2.48	0.43
3:D:1472:ILE:HG22	3:D:1474:ALA:O	2.19	0.43
3:D:369:ALA:HA	8:D:9461:HOH:O	2.19	0.43
3:D:772:PRO:HG3	3:D:1210:SER:OG	2.19	0.43
3:D:805:GLU:O	3:D:805:GLU:OE1	2.37	0.43
5:F:179:GLU:HG3	8:F:503:HOH:O	2.18	0.43
5:F:320:PRO:C	5:F:321:ILE:HD13	2.38	0.43
5:F:365:GLU:OE1	5:F:400:ILE:HD12	2.17	0.43
1:K:156:HIS:CD2	1:K:157:GLY:N	2.86	0.43
1:K:175:ARG:HE	1:K:175:ARG:HB2	1.64	0.43
1:K:198:ARG:HG3	1:K:198:ARG:H	1.65	0.43
1:L:101:LEU:HD21	1:L:113:ASP:HB3	1.99	0.43
2:M:1091:GLU:HA	3:N:520:LEU:HD13	2.00	0.43
2:M:196:LEU:O	2:M:199:VAL:HB	2.18	0.43
2:M:571:LEU:C	2:M:573:ARG:H	2.21	0.43
2:M:15:LEU:HD21	2:M:583:LEU:HD21	2.00	0.43
2:M:572:ILE:HG23	2:M:703:ILE:HD13	1.99	0.43
3:N:1059:SER:OG	3:N:1065:LEU:HA	2.17	0.43
3:N:1485:GLN:O	4:O:75:PHE:HA	2.19	0.43
3:N:568:ARG:O	3:N:569:ASN:C	2.57	0.43
3:N:789:LEU:O	3:N:792:ILE:HG23	2.18	0.43
3:N:89:ARG:NH2	8:N:9103:HOH:O	2.51	0.43
1:B:89:PHE:CD1	1:B:120:VAL:HG22	2.54	0.43
1:B:165:ILE:HA	1:B:166:PRO:HD3	1.87	0.43
1:A:215:VAL:HG11	1:B:225:PHE:CD1	2.53	0.43
2:C:1091:GLU:HG2	3:D:606:ILE:HG21	2.00	0.43
2:C:236:ILE:O	2:C:239:PHE:HB2	2.17	0.43
2:C:417:GLY:C	2:C:418:LEU:HD12	2.39	0.43
2:C:640:ARG:CB	2:C:640:ARG:HH11	2.32	0.43
3:D:1029:ARG:NH2	8:D:9488:HOH:O	2.52	0.43
3:D:1087:ARG:HG2	3:D:1087:ARG:HH11	1.83	0.43
3:D:1271:LYS:HE3	3:D:1334:GLN:NE2	2.33	0.43
3:D:133:ILE:HD11	8:D:9474:HOH:O	2.18	0.43
3:D:525:ARG:HA	3:D:538:SER:CB	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:853:VAL:HA	3:D:858:VAL:O	2.18	0.43
1:K:229:GLN:HB2	1:K:229:GLN:HE21	1.64	0.43
2:M:1019:GLN:OE1	3:N:621:LYS:HA	2.18	0.43
2:M:1051:GLU:CG	2:M:1056:LYS:HE3	2.40	0.43
2:M:1018:GLN:NE2	2:M:1063:ARG:NH2	2.66	0.43
2:M:186:VAL:HG23	2:M:187:ASN:N	2.26	0.43
2:M:203:ASP:OD1	2:M:206:THR:HG22	2.18	0.43
2:M:220:GLY:HA3	8:M:1170:HOH:O	2.18	0.43
2:M:302:VAL:C	2:M:305:PRO:HD2	2.39	0.43
2:M:553:ASP:HA	2:M:881:ASN:HA	1.99	0.43
3:N:1264:GLU:CD	3:N:1425:THR:HB	2.39	0.43
3:N:431:VAL:HG22	8:N:9550:HOH:O	2.18	0.43
3:N:47:GLU:HG2	8:N:9894:HOH:O	2.17	0.43
3:N:514:LEU:HA	8:N:9079:HOH:O	2.18	0.43
3:N:584:ASN:HB2	3:N:602:SER:OG	2.19	0.43
3:N:102:ILE:CG2	3:N:586:ARG:HD3	2.49	0.43
3:N:749:VAL:HA	3:N:750:PRO:HD3	1.90	0.43
4:O:54:LEU:N	8:O:4983:HOH:O	2.52	0.43
5:P:366:ALA:HB3	5:P:367:MET:CE	2.49	0.43
1:A:23:PHE:O	1:A:196:THR:HA	2.18	0.43
1:A:1:MET:O	1:A:6:LEU:HB2	2.18	0.43
1:A:85:LEU:HA	1:A:124:ASN:HD22	1.82	0.43
1:B:49:PRO:HA	8:B:322:HOH:O	2.19	0.43
2:C:1016:ILE:HD12	3:D:526:PRO:HG2	2.00	0.43
2:C:1042:ALA:HB1	8:D:9123:HOH:O	2.18	0.43
2:C:200:LEU:HD13	2:C:300:ASP:OD2	2.18	0.43
2:C:854:PRO:HD2	2:C:857:ASP:OD2	2.18	0.43
3:D:1102:THR:HG22	3:D:1102:THR:O	2.19	0.43
3:D:1434:TRP:CZ3	3:D:1457:ASP:HB2	2.53	0.43
3:D:57:GLU:HG2	3:D:58:CYS:O	2.19	0.43
3:D:606:ILE:O	3:D:613:ARG:HB2	2.18	0.43
3:D:819:GLY:HA2	8:D:9660:HOH:O	2.18	0.43
8:B:441:HOH:O	3:D:821:VAL:HG13	2.18	0.43
3:D:820:GLU:HG3	3:D:836:VAL:CG1	2.49	0.43
3:D:838:ARG:HG2	3:D:865:THR:OG1	2.18	0.43
5:F:313:GLU:HG2	5:F:313:GLU:H	1.42	0.43
1:K:193:ASP:HB2	8:K:3631:HOH:O	2.19	0.43
1:L:142:VAL:HG23	1:L:142:VAL:O	2.19	0.43
1:L:19:GLU:O	1:L:200:TRP:HA	2.18	0.43
2:M:274:ARG:CD	2:M:285:LEU:HB3	2.49	0.43
2:M:654:LEU:HD13	2:M:664:GLY:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:841:ASN:ND2	2:M:841:ASN:C	2.70	0.43
3:N:1237:THR:HB	3:N:1239:ARG:HH21	1.84	0.43
3:N:1425:THR:CG2	3:N:1426:LYS:N	2.82	0.43
3:N:210:ARG:HD3	8:N:9691:HOH:O	2.18	0.43
3:N:32:ILE:O	5:P:258:ILE:HG23	2.19	0.43
3:N:596:SER:OG	3:N:598:ARG:HB3	2.18	0.43
3:N:669:ASN:O	3:N:672:ALA:HB3	2.18	0.43
3:N:694:VAL:HG13	8:N:9146:HOH:O	2.18	0.43
3:N:910:SER:O	3:N:913:ASP:HB2	2.18	0.43
5:P:367:MET:HA	5:P:370:LYS:HZ3	1.84	0.43
5:P:77:THR:O	5:P:81:VAL:HG23	2.17	0.43
1:A:24:VAL:HG22	1:A:196:THR:CB	2.46	0.43
2:C:23:VAL:HA	2:C:121:MET:SD	2.59	0.43
2:C:43:GLY:HA2	2:C:341:THR:OG1	2.19	0.43
2:C:630:ARG:HH22	2:C:707:ARG:CB	2.32	0.43
2:C:588:VAL:HG21	2:C:664:GLY:O	2.17	0.43
2:C:816:LYS:O	2:C:819:VAL:HB	2.19	0.43
2:C:915:LYS:O	2:C:968:LEU:HD22	2.19	0.43
2:C:938:LYS:HD3	2:C:939:ARG:NH2	2.33	0.43
3:D:106:LYS:HA	3:D:106:LYS:HD3	1.83	0.43
3:D:1106:VAL:HG21	3:D:1474:ALA:HB2	2.00	0.43
3:D:641:GLN:O	3:D:716:PHE:HD2	2.01	0.43
3:D:677:LEU:HD21	3:D:687:VAL:HG21	2.01	0.43
3:D:699:VAL:CG2	3:D:760:ARG:HB3	2.45	0.43
3:D:965:GLU:HB2	8:D:2028:HOH:O	2.17	0.43
1:K:9:PRO:HB3	1:K:25:LEU:CG	2.48	0.43
1:L:137:ARG:CZ	1:L:137:ARG:HB3	2.49	0.43
2:M:1049:LEU:O	2:M:1049:LEU:HG	2.16	0.43
2:M:267:TYR:O	2:M:288:ARG:HD3	2.17	0.43
2:M:139:GLN:NE2	2:M:334:ARG:HH11	2.02	0.43
2:M:56:GLU:HB2	2:M:359:MET:SD	2.59	0.43
2:M:936:VAL:HG22	8:M:1450:HOH:O	2.18	0.43
3:N:1124:GLN:HA	3:N:1125:PRO:HD3	1.70	0.43
3:N:117:ASP:HB2	3:N:495:ARG:HH21	1.78	0.43
3:N:131:LYS:HE2	3:N:568:ARG:HB3	2.01	0.43
3:N:112:ILE:HD13	3:N:461:ILE:HG21	2.00	0.43
3:N:469:ASP:HB3	8:N:9566:HOH:O	2.18	0.43
3:N:629:SER:OG	3:N:630:VAL:N	2.50	0.43
3:N:684:LYS:HD3	3:N:686:GLU:CD	2.39	0.43
3:N:698:LYS:HA	3:N:756:GLN:HE21	1.84	0.43
3:N:798:GLU:HB2	3:N:828:LYS:HZ3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:9:LEU:HD21	4:O:69:LEU:HG	2.01	0.43
5:P:104:ARG:HD3	8:P:5106:HOH:O	2.18	0.43
5:P:223:ALA:HB2	5:P:242:TRP:CB	2.49	0.43
5:P:343:ASP:O	5:P:346:THR:HB	2.18	0.43
1:A:26:GLU:CB	1:A:194:LYS:HG3	2.49	0.43
1:A:86:VAL:CG1	1:A:124:ASN:HB2	2.49	0.43
1:B:143:ARG:CD	1:B:158:ILE:HG21	2.48	0.43
1:B:185:ARG:HG3	1:B:190:THR:HG22	2.01	0.43
1:B:191:ASP:O	1:B:192:LEU:HG	2.19	0.43
1:B:26:GLU:HG2	1:B:27:PRO:CA	2.49	0.43
2:C:974:LEU:HD11	2:C:989:VAL:HG11	2.01	0.43
2:C:98:LEU:N	2:C:98:LEU:HD12	2.33	0.43
3:D:210:ARG:HG3	3:D:398:ALA:N	2.32	0.43
3:D:32:ILE:HG22	5:F:258:ILE:HD12	2.00	0.43
3:D:445:ARG:HG2	3:D:445:ARG:NH1	2.33	0.43
3:D:478:LEU:HD21	3:D:500:ARG:HH22	1.77	0.43
3:D:805:GLU:HA	8:D:9801:HOH:O	2.18	0.43
3:D:907:GLU:OE1	3:D:908:LYS:N	2.52	0.43
1:K:101:LEU:HG	1:K:113:ASP:O	2.18	0.43
1:K:228:PRO:HA	1:L:11:PHE:O	2.19	0.43
2:M:1050:GLN:NE2	2:M:1079:PRO:HB2	2.33	0.43
2:M:1103:ASP:N	2:M:1107:ASN:O	2.52	0.43
2:M:289:THR:O	2:M:291:ALA:N	2.51	0.43
2:M:309:TYR:CE2	2:M:321:GLU:HB3	2.54	0.43
2:M:31:GLN:OE1	2:M:38:LYS:HB2	2.18	0.43
2:M:139:GLN:NE2	2:M:415:PRO:HG2	2.34	0.43
2:M:510:ALA:HB3	2:M:513:VAL:CG2	2.49	0.43
2:M:52:PHE:HB3	8:M:1173:HOH:O	2.18	0.43
2:M:773:LEU:HA	8:M:1485:HOH:O	2.19	0.43
1:K:152:PRO:HB3	2:M:832:LYS:NZ	2.34	0.43
2:M:89:THR:O	2:M:89:THR:HG23	2.19	0.43
2:M:984:GLU:O	3:N:946:GLY:HA3	2.18	0.43
3:N:1009:LYS:HG3	8:N:9857:HOH:O	2.18	0.43
3:N:1124:GLN:HG3	8:N:9303:HOH:O	2.19	0.43
3:N:1274:ILE:HA	8:N:9087:HOH:O	2.19	0.43
3:N:704:ARG:CD	3:N:705:ALA:H	2.24	0.43
3:N:806:PHE:O	3:N:807:ALA:C	2.56	0.43
3:N:829:VAL:H	3:N:835:SER:HB2	1.83	0.43
4:O:41:GLU:HG3	4:O:45:ARG:NH1	2.34	0.43
4:O:67:GLU:OE1	4:O:73:LEU:HD11	2.18	0.43
3:N:1485:GLN:NE2	4:O:79:LEU:H	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:337:HIS:CD2	5:P:337:HIS:N	2.86	0.43
5:P:340:SER:O	5:P:342:VAL:N	2.51	0.43
5:P:363:GLU:HA	5:P:367:MET:HE2	1.99	0.43
1:B:138:LEU:HB2	8:B:373:HOH:O	2.18	0.43
2:C:1059:ASP:OD2	2:C:1080:SER:N	2.48	0.43
2:C:10:ARG:HD3	2:C:10:ARG:HA	1.68	0.43
2:C:334:ARG:HB2	2:C:339:LEU:HD11	2.00	0.43
2:C:29:ALA:CB	2:C:337:GLY:HA2	2.49	0.43
2:C:480:THR:HG22	2:C:482:GLU:N	2.31	0.43
2:C:640:ARG:HA	2:C:641:PRO:HD3	1.90	0.43
2:C:680:ASP:HA	8:C:1147:HOH:O	2.18	0.43
2:C:745:ILE:HG13	8:C:1168:HOH:O	2.18	0.43
2:C:77:PRO:HD2	2:C:91:GLN:O	2.19	0.43
3:D:1144:LEU:O	3:D:1166:LEU:HG	2.18	0.43
3:D:1209:LEU:HD13	3:D:1211:MET:CE	2.41	0.43
3:D:1087:ARG:NH1	3:D:1234:THR:O	2.52	0.43
3:D:1303:TYR:CD1	3:D:1325:LEU:HD23	2.54	0.43
3:D:55:ASP:HB3	3:D:56:TYR:H	1.65	0.43
5:F:157:GLU:HG3	8:F:479:HOH:O	2.18	0.43
2:C:1010:THR:HG21	5:F:341:PRO:HB2	2.01	0.43
1:L:12:THR:OG1	1:L:24:VAL:HB	2.19	0.43
2:M:794:PRO:HB2	2:M:1027:PHE:CZ	2.54	0.43
2:M:443:THR:HA	2:M:444:PRO:HD3	1.80	0.43
2:M:570:PRO:HA	8:M:1348:HOH:O	2.18	0.43
2:M:582:GLY:N	2:M:584:GLU:OE2	2.48	0.43
2:M:6:PHE:CD1	2:M:909:ALA:HB2	2.53	0.43
3:N:1300:SER:HB3	8:N:9965:HOH:O	2.18	0.43
3:N:1413:THR:HG21	8:N:9344:HOH:O	2.18	0.43
3:N:185:VAL:HG12	3:N:191:LEU:HD21	2.01	0.43
3:N:397:LYS:HE3	8:N:9313:HOH:O	2.18	0.43
3:N:441:ARG:O	3:N:443:VAL:N	2.52	0.43
3:N:522:PRO:HA	3:N:525:ARG:NH1	2.34	0.43
3:N:760:ARG:HB2	4:O:3:GLU:OE2	2.19	0.43
2:M:1115:LEU:CG	3:N:85:VAL:HG13	2.49	0.43
3:N:87:ARG:HD2	3:N:88:TYR:CE2	2.50	0.43
3:N:898:GLU:HB3	3:N:921:ARG:NH2	2.34	0.43
3:N:781:PRO:HG2	3:N:911:LEU:HD23	2.01	0.43
3:N:950:GLY:H	3:N:953:ASP:CG	2.22	0.43
1:B:7:LYS:HD3	8:B:328:HOH:O	2.19	0.43
2:C:102:HIS:HD2	2:C:365:ASP:OD2	2.02	0.43
2:C:443:THR:HA	2:C:444:PRO:HD3	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:52:PHE:HB3	8:C:1475:HOH:O	2.18	0.43
2:C:744:ARG:HA	8:C:1168:HOH:O	2.18	0.43
2:C:975:TYR:N	2:C:975:TYR:CD1	2.86	0.43
3:D:154:THR:HG22	3:D:157:GLU:OE2	2.19	0.43
3:D:421:LEU:HD12	3:D:435:VAL:CG1	2.49	0.43
3:D:427:VAL:CB	3:D:435:VAL:HB	2.49	0.43
3:D:464:LEU:O	3:D:468:LEU:HG	2.19	0.43
3:D:508:ARG:HG2	3:D:508:ARG:HH11	1.84	0.43
3:D:566:ILE:HD13	5:F:217:ASN:HB3	2.01	0.43
3:D:633:VAL:C	3:D:635:PRO:HD3	2.39	0.43
3:D:708:LEU:HD23	3:D:708:LEU:HA	1.82	0.43
5:F:225:GLU:HG3	5:F:226:LYS:HG3	2.01	0.43
1:K:112:ARG:HH22	1:K:126:ASP:HB2	1.83	0.43
1:K:212:ASN:O	1:K:215:VAL:HG23	2.19	0.43
1:K:48:ILE:HG22	1:K:173:PRO:HD2	2.00	0.43
1:L:62:LEU:HD22	1:L:63:HIS:HE1	1.83	0.43
2:M:415:PRO:C	2:M:417:GLY:H	2.23	0.43
2:M:430:VAL:HG13	3:N:1075:HIS:ND1	2.34	0.43
2:M:495:THR:H	2:M:530:GLU:CD	2.22	0.43
2:M:666:LEU:HD12	2:M:667:ALA:H	1.84	0.43
3:N:1377:LYS:HB3	3:N:1378:TYR:CE1	2.53	0.43
3:N:493:ARG:NH1	3:N:1390:LEU:N	2.67	0.43
3:N:1476:THR:OG1	4:O:20:THR:HG21	2.19	0.43
3:N:828:LYS:N	3:N:828:LYS:HD3	2.33	0.43
2:M:1115:LEU:CB	3:N:85:VAL:HG13	2.49	0.43
5:P:278:LEU:HB3	5:P:286:PRO:CG	2.48	0.43
5:P:88:ILE:O	5:P:92:PRO:HG3	2.19	0.43
1:A:229:GLN:HB2	1:A:229:GLN:HE21	1.58	0.42
1:A:9:PRO:HB3	1:A:25:LEU:HD21	2.01	0.42
1:B:111:ALA:HB3	1:B:124:ASN:O	2.19	0.42
1:B:33:GLY:O	1:B:195:LEU:HD22	2.19	0.42
2:C:103:LYS:HE2	8:C:1421:HOH:O	2.19	0.42
2:C:1083:GLU:O	2:C:1087:VAL:HB	2.19	0.42
2:C:185:LYS:HE3	8:C:1838:HOH:O	2.19	0.42
2:C:524:VAL:HG22	2:C:528:GLU:CD	2.39	0.42
2:C:892:LEU:HD12	2:C:892:LEU:O	2.19	0.42
3:D:1107:VAL:O	3:D:1218:GLY:N	2.49	0.42
3:D:28:LYS:O	3:D:43:GLY:HA2	2.19	0.42
3:D:500:ARG:HD2	8:D:9527:HOH:O	2.18	0.42
3:D:568:ARG:O	3:D:569:ASN:C	2.57	0.42
3:D:638:LYS:C	3:D:729:HIS:HD2	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:1550:HOH:O	3:D:88:TYR:HB2	2.17	0.42
4:E:67:GLU:HG3	4:E:67:GLU:H	1.73	0.42
5:F:132:ARG:HG3	8:F:754:HOH:O	2.19	0.42
1:L:23:PHE:CE1	1:L:208:LEU:HD13	2.54	0.42
2:M:1016:ILE:HD13	2:M:1016:ILE:H	1.83	0.42
2:M:157:ARG:HD3	2:M:158:TYR:N	2.34	0.42
2:M:244:PRO:CD	2:M:245:GLY:N	2.82	0.42
2:M:34:VAL:CG1	2:M:38:LYS:HG3	2.49	0.42
2:M:631:SER:HG	2:M:635:THR:H	1.65	0.42
2:M:650:ARG:HB2	8:M:1333:HOH:O	2.17	0.42
2:M:68:PHE:HZ	2:M:71:TYR:HB3	1.84	0.42
3:N:1136:LYS:HG3	3:N:1139:ASP:HB2	2.01	0.42
3:N:125:GLN:NE2	8:N:9189:HOH:O	2.50	0.42
3:N:104:PHE:HE2	3:N:1448:THR:HA	1.84	0.42
3:N:1435:LEU:HB2	3:N:1457:ASP:OD2	2.19	0.42
3:N:552:ASN:O	3:N:556:LYS:HD3	2.19	0.42
3:N:794:GLN:NE2	3:N:795:VAL:O	2.52	0.42
1:A:101:LEU:HB2	1:A:114:PHE:CD2	2.54	0.42
1:A:224:TYR:CD2	1:B:9:PRO:HG2	2.54	0.42
2:C:1054:THR:C	2:C:1059:ASP:HB2	2.40	0.42
2:C:219:GLN:HA	2:C:222:MET:SD	2.58	0.42
2:C:321:GLU:HG2	2:C:321:GLU:H	1.57	0.42
2:C:498:GLN:CD	3:D:1068:LEU:HB2	2.39	0.42
2:C:676:ILE:O	2:C:676:ILE:HG23	2.18	0.42
2:C:834:GLN:HB3	8:C:1816:HOH:O	2.19	0.42
2:C:897:LEU:HD11	2:C:920:GLN:HG2	2.01	0.42
3:D:1057:VAL:HA	3:D:1069:GLU:HG2	2.00	0.42
3:D:1156:LEU:HG	3:D:1177:ALA:HB2	2.00	0.42
3:D:413:ASP:OD1	3:D:421:LEU:HD22	2.18	0.42
3:D:690:ALA:O	3:D:693:GLU:HB3	2.19	0.42
3:D:828:LYS:HD2	3:D:862:ASP:OD2	2.19	0.42
5:F:309:LYS:O	5:F:312:GLN:HG3	2.19	0.42
5:F:343:ASP:O	5:F:346:THR:HB	2.18	0.42
5:F:393:THR:O	5:F:397:ILE:HG13	2.19	0.42
5:F:84:TYR:CD2	5:F:192:LEU:HD13	2.54	0.42
1:L:23:PHE:CE1	1:L:208:LEU:HD22	2.55	0.42
2:M:1033:GLY:O	2:M:1037:VAL:HG23	2.19	0.42
2:M:400:PRO:HB3	8:M:1744:HOH:O	2.18	0.42
2:M:595:LEU:HD22	2:M:625:LEU:CD2	2.49	0.42
2:M:822:VAL:HG21	2:M:824:ARG:HH21	1.84	0.42
3:N:1241:PHE:HD1	3:N:1241:PHE:H	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:134:VAL:HG21	8:N:9491:HOH:O	2.19	0.42
3:N:737:ASN:N	8:N:9095:HOH:O	2.52	0.42
5:P:372:ARG:HA	8:P:3689:HOH:O	2.18	0.42
2:C:1034:GLU:CA	2:C:1037:VAL:HG23	2.49	0.42
2:C:91:GLN:HA	2:C:119:PRO:HA	2.02	0.42
2:C:238:LEU:HD23	2:C:241:LEU:HB3	2.01	0.42
2:C:254:VAL:O	2:C:257:VAL:HG23	2.18	0.42
2:C:430:VAL:O	2:C:430:VAL:HG13	2.19	0.42
2:C:460:ARG:HH11	2:C:460:ARG:CB	2.26	0.42
2:C:571:LEU:HD21	2:C:700:TYR:HD2	1.84	0.42
2:C:607:ASP:HB3	2:C:610:ARG:H	1.84	0.42
2:C:708:TYR:H	2:C:708:TYR:HD1	1.67	0.42
3:D:31:THR:HB	3:D:32:ILE:H	1.56	0.42
3:D:475:LYS:O	3:D:479:GLU:HG2	2.20	0.42
3:D:561:GLY:HA3	5:F:184:ARG:NH1	2.33	0.42
3:D:759:ALA:O	3:D:763:MET:HB3	2.19	0.42
3:D:917:GLN:NE2	3:D:917:GLN:HA	2.34	0.42
3:D:957:PRO:CD	3:D:1007:VAL:HG12	2.49	0.42
3:D:994:GLN:O	3:D:998:GLU:HG3	2.20	0.42
4:E:70:THR:HG22	4:E:71:GLY:N	2.34	0.42
5:F:348:SER:OG	5:F:349:LEU:N	2.52	0.42
5:F:368:VAL:HG13	5:F:388:ALA:O	2.20	0.42
1:L:51:THR:HA	1:L:145:ASP:O	2.19	0.42
1:L:165:ILE:HG13	1:L:165:ILE:O	2.19	0.42
1:L:179:PHE:HB2	1:L:195:LEU:HD11	2.00	0.42
2:M:184:MET:HB2	2:M:193:LEU:HD12	2.01	0.42
2:M:362:GLY:HA3	2:M:367:LEU:CD2	2.42	0.42
2:M:440:PRO:HG2	2:M:441:VAL:HG23	2.00	0.42
2:M:473:ARG:NH2	8:M:1124:HOH:O	2.52	0.42
2:M:732:ALA:O	2:M:735:ARG:HG3	2.19	0.42
2:M:959:PRO:O	2:M:963:LEU:HD23	2.19	0.42
3:N:1047:LYS:HB3	3:N:1048:PRO:HD2	2.01	0.42
3:N:1106:VAL:O	3:N:1108:ARG:HG2	2.20	0.42
3:N:1123:PHE:CD1	3:N:1134:LEU:HA	2.54	0.42
3:N:1145:TYR:CE2	3:N:1168:MET:HB2	2.54	0.42
3:N:1262:LEU:CD2	3:N:1351:GLU:HG3	2.50	0.42
3:N:1447:LEU:O	3:N:1448:THR:C	2.57	0.42
3:N:168:THR:O	3:N:393:ILE:N	2.52	0.42
3:N:675:ARG:O	3:N:678:GLU:HG2	2.19	0.42
3:N:681:ARG:HH11	3:N:681:ARG:HB3	1.84	0.42
3:N:78:VAL:HG12	3:N:78:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:850:LEU:H	3:N:850:LEU:CD1	2.23	0.42
5:P:419:ARG:O	5:P:421:PHE:N	2.52	0.42
2:C:1094:ALA:HB1	3:D:603:LEU:CD1	2.49	0.42
2:C:437:ARG:HG2	2:C:467:ILE:O	2.20	0.42
2:C:712:ALA:HB1	2:C:820:ARG:NH1	2.33	0.42
2:C:707:ARG:HG3	2:C:826:TYR:CE1	2.54	0.42
2:C:704:HIS:CG	2:C:831:ARG:HH21	2.37	0.42
3:D:1020:LEU:HD21	3:D:1038:LEU:HD13	2.01	0.42
3:D:1199:GLY:N	8:D:9253:HOH:O	2.51	0.42
3:D:1220:ALA:O	3:D:1224:VAL:HG23	2.19	0.42
3:D:1425:THR:CG2	3:D:1426:LYS:N	2.82	0.42
3:D:145:VAL:HG11	8:D:9724:HOH:O	2.18	0.42
3:D:163:TYR:O	3:D:447:VAL:HG21	2.19	0.42
3:D:507:ASN:HD22	3:D:507:ASN:HA	1.65	0.42
3:D:525:ARG:N	3:D:526:PRO:HD3	2.35	0.42
3:D:530:VAL:CG1	3:D:531:ASP:H	2.32	0.42
3:D:556:LYS:HD2	8:D:9348:HOH:O	2.19	0.42
3:D:655:PRO:HA	3:D:658:LEU:HD12	2.01	0.42
8:B:441:HOH:O	3:D:821:VAL:HG22	2.19	0.42
3:D:864:VAL:HG23	8:D:9288:HOH:O	2.18	0.42
2:C:1086:ARG:HD3	3:D:88:TYR:HH	1.83	0.42
5:F:262:VAL:O	5:F:266:GLU:HG3	2.17	0.42
1:L:161:ARG:HG3	8:L:3450:HOH:O	2.18	0.42
2:M:239:PHE:HE1	8:M:1543:HOH:O	2.02	0.42
2:M:549:PHE:CE2	2:M:886:LEU:HD12	2.55	0.42
2:M:652:GLY:HA2	8:M:1180:HOH:O	2.19	0.42
2:M:750:LYS:HG3	2:M:751:PRO:HD2	2.01	0.42
3:N:1007:VAL:CG2	3:N:1008:PHE:N	2.82	0.42
3:N:1112:CYS:CA	3:N:1195:GLN:HE22	2.31	0.42
3:N:1365:ASP:OD2	3:N:1365:ASP:N	2.53	0.42
3:N:1493:LYS:HZ3	3:N:1493:LYS:HA	1.83	0.42
3:N:759:ALA:HA	3:N:763:MET:CE	2.49	0.42
3:N:770:LEU:HD13	3:N:776:GLU:C	2.40	0.42
5:P:113:ILE:HG23	5:P:127:ILE:HG22	2.01	0.42
3:N:536:ALA:CA	5:P:315:VAL:O	2.68	0.42
3:D:1037:GLN:OE1	3:D:1042:ARG:NE	2.52	0.42
3:D:1120:VAL:HA	3:D:1121:PRO:HD3	1.83	0.42
3:D:112:ILE:HD13	3:D:461:ILE:HG21	2.01	0.42
3:D:1209:LEU:HD23	3:D:1210:SER:H	1.83	0.42
3:D:1432:LYS:HG3	3:D:1433:SER:H	1.83	0.42
3:D:421:LEU:HD12	3:D:435:VAL:HG11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:47:GLU:HG2	3:D:47:GLU:H	1.71	0.42
3:D:129:PHE:CD2	3:D:587:ARG:CZ	3.03	0.42
3:D:669:ASN:O	3:D:672:ALA:HB3	2.19	0.42
3:D:817:GLU:HB2	3:D:839:LEU:CD1	2.50	0.42
3:D:850:LEU:HD22	3:D:884:ARG:NH2	2.33	0.42
5:F:372:ARG:HD3	8:F:635:HOH:O	2.20	0.42
1:L:24:VAL:HG22	1:L:196:THR:OG1	2.20	0.42
2:M:1086:ARG:CB	2:M:1112:PHE:HE2	2.32	0.42
2:M:131:GLY:N	8:M:1593:HOH:O	2.53	0.42
2:M:507:ARG:HH11	2:M:507:ARG:CB	2.25	0.42
2:M:572:ILE:HD11	2:M:701:THR:CG2	2.49	0.42
2:M:577:PRO:HA	2:M:993:PHE:HD2	1.83	0.42
2:M:754:ILE:HD13	2:M:791:ARG:HD3	2.01	0.42
2:M:923:GLU:HA	2:M:923:GLU:OE1	2.19	0.42
3:N:1142:ALA:HB1	3:N:1365:ASP:OD2	2.19	0.42
3:N:115:LEU:HD13	3:N:499:VAL:HG22	2.01	0.42
3:N:553:ARG:HD2	3:N:570:GLU:OE2	2.19	0.42
3:N:661:MET:HE1	3:N:677:LEU:HD11	2.02	0.42
3:N:700:VAL:HG22	3:N:718:PRO:HG3	2.01	0.42
3:N:639:LEU:N	3:N:729:HIS:CD2	2.87	0.42
3:N:52:PRO:HG2	3:N:78:VAL:HG13	2.00	0.42
3:N:888:GLU:HA	3:N:891:GLU:OE1	2.19	0.42
3:N:1485:GLN:NE2	4:O:79:LEU:N	2.68	0.42
1:B:133:GLU:HG3	1:B:134:GLU:HG2	2.02	0.42
1:B:13:VAL:HG12	1:B:14:ARG:N	2.34	0.42
2:C:235:LEU:HD11	8:C:1777:HOH:O	2.20	0.42
2:C:135:VAL:N	2:C:393:GLN:O	2.50	0.42
2:C:421:GLU:HG3	8:C:1723:HOH:O	2.18	0.42
2:C:710:ILE:HD12	2:C:790:LEU:HB2	2.01	0.42
2:C:751:PRO:HA	2:C:792:VAL:HG12	2.01	0.42
3:D:1086:LEU:HB2	8:D:9637:HOH:O	2.20	0.42
3:D:1106:VAL:HG12	3:D:1107:VAL:N	2.34	0.42
3:D:1109:GLU:CG	3:D:1202:GLN:H	2.33	0.42
3:D:1259:VAL:O	3:D:1263:PHE:HD1	2.02	0.42
3:D:178:LEU:HD11	8:D:9071:HOH:O	2.19	0.42
3:D:183:GLU:HG3	8:D:9600:HOH:O	2.19	0.42
3:D:171:LEU:HD11	3:D:388:HIS:CB	2.50	0.42
