



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 11:24 pm BST

PDB ID : 3EQL
Title : Crystal structure of the T. Thermophilus RNA polymerase holoenzyme in complex with antibiotic myxopyronin
Authors : Vassilyev, D.G.; Vassilyeva, M.N.; Artsimovitch, I.
Deposited on : 2008-09-30
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

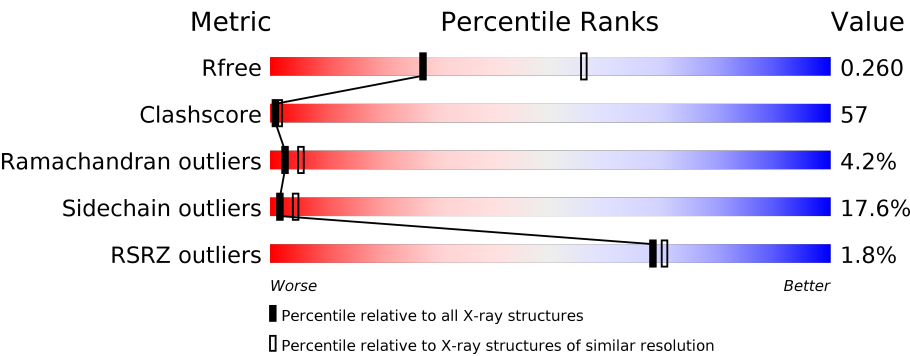
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	<div><div></div><div><div>18%</div><div>44%</div><div>10%</div><div>27%</div></div></div>
1	B	315	<div><div>3%</div><div><div>19%</div><div>44%</div><div>9%</div><div>27%</div></div></div>
1	K	315	<div><div></div><div><div>20%</div><div>42%</div><div>10%</div><div>27%</div></div></div>
1	L	315	<div><div>2%</div><div><div>17%</div><div>46%</div><div>9%</div><div>27%</div></div></div>
2	C	1119	<div><div>2%</div><div><div>25%</div><div>58%</div><div>16%</div></div></div>
2	M	1119	<div><div></div><div><div>24%</div><div>60%</div><div>15%</div></div></div>

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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>%24%51%11%•13%</div></div>
3	N	1524	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>%25%49%11%•13%</div></div>
4	E	99	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>2%21%61%11%••</div></div>
4	O	99	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>2%22%60%12%••</div></div>
5	F	423	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>%25%45%11%•18%</div></div>
5	P	423	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>2%27%44%9%•18%</div></div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 57340 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 subunit alpha.

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 subunit beta.

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 subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1321	Total	C	N	O	S	0	0	0
			10407	6585	1845	1944	33			
3	N	1321	Total	C	N	O	S	0	0	0
			10407	6585	1845	1944	33			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	95	Total	C	N	O	S	0	0	0
			770	491	133	142	4			
4	O	95	Total	C	N	O	S	0	0	0
			770	491	133	142	4			

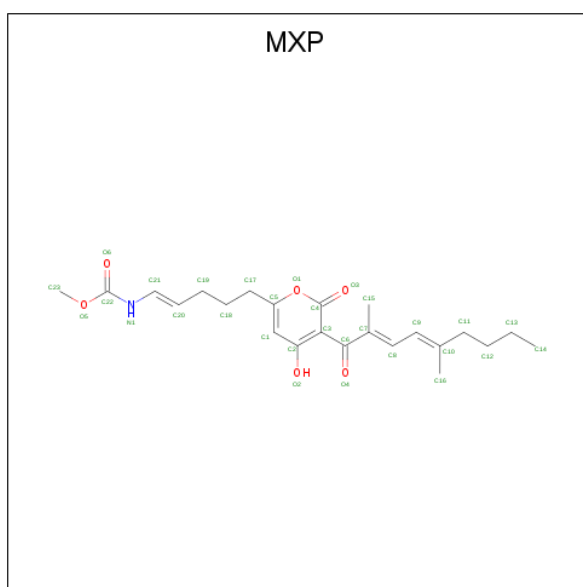
- Molecule 5 is a protein called RNA polymerase sigma factor rpoD.

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 Myxopyronin B (three-letter code: MXP) (formula: C₂₃H₃₁NO₆).



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

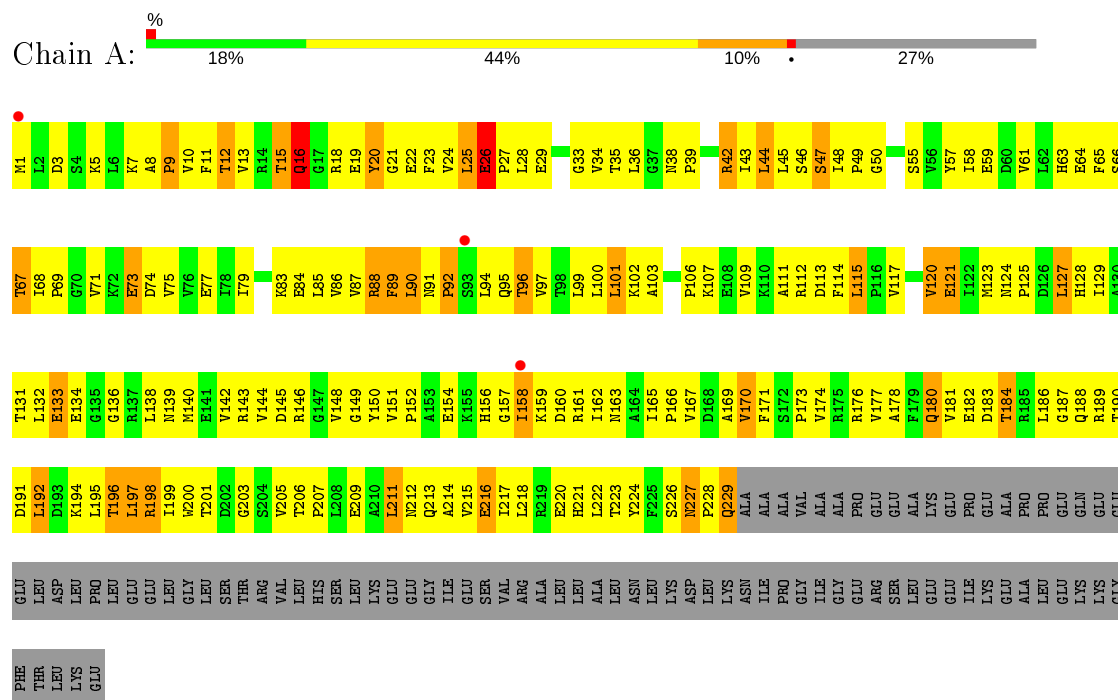
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	141	Total O 141 141	0	0
9	B	149	Total O 149 149	0	0
9	C	704	Total O 704 704	0	0
9	D	927	Total O 927 927	0	0
9	E	82	Total O 82 82	0	0
9	F	305	Total O 305 305	0	0
9	K	152	Total O 152 152	0	0
9	L	148	Total O 148 148	0	0
9	M	680	Total O 680 680	0	0
9	N	864	Total O 864 864	0	0
9	O	84	Total O 84 84	0	0
9	P	260	Total O 260 260	0	0

3 Residue-property plots

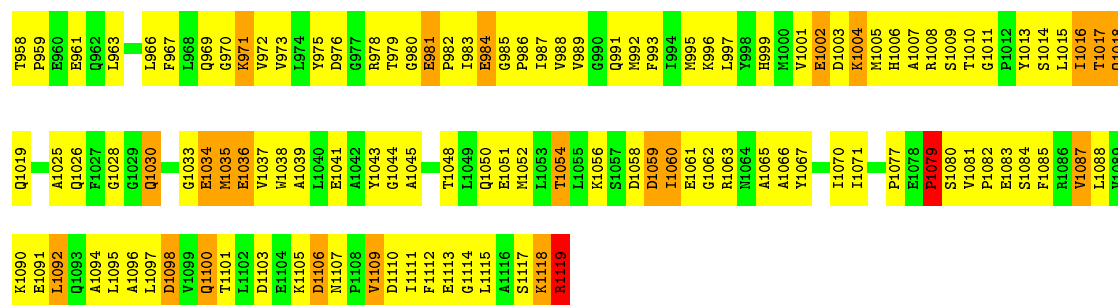
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 subunit alpha

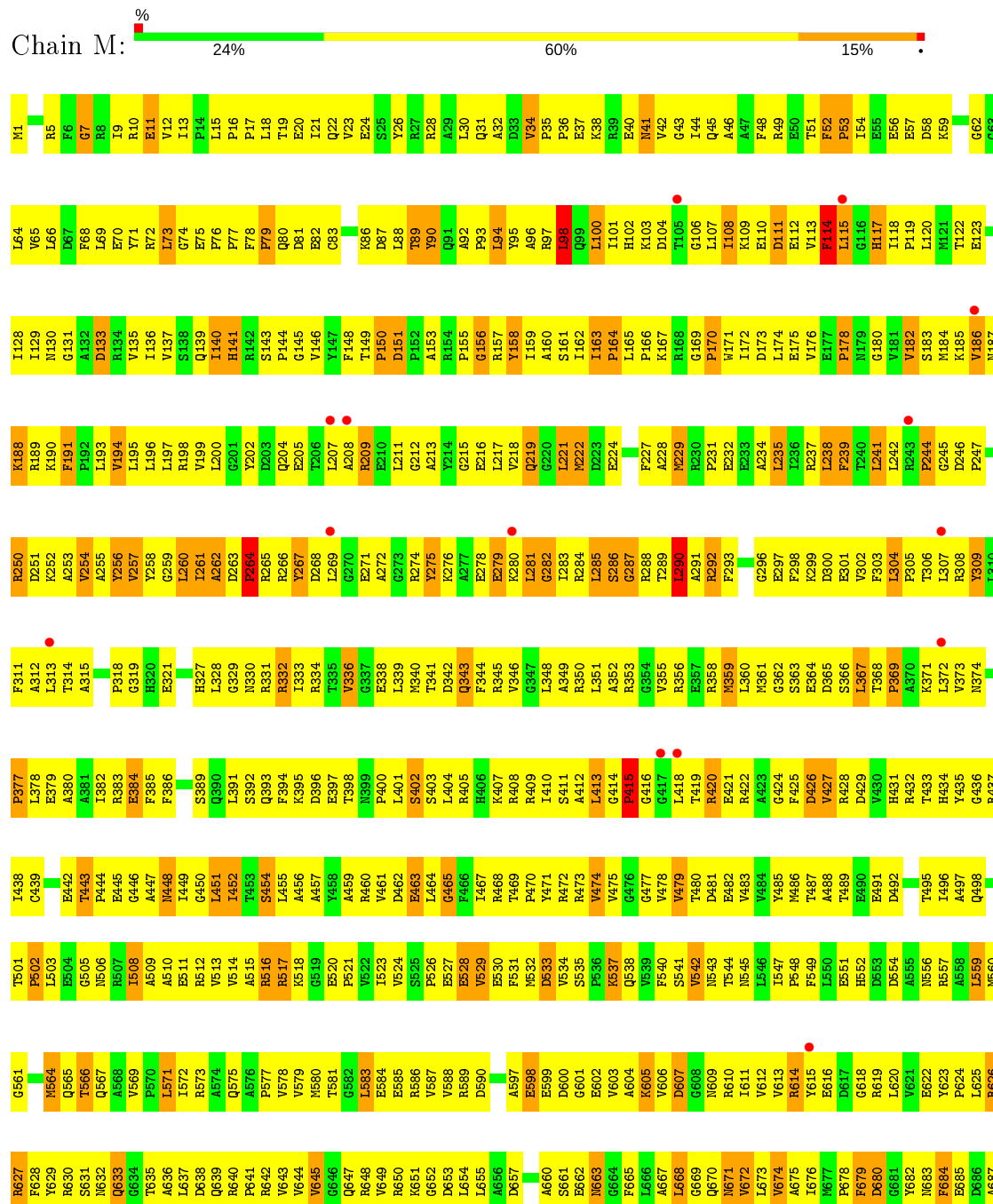


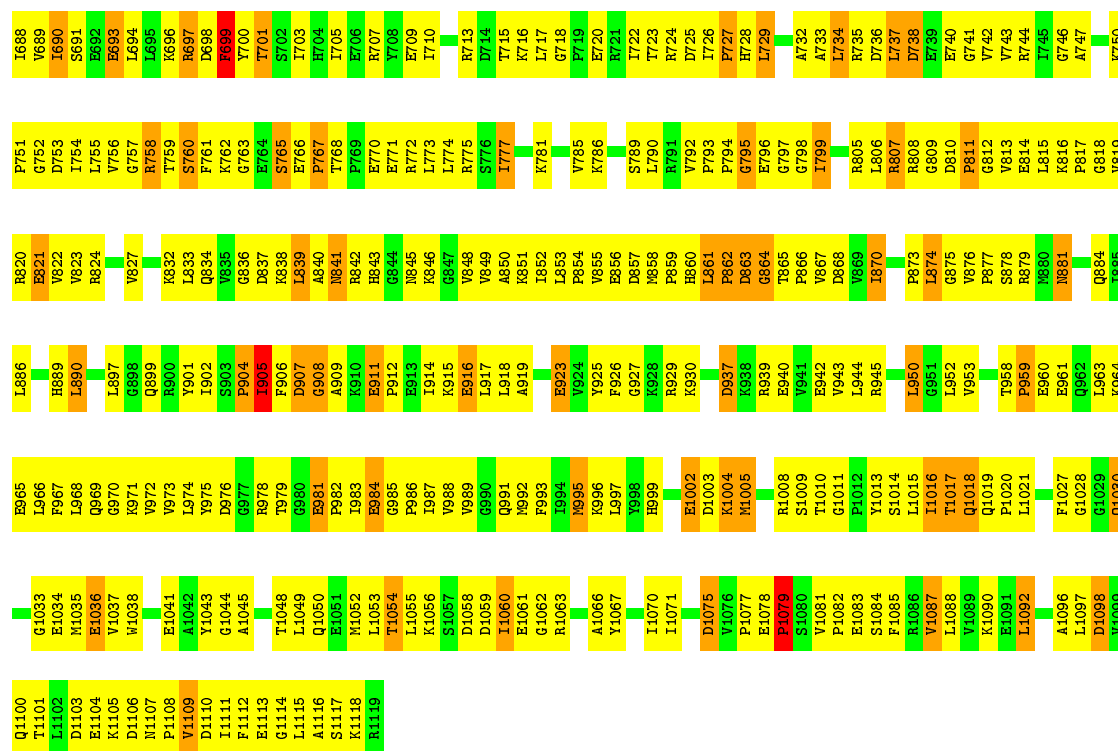


E887	E821	G752	I690	Y629	M564	A497	H434	V373	R308	P247	K185	T122	G62	H1
H888	V822	D753	S691	R630	Q565	Q498	V435	R374	Y309	R250	V186	EL23	G63	E2
H889	S631	L754	E693	S831	T566	T501	R437	R376	F311	R251	K188	D124	L64	I3
L890	R824	L755	E692	N632	Q567	P502	R438	R377	A312	K252	K189	S126	V65	K4
	V827	G757	L695	G634	A568	L503	Q439	L378	L313	A253	K190	G126	L66	R5
F886	A828	R758	K896	T835	V569	E504	P440	E379	T314	V254	F191	P127	D67	F6
L887	T759	S760	R697	A836	P570	G505	V441	A380		A255	F192	I128	F68	G7
G898	L637	D698	L637	D698	L571		A442	A381	V317	A256	F193	I129	L69	R8
Q899	K832	F761	F699	D638	S172	I508	T443	R382	P318	Y257	F194	G131	E70	I9
R900	L833	K762	R700	Q639	R573	A510	P444	R383		Y258	L195	A132	R72	R10
Y901	Q834	G763	T701	R640	A574	A510	G446	E321	E321	G259	L196	D133	L73	V11
I902	V836	S702	S702	P641	Q575	E511	A447	F384	V322	L260	L197	G174	G74	V12
S903	G836	S765	I703	R642	A576	R512	A447	F385			L198	V135	E75	F14
P904	D837	E766	H704	V643	P577	R513		F386	I325		R198	I136	P76	L15
I905	K838	F767	R705	V644	V578	V514	I449			A262	V199	V137	P77	P16
F906	L839	T768	E706	V645	V579	A515	I451	R390	L328	R265	G201	S138	F78	P17
D907	A840	R769	R707	G646	M580	R516	L451	L391	R264	R266	G202	Q139	F79	L18
G908	N841	E770	Y708	Q647	T581	R517	T452	S392	R331	Y267	D203	I140	Q80	T19
A909	R842	E771	E709	R648	G582	K518	T453	Q393	R332		Q204	H441	D81	E20
R910	H843	R772	I710	V649	L583	I523	S454	F394	I333	D268	E205	R142	S82	I21
E911	G844	L773	E711	R650	E584	E530	L455	K395	R334	L269	T206	S143	C83	Q22
P912	N845	L774	A712	K651	E585	P536	A456	D396	T335	G270	L207	P144	R84	V23
E913	K846	R775	R713	G652	R586	Q537	A457	E397	V336	A271	A208	G145	E85	E24
I914	G847	S776	D714	D653	V587	P526	V458	T398	G337	A272	R209	V146	K86	S25
K915	V848	I777	T715	L854	V588	E527	A459	R399	E338	G273	E210	Y147	D87	Y26
E916	V849	E780	K716	L855		E528	A459	P400	L339	R274	L211	F148	L88	Y26
L917	A850	E780	L717	A656	S591	V529	V461	L401	M340	Y275	G212	T149	T89	R28
I918	G851	G718	D657	D657	L592	E530	D462	S402	T341	K276	A213	P150	Y90	R28
K919	R852	V785	P719	G658		F531	E463	S403	D342	A277	Y214	D151	Q91	L30
L920	K853	K786	R720	P659	A597	M532	L464	L404	Q343	E278	G215		A92	Q31
A921	P854		E721	A660	E598	D533	G465	R405	F344	E279	E216	P155	P93	A32
F922	R855	S789	I722	S661	E599	V534	F466	H406	R345	K280	L217	G156	L94	D33
E923	E856	L790	R723	E662	D600	S535	L467	R407	V346	L281	V218	R157	Y95	V34
V924	R857	R791	R724	N663	G601	P536	R468	R408	G347	I282		G158	A96	P35
Y925	M858	V792	D725	G664	E602	K537	T469	R409	I283	I159		G159	R97	P36
F926	P859		I726	F665	V603	Q538	P470	L410	A349	N229	N222	A160	L98	E37
Q927	H860	G795	P727	L866	A604	V539	V471	S411	R350	L285	D223	S185	Q99	K38
	L861		H728	A667	R605	F540	R472	A412	L351	S286		I162	L100	R39
R928	L862	G798	L729	L668	V606	S541	R473	L413	A352	G287	V226	I163	I101	E40
R929	D863	I799	S730	G669	D607	V542	V474	G414	R353	R288	F227	P164	H102	N41
K930	G864		E731	Q670	G608	N543	V475	P415	G354	T289	A228	L165	V42	G43
	T865	R802	A732	N671	N609	T544	G476	G417	V355	L290	N229	D104	D104	G43
P866	V867	A733	V672	V672	R610	N545	G477		R356	A291	R230	T105	T105	I44
D868	L806	L734	V674	L946	I611	L946	V478	L418	E357	R292	P231	G169	G106	Q45
R869	R807	D736	A675	V612	V612	S547	V479	T419	R358	F293	E232	P170	L107	Q46
E940	R808	R808	R614	R614	R614	P548	T480	R420	M359	E294	E233	W171	I108	A47
V941	G809	D738	L737	V615	V615	F549	D481	E421	L360	D295	A234	I172	K109	F48
						L550	P482	R422	M361	G296	L235	D173	E110	R49
E942	D810	E739	V671	E551	E551	L550	V483	A423	G362	E297	T236	L174	D111	P50
V943	P811	E740	D680	H552	H552	H552	V484	G424	S363	F298	R237	E175	E112	T51
L944	G812	G741	G681	D553	D553	D553	V485	F425	E364	R299	L238	V176	V113	F52
R945	V813	V742	V621	D554	D554	D554	M486	D426	D365	D300	F239	E177	F114	F53
R946	E814	V743	N683	E622	A555	A555	T487	V427	S366	E301	T240	P178	F114	I54
S878	L815	F684	G684	V623	N556	N556	A488	R428	S367	V302	L241	G1179	G116	E45
R879	K816	I745	E685	P624	R557	R557		D429	T368	F303	L242	G180	H117	E56
L860		G746	D686	L625	A553	A553	E491	V430	P369	L304	R243	V181	I118	E57
G851			D687	R626	R626	R626		A431	A370	P305	P244	V182	P119	D58
L952			A687	R627	L559	L559	T495	R432	K371	G245		S183	L120	K59
V953			I688	V627	M560	M560		T433	L372	L307	D246	M184	M121	
	Q884	R820	P751	V689	F628	G561	I496							

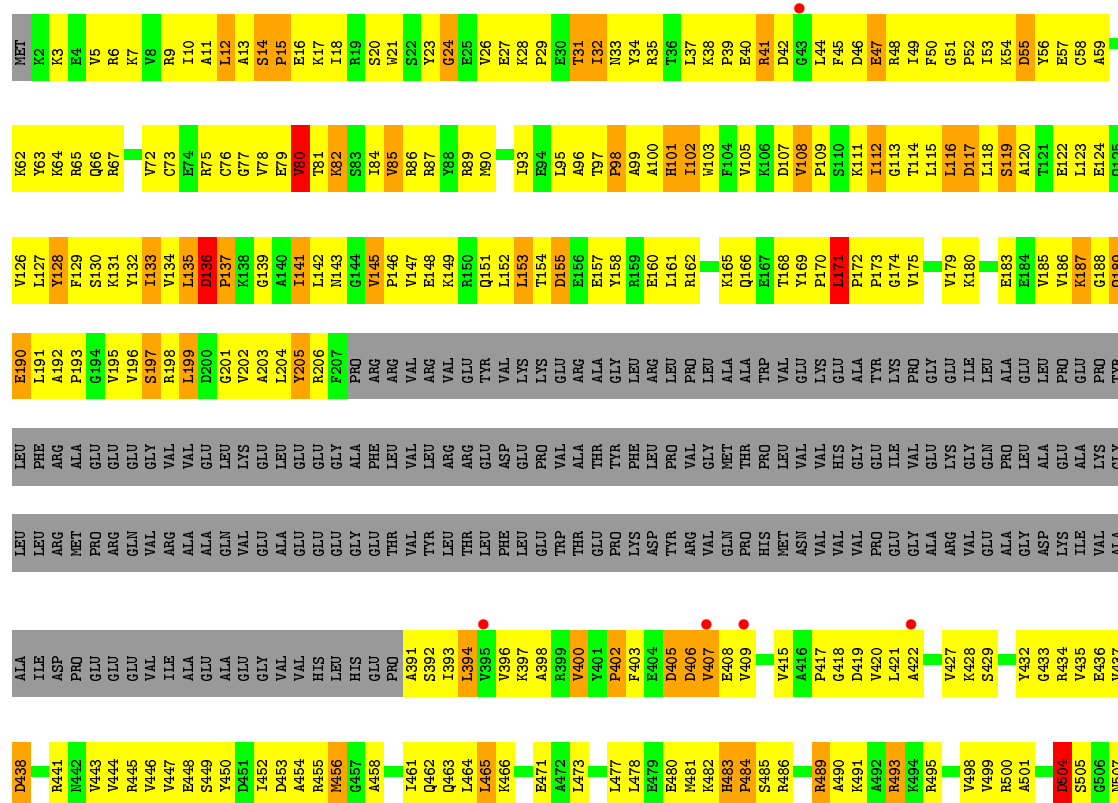


• Molecule 2: DNA-directed RNA polymerase subunit beta





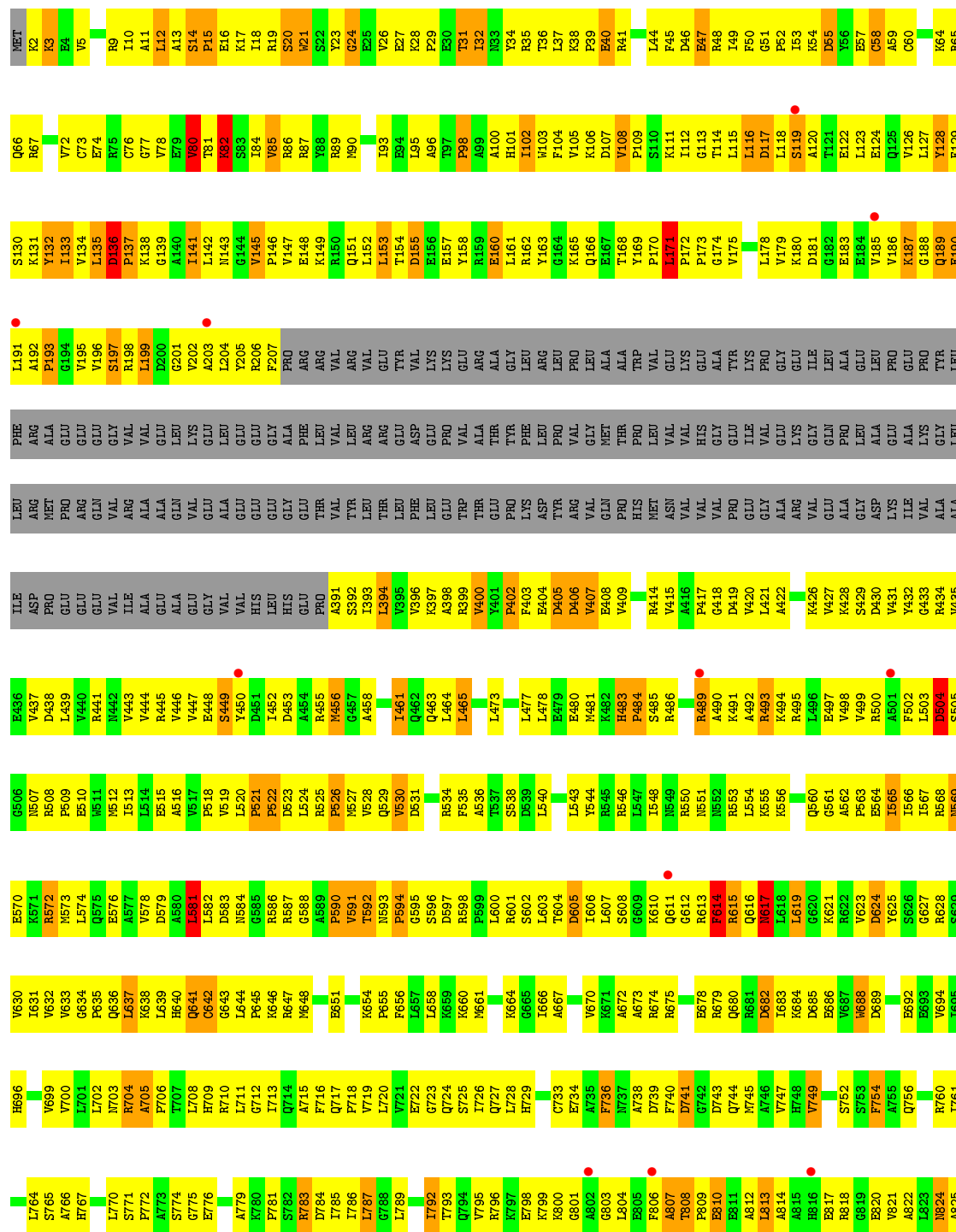
• Molecule 3: DNA-directed RNA polymerase subunit beta'

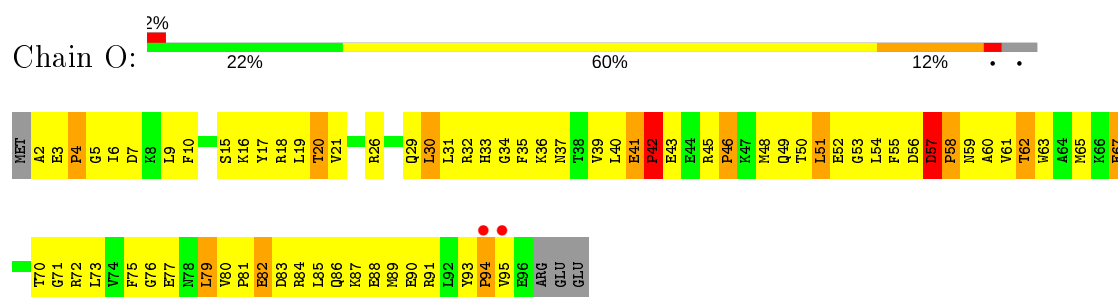


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K1412	E1351	E1284	G1222	V1155	G1092	I1031	V956	E888	A822	E758	I695	V633	R572	P509
T1413	I1352	E1285	I1223	E1156	Y1093	Q1032	I956	E889	L823	A759	G697	G634	M570	E510
P1414	Q1353	T1286	V1224	R1159	L1094	Q1033	P957	A899	R824	R760	G697	P635	L574	M511
V1415	K1354			L1160	T1095	Q1034	E958	V890	A825	I761	K698	Q636	Q575	M512
V1416	V1355		S1228	E1161	K1096	I1035	E959	E891	A826	Q762	V699	L637	E576	I513
V1417	V1356		I1229		K1097	R1036	K960	E892	R827	A763		K638	A577	L514
K1418	R1357		G1230		L1098	Q1037		E893	K828	L764	L702	L639	A578	E516
P1419	F1293		G1231		Y1099	L1038	Y963	E894	R829	S765	R703	H640		A516
L1420	Q1358		E1231		D1100	C1039	L964	R895	A830	A766	R704	Q641	L581	P517
E1294	E1295		P1232		V1101	G1040	E965	A896	G831	H767	A705	C642	L582	P518
M1422	T1234		G1233		T1102	G1041	E966	E897	G832	N768	P706	G643	D583	V519
G1423	L1361		L1235		H1103	R1042	D968	E898	E833	L769	T707	L644	N584	L520
V1424	L1362		L1236		E1104	G1043		L899	T834	L770	L708	P645	G585	P521
T1425	K1363		T1237		I1105	L1044	L972	I900	S835	S771	H709	R646	R586	P522
K1426	D1364		M1238		V1106	M1045		Q901	V836	A766	R710	R647	D523	E523
S1427	K1365		R1239		L1174	Q1046	E975	L902	G837	A773	G712	M648	G588	L524
A1428	H1367		T1240		R1108	K1047			R838	S774	G712	A649	A589	R525
L1429	F1241		R1241		E1109	P1048	M880	Q906	L839	G775	I713	L650	P590	P526
S1430	P1305		H1242		A1110	S1049		E907	K840	E776	Q714		E591	M527
T1431	K1307		E1243		D1111	G1050	L983	E908	T841	P777	A715		T592	V528
K1432	E1308		G1244		C1112	E1051	T984		H842	L778	F716	K654	N593	Q529
S1433	V1372		L1245		G1113	T1052	D985		F843		Q717	P655	P594	V530
V1434	R1373		V1246		T1114	F1053			F843		Q717	F656	G595	D531
	G1374		A1247		T1115		E887	I912	A844	F781	V719	L657	G596	G532
	M1375		G1248		N1116	P1056	R888	I914	R845	R783	L720	L658	D597	G533
	K1376		A1249		I1117	V1057	Y989	Y915	D847	D784	V721	K659	P599	R534
	K1377		L1250		L1118	R1058	Y990	Y916	E848	T785	E722	R660	G598	F535
	N1442		D1251		R1189	S1059	Q991		A849	T786	G723	M661	L600	L600
T1443	V1378		L1252		S1119	S1060	I992	L920	L850	L787	Q724	E662	R601	T537
T1444	E1380		T1253		P1121	F1061	L993	L921	L851	G788	S725	E663	S602	S638
	V1381		Q1254		L1122	R1062	Q994	L922	A852	L789	I726	K664	L603	D539
	T1448		G1255		F1123	E1063	L995	G923	V858		Q727	G665	T604	L540
E1449	P1384		L1256		C1201	G1064	M996	E925	L728		H729	I666	D605	L543
A1450	K1385		P1257		P1125	L1065	T997	E926	R924		P730	A667	I606	Y544
A1451	G1386		V1258		D1126	T1066	E998	I926	D859	V795	L731	V670	S608	R545
	S1387		R1259		E1127	V1067	T999	T927	L860	R796	V732	K671	G609	R546
K1455	R1388		E1261		V1128	L1068	T1000	A928	Q861	K797	C733	A672	K610	L547
K1456	L1389		L1262		T1129	E1069	E1001	I929	D862	E798		A673	Q611	L548
D1457	L1390		F1263		R1130	Y1070	K1002	L931	V864	K799		R674	G612	N549
			E1264		L1132	F1071	V1003	D932	T865	Q801	F736	R675	R613	R550
			A1265		R1133	I1072	A1006		V866	A802	A738	M676	F614	N551
			R1266		L1134	S1073	V1007	I935	R867	G803	D739	L677	R615	
			A1267			H1075	F1008		Y868	L804	F740	E678	Q616	L584
			P1268		R1137	G1076	K1009	Y937		E805	D741	R679	N617	K555
			K1269		A1138	A1077	N1010	G938					L618	
			A1270		D1139	R1078			K871				L619	L588
			R1271		I1140	K1079		F941	R872	L873	D743	R681	G620	A559
			S1210		E1141	G1080	P1019	S942	E874	T808	Q744	D682	K621	Q560
			M1211		A1142	G1081	L1020	T943	T875	P809	M745	I683	R622	G561
			A1212		L1143	A1082	I1021	T944	S876	E811	V746	D685	G623	A562
			E1275		L1144	D1083	M1022	S945	P877	H748	H748	E686	P563	E564
			P1214		V1145	T1084	M1023	G946	G878	L813	P749	V687	Y625	P563
			L1277		K1146	A1085	A1024	I947	R879	A814	P750	W688	S626	I565
			S1216		R1147	L1086	Q1025	T948	T880			D689	G627	I566
			L1217			R1087	S1026	I949	L861			A690	R628	I567
			G1218		R1151	T1088	A1027	G950	F882	E817	S753		R628	I567
			E1152		E1152	L1088	A1028	G950	F882	R818	F754	L691	S629	R568
			A1153		V1153	D1090	R1029	D952	R894	E820	Q756	E593	N569	E570