3:D:478:LEU:HD22	3:D:1388:ARG:NH2	2.35	0.42
3:D:502:PHE:CE1	3:D:509:PRO:HB3	2.54	0.42
3:D:49:ILE:HB	3:D:50:PHE:CE1	2.55	0.42
3:D:678:GLU:HG3	3:D:679:ARG:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:650:LEU:HD22	3:D:688:TRP:CH2	2.54	0.42
3:D:817:GLU:HG3	3:D:840:LYS:HZ1	1.85	0.42
2:C:1115:LEU:HB3	3:D:85:VAL:HG12	2.00	0.42
5:F:113:ILE:HG23	5:F:127:ILE:HG22	2.00	0.42
1:L:134:GLU:HA	8:L:3583:HOH:O	2.20	0.42
2:M:101:ILE:HG22	2:M:102:HIS:H	1.84	0.42
2:M:1067:TYR:CE2	5:P:342:VAL:HA	2.55	0.42
2:M:183:SER:HB2	2:M:190:LYS:HG2	2.00	0.42
2:M:240:THR:HG23	8:M:1647:HOH:O	2.19	0.42
2:M:345:ARG:HA	2:M:348:LEU:HB2	2.02	0.42
2:M:363:SER:HB3	8:M:1471:HOH:O	2.20	0.42
2:M:44:ILE:O	2:M:48:PHE:HB2	2.18	0.42
2:M:511:GLU:HG2	2:M:511:GLU:H	1.63	0.42
2:M:554:ASP:OD2	2:M:556:ASN:HB3	2.19	0.42
2:M:914:ILE:CD1	2:M:918:LEU:HD13	2.48	0.42
3:N:1110:ALA:O	3:N:1111:ASP:C	2.58	0.42
3:N:1209:LEU:CD2	3:N:1210:SER:H	2.29	0.42
3:N:65:ARG:HD2	3:N:65:ARG:HA	1.85	0.42
3:N:661:MET:HE1	3:N:673:ALA:HB1	2.00	0.42
3:N:860:LEU:HD23	3:N:877:PRO:HB2	2.00	0.42
1:L:176:ARG:HH12	3:N:884:ARG:HD3	1.84	0.42
5:P:338:LEU:HG	8:P:2822:HOH:O	2.19	0.42
1:A:216:GLU:O	1:A:220:GLU:HG3	2.20	0.42
1:B:18:ARG:HH12	1:B:123:MET:HE1	1.85	0.42
1:B:51:THR:HA	1:B:145:ASP:O	2.20	0.42
2:C:28:ARG:HG3	2:C:40:GLU:OE1	2.19	0.42
2:C:347:GLY:HA2	2:C:350:ARG:CD	2.43	0.42
2:C:388:ARG:HA	8:C:1349:HOH:O	2.19	0.42
2:C:437:ARG:NH1	2:C:488:ALA:HA	2.35	0.42
2:C:662:GLU:HB3	8:C:1359:HOH:O	2.19	0.42
2:C:7:GLY:HA3	2:C:907:ASP:O	2.20	0.42
2:C:95:TYR:CD1	2:C:95:TYR:N	2.88	0.42
3:D:1007:VAL:O	3:D:1010:ASN:HB3	2.20	0.42
3:D:10:ILE:HG13	3:D:1434:TRP:CE2	2.55	0.42
3:D:1123:PHE:CE2	3:D:1184:GLN:HA	2.55	0.42
3:D:1205:TYR:CE1	3:D:1221:VAL:CG1	3.02	0.42
3:D:39:PRO:HB2	8:D:9084:HOH:O	2.19	0.42
3:D:501:ALA:HB1	3:D:1453:ALA:CA	2.47	0.42
3:D:937:TYR:HE1	8:D:9501:HOH:O	2.02	0.42
1:K:41:ARG:HH11	1:K:41:ARG:HG3	1.83	0.42
1:K:46:SER:HB3	2:M:856:GLU:CG	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:159:LYS:NZ	8:L:3366:HOH:O	2.53	0.42
1:L:86:VAL:O	1:L:86:VAL:HG13	2.20	0.42
2:M:239:PHE:CZ	2:M:254:VAL:HB	2.55	0.42
2:M:367:LEU:HA	2:M:371:LYS:HB2	2.01	0.42
2:M:515:ALA:C	2:M:516:ARG:HD3	2.40	0.42
2:M:520:GLU:HA	2:M:521:PRO:HD3	1.90	0.42
2:M:751:PRO:HA	2:M:792:VAL:HB	2.02	0.42
3:N:1127:GLU:HB3	3:N:1128:VAL:H	1.68	0.42
3:N:135:LEU:HA	3:N:453:ASP:O	2.19	0.42
3:N:171:LEU:HB2	3:N:390:PRO:CA	2.46	0.42
3:N:610:LYS:CG	3:N:611:GLN:HE21	2.26	0.42
3:N:796:ARG:HG2	3:N:861:GLN:O	2.20	0.42
3:N:838:ARG:HD3	3:N:874:GLU:CG	2.50	0.42
3:N:865:THR:N	8:N:9349:HOH:O	2.52	0.42
3:N:948:THR:O	3:N:1019:PRO:CB	2.68	0.42
8:N:9099:HOH:O	4:O:84:ARG:HG2	2.20	0.42
1:A:209:GLU:HA	8:A:418:HOH:O	2.19	0.42
2:C:1015:LEU:HD13	5:F:334:PRO:O	2.20	0.42
2:C:30:LEU:O	2:C:30:LEU:HD12	2.20	0.42
2:C:724:ARG:HH22	2:C:734:LEU:HB3	1.85	0.42
3:D:1047:LYS:HA	3:D:1053:PHE:CZ	2.55	0.42
3:D:1132:LEU:HA	3:D:1132:LEU:HD12	1.80	0.42
3:D:1281:VAL:HG21	3:D:1313:VAL:CG2	2.50	0.42
3:D:1483:PHE:CD1	3:D:1483:PHE:N	2.88	0.42
3:D:591:VAL:CG1	3:D:597:ASP:HA	2.50	0.42
3:D:805:GLU:OE2	3:D:809:PRO:HG2	2.20	0.42
3:D:848:GLU:HA	3:D:851:LEU:HD12	2.02	0.42
3:D:971:LEU:CD1	3:D:992:ILE:HG23	2.50	0.42
5:F:213:ILE:HG22	5:F:217:ASN:HD21	1.84	0.42
5:F:401:GLU:HA	8:F:489:HOH:O	2.19	0.42
5:F:412:GLU:CD	5:F:418:LEU:HD13	2.40	0.42
1:K:111:ALA:HB3	1:K:124:ASN:O	2.20	0.42
1:K:191:ASP:O	1:K:192:LEU:HD23	2.20	0.42
1:K:176:ARG:O	1:K:200:TRP:HE3	2.02	0.42
1:L:111:ALA:HB3	1:L:124:ASN:O	2.20	0.42
1:L:123:MET:HA	8:L:3100:HOH:O	2.20	0.42
1:L:140:MET:HG2	1:L:142:VAL:HG13	2.01	0.42
2:M:1021:LEU:HD22	5:P:331:ASP:O	2.20	0.42
2:M:1060:ILE:HA	2:M:1063:ARG:HE	1.85	0.42
2:M:1060:ILE:CG1	2:M:1063:ARG:HH21	2.33	0.42
2:M:183:SER:C	2:M:193:LEU:HD11	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:212:GLY:C	2:M:215:GLY:H	2.23	0.42
2:M:249:LYS:HB2	2:M:249:LYS:NZ	2.35	0.42
2:M:257:VAL:HA	8:M:1429:HOH:O	2.20	0.42
2:M:439:CYS:HB3	2:M:442:GLU:HB2	2.00	0.42
2:M:54:ILE:HA	8:M:1389:HOH:O	2.19	0.42
2:M:694:LEU:O	2:M:699:PHE:HB2	2.20	0.42
2:M:910:LYS:HD2	2:M:910:LYS:N	2.35	0.42
3:N:1394:VAL:CG1	3:N:1397:LYS:HG3	2.50	0.42
3:N:408:GLU:HG2	8:N:9502:HOH:O	2.19	0.42
3:N:161:LEU:CD2	3:N:452:ILE:HG21	2.48	0.42
3:N:12:LEU:HD22	3:N:511:TRP:HB3	2.02	0.42
3:N:642:CYS:HA	8:N:9469:HOH:O	2.19	0.42
3:N:71:LYS:HE3	8:N:9783:HOH:O	2.19	0.42
3:N:83:SER:N	8:N:9092:HOH:O	2.53	0.42
2:C:1090:LYS:HA	2:C:1090:LYS:HD3	1.87	0.42
2:C:147:TYR:HE2	2:C:280:LYS:NZ	2.18	0.42
2:C:452:ILE:HG13	2:C:452:ILE:O	2.19	0.42
2:C:708:TYR:HE2	2:C:793:PRO:HD2	1.84	0.42
3:D:1152:GLU:CD	3:D:1159:ARG:NH1	2.73	0.42
3:D:1184:GLN:NE2	8:D:9269:HOH:O	2.52	0.42
3:D:1382:THR:HA	8:D:9579:HOH:O	2.20	0.42
3:D:15:PRO:CB	3:D:19:ARG:HH12	2.32	0.42
2:C:1031:ARG:HD3	3:D:619:LEU:HD23	2.02	0.42
3:D:978:TYR:CE1	3:D:985:ASP:HA	2.55	0.42
4:E:26:ARG:HG2	4:E:67:GLU:OE1	2.20	0.42
5:F:166:LEU:HD22	5:F:170:HIS:HB2	2.01	0.42
5:F:181:GLU:O	5:F:184:ARG:HB3	2.19	0.42
5:F:370:LYS:C	5:F:370:LYS:HD2	2.39	0.42
5:F:82:ARG:HG2	5:F:86:HIS:NE2	2.34	0.42
1:K:160:ASP:HB2	8:K:3421:HOH:O	2.20	0.42
1:K:198:ARG:C	1:K:199:ILE:HD12	2.41	0.42
1:L:108:GLU:HA	8:L:2956:HOH:O	2.20	0.42
2:M:1086:ARG:HB3	2:M:1112:PHE:HE2	1.84	0.42
2:M:503:LEU:HD12	8:M:1190:HOH:O	2.19	0.42
2:M:469:THR:HG23	2:M:538:GLN:OE1	2.20	0.42
2:M:565:GLN:HA	2:M:995:MET:HE3	2.01	0.42
2:M:922:PHE:CD2	2:M:964:LYS:HD3	2.54	0.42
3:N:1465:ASN:HD21	3:N:1470:ARG:HD3	1.85	0.42
3:N:65:ARG:HG3	3:N:66:GLN:HG2	2.00	0.42
3:N:82:LYS:HG2	5:P:337:HIS:HB3	2.01	0.42
3:N:83:SER:O	3:N:86:ARG:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1485:GLN:HE21	4:O:79:LEU:N	2.17	0.42
5:P:197:SER:O	5:P:200:LYS:HB3	2.20	0.42
5:P:273:ARG:O	5:P:276:ARG:HB2	2.20	0.42
5:P:328:PHE:HA	5:P:328:PHE:HD2	1.68	0.42
1:A:121:GLU:HG2	1:A:123:MET:SD	2.60	0.42
2:C:302:VAL:O	2:C:305:PRO:HD2	2.20	0.42
2:C:346:VAL:O	2:C:350:ARG:HG3	2.20	0.42
3:D:1086:LEU:HB3	3:D:1090:ASP:OD1	2.20	0.42
3:D:120:ALA:HB1	8:D:9091:HOH:O	2.18	0.42
3:D:1241:PHE:HB3	8:D:9758:HOH:O	2.19	0.42
3:D:154:THR:HG21	3:D:156:GLU:HG2	2.01	0.42
3:D:18:ILE:HD12	3:D:518:PRO:CG	2.49	0.42
3:D:613:ARG:O	3:D:617:ASN:HB2	2.20	0.42
3:D:828:LYS:N	3:D:828:LYS:HD3	2.35	0.42
3:D:860:LEU:HA	3:D:860:LEU:HD23	1.93	0.42
3:D:892:ASP:HB3	3:D:895:VAL:HB	2.01	0.42
4:E:42:PRO:HB2	4:E:43:GLU:OE2	2.20	0.42
5:F:291:ILE:HG23	5:F:304:VAL:HG21	2.01	0.42
3:D:671:LYS:CG	5:F:422:LEU:HA	2.46	0.42
5:F:96:LEU:HD12	5:F:97:GLU:OE2	2.20	0.42
1:K:26:GLU:N	1:K:26:GLU:OE2	2.53	0.42
2:M:1041:GLU:HG2	3:N:1462:LEU:HD13	2.01	0.42
2:M:397:GLU:H	2:M:633:GLN:CD	2.23	0.42
2:M:513:VAL:HG23	8:M:1203:HOH:O	2.19	0.42
2:M:18:LEU:HB2	2:M:590:ASP:HB3	2.01	0.42
2:M:865:THR:HA	2:M:866:PRO:HD3	1.78	0.42
2:M:993:PHE:CE1	2:M:995:MET:HG2	2.54	0.42
3:N:142:LEU:HD11	8:N:9478:HOH:O	2.19	0.42
3:N:144:GLY:HA3	8:N:9078:HOH:O	2.19	0.42
3:N:221:ALA:HB1	8:N:9440:HOH:O	2.20	0.42
3:N:482:LYS:HA	3:N:489:ARG:HH21	1.85	0.42
3:N:633:VAL:C	3:N:635:PRO:HD3	2.40	0.42
3:N:654:LYS:HD3	3:N:674:ARG:NH2	2.32	0.42
3:N:704:ARG:HD2	3:N:705:ALA:N	2.22	0.42
5:P:133:ALA:HA	5:P:142:ARG:NH2	2.35	0.42
5:P:247:ILE:HG22	5:P:251:ILE:CD1	2.45	0.42
2:M:1067:TYR:HE2	5:P:342:VAL:HA	1.85	0.42
1:A:38:ASN:HB3	1:A:39:PRO:HD3	2.01	0.41
1:B:26:GLU:HG3	1:B:194:LYS:NZ	2.35	0.41
1:B:211:LEU:O	1:B:214:ALA:HB3	2.20	0.41
2:C:110:GLU:OE2	2:C:369:PRO:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:142:ARG:NH2	2:C:325:ILE:HD13	2.35	0.41
2:C:216:GLU:HG2	8:C:1241:HOH:O	2.20	0.41
2:C:504:GLU:HG2	2:C:507:ARG:O	2.20	0.41
2:C:543:ASN:ND2	2:C:562:SER:O	2.50	0.41
2:C:901:TYR:CE2	2:C:917:LEU:HD13	2.55	0.41
3:D:955:VAL:O	3:D:1039:CYS:HB3	2.20	0.41
3:D:3:LYS:H	3:D:3:LYS:CD	2.33	0.41
3:D:470:LEU:HD12	3:D:508:ARG:NH2	2.34	0.41
3:D:628:ARG:HD3	8:D:9382:HOH:O	2.20	0.41
1:K:211:LEU:O	1:K:214:ALA:HB3	2.19	0.41
2:M:318:PRO:HD2	2:M:321:GLU:OE1	2.19	0.41
2:M:881:ASN:H	2:M:881:ASN:HD22	1.68	0.41
3:N:109:PRO:HG2	8:N:9287:HOH:O	2.20	0.41
3:N:123:LEU:HD21	8:N:9865:HOH:O	2.20	0.41
3:N:500:ARG:NH1	3:N:1388:ARG:HD2	2.35	0.41
3:N:438:ASP:OD1	3:N:440:VAL:HG23	2.20	0.41
3:N:488:ARG:CZ	3:N:488:ARG:HB3	2.50	0.41
3:N:62:LYS:HE2	3:N:75:ARG:HH11	1.84	0.41
3:N:630:VAL:HG12	3:N:631:ILE:N	2.35	0.41
3:N:972:LEU:HD12	8:N:9750:HOH:O	2.19	0.41
5:P:132:ARG:CZ	5:P:184:ARG:HH12	2.32	0.41
5:P:278:LEU:HB2	5:P:286:PRO:HG2	2.01	0.41
5:P:336:GLU:HG2	5:P:337:HIS:CD2	2.55	0.41
1:A:150:TYR:HB3	8:A:460:HOH:O	2.21	0.41
1:B:20:TYR:HD1	8:B:319:HOH:O	2.03	0.41
2:C:108:ILE:HB	2:C:368:THR:HG1	1.84	0.41
2:C:115:LEU:CD2	2:C:373:VAL:HG11	2.50	0.41
2:C:412:ALA:HB2	2:C:451:LEU:HB3	2.02	0.41
2:C:862:PRO:HA	2:C:975:TYR:CE1	2.55	0.41
3:D:1263:PHE:HD2	3:D:1375:MET:HE2	1.84	0.41
3:D:1299:PHE:N	3:D:1299:PHE:CD2	2.88	0.41
3:D:447:VAL:HG23	3:D:448:GLU:N	2.35	0.41
3:D:50:PHE:CD2	3:D:522:PRO:HG3	2.56	0.41
3:D:637:LEU:HD11	3:D:642:CYS:N	2.35	0.41
3:D:729:HIS:CE1	3:D:731:LEU:HG	2.56	0.41
3:D:820:GLU:HA	3:D:825:ALA:O	2.20	0.41
2:C:1115:LEU:HB3	3:D:85:VAL:CG1	2.49	0.41
3:D:961:LYS:HG2	3:D:962:GLN:N	2.35	0.41
5:F:282:LEU:CD1	5:F:286:PRO:HG3	2.47	0.41
1:K:158:ILE:HD11	8:K:4141:HOH:O	2.20	0.41
1:K:173:PRO:HA	1:K:202:ASP:OD1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:172:ILE:HG22	2:M:173:ASP:N	2.35	0.41
2:M:239:PHE:HZ	8:M:1251:HOH:O	2.01	0.41
2:M:352:ALA:HA	2:M:355:VAL:CG1	2.50	0.41
2:M:595:LEU:HD13	2:M:639:GLN:OE1	2.20	0.41
2:M:737:LEU:HD22	2:M:742:VAL:O	2.20	0.41
2:M:964:LYS:O	2:M:968:LEU:HG	2.20	0.41
3:N:1058:ARG:NH1	3:N:1058:ARG:HG3	2.30	0.41
3:N:1283:ILE:N	3:N:1315:ASP:OD1	2.53	0.41
3:N:1304:LYS:HB3	8:N:9093:HOH:O	2.20	0.41
3:N:223:LEU:N	3:N:365:ASP:O	2.51	0.41
3:N:603:LEU:HA	3:N:606:ILE:HG12	2.02	0.41
3:N:68:PHE:HA	3:N:71:LYS:NZ	2.34	0.41
3:N:827:ILE:HG23	3:N:837:GLY:HA3	2.02	0.41
3:N:853:VAL:HG22	3:N:858:VAL:HG23	2.01	0.41
3:N:868:TYR:HB2	3:N:873:LEU:HD13	2.01	0.41
2:M:984:GLU:OE1	3:N:945:SER:HA	2.20	0.41
4:O:94:PRO:HB3	8:O:4372:HOH:O	2.20	0.41
5:P:371:LEU:O	5:P:375:LEU:HB3	2.21	0.41
1:A:227:ASN:HB2	8:A:473:HOH:O	2.18	0.41
1:A:63:HIS:HA	8:A:326:HOH:O	2.19	0.41
2:C:1005:MET:O	2:C:1005:MET:HG3	2.20	0.41
2:C:378:LEU:HG	2:C:382:ILE:HD12	2.03	0.41
2:C:437:ARG:NH2	2:C:469:THR:HG22	2.36	0.41
2:C:620:LEU:N	2:C:620:LEU:HD13	2.36	0.41
2:C:569:VAL:HG23	2:C:635:THR:HG22	2.02	0.41
2:C:643:VAL:HG12	2:C:644:VAL:O	2.21	0.41
2:C:837:ASP:O	2:C:848:VAL:HG13	2.19	0.41
2:C:565:GLN:OE1	2:C:842:ARG:HG2	2.21	0.41
3:D:1487:VAL:CG1	3:D:1488:ASP:N	2.84	0.41
3:D:156:GLU:HG3	8:D:9239:HOH:O	2.18	0.41
3:D:211:VAL:HG22	3:D:393:ILE:HG23	2.02	0.41
3:D:521:PRO:C	3:D:525:ARG:HH11	2.24	0.41
3:D:890:VAL:HG13	3:D:926:LYS:CD	2.50	0.41
5:F:153:PRO:CG	5:F:154:LYS:H	2.33	0.41
5:F:370:LYS:O	5:F:370:LYS:HD2	2.19	0.41
5:F:370:LYS:NZ	5:F:371:LEU:HG	2.35	0.41
1:K:64:GLU:OE2	1:K:76:VAL:HA	2.20	0.41
1:L:81:ASN:ND2	1:L:128:HIS:O	2.53	0.41
2:M:132:ALA:HB1	2:M:632:ASN:ND2	2.36	0.41
2:M:19:THR:HG22	2:M:19:THR:O	2.20	0.41
2:M:371:LYS:HB2	8:M:1183:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:642:ARG:HG3	2:M:657:ASP:OD2	2.19	0.41
2:M:768:THR:HB	2:M:771:GLU:CB	2.49	0.41
2:M:861:LEU:HD21	2:M:925:TYR:HE2	1.85	0.41
2:M:874:LEU:O	3:N:1029:ARG:HD2	2.20	0.41
3:N:1076:GLY:O	3:N:1079:LYS:HG3	2.20	0.41
3:N:1482:ARG:HB2	3:N:1483:PHE:CD1	2.56	0.41
3:N:30:GLU:N	8:N:9867:HOH:O	2.52	0.41
3:N:421:LEU:O	3:N:421:LEU:HD23	2.20	0.41
2:M:1056:LYS:O	3:N:624:ASP:HB2	2.21	0.41
3:N:783:ARG:HH21	3:N:1029:ARG:HG3	1.82	0.41
3:N:974:ILE:HG13	3:N:974:ILE:H	1.75	0.41
4:O:54:LEU:HA	4:O:58:PRO:CG	2.51	0.41
5:P:156:VAL:HG23	5:P:157:GLU:N	2.36	0.41
5:P:370:LYS:HD2	5:P:370:LYS:C	2.40	0.41
1:A:26:GLU:HB2	1:A:194:LYS:HA	2.02	0.41
2:C:198:ARG:CZ	2:C:228:ALA:O	2.68	0.41
2:C:224:GLU:OE1	2:C:226:VAL:HG12	2.20	0.41
2:C:267:TYR:N	2:C:267:TYR:CD2	2.88	0.41
2:C:425:PHE:O	2:C:429:ASP:OD2	2.39	0.41
2:C:451:LEU:H	2:C:451:LEU:HD12	1.86	0.41
2:C:52:PHE:CD2	2:C:68:PHE:HB2	2.55	0.41
2:C:571:LEU:C	2:C:573:ARG:H	2.22	0.41
2:C:658:GLY:N	2:C:661:SER:OG	2.54	0.41
2:C:679:PHE:CZ	2:C:859:PRO:HD3	2.55	0.41
2:C:69:LEU:HD12	2:C:97:ARG:HB3	2.02	0.41
2:C:713:ARG:HG2	8:C:1811:HOH:O	2.20	0.41
2:C:909:ALA:HB1	2:C:914:ILE:CD1	2.50	0.41
2:C:925:TYR:C	2:C:925:TYR:CD1	2.94	0.41
2:C:9:ILE:HD11	2:C:537:LYS:NZ	2.35	0.41
3:D:1171:VAL:O	3:D:1175:ILE:HG13	2.21	0.41
3:D:1206:GLY:HA3	3:D:1366:LYS:HZ3	1.84	0.41
3:D:150:ARG:HG3	3:D:150:ARG:NH1	2.33	0.41
3:D:191:LEU:HD11	8:D:9536:HOH:O	2.19	0.41
3:D:404:GLU:HB3	3:D:414:ARG:CD	2.51	0.41
3:D:434:ARG:HB2	3:D:447:VAL:CG2	2.51	0.41
3:D:521:PRO:HA	3:D:522:PRO:HD3	1.84	0.41
4:E:29:GLN:CB	4:E:33:HIS:NE2	2.83	0.41
5:F:324:GLU:HA	8:F:663:HOH:O	2.19	0.41
1:K:150:TYR:CD1	2:M:696:LYS:HG2	2.55	0.41
2:M:1024:LYS:HG3	8:M:1569:HOH:O	2.21	0.41
2:M:620:LEU:HG	8:M:1346:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:821:GLU:HG2	2:M:822:VAL:N	2.35	0.41
2:M:832:LYS:HD2	8:M:1460:HOH:O	2.21	0.41
3:N:1314:LYS:NZ	3:N:1317:ASP:HB2	2.35	0.41
3:N:10:ILE:HG13	3:N:1434:TRP:CE2	2.55	0.41
3:N:404:GLU:HB3	3:N:414:ARG:CZ	2.50	0.41
3:N:592:THR:HA	8:N:9104:HOH:O	2.20	0.41
3:N:659:LYS:O	3:N:663:GLU:HG3	2.21	0.41
2:M:1044:GLY:N	3:N:762:GLN:OE1	2.52	0.41
3:N:770:LEU:HD12	3:N:775:GLY:O	2.21	0.41
3:N:875:THR:HG22	3:N:879:ARG:HB2	2.03	0.41
5:P:256:ARG:NE	5:P:260:ILE:HD12	2.35	0.41
5:P:392:VAL:HG12	5:P:396:ARG:HB2	2.02	0.41
1:A:29:GLU:HB3	1:A:30:ARG:H	1.70	0.41
1:B:27:PRO:HG2	1:B:186:LEU:CD1	2.50	0.41
2:C:1004:LYS:O	2:C:1005:MET:C	2.59	0.41
2:C:163:ILE:HG13	2:C:171:TRP:CH2	2.55	0.41
2:C:299:LYS:HD2	8:C:1273:HOH:O	2.20	0.41
2:C:335:THR:HG23	2:C:461:VAL:HG11	2.03	0.41
2:C:525:SER:O	2:C:529:VAL:HG23	2.19	0.41
2:C:557:ARG:CZ	2:C:879:ARG:HG2	2.50	0.41
2:C:693:GLU:OE1	2:C:693:GLU:HA	2.21	0.41
2:C:697:ARG:O	2:C:699:PHE:N	2.53	0.41
3:D:786:ILE:HG22	3:D:1026:SER:HB2	2.02	0.41
3:D:1063:GLU:HG3	8:D:9502:HOH:O	2.20	0.41
3:D:1211:MET:HG2	3:D:1213:ARG:H	1.85	0.41
3:D:1364:HIS:ND1	3:D:1365:ASP:N	2.67	0.41
3:D:13:ALA:O	3:D:511:TRP:HB3	2.21	0.41
3:D:1423:GLY:HA2	8:D:9248:HOH:O	2.19	0.41
3:D:187:LYS:HA	3:D:187:LYS:HD3	1.78	0.41
3:D:566:ILE:CG1	5:F:192:LEU:HD11	2.50	0.41
3:D:688:TRP:HA	3:D:688:TRP:CE3	2.55	0.41
3:D:817:GLU:HB2	3:D:839:LEU:HD13	2.01	0.41
4:E:46:PRO:HD3	8:E:180:HOH:O	2.20	0.41
4:E:93:TYR:HA	4:E:94:PRO:HD3	1.77	0.41
5:F:135:ILE:O	5:F:135:ILE:HD13	2.21	0.41
5:F:244:ARG:NH1	5:F:244:ARG:HG3	2.35	0.41
2:M:1090:LYS:HG2	2:M:1112:PHE:HZ	1.86	0.41
2:M:205:GLU:OE1	2:M:206:THR:N	2.53	0.41
2:M:327:HIS:O	2:M:330:ASN:HB2	2.20	0.41
2:M:601:GLY:HA3	2:M:615:TYR:HA	2.01	0.41
3:N:786:ILE:HD12	3:N:1028:ALA:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1175:ILE:O	3:N:1179:GLU:HG3	2.21	0.41
3:N:151:GLN:HB2	3:N:151:GLN:HE21	1.77	0.41
3:N:169:TYR:HA	3:N:392:SER:CB	2.50	0.41
3:N:171:LEU:HD11	3:N:388:HIS:CB	2.50	0.41
3:N:42:ASP:O	3:N:49:ILE:HD12	2.21	0.41
3:N:502:PHE:CE1	3:N:509:PRO:HB3	2.56	0.41
3:N:50:PHE:CB	3:N:522:PRO:HG2	2.50	0.41
3:N:519:VAL:HG13	3:N:544:TYR:CE1	2.55	0.41
3:N:565:ILE:HD12	3:N:565:ILE:N	2.20	0.41
3:N:637:LEU:HD11	3:N:642:CYS:CA	2.51	0.41
3:N:702:LEU:HD23	3:N:745:MET:CE	2.51	0.41
8:M:1645:HOH:O	3:N:940:THR:HG23	2.21	0.41
5:P:262:VAL:O	5:P:265:VAL:HB	2.21	0.41
1:A:178:ALA:HB3	1:A:198:ARG:HD3	2.03	0.41
1:A:211:LEU:O	1:A:214:ALA:HB3	2.21	0.41
1:B:29:GLU:HB3	1:B:30:ARG:H	1.75	0.41
1:B:42:ARG:NH1	1:B:42:ARG:HG2	2.35	0.41
2:C:162:ILE:CB	2:C:172:ILE:HD13	2.49	0.41
2:C:207:LEU:HD13	2:C:221:LEU:HD13	2.03	0.41
2:C:332:ARG:CB	2:C:332:ARG:HH11	2.15	0.41
2:C:365:ASP:O	2:C:367:LEU:N	2.54	0.41
2:C:710:ILE:HG12	2:C:758:ARG:HE	1.86	0.41
2:C:865:THR:HA	2:C:866:PRO:HD3	1.87	0.41
3:D:957:PRO:CG	3:D:1007:VAL:HG12	2.50	0.41
3:D:1208:ASP:OD1	3:D:1209:LEU:O	2.39	0.41
3:D:1274:ILE:CD1	3:D:1334:GLN:HB3	2.50	0.41
3:D:1262:LEU:HD23	3:D:1352:ILE:HA	2.02	0.41
3:D:397:LYS:HE2	3:D:399:ARG:NE	2.23	0.41
5:F:133:ALA:O	5:F:137:GLY:O	2.38	0.41
5:F:142:ARG:NH1	5:F:150:THR:HG21	2.36	0.41
1:K:109:VAL:O	1:K:129:ILE:HG12	2.21	0.41
1:K:97:VAL:HG12	1:K:99:LEU:HD12	2.01	0.41
1:L:100:LEU:HD12	1:L:115:LEU:HD11	2.03	0.41
1:L:95:GLN:N	1:L:95:GLN:HE21	2.12	0.41
2:M:1034:GLU:HA	2:M:1037:VAL:CG2	2.50	0.41
2:M:1054:THR:HB	2:M:1055:LEU:H	1.57	0.41
2:M:139:GLN:HE21	2:M:334:ARG:NH1	2.03	0.41
2:M:305:PRO:HG3	2:M:308:ARG:CZ	2.51	0.41
2:M:383:ARG:NH2	8:M:1405:HOH:O	2.54	0.41
2:M:473:ARG:HE	2:M:531:PHE:HE1	1.67	0.41
2:M:549:PHE:HE2	2:M:887:GLU:N	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:65:PHE:HE1	2:M:799:ILE:HD11	1.85	0.41
3:N:1485:GLN:HG2	3:N:1485:GLN:H	1.69	0.41
3:N:539:ASP:OD2	3:N:598:ARG:NH2	2.52	0.41
3:N:131:LYS:HZ3	3:N:568:ARG:HB2	1.86	0.41
4:O:31:LEU:HD23	4:O:35:PHE:CD1	2.55	0.41
5:P:394:ARG:HA	5:P:397:ILE:CD1	2.37	0.41
1:B:9:PRO:HB3	1:B:25:LEU:HG	2.03	0.41
2:C:123:GLU:HA	8:C:1818:HOH:O	2.21	0.41
2:C:30:LEU:HB3	2:C:44:ILE:CD1	2.44	0.41
2:C:460:ARG:HD2	2:C:485:TYR:CD2	2.56	0.41
2:C:676:ILE:CG2	2:C:988:VAL:HG22	2.50	0.41
2:C:952:LEU:HB3	2:C:966:LEU:HD11	2.02	0.41
3:D:1136:LYS:HE3	3:D:1139:ASP:OD2	2.21	0.41
3:D:1353:GLN:HB3	3:D:1357:ARG:NE	2.36	0.41
3:D:8:VAL:O	3:D:1434:TRP:HH2	2.04	0.41
3:D:1467:ILE:HD12	3:D:1467:ILE:H	1.86	0.41
3:D:587:ARG:HG2	8:D:9367:HOH:O	2.21	0.41
3:D:639:LEU:HD22	3:D:766:ALA:CA	2.50	0.41
3:D:806:PHE:O	3:D:806:PHE:CG	2.74	0.41
3:D:842:VAL:C	8:D:9557:HOH:O	2.59	0.41
3:D:86:ARG:HG3	3:D:86:ARG:O	2.20	0.41
3:D:893:GLU:O	3:D:896:ALA:HB3	2.21	0.41
5:F:113:ILE:O	5:F:116:LEU:HB2	2.21	0.41
5:F:329:TYR:HE1	8:F:541:HOH:O	2.02	0.41
5:F:421:PHE:C	5:F:423:ASP:N	2.72	0.41
1:K:85:LEU:HB2	1:K:127:LEU:HD21	2.01	0.41
1:K:197:LEU:HD23	1:K:197:LEU:N	2.33	0.41
1:L:105:GLY:HA2	8:L:3583:HOH:O	2.19	0.41
1:L:101:LEU:HD12	1:L:114:PHE:CE1	2.55	0.41
1:L:2:LEU:HD13	1:L:3:ASP:OD1	2.21	0.41
1:L:51:THR:HG22	1:L:89:PHE:CZ	2.56	0.41
2:M:612:VAL:HG22	2:M:622:GLU:HG3	2.03	0.41
2:M:671:ASN:N	2:M:671:ASN:ND2	2.69	0.41
2:M:86:LYS:HG3	2:M:813:VAL:HG12	2.03	0.41
2:M:983:ILE:O	2:M:984:GLU:C	2.59	0.41
2:M:425:PHE:HZ	3:N:1079:LYS:HB2	1.86	0.41
3:N:1310:ARG:H	3:N:1310:ARG:HG2	1.61	0.41
3:N:500:ARG:HH22	3:N:1388:ARG:HD3	1.85	0.41
3:N:1422:MET:CE	3:N:1426:LYS:HG3	2.50	0.41
3:N:783:ARG:CZ	3:N:783:ARG:HB3	2.50	0.41
5:P:142:ARG:H	5:P:142:ARG:HG2	1.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:303:ARG:NH2	8:P:3667:HOH:O	2.52	0.41
1:B:72:LYS:HB3	1:B:131:THR:OG1	2.21	0.41
2:C:25:SER:OG	2:C:337:GLY:N	2.50	0.41
2:C:34:VAL:HA	2:C:35:PRO:HD3	1.96	0.41
2:C:416:GLY:HA3	8:C:1572:HOH:O	2.21	0.41
2:C:547:ILE:HA	2:C:548:PRO:HD3	1.97	0.41
2:C:592:LEU:HA	2:C:592:LEU:HD23	1.91	0.41
2:C:860:HIS:N	8:C:1448:HOH:O	2.42	0.41
3:D:143:ASN:ND2	3:D:145:VAL:HG12	2.18	0.41
3:D:1472:ILE:HG22	3:D:1474:ALA:N	2.35	0.41
2:C:1109:VAL:CG2	3:D:3:LYS:HG2	2.49	0.41
3:D:729:HIS:ND1	3:D:730:PRO:N	2.68	0.41
3:D:761:ILE:HD13	4:E:20:THR:HA	2.02	0.41
3:D:794:GLN:HB3	3:D:794:GLN:HE21	1.50	0.41
3:D:907:GLU:N	3:D:910:SER:OG	2.53	0.41
2:C:873:PRO:HG2	3:D:947:ILE:O	2.20	0.41
3:D:965:GLU:HA	3:D:968:ASP:OD2	2.21	0.41
5:F:151:LEU:HB2	5:F:155:THR:OG1	2.21	0.41
5:F:192:LEU:O	5:F:192:LEU:HD23	2.21	0.41
5:F:292:ALA:HB1	5:F:299:TRP:O	2.21	0.41
5:F:95:THR:HG22	5:F:96:LEU:HD23	2.03	0.41
1:L:51:THR:HG23	8:L:4444:HOH:O	2.20	0.41
2:M:1013:TYR:HB2	5:P:335:ASP:OD2	2.21	0.41
2:M:253:ALA:O	2:M:256:TYR:HB2	2.21	0.41
2:M:137:VAL:HG22	2:M:391:LEU:O	2.20	0.41
2:M:575:GLN:HA	2:M:662:GLU:CD	2.41	0.41
2:M:87:ASP:HA	8:M:1593:HOH:O	2.20	0.41
2:M:899:GLN:HG3	2:M:901:TYR:OH	2.21	0.41
2:M:910:LYS:NZ	8:M:1254:HOH:O	2.51	0.41
2:M:964:LYS:HD3	8:M:1484:HOH:O	2.20	0.41
3:N:1465:ASN:OD1	3:N:1473:PRO:HG3	2.20	0.41
3:N:206:ARG:O	3:N:206:ARG:HD3	2.19	0.41
3:N:36:THR:O	3:N:38:LYS:N	2.51	0.41
3:N:704:ARG:HD3	3:N:738:ALA:HB2	2.03	0.41
3:N:820:GLU:HB2	3:N:836:VAL:HG11	2.01	0.41
3:N:826:PRO:HD2	3:N:829:VAL:HG13	2.03	0.41
3:N:960:LYS:O	3:N:964:LEU:HD12	2.20	0.41
4:O:5:GLY:HA2	8:O:3467:HOH:O	2.20	0.41
5:P:140:ARG:O	5:P:144:ILE:HG13	2.20	0.41
5:P:372:ARG:HA	8:P:4564:HOH:O	2.20	0.41
5:P:421:PHE:C	5:P:423:ASP:N	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ILE:O	1:A:83:LYS:HG3	2.20	0.41
2:C:166:PRO:HD3	2:C:265:ARG:NE	2.33	0.41
2:C:479:VAL:HG22	2:C:508:ILE:CD1	2.50	0.41
2:C:895:TYR:HD1	2:C:991:GLN:NE2	2.16	0.41
2:C:919:ALA:HA	8:C:1456:HOH:O	2.19	0.41
3:D:1023:MET:O	3:D:1028:ALA:HB3	2.21	0.41
3:D:783:ARG:NE	3:D:1029:ARG:NE	2.64	0.41
3:D:996:TRP:CE2	3:D:1056:PRO:HG2	2.56	0.41
3:D:1110:ALA:O	3:D:1111:ASP:C	2.60	0.41
3:D:1300:SER:HB3	8:D:9222:HOH:O	2.20	0.41
3:D:1352:ILE:HG21	3:D:1368:ILE:CG2	2.48	0.41
3:D:1101:VAL:HG12	3:D:1374:GLN:HB3	2.03	0.41
3:D:1462:LEU:HD22	3:D:1473:PRO:HD2	2.03	0.41
3:D:127:LEU:CD1	3:D:461:ILE:HD11	2.42	0.41
3:D:461:ILE:O	3:D:465:LEU:HB2	2.19	0.41
3:D:463:GLN:O	3:D:467:GLU:HG3	2.21	0.41
3:D:470:LEU:HD22	3:D:499:VAL:HG13	2.01	0.41
3:D:667:ALA:HB2	3:D:676:MET:CE	2.38	0.41
8:B:347:HOH:O	3:D:688:TRP:HB3	2.19	0.41
3:D:710:ARG:NE	8:D:9123:HOH:O	2.54	0.41
3:D:827:ILE:HB	3:D:828:LYS:HD3	2.01	0.41
3:D:762:GLN:HE21	4:E:20:THR:CB	2.33	0.41
5:F:74:LYS:HD3	5:F:74:LYS:HA	1.93	0.41
5:F:96:LEU:HB2	5:F:97:GLU:OE2	2.21	0.41
1:K:14:ARG:CG	1:K:22:GLU:HB2	2.49	0.41
1:L:71:VAL:HG22	1:L:132:LEU:CD1	2.51	0.41
2:M:1087:VAL:HG23	3:N:524:LEU:HD21	2.03	0.41
2:M:1097:LEU:HD22	2:M:1097:LEU:N	2.35	0.41
2:M:446:GLY:O	2:M:447:ALA:C	2.58	0.41
2:M:556:ASN:O	2:M:559:LEU:HB3	2.21	0.41
2:M:807:ARG:HB3	8:M:1400:HOH:O	2.21	0.41
2:M:833:LEU:CD1	2:M:837:ASP:HB2	2.51	0.41
3:N:1107:VAL:HA	3:N:1200:VAL:O	2.21	0.41
3:N:1292:VAL:O	3:N:1303:TYR:HB2	2.21	0.41
3:N:1380:GLU:HB3	3:N:1418:LYS:HB2	2.02	0.41
3:N:1437:ALA:O	3:N:1446:VAL:HG21	2.20	0.41
3:N:33:ASN:O	3:N:36:THR:O	2.39	0.41
3:N:443:VAL:HG12	3:N:445:ARG:HD2	2.02	0.41
2:M:769:PRO:HB2	3:N:65:ARG:NH1	2.36	0.41
3:N:881:LEU:O	3:N:881:LEU:HD12	2.21	0.41
3:N:948:THR:HG22	3:N:949:ILE:N	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:35:PHE:HZ	4:O:60:ALA:HA	1.86	0.41
2:C:1101:THR:OG1	2:C:1109:VAL:HG12	2.21	0.41
2:C:325:ILE:HA	8:C:1441:HOH:O	2.21	0.41
2:C:366:SER:O	2:C:371:LYS:HE3	2.20	0.41
2:C:881:ASN:ND2	8:C:1494:HOH:O	2.41	0.41
3:D:999:THR:O	3:D:1003:VAL:HG13	2.21	0.41
3:D:1353:GLN:OE1	3:D:1368:ILE:HD11	2.21	0.41
3:D:1365:ASP:O	3:D:1368:ILE:HG13	2.21	0.41
3:D:411:THR:HG23	8:D:9458:HOH:O	2.20	0.41
3:D:114:THR:HG21	3:D:498:VAL:HG11	2.01	0.41
3:D:569:ASN:O	3:D:573:MET:SD	2.78	0.41
3:D:631:ILE:HG21	3:D:745:MET:CG	2.51	0.41
3:D:65:ARG:CG	3:D:66:GLN:H	2.24	0.41
4:E:70:THR:HG21	4:E:72:ARG:NH2	2.36	0.41
5:F:109:GLY:O	5:F:113:ILE:HG13	2.21	0.41
5:F:352:GLU:O	5:F:356:LYS:HG3	2.21	0.41
5:F:84:TYR:O	5:F:88:ILE:HG13	2.20	0.41
1:K:100:LEU:HD12	8:K:3405:HOH:O	2.20	0.41
1:K:101:LEU:HG	1:K:113:ASP:C	2.40	0.41
1:K:132:LEU:HD12	1:K:132:LEU:N	2.36	0.41
2:M:1083:GLU:O	2:M:1087:VAL:HB	2.19	0.41
2:M:1109:VAL:CG1	3:N:5:VAL:HG22	2.51	0.41
2:M:116:GLY:N	8:M:1773:HOH:O	2.54	0.41
2:M:134:ARG:HE	2:M:393:GLN:C	2.23	0.41
2:M:144:PRO:HB2	2:M:267:TYR:HE1	1.86	0.41
2:M:340:MET:SD	2:M:344:PHE:HB2	2.61	0.41
2:M:353:ARG:HB2	2:M:353:ARG:HE	1.66	0.41
2:M:593:ALA:HB2	8:M:1744:HOH:O	2.20	0.41
2:M:682:TYR:HB3	2:M:689:VAL:HG22	2.02	0.41
2:M:772:ARG:HG3	2:M:773:LEU:N	2.36	0.41
2:M:975:TYR:N	2:M:975:TYR:CD1	2.88	0.41
3:N:1068:LEU:O	3:N:1069:GLU:C	2.59	0.41
3:N:110:SER:OG	3:N:113:GLY:N	2.51	0.41
3:N:112:ILE:O	3:N:116:LEU:HB2	2.21	0.41
3:N:1148:VAL:HG13	3:N:1163:GLY:O	2.20	0.41
3:N:1168:MET:HE3	3:N:1171:VAL:HB	2.02	0.41
3:N:1223:ILE:O	3:N:1224:VAL:C	2.60	0.41
3:N:1330:ILE:HD13	3:N:1347:TYR:OH	2.21	0.41
3:N:774:SER:HB3	3:N:1362:LYS:O	2.21	0.41
3:N:172:PRO:HA	3:N:173:PRO:HD3	1.67	0.41
3:N:212:ARG:HD3	3:N:445:ARG:NH1	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:1118:LYS:HA	3:N:23:TYR:OH	2.21	0.41
3:N:243:ALA:HB3	8:N:9487:HOH:O	2.20	0.41
3:N:701:LEU:C	3:N:702:LEU:HD12	2.41	0.41
3:N:705:ALA:CB	3:N:706:PRO:HD3	2.50	0.41
3:N:891:GLU:N	8:N:9462:HOH:O	2.54	0.41
5:P:261:PRO:HA	8:P:3364:HOH:O	2.20	0.41
5:P:338:LEU:HA	5:P:339:PRO:HD3	1.89	0.41
5:P:367:MET:SD	5:P:367:MET:N	2.94	0.41
1:A:64:GLU:OE2	1:A:76:VAL:HG13	2.21	0.41
1:B:73:GLU:HB3	1:B:77:GLU:HG2	1.98	0.41
2:C:101:ILE:HG23	2:C:107:LEU:CD2	2.45	0.41
2:C:1037:VAL:O	2:C:1041:GLU:HG3	2.20	0.41
2:C:1092:LEU:HD22	2:C:1099:VAL:CG2	2.51	0.41
2:C:137:VAL:O	2:C:391:LEU:HD11	2.21	0.41
2:C:139:GLN:HE22	2:C:415:PRO:HD3	1.86	0.41
2:C:308:ARG:HH11	2:C:308:ARG:HG2	1.85	0.41
2:C:313:LEU:HB2	2:C:321:GLU:HG3	2.03	0.41
2:C:41:ASN:N	2:C:41:ASN:ND2	2.57	0.41
2:C:328:LEU:H	2:C:433:THR:HG21	1.86	0.41
2:C:474:VAL:HG23	2:C:478:VAL:O	2.21	0.41
2:C:759:THR:HB	2:C:785:VAL:CG2	2.50	0.41
3:D:1133:ARG:HG2	3:D:1134:LEU:N	2.35	0.41
3:D:1155:VAL:HG11	3:D:1177:ALA:CB	2.51	0.41
3:D:1208:ASP:HB3	8:D:2063:HOH:O	2.21	0.41
3:D:120:ALA:HA	8:D:9188:HOH:O	2.20	0.41
3:D:1272:ALA:CB	3:D:1326:THR:HB	2.51	0.41
3:D:1342:GLU:HA	3:D:1346:ARG:NH2	2.36	0.41
3:D:135:LEU:HD11	3:D:139:GLY:HA3	2.02	0.41
3:D:1480:PHE:HD1	3:D:1480:PHE:O	2.02	0.41
3:D:393:ILE:HD12	3:D:393:ILE:N	2.32	0.41
3:D:804:LEU:N	8:D:9497:HOH:O	2.53	0.41
2:C:885:ILE:HD12	3:D:949:ILE:HB	2.02	0.41
5:F:160:ASP:O	5:F:163:LEU:HB2	2.22	0.41
5:F:192:LEU:O	5:F:196:VAL:HG23	2.21	0.41
5:F:287:THR:HG22	5:F:290:GLU:OE1	2.20	0.41
1:K:100:LEU:O	1:K:115:LEU:HG	2.21	0.41
1:K:150:TYR:HA	1:K:169:ALA:O	2.21	0.41
1:L:150:TYR:HA	1:L:169:ALA:O	2.21	0.41
2:M:261:ILE:HG22	2:M:262:ALA:N	2.36	0.41
2:M:304:LEU:HG	2:M:305:PRO:N	2.36	0.41
2:M:525:SER:O	2:M:529:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:401:LEU:HD21	2:M:565:GLN:HE21	1.86	0.41
2:M:592:LEU:HA	2:M:592:LEU:HD23	1.85	0.41
2:M:755:LEU:HD11	2:M:792:VAL:HG22	2.03	0.41
2:M:430:VAL:CG1	3:N:1075:HIS:HA	2.51	0.41
3:N:1173:LEU:HA	8:N:9311:HOH:O	2.21	0.41
3:N:1301:LYS:HD2	3:N:1301:LYS:HA	1.89	0.41
3:N:501:ALA:HA	3:N:504:ASP:HB2	2.03	0.41
3:N:787:LEU:HD21	3:N:947:ILE:CD1	2.51	0.41
4:O:49:GLN:HA	4:O:51:LEU:O	2.21	0.41
1:A:95:GLN:CG	1:A:146:ARG:HH22	2.19	0.40
1:B:106:PRO:HG3	1:B:133:GLU:O	2.22	0.40
1:B:55:SER:OG	1:B:158:ILE:HB	2.21	0.40
2:C:1018:GLN:HE21	2:C:1060:ILE:CD1	2.34	0.40
2:C:124:ASP:OD1	2:C:126:SER:N	2.48	0.40
2:C:13:ILE:HG13	2:C:458:TYR:HE2	1.86	0.40
2:C:722:ILE:HD12	2:C:805:ARG:NH2	2.36	0.40
2:C:897:LEU:HD21	2:C:920:GLN:HB3	2.02	0.40
3:D:1047:LYS:HE3	3:D:1051:GLU:HB2	2.03	0.40
3:D:1068:LEU:O	3:D:1068:LEU:HD23	2.21	0.40
3:D:1066:THR:CG2	3:D:1069:GLU:H	2.18	0.40
3:D:1243:THR:HG22	3:D:1244:GLY:H	1.87	0.40
3:D:1330:ILE:HD12	3:D:1347:TYR:HE1	1.86	0.40
3:D:613:ARG:HA	3:D:613:ARG:HD2	1.83	0.40
3:D:900:ILE:O	3:D:900:ILE:HD12	2.21	0.40
3:D:936:TYR:HD1	8:D:9501:HOH:O	2.03	0.40
3:D:988:ARG:O	3:D:992:ILE:HG13	2.20	0.40
5:F:115:LYS:HG3	5:F:173:TYR:CE2	2.56	0.40
5:F:272:SER:O	5:F:276:ARG:HG3	2.21	0.40
5:F:339:PRO:HB3	5:F:343:ASP:HB2	2.02	0.40
1:L:152:PRO:HD2	1:L:155:LYS:CD	2.47	0.40
1:L:145:ASP:O	1:L:171:PHE:HE1	2.05	0.40
1:L:48:ILE:HA	1:L:49:PRO:HD3	1.85	0.40
2:M:1043:TYR:HA	3:N:710:ARG:NH1	2.35	0.40
2:M:1115:LEU:N	2:M:1115:LEU:CD1	2.78	0.40
2:M:133:ASP:OD2	2:M:133:ASP:N	2.54	0.40
2:M:299:LYS:HG3	8:M:1137:HOH:O	2.21	0.40
2:M:415:PRO:HB2	2:M:418:LEU:CD1	2.52	0.40
2:M:419:THR:HA	2:M:420:ARG:NH1	2.35	0.40
2:M:510:ALA:CB	8:M:1203:HOH:O	2.67	0.40
2:M:575:GLN:HG2	2:M:662:GLU:OE2	2.21	0.40
2:M:753:ASP:O	2:M:792:VAL:HG23	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:920:GLN:HG3	8:M:1705:HOH:O	2.21	0.40
3:N:1209:LEU:C	3:N:1211:MET:N	2.75	0.40
3:N:122:GLU:OE1	3:N:126:VAL:HG23	2.21	0.40
3:N:1426:LYS:NZ	3:N:1430:SER:OG	2.54	0.40
3:N:558:LEU:HB2	8:N:9625:HOH:O	2.21	0.40
3:N:650:LEU:CD1	3:N:691:LEU:HD22	2.51	0.40
3:N:866:VAL:CG1	3:N:867:ARG:N	2.84	0.40
1:A:63:HIS:HB3	2:C:746:GLY:CA	2.44	0.40
2:C:367:LEU:CA	2:C:371:LYS:HB2	2.52	0.40
2:C:536:PRO:HD2	2:C:537:LYS:HD2	2.03	0.40
2:C:668:LEU:O	2:C:993:PHE:CZ	2.74	0.40
2:C:707:ARG:O	2:C:707:ARG:HG2	2.20	0.40
2:C:854:PRO:C	2:C:856:GLU:N	2.74	0.40
2:C:987:ILE:N	2:C:987:ILE:HD12	2.36	0.40
2:C:971:LYS:HB3	2:C:988:VAL:N	2.36	0.40
3:D:1047:LYS:HE3	3:D:1051:GLU:O	2.22	0.40
3:D:10:ILE:CD1	3:D:1434:TRP:NE1	2.84	0.40
3:D:118:LEU:CB	3:D:123:LEU:HD22	2.38	0.40
3:D:592:THR:H	3:D:600:LEU:HD21	1.86	0.40
3:D:613:ARG:HG3	8:D:9002:HOH:O	2.21	0.40
2:C:1020:PRO:O	3:D:622:ARG:HD2	2.20	0.40
3:D:637:LEU:HD21	3:D:642:CYS:CA	2.47	0.40
5:F:124:PRO:O	5:F:128:ARG:HB2	2.21	0.40
5:F:278:LEU:HB2	5:F:286:PRO:HG2	2.02	0.40
1:K:51:THR:HA	1:K:145:ASP:O	2.20	0.40
1:K:59:GLU:HG3	1:K:139:ASN:O	2.21	0.40
1:L:101:LEU:HG	1:L:113:ASP:O	2.21	0.40
1:L:180:GLN:HB2	1:L:198:ARG:NH2	2.22	0.40
1:L:211:LEU:O	1:L:214:ALA:HB3	2.21	0.40
1:L:91:ASN:O	1:L:94:LEU:HD12	2.20	0.40
2:M:1031:ARG:HD3	8:M:1668:HOH:O	2.21	0.40
2:M:1049:LEU:HG	2:M:1053:LEU:CD1	2.51	0.40
2:M:250:ARG:HG2	2:M:253:ALA:CB	2.46	0.40
2:M:455:LEU:O	2:M:541:SER:HB2	2.21	0.40
2:M:602:GLU:HG2	2:M:603:VAL:H	1.86	0.40
2:M:904:PRO:HG3	8:M:1508:HOH:O	2.21	0.40
3:N:1236:LEU:HD11	3:N:1356:TYR:CE1	2.57	0.40
3:N:1280:VAL:HG13	3:N:1316:GLY:O	2.21	0.40
3:N:138:LYS:HB2	3:N:138:LYS:HE3	1.87	0.40
3:N:156:GLU:O	3:N:159:ARG:HB3	2.21	0.40
3:N:432:TYR:HA	3:N:448:GLU:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:488:ARG:HH22	3:N:491:LYS:HZ1	1.70	0.40
3:N:13:ALA:O	3:N:511:TRP:HB3	2.21	0.40
3:N:948:THR:HB	8:N:9352:HOH:O	2.20	0.40
2:M:988:VAL:HG11	3:N:949:ILE:O	2.21	0.40
3:N:1480:PHE:O	4:O:18:ARG:NH2	2.55	0.40
5:P:220:LEU:HB2	5:P:243:ILE:HD11	2.03	0.40
8:M:1148:HOH:O	5:P:276:ARG:HD3	2.19	0.40
5:P:361:LEU:HD13	5:P:366:ALA:HB1	2.03	0.40
1:B:218:LEU:O	1:B:222:LEU:HG	2.21	0.40
1:B:39:PRO:O	1:B:43:ILE:HG12	2.21	0.40
2:C:1001:VAL:HG23	8:C:1823:HOH:O	2.21	0.40
2:C:440:PRO:HG2	2:C:441:VAL:HG23	2.02	0.40
2:C:75:GLU:HA	2:C:76:PRO:HD3	1.89	0.40
3:D:105:VAL:HG21	3:D:128:TYR:HE2	1.86	0.40
3:D:1167:SER:N	3:D:1170:ASP:OD2	2.48	0.40
3:D:1123:PHE:CZ	3:D:1178:ALA:HB1	2.57	0.40
3:D:1293:PHE:HD2	8:D:9222:HOH:O	2.03	0.40
3:D:1314:LYS:HZ1	3:D:1317:ASP:CB	2.34	0.40
3:D:1320:GLU:HG2	3:D:1339:LYS:NZ	2.36	0.40
3:D:1497:GLU:OE1	3:D:1500:LYS:HD2	2.21	0.40
3:D:150:ARG:O	3:D:150:ARG:HG2	2.20	0.40
3:D:27:GLU:O	3:D:28:LYS:HD2	2.21	0.40
3:D:646:LYS:HD3	8:D:2059:HOH:O	2.22	0.40
3:D:884:ARG:O	3:D:888:GLU:N	2.53	0.40
3:D:455:ARG:HH22	5:F:140:ARG:HD3	1.86	0.40
5:F:312:GLN:NE2	8:F:455:HOH:O	2.48	0.40
1:K:127:LEU:HD12	1:K:127:LEU:C	2.42	0.40
1:K:67:THR:OG1	2:M:627:ARG:NH2	2.53	0.40
1:L:100:LEU:HB2	1:L:115:LEU:CD2	2.49	0.40
2:M:167:LYS:HD2	2:M:168:ARG:NH1	2.35	0.40
2:M:207:LEU:HD22	2:M:221:LEU:CD2	2.51	0.40
2:M:621:VAL:HG13	8:M:1199:HOH:O	2.20	0.40
3:N:951:ILE:HD12	3:N:1062:ARG:NE	2.37	0.40
3:N:1209:LEU:HD23	3:N:1210:SER:N	2.28	0.40
3:N:1266:ARG:NH2	8:N:9590:HOH:O	2.54	0.40
3:N:396:VAL:CG1	3:N:447:VAL:HA	2.52	0.40
3:N:461:ILE:O	3:N:465:LEU:HB2	2.22	0.40
3:N:608:SER:O	3:N:615:ARG:NH1	2.54	0.40
3:N:85:VAL:HG12	3:N:89:ARG:CZ	2.51	0.40
3:N:861:GLN:H	3:N:861:GLN:CD	2.25	0.40
3:N:868:TYR:HB3	8:N:9527:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:875:THR:CG2	3:N:879:ARG:HE	2.33	0.40
4:O:59:ASN:HB3	4:O:62:THR:OG1	2.22	0.40
5:P:109:GLY:O	5:P:112:ALA:HB3	2.21	0.40
5:P:249:ARG:NH2	8:P:2663:HOH:O	2.52	0.40
5:P:273:ARG:HG3	8:P:2904:HOH:O	2.20	0.40
5:P:76:SER:O	5:P:80:PRO:CD	2.66	0.40
1:B:123:MET:O	1:B:125:PRO:HD3	2.21	0.40
1:B:180:GLN:HG3	1:B:196:THR:OG1	2.21	0.40
1:B:54:THR:CG2	1:B:158:ILE:HG13	2.50	0.40
2:C:150:PRO:HB2	8:C:1325:HOH:O	2.21	0.40
2:C:199:VAL:HG13	2:C:235:LEU:CD2	2.51	0.40
2:C:251:ASP:C	2:C:252:LYS:HD2	2.42	0.40
2:C:329:GLY:HA3	8:C:1467:HOH:O	2.21	0.40
2:C:367:LEU:HA	2:C:371:LYS:HB2	2.02	0.40
2:C:432:ARG:NE	2:C:519:GLY:HA3	2.37	0.40
2:C:730:SER:N	8:C:1699:HOH:O	2.54	0.40
2:C:871:LEU:HA	2:C:871:LEU:HD23	1.79	0.40
3:D:191:LEU:HB2	3:D:211:VAL:CG2	2.51	0.40
3:D:216:VAL:HG11	8:D:9324:HOH:O	2.22	0.40
3:D:500:ARG:HA	3:D:500:ARG:HD3	1.86	0.40
3:D:53:ILE:O	3:D:53:ILE:HG12	2.22	0.40
3:D:639:LEU:CD1	3:D:640:HIS:H	2.35	0.40
3:D:755:ALA:HA	3:D:758:GLU:OE2	2.21	0.40
4:E:57:ASP:N	4:E:58:PRO:HD3	2.37	0.40
5:F:225:GLU:OE1	5:F:226:LYS:HG2	2.21	0.40
5:F:325:LYS:HB2	8:F:519:HOH:O	2.22	0.40
5:F:359:SER:C	5:F:361:LEU:H	2.23	0.40
1:L:44:LEU:O	1:L:174:VAL:HG21	2.20	0.40
2:M:331:ARG:HG3	8:M:1502:HOH:O	2.22	0.40
2:M:496:ILE:HD12	2:M:496:ILE:N	2.36	0.40
2:M:478:VAL:HG13	2:M:506:ASN:ND2	2.36	0.40
2:M:507:ARG:NH1	8:M:1728:HOH:O	2.53	0.40
2:M:614:ARG:HG2	8:M:1443:HOH:O	2.20	0.40
2:M:666:LEU:HD12	2:M:667:ALA:N	2.35	0.40
2:M:724:ARG:O	2:M:734:LEU:HD11	2.22	0.40
2:M:908:GLY:C	2:M:910:LYS:HZ3	2.24	0.40
3:N:951:ILE:HD12	3:N:1062:ARG:HE	1.85	0.40
3:N:1103:HIS:CG	3:N:1104:GLU:N	2.90	0.40
3:N:1112:CYS:HB2	3:N:1195:GLN:CD	2.40	0.40
3:N:1114:THR:HG22	3:N:1195:GLN:HB3	2.02	0.40
3:N:159:ARG:NH1	3:N:159:ARG:HB2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:474:GLU:OE1	3:N:500:ARG:NE	2.54	0.40
3:N:583:ASP:HB2	3:N:604:THR:OG1	2.21	0.40
3:N:774:SER:C	3:N:776:GLU:N	2.75	0.40
3:N:970:LYS:O	3:N:974:ILE:HG13	2.21	0.40
3:N:99:ALA:HB1	3:N:575:GLN:CD	2.42	0.40
5:P:401:GLU:O	5:P:405:LEU:HD13	2.21	0.40
1:A:111:ALA:HB3	1:A:124:ASN:O	2.21	0.40
1:B:117:VAL:HG11	8:B:346:HOH:O	2.21	0.40
1:B:150:TYR:HA	1:B:169:ALA:O	2.21	0.40
1:B:61:VAL:HG11	1:B:75:VAL:HG21	2.03	0.40
2:C:585:GLU:HG2	2:C:665:PHE:HD2	1.87	0.40
2:C:693:GLU:OE1	2:C:696:LYS:HG3	2.22	0.40
2:C:966:LEU:HD12	2:C:966:LEU:HA	1.96	0.40
3:D:1161:GLU:HG2	3:D:1161:GLU:H	1.67	0.40
3:D:1320:GLU:HG3	8:D:9376:HOH:O	2.20	0.40
3:D:135:LEU:HD21	3:D:138:LYS:C	2.42	0.40
3:D:417:PRO:HB2	8:D:9616:HOH:O	2.21	0.40
3:D:570:GLU:OE2	3:D:573:MET:HE2	2.22	0.40
3:D:101:HIS:CE1	3:D:582:LEU:HD22	2.57	0.40
3:D:602:SER:O	3:D:606:ILE:HG12	2.22	0.40
5:F:421:PHE:C	5:F:423:ASP:H	2.25	0.40
1:K:57:TYR:CD2	1:K:161:ARG:NH1	2.90	0.40
1:K:26:GLU:HB2	1:K:27:PRO:HA	2.04	0.40
1:K:64:GLU:OE2	1:K:76:VAL:HG22	2.22	0.40
2:M:1008:ARG:NH2	2:M:1020:PRO:HB3	2.37	0.40
2:M:211:LEU:HD21	2:M:311:PHE:HE1	1.87	0.40
2:M:28:ARG:HG3	2:M:40:GLU:OE1	2.22	0.40
2:M:480:THR:HG22	2:M:481:ASP:H	1.86	0.40
2:M:513:VAL:HG12	8:M:1272:HOH:O	2.21	0.40
3:N:1102:THR:O	3:N:1102:THR:HG22	2.21	0.40
3:N:1422:MET:HE1	3:N:1426:LYS:HG3	2.02	0.40
3:N:14:SER:O	3:N:17:LYS:N	2.54	0.40
3:N:789:LEU:HA	3:N:789:LEU:HD23	1.84	0.40
3:N:960:LYS:HG2	3:N:964:LEU:HD12	2.04	0.40
5:P:315:VAL:HA	8:P:4638:HOH:O	2.21	0.40
5:P:348:SER:N	8:P:4815:HOH:O	2.53	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	227/315 (72%)	202 (89%)	21 (9%)	4 (2%)	9	30
1	B	227/315 (72%)	202 (89%)	21 (9%)	4 (2%)	9	30
1	K	227/315 (72%)	200 (88%)	23 (10%)	4 (2%)	9	30
1	L	227/315 (72%)	204 (90%)	19 (8%)	4 (2%)	9	30
2	C	1117/1119 (100%)	917 (82%)	150 (13%)	50 (4%)	3	9
2	M	1117/1119 (100%)	907 (81%)	159 (14%)	51 (5%)	2	8
3	D	1388/1524 (91%)	1123 (81%)	191 (14%)	74 (5%)	2	6
3	N	1388/1524 (91%)	1110 (80%)	195 (14%)	83 (6%)	2	4
4	E	93/99 (94%)	74 (80%)	16 (17%)	3 (3%)	4	15
4	O	93/99 (94%)	75 (81%)	15 (16%)	3 (3%)	4	15
5	F	341/423 (81%)	283 (83%)	42 (12%)	16 (5%)	2	8
5	P	341/423 (81%)	285 (84%)	40 (12%)	16 (5%)	2	8
All	All	6786/7590 (89%)	5582 (82%)	892 (13%)	312 (5%)	2	8