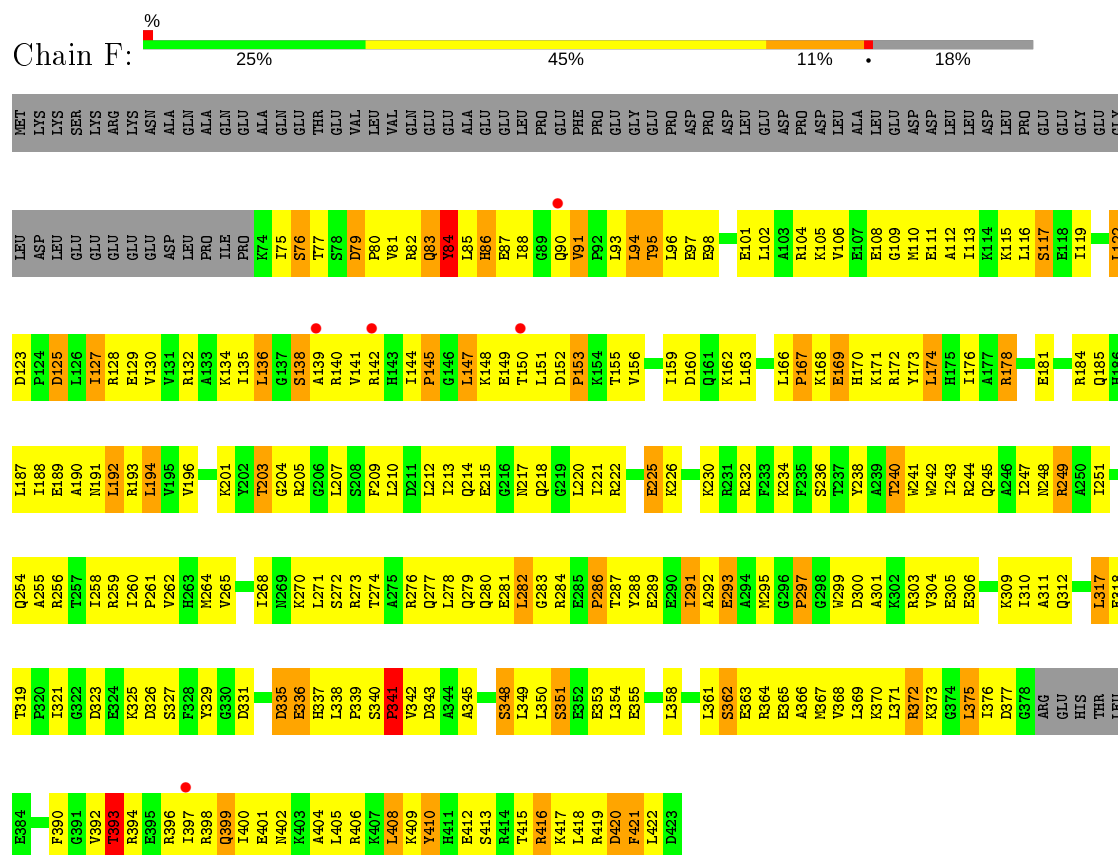


• Molecule 3: DNA-directed RNA polymerase subunit beta'

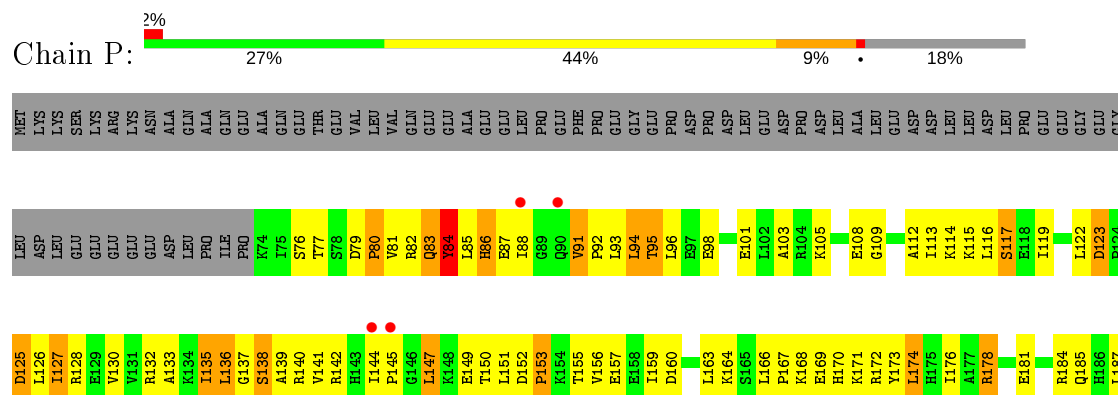




- Molecule 5: RNA polymerase sigma factor rpoD



- Molecule 5: RNA polymerase sigma factor rpoD



R393	R394	R395	R396	R397	R398	R399	I400	E401	N402	K403	A404	L405	R406	K407	L408	K409	Y410	R411	E412	S413	R414	R415	D416	D417	D418	D419	D420	F421	L422	D423	R259	I260	P261	V262	E263	M264	V265	E266	T267	L268	P269	K270	L271	T274	A275	R276	Q277	L278	Q279	Q280	E281	L282	G283	R284	E285	P286	T287	V288	E289	E290	I291	I292	A293	M295	G296	P297	G298	V299	D300	R303	V304	E305	E306	K309	I310	A311	Q312	V315	H316	L317	E318	I321	K325	P326	R327	R328	R329	R330	R331	R332	R333	R334	R335	R336	R337	R338	R339	R340	R341	R342	R343	S348	L349	K350	S351	E352	E353	L354	E355	K356	L357	L358	S359	K360	L361	E362	E363	R364	R365	A366	K367	V368	L369	K370	L371	R372	K373	G374	L375	L376	G377	ANG	GLU	HIS	THR	LEU	E384	E385	F390	G391	V392	I188	E189	A190	N191	L192	R193	L194	V195	K200	T203	G204	R205	G206	L207	S208	F209	L210	D211	L212	L213	Q214	E215	G216	N217	Q218	G219	L220	I221	A222	E223	V224	E225	K226	R232	F233	K234	F235	S236	T240	V241	V242	L243	R244	Q245	E246	I247	N248	R249	L250	L251	Q254	A255	R256	T257	L258
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4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	235.00Å 235.00Å 254.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.70 39.96 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.7 (40.00-2.70) 90.4 (39.96-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.240 , 0.270 0.238 , 0.260	Depositor DCC
R_{free} test set	18510 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	47.8	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 71.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.166 for -h,-k,l 0.048 for h,-h-k,-l 0.047 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	57340	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.84	2/1838 (0.1%)	1.04	9/2498 (0.4%)
1	B	0.74	1/1838 (0.1%)	0.95	9/2498 (0.4%)
1	K	0.81	2/1838 (0.1%)	1.00	8/2498 (0.3%)
1	L	0.75	1/1838 (0.1%)	0.96	10/2498 (0.4%)
2	C	0.73	0/8997	0.94	14/12164 (0.1%)
2	M	0.73	0/8997	0.94	14/12164 (0.1%)
3	D	0.75	2/10582 (0.0%)	0.97	15/14294 (0.1%)
3	N	0.75	1/10582 (0.0%)	0.97	18/14294 (0.1%)
4	E	0.73	0/784	1.23	5/1057 (0.5%)
4	O	0.71	0/784	1.08	3/1057 (0.3%)
5	F	0.65	0/2812	0.85	3/3781 (0.1%)
5	P	0.65	0/2812	0.86	2/3781 (0.1%)
All	All	0.74	9/53702 (0.0%)	0.96	110/72584 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	N	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	26	GLU	C-O	-11.04	1.02	1.23
1	K	26	GLU	C-O	-10.57	1.03	1.23
1	B	26	GLU	C-O	-10.23	1.03	1.23
1	L	26	GLU	C-O	-9.82	1.04	1.23
1	A	16	GLN	CB-CG	5.82	1.68	1.52
1	K	16	GLN	CB-CG	5.80	1.68	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	407	VAL	CB-CG2	-5.45	1.41	1.52
3	D	733	CYS	CB-SG	-5.41	1.73	1.81
3	D	407	VAL	CB-CG2	-5.33	1.41	1.52

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	94	PRO	CA-N-CD	-18.30	85.89	111.50
1	B	138	LEU	CA-CB-CG	12.41	143.84	115.30
1	L	138	LEU	CA-CB-CG	12.19	143.33	115.30
4	O	94	PRO	CA-N-CD	-9.89	97.65	111.50
1	K	26	GLU	CA-C-N	9.51	143.72	117.10
1	A	26	GLU	CA-C-N	9.00	142.30	117.10
3	N	1411	GLY	N-CA-C	-8.94	90.74	113.10
4	E	94	PRO	N-CA-C	8.91	135.26	112.10
3	D	1411	GLY	N-CA-C	-8.89	90.88	113.10
1	K	26	GLU	CA-C-O	-8.69	101.84	120.10
1	A	26	GLU	CA-C-O	-8.19	102.90	120.10
1	A	158	ILE	CG1-CB-CG2	-8.17	93.42	111.40
1	K	158	ILE	CG1-CB-CG2	-8.08	93.63	111.40
1	K	192	LEU	CA-CB-CG	7.83	133.31	115.30
1	A	42	ARG	NE-CZ-NH1	-7.74	116.43	120.30
3	D	614	PHE	CA-CB-CG	7.52	131.96	113.90
1	B	25	LEU	CA-CB-CG	7.34	132.17	115.30
3	N	581	LEU	CA-CB-CG	7.24	131.94	115.30
4	O	94	PRO	N-CA-C	7.03	130.37	112.10
1	L	26	GLU	CA-C-N	6.96	136.58	117.10
1	A	192	LEU	CA-CB-CG	6.92	131.22	115.30
5	F	136	LEU	CA-CB-CG	6.77	130.88	115.30
1	L	138	LEU	CB-CG-CD1	-6.65	99.70	111.00
3	D	637	LEU	CA-CB-CG	6.64	130.57	115.30
1	B	158	ILE	CB-CA-C	-6.64	98.33	111.60
1	L	25	LEU	CA-CB-CG	6.62	130.53	115.30
1	L	158	ILE	CB-CA-C	-6.57	98.47	111.60
1	A	197	LEU	CA-CB-CG	6.46	130.16	115.30
4	E	94	PRO	CA-CB-CG	-6.45	91.75	104.00
3	D	1207	TYR	CA-CB-CG	6.38	125.53	113.40
3	D	581	LEU	CA-CB-CG	6.38	129.98	115.30
5	P	84	TYR	CA-CB-CG	6.32	125.41	113.40
3	D	1109	GLU	CA-C-N	-6.30	103.34	117.20
3	N	813	LEU	CA-CB-CG	6.28	129.74	115.30
1	L	26	GLU	CA-C-O	-6.26	106.95	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	1109	GLU	C-N-CA	6.26	137.34	121.70
3	N	1389	LEU	CA-CB-CG	6.24	129.65	115.30
1	B	26	GLU	CA-C-N	6.23	134.55	117.10
3	D	171	LEU	CA-CB-CG	6.19	129.53	115.30
3	N	1207	TYR	CA-CB-CG	6.18	125.14	113.40
2	C	1119	ARG	CB-CA-C	6.17	122.75	110.40
3	N	80	VAL	CA-C-N	-6.13	103.70	117.20
2	C	114	PHE	CB-CG-CD1	6.13	125.09	120.80
3	N	1109	GLU	CA-C-N	-6.12	103.73	117.20
3	N	80	VAL	C-N-CA	6.05	136.82	121.70
3	D	1109	GLU	C-N-CA	6.04	136.79	121.70
1	B	138	LEU	CB-CG-CD1	-6.01	100.78	111.00
1	K	188	GLN	CA-CB-CG	-6.01	100.19	113.40
2	M	114	PHE	CB-CG-CD1	5.93	124.95	120.80
2	C	58	ASP	C-N-CA	5.91	136.48	121.70
2	C	100	LEU	CA-CB-CG	5.87	128.79	115.30
2	M	114	PHE	CB-CG-CD2	-5.83	116.72	120.80
2	M	503	LEU	CA-CB-CG	5.82	128.69	115.30
3	N	637	LEU	CA-CB-CG	5.82	128.68	115.30
3	N	572	ARG	NE-CZ-NH1	-5.81	117.40	120.30
4	E	94	PRO	N-CD-CG	5.78	111.87	103.20
3	D	80	VAL	CA-C-N	-5.77	104.50	117.20
2	M	58	ASP	C-N-CA	5.77	136.12	121.70
1	A	90	LEU	CA-CB-CG	-5.71	102.18	115.30
3	D	1389	LEU	CA-CB-CG	5.70	128.42	115.30
3	N	58	CYS	CA-CB-SG	5.69	124.25	114.00
2	C	728	HIS	CA-C-N	5.69	129.72	117.20
2	M	287	GLY	N-CA-C	-5.68	98.89	113.10
2	C	114	PHE	CB-CG-CD2	-5.68	116.83	120.80
2	M	571	LEU	CB-CG-CD2	-5.66	101.39	111.00
3	D	831	GLY	N-CA-C	-5.65	98.97	113.10
3	N	831	GLY	N-CA-C	-5.65	98.98	113.10
3	N	171	LEU	CA-CB-CG	5.63	128.25	115.30
1	L	188	GLN	CA-CB-CG	5.62	125.78	113.40
1	B	26	GLU	CA-C-O	-5.60	108.33	120.10
2	C	287	GLY	N-CA-C	-5.60	99.10	113.10
4	E	50	THR	C-N-CA	5.59	135.68	121.70
1	L	146	ARG	CA-CB-CG	5.58	125.69	113.40
5	P	136	LEU	CA-CB-CG	5.58	128.14	115.30
2	M	728	HIS	CA-C-N	5.58	129.48	117.20
4	O	50	THR	C-N-CA	5.53	135.51	121.70
1	K	90	LEU	CA-CB-CG	-5.50	102.66	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	198	ARG	C-N-CA	5.48	135.40	121.70
2	C	98	LEU	CA-CB-CG	5.48	127.90	115.30
3	N	198	ARG	C-N-CA	5.47	135.39	121.70
1	K	25	LEU	C-N-CA	-5.46	108.06	121.70
3	D	564	GLU	CA-CB-CG	-5.43	101.45	113.40
2	C	264	PRO	C-N-CA	-5.43	108.13	121.70
1	B	188	GLN	CA-CB-CG	5.41	125.31	113.40
5	F	84	TYR	CA-CB-CG	5.41	123.68	113.40
2	C	795	GLY	N-CA-C	-5.41	99.58	113.10
2	M	264	PRO	C-N-CA	-5.40	108.20	121.70
2	M	795	GLY	N-CA-C	-5.37	99.67	113.10
2	M	98	LEU	CA-CB-CG	5.37	127.64	115.30
1	A	188	GLN	CA-CB-CG	-5.35	101.63	113.40
3	N	21	TRP	CA-CB-CG	5.29	123.76	113.70
2	M	974	LEU	CA-CB-CG	5.26	127.39	115.30
1	B	146	ARG	CA-CB-CG	5.26	124.97	113.40
2	C	58	ASP	CA-C-N	-5.22	105.72	117.20
1	L	132	LEU	CA-CB-CG	5.21	127.29	115.30
2	M	58	ASP	CA-C-N	-5.20	105.77	117.20
1	L	2	LEU	CA-CB-CG	5.20	127.25	115.30
1	K	127	LEU	CA-CB-CG	5.17	127.20	115.30
5	F	377	ASP	CB-CG-OD2	5.17	122.96	118.30
3	D	41	ARG	NE-CZ-NH2	-5.17	117.72	120.30
3	D	80	VAL	C-N-CA	5.16	134.60	121.70
3	N	1351	GLU	CA-CB-CG	-5.16	102.05	113.40
2	C	260	LEU	CA-CB-CG	5.10	127.03	115.30
3	N	614	PHE	CB-CG-CD1	5.09	124.37	120.80
2	C	207	LEU	CA-CB-CG	5.09	127.01	115.30
1	A	25	LEU	C-N-CA	-5.07	109.03	121.70
2	M	728	HIS	C-N-CA	-5.05	109.07	121.70
1	B	132	LEU	CA-CB-CG	5.02	126.85	115.30
2	M	1027	PHE	CA-C-N	5.02	126.25	116.20
2	C	763	GLY	C-N-CA	-5.02	109.16	121.70

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	184	0
1	B	1806	0	1861	197	0
1	K	1806	0	1861	212	0
1	L	1806	0	1861	198	0
2	C	8829	0	8933	1145	0
2	M	8829	0	8933	1073	0
3	D	10407	0	10633	1296	0
3	N	10407	0	10633	1283	0
4	E	770	0	784	121	0
4	O	770	0	784	113	0
5	F	2771	0	2844	316	0
5	P	2771	0	2844	312	0
6	D	2	0	0	0	0
6	N	2	0	0	0	0
7	D	30	0	31	18	0
7	N	30	0	31	18	0
8	D	1	0	0	0	0
8	N	1	0	0	0	0
9	A	141	0	0	28	0
9	B	149	0	0	30	0
9	C	704	0	0	215	0
9	D	927	0	0	239	0
9	E	82	0	0	29	0
9	F	305	0	0	77	0
9	K	152	0	0	41	0
9	L	148	0	0	34	0
9	M	680	0	0	180	0
9	N	864	0	0	235	0
9	O	84	0	0	26	0
9	P	260	0	0	71	0
All	All	57340	0	53894	6054	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 57.