All (312) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	B	29	GLU
1	B	48	ILE
2	C	152	PRO
2	C	178	PRO
2	C	231	PRO
2	C	244	PRO
2	C	261	ILE
2	C	262	ALA
2	C	288	ARG
2	C	369	PRO
2	C	425	PHE

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Mol	Chain	Res	Type
2	C	462	ASP
2	C	465	GLY
2	C	548	PRO
2	C	680	ASP
2	C	864	GLY
2	C	908	GLY
2	C	1004	LYS
2	C	1106	ASP
3	D	40	GLU
3	D	43	GLY
3	D	55	ASP
3	D	82	LYS
3	D	137	PRO
3	D	208	PRO
3	D	209	ARG
3	D	238	PRO
3	D	246	PRO
3	D	370	ALA
3	D	373	PRO
3	D	385	VAL
3	D	440	VAL
3	D	451	ASP
3	D	504	ASP
3	D	832	ARG
3	D	844	ALA
3	D	1028	ALA
3	D	1129	THR
3	D	1208	ASP
3	D	1213	ARG
3	D	1243	THR
3	D	1441	GLN
4	E	42	PRO
4	E	58	PRO
5	F	147	LEU
5	F	153	PRO
5	F	324	GLU
5	F	326	ASP
5	F	341	PRO
5	F	390	PHE
1	K	29	GLU
1	L	29	GLU
2	M	152	PRO

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Mol	Chain	Res	Type
2	M	178	PRO
2	M	231	PRO
2	M	244	PRO
2	M	261	ILE
2	M	262	ALA
2	M	288	ARG
2	M	369	PRO
2	M	425	PHE
2	M	462	ASP
2	M	465	GLY
2	M	548	PRO
2	M	680	ASP
2	M	864	GLY
2	M	908	GLY
2	M	1106	ASP
3	N	31	THR
3	N	40	GLU
3	N	43	GLY
3	N	55	ASP
3	N	82	LYS
3	N	137	PRO
3	N	208	PRO
3	N	209	ARG
3	N	217	LYS
3	N	238	PRO
3	N	246	PRO
3	N	370	ALA
3	N	373	PRO
3	N	385	VAL
3	N	440	VAL
3	N	504	ASP
3	N	832	ARG
3	N	844	ALA
3	N	1028	ALA
3	N	1125	PRO
3	N	1129	THR
3	N	1208	ASP
3	N	1213	ARG
3	N	1243	THR
3	N	1441	GLN
4	O	42	PRO
4	O	58	PRO

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Mol	Chain	Res	Type
5	P	147	LEU
5	P	153	PRO
5	P	324	GLU
5	P	326	ASP
5	P	390	PHE
1	A	187	GLY
1	B	187	GLY
2	C	59	LYS
2	C	156	GLY
2	C	170	PRO
2	C	290	LEU
2	C	363	SER
2	C	517	ARG
2	C	626	ARG
2	C	627	ARG
3	D	31	THR
3	D	96	ALA
3	D	120	ALA
3	D	231	VAL
3	D	381	ALA
3	D	415	VAL
3	D	417	PRO
3	D	594	PRO
3	D	609	GLY
3	D	766	ALA
3	D	783	ARG
3	D	803	GLY
3	D	822	ALA
3	D	1389	LEU
4	E	53	GLY
5	F	393	THR
5	F	420	ASP
1	K	187	GLY
1	L	187	GLY
2	M	59	LYS
2	M	156	GLY
2	M	170	PRO
2	M	290	LEU
2	M	363	SER
2	M	517	ARG
2	M	626	ARG
2	M	781	LYS