All (6054) 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)
3:D:610:LYS:HD3	7:D:1527:MXP:C15	1.49	1.41
3:N:610:LYS:HD3	7:N:1527:MXP:C15	1.55	1.37
3:N:136:ASP:HB3	3:N:137:PRO:HD3	1.27	1.15
3:D:136:ASP:HB3	3:D:137:PRO:HD3	1.27	1.13
3:D:610:LYS:HD3	7:D:1527:MXP:H15B	1.19	1.10
1:L:109:VAL:HG21	1:L:138:LEU:HD11	1.33	1.08
3:N:610:LYS:HD3	7:N:1527:MXP:H15	1.08	1.06
1:B:109:VAL:HG21	1:B:138:LEU:HD11	1.35	1.06
1:A:42:ARG:HH12	1:B:34:VAL:HB	1.00	1.06
2:M:877:PRO:HG2	3:N:1023:MET:HE2	1.27	1.06
3:D:611:GLN:HE22	3:D:1463:LYS:HE2	1.20	1.05
3:N:613:ARG:HG3	3:N:1441:GLN:HB2	1.39	1.04
3:N:101:HIS:HD1	3:N:103:TRP:HB2	1.21	1.04
3:N:180:LYS:HG2	3:N:183:GLU:HB2	1.35	1.04
2:C:395:LYS:HE2	2:C:403:SER:HB2	1.34	1.04
3:D:180:LYS:HG2	3:D:183:GLU:HB2	1.37	1.03
2:C:795:GLY:HA3	2:C:1004:LYS:HE2	1.41	1.02
3:D:1335:LEU:HD23	3:D:1344:VAL:HA	1.41	1.02
3:N:610:LYS:CD	7:N:1527:MXP:C15	2.37	1.02
3:D:187:LYS:HE2	3:D:199:LEU:HB3	1.42	1.02
1:K:67:THR:HG21	2:M:609:ASN:HD21	1.24	1.02
2:M:150:PRO:HA	2:M:158:TYR:HB3	1.40	1.01
3:N:100:ALA:HB2	3:N:513:ILE:HD13	1.41	1.01
2:C:1054:THR:HG21	2:C:1079:PRO:HB3	1.42	1.01
3:D:610:LYS:CD	7:D:1527:MXP:C15	2.38	1.01
1:A:7:LYS:HE2	1:A:186:LEU:HD11	1.42	1.01
4:E:94:PRO:HD3	9:E:180:HOH:O	1.60	1.00
1:K:7:LYS:HE2	1:K:186:LEU:HD11	1.40	1.00
3:N:1209:LEU:HD21	4:O:16:LYS:HD2	1.38	1.00
3:N:1160:LEU:HD11	3:N:1174:LEU:HD21	1.45	0.98
2:C:150:PRO:HA	2:C:158:TYR:HB3	1.42	0.98
3:D:907:GLU:HA	9:D:2416:HOH:O	1.65	0.97
3:N:148:GLU:HB3	3:N:151:GLN:HB2	1.43	0.97
2:C:2:GLU:HG3	2:C:899:GLN:HB3	1.46	0.97
3:D:1101:VAL:HG21	3:D:1424:VAL:HG22	1.44	0.96
1:A:152:PRO:HA	9:A:351:HOH:O	1.66	0.95
3:N:957:PRO:HG2	3:N:1007:VAL:HA	1.49	0.95
2:M:169:GLY:HA2	2:M:263:ASP:HB3	1.45	0.95
3:N:610:LYS:CD	7:N:1527:MXP:H15	1.96	0.95
1:K:42:ARG:HH12	1:L:34:VAL:HB	1.31	0.95
3:N:1405:GLU:O	3:N:1410:GLU:HA	1.67	0.95
3:D:148:GLU:HB3	3:D:151:GLN:HB2	1.49	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1465:ASN:HD21	3:N:1470:ARG:HD3	1.33	0.94
3:D:1393:GLN:HB2	3:D:1398:TRP:HE1	1.32	0.94
1:A:42:ARG:NH1	1:B:34:VAL:HB	1.82	0.94
3:D:581:LEU:HD12	3:D:603:LEU:HD11	1.50	0.94
2:C:12:VAL:HG21	2:C:472:ARG:HD3	1.48	0.94
5:P:268:ILE:HA	5:P:271:LEU:HD12	1.49	0.94
1:A:42:ARG:HH12	1:B:34:VAL:CB	1.80	0.93
1:L:152:PRO:HD2	1:L:155:LYS:HD3	1.46	0.93
3:D:18:ILE:HG23	3:D:518:PRO:HG3	1.50	0.93
2:C:862:PRO:HA	2:C:975:TYR:HE1	1.32	0.93
2:C:890:LEU:HA	2:C:914:ILE:HD11	1.50	0.93
5:P:361:LEU:HD22	5:P:366:ALA:HB2	1.48	0.93
2:C:66:LEU:HD22	2:C:372:LEU:HD23	1.52	0.92
3:D:957:PRO:HG2	3:D:1007:VAL:HA	1.52	0.92
2:M:757:GLY:HA2	2:M:789:SER:HB3	1.52	0.92
3:D:1194:CYS:HB2	9:D:1762:HOH:O	1.70	0.92
2:M:890:LEU:HA	2:M:914:ILE:HD11	1.52	0.92
3:D:610:LYS:HD3	7:D:1527:MXP:H15	1.52	0.92
2:M:1054:THR:HG23	2:M:1082:PRO:HG3	1.48	0.92
5:F:268:ILE:HA	5:F:271:LEU:HD12	1.51	0.91
3:N:581:LEU:HD12	3:N:603:LEU:HD11	1.51	0.91
3:D:611:GLN:HE22	3:D:1463:LYS:CE	1.84	0.91
2:M:437:ARG:CZ	2:M:488:ALA:HA	2.01	0.91
3:D:508:ARG:HG2	3:D:509:PRO:HD2	1.52	0.91
2:M:66:LEU:HD22	2:M:372:LEU:HD23	1.53	0.91
3:D:100:ALA:HB2	3:D:513:ILE:HD13	1.50	0.91
3:D:611:GLN:NE2	3:D:1463:LYS:HE2	1.84	0.91
3:N:675:ARG:HH12	5:P:421:PHE:HD2	1.15	0.91
2:M:409:ARG:HA	2:M:454:SER:HA	1.53	0.91
3:D:1405:GLU:O	3:D:1410:GLU:HA	1.71	0.90
2:C:41:ASN:HD22	2:C:41:ASN:H	1.16	0.90
2:M:862:PRO:HA	2:M:975:TYR:HE1	1.34	0.90
2:C:1114:GLY:H	2:C:1115:LEU:HD12	1.35	0.90
1:K:190:THR:HA	9:K:1309:HOH:O	1.70	0.90
3:D:520:LEU:HD12	3:D:521:PRO:HD2	1.53	0.90
3:D:406:ASP:HB3	5:F:168:LYS:HE2	1.54	0.89
3:D:87:ARG:HA	9:D:1713:HOH:O	1.71	0.89
1:B:152:PRO:HD2	1:B:155:LYS:HD3	1.54	0.89
3:N:18:ILE:HG23	3:N:518:PRO:HG3	1.54	0.89
1:A:24:VAL:HG22	1:A:196:THR:HB	1.54	0.88
3:D:204:LEU:HA	3:D:441:ARG:HH22	1.36	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:508:ARG:HG2	3:N:509:PRO:HD2	1.54	0.88
2:M:874:LEU:HD21	3:N:787:LEU:HD22	1.53	0.88
5:P:128:ARG:O	5:P:132:ARG:HG3	1.72	0.88
1:B:87:VAL:HG21	1:B:144:VAL:HG11	1.56	0.88
3:D:1383:ASP:HB2	3:D:1416:ALA:HB3	1.54	0.88
2:C:367:LEU:HA	2:C:371:LYS:HG3	1.53	0.88
2:C:1087:VAL:CG1	3:D:610:LYS:NZ	2.36	0.88
3:N:400:VAL:HG22	3:N:443:VAL:HG21	1.54	0.88
2:C:1054:THR:HG22	2:C:1059:ASP:HB2	1.52	0.88
5:P:205:ARG:HD2	5:P:251:ILE:HD13	1.56	0.88
2:C:191:PHE:HZ	2:C:196:LEU:HB2	1.37	0.88
3:N:165:LYS:HB2	3:N:397:LYS:HB3	1.56	0.88
2:C:431:HIS:HB3	2:C:434:HIS:HD2	1.39	0.88
2:C:1008:ARG:HH11	2:C:1028:GLY:HA2	1.39	0.88
2:C:952:LEU:HD12	2:C:969:GLN:HE22	1.35	0.88
5:F:128:ARG:O	5:F:132:ARG:HG3	1.74	0.88
1:L:184:THR:HG23	1:L:192:LEU:HB3	1.55	0.87
2:M:41:ASN:HD22	2:M:41:ASN:H	1.17	0.87
1:B:86:VAL:HG12	1:B:124:ASN:HD22	1.39	0.87
2:C:671:ASN:HD22	2:C:671:ASN:N	1.70	0.87
4:O:41:GLU:HA	4:O:45:ARG:HD3	1.57	0.87
3:N:131:LYS:HG2	3:N:568:ARG:HG2	1.56	0.87
1:L:194:LYS:HG2	9:L:1676:HOH:O	1.74	0.87
2:M:367:LEU:HA	2:M:371:LYS:HG3	1.57	0.87
3:N:1406:ARG:HA	3:N:1410:GLU:HG2	1.56	0.87
3:N:1393:GLN:HB2	3:N:1398:TRP:HE1	1.40	0.87
1:L:132:LEU:HG	1:L:136:GLY:HA3	1.57	0.86
1:L:86:VAL:HG12	1:L:124:ASN:HD22	1.39	0.86
3:N:494:LYS:HA	9:N:1731:HOH:O	1.73	0.86
3:N:59:ALA:HB3	3:N:76:CYS:SG	2.14	0.86
3:N:116:LEU:HD21	3:N:464:LEU:HB3	1.56	0.86
1:A:20:TYR:HD2	1:A:21:GLY:N	1.72	0.86
2:C:121:MET:HA	9:C:1509:HOH:O	1.73	0.86
2:M:140:ILE:HD11	2:M:412:ALA:HA	1.56	0.86
2:M:762:LYS:HB2	2:M:786:LYS:HD2	1.55	0.86
2:M:597:ALA:HB2	2:M:655:LEU:HD21	1.56	0.86
1:L:94:LEU:HD21	1:L:119:ASP:HB2	1.55	0.86
3:N:1383:ASP:HB2	3:N:1416:ALA:HB3	1.56	0.86
1:K:222:LEU:HD21	1:L:218:LEU:HD23	1.58	0.86
3:N:1232:PRO:HB3	3:N:1361:VAL:HG21	1.58	0.85
3:N:489:ARG:HH22	3:N:1389:LEU:HD21	1.40	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:LEU:HD21	1:B:119:ASP:HB2	1.56	0.85
2:M:1054:THR:HG22	2:M:1059:ASP:HB2	1.58	0.85
3:N:187:LYS:HE2	3:N:199:LEU:HB3	1.56	0.85
3:N:201:GLY:HA2	3:N:396:VAL:O	1.74	0.85
5:P:291:ILE:HG21	5:P:304:VAL:HG11	1.57	0.85
3:D:201:GLY:HA2	3:D:396:VAL:O	1.76	0.85
3:D:400:VAL:HG22	3:D:443:VAL:HG21	1.57	0.85
2:C:1087:VAL:CG1	3:D:610:LYS:HZ1	1.87	0.85
5:F:205:ARG:HD2	5:F:251:ILE:HD13	1.56	0.85
3:N:204:LEU:HA	3:N:441:ARG:HH22	1.40	0.85
4:E:41:GLU:HA	4:E:45:ARG:HD3	1.56	0.85
2:M:302:VAL:HG12	9:M:1862:HOH:O	1.75	0.85
5:P:166:LEU:HB3	5:P:170:HIS:HB2	1.57	0.85
1:B:184:THR:HG23	1:B:192:LEU:HB3	1.57	0.85
2:C:1084:SER:HB2	7:D:1527:MXP:O4	1.76	0.85
3:D:561:GLY:HA3	5:F:184:ARG:HH12	1.42	0.85
3:D:1160:LEU:HD11	3:D:1174:LEU:HD21	1.57	0.85
2:M:710:ILE:HB	2:M:790:LEU:HD13	1.59	0.85
1:A:103:ALA:HB1	1:A:107:LYS:HE2	1.57	0.84
3:N:908:LYS:HB3	3:N:1027:GLY:HA3	1.58	0.84
1:B:58:ILE:HG22	1:B:137:ARG:HH21	1.41	0.84
3:D:59:ALA:HB3	3:D:76:CYS:SG	2.17	0.84
3:N:617:ASN:N	3:N:617:ASN:OD1	2.09	0.84
5:F:166:LEU:HB3	5:F:170:HIS:HB2	1.59	0.84
3:D:558:LEU:HD13	5:F:145:PRO:HB3	1.58	0.84
3:D:1232:PRO:HB3	3:D:1361:VAL:HG21	1.59	0.84
3:D:101:HIS:HD1	3:D:103:TRP:HB2	1.42	0.84
3:D:611:GLN:OE1	7:D:1527:MXP:H16B	1.78	0.84
4:O:95:VAL:HG13	9:O:1302:HOH:O	1.75	0.84
3:D:119:SER:HB2	3:D:123:LEU:HB2	1.59	0.84
4:E:25:LYS:HE2	9:E:136:HOH:O	1.78	0.83
2:M:733:ALA:HB2	3:N:679:ARG:NH2	1.93	0.83
1:B:158:ILE:HD11	1:B:166:PRO:HA	1.59	0.83
1:L:158:ILE:HD11	1:L:166:PRO:HA	1.60	0.83
3:D:1465:ASN:HD21	3:D:1470:ARG:HD3	1.43	0.83
2:C:461:VAL:HG13	2:C:465:GLY:HA2	1.58	0.83
4:O:54:LEU:HG	4:O:58:PRO:HG2	1.61	0.83
1:A:35:THR:HG21	1:B:43:ILE:HD11	1.58	0.83
2:C:1009:SER:HB2	3:D:651:GLU:O	1.78	0.83
2:M:18:LEU:HD23	2:M:404:LEU:HD21	1.59	0.83
2:M:1114:GLY:H	2:M:1115:LEU:HD12	1.42	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:108:VAL:HB	3:N:109:PRO:HD3	1.60	0.83
1:K:42:ARG:HH21	2:M:857:ASP:HB3	1.44	0.83
3:D:1466:VAL:HG23	3:D:1472:ILE:HD11	1.60	0.83
2:M:952:LEU:HD12	2:M:969:GLN:HE22	1.41	0.83
3:N:611:GLN:HG2	3:N:619:LEU:CD1	2.09	0.82
2:M:1005:MET:HE1	3:N:648:MET:HB2	1.61	0.82
1:B:132:LEU:HD13	1:B:138:LEU:HD12	1.61	0.82
5:F:291:ILE:HG21	5:F:304:VAL:HG11	1.59	0.82
2:C:148:PHE:HZ	2:C:281:LEU:HD13	1.43	0.82
1:L:87:VAL:HG21	1:L:144:VAL:HG11	1.59	0.82
3:N:520:LEU:HD12	3:N:521:PRO:HD2	1.61	0.82
3:N:615:ARG:HH21	3:N:1089:ALA:HB2	1.44	0.82
2:C:409:ARG:HA	2:C:454:SER:HA	1.61	0.82
2:C:877:PRO:HG2	3:D:1023:MET:HE2	1.59	0.82
2:C:114:PHE:HD1	2:C:114:PHE:H	1.25	0.82
3:D:1406:ARG:HA	3:D:1410:GLU:HG2	1.61	0.82
3:N:32:ILE:HA	9:N:1836:HOH:O	1.79	0.82
2:C:1044:GLY:HA3	4:E:17:TYR:HE1	1.45	0.82
3:D:614:PHE:CD1	3:D:617:ASN:HA	2.14	0.82
3:N:465:LEU:HD21	9:N:1664:HOH:O	1.80	0.82
2:M:571:LEU:HD21	2:M:700:TYR:HA	1.60	0.82
3:N:152:LEU:HD23	3:N:152:LEU:H	1.43	0.82
3:N:1057:VAL:HG13	3:N:1069:GLU:HB3	1.60	0.82
2:C:750:LYS:HG3	3:D:681:ARG:HH21	1.45	0.82
2:M:603:VAL:HG21	2:M:643:VAL:HG11	1.60	0.82
2:M:643:VAL:HG23	9:M:1789:HOH:O	1.80	0.82
2:C:874:LEU:HD21	3:D:787:LEU:HD22	1.61	0.81
3:N:119:SER:HB2	3:N:123:LEU:HB2	1.58	0.81
2:M:1054:THR:HG21	2:M:1079:PRO:HB3	1.62	0.81
3:N:1466:VAL:HG23	3:N:1472:ILE:HD11	1.60	0.81
3:D:798:GLU:HB2	3:D:828:LYS:HE3	1.62	0.81
2:M:114:PHE:H	2:M:114:PHE:HD1	1.23	0.81
3:N:1115:THR:HB	9:N:1624:HOH:O	1.80	0.81
3:D:136:ASP:HB3	3:D:137:PRO:CD	2.10	0.81
3:N:136:ASP:HB3	3:N:137:PRO:CD	2.10	0.81
2:M:513:VAL:HB	9:M:1622:HOH:O	1.80	0.81
4:O:10:PHE:HE2	4:O:16:LYS:HG3	1.45	0.81
3:N:795:VAL:HG11	3:N:863:VAL:HG13	1.61	0.81
5:P:117:SER:HA	9:P:595:HOH:O	1.81	0.81
1:B:132:LEU:HG	1:B:136:GLY:HA3	1.60	0.80
2:C:169:GLY:HA2	2:C:263:ASP:HB3	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:860:HIS:HB2	9:C:1269:HOH:O	1.81	0.80
3:D:633:VAL:HG22	3:D:635:PRO:HD3	1.62	0.80
3:N:610:LYS:HD3	7:N:1527:MXP:H15B	1.58	0.80
3:N:843:PHE:HE1	3:N:864:VAL:HG11	1.44	0.80
2:C:436:GLY:O	2:C:459:ALA:HB2	1.81	0.80
3:D:592:THR:H	3:D:600:LEU:HD21	1.46	0.80
5:F:350:LEU:HD12	5:F:422:LEU:HD12	1.63	0.80
2:C:413:LEU:HD12	2:C:413:LEU:H	1.45	0.80
1:L:4:SER:HA	1:L:7:LYS:HE2	1.63	0.80
2:M:675:ALA:HA	2:M:989:VAL:HG12	1.63	0.80
3:N:699:VAL:H	3:N:756:GLN:NE2	1.80	0.80
3:D:1161:GLU:HG3	3:D:1164:ARG:HB2	1.64	0.80
2:M:599:GLU:HG3	2:M:600:ASP:H	1.46	0.80
2:M:786:LYS:HA	9:M:1657:HOH:O	1.80	0.80
3:N:1277:ILE:HD12	3:N:1301:LYS:HB2	1.63	0.80
3:N:135:LEU:HD11	9:N:2226:HOH:O	1.82	0.80
2:M:675:ALA:HB2	2:M:867:VAL:HG11	1.62	0.80
2:M:943:VAL:HG23	2:M:985:GLY:H	1.46	0.80
2:M:611:ILE:HD11	2:M:641:PRO:HG3	1.64	0.80
3:D:1220:ALA:HB1	3:D:1223:ILE:HD13	1.63	0.80
3:D:1223:ILE:HD12	3:D:1223:ILE:H	1.47	0.80
1:K:100:LEU:HB2	1:K:115:LEU:HD11	1.64	0.80
1:K:185:ARG:HA	9:K:1309:HOH:O	1.82	0.80
2:C:76:PRO:HB3	9:C:1229:HOH:O	1.83	0.79
3:D:1393:GLN:HB2	3:D:1398:TRP:NE1	1.96	0.79
3:D:890:VAL:HG11	3:D:922:LEU:HD13	1.64	0.79
1:K:87:VAL:HG21	1:K:144:VAL:HG11	1.64	0.79
1:L:55:SER:HB3	1:L:143:ARG:HB3	1.64	0.79
2:C:54:ILE:HD11	2:C:356:ARG:HG2	1.63	0.79
1:K:20:TYR:HD2	1:K:21:GLY:N	1.80	0.79
2:M:260:LEU:HB2	2:M:291:ALA:HB1	1.62	0.79
3:N:1095:THR:HG23	3:N:1230:GLY:HA3	1.62	0.79
5:P:132:ARG:HG2	5:P:181:GLU:OE1	1.81	0.79
3:N:613:ARG:NH2	3:N:1097:LYS:HE2	1.97	0.79
1:B:4:SER:HA	1:B:7:LYS:HE2	1.64	0.79
2:C:199:VAL:HG21	9:C:1705:HOH:O	1.82	0.79
2:M:1008:ARG:HH11	2:M:1028:GLY:HA2	1.47	0.79
1:A:87:VAL:HG21	1:A:144:VAL:HG11	1.63	0.79
4:E:94:PRO:CD	9:E:180:HOH:O	2.25	0.79
2:M:578:VAL:HG11	2:M:991:GLN:HB3	1.62	0.79
3:D:119:SER:H	3:D:123:LEU:HD22	1.46	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:1937:HOH:O	3:N:1068:LEU:HD11	1.82	0.79
3:N:783:ARG:NH1	3:N:1029:ARG:HG3	1.96	0.79
3:D:1095:THR:HG23	3:D:1230:GLY:HA3	1.64	0.79
2:M:774:LEU:HA	2:M:777:ILE:HD12	1.64	0.79
1:A:222:LEU:HD23	1:B:215:VAL:HB	1.64	0.79
2:C:512:ARG:HD3	2:C:523:ILE:HD11	1.65	0.79
3:D:162:ARG:HB3	9:D:2186:HOH:O	1.81	0.79
5:F:293:GLU:HB3	9:F:578:HOH:O	1.82	0.79
2:C:457:ALA:HB3	2:C:538:GLN:HA	1.65	0.78
2:C:675:ALA:HB2	2:C:867:VAL:HG11	1.64	0.78
4:E:54:LEU:HG	4:E:58:PRO:HG2	1.65	0.78
2:M:148:PHE:HZ	2:M:281:LEU:HD13	1.47	0.78
2:M:630:ARG:NH1	2:M:707:ARG:H	1.81	0.78
3:N:546:ARG:O	3:N:550:ARG:HG2	1.81	0.78
1:K:150:TYR:CE1	2:M:696:LYS:HA	2.19	0.78
1:K:206:THR:HG22	1:K:209:GLU:HG3	1.64	0.78
3:N:1273:VAL:HG22	3:N:1326:THR:OG1	1.84	0.78
3:N:798:GLU:HB2	3:N:828:LYS:HE3	1.65	0.78
2:C:256:TYR:CE1	2:C:293:PHE:HB2	2.18	0.78
2:C:474:VAL:HG11	2:C:529:VAL:HG12	1.64	0.78
2:M:571:LEU:HD21	2:M:700:TYR:HD2	1.47	0.78
3:N:493:ARG:HD2	3:N:1390:LEU:O	1.83	0.78
3:N:592:THR:H	3:N:600:LEU:HD21	1.47	0.78
4:O:46:PRO:HB3	4:O:54:LEU:HD22	1.64	0.78
2:M:413:LEU:H	2:M:413:LEU:HD12	1.48	0.78
3:N:630:VAL:HA	3:N:744:GLN:HG2	1.64	0.78
2:C:143:SER:HB2	2:C:276:LYS:HZ1	1.49	0.78
3:D:908:LYS:HB3	3:D:1027:GLY:HA3	1.64	0.78
3:D:1277:ILE:HD12	3:D:1301:LYS:HB2	1.65	0.78
5:F:85:LEU:HA	5:F:88:ILE:HD12	1.66	0.78
1:L:58:ILE:HG22	1:L:137:ARG:HH21	1.48	0.78
3:N:55:ASP:HB3	9:N:1551:HOH:O	1.84	0.78
1:A:88:ARG:HA	9:A:344:HOH:O	1.82	0.78
2:C:578:VAL:HG23	2:C:579:VAL:HG12	1.64	0.78
3:D:1198:TYR:HA	9:D:2099:HOH:O	1.83	0.78
2:C:1087:VAL:HG13	3:D:610:LYS:HZ1	1.48	0.78
2:M:862:PRO:HA	2:M:975:TYR:CE1	2.19	0.78
2:C:100:LEU:HD23	2:C:368:THR:HA	1.66	0.78
4:E:31:LEU:HD21	4:E:60:ALA:HB2	1.65	0.78
5:P:130:VAL:HG21	5:P:159:ILE:HG21	1.65	0.78
1:B:41:ARG:HG3	1:B:177:VAL:HG21	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:HIS:HA	1:B:224:TYR:HD2	1.46	0.78
2:C:178:PRO:HA	9:C:1213:HOH:O	1.82	0.78
2:C:470:PRO:HB2	2:C:534:VAL:HG21	1.65	0.78
3:N:1312:LEU:HB2	9:N:2368:HOH:O	1.84	0.78
2:C:312:ALA:HB1	2:C:318:PRO:HG2	1.65	0.77
2:M:12:VAL:HG12	2:M:534:VAL:HG13	1.64	0.77
3:N:1291:SER:HB2	3:N:1293:PHE:HE1	1.48	0.77
1:B:32:PHE:HB2	9:B:398:HOH:O	1.84	0.77
3:D:610:LYS:CD	7:D:1527:MXP:H15B	2.06	0.77
3:N:116:LEU:HD22	3:N:118:LEU:HD11	1.67	0.77
2:C:1083:GLU:HG2	9:D:1751:HOH:O	1.82	0.77
2:M:797:GLY:HA2	9:M:1828:HOH:O	1.83	0.77
1:A:186:LEU:HB2	1:A:192:LEU:HD11	1.67	0.77
3:D:116:LEU:HD21	3:D:464:LEU:HB3	1.66	0.77
3:D:615:ARG:O	3:D:617:ASN:N	2.17	0.77
1:A:9:PRO:HB2	1:B:224:TYR:HB3	1.67	0.77
3:D:403:PHE:HD1	3:D:405:ASP:O	1.67	0.77
2:C:163:ILE:HB	2:C:171:TRP:CH2	2.18	0.77
2:C:157:ARG:HD2	2:C:314:THR:HG22	1.67	0.77
2:C:597:ALA:HB2	2:C:655:LEU:HD21	1.64	0.77
2:M:115:LEU:HD22	2:M:373:VAL:HG11	1.64	0.77
3:N:32:ILE:HG22	5:P:258:ILE:HD12	1.66	0.77
2:C:766:GLU:HG2	2:C:772:ARG:HH12	1.50	0.77
3:D:400:VAL:CG2	3:D:443:VAL:HG21	2.15	0.77
2:M:512:ARG:HD3	2:M:523:ILE:HD11	1.65	0.77
2:M:87:ASP:HA	9:M:1651:HOH:O	1.83	0.77
3:D:1495:ILE:HG12	4:E:80:VAL:HG11	1.66	0.77
5:F:132:ARG:HG2	5:F:181:GLU:OE1	1.85	0.77
2:M:1115:LEU:HD23	3:N:85:VAL:HG13	1.65	0.77
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.67	0.77
3:D:1389:LEU:HD12	3:D:1390:LEU:H	1.49	0.77
2:M:431:HIS:HB3	2:M:434:HIS:HD2	1.48	0.77
3:N:1223:ILE:H	3:N:1223:ILE:HD12	1.49	0.77
5:P:142:ARG:HD2	9:P:502:HOH:O	1.85	0.77
5:P:144:ILE:HB	5:P:145:PRO:HD3	1.67	0.77
2:C:760:SER:HA	9:C:1430:HOH:O	1.85	0.76
3:D:135:LEU:HD23	9:D:1592:HOH:O	1.86	0.76
2:M:1019:GLN:HE22	3:N:621:LYS:HA	1.49	0.76
3:D:108:VAL:HB	3:D:109:PRO:HD3	1.66	0.76
3:D:1112:CYS:HB2	3:D:1195:GLN:HG2	1.67	0.76
3:D:630:VAL:HA	3:D:744:GLN:HG2	1.65	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:654:LYS:HB3	3:N:655:PRO:HD3	1.66	0.76
3:D:1191:PRO:HA	9:D:1762:HOH:O	1.86	0.76
3:D:478:LEU:HD21	3:D:500:ARG:NH2	2.01	0.76
2:C:468:ARG:HB2	2:C:486:MET:O	1.85	0.76
3:D:1057:VAL:HG13	3:D:1069:GLU:HB3	1.65	0.76
2:C:1103:ASP:OD1	3:D:3:LYS:HB2	1.85	0.76
1:L:60:ASP:HB2	1:L:137:ARG:CZ	2.16	0.76
3:N:611:GLN:HG2	3:N:619:LEU:HG	1.66	0.76
3:N:863:VAL:HG23	9:N:1635:HOH:O	1.85	0.76
3:D:1262:LEU:HD23	3:D:1352:ILE:HG13	1.66	0.76
3:D:152:LEU:HD23	3:D:152:LEU:H	1.50	0.76
5:F:260:ILE:HG23	5:F:264:MET:HB2	1.66	0.76
3:N:1040:GLY:O	3:N:1060:SER:HB3	1.85	0.76
2:M:914:ILE:HB	9:M:1825:HOH:O	1.85	0.76
2:C:862:PRO:HA	2:C:975:TYR:CE1	2.17	0.76
1:K:117:VAL:HB	1:K:120:VAL:HG12	1.66	0.76
3:N:1041:LEU:HD12	3:N:1058:ARG:HA	1.68	0.76
3:N:489:ARG:NH2	3:N:1389:LEU:HD21	2.00	0.76
3:D:544:TYR:O	3:D:548:ILE:HG12	1.85	0.76
5:F:144:ILE:HB	5:F:145:PRO:HD3	1.68	0.76
3:N:850:LEU:H	3:N:850:LEU:HD12	1.48	0.76
1:K:103:ALA:HB1	1:K:107:LYS:HE2	1.67	0.76
2:C:108:ILE:HB	2:C:368:THR:OG1	1.86	0.76
2:C:260:LEU:HB2	2:C:291:ALA:HB1	1.66	0.76
2:C:905:ILE:H	2:C:905:ILE:HD12	1.50	0.76
3:D:1205:TYR:CD2	3:D:1215:VAL:HG21	2.21	0.76
3:D:28:LYS:HG3	3:D:41:ARG:HH11	1.50	0.76
3:N:1094:LEU:O	3:N:1098:LEU:HD13	1.86	0.76
3:N:608:SER:HA	3:N:1443:THR:HG21	1.66	0.76
3:N:1495:ILE:HG12	4:O:80:VAL:HG11	1.66	0.76
4:O:31:LEU:HD21	4:O:60:ALA:HB2	1.67	0.76
5:F:155:THR:O	5:F:159:ILE:HG12	1.86	0.75
2:M:199:VAL:HG13	2:M:235:LEU:HG	1.66	0.75
3:N:1062:ARG:HB2	9:N:1637:HOH:O	1.84	0.75
3:N:400:VAL:CG2	3:N:443:VAL:HG21	2.17	0.75
3:N:637:LEU:HD21	3:N:642:CYS:HA	1.67	0.75
3:D:13:ALA:HA	9:D:1541:HOH:O	1.86	0.75
3:D:804:LEU:HB2	3:D:830:ALA:O	1.86	0.75
2:M:983:ILE:HG21	2:M:987:ILE:HD11	1.68	0.75
3:N:101:HIS:ND1	3:N:103:TRP:HB2	1.99	0.75
2:C:1081:VAL:HG21	2:C:1111:ILE:HG22	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:232:GLU:HA	2:C:235:LEU:HD12	1.67	0.75
2:M:163:ILE:HB	2:M:171:TRP:CH2	2.22	0.75
2:C:54:ILE:HG21	9:C:1578:HOH:O	1.86	0.75
2:M:534:VAL:HB	9:M:1660:HOH:O	1.87	0.75
2:M:18:LEU:HB2	2:M:590:ASP:HB3	1.69	0.75
3:N:100:ALA:HB2	3:N:513:ILE:CD1	2.16	0.75
5:P:139:ALA:HA	5:P:152:ASP:CG	2.06	0.75
5:P:155:THR:O	5:P:159:ILE:HG12	1.86	0.75
1:A:224:TYR:HB3	1:B:9:PRO:HB2	1.66	0.75
2:C:197:LEU:HD22	2:C:202:TYR:HD2	1.51	0.75
3:D:1040:GLY:O	3:D:1060:SER:HB3	1.86	0.75
2:M:129:ILE:HG12	2:M:386:PHE:HB3	1.68	0.75
2:M:671:ASN:HD22	2:M:671:ASN:N	1.83	0.75
2:M:691:SER:HB2	2:M:858:MET:SD	2.26	0.75
1:B:55:SER:HB3	1:B:143:ARG:HB3	1.68	0.75
3:D:508:ARG:HB3	9:D:1761:HOH:O	1.86	0.75
3:D:850:LEU:HD12	3:D:850:LEU:H	1.49	0.75
5:F:87:GLU:O	5:F:91:VAL:HG23	1.85	0.75
1:K:18:ARG:HH11	1:K:123:MET:HE2	1.52	0.75
2:C:325:ILE:HG23	9:C:1315:HOH:O	1.86	0.75
3:N:611:GLN:HE22	7:N:1527:MXP:H16B	1.50	0.75
5:P:132:ARG:O	5:P:136:LEU:HG	1.87	0.75
1:B:34:VAL:HG22	1:B:181:VAL:HG21	1.68	0.74
4:E:45:ARG:HE	4:E:55:PHE:HD2	1.33	0.74
3:N:611:GLN:HG2	3:N:619:LEU:CG	2.17	0.74
3:D:458:ALA:HB1	3:D:513:ILE:HD12	1.67	0.74
5:F:130:VAL:HG21	5:F:159:ILE:HG21	1.68	0.74
3:N:1101:VAL:HG22	3:N:1428:ALA:HB2	1.70	0.74
3:N:171:LEU:HG	9:N:1934:HOH:O	1.86	0.74
3:N:1420:LEU:HD12	3:N:1421:LEU:H	1.51	0.74
2:C:979:THR:HG23	2:C:981:GLU:H	1.52	0.74
3:D:1045:MET:HB2	3:D:1072:ILE:HG22	1.70	0.74
2:C:101:ILE:HG23	2:C:107:LEU:HD22	1.69	0.74
3:N:890:VAL:HG11	3:N:922:LEU:HD13	1.70	0.74
3:D:586:ARG:NH1	3:D:1444:THR:HG21	2.02	0.74
2:C:1056:LYS:O	3:D:624:ASP:HB2	1.87	0.74
5:F:274:THR:O	5:F:278:LEU:HG	1.88	0.74
1:K:221:HIS:HA	1:K:224:TYR:CD2	2.22	0.74
3:N:1264:GLU:HG3	3:N:1424:VAL:HG12	1.69	0.74
1:A:206:THR:HG22	1:A:209:GLU:HG3	1.69	0.74
1:K:226:SER:O	1:K:228:PRO:HD3	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1147:ARG:HB3	3:N:1188:VAL:HG21	1.68	0.74
3:D:1273:VAL:HG22	3:D:1326:THR:OG1	1.88	0.74
1:L:221:HIS:HA	1:L:224:TYR:HD2	1.51	0.74
2:M:139:GLN:OE1	2:M:415:PRO:HD2	1.88	0.74
3:N:1324:PRO:HA	9:N:1761:HOH:O	1.87	0.74
3:N:458:ALA:HB1	3:N:513:ILE:HD12	1.68	0.74
3:D:171:LEU:HB2	3:D:391:ALA:O	1.86	0.74
9:M:2128:HOH:O	3:N:1047:LYS:HE2	1.86	0.74
5:P:101:GLU:HB3	5:P:105:LYS:HE3	1.69	0.74
2:M:431:HIS:HB3	2:M:434:HIS:CD2	2.23	0.74
3:N:489:ARG:HG3	3:N:1388:ARG:HH22	1.53	0.74
1:B:201:THR:HG22	1:B:203:GLY:H	1.53	0.73
2:C:683:ASN:HA	2:C:687:ALA:HB3	1.70	0.73
9:C:1263:HOH:O	5:F:331:ASP:HA	1.88	0.73
3:N:206:ARG:HH12	5:P:98:GLU:HA	1.50	0.73
2:M:256:TYR:CE1	2:M:293:PHE:HB2	2.23	0.73
1:K:42:ARG:HH21	2:M:857:ASP:CB	2.00	0.73
3:N:1209:LEU:HD23	3:N:1211:MET:SD	2.28	0.73
2:C:1014:SER:HB3	2:C:1017:THR:O	1.88	0.73
2:C:222:MET:HB3	9:C:1633:HOH:O	1.88	0.73
1:B:176:ARG:HH21	3:D:850:LEU:HD13	1.53	0.73
3:N:37:LEU:HB3	9:N:1894:HOH:O	1.88	0.73
2:C:191:PHE:CZ	2:C:196:LEU:HB2	2.22	0.73
3:D:569:ASN:HB3	5:F:214:GLN:NE2	2.03	0.73
5:F:400:ILE:HG22	9:F:568:HOH:O	1.88	0.73
3:D:677:LEU:HD11	9:D:2185:HOH:O	1.88	0.73
4:E:46:PRO:HB3	4:E:54:LEU:HD22	1.71	0.73
1:K:22:GLU:HB3	9:K:1055:HOH:O	1.88	0.73
3:N:171:LEU:HB2	3:N:391:ALA:O	1.87	0.73
3:N:804:LEU:HB2	3:N:830:ALA:O	1.87	0.73
2:C:1008:ARG:HD2	2:C:1028:GLY:H	1.53	0.73
5:F:394:ARG:CZ	5:F:398:ARG:HB2	2.19	0.73
2:M:169:GLY:HA2	2:M:263:ASP:CB	2.19	0.73
2:C:654:LEU:HD11	2:C:663:ASN:ND2	2.03	0.73
3:D:477:LEU:HD11	3:D:495:ARG:HD3	1.69	0.73
1:L:213:GLN:O	1:L:217:ILE:HD12	1.88	0.73
1:B:60:ASP:HB2	1:B:137:ARG:CZ	2.19	0.73
2:C:109:LYS:HE2	2:C:111:ASP:OD1	1.88	0.73
5:P:112:ALA:HA	5:P:173:TYR:HD2	1.54	0.73
1:A:226:SER:O	1:A:228:PRO:HD3	1.89	0.73
2:C:431:HIS:HB3	2:C:434:HIS:CD2	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:603:VAL:HG21	2:C:643:VAL:HG11	1.69	0.73
2:M:431:HIS:CD2	2:M:433:THR:H	2.07	0.73
1:A:49:PRO:HB3	1:A:148:VAL:HG22	1.71	0.73
1:B:138:LEU:HD23	1:B:140:MET:SD	2.28	0.73
1:B:58:ILE:HG22	1:B:137:ARG:NH2	2.03	0.73
3:D:453:ASP:HB2	9:D:1592:HOH:O	1.87	0.73
2:M:232:GLU:HA	2:M:235:LEU:HD12	1.70	0.73
3:N:536:ALA:HA	5:P:315:VAL:O	1.88	0.73
2:C:42:VAL:HG12	2:C:43:GLY:H	1.54	0.72
2:C:943:VAL:HG23	2:C:985:GLY:H	1.54	0.72
3:D:80:VAL:HG23	9:D:1536:HOH:O	1.87	0.72
2:C:1010:THR:HG21	5:F:341:PRO:HB2	1.69	0.72
2:M:256:TYR:HE1	2:M:293:PHE:HB2	1.52	0.72
2:M:140:ILE:HA	2:M:332:ARG:O	1.88	0.72
1:B:36:LEU:O	1:B:39:PRO:HD2	1.90	0.72
2:M:738:ASP:HB2	2:M:744:ARG:HB3	1.70	0.72
5:P:260:ILE:HG23	5:P:264:MET:HB2	1.69	0.72
2:C:140:ILE:HD11	2:C:412:ALA:HA	1.71	0.72
3:D:705:ALA:HB3	3:D:706:PRO:HD3	1.70	0.72
5:F:394:ARG:HA	5:F:397:ILE:HD12	1.69	0.72
1:K:67:THR:CG2	2:M:609:ASN:HD21	1.98	0.72
1:L:80:LEU:HD12	9:L:3794:HOH:O	1.88	0.72
2:C:276:LYS:HB3	9:C:1337:HOH:O	1.87	0.72
2:C:115:LEU:HD22	2:C:373:VAL:HG11	1.70	0.72
2:M:139:GLN:NE2	2:M:418:LEU:HD22	2.04	0.72
2:M:437:ARG:NH2	2:M:488:ALA:HA	2.05	0.72
2:M:549:PHE:HB3	2:M:552:HIS:HD2	1.54	0.72
5:P:260:ILE:HD11	5:P:310:ILE:HG22	1.71	0.72
1:A:150:TYR:HE2	1:A:152:PRO:HG3	1.54	0.72
2:C:274:ARG:HD2	2:C:285:LEU:O	1.90	0.72
2:C:147:TYR:HE2	2:C:280:LYS:HZ3	1.36	0.72
2:C:768:THR:HB	2:C:771:GLU:HB3	1.71	0.72
2:C:904:PRO:HD2	2:C:908:GLY:HA2	1.72	0.72
3:D:400:VAL:HG12	9:D:2306:HOH:O	1.87	0.72
3:D:806:PHE:CE1	3:D:813:LEU:HB3	2.25	0.72
2:M:191:PHE:HZ	2:M:196:LEU:HB2	1.53	0.72
2:M:958:THR:HA	9:M:1887:HOH:O	1.89	0.72
3:N:808:THR:HB	3:N:809:PRO:HD3	1.70	0.72
3:N:570:GLU:N	5:P:214:GLN:HE22	1.88	0.72
2:C:1044:GLY:HA3	4:E:17:TYR:CE1	2.24	0.72
2:C:352:ALA:O	2:C:356:ARG:HG3	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:1115:LEU:HB3	3:N:85:VAL:HG13	1.71	0.72
3:N:1393:GLN:HB2	3:N:1398:TRP:NE1	2.04	0.72
3:N:572:ARG:HH12	5:P:79:ASP:CG	1.92	0.72
5:P:92:PRO:HB3	9:P:672:HOH:O	1.88	0.72
2:C:305:PRO:HA	2:C:308:ARG:HB2	1.70	0.72
1:A:10:VAL:HG12	1:A:12:THR:HG22	1.70	0.72
2:C:952:LEU:HD12	2:C:969:GLN:NE2	2.04	0.72
3:D:810:GLU:O	3:D:813:LEU:HG	1.88	0.72
2:C:603:VAL:HG12	9:C:1531:HOH:O	1.90	0.72
3:D:546:ARG:O	3:D:550:ARG:HG2	1.90	0.72
2:M:683:ASN:HA	2:M:687:ALA:HB3	1.71	0.72
1:B:97:VAL:HG11	1:B:120:VAL:HG21	1.72	0.71
3:D:1377:LYS:HA	9:D:2039:HOH:O	1.89	0.71
3:D:206:ARG:HH12	5:F:98:GLU:CA	2.03	0.71
5:F:218:GLN:HA	5:F:221:ILE:HD12	1.69	0.71
2:M:305:PRO:HA	2:M:308:ARG:HB2	1.70	0.71
2:M:535:SER:HB2	2:M:537:LYS:HE3	1.72	0.71
5:P:132:ARG:HD2	9:P:505:HOH:O	1.89	0.71
2:C:630:ARG:HA	9:C:1414:HOH:O	1.90	0.71
2:C:654:LEU:HD11	2:C:663:ASN:HD22	1.56	0.71
1:K:28:LEU:HD12	9:K:2517:HOH:O	1.88	0.71
2:M:31:GLN:HB3	2:M:71:TYR:OH	1.90	0.71
2:M:408:ARG:HH21	2:M:542:VAL:HG22	1.55	0.71
3:N:406:ASP:HB3	5:P:168:LYS:HE2	1.70	0.71
4:O:45:ARG:HG2	9:O:1147:HOH:O	1.90	0.71
3:D:1239:ARG:HG3	9:D:2068:HOH:O	1.91	0.71
5:F:139:ALA:HA	5:F:152:ASP:CG	2.11	0.71
3:N:705:ALA:HB3	3:N:706:PRO:HD3	1.73	0.71
5:P:204:GLY:HA3	9:P:572:HOH:O	1.89	0.71
1:K:150:TYR:HE1	2:M:696:LYS:HA	1.54	0.71
2:M:461:VAL:HG13	2:M:465:GLY:HA2	1.71	0.71
2:M:569:VAL:HG12	2:M:996:LYS:O	1.89	0.71
3:N:1210:SER:HA	9:N:1732:HOH:O	1.90	0.71
1:B:61:VAL:HG23	1:B:137:ARG:HH22	1.56	0.71
2:C:713:ARG:NH2	3:D:531:ASP:HB3	2.06	0.71
5:F:88:ILE:HG21	5:F:193:ARG:HD3	1.73	0.71
1:L:83:LYS:HE2	1:L:168:ASP:HB2	1.71	0.71
1:A:221:HIS:HA	1:A:224:TYR:HD2	1.55	0.71
2:C:685:GLU:N	9:C:1222:HOH:O	2.23	0.71
2:M:298:PHE:HA	9:M:2058:HOH:O	1.90	0.71
2:C:724:ARG:HG2	2:C:734:LEU:HD23	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:738:ASP:HB2	2:C:744:ARG:HB3	1.71	0.71
3:N:86:ARG:O	3:N:522:PRO:HD2	1.91	0.71
2:C:157:ARG:HA	9:C:1318:HOH:O	1.90	0.71
2:C:671:ASN:HD22	2:C:671:ASN:H	1.36	0.71
2:C:139:GLN:HE22	2:C:415:PRO:HD2	1.56	0.71
3:D:105:VAL:HG21	3:D:128:TYR:HE2	1.55	0.71
3:D:894:LYS:HA	9:D:1776:HOH:O	1.91	0.71
5:F:151:LEU:O	5:F:155:THR:HB	1.90	0.71
2:M:1021:LEU:HD21	5:P:332:PHE:O	1.91	0.71
2:M:420:ARG:HB2	9:M:1926:HOH:O	1.90	0.71
3:N:611:GLN:O	3:N:1439:SER:O	2.09	0.71
2:C:676:ILE:O	2:C:676:ILE:HG23	1.91	0.71
3:D:574:LEU:O	3:D:578:VAL:HG23	1.90	0.71
2:M:428:ARG:HE	2:M:451:LEU:HD21	1.54	0.71
2:M:551:GLU:HG3	2:M:552:HIS:CD2	2.25	0.71
3:N:15:PRO:HB3	9:N:1827:HOH:O	1.90	0.71
3:N:574:LEU:O	3:N:578:VAL:HG23	1.91	0.71
1:A:35:THR:HG21	1:B:43:ILE:CD1	2.21	0.70
2:C:83:CYS:HA	2:C:88:LEU:HB3	1.73	0.70
3:D:131:LYS:HG2	3:D:568:ARG:HG2	1.72	0.70
1:L:56:VAL:HG13	1:L:142:VAL:HG12	1.73	0.70
2:M:514:VAL:HB	9:M:2025:HOH:O	1.91	0.70
3:N:1472:ILE:HG22	3:N:1474:ALA:H	1.56	0.70
1:A:20:TYR:CE2	1:A:22:GLU:HG3	2.26	0.70
2:M:904:PRO:HD2	2:M:908:GLY:HA2	1.72	0.70
3:N:611:GLN:CD	3:N:619:LEU:HD21	2.12	0.70
2:C:76:PRO:HB2	9:C:1121:HOH:O	1.91	0.70
3:D:185:VAL:HG22	3:D:191:LEU:HD21	1.71	0.70
2:M:12:VAL:HG21	2:M:472:ARG:HD3	1.74	0.70
2:M:716:LYS:HB2	9:M:2121:HOH:O	1.91	0.70
3:N:1161:GLU:HG3	3:N:1164:ARG:HB2	1.73	0.70
1:B:55:SER:CB	1:B:158:ILE:HD13	2.21	0.70
2:C:163:ILE:HD13	9:C:1347:HOH:O	1.90	0.70
5:F:361:LEU:HD12	5:F:408:LEU:HD11	1.74	0.70
1:L:197:LEU:HD21	1:L:199:ILE:HD11	1.73	0.70
2:M:789:SER:HB2	9:M:1726:HOH:O	1.90	0.70
3:N:1215:VAL:HG13	9:N:1985:HOH:O	1.90	0.70
2:C:399:ASN:O	2:C:402:SER:HB2	1.92	0.70
5:F:358:LEU:HD21	5:F:370:LYS:HZ2	1.54	0.70
2:M:889:HIS:HE1	3:N:951:ILE:H	1.37	0.70
2:M:890:LEU:HD12	2:M:914:ILE:HD13	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1077:ALA:HA	9:N:1738:HOH:O	1.90	0.70
3:N:1481:VAL:HG11	4:O:18:ARG:HA	1.74	0.70
1:A:107:LYS:HG2	9:A:404:HOH:O	1.91	0.70
3:D:614:PHE:C	3:D:615:ARG:O	2.26	0.70
1:L:132:LEU:HD13	1:L:138:LEU:HD12	1.74	0.70
2:M:157:ARG:HD2	2:M:314:THR:HG22	1.72	0.70
2:M:45:GLN:HA	9:M:1991:HOH:O	1.89	0.70
3:N:1205:TYR:CD2	3:N:1215:VAL:HG21	2.25	0.70
3:N:785:ILE:HD13	3:N:935:LYS:HA	1.74	0.70
1:A:117:VAL:HB	1:A:120:VAL:HG12	1.72	0.70
1:B:85:LEU:HD12	1:B:124:ASN:HB3	1.72	0.70
2:C:156:GLY:HA3	9:C:1282:HOH:O	1.90	0.70
2:C:611:ILE:HD11	2:C:641:PRO:HG3	1.72	0.70
3:D:206:ARG:HH12	5:F:98:GLU:N	1.90	0.70
2:M:83:CYS:HA	2:M:88:LEU:HB3	1.73	0.70
3:N:433:GLY:HA3	3:N:447:VAL:O	1.90	0.70
2:C:838:LYS:HE3	2:C:846:LYS:HE2	1.71	0.70
2:C:3:ILE:HA	2:C:900:ARG:O	1.91	0.70
3:D:1101:VAL:HA	3:D:1428:ALA:HB2	1.72	0.70
3:D:433:GLY:HA3	3:D:447:VAL:O	1.90	0.70
1:K:186:LEU:HB2	1:K:192:LEU:HD11	1.73	0.70
2:M:163:ILE:HG13	2:M:163:ILE:O	1.91	0.70
2:M:855:VAL:HG12	9:M:1977:HOH:O	1.90	0.70
3:N:1147:ARG:HB3	3:N:1188:VAL:CG2	2.21	0.70
1:B:59:GLU:HG3	1:B:139:ASN:HD22	1.57	0.70
2:C:276:LYS:HD2	9:C:1736:HOH:O	1.90	0.70
3:D:1114:THR:H	3:D:1195:GLN:HE21	1.39	0.70
3:D:105:VAL:HG21	3:D:128:TYR:CE2	2.27	0.70
4:E:10:PHE:HE2	4:E:16:LYS:HG3	1.55	0.70
1:L:201:THR:HG22	1:L:203:GLY:H	1.55	0.70
1:L:55:SER:CB	1:L:158:ILE:HD13	2.21	0.70
2:M:1009:SER:HB2	3:N:651:GLU:O	1.91	0.70
2:M:191:PHE:HB2	2:M:241:LEU:HD13	1.74	0.70
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.74	0.70
1:A:221:HIS:HA	1:A:224:TYR:CD2	2.27	0.70
3:D:1356:TYR:CD2	3:D:1363:LEU:HD23	2.27	0.70
1:L:148:VAL:HG22	9:L:3229:HOH:O	1.92	0.70
2:M:312:ALA:HB1	2:M:318:PRO:HG2	1.73	0.70
2:M:436:GLY:HA2	2:M:538:GLN:O	1.92	0.70
3:N:1498:ALA:HB2	4:O:88:GLU:OE1	1.92	0.70
3:N:584:ASN:ND2	3:N:590:PRO:HD2	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:810:GLU:O	3:N:813:LEU:HG	1.92	0.70
5:P:394:ARG:CZ	5:P:398:ARG:HB2	2.21	0.70
1:B:158:ILE:HD11	1:B:166:PRO:CA	2.22	0.69
2:C:139:GLN:NE2	2:C:415:PRO:HD2	2.07	0.69
3:D:1279:GLY:O	3:D:1318:TYR:HA	1.91	0.69
3:D:73:CYS:HB3	3:D:76:CYS:O	1.92	0.69
2:M:511:GLU:O	2:M:526:PRO:HD3	1.92	0.69
3:N:481:MET:HG3	3:N:1388:ARG:CZ	2.22	0.69
4:O:45:ARG:HD2	9:O:1011:HOH:O	1.92	0.69
2:C:572:ILE:HG13	9:C:1310:HOH:O	1.92	0.69
2:M:219:GLN:HG3	9:M:1965:HOH:O	1.90	0.69
2:C:671:ASN:ND2	2:C:671:ASN:N	2.40	0.69
3:D:607:LEU:O	3:D:610:LYS:HB2	1.92	0.69
1:K:50:GLY:HA3	1:K:173:PRO:HG3	1.74	0.69
2:M:578:VAL:HG23	2:M:579:VAL:HG12	1.73	0.69
3:N:10:ILE:HG13	3:N:1434:TRP:CZ2	2.27	0.69
3:N:680:GLN:HB2	9:N:2087:HOH:O	1.92	0.69
4:O:45:ARG:HB2	4:O:46:PRO:HD2	1.74	0.69
9:N:2060:HOH:O	5:P:147:LEU:HD21	1.91	0.69
1:B:221:HIS:HA	1:B:224:TYR:CD2	2.26	0.69
2:C:307:LEU:HG	2:C:311:PHE:HE2	1.57	0.69
3:D:1243:THR:OG1	3:D:1253:THR:HB	1.92	0.69
3:D:611:GLN:HB2	7:D:1527:MXP:H11A	1.73	0.69
5:F:279:GLN:HA	9:F:487:HOH:O	1.91	0.69
1:K:184:THR:HG23	1:K:192:LEU:HB2	1.74	0.69
1:K:24:VAL:HG22	1:K:196:THR:HB	1.74	0.69
3:N:705:ALA:CB	3:N:706:PRO:HD3	2.22	0.69
5:P:367:MET:HB2	9:P:493:HOH:O	1.92	0.69
2:C:276:LYS:O	2:C:280:LYS:HB2	1.93	0.69
3:D:795:VAL:HG11	3:D:863:VAL:HG13	1.73	0.69
1:K:7:LYS:NZ	1:K:186:LEU:HD21	2.07	0.69
3:N:1274:ILE:HD11	3:N:1334:GLN:NE2	2.08	0.69
1:A:58:ILE:HG21	1:A:68:ILE:HD11	1.75	0.69
1:B:158:ILE:HG22	1:B:160:ASP:H	1.56	0.69
2:C:139:GLN:OE1	2:C:415:PRO:HD2	1.92	0.69
2:C:436:GLY:HA2	2:C:538:GLN:O	1.92	0.69
2:C:603:VAL:HG13	9:C:1654:HOH:O	1.93	0.69
2:C:732:ALA:HB3	9:C:1588:HOH:O	1.93	0.69
3:N:1086:LEU:HB2	9:N:2385:HOH:O	1.91	0.69
4:E:47:LYS:HA	9:E:150:HOH:O	1.93	0.69
5:F:171:LYS:HD3	9:F:640:HOH:O	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:183:ASP:HB3	9:K:3288:HOH:O	1.93	0.69
2:M:143:SER:HB2	2:M:276:LYS:NZ	2.07	0.69
2:M:838:LYS:HE3	2:M:846:LYS:HE2	1.72	0.69
3:N:1001:GLU:HG2	9:N:2222:HOH:O	1.93	0.69
5:P:160:ASP:HA	5:P:163:LEU:HD12	1.73	0.69
5:P:166:LEU:O	5:P:171:LYS:HB2	1.93	0.69
2:C:909:ALA:HB1	9:C:1225:HOH:O	1.92	0.69
5:F:392:VAL:HG12	9:F:496:HOH:O	1.92	0.69
1:K:9:PRO:HD2	1:L:224:TYR:CD1	2.27	0.69
2:M:311:PHE:HB3	9:M:1792:HOH:O	1.92	0.69
2:M:468:ARG:HB2	2:M:486:MET:O	1.92	0.69
2:M:905:ILE:HD12	2:M:905:ILE:H	1.57	0.69
3:N:1095:THR:O	3:N:1099:VAL:HG23	1.91	0.69
3:N:877:PRO:O	3:N:880:ILE:HG22	1.93	0.69
3:N:675:ARG:NH1	5:P:421:PHE:HD2	1.90	0.69
3:D:654:LYS:HB3	3:D:655:PRO:HD3	1.73	0.69
2:M:141:HIS:HB3	2:M:418:LEU:HG	1.75	0.69
2:M:352:ALA:O	2:M:356:ARG:HG3	1.93	0.69
3:N:149:LYS:HG3	9:N:2241:HOH:O	1.91	0.69
5:P:85:LEU:HA	5:P:88:ILE:HD12	1.74	0.69
1:A:58:ILE:HB	1:A:61:VAL:HB	1.75	0.69
2:C:218:VAL:HG22	2:C:221:LEU:HD23	1.75	0.69
2:C:541:SER:HB2	9:C:1523:HOH:O	1.93	0.69
2:C:86:LYS:HD3	2:C:813:VAL:HG12	1.74	0.69
3:D:799:LYS:H	3:D:826:PRO:HG2	1.58	0.69
4:E:33:HIS:HB2	4:E:37:ASN:HD21	1.58	0.69
2:M:139:GLN:HE22	2:M:415:PRO:HG2	1.56	0.69
2:M:343:GLN:HG2	2:M:385:PHE:HB2	1.75	0.69
2:M:521:PRO:HG3	3:N:1068:LEU:HD23	1.75	0.69
2:M:751:PRO:HG3	2:M:795:GLY:O	1.92	0.69
3:N:484:PRO:HB3	9:N:1630:HOH:O	1.91	0.69
5:P:132:ARG:HG2	5:P:181:GLU:CD	2.14	0.69
1:A:97:VAL:HG23	9:A:349:HOH:O	1.92	0.69
2:C:176:VAL:HG12	2:C:182:VAL:HG13	1.73	0.69
2:C:396:ASP:HA	2:C:633:GLN:NE2	2.08	0.69
3:D:584:ASN:ND2	3:D:590:PRO:HD2	2.07	0.69
2:M:28:ARG:NH1	2:M:463:GLU:HG2	2.07	0.69
3:N:124:GLU:O	3:N:128:TYR:HB2	1.93	0.69
1:A:111:ALA:HB2	1:A:127:LEU:HG	1.75	0.68
2:C:634:GLY:HA3	9:C:1157:HOH:O	1.92	0.68
3:D:206:ARG:HH12	5:F:98:GLU:HA	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:69:PRO:HB3	9:M:1747:HOH:O	1.93	0.68
3:N:1354:LYS:HA	9:N:1826:HOH:O	1.92	0.68
3:N:36:THR:HA	9:N:2104:HOH:O	1.93	0.68
4:O:46:PRO:HD2	9:O:1011:HOH:O	1.92	0.68
1:B:58:ILE:HB	1:B:61:VAL:HB	1.73	0.68
2:C:399:ASN:HB3	2:C:568:ALA:O	1.93	0.68
3:D:29:PRO:HG2	3:D:549:ASN:ND2	2.07	0.68
3:D:483:HIS:HB2	3:D:484:PRO:HD3	1.75	0.68
4:E:17:TYR:O	4:E:21:VAL:HG23	1.92	0.68
2:M:575:GLN:OE1	2:M:670:GLN:HB3	1.93	0.68
2:M:838:LYS:HE3	2:M:997:LEU:HD12	1.75	0.68
3:N:1146:GLY:HA3	3:N:1207:TYR:HB2	1.74	0.68
3:N:1162:GLU:HB3	9:N:1922:HOH:O	1.92	0.68
3:N:428:LYS:HD3	9:N:2334:HOH:O	1.93	0.68
3:N:646:LYS:HE2	3:N:722:GLU:HG2	1.75	0.68
5:P:87:GLU:O	5:P:91:VAL:HG23	1.92	0.68
3:D:1472:ILE:HG22	3:D:1474:ALA:H	1.58	0.68
1:L:101:LEU:HG	9:L:2708:HOH:O	1.91	0.68
3:N:1112:CYS:HB2	3:N:1195:GLN:HG2	1.75	0.68
3:N:1317:ASP:HB2	9:N:1639:HOH:O	1.93	0.68
3:N:555:LYS:HB3	9:N:1956:HOH:O	1.93	0.68
4:O:45:ARG:HE	4:O:55:PHE:HD2	1.40	0.68
1:B:52:ALA:HB2	1:B:170:VAL:O	1.93	0.68
2:C:73:LEU:HD22	2:C:118:ILE:HD11	1.75	0.68
1:L:97:VAL:HG11	1:L:120:VAL:HG21	1.73	0.68
2:M:69:LEU:HB2	2:M:97:ARG:HB2	1.76	0.68
3:N:403:PHE:HD1	3:N:405:ASP:O	1.76	0.68
3:N:523:ASP:HB3	9:N:1572:HOH:O	1.93	0.68
2:C:256:TYR:HE1	2:C:293:PHE:HB2	1.57	0.68
2:C:811:PRO:HB2	2:C:813:VAL:HG13	1.74	0.68
5:F:88:ILE:HD13	5:F:193:ARG:HD2	1.75	0.68
2:M:750:LYS:HD3	9:N:2087:HOH:O	1.93	0.68
3:N:119:SER:H	3:N:123:LEU:HD22	1.56	0.68
1:B:109:VAL:HG21	1:B:138:LEU:CD1	2.19	0.68
2:C:1107:ASN:HB3	9:C:1226:HOH:O	1.94	0.68
2:C:619:ARG:HG2	9:C:1584:HOH:O	1.94	0.68
3:D:565:ILE:HD12	5:F:192:LEU:HD13	1.75	0.68
5:P:248:ASN:HA	5:P:251:ILE:HD12	1.74	0.68
1:B:213:GLN:O	1:B:217:ILE:HD12	1.94	0.68
2:C:299:LYS:HB3	9:C:1267:HOH:O	1.94	0.68
3:D:704:ARG:HG2	3:D:705:ALA:H	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:147:LEU:HB2	9:F:2238:HOH:O	1.94	0.68
3:N:46:ASP:OD2	3:N:48:ARG:HG2	1.94	0.68
3:N:607:LEU:O	3:N:610:LYS:HB2	1.93	0.68
3:N:610:LYS:HB3	9:N:1557:HOH:O	1.94	0.68
5:P:77:THR:O	5:P:81:VAL:HG23	1.93	0.68
2:C:554:ASP:OD2	2:C:556:ASN:HB3	1.91	0.68
3:D:1239:ARG:HB2	9:D:2065:HOH:O	1.94	0.68
3:D:153:LEU:HD11	3:D:158:TYR:N	2.09	0.68
5:F:129:GLU:HG2	9:F:492:HOH:O	1.93	0.68
1:L:158:ILE:HG13	1:L:166:PRO:HB3	1.76	0.68
2:M:108:ILE:HB	2:M:368:THR:OG1	1.94	0.68
2:M:571:LEU:HD21	2:M:700:TYR:CD2	2.29	0.68
3:N:672:ALA:HB1	9:N:1656:HOH:O	1.93	0.68
1:A:100:LEU:HB2	1:A:115:LEU:HD11	1.76	0.68
1:A:136:GLY:HA3	9:A:320:HOH:O	1.93	0.68
2:C:145:GLY:O	2:C:163:ILE:HG23	1.93	0.68
3:D:1141:GLU:HG2	3:D:1168:MET:HE1	1.75	0.68
3:D:162:ARG:HA	3:D:449:SER:CB	2.24	0.68
1:K:133:GLU:HG2	1:K:134:GLU:N	2.07	0.68
1:L:128:HIS:HB2	9:L:3368:HOH:O	1.93	0.68
2:M:148:PHE:CZ	2:M:281:LEU:HD13	2.29	0.68
3:N:535:PHE:O	5:P:315:VAL:N	2.26	0.68
5:P:133:ALA:HA	9:P:567:HOH:O	1.92	0.68
5:P:218:GLN:HA	5:P:221:ILE:HD12	1.75	0.68
2:C:599:GLU:HG3	2:C:600:ASP:H	1.59	0.68
2:C:578:VAL:HG13	2:C:671:ASN:OD1	1.93	0.68
2:C:815:LEU:HD13	9:C:1286:HOH:O	1.94	0.68
2:C:874:LEU:HD12	3:D:784:ASP:OD2	1.94	0.68
2:C:915:LYS:HE3	9:C:1136:HOH:O	1.94	0.68
2:C:1096:ALA:O	3:D:13:ALA:HB2	1.94	0.68
3:D:723:GLY:HA3	9:D:1680:HOH:O	1.94	0.68
5:F:160:ASP:HA	5:F:163:LEU:HD12	1.75	0.68
2:M:492:ASP:HA	9:M:1901:HOH:O	1.92	0.68
3:N:108:VAL:HG21	9:N:2073:HOH:O	1.94	0.68
5:P:368:VAL:HG22	9:P:506:HOH:O	1.93	0.68
1:A:198:ARG:HB2	1:A:200:TRP:CZ3	2.29	0.67
1:B:158:ILE:HG13	1:B:166:PRO:HB3	1.76	0.67
2:C:333:ILE:HD13	2:C:467:ILE:HG13	1.76	0.67
3:D:586:ARG:HH12	3:D:1444:THR:HG21	1.58	0.67
2:M:145:GLY:O	2:M:163:ILE:HG23	1.94	0.67
3:N:1430:SER:HA	9:N:2035:HOH:O	1.92	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:339:LEU:HD11	9:C:1322:HOH:O	1.94	0.67
3:D:1146:GLY:HA3	3:D:1207:TYR:HB2	1.76	0.67
3:D:805:GLU:HG3	9:D:1779:HOH:O	1.93	0.67
2:M:292:ARG:HB3	9:M:2058:HOH:O	1.93	0.67
2:M:93:PRO:HG3	2:M:117:HIS:CE1	2.29	0.67
3:N:611:GLN:NE2	7:N:1527:MXP:H16B	2.09	0.67
3:N:1476:THR:HG23	4:O:21:VAL:HG22	1.75	0.67
4:O:88:GLU:HG3	9:O:2559:HOH:O	1.93	0.67
4:O:9:LEU:HB3	4:O:19:LEU:HD21	1.76	0.67
1:A:103:ALA:CB	1:A:107:LYS:HE2	2.24	0.67
2:C:914:ILE:HB	9:C:1225:HOH:O	1.93	0.67
2:C:983:ILE:HG21	2:C:987:ILE:HD11	1.75	0.67
1:L:180:GLN:HB3	9:L:1094:HOH:O	1.95	0.67
2:M:283:ILE:HD11	9:M:2124:HOH:O	1.95	0.67
2:M:445:GLU:HG2	9:M:1876:HOH:O	1.94	0.67
2:M:660:ALA:HB1	2:M:667:ALA:O	1.93	0.67
2:M:793:PRO:HD2	9:M:2061:HOH:O	1.93	0.67
2:M:966:LEU:HD11	2:M:986:PRO:HG2	1.74	0.67
3:N:1243:THR:OG1	3:N:1253:THR:HB	1.94	0.67
3:N:130:SER:HB3	3:N:132:TYR:CE1	2.30	0.67
3:N:483:HIS:HB2	3:N:484:PRO:HD3	1.77	0.67
3:N:658:LEU:O	3:N:661:MET:HB2	1.94	0.67
5:F:408:LEU:O	5:F:412:GLU:HG2	1.95	0.67
1:K:10:VAL:HG12	1:K:12:THR:HG22	1.77	0.67
2:M:979:THR:HG23	2:M:981:GLU:H	1.59	0.67
3:N:956:ILE:HG12	3:N:1039:CYS:O	1.95	0.67
3:N:28:LYS:HG3	3:N:41:ARG:HH11	1.59	0.67
2:M:318:PRO:HA	9:M:1903:HOH:O	1.94	0.67
3:N:1152:GLU:CD	3:N:1159:ARG:HH12	1.97	0.67
3:N:544:TYR:O	3:N:548:ILE:HG12	1.93	0.67
4:O:48:MET:O	4:O:52:GLU:HA	1.94	0.67
5:P:408:LEU:O	5:P:412:GLU:HG2	1.93	0.67
5:F:361:LEU:HD23	5:F:362:SER:H	1.58	0.67
2:M:724:ARG:HG2	2:M:734:LEU:HD23	1.77	0.67
3:N:141:ILE:CG2	3:N:450:TYR:H	2.08	0.67
5:P:268:ILE:HD13	5:P:311:ALA:HB2	1.77	0.67
2:C:551:GLU:HG3	2:C:552:HIS:CD2	2.30	0.67
2:C:944:LEU:HD21	2:C:963:LEU:HD23	1.77	0.67
3:D:1041:LEU:HD12	3:D:1058:ARG:HA	1.77	0.67
3:D:809:PRO:HB2	3:D:812:ALA:HB2	1.76	0.67
3:D:906:GLN:HB3	3:D:911:LEU:CD1	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:61:VAL:HG23	1:L:137:ARG:HH22	1.59	0.67
3:N:1277:ILE:HA	9:N:1570:HOH:O	1.95	0.67
3:N:764:LEU:HD23	3:N:767:HIS:ND1	2.10	0.67
1:B:38:ASN:HB3	1:B:39:PRO:HD3	1.77	0.67
2:C:328:LEU:HD13	2:C:433:THR:HB	1.76	0.67
2:C:464:LEU:HG	9:C:1551:HOH:O	1.94	0.67
2:C:889:HIS:CD2	2:C:970:GLY:HA3	2.30	0.67
3:D:1432:LYS:HG2	9:D:1537:HOH:O	1.93	0.67
3:D:617:ASN:HB2	3:D:618:LEU:HD12	1.77	0.67
2:M:722:ILE:HG21	2:M:821:GLU:OE1	1.94	0.67
3:N:1220:ALA:HB1	3:N:1223:ILE:HD13	1.77	0.67
3:N:1279:GLY:O	3:N:1318:TYR:HA	1.94	0.67
3:N:508:ARG:HB3	9:N:1796:HOH:O	1.95	0.67
3:N:65:ARG:CG	3:N:66:GLN:H	2.07	0.67
3:N:804:LEU:HD23	3:N:804:LEU:H	1.60	0.67
1:A:48:ILE:HG22	1:A:173:PRO:HD2	1.75	0.67
1:B:60:ASP:H	1:B:137:ARG:NH2	1.92	0.67
2:C:244:PRO:HG2	2:C:246:ASP:OD2	1.95	0.67
3:D:637:LEU:HD21	3:D:642:CYS:HA	1.75	0.67
3:D:658:LEU:O	3:D:661:MET:HB2	1.95	0.67
5:F:191:ASN:HB3	5:F:220:LEU:HD11	1.76	0.67
1:K:123:MET:O	1:K:125:PRO:HD3	1.95	0.67
3:N:996:TRP:HA	3:N:999:THR:HG22	1.77	0.67
3:D:16:GLU:HA	9:D:2072:HOH:O	1.95	0.67
3:D:613:ARG:HB2	9:D:1834:HOH:O	1.95	0.67
3:D:785:ILE:HD13	3:D:935:LYS:HA	1.75	0.67
3:D:1481:VAL:HG11	4:E:18:ARG:HA	1.77	0.67
5:F:110:MET:HB2	9:F:483:HOH:O	1.94	0.67
2:M:156:GLY:HA3	9:M:2199:HOH:O	1.95	0.67
2:M:770:GLU:HG2	9:M:2011:HOH:O	1.94	0.67
2:M:805:ARG:HG3	2:M:823:VAL:HG22	1.77	0.67
1:K:46:SER:HB3	2:M:856:GLU:HG2	1.76	0.67
3:N:178:LEU:HD12	9:N:2234:HOH:O	1.94	0.67
3:N:556:LYS:HB3	5:P:218:GLN:HE22	1.59	0.67
5:P:295:MET:HG2	5:P:299:TRP:CD2	2.30	0.67
2:C:136:ILE:HG21	2:C:336:VAL:HG13	1.77	0.66
3:D:1094:LEU:O	3:D:1098:LEU:HD13	1.95	0.66
3:D:808:THR:HB	3:D:809:PRO:HD3	1.76	0.66
1:L:123:MET:C	1:L:125:PRO:HD3	2.15	0.66
2:M:1108:PRO:HD3	9:M:2055:HOH:O	1.95	0.66
2:M:204:GLN:NE2	2:M:222:MET:HA	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:ALA:HB1	1:B:171:PHE:CD2	2.30	0.66
2:C:310:LEU:HD12	9:C:1562:HOH:O	1.94	0.66
2:C:397:GLU:HB2	9:C:1153:HOH:O	1.94	0.66
2:C:859:PRO:O	2:C:867:VAL:HG22	1.95	0.66
3:D:1410:GLU:OE2	3:D:1414:PRO:HG3	1.95	0.66
2:M:1096:ALA:HB1	9:N:1592:HOH:O	1.94	0.66
2:M:64:LEU:HD13	2:M:359:MET:HG3	1.76	0.66
3:N:1321:ALA:O	3:N:1339:LYS:HE3	1.96	0.66
3:N:188:GLY:N	3:N:199:LEU:HD23	2.11	0.66
3:D:609:GLY:O	3:D:617:ASN:ND2	2.28	0.66
3:D:705:ALA:CB	3:D:706:PRO:HD3	2.25	0.66
3:D:965:GLU:HB2	9:D:1794:HOH:O	1.96	0.66