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Mol	Chain	Res	Type
3	N	96	ALA
3	N	231	VAL
3	N	381	ALA
3	N	415	VAL
3	N	417	PRO
3	N	451	ASP
3	N	594	PRO
3	N	609	GLY
3	N	803	GLY
3	N	822	ALA
3	N	1342	GLU
4	O	53	GLY
5	P	288	TYR
5	P	341	PRO
1	A	106	PRO
1	B	106	PRO
2	C	18	LEU
2	C	40	GLU
2	C	164	PRO
2	C	419	THR
2	C	727	PRO
2	C	781	LYS
3	D	37	LEU
3	D	98	PRO
3	D	161	LEU
3	D	165	LYS
3	D	170	PRO
3	D	424	GLY
3	D	1388	ARG
5	F	97	GLU
5	F	286	PRO
5	F	288	TYR
1	K	106	PRO
2	M	40	GLU
2	M	164	PRO
2	M	419	THR
2	M	455	LEU
2	M	627	ARG
2	M	727	PRO
2	M	1004	LYS
3	N	37	LEU
3	N	98	PRO

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Mol	Chain	Res	Type
3	N	120	ALA
3	N	161	LEU
3	N	165	LYS
3	N	170	PRO
3	N	424	GLY
3	N	533	GLY
3	N	705	ALA
3	N	766	ALA
3	N	783	ARG
3	N	1341	PRO
3	N	1349	VAL
3	N	1385	GLY
3	N	1389	LEU
5	P	97	GLU
5	P	232	ARG
5	P	286	PRO
5	P	393	THR
1	A	188	GLN
2	C	74	GLY
2	C	144	PRO
2	C	180	GLY
2	C	400	PRO
2	C	529	VAL
2	C	905	ILE
3	D	220	ARG
3	D	416	ALA
3	D	522	PRO
3	D	696	HIS
3	D	705	ALA
3	D	808	THR
3	D	1020	LEU
3	D	1137	ARG
3	D	1366	LYS
3	D	1385	GLY
3	D	1446	VAL
5	F	232	ARG
1	K	188	GLN
1	L	106	PRO
2	M	74	GLY
2	M	180	GLY
2	M	413	LEU
2	M	529	VAL

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Mol	Chain	Res	Type
3	N	24	GLY
3	N	110	SER
3	N	220	ARG
3	N	416	ALA
3	N	526	PRO
3	N	530	VAL
3	N	808	THR
3	N	1019	PRO
3	N	1366	LYS
3	N	1388	ARG
5	P	420	ASP
2	C	251	ASP
2	C	272	ALA
2	C	420	ARG
2	C	422	ARG
2	C	1097	LEU
3	D	521	PRO
3	D	526	PRO
3	D	530	VAL
3	D	615	ARG
3	D	924	MET
3	D	1019	PRO
3	D	1390	LEU
5	F	184	ARG
5	F	360	LYS
1	L	188	GLN
2	M	223	ASP
2	M	272	ALA
2	M	574	ALA
2	M	705	ILE
2	M	905	ILE
2	M	1097	LEU
3	N	34	TYR
3	N	407	VAL
3	N	522	PRO
3	N	1137	ARG
3	N	1390	LEU
3	N	1432	LYS
3	N	1446	VAL
2	C	779	GLY
2	C	784	ASP
3	D	24	GLY

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Mol	Chain	Res	Type
3	D	136	ASP
3	D	368	VAL
3	D	1248	GLY
3	D	1306	PRO
5	F	297	PRO
2	M	144	PRO
2	M	251	ASP
2	M	779	GLY
3	N	615	ARG
3	N	833	GLU
3	N	1226	ALA
3	N	1268	PRO
5	P	360	LYS
2	C	53	PRO
2	C	270	GLY
2	C	336	VAL
3	D	407	VAL
2	M	53	PRO
2	M	270	GLY
3	N	670	VAL
3	N	1248	GLY
3	N	1306	PRO
5	P	297	PRO
2	C	79	PRO
3	D	425	GLY
3	D	1064	GLY
3	D	1349	VAL
5	F	167	PRO
3	N	1064	GLY
5	P	167	PRO
2	C	273	GLY
3	D	670	VAL
3	D	1050	GLY
3	D	1379	VAL
2	M	424	GLY
2	M	1079	PRO
3	N	173	PRO
3	N	425	GLY
5	P	314	PRO
2	M	79	PRO
2	M	273	GLY
2	M	336	VAL

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Mol	Chain	Res	Type
3	N	136	ASP
3	N	368	VAL
3	N	521	PRO
3	N	1050	GLY
3	N	509	PRO
2	C	166	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	202/273 (74%)	147 (73%)	55 (27%)	0	1
1	B	202/273 (74%)	163 (81%)	39 (19%)	1	5
1	K	202/273 (74%)	152 (75%)	50 (25%)	0	2
1	L	202/273 (74%)	158 (78%)	44 (22%)	1	3
2	C	941/941 (100%)	734 (78%)	207 (22%)	1	3
2	M	941/941 (100%)	730 (78%)	211 (22%)	1	3
3	D	1123/1279 (88%)	846 (75%)	277 (25%)	0	2
3	N	1123/1279 (88%)	866 (77%)	257 (23%)	1	2
4	E	83/87 (95%)	58 (70%)	25 (30%)	0	1
4	O	83/87 (95%)	64 (77%)	19 (23%)	1	2
5	F	295/370 (80%)	228 (77%)	67 (23%)	1	3
5	P	295/370 (80%)	249 (84%)	46 (16%)	3	9
All	All	5692/6446 (88%)	4395 (77%)	1297 (23%)	1	2

All (1297) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	5	LYS
1	A	9	PRO
1	A	12	THR

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Mol	Chain	Res	Type
1	A	15	THR
1	A	16	GLN
1	A	19	GLU
1	A	20	TYR
1	A	26	GLU
1	A	28	LEU
1	A	32	PHE
1	A	34	VAL
1	A	44	LEU
1	A	47	SER
1	A	54	THR
1	A	60	ASP
1	A	62	LEU
1	A	66	SER
1	A	73	GLU
1	A	74	ASP
1	A	76	VAL
1	A	77	GLU
1	A	84	GLU
1	A	88	ARG
1	A	89	PHE
1	A	96	THR
1	A	101	LEU
1	A	104	GLU
1	A	113	ASP
1	A	120	VAL
1	A	127	LEU
1	A	137	ARG
1	A	142	VAL
1	A	143	ARG
1	A	156	HIS
1	A	161	ARG
1	A	163	ASN
1	A	165	ILE
1	A	167	VAL
1	A	176	ARG
1	A	180	GLN
1	A	183	ASP
1	A	186	LEU
1	A	188	GLN
1	A	191	ASP
1	A	196	THR

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Mol	Chain	Res	Type
1	A	197	LEU
1	A	198	ARG
1	A	201	THR
1	A	205	VAL
1	A	206	THR
1	A	211	LEU
1	A	216	GLU
1	A	227	ASN
1	A	229	GLN
1	B	1	MET
1	B	5	LYS
1	B	26	GLU
1	B	38	ASN
1	B	55	SER
1	B	62	LEU
1	B	65	PHE
1	B	68	ILE
1	B	73	GLU
1	B	77	GLU
1	B	81	ASN
1	B	87	VAL
1	B	88	ARG
1	B	89	PHE
1	B	92	PRO
1	B	94	LEU
1	B	95	GLN
1	B	96	THR
1	B	99	LEU
1	B	101	LEU
1	B	112	ARG
1	B	119	ASP
1	B	121	GLU
1	B	124	ASN
1	B	128	HIS
1	B	133	GLU
1	B	140	MET
1	B	159	LYS
1	B	161	ARG
1	B	176	ARG
1	B	192	LEU
1	B	197	LEU
1	B	200	TRP

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Mol	Chain	Res	Type
1	B	201	THR
1	B	206	THR
1	B	208	LEU
1	B	209	GLU
1	B	220	GLU
1	B	224	TYR
2	C	5	ARG
2	C	10	ARG
2	C	12	VAL
2	C	15	LEU
2	C	20	GLU
2	C	22	GLN
2	C	26	TYR
2	C	30	LEU
2	C	31	GLN
2	C	34	VAL
2	C	41	ASN
2	C	48	PHE
2	C	49	ARG
2	C	51	THR
2	C	52	PHE
2	C	71	TYR
2	C	72	ARG
2	C	73	LEU
2	C	81	ASP
2	C	89	THR
2	C	95	TYR
2	C	98	LEU
2	C	100	LEU
2	C	104	ASP
2	C	108	ILE
2	C	110	GLU
2	C	111	ASP
2	C	114	PHE
2	C	115	LEU
2	C	140	ILE
2	C	141	HIS
2	C	149	THR
2	C	152	PRO
2	C	157	ARG
2	C	158	TYR
2	C	168	ARG

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Mol	Chain	Res	Type
2	C	170	PRO
2	C	177	GLU
2	C	178	PRO
2	C	193	LEU
2	C	198	ARG
2	C	205	GLU
2	C	209	ARG
2	C	216	GLU
2	C	221	LEU
2	C	222	MET
2	C	224	GLU
2	C	229	MET
2	C	237	ARG
2	C	238	LEU
2	C	239	PHE
2	C	243	ARG
2	C	250	ARG
2	C	252	LYS
2	C	257	VAL
2	C	266	ARG
2	C	267	TYR
2	C	275	TYR
2	C	279	GLU
2	C	281	LEU
2	C	285	LEU
2	C	286	SER
2	C	288	ARG
2	C	290	LEU
2	C	303	PHE
2	C	304	LEU
2	C	309	TYR
2	C	321	GLU
2	C	332	ARG
2	C	334	ARG
2	C	340	MET
2	C	342	ASP
2	C	343	GLN
2	C	357	GLU
2	C	359	MET
2	C	360	LEU
2	C	365	ASP
2	C	368	THR