4:E:48:MET:O	4:E:52:GLU:HA	1.96	0.66
2:M:909:ALA:HB1	9:M:1825:HOH:O	1.94	0.66
2:M:952:LEU:HD12	2:M:969:GLN:NE2	2.08	0.66
2:M:1096:ALA:O	3:N:13:ALA:HB2	1.95	0.66
1:B:78:ILE:HA	9:B:438:HOH:O	1.95	0.66
3:D:116:LEU:HD22	3:D:118:LEU:HD11	1.76	0.66
3:D:805:GLU:HG2	9:D:1726:HOH:O	1.95	0.66
3:D:843:PHE:HE1	3:D:864:VAL:HG11	1.60	0.66
2:M:1:MET:HE2	9:M:2228:HOH:O	1.94	0.66
3:N:185:VAL:HG22	3:N:191:LEU:HD21	1.76	0.66
5:P:303:ARG:HB2	9:P:433:HOH:O	1.94	0.66
2:C:431:HIS:CD2	2:C:433:THR:H	2.13	0.66
2:C:693:GLU:HA	2:C:696:LYS:HG3	1.76	0.66
3:D:1147:ARG:HB3	3:D:1188:VAL:CG2	2.25	0.66
3:D:817:GLU:O	3:D:821:VAL:HG23	1.94	0.66
5:F:336:GLU:HA	9:F:469:HOH:O	1.94	0.66
3:N:82:LYS:HE2	9:N:1551:HOH:O	1.95	0.66
5:P:234:LYS:HG2	9:P:475:HOH:O	1.95	0.66
3:N:569:ASN:OD1	5:P:80:PRO:HB3	1.96	0.66
1:A:180:GLN:HB3	9:A:352:HOH:O	1.95	0.66
1:B:173:PRO:HG3	9:B:480:HOH:O	1.95	0.66
1:B:18:ARG:O	1:B:207:PRO:HD3	1.96	0.66
1:B:199:ILE:HD11	1:B:211:LEU:HD13	1.76	0.66
3:D:1166:LEU:HD12	3:D:1171:VAL:HG22	1.78	0.66
1:L:76:VAL:HG23	9:L:1317:HOH:O	1.95	0.66
2:M:1033:GLY:O	2:M:1036:GLU:HG2	1.96	0.66
2:M:1083:GLU:HG2	9:M:1724:HOH:O	1.96	0.66
2:M:21:ILE:HD12	2:M:21:ILE:H	1.60	0.66
3:N:126:VAL:HG21	9:N:2194:HOH:O	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:161:LEU:O	3:N:449:SER:HB3	1.95	0.66
5:P:335:ASP:OD1	5:P:338:LEU:HB2	1.95	0.66
2:C:15:LEU:CD2	2:C:583:LEU:HD11	2.26	0.66
2:C:498:GLN:O	2:C:501:THR:HG23	1.96	0.66
3:D:1498:ALA:HB2	4:E:88:GLU:OE1	1.96	0.66
3:D:100:ALA:HB2	3:D:513:ILE:CD1	2.24	0.66
4:E:6:ILE:HA	4:E:9:LEU:HD12	1.77	0.66
2:M:42:VAL:HG12	2:M:43:GLY:H	1.59	0.66
2:M:768:THR:HB	2:M:771:GLU:HB3	1.77	0.66
3:N:996:TRP:CD2	3:N:1056:PRO:HG2	2.31	0.66
3:N:1101:VAL:HG21	3:N:1424:VAL:HG22	1.77	0.66
3:N:133:ILE:HD11	3:N:155:ASP:OD1	1.96	0.66
3:N:58:CYS:HA	3:N:78:VAL:HG11	1.77	0.66
3:N:924:MET:O	3:N:927:THR:HB	1.96	0.66
2:C:1018:GLN:OE1	2:C:1060:ILE:HD11	1.95	0.66
2:C:198:ARG:NE	2:C:228:ALA:HA	2.11	0.66
2:C:141:HIS:HB3	2:C:418:LEU:HG	1.77	0.66
3:D:1310:ARG:HG3	3:D:1327:ARG:HB3	1.78	0.66
2:C:713:ARG:HH22	3:D:531:ASP:HB3	1.60	0.66
2:C:1019:GLN:HE22	3:D:621:LYS:HA	1.61	0.66
5:F:260:ILE:HD11	5:F:310:ILE:HG22	1.77	0.66
2:M:781:LYS:HG3	9:M:1700:HOH:O	1.95	0.66
3:N:1087:ARG:HB3	9:N:1678:HOH:O	1.95	0.66
3:N:633:VAL:HG22	3:N:635:PRO:HD3	1.76	0.66
3:N:704:ARG:HG2	3:N:705:ALA:H	1.59	0.66
2:C:864:GLY:O	2:C:866:PRO:HD3	1.96	0.66
2:M:1014:SER:HB3	2:M:1017:THR:O	1.96	0.66
2:M:350:ARG:HA	2:M:353:ARG:HD2	1.78	0.66
2:M:627:ARG:HA	9:M:1936:HOH:O	1.95	0.66
2:M:976:ASP:CB	2:M:979:THR:HG22	2.25	0.66
3:N:806:PHE:CE1	3:N:813:LEU:HB3	2.30	0.66
4:O:17:TYR:O	4:O:21:VAL:HG23	1.95	0.66
2:C:289:THR:HB	9:C:1392:HOH:O	1.96	0.66
3:D:1044:LEU:HD23	9:D:1976:HOH:O	1.95	0.66
3:D:679:ARG:HB2	3:D:682:ASP:OD2	1.95	0.66
5:F:321:ILE:HB	5:F:327:SER:OG	1.96	0.66
1:K:206:THR:HG22	1:K:209:GLU:H	1.61	0.66
3:N:1258:ARG:CZ	3:N:1262:LEU:HD11	2.26	0.66
5:P:292:ALA:HB1	5:P:299:TRP:O	1.96	0.66
2:C:1015:LEU:HD11	9:F:451:HOH:O	1.95	0.65
2:C:439:CYS:HB3	9:C:1185:HOH:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1141:GLU:CG	3:D:1168:MET:HE1	2.26	0.65
1:L:158:ILE:HG22	1:L:160:ASP:H	1.60	0.65
2:M:197:LEU:HD22	2:M:202:TYR:HD2	1.61	0.65
2:M:304:LEU:HD23	2:M:305:PRO:HD3	1.78	0.65
5:P:295:MET:HG2	5:P:299:TRP:CE2	2.31	0.65
5:P:407:LYS:HG2	9:P:600:HOH:O	1.95	0.65
3:D:403:PHE:CE1	3:D:407:VAL:HG23	2.31	0.65
5:F:273:ARG:HD3	9:F:735:HOH:O	1.96	0.65
2:M:312:ALA:HA	9:M:1882:HOH:O	1.96	0.65
3:N:139:GLY:HA3	9:N:2226:HOH:O	1.95	0.65
2:C:805:ARG:HG3	2:C:823:VAL:HG22	1.78	0.65
3:D:1102:THR:HG22	3:D:1222:GLY:HA2	1.78	0.65
5:F:415:THR:HG21	9:F:598:HOH:O	1.95	0.65
2:M:1081:VAL:HG21	2:M:1111:ILE:HG22	1.78	0.65
2:M:368:THR:HB	2:M:369:PRO:HD3	1.77	0.65
3:N:1035:ILE:HA	3:N:1038:LEU:CD1	2.26	0.65
3:N:154:THR:HG23	3:N:157:GLU:H	1.60	0.65
3:N:493:ARG:HH11	3:N:1390:LEU:C	1.99	0.65
5:P:151:LEU:O	5:P:155:THR:HB	1.96	0.65
5:P:261:PRO:HB3	9:P:570:HOH:O	1.94	0.65
3:D:1211:MET:HB3	9:D:2053:HOH:O	1.95	0.65
3:D:128:TYR:HE1	3:D:461:ILE:HG13	1.61	0.65
3:D:611:GLN:NE2	3:D:1463:LYS:CE	2.53	0.65
5:F:125:ASP:HA	9:F:652:HOH:O	1.97	0.65
1:L:206:THR:HG22	1:L:209:GLU:HB2	1.78	0.65
1:L:58:ILE:HB	1:L:61:VAL:HB	1.77	0.65
2:M:150:PRO:CA	2:M:158:TYR:HB3	2.22	0.65
2:M:528:GLU:HB3	9:M:1626:HOH:O	1.97	0.65
3:N:59:ALA:HB1	9:N:1806:HOH:O	1.96	0.65
3:N:644:LEU:HD12	3:N:645:PRO:HD2	1.78	0.65
3:N:65:ARG:HG3	3:N:66:GLN:H	1.62	0.65
2:C:237:ARG:HD2	9:C:1406:HOH:O	1.97	0.65
3:D:611:GLN:HE21	3:D:1439:SER:HB3	1.61	0.65
3:D:1502:ALA:HB1	9:D:2407:HOH:O	1.95	0.65
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.78	0.65
1:L:158:ILE:HD11	1:L:166:PRO:CA	2.25	0.65
2:M:571:LEU:CD2	2:M:700:TYR:HA	2.26	0.65
3:N:1301:LYS:HG2	9:N:2327:HOH:O	1.95	0.65
1:L:176:ARG:HD3	3:N:884:ARG:NH2	2.11	0.65
1:B:59:GLU:HG3	1:B:139:ASN:ND2	2.12	0.65
2:C:292:ARG:HD2	2:C:299:LYS:HG2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:511:GLU:O	2:C:526:PRO:HD3	1.95	0.65
3:D:1109:GLU:OE1	3:D:1201:CYS:HB2	1.95	0.65
2:C:1098:ASP:HB2	3:D:21:TRP:HZ2	1.60	0.65
3:D:583:ASP:OD2	3:D:604:THR:HG21	1.96	0.65
2:C:1030:GLN:NE2	3:D:628:ARG:HB3	2.11	0.65
1:L:46:SER:O	1:L:148:VAL:HB	1.96	0.65
2:M:422:ARG:HA	9:M:1913:HOH:O	1.97	0.65
2:M:471:TYR:CE2	2:M:496:ILE:HG21	2.31	0.65
2:M:52:PHE:CD2	2:M:68:PHE:HB2	2.31	0.65
3:N:1109:GLU:OE1	3:N:1201:CYS:HB2	1.96	0.65
5:P:392:VAL:HG21	9:P:614:HOH:O	1.97	0.65
1:A:206:THR:CG2	1:A:209:GLU:H	2.10	0.65
2:C:1118:LYS:HG3	9:C:1317:HOH:O	1.95	0.65
3:D:1095:THR:O	3:D:1099:VAL:HG23	1.96	0.65
1:K:9:PRO:HB2	1:L:224:TYR:HB3	1.77	0.65
1:L:109:VAL:HG12	9:L:1850:HOH:O	1.96	0.65
1:L:12:THR:HB	9:L:1867:HOH:O	1.96	0.65
2:M:289:THR:HB	9:M:1685:HOH:O	1.97	0.65
2:M:724:ARG:O	2:M:734:LEU:HD21	1.97	0.65
3:N:1046:GLN:HA	3:N:1052:THR:HA	1.79	0.65
3:N:105:VAL:HG21	3:N:128:TYR:CE2	2.30	0.65
1:B:179:PHE:HB2	1:B:195:LEU:HD11	1.77	0.65
2:C:1103:ASP:HB2	2:C:1107:ASN:O	1.96	0.65
2:C:442:GLU:HG2	2:C:454:SER:OG	1.96	0.65
3:D:493:ARG:NH1	3:D:1390:LEU:HB3	2.12	0.65
3:D:833:GLU:HG2	9:D:1935:HOH:O	1.97	0.65
1:K:16:GLN:HB3	9:K:1964:HOH:O	1.97	0.65
2:M:101:ILE:HG23	2:M:107:LEU:HD22	1.77	0.65
3:N:134:VAL:HG12	3:N:152:LEU:HB3	1.77	0.65
3:N:614:PHE:HD1	3:N:615:ARG:N	1.94	0.65
3:N:664:LYS:HE2	9:N:2324:HOH:O	1.96	0.65
2:C:610:ARG:HB2	9:C:1140:HOH:O	1.97	0.65
3:D:1264:GLU:HG2	3:D:1425:THR:HG22	1.78	0.65
3:D:1422:MET:HE2	3:D:1427:SER:HA	1.79	0.65
3:D:161:LEU:HD22	3:D:452:ILE:HG21	1.79	0.65
3:D:957:PRO:CG	3:D:1007:VAL:HA	2.25	0.65
1:L:221:HIS:HA	1:L:224:TYR:CD2	2.31	0.65
2:M:607:ASP:HB3	2:M:609:ASN:H	1.62	0.65
2:M:755:LEU:HB2	9:M:1781:HOH:O	1.97	0.65
3:N:508:ARG:CG	3:N:509:PRO:HD2	2.26	0.65
3:N:760:ARG:HH21	4:O:61:VAL:HG12	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:274:THR:O	5:P:278:LEU:HG	1.97	0.65
5:P:291:ILE:HG23	5:P:304:VAL:HG21	1.78	0.65
1:B:2:LEU:HD12	1:B:3:ASP:N	2.11	0.65
2:C:141:HIS:HB3	2:C:418:LEU:CG	2.27	0.65
2:C:627:ARG:HG3	2:C:628:PHE:H	1.61	0.65
3:D:1441:GLN:HB3	9:D:1557:HOH:O	1.97	0.65
5:F:166:LEU:O	5:F:171:LYS:HB2	1.96	0.65
2:M:916:GLU:HG2	9:M:2028:HOH:O	1.96	0.65
3:N:1166:LEU:HD12	3:N:1171:VAL:HG22	1.79	0.65
2:C:905:ILE:HB	9:C:1738:HOH:O	1.96	0.64
3:D:812:ALA:HB1	9:D:1779:HOH:O	1.98	0.64
3:D:906:GLN:HB3	3:D:911:LEU:HD11	1.78	0.64
5:F:187:LEU:O	5:F:187:LEU:HD23	1.97	0.64
1:K:38:ASN:HB3	1:K:39:PRO:HD3	1.77	0.64
1:L:54:THR:HG22	9:L:3428:HOH:O	1.96	0.64
1:L:61:VAL:N	1:L:137:ARG:HH22	1.95	0.64
2:M:838:LYS:HB2	2:M:848:VAL:HG22	1.78	0.64
3:N:611:GLN:HG2	3:N:619:LEU:HD11	1.77	0.64
3:D:1209:LEU:HD23	3:D:1211:MET:SD	2.37	0.64
2:M:429:ASP:HB3	9:M:2136:HOH:O	1.96	0.64
2:M:54:ILE:HD11	2:M:356:ARG:HG2	1.79	0.64
2:M:73:LEU:HD22	2:M:118:ILE:HD11	1.79	0.64
3:N:445:ARG:HB3	9:N:2112:HOH:O	1.98	0.64
3:N:817:GLU:O	3:N:821:VAL:HG23	1.96	0.64
1:A:13:VAL:HG12	1:A:15:THR:HG22	1.78	0.64
1:A:20:TYR:HB3	9:A:413:HOH:O	1.97	0.64
3:D:1237:THR:HG22	9:D:2068:HOH:O	1.98	0.64
3:D:534:ARG:HG2	9:F:611:HOH:O	1.97	0.64
5:F:401:GLU:O	5:F:405:LEU:HB2	1.97	0.64
1:K:13:VAL:HG12	1:K:15:THR:HG22	1.80	0.64
1:L:38:ASN:HB3	1:L:39:PRO:HD3	1.78	0.64
2:M:100:LEU:HD23	2:M:368:THR:HA	1.78	0.64
2:M:811:PRO:HB2	2:M:813:VAL:HG13	1.78	0.64
3:N:141:ILE:HD12	9:N:2046:HOH:O	1.97	0.64
3:N:175:VAL:HG11	3:N:193:PRO:HB2	1.80	0.64
3:N:131:LYS:CG	3:N:568:ARG:HG2	2.26	0.64
3:N:722:GLU:HA	9:N:1930:HOH:O	1.97	0.64
1:B:124:ASN:OD1	1:B:127:LEU:HB2	1.97	0.64
1:B:226:SER:O	1:B:228:PRO:HD3	1.97	0.64
2:C:645:VAL:HA	9:C:1531:HOH:O	1.96	0.64
2:C:976:ASP:CB	2:C:979:THR:HG22	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1046:GLN:HA	3:D:1052:THR:HA	1.80	0.64
3:D:149:LYS:HA	9:D:1632:HOH:O	1.98	0.64
3:D:55:ASP:HB3	3:D:82:LYS:HE2	1.79	0.64
5:F:349:LEU:HB2	9:F:433:HOH:O	1.98	0.64
2:M:263:ASP:HB2	2:M:264:PRO:HD3	1.78	0.64
3:N:1013:GLU:HB3	9:N:2351:HOH:O	1.97	0.64
2:C:691:SER:HB2	2:C:858:MET:SD	2.38	0.64
2:C:890:LEU:HD23	9:C:1640:HOH:O	1.97	0.64
3:D:124:GLU:O	3:D:128:TYR:HB2	1.97	0.64
1:K:41:ARG:HH22	2:M:866:PRO:HG3	1.63	0.64
1:L:109:VAL:HG21	1:L:138:LEU:CD1	2.18	0.64
1:L:52:ALA:HB1	9:L:1023:HOH:O	1.98	0.64
1:L:9:PRO:HD3	9:L:1857:HOH:O	1.98	0.64
2:M:170:PRO:HG2	2:M:258:TYR:CD2	2.32	0.64
2:M:176:VAL:HG12	2:M:182:VAL:HG13	1.78	0.64
2:M:549:PHE:CE2	2:M:886:LEU:HB3	2.32	0.64
3:N:1209:LEU:HD12	3:N:1219:GLU:OE1	1.97	0.64
3:N:565:ILE:HB	5:P:84:TYR:HD2	1.63	0.64
3:N:702:LEU:HD13	3:N:716:PHE:CD1	2.33	0.64
3:N:799:LYS:HB3	3:N:826:PRO:HG2	1.77	0.64
4:O:54:LEU:HG	4:O:58:PRO:CG	2.26	0.64
5:P:112:ALA:O	5:P:116:LEU:HG	1.98	0.64
5:P:315:VAL:HA	9:P:479:HOH:O	1.97	0.64
1:B:71:VAL:HG22	1:B:132:LEU:HD12	1.80	0.64
2:C:84:ARG:HH21	2:C:128:ILE:HD11	1.63	0.64
2:C:265:ARG:HG2	2:C:266:ARG:N	2.11	0.64
2:C:140:ILE:CD1	2:C:412:ALA:HA	2.27	0.64
2:C:57:GLU:HB2	9:C:1254:HOH:O	1.97	0.64
2:C:79:PRO:HA	9:C:1251:HOH:O	1.97	0.64
3:D:1035:ILE:HA	3:D:1038:LEU:HD12	1.80	0.64
3:D:583:ASP:HB2	3:D:604:THR:OG1	1.97	0.64
2:M:720:GLU:HA	2:M:759:THR:O	1.98	0.64
3:N:426:LYS:HD2	9:N:2209:HOH:O	1.96	0.64
4:O:67:GLU:OE1	4:O:73:LEU:HD11	1.97	0.64
2:C:218:VAL:HG22	2:C:221:LEU:CD2	2.28	0.64
2:C:549:PHE:HB3	2:C:552:HIS:HD2	1.63	0.64
2:C:573:ARG:HB2	9:C:1310:HOH:O	1.97	0.64
2:C:671:ASN:ND2	2:C:671:ASN:H	1.94	0.64
3:D:188:GLY:N	3:D:199:LEU:HD23	2.13	0.64
3:D:564:GLU:HA	3:D:567:ILE:HD13	1.80	0.64
3:D:891:GLU:HG2	9:D:2400:HOH:O	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:614:PHE:CZ	5:F:326:ASP:HB3	2.33	0.64
5:F:327:SER:HA	9:F:456:HOH:O	1.96	0.64
2:M:603:VAL:HG22	2:M:613:VAL:HG12	1.79	0.64
2:M:545:ASN:OD1	2:M:905:ILE:HG12	1.96	0.64
4:O:88:GLU:HB3	9:O:2455:HOH:O	1.97	0.64
2:C:41:ASN:N	2:C:41:ASN:HD22	1.91	0.64
2:C:69:LEU:HB2	2:C:97:ARG:HB2	1.80	0.64
3:D:175:VAL:HG11	3:D:193:PRO:HB2	1.80	0.64
5:F:112:ALA:HA	5:F:173:TYR:HD2	1.63	0.64
2:M:118:ILE:HB	9:M:2032:HOH:O	1.98	0.64
2:M:331:ARG:CZ	2:M:427:VAL:HG12	2.28	0.64
3:N:1065:LEU:HG	3:N:1070:TYR:HD2	1.63	0.64
3:N:148:GLU:HG2	3:N:151:GLN:NE2	2.11	0.64
3:N:546:ARG:HA	9:N:1614:HOH:O	1.98	0.64
3:N:679:ARG:HB2	3:N:682:ASP:OD2	1.98	0.64
2:C:150:PRO:CA	2:C:158:TYR:HB3	2.23	0.64
2:C:314:THR:HG23	9:C:1562:HOH:O	1.98	0.64
2:C:773:LEU:HB2	9:C:1139:HOH:O	1.96	0.64
3:D:148:GLU:HG2	3:D:151:GLN:NE2	2.12	0.64
1:K:197:LEU:HD23	1:K:197:LEU:H	1.62	0.64
1:K:201:THR:HG22	1:K:203:GLY:H	1.63	0.64
3:N:153:LEU:HD11	3:N:158:TYR:N	2.13	0.64
3:N:595:GLY:HA2	9:N:2178:HOH:O	1.98	0.64
2:C:144:PRO:O	2:C:276:LYS:HD3	1.96	0.64
2:C:472:ARG:HB3	2:C:480:THR:O	1.97	0.64
3:D:1434:TRP:CZ3	3:D:1457:ASP:HB2	2.33	0.64
3:D:154:THR:HG23	3:D:157:GLU:H	1.63	0.64
1:K:117:VAL:HB	1:K:120:VAL:CG1	2.27	0.64
1:L:61:VAL:HG23	1:L:137:ARG:NH2	2.13	0.64
2:M:19:THR:O	2:M:23:VAL:HG23	1.97	0.64
3:N:1023:MET:HB2	3:N:1029:ARG:O	1.98	0.64
3:N:615:ARG:HB3	9:N:2387:HOH:O	1.97	0.64
4:O:59:ASN:HB3	4:O:62:THR:OG1	1.98	0.64
2:C:129:ILE:HG12	2:C:386:PHE:HB3	1.80	0.63
3:D:1147:ARG:HB3	3:D:1188:VAL:HG21	1.80	0.63
1:K:99:LEU:HB3	1:K:114:PHE:CD2	2.33	0.63
3:N:189:GLN:HG3	3:N:190:GLU:N	2.13	0.63
3:N:610:LYS:O	3:N:611:GLN:HG3	1.98	0.63
2:C:1014:SER:O	2:C:1018:GLN:HG3	1.97	0.63
2:C:439:CYS:SG	2:C:441:VAL:HB	2.39	0.63
3:D:558:LEU:HD13	5:F:145:PRO:CB	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:52:PRO:HB2	3:D:80:VAL:HG13	1.79	0.63
1:K:150:TYR:HE2	1:K:152:PRO:HG3	1.62	0.63
3:N:131:LYS:HE2	3:N:456:MET:HE1	1.80	0.63
3:N:569:ASN:HD21	5:P:210:LEU:HD22	1.62	0.63
1:B:61:VAL:N	1:B:137:ARG:HH22	1.96	0.63
2:C:200:LEU:HB2	9:C:1462:HOH:O	1.97	0.63
9:K:1622:HOH:O	2:M:640:ARG:HB2	1.98	0.63
5:P:166:LEU:HD11	9:P:491:HOH:O	1.98	0.63
3:D:764:LEU:HD23	3:D:767:HIS:CE1	2.33	0.63
1:K:120:VAL:HG13	9:K:2485:HOH:O	1.99	0.63
2:M:1016:ILE:HG23	3:N:526:PRO:HG2	1.79	0.63
2:M:1098:ASP:HB2	3:N:21:TRP:HZ2	1.63	0.63
2:M:693:GLU:HA	2:M:696:LYS:HG3	1.80	0.63
3:N:147:VAL:HA	9:N:1777:HOH:O	1.98	0.63
3:N:72:VAL:HG23	3:N:78:VAL:H	1.63	0.63
2:C:18:LEU:HD21	2:C:542:VAL:HG11	1.80	0.63
3:D:1397:LYS:HE3	9:D:2203:HOH:O	1.98	0.63
3:D:1439:SER:HB3	3:D:1463:LYS:HE2	1.79	0.63
1:K:177:VAL:HG12	9:K:1774:HOH:O	1.99	0.63
1:L:41:ARG:HG3	1:L:177:VAL:HG21	1.80	0.63
2:M:437:ARG:HG2	2:M:467:ILE:O	1.97	0.63
2:M:474:VAL:HG11	2:M:529:VAL:HG12	1.79	0.63
2:M:944:LEU:HD21	2:M:963:LEU:HD23	1.80	0.63
2:M:968:LEU:HB3	9:M:2164:HOH:O	1.98	0.63
3:N:169:TYR:CG	3:N:195:VAL:HG11	2.34	0.63
3:N:614:PHE:C	3:N:615:ARG:O	2.33	0.63
3:N:720:LEU:H	3:N:720:LEU:HD12	1.63	0.63
5:P:372:ARG:N	5:P:372:ARG:HD2	2.12	0.63
1:A:191:ASP:O	1:A:192:LEU:HD23	1.99	0.63
1:A:20:TYR:HE2	1:A:22:GLU:HG3	1.62	0.63
2:C:243:ARG:HG2	9:C:1218:HOH:O	1.99	0.63
2:C:358:ARG:HB3	2:C:371:LYS:O	1.98	0.63
3:D:1266:ARG:O	3:D:1268:PRO:HD3	1.98	0.63
3:D:562:ALA:HB1	3:D:567:ILE:HD11	1.80	0.63
3:D:614:PHE:HZ	5:F:326:ASP:HB3	1.63	0.63
3:D:785:ILE:HG22	3:D:789:LEU:HD12	1.80	0.63
5:F:132:ARG:O	5:F:136:LEU:HG	1.99	0.63
5:F:115:LYS:HD2	5:F:173:TYR:CE2	2.33	0.63
1:L:138:LEU:HD23	1:L:140:MET:SD	2.37	0.63
2:M:307:LEU:HG	2:M:311:PHE:HE2	1.62	0.63
3:N:890:VAL:HG13	3:N:926:LYS:HG2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:34:GLY:HA2	9:O:3283:HOH:O	1.98	0.63
1:A:109:VAL:HG23	1:A:132:LEU:HD13	1.80	0.63
2:C:304:LEU:HD23	2:C:305:PRO:HD3	1.80	0.63
3:D:799:LYS:N	3:D:826:PRO:HG2	2.12	0.63
1:L:72:LYS:HD2	9:L:2772:HOH:O	1.98	0.63
2:M:397:GLU:HB2	9:M:1672:HOH:O	1.97	0.63
2:M:820:ARG:HG3	9:M:1785:HOH:O	1.99	0.63
3:N:161:LEU:HD22	3:N:452:ILE:HG21	1.79	0.63
3:N:478:LEU:HD21	3:N:500:ARG:NH2	2.13	0.63
3:N:925:GLU:HB3	4:O:2:ALA:HB3	1.79	0.63
4:O:60:ALA:O	4:O:63:TRP:HB2	1.97	0.63
2:C:185:LYS:HE2	2:C:190:LYS:HE2	1.80	0.63
2:C:660:ALA:HB1	2:C:667:ALA:O	1.98	0.63
3:D:1046:GLN:HG3	9:D:1606:HOH:O	1.98	0.63
3:D:1432:LYS:HG3	3:D:1433:SER:H	1.64	0.63
3:D:1465:ASN:ND2	3:D:1470:ARG:HD3	2.12	0.63
3:D:65:ARG:HG3	3:D:66:GLN:H	1.64	0.63
4:E:54:LEU:HG	4:E:58:PRO:CG	2.27	0.63
1:L:182:GLU:O	1:L:194:LYS:HB3	1.98	0.63
3:N:610:LYS:HG2	7:N:1527:MXP:H15A	1.80	0.63
5:P:401:GLU:O	5:P:405:LEU:HB2	1.99	0.63
1:B:61:VAL:HG23	1:B:137:ARG:NH2	2.13	0.63
2:C:599:GLU:HB2	9:C:1216:HOH:O	1.99	0.63
2:C:659:PRO:HD3	9:C:1639:HOH:O	1.98	0.63
5:F:88:ILE:HB	5:F:193:ARG:HH11	1.63	0.63
2:M:265:ARG:HG2	2:M:266:ARG:N	2.14	0.63
3:N:1272:ALA:HA	3:N:1326:THR:HB	1.81	0.63
3:N:1356:TYR:CD2	3:N:1363:LEU:HD23	2.33	0.63
3:N:403:PHE:CE1	3:N:407:VAL:HG23	2.34	0.63
3:N:906:GLN:HB3	3:N:911:LEU:CD1	2.29	0.63
3:N:961:LYS:HA	9:N:2211:HOH:O	1.99	0.63
1:A:91:ASN:OD1	1:A:92:PRO:HD2	1.98	0.62
2:C:142:ARG:HH21	2:C:325:ILE:CD1	2.12	0.62
3:D:1109:GLU:HG2	3:D:1201:CYS:HA	1.81	0.62
5:F:372:ARG:N	5:F:372:ARG:HD2	2.14	0.62
2:M:1103:ASP:HB2	2:M:1107:ASN:O	1.99	0.62
2:M:790:LEU:HG	9:M:1781:HOH:O	1.99	0.62
5:P:356:LYS:HB2	9:P:473:HOH:O	1.99	0.62
1:A:18:ARG:O	1:A:207:PRO:HD3	1.98	0.62
1:B:182:GLU:O	1:B:194:LYS:HB3	1.98	0.62
2:C:343:GLN:HG2	2:C:385:PHE:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:367:LEU:O	2:C:372:LEU:HD13	1.99	0.62
3:D:1037:GLN:HG2	3:D:1042:ARG:HB3	1.81	0.62
3:D:1488:ASP:HA	9:E:110:HOH:O	1.99	0.62
3:D:179:VAL:HG13	3:D:183:GLU:HB3	1.81	0.62
3:D:55:ASP:HB3	9:D:1577:HOH:O	1.99	0.62
3:D:996:TRP:CE2	3:D:1056:PRO:HG2	2.34	0.62
1:L:55:SER:OG	1:L:158:ILE:HD13	2.00	0.62
2:M:1067:TYR:HE1	3:N:655:PRO:HG3	1.62	0.62
2:M:276:LYS:O	2:M:280:LYS:HB2	1.99	0.62
2:M:676:ILE:O	2:M:676:ILE:HG23	1.99	0.62
3:N:1109:GLU:HG2	3:N:1201:CYS:HA	1.81	0.62
3:N:188:GLY:HA2	9:N:1751:HOH:O	1.98	0.62
4:O:37:ASN:HA	4:O:93:TYR:CE2	2.34	0.62
5:P:152:ASP:HA	9:P:502:HOH:O	1.98	0.62
2:C:162:ILE:O	2:C:164:PRO:HD3	1.99	0.62
2:C:1109:VAL:HG11	3:D:5:VAL:HG13	1.79	0.62
3:D:58:CYS:HA	3:D:78:VAL:HG11	1.80	0.62
4:E:45:ARG:HB2	4:E:46:PRO:HD2	1.80	0.62
4:E:95:VAL:HG12	4:E:95:VAL:O	1.99	0.62
2:M:166:PRO:HD3	2:M:265:ARG:HG3	1.79	0.62
2:M:709:GLU:HG3	2:M:824:ARG:HG2	1.82	0.62
3:N:1262:LEU:HD23	3:N:1352:ILE:CG1	2.29	0.62
3:N:538:SER:HB3	9:P:565:HOH:O	1.97	0.62
3:N:860:LEU:HD22	3:N:878:GLY:HA2	1.81	0.62
4:O:83:ASP:O	4:O:86:GLN:HG2	1.99	0.62
2:C:1005:MET:O	2:C:1005:MET:HG3	1.99	0.62
2:C:165:LEU:O	2:C:265:ARG:HD2	1.99	0.62
1:L:18:ARG:O	1:L:207:PRO:HD3	1.99	0.62
1:L:52:ALA:HB2	1:L:170:VAL:O	1.99	0.62
1:L:59:GLU:HG3	1:L:139:ASN:ND2	2.14	0.62
3:N:1264:GLU:CD	3:N:1425:THR:HB	2.19	0.62
3:N:1290:LEU:CD2	3:N:1291:SER:H	2.12	0.62
3:N:40:GLU:N	9:N:1836:HOH:O	2.31	0.62
3:N:643:GLY:HA3	3:N:727:GLN:HB2	1.80	0.62
2:C:1001:VAL:HG13	9:C:1323:HOH:O	1.98	0.62
2:C:263:ASP:HB2	2:C:264:PRO:HD3	1.81	0.62
2:C:395:LYS:HE2	2:C:403:SER:CB	2.20	0.62
2:C:838:LYS:CE	2:C:846:LYS:HE2	2.29	0.62
3:D:187:LYS:HG3	3:D:199:LEU:HD22	1.81	0.62
3:D:165:LYS:HB2	3:D:397:LYS:HB3	1.81	0.62
3:D:47:GLU:HG2	3:D:53:ILE:HG22	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:865:THR:HG22	9:D:1855:HOH:O	1.99	0.62
5:F:119:ILE:HD13	5:F:170:HIS:ND1	2.15	0.62
2:M:110:GLU:CB	2:M:369:PRO:HG3	2.30	0.62
2:M:741:GLY:HA3	9:M:1665:HOH:O	1.99	0.62
3:N:185:VAL:HG23	3:N:202:VAL:C	2.18	0.62
3:N:510:GLU:HB3	9:N:2186:HOH:O	1.99	0.62
3:N:12:LEU:HD11	3:N:512:MET:HG2	1.80	0.62
3:N:52:PRO:HG3	3:N:78:VAL:HG13	1.81	0.62
3:N:583:ASP:OD2	3:N:604:THR:HG21	1.99	0.62
5:P:375:LEU:HG	5:P:376:ILE:HG13	1.82	0.62
1:B:79:ILE:HD12	9:B:474:HOH:O	1.98	0.62
2:C:971:LYS:HA	2:C:988:VAL:HA	1.82	0.62
3:D:834:THR:HB	3:D:838:ARG:HB2	1.81	0.62
3:D:860:LEU:HA	3:D:877:PRO:HB2	1.82	0.62
2:M:333:ILE:HD13	2:M:467:ILE:HG13	1.81	0.62
2:M:472:ARG:HB3	2:M:480:THR:O	2.00	0.62
2:M:480:THR:HG22	2:M:481:ASP:H	1.64	0.62
3:N:1189:ARG:HH11	3:N:1203:LYS:HB2	1.64	0.62
3:N:775:GLY:HA2	9:N:2264:HOH:O	2.00	0.62
3:N:864:VAL:HG12	3:N:865:THR:H	1.65	0.62
5:P:172:ARG:O	5:P:176:ILE:HD13	1.99	0.62
2:C:877:PRO:HG2	3:D:1023:MET:CE	2.27	0.62
3:D:1114:THR:CG2	3:D:1195:GLN:HB3	2.29	0.62
3:D:1231:GLU:HB3	3:D:1232:PRO:HD3	1.82	0.62
3:D:1356:TYR:HD2	3:D:1363:LEU:HD23	1.65	0.62
3:D:493:ARG:HH11	3:D:1390:LEU:HB3	1.63	0.62
3:D:1467:ILE:HG23	7:D:1527:MXP:H16A	1.81	0.62
3:D:877:PRO:O	3:D:880:ILE:HG22	1.99	0.62
1:K:48:ILE:HG22	1:K:173:PRO:HD2	1.80	0.62
1:L:223:THR:HG22	9:L:4161:HOH:O	1.98	0.62
2:M:1002:GLU:HG2	2:M:1003:ASP:N	2.14	0.62
2:M:146:VAL:HG11	2:M:306:THR:HG22	1.81	0.62
2:M:431:HIS:HD2	2:M:433:THR:H	1.45	0.62
2:M:80:GLN:O	2:M:83:CYS:HB2	1.99	0.62
2:C:244:PRO:HG3	9:C:1642:HOH:O	1.98	0.62
3:D:1321:ALA:O	3:D:1339:LYS:HE3	2.00	0.62
3:D:491:LYS:HD3	9:D:1938:HOH:O	1.99	0.62
9:D:1795:HOH:O	4:E:50:THR:HB	2.00	0.62
3:N:957:PRO:CG	3:N:1007:VAL:HA	2.27	0.62
3:N:723:GLY:HA3	9:N:1625:HOH:O	2.00	0.62
4:O:30:LEU:O	4:O:35:PHE:HA	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:THR:HG22	1:B:209:GLU:HB2	1.81	0.62
3:D:1056:PRO:HD3	9:D:1650:HOH:O	1.99	0.62
3:D:1111:ASP:HB3	3:D:1203:LYS:HG3	1.82	0.62
3:D:49:ILE:HG21	9:D:2241:HOH:O	2.00	0.62
5:F:396:ARG:HB2	9:F:496:HOH:O	1.98	0.62
2:M:498:GLN:O	2:M:501:THR:HG23	2.00	0.62
2:M:559:LEU:HD23	2:M:560:MET:N	2.14	0.62
2:M:567:GLN:HB2	2:M:997:LEU:HD22	1.80	0.62
2:M:715:THR:HG22	2:M:717:LEU:HG	1.82	0.62
2:M:722:ILE:CD1	2:M:823:VAL:HG21	2.29	0.62
2:M:86:LYS:CD	2:M:813:VAL:HG12	2.30	0.62
2:M:557:ARG:NH1	2:M:879:ARG:HG2	2.15	0.62
3:N:1192:LEU:HD13	3:N:1345:GLU:HG2	1.81	0.62
2:C:274:ARG:HG2	9:C:1142:HOH:O	1.99	0.62
2:C:307:LEU:HG	2:C:311:PHE:CE2	2.35	0.62
3:D:428:LYS:HE2	9:D:1881:HOH:O	2.00	0.62
3:N:1013:GLU:HB2	9:N:1747:HOH:O	2.00	0.62
3:N:1258:ARG:NH2	3:N:1262:LEU:HD11	2.15	0.62
3:N:1293:PHE:CZ	3:N:1302:GLU:HB3	2.34	0.62
3:N:394:LEU:HD21	9:N:2081:HOH:O	2.00	0.62
1:B:83:LYS:HE2	1:B:168:ASP:HB2	1.81	0.61
2:C:137:VAL:HG22	2:C:391:LEU:O	2.00	0.61
2:C:141:HIS:CB	2:C:418:LEU:HG	2.29	0.61
2:C:420:ARG:HA	9:C:1293:HOH:O	1.98	0.61
2:C:738:ASP:CB	2:C:744:ARG:HB3	2.29	0.61
2:C:902:ILE:O	2:C:904:PRO:HD3	2.00	0.61
3:D:107:ASP:O	3:D:108:VAL:C	2.37	0.61
3:D:1269:LYS:HD3	9:D:2029:HOH:O	1.99	0.61
3:D:1291:SER:HB2	3:D:1293:PHE:HE1	1.65	0.61
1:L:128:HIS:HE1	1:L:131:THR:HG23	1.64	0.61
1:L:169:ALA:HB1	1:L:171:PHE:CD2	2.35	0.61
3:N:1295:GLU:HB3	3:N:1300:SER:CB	2.30	0.61
3:N:683:ILE:HG22	9:N:1566:HOH:O	2.00	0.61
3:N:717:GLN:HG2	9:N:1629:HOH:O	2.00	0.61
3:N:80:VAL:HA	9:N:2248:HOH:O	1.99	0.61
2:C:528:GLU:HG2	9:C:1477:HOH:O	1.99	0.61
2:C:63:GLY:HA3	9:C:1168:HOH:O	1.98	0.61
2:C:31:GLN:HB3	2:C:71:TYR:OH	2.00	0.61
3:D:400:VAL:HG22	3:D:443:VAL:CG2	2.29	0.61
3:D:613:ARG:HG3	3:D:1441:GLN:HB2	1.82	0.61
3:D:955:VAL:HA	9:D:2261:HOH:O	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:30:LEU:O	4:E:35:PHE:HA	2.00	0.61
2:M:864:GLY:O	2:M:866:PRO:HD3	2.00	0.61
3:N:1036:ARG:HH21	3:N:1042:ARG:HA	1.64	0.61
3:N:1274:ILE:HA	9:N:1761:HOH:O	2.00	0.61
3:N:1304:LYS:HA	9:N:1838:HOH:O	1.99	0.61
3:N:491:LYS:HD3	9:N:2284:HOH:O	1.98	0.61
3:N:611:GLN:CG	3:N:619:LEU:HG	2.29	0.61
4:O:86:GLN:O	4:O:90:GLU:HG3	2.00	0.61
5:P:88:ILE:HG21	5:P:193:ARG:HD3	1.83	0.61
2:C:151:ASP:OD2	2:C:159:ILE:HG23	2.00	0.61
2:C:512:ARG:HB2	9:C:1201:HOH:O	2.00	0.61
3:D:50:PHE:CB	3:D:522:PRO:HG2	2.29	0.61
2:M:274:ARG:HD2	2:M:285:LEU:O	1.99	0.61
2:M:838:LYS:CE	2:M:846:LYS:HE2	2.29	0.61
2:M:926:PHE:CE1	2:M:929:ARG:HD3	2.35	0.61
5:P:284:ARG:HD2	9:P:504:HOH:O	1.99	0.61
2:C:305:PRO:HA	2:C:308:ARG:HD2	1.82	0.61
3:D:1097:LYS:HE3	9:D:2031:HOH:O	2.01	0.61
3:D:1430:SER:HA	9:D:1920:HOH:O	1.99	0.61
1:K:109:VAL:HG23	1:K:132:LEU:HD13	1.81	0.61
1:K:67:THR:HG21	2:M:609:ASN:ND2	2.07	0.61
2:M:144:PRO:HA	2:M:163:ILE:HG13	1.82	0.61
2:M:239:PHE:HB3	9:M:1968:HOH:O	2.00	0.61
3:N:1042:ARG:O	3:N:1057:VAL:HB	2.00	0.61
3:N:702:LEU:HD13	3:N:716:PHE:HD1	1.64	0.61
9:N:1961:HOH:O	5:P:168:LYS:HG2	2.01	0.61
9:N:2314:HOH:O	5:P:376:ILE:HD11	1.99	0.61
1:A:125:PRO:HD2	9:A:394:HOH:O	2.00	0.61
1:A:184:THR:HG23	1:A:192:LEU:HB2	1.82	0.61
2:C:1002:GLU:HG2	2:C:1003:ASP:N	2.14	0.61
2:C:1056:LYS:NZ	3:D:749:VAL:O	2.33	0.61
2:C:143:SER:HB2	2:C:276:LYS:NZ	2.14	0.61
2:C:399:ASN:ND2	2:C:568:ALA:HB3	2.15	0.61
2:C:625:LEU:HB3	2:C:639:GLN:HB2	1.82	0.61
3:D:847:ASP:O	3:D:851:LEU:HG	2.01	0.61
5:F:230:LYS:HD3	9:F:439:HOH:O	1.99	0.61
9:D:1675:HOH:O	5:F:337:HIS:HB3	2.01	0.61
5:F:361:LEU:HD23	5:F:362:SER:N	2.15	0.61
2:M:267:TYR:HB2	2:M:272:ALA:HB1	1.82	0.61
2:M:367:LEU:O	2:M:372:LEU:HD13	2.01	0.61
2:M:358:ARG:HB3	2:M:371:LYS:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1102:THR:HG22	3:N:1222:GLY:HA2	1.82	0.61
3:N:1173:LEU:HD23	3:N:1174:LEU:HD23	1.83	0.61
3:N:1389:LEU:HD12	3:N:1390:LEU:H	1.65	0.61
3:N:996:TRP:CE3	3:N:999:THR:HG21	2.35	0.61
1:B:108:GLU:HB2	9:B:409:HOH:O	2.00	0.61
2:C:1007:ALA:HB2	3:D:648:MET:HG3	1.82	0.61
2:C:1066:ALA:O	2:C:1070:ILE:HG13	1.99	0.61
2:C:123:GLU:HB2	9:C:1197:HOH:O	2.00	0.61
2:C:675:ALA:HA	2:C:989:VAL:HG12	1.83	0.61
2:C:6:PHE:CG	2:C:909:ALA:HA	2.35	0.61
3:D:119:SER:HB2	3:D:123:LEU:HD13	1.81	0.61
2:M:15:LEU:H	2:M:15:LEU:HD12	1.66	0.61
2:M:176:VAL:HG12	2:M:182:VAL:CG1	2.31	0.61
2:M:57:GLU:HG3	9:M:1902:HOH:O	1.99	0.61
3:N:119:SER:HB2	3:N:123:LEU:HD13	1.81	0.61
3:N:1377:LYS:HG3	3:N:1394:VAL:HG13	1.81	0.61
3:N:400:VAL:HG13	3:N:402:PRO:HD3	1.83	0.61
3:N:52:PRO:HG2	3:N:80:VAL:HG13	1.81	0.61
2:C:333:ILE:CD1	2:C:467:ILE:HG13	2.30	0.61
2:C:64:LEU:HD13	2:C:359:MET:HG3	1.82	0.61
2:C:108:ILE:HB	2:C:368:THR:HG1	1.65	0.61
3:D:204:LEU:HG	3:D:441:ARG:HH12	1.66	0.61
3:D:637:LEU:HD11	3:D:642:CYS:N	2.15	0.61
3:D:715:ALA:HB3	3:D:764:LEU:HA	1.82	0.61
5:F:335:ASP:OD1	5:F:338:LEU:HB2	2.01	0.61
3:N:128:TYR:HE1	3:N:461:ILE:HG13	1.65	0.61
3:N:187:LYS:HG3	3:N:199:LEU:HD22	1.83	0.61
3:N:674:ARG:HD3	9:N:1957:HOH:O	2.01	0.61
5:P:203:THR:HG22	5:P:204:GLY:N	2.16	0.61
1:A:150:TYR:CE2	1:A:152:PRO:HG3	2.35	0.61
2:C:455:LEU:HD12	2:C:456:ALA:O	2.00	0.61
3:D:1384:PRO:HG3	3:D:1389:LEU:HA	1.83	0.61
3:D:65:ARG:CG	3:D:66:GLN:H	2.13	0.61
1:K:20:TYR:HD2	1:K:21:GLY:H	1.49	0.61
1:L:143:ARG:HD2	1:L:160:ASP:OD2	2.00	0.61
1:L:83:LYS:HA	9:L:2646:HOH:O	2.00	0.61
2:M:479:VAL:HG11	2:M:532:MET:HE2	1.81	0.61
3:N:500:ARG:HD2	9:N:2131:HOH:O	2.00	0.61
3:N:799:LYS:H	3:N:826:PRO:HG2	1.66	0.61
1:A:20:TYR:CD2	1:A:21:GLY:N	2.63	0.61
2:C:775:ARG:HG3	9:C:1214:HOH:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:919:ALA:HA	9:C:1166:HOH:O	2.00	0.61
3:D:169:TYR:CG	3:D:195:VAL:HG11	2.36	0.61
3:D:486:ARG:HD3	3:D:489:ARG:HD3	1.81	0.61
3:D:206:ARG:HH11	5:F:97:GLU:HB3	1.65	0.61
1:L:57:TYR:HE1	1:L:163:ASN:HB2	1.65	0.61
2:M:307:LEU:HG	2:M:311:PHE:CE2	2.36	0.61
3:N:1420:LEU:HD12	3:N:1421:LEU:N	2.14	0.61
3:N:31:THR:HG23	3:N:45:PHE:CE2	2.35	0.61
3:N:824:ASN:HB2	9:N:1978:HOH:O	2.01	0.61
1:L:176:ARG:HH21	3:N:850:LEU:HD13	1.65	0.61
2:C:1067:TYR:O	2:C:1071:ILE:HG12	2.01	0.61
2:C:1065:ALA:HB1	2:C:1077:PRO:HG2	1.83	0.61
2:C:325:ILE:HG12	9:C:1558:HOH:O	2.00	0.61
2:C:73:LEU:HD23	2:C:94:LEU:HB2	1.83	0.61
3:D:1127:GLU:HB2	9:D:1604:HOH:O	2.00	0.61
3:D:1394:VAL:HG11	9:D:2203:HOH:O	2.00	0.61
3:D:400:VAL:HG13	3:D:402:PRO:HD3	1.83	0.61
3:D:633:VAL:HG22	3:D:635:PRO:CD	2.30	0.61
3:D:850:LEU:HD12	3:D:850:LEU:N	2.15	0.61
2:M:41:ASN:ND2	2:M:41:ASN:H	1.94	0.61
3:N:860:LEU:HA	3:N:877:PRO:HB2	1.82	0.61
1:B:90:LEU:HD23	9:B:496:HOH:O	1.99	0.60
2:C:926:PHE:CE1	2:C:929:ARG:HD3	2.36	0.60
2:C:969:GLN:HA	9:D:1915:HOH:O	2.00	0.60
3:D:10:ILE:HG13	3:D:1434:TRP:CZ2	2.35	0.60
3:D:130:SER:HB3	3:D:132:TYR:CE1	2.36	0.60
3:D:1393:GLN:CB	3:D:1398:TRP:HE1	2.10	0.60
3:D:1462:LEU:HD22	3:D:1472:ILE:HG23	1.83	0.60
3:D:471:GLU:HG3	9:D:1589:HOH:O	2.01	0.60
3:D:631:ILE:HG12	3:D:743:ASP:O	2.00	0.60
1:K:206:THR:CG2	1:K:209:GLU:H	2.14	0.60
1:K:221:HIS:HA	1:K:224:TYR:HD2	1.64	0.60
3:N:204:LEU:HD21	3:N:445:ARG:HH12	1.65	0.60
2:C:331:ARG:HB2	9:C:1737:HOH:O	1.99	0.60
2:C:1118:LYS:HG2	3:D:23:TYR:CE1	2.36	0.60
2:C:1067:TYR:HE1	3:D:655:PRO:HG3	1.65	0.60
1:L:2:LEU:HD12	1:L:3:ASP:N	2.16	0.60
3:N:1291:SER:HB2	3:N:1293:PHE:CE1	2.35	0.60
3:N:131:LYS:HE3	3:N:568:ARG:CB	2.31	0.60
3:N:809:PRO:HB2	3:N:812:ALA:HB2	1.82	0.60
5:P:247:ILE:HG22	5:P:251:ILE:HD11	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:95:THR:HG21	9:P:531:HOH:O	2.01	0.60
1:B:106:PRO:HG3	1:B:134:GLU:HG2	1.82	0.60
1:B:206:THR:HG22	1:B:209:GLU:H	1.66	0.60
2:C:193:LEU:HD21	9:C:1526:HOH:O	2.02	0.60
3:D:507:ASN:HA	9:D:2352:HOH:O	2.01	0.60
3:D:728:LEU:HD22	3:D:745:MET:SD	2.42	0.60
1:K:157:GLY:HA3	9:K:2579:HOH:O	2.01	0.60
1:K:42:ARG:NH2	2:M:857:ASP:HB3	2.15	0.60
2:M:341:THR:O	2:M:345:ARG:HG3	2.00	0.60
3:N:1434:TRP:CZ3	3:N:1457:ASP:HB2	2.36	0.60
3:N:27:GLU:HB2	9:N:2072:HOH:O	2.00	0.60
3:N:509:PRO:HB2	9:N:1664:HOH:O	2.00	0.60
3:D:1299:PHE:HB2	9:D:2455:HOH:O	2.00	0.60
3:D:86:ARG:O	3:D:522:PRO:HD2	2.01	0.60
3:D:559:ALA:HA	9:F:646:HOH:O	2.01	0.60
3:D:829:VAL:H	3:D:835:SER:HB2	1.66	0.60
3:D:860:LEU:HD22	3:D:878:GLY:HA2	1.84	0.60
1:K:213:GLN:O	1:K:217:ILE:HG13	2.02	0.60
2:M:811:PRO:HG2	9:M:1891:HOH:O	2.00	0.60
3:N:107:ASP:O	3:N:108:VAL:C	2.39	0.60
3:N:52:PRO:CG	3:N:78:VAL:HG13	2.31	0.60
3:N:95:LEU:HA	3:N:551:ASN:ND2	2.16	0.60
3:N:566:ILE:HG23	5:P:217:ASN:HD22	1.66	0.60
2:C:1101:THR:HB	3:D:5:VAL:HG13	1.83	0.60
2:C:720:GLU:HA	2:C:759:THR:O	2.02	0.60
3:D:29:PRO:HB3	3:D:545:ARG:HG2	1.84	0.60
3:D:517:VAL:HG11	3:D:581:LEU:HD21	1.83	0.60
3:D:569:ASN:HB3	5:F:214:GLN:HE21	1.65	0.60
2:M:554:ASP:OD2	2:M:556:ASN:HB3	2.01	0.60
2:M:747:ALA:O	2:M:799:ILE:HA	2.01	0.60
2:M:971:LYS:HA	2:M:988:VAL:HA	1.84	0.60
3:N:799:LYS:N	3:N:826:PRO:HG2	2.16	0.60
3:N:80:VAL:HG12	3:N:81:THR:O	2.02	0.60
5:P:209:PHE:CE2	5:P:213:ILE:HD11	2.37	0.60
1:A:38:ASN:HB3	1:A:39:PRO:HD3	1.83	0.60
2:C:93:PRO:HG3	2:C:117:HIS:CE1	2.37	0.60
2:C:132:ALA:HB1	2:C:632:ASN:ND2	2.16	0.60
2:C:571:LEU:HD21	2:C:700:TYR:HA	1.82	0.60
5:F:369:LEU:HB2	9:F:426:HOH:O	2.02	0.60
9:K:3509:HOH:O	1:L:155:LYS:HE2	2.00	0.60
2:M:265:ARG:HB3	2:M:267:TYR:CD2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:518:LYS:HA	9:M:1901:HOH:O	2.02	0.60
2:M:890:LEU:CA	2:M:914:ILE:HD11	2.31	0.60
3:N:1109:GLU:HG2	3:N:1202:GLN:H	1.66	0.60
4:O:54:LEU:CD2	4:O:63:TRP:HE1	2.14	0.60
5:P:325:LYS:HB2	9:P:652:HOH:O	2.01	0.60
2:C:169:GLY:HA3	9:C:1253:HOH:O	2.01	0.60
2:C:52:PHE:CD2	2:C:68:PHE:HB2	2.37	0.60
2:C:559:LEU:HD23	2:C:560:MET:N	2.17	0.60
3:D:519:VAL:HG13	3:D:544:TYR:CZ	2.36	0.60
3:D:984:THR:HG22	3:D:987:GLU:H	1.66	0.60
5:F:132:ARG:HD2	9:F:492:HOH:O	2.02	0.60
5:F:375:LEU:HG	5:F:376:ILE:HG13	1.83	0.60
1:K:18:ARG:HD2	1:K:123:MET:HE1	1.84	0.60
1:L:5:LYS:O	1:L:8:ALA:HB2	2.01	0.60
2:M:1104:GLU:HG3	9:M:1982:HOH:O	2.01	0.60
2:M:218:VAL:HA	2:M:221:LEU:HD23	1.84	0.60
2:M:218:VAL:HG22	2:M:221:LEU:HD23	1.84	0.60
3:N:142:LEU:HD11	9:N:2326:HOH:O	2.01	0.60
3:N:439:LEU:HB3	9:N:2015:HOH:O	1.99	0.60
3:N:583:ASP:OD1	3:N:586:ARG:HG3	2.01	0.60
3:N:647:ARG:HB3	9:N:2056:HOH:O	1.99	0.60
5:P:88:ILE:HD13	5:P:193:ARG:HB2	1.82	0.60
1:B:175:ARG:O	1:B:176:ARG:HG3	2.01	0.60
2:C:712:ALA:O	2:C:820:ARG:CB	2.50	0.60
2:C:818:GLY:N	5:F:309:LYS:HE2	2.17	0.60
3:D:1123:PHE:HA	3:D:1133:ARG:O	2.01	0.60
5:F:151:LEU:HB3	9:F:614:HOH:O	2.00	0.60
1:L:7:LYS:O	1:L:7:LYS:HG3	2.02	0.60
2:M:565:GLN:HA	2:M:995:MET:HE1	1.84	0.60
3:N:477:LEU:HD11	3:N:495:ARG:HD3	1.84	0.60
3:N:961:LYS:HB3	9:N:2007:HOH:O	2.00	0.60
1:B:132:LEU:HD21	1:B:136:GLY:O	2.01	0.60
2:C:1017:THR:HG23	9:C:1263:HOH:O	2.00	0.60
2:C:260:LEU:HA	2:C:291:ALA:CB	2.31	0.60
2:C:591:SER:HA	9:C:1421:HOH:O	2.02	0.60
2:C:816:LYS:HB2	2:C:819:VAL:HG21	1.84	0.60
3:D:408:GLU:HA	5:F:171:LYS:NZ	2.16	0.60
1:K:7:LYS:HZ1	1:K:186:LEU:HD21	1.67	0.60
1:K:18:ARG:NH1	1:K:88:ARG:HD3	2.16	0.60
2:M:9:ILE:HG13	2:M:9:ILE:O	2.02	0.60
3:N:1114:THR:CG2	3:N:1195:GLN:HB3	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:141:ILE:HG22	3:N:450:TYR:H	1.66	0.60
3:N:161:LEU:O	3:N:161:LEU:HD23	2.02	0.60
3:N:73:CYS:HB3	3:N:76:CYS:O	2.02	0.60
2:C:1008:ARG:HD2	2:C:1028:GLY:N	2.17	0.60
2:C:137:VAL:HG23	2:C:391:LEU:HG	1.83	0.60
3:D:1125:PRO:HB2	9:D:2360:HOH:O	2.01	0.60
3:D:1295:GLU:HB3	3:D:1300:SER:CB	2.32	0.60
3:D:1326:THR:HG23	9:D:2026:HOH:O	2.01	0.60
3:D:776:GLU:HB3	3:D:912:LYS:HE2	1.84	0.60
1:L:217:ILE:O	1:L:221:HIS:ND1	2.33	0.60
2:M:710:ILE:HD11	2:M:758:ARG:HD3	1.84	0.60
2:M:833:LEU:HD12	2:M:834:GLN:H	1.67	0.60
2:M:874:LEU:HD12	3:N:784:ASP:OD2	2.02	0.60
3:N:1114:THR:H	3:N:1195:GLN:HE21	1.50	0.60
3:N:10:ILE:HG13	3:N:1434:TRP:CE2	2.37	0.60
3:N:130:SER:O	3:N:568:ARG:NH2	2.35	0.60
4:O:61:VAL:O	4:O:65:MET:HG3	2.02	0.60
4:O:9:LEU:HD22	4:O:19:LEU:HD11	1.83	0.60
1:A:123:MET:C	1:A:125:PRO:HD3	2.22	0.59
1:B:123:MET:C	1:B:125:PRO:HD3	2.22	0.59
2:C:244:PRO:HD2	2:C:245:GLY:H	1.65	0.59
2:C:431:HIS:H	2:C:434:HIS:CD2	2.20	0.59
3:D:1117:TYR:HB3	9:D:2262:HOH:O	2.02	0.59
3:D:438:ASP:HB3	9:D:1574:HOH:O	2.02	0.59
3:D:519:VAL:HG13	3:D:544:TYR:CE1	2.37	0.59
1:K:191:ASP:O	1:K:192:LEU:HD23	2.01	0.59
2:M:1018:GLN:OE1	2:M:1060:ILE:HD11	2.02	0.59
2:M:1066:ALA:O	2:M:1070:ILE:HG13	2.02	0.59
2:M:139:GLN:NE2	2:M:415:PRO:HD2	2.17	0.59
3:N:204:LEU:HB2	3:N:394:LEU:HG	1.83	0.59
5:P:93:LEU:HG	5:P:190:ALA:CB	2.32	0.59
2:C:139:GLN:HE22	2:C:415:PRO:CD	2.15	0.59
2:C:712:ALA:O	2:C:820:ARG:HB2	2.02	0.59
2:C:933:GLY:HA2	9:C:1525:HOH:O	2.02	0.59
3:D:133:ILE:HG21	9:D:1764:HOH:O	2.02	0.59
3:D:409:VAL:CG1	3:D:435:VAL:HG11	2.31	0.59
3:D:37:LEU:HD13	3:D:535:PHE:HZ	1.68	0.59
3:D:786:ILE:HD13	3:D:1027:GLY:HA3	1.83	0.59
5:F:372:ARG:HG3	9:F:595:HOH:O	2.01	0.59
1:K:198:ARG:HG2	9:K:1904:HOH:O	2.01	0.59
1:L:59:GLU:HG3	1:L:139:ASN:HD22	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:169:TYR:O	3:N:392:SER:HB2	2.01	0.59
3:N:550:ARG:HH11	3:N:573:MET:HB3	1.67	0.59
3:N:675:ARG:HG2	3:N:678:GLU:OE2	2.02	0.59
3:N:865:THR:HG22	9:N:1713:HOH:O	2.03	0.59
1:A:117:VAL:HB	1:A:120:VAL:CG1	2.31	0.59
1:B:89:PHE:HB3	1:B:94:LEU:HD22	1.84	0.59
2:C:471:TYR:CE2	2:C:496:ILE:HG21	2.36	0.59
3:D:133:ILE:HG22	3:D:455:ARG:N	2.17	0.59
3:D:47:GLU:HG2	9:D:1900:HOH:O	2.02	0.59
3:D:617:ASN:OD1	3:D:617:ASN:N	2.36	0.59
3:D:704:ARG:HD2	3:D:738:ALA:HB2	1.84	0.59
4:E:47:LYS:HE2	9:E:154:HOH:O	2.03	0.59
2:M:833:LEU:HD12	2:M:834:GLN:N	2.17	0.59
3:N:1087:ARG:HG2	3:N:1238:MET:HB3	1.83	0.59
3:N:1264:GLU:O	3:N:1266:ARG:HG3	2.02	0.59
2:M:1085:PHE:CD2	3:N:1468:LEU:HA	2.36	0.59
3:N:50:PHE:HB3	3:N:522:PRO:HG2	1.83	0.59
3:N:565:ILE:HD12	5:P:192:LEU:HD13	1.84	0.59
3:N:704:ARG:HD2	3:N:738:ALA:HB2	1.83	0.59
3:N:770:LEU:HB3	9:N:1689:HOH:O	2.01	0.59
3:N:95:LEU:HA	3:N:551:ASN:HD21	1.66	0.59
1:B:169:ALA:HB1	1:B:171:PHE:CE2	2.37	0.59
3:D:1023:MET:HB2	3:D:1029:ARG:O	2.03	0.59
3:D:1272:ALA:HA	3:D:1326:THR:HB	1.83	0.59
3:D:486:ARG:HD2	9:D:1689:HOH:O	2.03	0.59
3:D:644:LEU:HD12	3:D:645:PRO:HD2	1.83	0.59
3:D:804:LEU:HD23	3:D:804:LEU:H	1.68	0.59
3:D:980:MET:HG3	9:D:1653:HOH:O	2.01	0.59
5:F:295:MET:HG2	5:F:299:TRP:CE2	2.37	0.59
1:K:88:ARG:HG2	1:K:121:GLU:HG2	1.84	0.59
1:K:50:GLY:O	1:K:146:ARG:HA	2.02	0.59
1:L:226:SER:O	1:L:228:PRO:HD3	2.02	0.59
2:M:1038:TRP:HA	2:M:1041:GLU:HB2	1.84	0.59
2:M:328:LEU:HD22	2:M:437:ARG:HB3	1.83	0.59
2:M:468:ARG:HD3	9:M:2184:HOH:O	2.01	0.59
3:N:165:LYS:HG3	3:N:397:LYS:HD3	1.84	0.59
3:N:734:GLU:HB2	9:N:1648:HOH:O	2.01	0.59
4:O:33:HIS:HB2	4:O:37:ASN:HD21	1.66	0.59
2:C:510:ALA:HB3	2:C:513:VAL:CG2	2.32	0.59
2:C:966:LEU:HD21	2:C:986:PRO:HG3	1.85	0.59
3:D:1088:THR:HG21	9:D:1813:HOH:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:192:ALA:HB1	9:D:2083:HOH:O	2.02	0.59
1:K:89:PHE:HB3	1:K:94:LEU:HD22	1.84	0.59
2:M:208:ALA:O	2:M:218:VAL:HG21	2.02	0.59
2:M:305:PRO:HA	2:M:308:ARG:HD2	1.84	0.59
3:N:1342:GLU:HG3	9:N:1945:HOH:O	2.03	0.59
3:N:1357:ARG:HB2	9:N:1826:HOH:O	2.01	0.59
3:N:570:GLU:HB2	5:P:214:GLN:OE1	2.02	0.59
1:A:123:MET:O	1:A:125:PRO:HD3	2.03	0.59
1:B:40:LEU:HD21	1:B:215:VAL:HG12	1.84	0.59
3:D:169:TYR:O	3:D:392:SER:HB2	2.02	0.59
3:D:926:LYS:HE2	9:D:1617:HOH:O	2.01	0.59
2:C:984:GLU:HG3	3:D:944:THR:O	2.02	0.59
4:E:9:LEU:HB3	4:E:19:LEU:HD21	1.85	0.59
3:D:408:GLU:HA	5:F:171:LYS:HZ1	1.67	0.59
5:F:220:LEU:HD12	5:F:243:ILE:HD11	1.83	0.59
5:F:256:ARG:HD3	9:F:585:HOH:O	2.03	0.59
5:F:268:ILE:HD13	5:F:311:ALA:HB2	1.83	0.59
2:M:200:LEU:HD13	2:M:300:ASP:CG	2.23	0.59
2:M:404:LEU:HA	2:M:407:LYS:HD2	1.84	0.59
2:M:750:LYS:HB3	9:N:2087:HOH:O	2.02	0.59
3:N:1117:TYR:HB3	9:N:1591:HOH:O	2.03	0.59
3:N:133:ILE:HG22	3:N:455:ARG:N	2.18	0.59
3:N:1403:LEU:HD23	9:N:1794:HOH:O	2.02	0.59
3:N:434:ARG:HG2	9:N:2229:HOH:O	2.03	0.59
3:N:562:ALA:HB1	3:N:567:ILE:HD11	1.85	0.59
3:N:560:GLN:OE1	5:P:218:GLN:HG3	2.01	0.59
5:P:361:LEU:CD2	5:P:366:ALA:HB2	2.27	0.59
2:C:230:ARG:HG3	9:C:1406:HOH:O	2.01	0.59
2:C:260:LEU:HD21	9:C:1182:HOH:O	2.02	0.59
2:C:346:VAL:O	2:C:350:ARG:HG3	2.03	0.59
3:D:31:THR:HG23	3:D:45:PHE:CE2	2.37	0.59
3:D:490:ALA:HA	9:D:1529:HOH:O	2.03	0.59
2:C:987:ILE:HG23	3:D:948:THR:HG21	1.84	0.59
4:E:41:GLU:N	4:E:42:PRO:HD2	2.17	0.59
2:M:1034:GLU:HA	2:M:1037:VAL:HG23	1.83	0.59
2:M:208:ALA:HB1	2:M:218:VAL:HG13	1.84	0.59
2:M:482:GLU:HB3	9:M:2150:HOH:O	2.02	0.59
2:M:627:ARG:HG3	2:M:628:PHE:H	1.68	0.59
2:M:738:ASP:CB	2:M:744:ARG:HB3	2.31	0.59
2:M:816:LYS:HB2	2:M:819:VAL:HG21	1.84	0.59
2:M:92:ALA:HB2	2:M:120:LEU:HD11	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:113:ILE:HG23	5:P:127:ILE:HB	1.85	0.59
5:P:400:ILE:HD11	9:P:513:HOH:O	2.02	0.59
1:A:26:GLU:HG3	1:A:27:PRO:HD3	1.85	0.59
2:C:19:THR:O	2:C:23:VAL:HG23	2.02	0.59
2:C:69:LEU:HD12	2:C:97:ARG:HB3	1.85	0.59
2:C:773:LEU:O	2:C:777:ILE:HG13	2.03	0.59
3:D:47:GLU:HA	3:D:51:GLY:O	2.03	0.59
3:D:824:ASN:HB3	9:D:2122:HOH:O	2.01	0.59
4:E:7:ASP:HB2	9:E:100:HOH:O	2.03	0.59
5:F:369:LEU:O	5:F:373:LYS:HB2	2.02	0.59
5:F:400:ILE:HD11	9:F:643:HOH:O	2.03	0.59
2:M:191:PHE:CZ	2:M:196:LEU:HB2	2.35	0.59
2:M:579:VAL:HB	2:M:890:LEU:CD2	2.33	0.59
3:N:404:GLU:HB2	9:N:1640:HOH:O	2.03	0.59
2:C:185:LYS:HE2	2:C:190:LYS:HG2	1.84	0.59
2:C:200:LEU:HD13	2:C:300:ASP:CG	2.23	0.59
2:C:408:ARG:HH21	2:C:542:VAL:HG22	1.66	0.59
2:C:564:MET:HG3	2:C:997:LEU:HD11	1.84	0.59
2:C:841:ASN:HD21	2:C:845:ASN:H	1.50	0.59
3:D:1102:THR:HG22	3:D:1222:GLY:CA	2.32	0.59
3:D:646:LYS:HE2	3:D:722:GLU:HG2	1.84	0.59
2:C:1115:LEU:HB3	3:D:85:VAL:HG13	1.85	0.59
1:L:182:GLU:HB2	9:L:2617:HOH:O	2.01	0.59
2:M:1053:LEU:HB3	9:N:2033:HOH:O	2.03	0.59
2:M:585:GLU:HB3	9:M:1636:HOH:O	2.01	0.59
3:N:1108:ARG:NH2	3:N:1198:TYR:HB2	2.16	0.59
3:N:1299:PHE:HB2	9:N:1861:HOH:O	2.02	0.59
3:N:1351:GLU:HG2	9:N:1724:HOH:O	2.02	0.59
3:N:847:ASP:O	3:N:851:LEU:HG	2.02	0.59
3:N:897:TRP:CH2	3:N:902:LEU:HD21	2.38	0.59
5:P:130:VAL:HA	5:P:142:ARG:NH2	2.17	0.59
2:C:163:ILE:HG13	2:C:163:ILE:O	2.01	0.59
2:C:362:GLY:HA3	2:C:367:LEU:CD2	2.33	0.59
2:C:410:ILE:HD11	2:C:455:LEU:HB3	1.84	0.59
2:C:705:ILE:HG12	2:C:828:ALA:HB2	1.85	0.59
2:C:36:PRO:HG3	2:C:71:TYR:CE2	2.38	0.59
3:D:187:LYS:CE	3:D:199:LEU:HB3	2.27	0.59
3:D:448:GLU:HG2	3:D:448:GLU:O	2.02	0.59
5:F:361:LEU:HD22	5:F:366:ALA:HB2	1.85	0.59
1:K:158:ILE:H	1:K:166:PRO:HG3	1.68	0.59
1:L:101:LEU:HD11	9:L:1850:HOH:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:489:ARG:HH21	3:N:1389:LEU:HD11	1.67	0.59
5:P:406:ARG:O	5:P:409:LYS:HG2	2.02	0.59
1:A:161:ARG:HB2	1:A:161:ARG:NH1	2.18	0.58
2:C:294:GLU:HB3	9:C:1227:HOH:O	2.03	0.58
2:C:437:ARG:CZ	2:C:488:ALA:HA	2.33	0.58
2:C:402:SER:OG	2:C:566:THR:HG22	2.02	0.58
3:D:1243:THR:HB	3:D:1253:THR:HG22	1.85	0.58
3:D:1311:LEU:HD22	9:D:1836:HOH:O	2.03	0.58
3:D:153:LEU:CD1	3:D:157:GLU:HB2	2.33	0.58
3:D:481:MET:HG3	3:D:1388:ARG:CZ	2.32	0.58
3:D:498:VAL:HG23	3:D:499:VAL:N	2.18	0.58
3:D:592:THR:N	3:D:600:LEU:HD21	2.15	0.58
2:C:1087:VAL:HG13	3:D:610:LYS:NZ	2.13	0.58
4:E:83:ASP:O	4:E:86:GLN:HG2	2.03	0.58
2:M:185:LYS:HE2	2:M:190:LYS:HE2	1.84	0.58
2:M:218:VAL:HG22	2:M:221:LEU:CD2	2.32	0.58
2:M:292:ARG:HG2	9:M:1952:HOH:O	2.01	0.58
3:N:117:ASP:HB2	3:N:495:ARG:NH2	2.17	0.58
2:M:1056:LYS:NZ	3:N:749:VAL:O	2.35	0.58
3:N:715:ALA:HB3	3:N:764:LEU:HA	1.84	0.58
3:N:84:ILE:HG13	3:N:85:VAL:N	2.18	0.58
5:P:140:ARG:HG3	5:P:141:VAL:H	1.68	0.58
5:P:361:LEU:HD13	5:P:366:ALA:CB	2.33	0.58
1:A:36:LEU:O	1:A:39:PRO:HD2	2.02	0.58
3:D:1109:GLU:HG2	3:D:1202:GLN:H	1.66	0.58
3:D:1177:ALA:HB3	3:D:1183:ILE:HD11	1.85	0.58
3:D:702:LEU:HD23	3:D:745:MET:HE2	1.85	0.58
3:D:799:LYS:HB3	3:D:826:PRO:HG2	1.84	0.58
5:F:270:LYS:HG3	9:F:511:HOH:O	2.02	0.58
2:M:194:VAL:HG21	2:M:221:LEU:O	2.02	0.58
2:M:300:ASP:HA	9:M:2239:HOH:O	2.03	0.58
2:M:140:ILE:CD1	2:M:412:ALA:HA	2.32	0.58
2:M:710:ILE:HD12	2:M:790:LEU:HB2	1.85	0.58
3:N:1114:THR:H	3:N:1195:GLN:NE2	2.01	0.58
3:N:206:ARG:HH12	5:P:98:GLU:CA	2.15	0.58