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Mol	Chain	Res	Type
2	C	384	GLU
2	C	388	ARG
2	C	392	SER
2	C	393	GLN
2	C	394	PHE
2	C	399	ASN
2	C	400	PRO
2	C	408	ARG
2	C	409	ARG
2	C	413	LEU
2	C	420	ARG
2	C	425	PHE
2	C	432	ARG
2	C	451	LEU
2	C	453	THR
2	C	460	ARG
2	C	474	VAL
2	C	479	VAL
2	C	481	ASP
2	C	487	THR
2	C	492	ASP
2	C	496	ILE
2	C	500	ASN
2	C	503	LEU
2	C	504	GLU
2	C	508	ILE
2	C	513	VAL
2	C	523	ILE
2	C	524	VAL
2	C	527	GLU
2	C	532	MET
2	C	533	ASP
2	C	542	VAL
2	C	543	ASN
2	C	548	PRO
2	C	559	LEU
2	C	563	ASN
2	C	564	MET
2	C	566	THR
2	C	575	GLN
2	C	584	GLU
2	C	589	ARG

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Mol	Chain	Res	Type
2	C	605	LYS
2	C	620	LEU
2	C	622	GLU
2	C	633	GLN
2	C	639	GLN
2	C	640	ARG
2	C	645	VAL
2	C	653	ASP
2	C	657	ASP
2	C	663	ASN
2	C	668	LEU
2	C	671	ASN
2	C	672	VAL
2	C	679	PHE
2	C	691	SER
2	C	693	GLU
2	C	697	ARG
2	C	699	PHE
2	C	701	THR
2	C	707	ARG
2	C	722	ILE
2	C	724	ARG
2	C	727	PRO
2	C	729	LEU
2	C	737	LEU
2	C	740	GLU
2	C	749	VAL
2	C	785	VAL
2	C	791	ARG
2	C	799	ILE
2	C	803	THR
2	C	804	VAL
2	C	808	ARG
2	C	814	GLU
2	C	821	GLU
2	C	839	LEU
2	C	841	ASN
2	C	853	LEU
2	C	858	MET
2	C	862	PRO
2	C	863	ASP
2	C	868	ASP

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Mol	Chain	Res	Type
2	C	870	ILE
2	C	878	SER
2	C	881	ASN
2	C	882	LEU
2	C	886	LEU
2	C	900	ARG
2	C	901	TYR
2	C	904	PRO
2	C	907	ASP
2	C	923	GLU
2	C	925	TYR
2	C	934	PHE
2	C	948	GLU
2	C	950	LEU
2	C	953	VAL
2	C	959	PRO
2	C	969	GLN
2	C	971	LYS
2	C	975	TYR
2	C	978	ARG
2	C	981	GLU
2	C	982	PRO
2	C	984	GLU
2	C	988	VAL
2	C	995	MET
2	C	1006	HIS
2	C	1008	ARG
2	C	1016	ILE
2	C	1017	THR
2	C	1019	GLN
2	C	1021	LEU
2	C	1035	MET
2	C	1052	MET
2	C	1076	VAL
2	C	1079	PRO
2	C	1085	PHE
2	C	1087	VAL
2	C	1092	LEU
2	C	1095	LEU
2	C	1098	ASP
2	C	1103	ASP
2	C	1104	GLU

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Mol	Chain	Res	Type
2	C	1106	ASP
2	C	1109	VAL
2	C	1115	LEU
3	D	3	LYS
3	D	6	ARG
3	D	12	LEU
3	D	17	LYS
3	D	25	GLU
3	D	27	GLU
3	D	29	PRO
3	D	30	GLU
3	D	32	ILE
3	D	41	ARG
3	D	42	ASP
3	D	47	GLU
3	D	48	ARG
3	D	56	TYR
3	D	58	CYS
3	D	62	LYS
3	D	71	LYS
3	D	74	GLU
3	D	76	CYS
3	D	80	VAL
3	D	82	LYS
3	D	85	VAL
3	D	86	ARG
3	D	87	ARG
3	D	89	ARG
3	D	90	MET
3	D	97	THR
3	D	101	HIS
3	D	103	TRP
3	D	107	ASP
3	D	112	ILE
3	D	115	LEU
3	D	117	ASP
3	D	118	LEU
3	D	121	THR
3	D	133	ILE
3	D	136	ASP
3	D	145	VAL
3	D	148	GLU

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Mol	Chain	Res	Type
3	D	153	LEU
3	D	155	ASP
3	D	156	GLU
3	D	162	ARG
3	D	170	PRO
3	D	171	LEU
3	D	176	ASP
3	D	185	VAL
3	D	199	LEU
3	D	200	ASP
3	D	204	LEU
3	D	205	TYR
3	D	206	ARG
3	D	208	PRO
3	D	209	ARG
3	D	210	ARG
3	D	389	GLU
3	D	394	LEU
3	D	395	VAL
3	D	411	THR
3	D	413	ASP
3	D	421	LEU
3	D	432	TYR
3	D	444	VAL
3	D	445	ARG
3	D	451	ASP
3	D	455	ARG
3	D	456	MET
3	D	465	LEU
3	D	466	LYS
3	D	469	ASP
3	D	479	GLU
3	D	481	MET
3	D	483	HIS
3	D	489	ARG
3	D	493	ARG
3	D	497	GLU
3	D	503	LEU
3	D	513	ILE
3	D	521	PRO
3	D	525	ARG
3	D	528	VAL

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Mol	Chain	Res	Type
3	D	529	GLN
3	D	535	PHE
3	D	540	LEU
3	D	542	ASP
3	D	548	ILE
3	D	549	ASN
3	D	565	ILE
3	D	573	MET
3	D	590	PRO
3	D	594	PRO
3	D	597	ASP
3	D	598	ARG
3	D	607	LEU
3	D	613	ARG
3	D	615	ARG
3	D	616	GLN
3	D	617	ASN
3	D	624	ASP
3	D	636	GLN
3	D	639	LEU
3	D	641	GLN
3	D	651	GLU
3	D	652	LEU
3	D	653	PHE
3	D	655	PRO
3	D	660	LYS
3	D	666	ILE
3	D	675	ARG
3	D	676	MET
3	D	681	ARG
3	D	685	ASP
3	D	687	VAL
3	D	688	TRP
3	D	692	GLU
3	D	695	ILE
3	D	702	LEU
3	D	703	ASN
3	D	704	ARG
3	D	710	ARG
3	D	713	ILE
3	D	717	GLN
3	D	719	VAL

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Mol	Chain	Res	Type
3	D	724	GLN
3	D	725	SER
3	D	736	PHE
3	D	739	ASP
3	D	749	VAL
3	D	754	PHE
3	D	762	GLN
3	D	763	MET
3	D	765	SER
3	D	768	ASN
3	D	778	LEU
3	D	783	ARG
3	D	794	GLN
3	D	796	ARG
3	D	797	LYS
3	D	800	LYS
3	D	805	GLU
3	D	810	GLU
3	D	824	ASN
3	D	828	LYS
3	D	829	VAL
3	D	832	ARG
3	D	833	GLU
3	D	838	ARG
3	D	839	LEU
3	D	847	ASP
3	D	858	VAL
3	D	859	ASP
3	D	862	ASP
3	D	863	VAL
3	D	865	THR
3	D	867	ARG
3	D	879	ARG
3	D	880	ILE
3	D	888	GLU
3	D	897	TRP
3	D	898	GLU
3	D	902	LEU
3	D	907	GLU
3	D	910	SER
3	D	911	LEU
3	D	914	LEU

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Mol	Chain	Res	Type
3	D	915	VAL
3	D	916	TYR
3	D	922	LEU
3	D	944	THR
3	D	952	ASP
3	D	959	GLU
3	D	961	LYS
3	D	969	ARG
3	D	972	LEU
3	D	985	ASP
3	D	987	GLU
3	D	988	ARG
3	D	997	THR
3	D	1000	THR
3	D	1001	GLU
3	D	1032	PRO
3	D	1033	GLN
3	D	1038	LEU
3	D	1039	CYS
3	D	1042	ARG
3	D	1049	SER
3	D	1051	GLU
3	D	1058	ARG
3	D	1060	SER
3	D	1062	ARG
3	D	1068	LEU
3	D	1083	ASP
3	D	1087	ARG
3	D	1093	TYR
3	D	1095	THR
3	D	1096	ARG
3	D	1104	GLU
3	D	1109	GLU
3	D	1112	CYS
3	D	1116	ASN
3	D	1124	GLN
3	D	1129	THR
3	D	1144	LEU
3	D	1160	LEU
3	D	1161	GLU
3	D	1164	ARG
3	D	1166	LEU

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Mol	Chain	Res	Type
3	D	1176	LYS
3	D	1182	GLU
3	D	1183	ILE
3	D	1190	SER
3	D	1195	GLN
3	D	1207	TYR
3	D	1210	SER
3	D	1211	MET
3	D	1213	ARG
3	D	1238	MET
3	D	1243	THR
3	D	1251	ASP
3	D	1258	ARG
3	D	1260	ILE
3	D	1262	LEU
3	D	1267	ARG
3	D	1269	LYS
3	D	1280	VAL
3	D	1290	LEU
3	D	1295	GLU
3	D	1299	PHE
3	D	1302	GLU
3	D	1305	LEU
3	D	1306	PRO
3	D	1307	LYS
3	D	1310	ARG
3	D	1314	LYS
3	D	1317	ASP
3	D	1318	TYR
3	D	1320	GLU
3	D	1331	ASP
3	D	1332	PRO
3	D	1337	GLU
3	D	1339	LYS
3	D	1344	VAL
3	D	1346	ARG
3	D	1348	LEU
3	D	1359	GLN
3	D	1363	LEU
3	D	1368	ILE
3	D	1382	THR
3	D	1401	GLU

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Mol	Chain	Res	Type
3	D	1403	LEU
3	D	1406	ARG
3	D	1407	LEU
3	D	1410	GLU
3	D	1415	VAL
3	D	1419	PRO
3	D	1420	LEU
3	D	1421	LEU
3	D	1424	VAL
3	D	1425	THR
3	D	1432	LYS
3	D	1433	SER
3	D	1440	PHE
3	D	1444	THR
3	D	1447	LEU
3	D	1462	LEU
3	D	1463	LYS
3	D	1464	GLU
3	D	1465	ASN
3	D	1466	VAL
3	D	1470	ARG
3	D	1480	PHE
3	D	1481	VAL
3	D	1483	PHE
3	D	1485	GLN
3	D	1488	ASP
3	D	1496	GLU
3	D	1501	GLU
4	E	7	ASP
4	E	10	PHE
4	E	12	MET
4	E	14	ASP
4	E	15	SER
4	E	20	THR
4	E	28	GLN
4	E	29	GLN
4	E	30	LEU
4	E	31	LEU
4	E	32	ARG
4	E	33	HIS
4	E	40	LEU
4	E	42	PRO

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Mol	Chain	Res	Type
4	E	45	ARG
4	E	51	LEU
4	E	57	ASP
4	E	58	PRO
4	E	59	ASN
4	E	61	GLU
4	E	66	LYS
4	E	67	GLU
4	E	81	PRO
4	E	84	ARG
4	E	89	MET
5	F	80	PRO
5	F	83	GLN
5	F	84	TYR
5	F	91	VAL
5	F	96	LEU
5	F	101	GLU
5	F	117	SER
5	F	120	THR
5	F	124	PRO
5	F	125	ASP
5	F	135	ILE
5	F	136	LEU
5	F	142	ARG
5	F	149	GLU
5	F	170	HIS
5	F	174	LEU
5	F	181	GLU
5	F	185	GLN
5	F	186	HIS
5	F	192	LEU
5	F	194	LEU
5	F	208	SER
5	F	209	PHE
5	F	218	GLN
5	F	220	LEU
5	F	225	GLU
5	F	228	GLU
5	F	233	PHE
5	F	236	SER
5	F	240	THR
5	F	245	GLN

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Mol	Chain	Res	Type
5	F	269	ASN
5	F	273	ARG
5	F	281	GLU
5	F	282	LEU
5	F	285	GLU
5	F	288	TYR
5	F	289	GLU
5	F	295	MET
5	F	302	LYS
5	F	313	GLU
5	F	317	LEU
5	F	328	PHE
5	F	329	TYR
5	F	331	ASP
5	F	335	ASP
5	F	336	GLU
5	F	340	SER
5	F	341	PRO
5	F	342	VAL
5	F	347	GLN
5	F	349	LEU
5	F	350	LEU
5	F	353	GLU
5	F	355	GLU
5	F	361	LEU
5	F	365	GLU
5	F	370	LYS
5	F	393	THR
5	F	398	ARG
5	F	399	GLN
5	F	403	LYS
5	F	410	TYR
5	F	412	GLU
5	F	414	ARG
5	F	419	ARG
5	F	420	ASP
1	K	5	LYS
1	K	9	PRO
1	K	12	THR
1	K	14	ARG
1	K	15	THR
1	K	18	ARG

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Mol	Chain	Res	Type
1	K	25	LEU
1	K	44	LEU
1	K	45	LEU
1	K	62	LEU
1	K	66	SER
1	K	80	LEU
1	K	88	ARG
1	K	92	PRO
1	K	94	LEU
1	K	96	THR
1	K	100	LEU
1	K	101	LEU
1	K	107	LYS
1	K	108	GLU
1	K	113	ASP
1	K	116	PRO
1	K	119	ASP
1	K	120	VAL
1	K	121	GLU
1	K	127	LEU
1	K	131	THR
1	K	133	GLU
1	K	138	LEU
1	K	140	MET
1	K	154	GLU
1	K	156	HIS
1	K	165	ILE
1	K	167	VAL
1	K	176	ARG
1	K	180	GLN
1	K	184	THR
1	K	185	ARG
1	K	186	LEU
1	K	190	THR
1	K	191	ASP
1	K	193	ASP
1	K	196	THR
1	K	198	ARG
1	K	206	THR
1	K	211	LEU
1	K	219	ARG
1	K	221	HIS

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Mol	Chain	Res	Type
1	K	223	THR
1	K	227	ASN
1	L	1	MET
1	L	2	LEU
1	L	3	ASP
1	L	5	LYS
1	L	7	LYS
1	L	9	PRO
1	L	25	LEU
1	L	29	GLU
1	L	30	ARG
1	L	38	ASN
1	L	47	SER
1	L	55	SER
1	L	62	LEU
1	L	63	HIS
1	L	65	PHE
1	L	67	THR
1	L	73	GLU
1	L	77	GLU
1	L	81	ASN
1	L	88	ARG
1	L	89	PHE
1	L	91	ASN
1	L	94	LEU
1	L	95	GLN
1	L	99	LEU
1	L	101	LEU
1	L	110	LYS
1	L	121	GLU
1	L	138	LEU
1	L	140	MET
1	L	141	GLU
1	L	159	LYS
1	L	167	VAL
1	L	176	ARG
1	L	177	VAL
1	L	184	THR
1	L	193	ASP
1	L	201	THR
1	L	206	THR
1	L	213	GLN

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Mol	Chain	Res	Type
1	L	216	GLU
1	L	220	GLU
1	L	227	ASN
1	L	229	GLN
2	M	5	ARG
2	M	9	ILE
2	M	22	GLN
2	M	26	TYR
2	M	30	LEU
2	M	31	GLN
2	M	33	ASP
2	M	34	VAL
2	M	39	ARG
2	M	48	PHE
2	M	49	ARG
2	M	51	THR
2	M	55	GLU
2	M	71	TYR
2	M	81	ASP
2	M	91	GLN
2	M	94	LEU
2	M	95	TYR
2	M	98	LEU
2	M	99	GLN
2	M	100	LEU
2	M	105	THR
2	M	107	LEU
2	M	108	ILE
2	M	114	PHE
2	M	115	LEU
2	M	133	ASP
2	M	134	ARG
2	M	140	ILE
2	M	141	HIS
2	M	149	THR
2	M	152	PRO
2	M	157	ARG
2	M	158	TYR
2	M	163	ILE
2	M	175	GLU
2	M	177	GLU
2	M	178	PRO

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Mol	Chain	Res	Type
2	M	185	LYS
2	M	193	LEU
2	M	196	LEU
2	M	198	ARG
2	M	205	GLU
2	M	209	ARG
2	M	211	LEU
2	M	221	LEU
2	M	223	ASP
2	M	229	MET
2	M	230	ARG
2	M	233	GLU
2	M	235	LEU
2	M	237	ARG
2	M	239	PHE
2	M	242	LEU
2	M	243	ARG
2	M	246	ASP
2	M	249	LYS
2	M	252	LYS
2	M	254	VAL
2	M	257	VAL
2	M	260	LEU
2	M	267	TYR
2	M	268	ASP
2	M	279	GLU
2	M	281	LEU
2	M	285	LEU
2	M	290	LEU
2	M	297	GLU
2	M	303	PHE
2	M	304	LEU
2	M	309	TYR
2	M	313	LEU
2	M	321	GLU
2	M	322	VAL
2	M	327	HIS
2	M	328	LEU
2	M	332	ARG
2	M	335	THR
2	M	343	GLN
2	M	345	ARG

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Mol	Chain	Res	Type
2	M	348	LEU
2	M	359	MET
2	M	367	LEU
2	M	371	LYS
2	M	379	GLU
2	M	383	ARG
2	M	392	SER
2	M	397	GLU
2	M	400	PRO
2	M	405	ARG
2	M	408	ARG
2	M	413	LEU
2	M	420	ARG
2	M	425	PHE
2	M	426	ASP
2	M	427	VAL
2	M	443	THR
2	M	448	ASN
2	M	451	LEU
2	M	455	LEU
2	M	460	ARG
2	M	468	ARG
2	M	469	THR
2	M	470	PRO
2	M	480	THR
2	M	481	ASP
2	M	496	ILE
2	M	503	LEU
2	M	507	ARG
2	M	517	ARG
2	M	524	VAL
2	M	527	GLU
2	M	528	GLU
2	M	533	ASP
2	M	544	THR
2	M	545	ASN
2	M	554	ASP
2	M	559	LEU
2	M	564	MET
2	M	571	LEU
2	M	579	VAL
2	M	581	THR