3:N:634:GLY:O	3:N:637:LEU:HB3	2.03	0.58
3:N:640:HIS:HE1	4:O:3:GLU:HG2	1.68	0.58
3:N:767:HIS:CD2	4:O:6:ILE:HG12	2.37	0.58
3:N:957:PRO:HG2	3:N:1007:VAL:CA	2.29	0.58
1:A:39:PRO:CG	1:B:39:PRO:HG3	2.33	0.58
2:C:208:ALA:O	2:C:218:VAL:HG21	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:838:LYS:HE3	2:C:997:LEU:HD12	1.86	0.58
2:C:80:GLN:O	2:C:83:CYS:HB2	2.03	0.58
3:D:481:MET:HG2	3:D:482:LYS:N	2.18	0.58
3:D:992:ILE:O	3:D:995:LEU:HB3	2.03	0.58
4:E:69:LEU:HB3	9:E:140:HOH:O	2.02	0.58
5:F:132:ARG:HG2	5:F:181:GLU:CD	2.22	0.58
5:F:207:LEU:HB3	5:F:212:LEU:HG	1.84	0.58
1:L:99:LEU:HG	9:L:1066:HOH:O	2.03	0.58
2:M:212:GLY:HA3	2:M:218:VAL:HG23	1.85	0.58
2:M:654:LEU:HD11	2:M:663:ASN:ND2	2.18	0.58
2:M:838:LYS:NZ	2:M:846:LYS:HE2	2.18	0.58
2:M:859:PRO:O	2:M:867:VAL:HG22	2.03	0.58
2:M:694:LEU:HD11	2:M:868:ASP:HB3	1.85	0.58
3:N:169:TYR:CB	3:N:195:VAL:HG11	2.33	0.58
3:N:610:LYS:O	3:N:611:GLN:CG	2.50	0.58
1:B:46:SER:O	1:B:148:VAL:HB	2.03	0.58
2:C:110:GLU:CB	2:C:369:PRO:HG3	2.33	0.58
2:C:641:PRO:O	2:C:642:ARG:HD2	2.02	0.58
2:C:730:SER:HB2	9:C:1128:HOH:O	2.02	0.58
3:D:527:MET:CE	5:F:258:ILE:HD11	2.33	0.58
3:D:560:GLN:HB2	9:D:1923:HOH:O	2.03	0.58
3:D:52:PRO:HG3	3:D:78:VAL:HG13	1.85	0.58
2:M:137:VAL:HG23	2:M:391:LEU:HG	1.85	0.58
5:P:282:LEU:HD22	9:P:504:HOH:O	2.03	0.58
2:C:150:PRO:HD3	9:C:1150:HOH:O	2.04	0.58
2:C:328:LEU:HB2	2:C:433:THR:HG21	1.84	0.58
3:D:1152:GLU:CD	3:D:1159:ARG:HH12	2.06	0.58
3:D:1145:TYR:HE2	3:D:1168:MET:HB2	1.69	0.58
3:D:523:ASP:N	9:D:1713:HOH:O	2.30	0.58
3:D:957:PRO:HG2	3:D:1007:VAL:CA	2.30	0.58
4:E:59:ASN:HB3	4:E:62:THR:OG1	2.03	0.58
2:M:15:LEU:HD22	2:M:583:LEU:HD21	1.85	0.58
2:M:742:VAL:HG12	2:M:743:VAL:N	2.19	0.58
3:N:783:ARG:CZ	3:N:1029:ARG:HG3	2.32	0.58
1:L:188:GLN:HG3	3:N:685:ASP:OD2	2.03	0.58
3:N:813:LEU:O	3:N:817:GLU:HB2	2.03	0.58
1:A:218:LEU:O	1:A:222:LEU:HD12	2.04	0.58
2:C:429:ASP:HB3	9:C:1177:HOH:O	2.04	0.58
2:C:911:GLU:O	2:C:914:ILE:HG22	2.03	0.58
2:C:980:GLY:HA2	9:C:1431:HOH:O	2.03	0.58
5:F:323:ASP:HA	9:F:481:HOH:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:257:VAL:HG12	2:M:263:ASP:OD1	2.04	0.58
2:M:723:THR:HG21	9:M:1850:HOH:O	2.03	0.58
3:N:1018:ASN:HB3	3:N:1021:TYR:HB3	1.85	0.58
3:N:481:MET:SD	3:N:1388:ARG:HD2	2.44	0.58
3:N:829:VAL:H	3:N:835:SER:HB2	1.69	0.58
3:N:965:GLU:HA	3:N:968:ASP:HB2	1.84	0.58
2:C:1034:GLU:HA	2:C:1037:VAL:HG23	1.84	0.58
2:C:265:ARG:HG2	2:C:267:TYR:H	1.68	0.58
3:D:1026:SER:HA	9:D:2416:HOH:O	2.02	0.58
3:D:1063:GLU:HB3	9:D:1948:HOH:O	2.03	0.58
3:D:1422:MET:CE	3:D:1427:SER:HA	2.34	0.58
3:D:586:ARG:CZ	3:D:1444:THR:HG21	2.34	0.58
3:D:710:ARG:HH21	3:D:1210:SER:HB2	1.69	0.58
3:D:792:ILE:O	3:D:878:GLY:HA3	2.04	0.58
5:F:292:ALA:HB1	5:F:299:TRP:O	2.03	0.58
2:M:1037:VAL:HG13	2:M:1049:LEU:HD11	1.86	0.58
2:M:139:GLN:CD	2:M:415:PRO:HD2	2.24	0.58
2:M:151:ASP:OD2	2:M:159:ILE:HG23	2.03	0.58
3:N:1035:ILE:HA	3:N:1038:LEU:HD12	1.84	0.58
3:N:1145:TYR:HE2	3:N:1168:MET:HB2	1.67	0.58
3:N:116:LEU:HD21	3:N:464:LEU:CB	2.31	0.58
3:N:699:VAL:HG21	3:N:760:ARG:HB3	1.86	0.58
3:N:787:LEU:HD21	3:N:947:ILE:CD1	2.33	0.58
3:N:984:THR:HG22	3:N:987:GLU:H	1.68	0.58
1:B:108:GLU:HB3	9:B:522:HOH:O	2.02	0.58
2:C:137:VAL:O	2:C:391:LEU:HD21	2.04	0.58
2:C:139:GLN:CD	2:C:415:PRO:HD2	2.24	0.58
2:C:208:ALA:HB1	2:C:218:VAL:HG13	1.85	0.58
2:C:267:TYR:HB2	2:C:272:ALA:HB1	1.84	0.58
2:C:56:GLU:OE1	2:C:64:LEU:HD22	2.03	0.58
2:C:86:LYS:CD	2:C:813:VAL:HG12	2.33	0.58
5:F:406:ARG:HA	5:F:409:LYS:HG2	1.85	0.58
5:F:77:THR:O	5:F:81:VAL:HG23	2.03	0.58
1:K:96:THR:HG21	9:K:4199:HOH:O	2.03	0.58
2:M:101:ILE:HD11	9:M:1739:HOH:O	2.04	0.58
2:M:583:LEU:O	2:M:587:VAL:HG23	2.04	0.58
3:N:1102:THR:HG22	3:N:1222:GLY:CA	2.34	0.58
3:N:631:ILE:HG21	3:N:745:MET:SD	2.43	0.58
1:B:105:GLY:O	1:B:132:LEU:HB3	2.04	0.58
1:B:57:TYR:HE1	1:B:163:ASN:HB2	1.69	0.58
2:C:9:ILE:O	2:C:9:ILE:HG13	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1114:THR:H	3:D:1195:GLN:NE2	2.01	0.58
3:D:1357:ARG:HG2	9:D:2067:HOH:O	2.04	0.58
3:D:1206:GLY:HA3	3:D:1366:LYS:HZ1	1.68	0.58
3:D:185:VAL:HG23	3:D:202:VAL:C	2.24	0.58
3:D:686:GLU:HA	3:D:689:ASP:OD2	2.04	0.58
5:F:95:THR:HG23	9:F:465:HOH:O	2.02	0.58
1:K:182:GLU:O	1:K:194:LYS:HB3	2.04	0.58
2:M:1111:ILE:HG13	2:M:1112:PHE:H	1.69	0.58
2:M:260:LEU:HA	2:M:291:ALA:CB	2.34	0.58
2:M:902:ILE:O	2:M:904:PRO:HD3	2.03	0.58
2:M:1056:LYS:O	3:N:624:ASP:HB2	2.04	0.58
1:A:133:GLU:HB3	9:C:1680:HOH:O	2.02	0.58
2:C:182:VAL:HB	2:C:193:LEU:HD13	1.85	0.58
2:C:72:ARG:HB2	9:C:1804:HOH:O	2.04	0.58
3:D:171:LEU:HD21	9:D:2083:HOH:O	2.03	0.58
3:D:633:VAL:HB	3:D:740:PHE:CE1	2.39	0.58
5:F:79:ASP:OD2	5:F:80:PRO:HD3	2.04	0.58
2:M:77:PRO:HD3	2:M:93:PRO:HD3	1.85	0.58
3:N:1286:THR:HG22	9:N:1537:HOH:O	2.02	0.58
4:O:31:LEU:HD23	4:O:35:PHE:HE1	1.68	0.58
2:C:102:HIS:HB2	2:C:106:GLY:O	2.04	0.57
2:C:184:MET:SD	2:C:303:PHE:HE2	2.27	0.57
2:C:242:LEU:HD23	9:C:1218:HOH:O	2.03	0.57
2:C:404:LEU:O	2:C:407:LYS:HB2	2.04	0.57
2:C:52:PHE:CG	2:C:68:PHE:HB2	2.39	0.57
2:C:705:ILE:HA	2:C:827:VAL:O	2.04	0.57
3:D:1290:LEU:CD2	3:D:1291:SER:H	2.17	0.57
3:D:561:GLY:HA3	5:F:184:ARG:NH1	2.17	0.57
3:D:813:LEU:O	3:D:817:GLU:HB2	2.04	0.57
3:D:81:THR:HB	3:D:85:VAL:CG2	2.34	0.57
2:M:420:ARG:NH1	2:M:422:ARG:HH21	2.02	0.57
2:M:768:THR:HG21	9:P:562:HOH:O	2.04	0.57
3:N:572:ARG:HH21	5:P:83:GLN:HE21	1.50	0.57
2:M:1005:MET:CE	3:N:648:MET:HB2	2.33	0.57
2:C:165:LEU:HD12	2:C:166:PRO:HA	1.84	0.57
3:D:1045:MET:HG3	3:D:1073:SER:HA	1.86	0.57
3:D:1141:GLU:CD	3:D:1168:MET:HE1	2.25	0.57
3:D:15:PRO:HG3	9:D:1709:HOH:O	2.04	0.57
3:D:204:LEU:HB2	3:D:394:LEU:HG	1.84	0.57
2:M:671:ASN:N	2:M:671:ASN:ND2	2.48	0.57
2:M:697:ARG:HD2	2:M:699:PHE:CD1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1209:LEU:HD23	3:N:1211:MET:CG	2.34	0.57
3:N:415:VAL:HG13	3:N:419:ASP:HB2	1.86	0.57
3:N:525:ARG:N	3:N:526:PRO:HD3	2.18	0.57
2:M:733:ALA:HB2	3:N:679:ARG:HH21	1.69	0.57
5:P:365:GLU:OE1	5:P:400:ILE:HD12	2.04	0.57
1:B:206:THR:CG2	1:B:209:GLU:H	2.17	0.57
1:A:224:TYR:CD1	1:B:9:PRO:HD2	2.39	0.57
2:C:676:ILE:CG2	2:C:988:VAL:HG22	2.33	0.57
2:C:715:THR:HG22	2:C:717:LEU:HG	1.86	0.57
3:D:1112:CYS:HB2	3:D:1195:GLN:CG	2.33	0.57
3:D:1232:PRO:HB3	3:D:1361:VAL:CG2	2.34	0.57
3:D:1282:ARG:HA	3:D:1315:ASP:OD1	2.03	0.57
3:D:582:LEU:HA	3:D:603:LEU:HD12	1.87	0.57
3:D:996:TRP:CE3	3:D:999:THR:HG21	2.39	0.57
1:K:58:ILE:HB	1:K:61:VAL:HB	1.85	0.57
1:L:101:LEU:HD12	1:L:114:PHE:N	2.18	0.57
1:L:99:LEU:HD21	1:L:122:ILE:HD11	1.86	0.57
1:L:62:LEU:HD12	1:L:62:LEU:H	1.69	0.57
2:M:144:PRO:O	2:M:276:LYS:HD3	2.04	0.57
3:N:1293:PHE:CE2	3:N:1302:GLU:HB3	2.39	0.57
3:N:152:LEU:HD23	3:N:152:LEU:N	2.18	0.57
3:N:493:ARG:HB2	3:N:1388:ARG:CZ	2.34	0.57
5:P:130:VAL:HG11	5:P:159:ILE:HB	1.86	0.57
1:A:186:LEU:CB	1:A:192:LEU:HD11	2.34	0.57
1:B:209:GLU:HB3	9:B:448:HOH:O	2.04	0.57
1:B:55:SER:OG	1:B:158:ILE:HD13	2.05	0.57
2:C:94:LEU:HD12	9:C:1545:HOH:O	2.04	0.57
1:K:42:ARG:HH12	1:L:34:VAL:CB	2.13	0.57
1:K:9:PRO:HB3	1:K:25:LEU:HG	1.86	0.57
2:M:139:GLN:O	2:M:333:ILE:HA	2.04	0.57
2:M:136:ILE:HG22	2:M:336:VAL:HG22	1.86	0.57
2:M:334:ARG:NH1	2:M:415:PRO:HG2	2.19	0.57
3:N:1115:THR:HG22	9:N:1591:HOH:O	2.04	0.57
3:N:18:ILE:HD12	3:N:518:PRO:CG	2.34	0.57
1:A:227:ASN:H	1:A:227:ASN:ND2	2.03	0.57
2:C:100:LEU:HD12	2:C:101:ILE:O	2.05	0.57
2:C:166:PRO:HD3	2:C:265:ARG:CG	2.34	0.57
2:C:611:ILE:HG22	2:C:613:VAL:HG13	1.86	0.57
3:D:189:GLN:HG3	3:D:190:GLU:N	2.20	0.57
3:D:195:VAL:HG13	9:D:2268:HOH:O	2.04	0.57
3:D:434:ARG:HB2	3:D:447:VAL:CG2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:81:THR:O	3:D:82:LYS:O	2.21	0.57
4:E:63:TRP:O	4:E:67:GLU:HG3	2.05	0.57
9:C:1139:HOH:O	5:F:373:LYS:HB3	2.03	0.57
1:K:16:GLN:O	1:K:16:GLN:HG2	2.05	0.57
1:K:18:ARG:O	1:K:207:PRO:HD3	2.05	0.57
1:L:132:LEU:HD21	1:L:136:GLY:O	2.04	0.57
2:M:480:THR:HB	9:M:2150:HOH:O	2.03	0.57
2:M:56:GLU:OE1	2:M:64:LEU:HD22	2.05	0.57
3:N:480:GLU:O	3:N:480:GLU:HG3	2.04	0.57
3:N:614:PHE:CD1	3:N:615:ARG:N	2.72	0.57
4:O:41:GLU:N	4:O:42:PRO:HD2	2.20	0.57
1:B:143:ARG:HD2	1:B:160:ASP:OD2	2.04	0.57
2:C:142:ARG:HD3	9:C:1347:HOH:O	2.04	0.57
2:C:15:LEU:HD22	2:C:583:LEU:HD11	1.85	0.57
2:C:480:THR:HG22	2:C:481:ASP:N	2.19	0.57
3:D:1109:GLU:CD	3:D:1202:GLN:H	2.07	0.57
3:D:1179:GLU:HA	9:D:2069:HOH:O	2.05	0.57
3:D:576:GLU:HB2	9:D:1696:HOH:O	2.03	0.57
3:D:610:LYS:CD	7:D:1527:MXP:H15A	2.34	0.57
5:F:278:LEU:HB2	5:F:286:PRO:HG2	1.85	0.57
2:M:41:ASN:N	2:M:41:ASN:HD22	1.89	0.57
2:M:420:ARG:HG3	2:M:422:ARG:HG2	1.87	0.57
2:M:959:PRO:HD3	9:M:1887:HOH:O	2.04	0.57
3:N:455:ARG:HD2	9:N:2063:HOH:O	2.05	0.57
3:N:827:ILE:HB	9:N:2048:HOH:O	2.04	0.57
3:N:850:LEU:N	3:N:850:LEU:HD12	2.15	0.57
5:P:147:LEU:HB3	9:P:604:HOH:O	2.04	0.57
5:P:394:ARG:HA	5:P:397:ILE:HD12	1.87	0.57
2:C:21:ILE:HD12	2:C:21:ILE:H	1.70	0.57
2:C:705:ILE:HB	9:C:1287:HOH:O	2.04	0.57
2:C:897:LEU:HD23	2:C:899:GLN:NE2	2.19	0.57
2:C:430:VAL:HG11	3:D:1074:SER:OG	2.04	0.57
3:D:82:LYS:HE2	9:D:1577:HOH:O	2.05	0.57
2:M:1002:GLU:HG3	3:N:744:GLN:NE2	2.20	0.57
3:N:1037:GLN:HG2	3:N:1042:ARG:HB3	1.85	0.57
3:N:1189:ARG:NH1	3:N:1203:LYS:HB2	2.20	0.57
2:C:1008:ARG:NH1	2:C:1028:GLY:HA2	2.15	0.57
2:C:238:LEU:HD12	9:C:1705:HOH:O	2.05	0.57
2:C:495:THR:H	2:C:530:GLU:CD	2.08	0.57
2:C:724:ARG:O	2:C:734:LEU:HD21	2.05	0.57
2:C:774:LEU:HA	2:C:777:ILE:HD12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:113:ILE:HG23	5:F:127:ILE:HB	1.87	0.57
1:K:227:ASN:ND2	1:K:227:ASN:H	2.02	0.57
1:L:39:PRO:O	1:L:43:ILE:HG12	2.05	0.57
2:M:189:ARG:HD2	9:M:2270:HOH:O	2.04	0.57
1:K:178:ALA:HB2	2:M:864:GLY:H	1.69	0.57
3:N:992:ILE:O	3:N:995:LEU:HB3	2.05	0.57
1:B:7:LYS:O	1:B:7:LYS:HG3	2.05	0.57
2:C:206:THR:HG21	9:C:1559:HOH:O	2.04	0.57
2:C:322:VAL:HG21	9:C:1390:HOH:O	2.04	0.57
2:C:341:THR:HG21	9:C:1365:HOH:O	2.05	0.57
2:C:615:TYR:HB2	9:C:1584:HOH:O	2.05	0.57
3:D:956:ILE:HG12	3:D:1039:CYS:O	2.05	0.57
3:D:1376:MET:HG2	3:D:1421:LEU:HD12	1.86	0.57
3:D:546:ARG:HA	9:D:1595:HOH:O	2.05	0.57
3:D:820:GLU:HG3	3:D:836:VAL:CG1	2.34	0.57
3:D:820:GLU:HG3	3:D:836:VAL:HG11	1.86	0.57
2:M:395:LYS:HE2	2:M:403:SER:HB2	1.86	0.57
2:M:876:VAL:HA	9:M:1870:HOH:O	2.03	0.57
2:M:939:ARG:HD3	2:M:975:TYR:CE2	2.40	0.57
3:N:77:GLY:O	3:N:78:VAL:HG23	2.05	0.57
3:N:834:THR:HB	3:N:838:ARG:HB2	1.86	0.57
4:O:54:LEU:O	4:O:54:LEU:HD23	2.05	0.57
5:P:138:SER:O	5:P:141:VAL:HG12	2.03	0.57
1:B:101:LEU:HD11	1:B:113:ASP:HB2	1.87	0.57
2:C:477:GLY:O	2:C:508:ILE:HG12	2.05	0.57
2:C:838:LYS:NZ	2:C:846:LYS:HE2	2.20	0.57
3:D:1443:THR:HG22	9:D:1543:HOH:O	2.03	0.57
1:K:18:ARG:HD2	1:K:123:MET:CE	2.35	0.57
1:K:91:ASN:OD1	1:K:92:PRO:HD2	2.05	0.57
1:L:44:LEU:HD21	1:L:199:ILE:HD13	1.85	0.57
3:N:1295:GLU:HB3	3:N:1300:SER:HB3	1.87	0.57
3:N:1390:LEU:HB2	9:N:1897:HOH:O	2.05	0.57
3:N:171:LEU:HD13	9:N:1797:HOH:O	2.05	0.57
3:N:409:VAL:CG1	3:N:435:VAL:HG11	2.33	0.57
4:O:33:HIS:CE1	4:O:89:MET:HG2	2.39	0.57
5:P:361:LEU:HD13	5:P:366:ALA:HB2	1.86	0.57
5:P:393:THR:O	5:P:397:ILE:HG13	2.05	0.57
1:A:178:ALA:HB1	9:C:1688:HOH:O	2.05	0.56
1:B:201:THR:HG21	1:B:205:VAL:O	2.05	0.56
1:A:34:VAL:HB	1:B:42:ARG:HH21	1.69	0.56
2:C:1038:TRP:HA	2:C:1041:GLU:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:207:LEU:HD22	2:C:221:LEU:HD22	1.87	0.56
2:C:457:ALA:N	2:C:540:PHE:O	2.36	0.56
2:C:857:ASP:HB2	2:C:978:ARG:HB3	1.85	0.56
3:D:101:HIS:ND1	3:D:103:TRP:HB2	2.16	0.56
3:D:1090:ASP:HA	3:D:1093:TYR:HB2	1.87	0.56
3:D:1258:ARG:CZ	3:D:1262:LEU:HD11	2.36	0.56
3:D:32:ILE:HG22	5:F:258:ILE:HD12	1.87	0.56
9:C:1255:HOH:O	5:F:354:LEU:HD11	2.04	0.56
2:M:1105:LYS:HG3	9:M:1731:HOH:O	2.04	0.56
2:M:144:PRO:HA	2:M:163:ILE:CG1	2.35	0.56
2:M:404:LEU:O	2:M:407:LYS:HB2	2.05	0.56
2:M:665:PHE:HB2	9:M:1978:HOH:O	2.04	0.56
3:N:1231:GLU:HB3	3:N:1232:PRO:HD3	1.87	0.56
3:N:1384:PRO:HG3	3:N:1389:LEU:HA	1.86	0.56
3:N:1462:LEU:HD22	3:N:1472:ILE:HG23	1.87	0.56
3:N:957:PRO:HG3	3:N:1010:ASN:HD22	1.70	0.56
1:A:149:GLY:O	1:A:171:PHE:HB2	2.06	0.56
1:A:158:ILE:H	1:A:166:PRO:HG3	1.70	0.56
1:A:206:THR:HG22	1:A:209:GLU:H	1.69	0.56
2:C:252:LYS:HE2	9:C:1771:HOH:O	2.04	0.56
2:C:766:GLU:HG2	2:C:772:ARG:NH1	2.19	0.56
3:D:1410:GLU:HG3	9:D:1966:HOH:O	2.04	0.56
3:D:428:LYS:HD3	9:D:1840:HOH:O	2.05	0.56
2:C:1115:LEU:HD23	3:D:85:VAL:HA	1.85	0.56
3:D:894:LYS:HB3	9:D:2117:HOH:O	2.05	0.56
1:K:103:ALA:CB	1:K:107:LYS:HE2	2.35	0.56
1:L:123:MET:O	1:L:125:PRO:HD3	2.05	0.56
1:L:57:TYR:O	1:L:140:MET:HA	2.05	0.56
1:K:224:TYR:HB3	1:L:9:PRO:HB2	1.87	0.56
2:M:102:HIS:HB2	2:M:106:GLY:O	2.05	0.56
2:M:110:GLU:H	2:M:368:THR:HG21	1.69	0.56
2:M:141:HIS:HB3	2:M:418:LEU:CG	2.35	0.56
2:M:722:ILE:O	2:M:722:ILE:HG23	2.04	0.56
3:N:106:LYS:HB3	9:N:2026:HOH:O	2.05	0.56
3:N:1087:ARG:HG2	3:N:1238:MET:CB	2.34	0.56
3:N:1288:GLU:HA	9:N:1542:HOH:O	2.04	0.56
3:N:2:LYS:HD3	9:N:2388:HOH:O	2.04	0.56
4:O:45:ARG:NH2	4:O:55:PHE:HB3	2.20	0.56
1:A:198:ARG:HB2	1:A:200:TRP:CH2	2.41	0.56
1:A:88:ARG:NH2	1:A:90:LEU:HD21	2.20	0.56
3:D:165:LYS:HA	9:D:2176:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:169:TYR:CE1	3:D:197:SER:HB2	2.40	0.56
3:D:81:THR:HG22	3:D:82:LYS:N	2.21	0.56
4:E:45:ARG:NH2	4:E:55:PHE:HB3	2.20	0.56
5:F:88:ILE:HG12	5:F:193:ARG:HB2	1.87	0.56
1:K:161:ARG:NH1	1:K:161:ARG:HB2	2.19	0.56
1:K:5:LYS:O	1:K:8:ALA:HB2	2.05	0.56
1:L:169:ALA:HB1	1:L:171:PHE:CE2	2.40	0.56
2:M:328:LEU:HD23	2:M:467:ILE:HB	1.87	0.56
2:M:52:PHE:CG	2:M:68:PHE:HB2	2.40	0.56
2:M:631:SER:HB3	2:M:637:LEU:HD21	1.87	0.56
3:N:1388:ARG:HG3	3:N:1389:LEU:N	2.19	0.56
3:N:799:LYS:HB3	3:N:826:PRO:CG	2.34	0.56
2:C:1018:GLN:NE2	3:D:87:ARG:HH12	2.03	0.56
2:C:1097:LEU:HD12	2:C:1097:LEU:N	2.20	0.56
2:C:8:ARG:HB3	9:C:1721:HOH:O	2.05	0.56
3:D:1007:VAL:HG23	3:D:1008:PHE:N	2.21	0.56
3:D:611:GLN:NE2	3:D:1439:SER:HB3	2.20	0.56
4:E:54:LEU:CD2	4:E:63:TRP:HE1	2.18	0.56
5:F:203:THR:HG22	5:F:204:GLY:N	2.20	0.56
5:F:271:LEU:HG	5:F:295:MET:HE1	1.87	0.56
1:L:71:VAL:HG22	1:L:132:LEU:HD12	1.87	0.56
1:L:34:VAL:HG22	1:L:181:VAL:HG21	1.85	0.56
1:L:36:LEU:O	1:L:39:PRO:HD2	2.04	0.56
2:M:1015:LEU:HD12	9:P:651:HOH:O	2.04	0.56
2:M:378:LEU:HG	2:M:382:ILE:HD11	1.87	0.56
2:M:480:THR:HG22	2:M:481:ASP:N	2.19	0.56
2:M:733:ALA:HB2	3:N:679:ARG:HH22	1.66	0.56
2:M:863:ASP:O	2:M:865:THR:N	2.37	0.56
3:N:1169:ASP:HA	9:N:1842:HOH:O	2.04	0.56
3:N:1232:PRO:HB3	3:N:1361:VAL:CG2	2.33	0.56
3:N:1356:TYR:HD2	3:N:1363:LEU:HD23	1.69	0.56
3:N:114:THR:O	3:N:495:ARG:HG3	2.06	0.56
1:B:132:LEU:CD1	1:B:138:LEU:HD12	2.35	0.56
2:C:176:VAL:C	2:C:178:PRO:HD3	2.25	0.56
3:D:394:LEU:HD21	9:D:1995:HOH:O	2.06	0.56
3:D:640:HIS:HB2	9:E:156:HOH:O	2.05	0.56
2:C:770:GLU:CG	3:D:65:ARG:HH12	2.17	0.56
2:M:292:ARG:HD2	2:M:299:LYS:HG2	1.86	0.56
2:M:662:GLU:HB3	9:M:1978:HOH:O	2.05	0.56
2:M:565:GLN:OE1	2:M:842:ARG:HG2	2.05	0.56
3:N:113:GLY:HA3	3:N:120:ALA:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:560:GLN:HG2	5:P:221:ILE:HG21	1.86	0.56
1:A:66:SER:O	1:A:75:VAL:HG23	2.05	0.56
2:C:350:ARG:HA	2:C:353:ARG:HD2	1.87	0.56
2:C:413:LEU:HB3	9:C:1518:HOH:O	2.05	0.56
2:C:838:LYS:HB2	2:C:848:VAL:HG22	1.86	0.56
2:C:979:THR:HG23	2:C:981:GLU:N	2.18	0.56
3:D:1092:GLY:HA3	9:D:2012:HOH:O	2.05	0.56
3:D:1389:LEU:HD12	3:D:1390:LEU:N	2.19	0.56
3:D:55:ASP:O	3:D:80:VAL:HG11	2.06	0.56
5:F:140:ARG:HG3	5:F:141:VAL:H	1.69	0.56
1:K:34:VAL:HG13	2:M:939:ARG:HH21	1.70	0.56
1:K:91:ASN:CG	1:K:92:PRO:HD2	2.26	0.56
1:L:58:ILE:HG22	1:L:137:ARG:NH2	2.17	0.56
2:M:114:PHE:CE2	5:P:283:GLY:HA3	2.40	0.56
2:M:418:LEU:HD12	2:M:418:LEU:N	2.20	0.56
2:M:464:LEU:HD12	2:M:465:GLY:H	1.70	0.56
2:M:611:ILE:HG22	2:M:613:VAL:HG13	1.88	0.56
2:M:69:LEU:HD12	2:M:97:ARG:HB3	1.86	0.56
3:N:102:ILE:HD12	3:N:579:ASP:HB3	1.86	0.56
3:N:119:SER:HB2	3:N:123:LEU:CB	2.34	0.56
3:N:1243:THR:HG22	3:N:1244:GLY:H	1.71	0.56
3:N:143:ASN:HD21	3:N:145:VAL:HG12	1.70	0.56
3:N:45:PHE:HD1	3:N:86:ARG:HH22	1.52	0.56
3:N:592:THR:N	3:N:600:LEU:HD21	2.18	0.56
3:N:814:ALA:O	3:N:818:ARG:HG3	2.05	0.56
1:B:15:THR:HB	9:B:419:HOH:O	2.05	0.56
1:B:2:LEU:HD12	1:B:3:ASP:HB2	1.86	0.56
2:C:470:PRO:HD3	2:C:485:TYR:CE2	2.41	0.56
2:C:785:VAL:HG21	9:C:1244:HOH:O	2.05	0.56
3:D:1495:ILE:HG12	4:E:80:VAL:CG1	2.35	0.56
3:D:169:TYR:CB	3:D:195:VAL:HG11	2.34	0.56
3:D:842:VAL:HG23	9:D:1531:HOH:O	2.06	0.56
3:D:996:TRP:HE3	3:D:999:THR:HG21	1.70	0.56
5:F:291:ILE:HG23	5:F:304:VAL:HG21	1.87	0.56
2:M:141:HIS:HB2	9:M:2163:HOH:O	2.06	0.56
2:M:369:PRO:HD2	9:M:1905:HOH:O	2.06	0.56
2:M:510:ALA:HB3	2:M:513:VAL:CG2	2.36	0.56
2:M:510:ALA:HB3	2:M:513:VAL:HG23	1.88	0.56
2:M:408:ARG:HH21	2:M:542:VAL:CG2	2.17	0.56
2:M:660:ALA:HB3	9:M:1638:HOH:O	2.06	0.56
3:N:1113:GLY:N	3:N:1195:GLN:HE22	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:485:SER:O	3:N:489:ARG:HB3	2.05	0.56
3:N:564:GLU:HA	3:N:567:ILE:HD13	1.88	0.56
3:N:637:LEU:HD11	3:N:642:CYS:N	2.21	0.56
3:N:72:VAL:HG13	9:N:1744:HOH:O	2.05	0.56
5:P:113:ILE:HA	5:P:116:LEU:HD12	1.88	0.56
1:A:133:GLU:HG2	1:A:134:GLU:N	2.20	0.56
1:B:115:LEU:HD23	9:B:435:HOH:O	2.04	0.56
2:C:176:VAL:HG12	2:C:182:VAL:CG1	2.36	0.56
2:C:28:ARG:NH1	2:C:463:GLU:HG2	2.21	0.56
2:C:607:ASP:HB3	2:C:609:ASN:H	1.70	0.56
2:C:80:GLN:HB2	9:C:1803:HOH:O	2.04	0.56
2:C:818:GLY:HA2	5:F:309:LYS:NZ	2.20	0.56
3:D:1336:LEU:HA	3:D:1344:VAL:HG22	1.87	0.56
2:M:34:VAL:HG21	2:M:38:LYS:HD3	1.87	0.56
2:M:15:LEU:HD21	2:M:583:LEU:HD11	1.88	0.56
2:M:599:GLU:HG3	2:M:600:ASP:N	2.18	0.56
2:M:857:ASP:HB2	2:M:978:ARG:HB3	1.87	0.56
2:M:97:ARG:HG3	9:M:2157:HOH:O	2.05	0.56
3:N:1007:VAL:HG23	3:N:1008:PHE:N	2.21	0.56
3:N:602:SER:O	3:N:606:ILE:HG13	2.06	0.56
3:N:800:LYS:HE2	3:N:804:LEU:HD13	1.88	0.56
3:N:1495:ILE:HG12	4:O:80:VAL:CG1	2.35	0.56
5:P:108:GLU:HG3	5:P:176:ILE:HG21	1.88	0.56
5:P:138:SER:HB2	5:P:140:ARG:HG2	1.88	0.56
2:C:1101:THR:HB	3:D:5:VAL:CG1	2.35	0.56
9:A:318:HOH:O	2:C:627:ARG:HA	2.05	0.56
3:D:485:SER:O	3:D:489:ARG:HB3	2.06	0.56
5:F:101:GLU:HB3	5:F:105:LYS:HE3	1.87	0.56
5:F:225:GLU:HB3	9:F:605:HOH:O	2.06	0.56
1:K:20:TYR:CE2	1:K:22:GLU:HG3	2.41	0.56
2:M:167:LYS:HB2	9:M:1774:HOH:O	2.06	0.56
3:N:1047:LYS:HA	3:N:1053:PHE:CE1	2.41	0.56
3:N:1091:SER:HA	9:N:1706:HOH:O	2.06	0.56
3:N:443:VAL:HG22	3:N:444:VAL:N	2.20	0.56
4:O:84:ARG:HG3	9:O:2468:HOH:O	2.06	0.56
2:C:165:LEU:HD13	9:C:1292:HOH:O	2.05	0.56
2:C:580:MET:SD	2:C:584:GLU:HG3	2.46	0.56
3:D:403:PHE:CD1	3:D:405:ASP:O	2.53	0.56
2:C:750:LYS:HD2	3:D:681:ARG:HE	1.70	0.56
3:D:696:HIS:HB2	4:E:48:MET:HE3	1.87	0.56
4:E:33:HIS:HB2	4:E:37:ASN:ND2	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:72:LYS:HE2	9:M:2012:HOH:O	2.05	0.56
2:M:1115:LEU:HB3	3:N:85:VAL:CG1	2.35	0.56
2:M:193:LEU:HD11	9:M:1951:HOH:O	2.04	0.56
2:M:625:LEU:HB3	2:M:639:GLN:HB2	1.86	0.56
3:N:1492:LEU:HD23	9:N:2099:HOH:O	2.04	0.56
4:O:95:VAL:HG22	9:O:1302:HOH:O	2.06	0.56
5:P:193:ARG:HD2	9:P:514:HOH:O	2.05	0.56
5:P:375:LEU:HD23	9:P:476:HOH:O	2.05	0.56
1:A:138:LEU:HD21	9:A:355:HOH:O	2.05	0.56
2:C:365:ASP:HB3	9:C:1410:HOH:O	2.06	0.56
2:C:729:LEU:HD22	9:D:1907:HOH:O	2.06	0.56
3:D:1113:GLY:N	3:D:1195:GLN:NE2	2.53	0.56
3:D:1204:CYS:HB3	9:D:1762:HOH:O	2.06	0.56
3:D:126:VAL:O	3:D:132:TYR:HD1	1.89	0.56
3:D:925:GLU:HB3	4:E:2:ALA:HB3	1.88	0.56
1:K:88:ARG:HG3	1:K:88:ARG:O	2.06	0.56
2:M:235:LEU:HD11	9:M:2260:HOH:O	2.06	0.56
2:M:158:TYR:CE1	2:M:313:LEU:HG	2.40	0.56
2:M:328:LEU:CD2	2:M:437:ARG:HB3	2.36	0.56
2:M:626:ARG:HB2	2:M:639:GLN:HE21	1.70	0.56
2:M:670:GLN:HE22	2:M:699:PHE:CA	2.19	0.56
3:N:118:LEU:O	3:N:120:ALA:N	2.39	0.56
3:N:1466:VAL:HG23	3:N:1472:ILE:CD1	2.35	0.56
3:N:486:ARG:HD3	3:N:489:ARG:HD3	1.87	0.56
2:M:1109:VAL:HG11	3:N:5:VAL:HG22	1.87	0.56
1:B:158:ILE:HG22	1:B:159:LYS:N	2.20	0.55
1:B:99:LEU:HD13	9:B:416:HOH:O	2.06	0.55