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Mol	Chain	Res	Type
2	M	586	ARG
2	M	589	ARG
2	M	607	ASP
2	M	614	ARG
2	M	617	ASP
2	M	620	LEU
2	M	627	ARG
2	M	630	ARG
2	M	632	ASN
2	M	633	GLN
2	M	635	THR
2	M	637	LEU
2	M	640	ARG
2	M	654	LEU
2	M	663	ASN
2	M	668	LEU
2	M	672	VAL
2	M	676	ILE
2	M	697	ARG
2	M	699	PHE
2	M	715	THR
2	M	717	LEU
2	M	725	ASP
2	M	727	PRO
2	M	728	HIS
2	M	729	LEU
2	M	737	LEU
2	M	748	GLU
2	M	762	LYS
2	M	772	ARG
2	M	780	GLU
2	M	785	VAL
2	M	788	THR
2	M	799	ILE
2	M	807	ARG
2	M	808	ARG
2	M	820	ARG
2	M	821	GLU
2	M	829	GLN
2	M	834	GLN
2	M	839	LEU
2	M	841	ASN

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Mol	Chain	Res	Type
2	M	861	LEU
2	M	862	PRO
2	M	870	ILE
2	M	881	ASN
2	M	886	LEU
2	M	900	ARG
2	M	907	ASP
2	M	910	LYS
2	M	914	ILE
2	M	916	GLU
2	M	917	LEU
2	M	918	LEU
2	M	923	GLU
2	M	925	TYR
2	M	938	LYS
2	M	939	ARG
2	M	950	LEU
2	M	975	TYR
2	M	981	GLU
2	M	984	GLU
2	M	988	VAL
2	M	991	GLN
2	M	999	HIS
2	M	1000	MET
2	M	1002	GLU
2	M	1003	ASP
2	M	1008	ARG
2	M	1016	ILE
2	M	1017	THR
2	M	1035	MET
2	M	1041	GLU
2	M	1053	LEU
2	M	1054	THR
2	M	1058	ASP
2	M	1074	GLU
2	M	1076	VAL
2	M	1079	PRO
2	M	1081	VAL
2	M	1087	VAL
2	M	1088	LEU
2	M	1091	GLU
2	M	1092	LEU

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Mol	Chain	Res	Type
2	M	1097	LEU
2	M	1098	ASP
2	M	1099	VAL
2	M	1100	GLN
2	M	1111	ILE
3	N	2	LYS
3	N	3	LYS
3	N	6	ARG
3	N	12	LEU
3	N	15	PRO
3	N	34	TYR
3	N	36	THR
3	N	41	ARG
3	N	52	PRO
3	N	55	ASP
3	N	56	TYR
3	N	71	LYS
3	N	76	CYS
3	N	80	VAL
3	N	82	LYS
3	N	85	VAL
3	N	86	ARG
3	N	87	ARG
3	N	101	HIS
3	N	102	ILE
3	N	107	ASP
3	N	108	VAL
3	N	111	LYS
3	N	112	ILE
3	N	117	ASP
3	N	118	LEU
3	N	123	LEU
3	N	128	TYR
3	N	145	VAL
3	N	147	VAL
3	N	152	LEU
3	N	153	LEU
3	N	162	ARG
3	N	165	LYS
3	N	169	TYR
3	N	170	PRO
3	N	171	LEU

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Mol	Chain	Res	Type
3	N	172	PRO
3	N	185	VAL
3	N	199	LEU
3	N	200	ASP
3	N	205	TYR
3	N	206	ARG
3	N	208	PRO
3	N	389	GLU
3	N	394	LEU
3	N	395	VAL
3	N	405	ASP
3	N	411	THR
3	N	413	ASP
3	N	414	ARG
3	N	419	ASP
3	N	421	LEU
3	N	427	VAL
3	N	430	ASP
3	N	432	TYR
3	N	442	ASN
3	N	445	ARG
3	N	448	GLU
3	N	449	SER
3	N	455	ARG
3	N	456	MET
3	N	459	GLU
3	N	463	GLN
3	N	465	LEU
3	N	470	LEU
3	N	473	LEU
3	N	475	LYS
3	N	488	ARG
3	N	493	ARG
3	N	502	PHE
3	N	503	LEU
3	N	513	ILE
3	N	521	PRO
3	N	528	VAL
3	N	530	VAL
3	N	534	ARG
3	N	535	PHE
3	N	549	ASN

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Mol	Chain	Res	Type
3	N	554	LEU
3	N	560	GLN
3	N	567	ILE
3	N	569	ASN
3	N	581	LEU
3	N	590	PRO
3	N	592	THR
3	N	594	PRO
3	N	596	SER
3	N	597	ASP
3	N	601	ARG
3	N	602	SER
3	N	613	ARG
3	N	624	ASP
3	N	628	ARG
3	N	629	SER
3	N	635	PRO
3	N	636	GLN
3	N	639	LEU
3	N	641	GLN
3	N	651	GLU
3	N	666	ILE
3	N	676	MET
3	N	681	ARG
3	N	682	ASP
3	N	688	TRP
3	N	692	GLU
3	N	695	ILE
3	N	703	ASN
3	N	704	ARG
3	N	709	HIS
3	N	710	ARG
3	N	717	GLN
3	N	719	VAL
3	N	721	VAL
3	N	725	SER
3	N	732	VAL
3	N	734	GLU
3	N	736	PHE
3	N	739	ASP
3	N	744	GLN
3	N	754	PHE

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Mol	Chain	Res	Type
3	N	770	LEU
3	N	780	LYS
3	N	781	PRO
3	N	783	ARG
3	N	786	ILE
3	N	787	LEU
3	N	792	ILE
3	N	794	GLN
3	N	796	ARG
3	N	797	LYS
3	N	799	LYS
3	N	800	LYS
3	N	804	LEU
3	N	805	GLU
3	N	823	LEU
3	N	828	LYS
3	N	829	VAL
3	N	832	ARG
3	N	839	LEU
3	N	841	TYR
3	N	846	PRO
3	N	847	ASP
3	N	850	LEU
3	N	858	VAL
3	N	863	VAL
3	N	865	THR
3	N	867	ARG
3	N	876	SER
3	N	880	ILE
3	N	888	GLU
3	N	892	ASP
3	N	899	LEU
3	N	901	GLN
3	N	914	LEU
3	N	917	GLN
3	N	951	ILE
3	N	952	ASP
3	N	959	GLU
3	N	972	LEU
3	N	975	GLU
3	N	984	THR
3	N	994	GLN

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Mol	Chain	Res	Type
3	N	1005	GLN
3	N	1029	ARG
3	N	1031	ASN
3	N	1042	ARG
3	N	1045	MET
3	N	1051	GLU
3	N	1052	THR
3	N	1058	ARG
3	N	1059	SER
3	N	1062	ARG
3	N	1065	LEU
3	N	1066	THR
3	N	1068	LEU
3	N	1070	TYR
3	N	1071	PHE
3	N	1079	LYS
3	N	1087	ARG
3	N	1090	ASP
3	N	1095	THR
3	N	1096	ARG
3	N	1109	GLU
3	N	1111	ASP
3	N	1112	CYS
3	N	1127	GLU
3	N	1129	THR
3	N	1133	ARG
3	N	1137	ARG
3	N	1144	LEU
3	N	1162	GLU
3	N	1166	LEU
3	N	1173	LEU
3	N	1176	LYS
3	N	1182	GLU
3	N	1183	ILE
3	N	1195	GLN
3	N	1202	GLN
3	N	1207	TYR
3	N	1211	MET
3	N	1219	GLU
3	N	1231	GLU
3	N	1238	MET
3	N	1243	THR

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Mol	Chain	Res	Type
3	N	1252	ILE
3	N	1254	GLN
3	N	1260	ILE
3	N	1262	LEU
3	N	1264	GLU
3	N	1267	ARG
3	N	1278	ASP
3	N	1285	GLU
3	N	1295	GLU
3	N	1297	GLU
3	N	1299	PHE
3	N	1305	LEU
3	N	1314	LYS
3	N	1331	ASP
3	N	1344	VAL
3	N	1346	ARG
3	N	1348	LEU
3	N	1350	GLU
3	N	1353	GLN
3	N	1355	VAL
3	N	1359	GLN
3	N	1363	LEU
3	N	1365	ASP
3	N	1368	ILE
3	N	1378	TYR
3	N	1380	GLU
3	N	1382	THR
3	N	1383	ASP
3	N	1388	ARG
3	N	1396	GLU
3	N	1401	GLU
3	N	1406	ARG
3	N	1410	GLU
3	N	1415	VAL
3	N	1419	PRO
3	N	1424	VAL
3	N	1432	LYS
3	N	1433	SER
3	N	1440	PHE
3	N	1441	GLN
3	N	1442	ASN
3	N	1460	ILE

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Mol	Chain	Res	Type
3	N	1463	LYS
3	N	1465	ASN
3	N	1466	VAL
3	N	1467	ILE
3	N	1468	LEU
3	N	1485	GLN
3	N	1487	VAL
3	N	1488	ASP
3	N	1493	LYS
3	N	1496	GLU
4	O	10	PHE
4	O	12	MET
4	O	20	THR
4	O	32	ARG
4	O	42	PRO
4	O	43	GLU
4	O	45	ARG
4	O	47	LYS
4	O	51	LEU
4	O	57	ASP
4	O	59	ASN
4	O	61	GLU
4	O	66	LYS
4	O	69	LEU
4	O	70	THR
4	O	84	ARG
4	O	85	LEU
4	O	86	GLN
4	O	89	MET
5	P	83	GLN
5	P	84	TYR
5	P	85	LEU
5	P	91	VAL
5	P	96	LEU
5	P	101	GLU
5	P	108	GLU
5	P	125	ASP
5	P	126	LEU
5	P	135	ILE
5	P	136	LEU
5	P	138	SER
5	P	142	ARG

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Mol	Chain	Res	Type
5	P	144	ILE
5	P	149	GLU
5	P	150	THR
5	P	168	LYS
5	P	174	LEU
5	P	176	ILE
5	P	186	HIS
5	P	214	GLN
5	P	218	GLN
5	P	220	LEU
5	P	221	ILE
5	P	241	TRP
5	P	280	GLN
5	P	295	MET
5	P	302	LYS
5	P	318	GLU
5	P	328	PHE
5	P	337	HIS
5	P	338	LEU
5	P	341	PRO
5	P	347	GLN
5	P	350	LEU
5	P	353	GLU
5	P	365	GLU
5	P	370	LYS
5	P	393	THR
5	P	394	ARG
5	P	396	ARG
5	P	399	GLN
5	P	403	LYS
5	P	410	TYR
5	P	419	ARG
5	P	420	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (179) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	38	ASN
1	A	139	ASN
1	A	156	HIS
1	A	163	ASN

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Mol	Chain	Res	Type
1	A	180	GLN
1	A	188	GLN
1	A	227	ASN
1	A	229	GLN
1	B	95	GLN
1	B	124	ASN
1	B	128	HIS
1	B	163	ASN
2	C	22	GLN
2	C	41	ASN
2	C	102	HIS
2	C	117	HIS
2	C	130	ASN
2	C	139	GLN
2	C	327	HIS
2	C	343	GLN
2	C	374	ASN
2	C	393	GLN
2	C	399	ASN
2	C	431	HIS
2	C	434	HIS
2	C	448	ASN
2	C	538	GLN
2	C	545	ASN
2	C	563	ASN
2	C	565	GLN
2	C	609	ASN
2	C	633	GLN
2	C	639	GLN
2	C	663	ASN
2	C	834	GLN
2	C	841	ASN
2	C	881	ASN
2	C	889	HIS
2	C	899	GLN
2	C	920	GLN
2	C	991	GLN
2	C	1018	GLN
2	C	1019	GLN
2	C	1047	HIS
2	C	1107	ASN
3	D	66	GLN

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Mol	Chain	Res	Type
3	D	143	ASN
3	D	151	GLN
3	D	507	ASN
3	D	549	ASN
3	D	560	GLN
3	D	575	GLN
3	D	640	HIS
3	D	669	ASN
3	D	703	ASN
3	D	709	HIS
3	D	717	GLN
3	D	748	HIS
3	D	756	GLN
3	D	768	ASN
3	D	794	GLN
3	D	855	HIS
3	D	906	GLN
3	D	917	GLN
3	D	1033	GLN
3	D	1075	HIS
3	D	1116	ASN
3	D	1124	GLN
3	D	1202	GLN
3	D	1242	HIS
3	D	1323	GLN
3	D	1333	HIS
3	D	1353	GLN
3	D	1359	GLN
3	D	1374	GLN
3	D	1404	ASN
3	D	1465	ASN
4	E	28	GLN
4	E	37	ASN
4	E	86	GLN
5	F	161	GLN
5	F	218	GLN
5	F	337	HIS
5	F	399	GLN
5	F	402	ASN
1	K	16	GLN
1	K	63	HIS
1	K	81	ASN

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Mol	Chain	Res	Type
1	K	124	ASN
1	K	156	HIS
1	K	213	GLN
1	K	227	ASN
1	K	229	GLN
1	L	16	GLN
1	L	38	ASN
1	L	81	ASN
1	L	91	ASN
1	L	95	GLN
1	L	124	ASN
1	L	212	ASN
2	M	22	GLN
2	M	99	GLN
2	M	117	HIS
2	M	139	GLN
2	M	187	ASN
2	M	204	GLN
2	M	343	GLN
2	M	390	GLN
2	M	393	GLN
2	M	431	HIS
2	M	498	GLN
2	M	538	GLN
2	M	543	ASN
2	M	545	ASN
2	M	563	ASN
2	M	565	GLN
2	M	609	ASN
2	M	639	GLN
2	M	663	ASN
2	M	671	ASN
2	M	704	HIS
2	M	834	GLN
2	M	841	ASN
2	M	843	HIS
2	M	860	HIS
2	M	872	ASN
2	M	881	ASN
2	M	889	HIS
2	M	920	GLN
2	M	969	GLN

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Mol	Chain	Res	Type
2	M	991	GLN
2	M	999	HIS
2	M	1018	GLN
2	M	1050	GLN
2	M	1100	GLN
2	M	1107	ASN
3	N	125	GLN
3	N	151	GLN
3	N	166	GLN
3	N	463	GLN
3	N	507	ASN
3	N	552	ASN
3	N	560	GLN
3	N	569	ASN
3	N	703	ASN
3	N	724	GLN
3	N	756	GLN
3	N	768	ASN
3	N	794	GLN
3	N	909	ASN
3	N	917	GLN
3	N	976	GLN
3	N	994	GLN
3	N	1005	GLN
3	N	1010	ASN
3	N	1014	ASN
3	N	1033	GLN
3	N	1103	HIS
3	N	1172	HIS
3	N	1202	GLN
3	N	1333	HIS
3	N	1334	GLN
3	N	1353	GLN
3	N	1359	GLN
3	N	1374	GLN
3	N	1404	ASN
3	N	1441	GLN
3	N	1465	ASN
3	N	1485	GLN
4	O	28	GLN
4	O	29	GLN
4	O	59	ASN

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Mol	Chain	Res	Type
5	P	191	ASN
5	P	217	ASN
5	P	218	GLN
5	P	269	ASN
5	P	337	HIS
5	P	399	GLN

### 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 carbohydrates in this entry.

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

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	229/315 (72%)	-0.38	0 <span>100</span> <span>100</span>	38, 65, 92, 117	0
1	B	229/315 (72%)	-0.27	8 (3%) <span>44</span> <span>33</span>	53, 95, 115, 121	0
1	K	229/315 (72%)	-0.37	0 <span>100</span> <span>100</span>	41, 66, 93, 122	0
1	L	229/315 (72%)	-0.39	3 (1%) <span>77</span> <span>71</span>	52, 94, 114, 127	0
2	C	1119/1119 (100%)	-0.35	8 (0%) <span>87</span> <span>83</span>	23, 81, 110, 119	0
2	M	1119/1119 (100%)	-0.39	6 (0%) <span>90</span> <span>88</span>	27, 79, 109, 122	0
3	D	1392/1524 (91%)	-0.33	12 (0%) <span>84</span> <span>79</span>	17, 68, 113, 130	0
3	N	1392/1524 (91%)	-0.35	16 (1%) <span>80</span> <span>75</span>	27, 69, 110, 138	0
4	E	95/99 (95%)	-0.35	0 <span>100</span> <span>100</span>	47, 85, 115, 133	0
4	O	95/99 (95%)	-0.49	1 (1%) <span>80</span> <span>75</span>	40, 76, 97, 111	0
5	F	345/423 (81%)	-0.40	3 (0%) <span>84</span> <span>79</span>	46, 84, 112, 131	0
5	P	345/423 (81%)	-0.39	5 (1%) <span>75</span> <span>69</span>	54, 87, 112, 125	0
All	All	6818/7590 (89%)	-0.36	62 (0%) <span>84</span> <span>79</span>	17, 77, 111, 138	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	130	ALA	5.1
3	D	1240	THR	4.7
3	N	1243	THR	4.7
3	D	1243	THR	4.5
5	F	145	PRO	4.4
3	N	1248	GLY	4.4
2	C	307	LEU	4.4
1	L	6	LEU	4.0
3	D	1244	GLY	3.8
3	N	1242	HIS	3.5
2	C	92	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
3	N	1249	ALA	3.4
5	P	365	GLU	3.3
5	F	144	ILE	3.2
3	N	802	ALA	3.2
1	L	109	VAL	3.0
4	O	2	ALA	2.9
1	B	5	LYS	2.9
1	B	109	VAL	2.9
2	C	372	LEU	2.9
2	M	372	LEU	2.9
2	C	152	PRO	2.9
3	N	533	GLY	2.7
1	L	1	MET	2.7
5	P	369	LEU	2.7
3	D	128	TYR	2.7
1	B	6	LEU	2.6
1	B	118	ALA	2.6
3	N	1240	THR	2.6
3	N	1246	VAL	2.6
2	M	281	LEU	2.6
2	M	307	LEU	2.6
2	M	306	THR	2.5
5	P	378	GLY	2.5
2	M	101	ILE	2.5
2	C	311	PHE	2.5
3	D	439	LEU	2.5
3	N	179	VAL	2.4
3	N	1398	TRP	2.4
5	P	357	ALA	2.4
5	P	145	PRO	2.4
2	C	819	VAL	2.3
3	N	394	LEU	2.3
3	N	205	TYR	2.3
3	N	165	LYS	2.3
1	B	82	LEU	2.2
1	B	120	VAL	2.2
2	C	281	LEU	2.2
3	N	381	ALA	2.2
3	N	242	LEU	2.2
2	M	359	MET	2.2
3	D	238	PRO	2.2
3	D	446	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
3	D	127	LEU	2.1
5	F	93	LEU	2.1
2	C	153	ALA	2.1
3	D	1245	GLY	2.1
3	D	505	SER	2.1
1	B	61	VAL	2.1
3	D	177	ALA	2.0
3	N	425	GLY	2.0
3	D	1305	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	MG	N	9002	1/1	0.94	0.13	64,64,64,64	0
7	MG	D	9001	1/1	0.97	0.15	67,67,67,67	0
6	ZN	N	7113	1/1	0.98	0.10	87,87,87,87	0
6	ZN	D	7058	1/1	0.98	0.07	109,109,109,109	0
6	ZN	D	7112	1/1	0.99	0.14	75,75,75,75	0
6	ZN	N	7059	1/1	0.99	0.11	100,100,100,100	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.