2:C:630:ARG:HG3	9:C:1287:HOH:O	2.07	0.55
3:D:1035:ILE:HA	3:D:1038:LEU:CD1	2.36	0.55
3:D:1087:ARG:HD3	3:D:1236:LEU:O	2.06	0.55
3:D:806:PHE:HE1	3:D:813:LEU:HB3	1.70	0.55
3:D:80:VAL:N	9:D:1536:HOH:O	2.40	0.55
5:F:416:ARG:HD3	5:F:419:ARG:HD3	1.89	0.55
1:K:88:ARG:NH2	1:K:90:LEU:HD21	2.21	0.55
1:L:206:THR:HG22	1:L:209:GLU:H	1.71	0.55
1:L:85:LEU:HD13	1:L:127:LEU:HD23	1.88	0.55
2:M:100:LEU:HD12	2:M:101:ILE:O	2.06	0.55
2:M:172:ILE:HA	2:M:185:LYS:O	2.07	0.55
2:M:208:ALA:HB1	2:M:218:VAL:CG1	2.36	0.55
2:M:12:VAL:CG1	2:M:534:VAL:HG13	2.35	0.55
3:N:421:LEU:HG	3:N:429:SER:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:592:THR:HG23	9:N:1987:HOH:O	2.06	0.55
4:O:54:LEU:HA	4:O:58:PRO:HG2	1.88	0.55
5:P:271:LEU:HG	5:P:295:MET:HE1	1.88	0.55
5:P:95:THR:HB	9:P:638:HOH:O	2.05	0.55
2:C:34:VAL:HG21	2:C:38:LYS:HD3	1.88	0.55
2:C:416:GLY:HA3	9:C:1419:HOH:O	2.06	0.55
2:C:605:LYS:HG3	2:C:612:VAL:HB	1.88	0.55
2:C:657:ASP:OD1	2:C:661:SER:HB2	2.06	0.55
2:C:670:GLN:O	2:C:672:VAL:HG12	2.06	0.55
3:D:1305:LEU:HD13	9:D:1836:HOH:O	2.06	0.55
3:D:408:GLU:HB3	9:D:2146:HOH:O	2.05	0.55
3:D:1486:VAL:HG12	4:E:73:LEU:HD22	1.89	0.55
4:E:76:GLY:HA3	4:E:79:LEU:HD12	1.88	0.55
5:F:234:LYS:HG3	5:F:236:SER:H	1.71	0.55
2:M:1008:ARG:NH1	2:M:1028:GLY:HA2	2.17	0.55
2:M:473:ARG:HB3	9:M:2150:HOH:O	2.05	0.55
2:M:598:GLU:O	2:M:651:LYS:HG3	2.06	0.55
3:N:1422:MET:CE	3:N:1427:SER:HA	2.36	0.55
3:N:561:GLY:HA3	5:P:184:ARG:HH12	1.71	0.55
2:M:987:ILE:HG23	3:N:948:THR:HG21	1.87	0.55
5:P:261:PRO:O	5:P:265:VAL:HG23	2.07	0.55
1:B:111:ALA:HB2	9:B:460:HOH:O	2.05	0.55
2:C:1105:LYS:O	2:C:1107:ASN:N	2.38	0.55
2:C:149:THR:HA	9:C:1150:HOH:O	2.05	0.55
2:C:144:PRO:HA	2:C:163:ILE:CG1	2.37	0.55
2:C:172:ILE:HA	2:C:185:LYS:O	2.07	0.55
2:C:197:LEU:HD22	2:C:202:TYR:CD2	2.38	0.55
2:C:22:GLN:HE22	2:C:135:VAL:HG12	1.71	0.55
3:D:421:LEU:HG	3:D:429:SER:HB3	1.87	0.55
3:D:646:LYS:HD3	9:D:1609:HOH:O	2.06	0.55
9:D:1806:HOH:O	5:F:309:LYS:HB3	2.07	0.55
1:K:184:THR:HG23	1:K:192:LEU:HD12	1.87	0.55
1:L:58:ILE:HD13	1:L:140:MET:HB3	1.88	0.55
2:M:654:LEU:HD11	2:M:663:ASN:HD22	1.70	0.55
3:N:1463:LYS:O	3:N:1467:ILE:HG13	2.06	0.55
3:N:19:ARG:NH2	9:N:1827:HOH:O	2.40	0.55
2:M:770:GLU:HG3	3:N:65:ARG:HH12	1.70	0.55
1:B:212:ASN:O	1:B:215:VAL:HG22	2.05	0.55
1:B:59:GLU:HG2	9:B:405:HOH:O	2.05	0.55
2:C:1019:GLN:NE2	3:D:621:LYS:HA	2.20	0.55
2:C:1094:ALA:HB1	3:D:603:LEU:HD22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:139:GLN:HG2	2:C:140:ILE:H	1.71	0.55
2:C:208:ALA:HB1	2:C:218:VAL:CG1	2.36	0.55
2:C:583:LEU:O	2:C:587:VAL:HG23	2.06	0.55
3:D:82:LYS:HG2	9:D:1675:HOH:O	2.06	0.55
4:E:86:GLN:O	4:E:90:GLU:HG3	2.06	0.55
5:F:138:SER:O	5:F:141:VAL:HG12	2.07	0.55
1:L:199:ILE:HD11	1:L:211:LEU:HD13	1.89	0.55
2:M:261:ILE:HG21	9:M:2030:HOH:O	2.05	0.55
2:M:410:ILE:N	2:M:410:ILE:HD12	2.22	0.55
2:M:578:VAL:HG11	2:M:991:GLN:CB	2.35	0.55
2:M:589:ARG:HD2	9:M:1929:HOH:O	2.05	0.55
2:M:641:PRO:O	2:M:642:ARG:HD2	2.07	0.55
2:M:726:ILE:HG22	2:M:726:ILE:O	2.06	0.55
2:M:80:GLN:HB2	9:M:1668:HOH:O	2.07	0.55
3:N:1243:THR:HB	3:N:1253:THR:HG22	1.87	0.55
3:N:1281:VAL:HG23	3:N:1317:ASP:O	2.07	0.55
3:N:128:TYR:HB3	3:N:129:PHE:HD1	1.71	0.55
3:N:111:LYS:HE3	3:N:1449:GLU:HG2	1.88	0.55
3:N:703:ASN:HB2	3:N:713:ILE:HG12	1.89	0.55
5:P:317:LEU:O	5:P:329:TYR:HB3	2.07	0.55
1:B:65:PHE:HB2	9:B:397:HOH:O	2.05	0.55
2:C:36:PRO:HB3	9:C:1632:HOH:O	2.06	0.55
3:D:1398:TRP:HB2	9:D:2042:HOH:O	2.07	0.55
3:D:16:GLU:HG3	9:D:1656:HOH:O	2.06	0.55
2:C:770:GLU:HG3	3:D:65:ARG:HH12	1.70	0.55
1:K:16:GLN:O	1:K:16:GLN:CG	2.55	0.55
2:M:701:THR:HG23	2:M:832:LYS:HA	1.88	0.55
2:M:877:PRO:HG3	3:N:1020:LEU:HD12	1.89	0.55
2:M:73:LEU:HD23	2:M:94:LEU:HB2	1.88	0.55
3:N:1066:THR:HG22	3:N:1069:GLU:HG3	1.86	0.55
3:N:741:ASP:N	3:N:741:ASP:OD2	2.33	0.55
3:N:829:VAL:HG11	9:N:1877:HOH:O	2.07	0.55
2:C:199:VAL:HG13	2:C:235:LEU:HG	1.89	0.55
2:C:318:PRO:HD2	9:C:1596:HOH:O	2.07	0.55
3:D:1095:THR:CG2	3:D:1230:GLY:HA3	2.36	0.55
3:D:187:LYS:HG3	3:D:199:LEU:HB3	1.89	0.55
5:F:373:LYS:HG3	9:F:450:HOH:O	2.06	0.55
1:K:198:ARG:HB2	1:K:200:TRP:CZ3	2.42	0.55
1:K:74:ASP:O	1:K:78:ILE:HG13	2.06	0.55
2:M:128:ILE:HG22	9:M:1824:HOH:O	2.06	0.55
2:M:139:GLN:HE22	2:M:415:PRO:CG	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:53:PRO:HD3	9:M:1709:HOH:O	2.06	0.55
2:M:918:LEU:HD23	2:M:967:PHE:O	2.07	0.55
3:N:586:ARG:HB2	9:N:1869:HOH:O	2.06	0.55
2:C:172:ILE:H	2:C:172:ILE:HD12	1.72	0.55
2:C:362:GLY:HA3	2:C:367:LEU:HD23	1.89	0.55
2:C:9:ILE:HG12	2:C:907:ASP:OD2	2.07	0.55
3:D:1277:ILE:HD11	3:D:1301:LYS:HD2	1.89	0.55
3:D:924:MET:O	3:D:927:THR:HB	2.06	0.55
2:C:889:HIS:HE1	3:D:951:ILE:H	1.54	0.55
5:F:256:ARG:HB2	9:F:658:HOH:O	2.07	0.55
1:K:176:ARG:O	1:K:200:TRP:HE3	1.88	0.55
1:K:94:LEU:HD13	9:K:1900:HOH:O	2.06	0.55
2:M:114:PHE:CD1	2:M:114:PHE:N	2.73	0.55
2:M:195:LEU:HD12	2:M:234:ALA:HB1	1.89	0.55
2:M:346:VAL:O	2:M:350:ARG:HG3	2.07	0.55
2:M:557:ARG:HD2	2:M:879:ARG:HG2	1.89	0.55
2:M:580:MET:O	2:M:902:ILE:HA	2.07	0.55
2:M:937:ASP:OD2	2:M:939:ARG:HD2	2.06	0.55
3:N:1312:LEU:HD22	9:N:2126:HOH:O	2.06	0.55
3:N:1432:LYS:HG3	3:N:1433:SER:H	1.72	0.55
3:N:906:GLN:HB3	3:N:911:LEU:HD11	1.87	0.55
2:M:1010:THR:HG21	5:P:341:PRO:HB2	1.89	0.55
3:D:111:LYS:HE2	3:D:498:VAL:HG12	1.88	0.55
3:D:1311:LEU:HD23	3:D:1311:LEU:H	1.71	0.55
3:D:1397:LYS:HG2	9:D:1681:HOH:O	2.06	0.55
3:D:482:LYS:HD2	9:D:2211:HOH:O	2.07	0.55
3:D:634:GLY:O	3:D:637:LEU:HB3	2.05	0.55
3:D:760:ARG:HD2	4:E:3:GLU:OE2	2.06	0.55
2:M:368:THR:HG22	9:M:2230:HOH:O	2.05	0.55
2:M:49:ARG:HA	9:M:1709:HOH:O	2.07	0.55
2:M:86:LYS:HD3	2:M:813:VAL:HG12	1.89	0.55
2:M:966:LEU:HD21	2:M:986:PRO:HG3	1.88	0.55
3:N:1177:ALA:HB3	3:N:1183:ILE:HD11	1.88	0.55
3:N:1220:ALA:O	3:N:1224:VAL:HG23	2.07	0.55
3:N:126:VAL:O	3:N:132:TYR:HD1	1.90	0.55
3:N:1281:VAL:HG21	3:N:1313:VAL:CG2	2.37	0.55
3:N:1396:GLU:O	3:N:1400:VAL:HG23	2.07	0.55
3:N:126:VAL:HG11	3:N:152:LEU:HD12	1.88	0.55
3:N:646:LYS:HD3	9:N:2006:HOH:O	2.06	0.55
3:N:774:SER:C	3:N:776:GLU:H	2.10	0.55
3:N:843:PHE:CD2	3:N:849:ALA:HA	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:843:PHE:CE1	3:N:864:VAL:HG11	2.32	0.55
1:A:99:LEU:HB3	1:A:114:PHE:CD2	2.41	0.55
2:C:1054:THR:CG2	2:C:1079:PRO:HB3	2.28	0.55
2:C:2:GLU:HG3	2:C:899:GLN:CB	2.29	0.55
2:C:567:GLN:HB2	2:C:997:LEU:HD22	1.89	0.55
2:C:575:GLN:OE1	2:C:670:GLN:HB3	2.07	0.55
2:C:737:LEU:HD12	2:C:754:ILE:HB	1.88	0.55
2:C:551:GLU:OE1	2:C:906:PHE:HA	2.07	0.55
3:D:1147:ARG:O	3:D:1166:LEU:HD23	2.06	0.55
3:D:1293:PHE:CE2	3:D:1302:GLU:HB3	2.42	0.55
3:D:714:GLN:OE1	3:D:765:SER:HB2	2.07	0.55
3:D:890:VAL:HA	9:D:1617:HOH:O	2.07	0.55
5:F:172:ARG:O	5:F:176:ILE:HD13	2.07	0.55
1:L:179:PHE:HB2	1:L:195:LEU:HD11	1.88	0.55
2:M:137:VAL:CG2	2:M:391:LEU:HG	2.36	0.55
3:N:481:MET:HG3	3:N:1388:ARG:NH1	2.22	0.55
3:N:561:GLY:HA3	5:P:184:ARG:NH2	2.22	0.55
3:N:576:GLU:HB2	9:N:1886:HOH:O	2.06	0.55
3:N:989:TYR:CZ	3:N:993:LEU:HD11	2.42	0.55
3:N:561:GLY:HA3	5:P:184:ARG:HH22	1.71	0.55
1:A:127:LEU:HD12	1:A:127:LEU:C	2.27	0.55
1:A:132:LEU:HD21	1:A:138:LEU:HB2	1.89	0.55
2:C:56:GLU:OE2	2:C:356:ARG:HG2	2.07	0.55
2:C:57:GLU:O	2:C:62:GLY:HA3	2.06	0.55
2:C:670:GLN:HE22	2:C:699:PHE:CA	2.20	0.55
2:C:553:ASP:OD1	2:C:843:HIS:ND1	2.40	0.55
3:D:1090:ASP:HA	3:D:1093:TYR:CB	2.36	0.55
3:D:1431:THR:HB	9:D:1537:HOH:O	2.06	0.55
4:E:39:VAL:CG2	4:E:72:ARG:HD2	2.36	0.55
5:F:393:THR:HG22	9:F:485:HOH:O	2.07	0.55
2:M:1060:ILE:CG2	2:M:1061:GLU:N	2.69	0.55
2:M:632:ASN:N	9:M:1672:HOH:O	2.39	0.55
2:M:770:GLU:HA	9:M:1880:HOH:O	2.06	0.55
3:N:1225:ALA:HB2	9:N:1769:HOH:O	2.06	0.55
3:N:561:GLY:HA3	5:P:184:ARG:NH1	2.22	0.55
5:P:292:ALA:HB2	9:P:522:HOH:O	2.05	0.55
1:B:33:GLY:O	1:B:195:LEU:HD22	2.06	0.54
2:C:194:VAL:HG21	2:C:221:LEU:O	2.07	0.54
2:C:260:LEU:HG	2:C:261:ILE:HG13	1.89	0.54
2:C:136:ILE:HG22	2:C:336:VAL:HG22	1.89	0.54
2:C:54:ILE:HD11	2:C:356:ARG:CG	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1336:LEU:HB2	3:D:1344:VAL:HG21	1.89	0.54
3:D:1382:THR:HG23	9:D:1608:HOH:O	2.07	0.54
3:D:1413:THR:HG23	9:D:1816:HOH:O	2.07	0.54
3:D:1101:VAL:CG2	3:D:1424:VAL:HG22	2.29	0.54
3:D:149:LYS:HD2	9:D:1914:HOH:O	2.07	0.54
3:D:583:ASP:OD1	3:D:586:ARG:HG3	2.07	0.54
3:D:80:VAL:HG12	3:D:81:THR:O	2.06	0.54
5:F:152:ASP:HB3	5:F:153:PRO:HD3	1.87	0.54
1:K:24:VAL:HG23	9:K:1055:HOH:O	2.06	0.54
1:L:105:GLY:O	1:L:132:LEU:HB3	2.07	0.54
1:L:175:ARG:O	1:L:176:ARG:HG3	2.07	0.54
1:L:52:ALA:HB2	1:L:170:VAL:C	2.28	0.54
2:M:1075:ASP:HA	9:M:2290:HOH:O	2.06	0.54
2:M:254:VAL:O	2:M:257:VAL:HG23	2.07	0.54
2:M:413:LEU:CD1	2:M:413:LEU:H	2.13	0.54
2:M:455:LEU:HD12	2:M:456:ALA:O	2.07	0.54
3:N:1083:ASP:O	3:N:1087:ARG:HG3	2.07	0.54
3:N:1147:ARG:O	3:N:1166:LEU:HD23	2.08	0.54
3:N:1467:ILE:HG23	7:N:1527:MXP:H16A	1.89	0.54
2:M:1084:SER:HB2	7:N:1527:MXP:O4	2.07	0.54
3:N:527:MET:HE3	3:N:535:PHE:HB3	1.89	0.54
1:A:88:ARG:HG2	1:A:121:GLU:HG2	1.89	0.54
2:C:41:ASN:O	2:C:46:ALA:HB2	2.08	0.54
2:C:510:ALA:HB3	2:C:513:VAL:HG23	1.89	0.54
2:C:580:MET:HB3	2:C:584:GLU:CD	2.28	0.54
2:C:805:ARG:HD2	9:C:1160:HOH:O	2.07	0.54
3:D:400:VAL:C	3:D:402:PRO:HD3	2.26	0.54
3:D:611:GLN:OE1	7:D:1527:MXP:C16	2.53	0.54
2:C:1056:LYS:HB3	3:D:623:VAL:HG13	1.89	0.54
3:D:675:ARG:HH12	5:F:421:PHE:HD2	1.55	0.54
3:D:786:ILE:HD13	3:D:908:LYS:HB3	1.87	0.54
5:F:84:TYR:O	5:F:88:ILE:HD12	2.07	0.54
5:F:94:LEU:HD23	9:F:642:HOH:O	2.07	0.54
1:L:85:LEU:HD12	1:L:124:ASN:HB3	1.89	0.54
2:M:197:LEU:HD12	2:M:207:LEU:HD11	1.89	0.54
3:N:996:TRP:CE2	3:N:1056:PRO:HG2	2.42	0.54
3:N:1144:LEU:HB3	3:N:1166:LEU:HD11	1.89	0.54
3:N:679:ARG:HB3	9:N:2172:HOH:O	2.06	0.54
3:N:77:GLY:HA3	9:N:2213:HOH:O	2.07	0.54
4:O:17:TYR:CD2	4:O:17:TYR:N	2.74	0.54
5:P:278:LEU:HB2	5:P:286:PRO:HG2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:TYR:HD2	1:A:21:GLY:H	1.53	0.54
1:A:213:GLN:O	1:A:217:ILE:HG13	2.07	0.54
1:A:57:TYR:CE2	1:A:59:GLU:HA	2.42	0.54
1:B:107:LYS:HG3	1:B:108:GLU:N	2.22	0.54
1:B:56:VAL:HG13	1:B:142:VAL:HG12	1.89	0.54
2:C:272:ALA:HB1	9:C:1127:HOH:O	2.06	0.54
2:C:724:ARG:HE	2:C:734:LEU:HD23	1.72	0.54
2:C:816:LYS:HE2	2:C:819:VAL:HG21	1.89	0.54
3:D:1286:THR:HG22	9:D:1533:HOH:O	2.07	0.54
3:D:165:LYS:HG3	3:D:397:LYS:HD3	1.90	0.54
3:D:533:GLY:HA3	9:D:1806:HOH:O	2.07	0.54
3:D:568:ARG:O	3:D:572:ARG:HG3	2.06	0.54
3:D:675:ARG:HG2	3:D:678:GLU:OE2	2.06	0.54
5:F:254:GLN:HA	9:F:443:HOH:O	2.08	0.54
1:L:106:PRO:HG3	1:L:134:GLU:HG2	1.88	0.54
1:L:158:ILE:HG22	1:L:159:LYS:N	2.21	0.54
2:M:1084:SER:O	2:M:1087:VAL:HG12	2.08	0.54
3:N:1087:ARG:HD3	3:N:1237:THR:HA	1.90	0.54
3:N:1351:GLU:HG3	3:N:1354:LYS:HD2	1.90	0.54
3:N:98:PRO:HG3	3:N:515:GLU:HB3	1.89	0.54
3:N:583:ASP:HB2	3:N:604:THR:OG1	2.07	0.54
3:N:820:GLU:HG3	3:N:836:VAL:CG1	2.36	0.54
5:P:205:ARG:HD3	5:P:251:ILE:HG21	1.89	0.54
5:P:358:LEU:O	5:P:358:LEU:HG	2.06	0.54
1:A:132:LEU:HD12	1:A:132:LEU:N	2.23	0.54
1:B:175:ARG:HA	9:B:492:HOH:O	2.08	0.54
1:B:211:LEU:O	1:B:214:ALA:HB3	2.07	0.54
2:C:1087:VAL:CG1	3:D:610:LYS:HZ3	2.17	0.54
2:C:120:LEU:HD23	9:C:1499:HOH:O	2.06	0.54
2:C:577:PRO:HG3	2:C:993:PHE:CE2	2.43	0.54
2:C:710:ILE:HD11	2:C:758:ARG:HD3	1.88	0.54
2:C:84:ARG:NH2	2:C:128:ILE:HD11	2.23	0.54
3:D:1042:ARG:O	3:D:1057:VAL:HB	2.08	0.54
3:D:1293:PHE:CZ	3:D:1302:GLU:HB3	2.43	0.54
3:D:1381:VAL:HB	3:D:1389:LEU:O	2.08	0.54
3:D:49:ILE:HB	3:D:50:PHE:CD1	2.42	0.54
3:D:570:GLU:N	5:F:214:GLN:HE22	2.05	0.54
3:D:711:LEU:C	3:D:713:ILE:H	2.11	0.54
5:F:305:GLU:O	5:F:309:LYS:HG3	2.07	0.54
2:M:889:HIS:CD2	2:M:970:GLY:HA3	2.43	0.54
2:M:565:GLN:HG2	2:M:995:MET:CE	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1009:LYS:HE2	9:N:1963:HOH:O	2.07	0.54
3:N:1041:LEU:CD1	3:N:1058:ARG:HA	2.36	0.54
3:N:1262:LEU:HD23	3:N:1352:ILE:HG13	1.90	0.54
3:N:1472:ILE:O	3:N:1477:GLY:HA3	2.08	0.54
3:N:32:ILE:HD11	9:N:1596:HOH:O	2.06	0.54
3:N:566:ILE:HG12	5:P:192:LEU:HD21	1.88	0.54
3:N:610:LYS:C	3:N:611:GLN:HG3	2.28	0.54
5:P:88:ILE:HB	9:P:514:HOH:O	2.06	0.54
1:A:184:THR:HG23	1:A:192:LEU:HD12	1.89	0.54
2:C:17:PRO:HB2	9:C:1289:HOH:O	2.07	0.54
2:C:292:ARG:NH1	2:C:299:LYS:HD3	2.22	0.54
3:D:1045:MET:HG3	3:D:1073:SER:OG	2.07	0.54
3:D:1112:CYS:HA	9:D:2179:HOH:O	2.08	0.54
3:D:1142:ALA:HB3	9:D:2234:HOH:O	2.06	0.54
3:D:118:LEU:O	3:D:120:ALA:N	2.41	0.54
3:D:41:ARG:HD2	9:D:2449:HOH:O	2.07	0.54
3:D:72:VAL:HG23	3:D:78:VAL:H	1.71	0.54
3:D:957:PRO:CD	3:D:1007:VAL:HG12	2.37	0.54
5:F:88:ILE:CB	5:F:193:ARG:HH11	2.20	0.54
2:M:362:GLY:HA3	2:M:367:LEU:CD2	2.37	0.54
2:M:137:VAL:HG22	2:M:391:LEU:O	2.08	0.54
3:N:1080:GLY:O	3:N:1084:THR:HG23	2.07	0.54
3:N:764:LEU:HD23	3:N:767:HIS:CE1	2.42	0.54
3:N:799:LYS:O	3:N:826:PRO:HD2	2.08	0.54
1:B:122:ILE:HG23	9:B:527:HOH:O	2.08	0.54
1:B:123:MET:O	1:B:125:PRO:HD3	2.08	0.54
2:C:420:ARG:CZ	2:C:422:ARG:HH21	2.20	0.54
2:C:481:ASP:O	2:C:483:VAL:HG23	2.06	0.54
2:C:398:THR:O	2:C:570:PRO:HD3	2.08	0.54
2:C:725:ASP:HA	9:C:1479:HOH:O	2.08	0.54
3:D:478:LEU:HD21	3:D:500:ARG:HH21	1.71	0.54
3:D:534:ARG:HE	5:F:312:GLN:HE22	1.56	0.54
1:K:86:VAL:HG13	1:K:124:ASN:HB2	1.89	0.54
2:M:1049:LEU:O	2:M:1053:LEU:HG	2.07	0.54
2:M:157:ARG:NH1	2:M:314:THR:HB	2.22	0.54
2:M:252:LYS:HD3	2:M:296:GLY:HA2	1.89	0.54
3:N:172:PRO:HA	9:N:2177:HOH:O	2.06	0.54
3:N:493:ARG:HB2	3:N:1388:ARG:NE	2.23	0.54
3:N:584:ASN:CG	3:N:590:PRO:HD2	2.27	0.54
2:C:191:PHE:HD2	2:C:195:LEU:HD23	1.72	0.54
2:C:502:PRO:HB2	2:C:509:ALA:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1109:GLU:CG	3:D:1202:GLN:H	2.21	0.54
3:D:1466:VAL:HG23	3:D:1472:ILE:CD1	2.33	0.54
3:D:117:ASP:HB2	3:D:495:ARG:NH2	2.23	0.54
3:D:99:ALA:HB1	3:D:575:GLN:CD	2.28	0.54
1:K:111:ALA:HB2	1:K:127:LEU:HG	1.90	0.54
1:K:193:ASP:HA	9:K:2597:HOH:O	2.07	0.54
1:L:206:THR:CG2	1:L:209:GLU:H	2.21	0.54
2:M:185:LYS:HB3	2:M:188:LYS:O	2.07	0.54
2:M:281:LEU:CD1	2:M:306:THR:HA	2.38	0.54
2:M:669:GLY:HA3	2:M:995:MET:HA	1.90	0.54
3:N:1005:GLN:HB2	9:N:1763:HOH:O	2.07	0.54
3:N:1104:GLU:O	3:N:1106:VAL:HG23	2.08	0.54
3:N:1290:LEU:HD22	3:N:1291:SER:H	1.73	0.54
1:A:101:LEU:HD12	1:A:114:PHE:CD1	2.43	0.54
2:C:334:ARG:NH2	2:C:418:LEU:HD11	2.23	0.54
2:C:740:GLU:HB3	9:C:1664:HOH:O	2.08	0.54
3:D:1195:GLN:HG3	3:D:1196:THR:N	2.22	0.54
1:K:173:PRO:O	1:K:201:THR:HG23	2.08	0.54
2:M:250:ARG:HG3	9:M:2168:HOH:O	2.06	0.54
2:M:338:GLU:HA	2:M:341:THR:HG22	1.89	0.54
2:M:129:ILE:CG1	2:M:386:PHE:HB3	2.35	0.54
2:M:420:ARG:CZ	2:M:422:ARG:HH21	2.20	0.54
2:M:841:ASN:HD21	2:M:845:ASN:H	1.56	0.54
3:N:127:LEU:HD11	3:N:461:ILE:HD11	1.89	0.54
3:N:187:LYS:HG3	3:N:199:LEU:HB3	1.89	0.54
3:N:477:LEU:HD23	9:N:1890:HOH:O	2.07	0.54
2:M:1034:GLU:OE2	3:N:616:GLN:HG2	2.08	0.54
4:O:46:PRO:CB	4:O:54:LEU:HD22	2.35	0.54
4:O:70:THR:HG21	4:O:72:ARG:NE	2.23	0.54
5:P:142:ARG:CZ	5:P:156:VAL:HG22	2.38	0.54
5:P:207:LEU:HB3	5:P:212:LEU:HG	1.90	0.54
1:B:185:ARG:HD2	9:D:1847:HOH:O	2.08	0.54
2:C:1115:LEU:HD12	2:C:1115:LEU:N	2.22	0.54
2:C:130:ASN:HA	9:C:1363:HOH:O	2.07	0.54
2:C:438:ILE:HD11	2:C:467:ILE:HD12	1.89	0.54
2:C:51:THR:HB	2:C:348:LEU:HD23	1.89	0.54
2:C:774:LEU:HB2	9:C:1255:HOH:O	2.07	0.54
2:C:77:PRO:HD3	2:C:93:PRO:HD3	1.89	0.54
3:D:1113:GLY:HA2	9:D:1697:HOH:O	2.07	0.54
3:D:1137:ARG:O	3:D:1141:GLU:HG3	2.08	0.54
3:D:119:SER:H	3:D:123:LEU:CD2	2.17	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:148:GLU:HG2	3:D:151:GLN:HE21	1.73	0.54
3:D:24:GLY:HA2	9:D:2024:HOH:O	2.07	0.54
4:E:35:PHE:HZ	4:E:60:ALA:HA	1.73	0.54
5:F:94:LEU:HB2	5:F:98:GLU:OE2	2.08	0.54
1:K:184:THR:HG23	1:K:192:LEU:CB	2.36	0.54
1:L:173:PRO:O	1:L:201:THR:HG23	2.07	0.54
2:M:1008:ARG:HH11	2:M:1028:GLY:CA	2.20	0.54
2:M:229:MET:HG3	9:M:1707:HOH:O	2.07	0.54
3:N:1389:LEU:HD22	9:N:1771:HOH:O	2.08	0.54
3:N:187:LYS:CE	3:N:199:LEU:HB3	2.34	0.54
3:N:800:LYS:HD3	9:N:1722:HOH:O	2.08	0.54
3:N:891:GLU:HB2	9:N:2068:HOH:O	2.07	0.54
4:O:6:ILE:HA	4:O:9:LEU:HD12	1.89	0.54
1:B:83:LYS:O	1:B:170:VAL:HG21	2.08	0.54
2:C:602:GLU:HA	2:C:647:GLN:O	2.07	0.54
2:C:650:ARG:HG3	9:C:1791:HOH:O	2.08	0.54
2:C:863:ASP:O	2:C:865:THR:N	2.41	0.54
3:D:1176:LYS:O	3:D:1179:GLU:HB2	2.08	0.54
3:D:1369:GLU:O	3:D:1372:VAL:HG12	2.08	0.54
3:D:169:TYR:HB3	3:D:195:VAL:HG11	1.89	0.54
3:D:52:PRO:HG2	3:D:79:GLU:O	2.08	0.54
5:F:301:ALA:HB2	9:F:602:HOH:O	2.08	0.54
1:K:23:PHE:HE1	1:K:208:LEU:HD13	1.73	0.54
2:M:182:VAL:HG11	9:M:2050:HOH:O	2.08	0.54
2:M:216:GLU:HB3	9:M:1627:HOH:O	2.08	0.54
2:M:137:VAL:O	2:M:391:LEU:HD21	2.08	0.54
2:M:481:ASP:O	2:M:483:VAL:HG23	2.07	0.54
3:N:1277:ILE:HD11	3:N:1301:LYS:HD2	1.89	0.54
3:N:400:VAL:C	3:N:402:PRO:HD3	2.28	0.54
2:C:1111:ILE:HG13	2:C:1112:PHE:H	1.73	0.53
2:C:860:HIS:HE1	9:C:1431:HOH:O	1.91	0.53
3:D:1213:ARG:HG3	9:D:2053:HOH:O	2.06	0.53
3:D:550:ARG:HH11	3:D:573:MET:HB3	1.73	0.53
3:D:699:VAL:HG12	3:D:717:GLN:HA	1.88	0.53
3:D:820:GLU:HG2	3:D:825:ALA:O	2.08	0.53
3:D:1485:GLN:O	4:E:75:PHE:HA	2.08	0.53
5:F:399:GLN:HG3	9:F:571:HOH:O	2.08	0.53
1:K:123:MET:C	1:K:125:PRO:HD3	2.29	0.53
1:L:57:TYR:CE1	1:L:163:ASN:HB2	2.43	0.53
2:M:191:PHE:HD2	2:M:195:LEU:HD23	1.72	0.53
2:M:315:ALA:HB3	9:M:1882:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:352:ALA:HA	2:M:355:VAL:HG12	1.89	0.53
2:M:689:VAL:HB	2:M:870:ILE:HG13	1.89	0.53
3:N:81:THR:O	3:N:82:LYS:O	2.26	0.53
1:B:106:PRO:HG2	9:B:483:HOH:O	2.07	0.53
3:D:131:LYS:HD2	5:F:83:GLN:NE2	2.23	0.53
3:D:139:GLY:O	3:D:147:VAL:HB	2.08	0.53
3:D:161:LEU:HD23	3:D:161:LEU:O	2.08	0.53
3:D:1476:THR:HG23	4:E:21:VAL:HG22	1.90	0.53
4:E:49:GLN:HG2	9:E:108:HOH:O	2.09	0.53
5:F:271:LEU:HG	5:F:295:MET:CE	2.37	0.53
1:L:68:ILE:HG23	1:L:137:ARG:NH1	2.24	0.53
1:L:14:ARG:HA	9:L:3344:HOH:O	2.07	0.53
1:L:212:ASN:O	1:L:215:VAL:HG22	2.07	0.53
2:M:89:THR:HA	2:M:129:ILE:O	2.08	0.53
2:M:411:SER:HA	2:M:452:ILE:HA	1.90	0.53
2:M:41:ASN:O	2:M:46:ALA:HB2	2.09	0.53
2:M:685:GLU:CG	3:N:783:ARG:HD2	2.38	0.53
2:M:911:GLU:O	2:M:914:ILE:HG22	2.08	0.53
3:N:1049:SER:OG	3:N:1051:GLU:HG3	2.08	0.53
3:N:1381:VAL:HB	3:N:1389:LEU:O	2.07	0.53
3:N:610:LYS:CG	7:N:1527:MXR:C15	2.85	0.53
3:N:615:ARG:O	3:N:616:GLN:C	2.46	0.53
3:N:820:GLU:HB2	3:N:836:VAL:HG11	1.90	0.53
3:N:983:LEU:HD13	3:N:991:GLN:OE1	2.08	0.53
5:P:234:LYS:HG3	5:P:236:SER:H	1.74	0.53
1:B:44:LEU:HD21	1:B:199:ILE:HD13	1.89	0.53
2:C:254:VAL:O	2:C:257:VAL:HG23	2.09	0.53
2:C:736:ASP:C	2:C:738:ASP:H	2.12	0.53
3:D:1273:VAL:HG13	9:D:2190:HOH:O	2.08	0.53
3:D:454:ALA:HB3	9:D:2225:HOH:O	2.08	0.53
3:D:57:GLU:HG3	3:D:64:LYS:HG2	1.91	0.53
3:D:764:LEU:HD23	3:D:767:HIS:ND1	2.24	0.53
3:D:787:LEU:HD21	3:D:947:ILE:HD13	1.90	0.53
3:D:959:GLU:O	3:D:963:TYR:HD1	1.91	0.53
4:E:19:LEU:HB3	9:E:116:HOH:O	2.08	0.53
5:F:95:THR:HG22	5:F:96:LEU:HD23	1.90	0.53
1:K:126:ASP:HB2	9:K:1975:HOH:O	2.06	0.53
1:L:83:LYS:O	1:L:170:VAL:HG21	2.07	0.53
1:L:86:VAL:HG12	1:L:124:ASN:ND2	2.16	0.53
2:M:1103:ASP:OD1	3:N:3:LYS:HB2	2.09	0.53
2:M:673:LEU:HD22	2:M:867:VAL:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:766:GLU:HG2	2:M:772:ARG:HH12	1.73	0.53
2:M:690:ILE:CG2	2:M:852:ILE:HG13	2.38	0.53
3:N:1209:LEU:HD23	3:N:1211:MET:HG3	1.90	0.53
3:N:1278:ASP:HA	3:N:1319:VAL:O	2.08	0.53
3:N:1395:LEU:HD21	9:N:1988:HOH:O	2.08	0.53
3:N:407:VAL:HG13	3:N:421:LEU:O	2.09	0.53
3:D:1080:GLY:O	3:D:1084:THR:HG23	2.08	0.53
3:D:1258:ARG:HG3	3:D:1262:LEU:HD13	1.89	0.53
3:D:1264:GLU:O	3:D:1266:ARG:HG3	2.07	0.53
3:D:408:GLU:O	3:D:408:GLU:HG2	2.07	0.53
3:D:662:GLU:HB2	9:D:1987:HOH:O	2.09	0.53
4:E:29:GLN:HB2	4:E:33:HIS:CD2	2.43	0.53
5:F:162:LYS:HE2	9:F:641:HOH:O	2.08	0.53
5:F:345:ALA:HB1	9:F:710:HOH:O	2.08	0.53
1:K:63:HIS:HB3	2:M:746:GLY:HA2	1.89	0.53
2:M:182:VAL:CG1	2:M:193:LEU:HD13	2.38	0.53
2:M:227:PHE:HA	2:M:237:ARG:NH1	2.23	0.53
2:M:52:PHE:O	2:M:54:ILE:N	2.41	0.53
2:M:571:LEU:HD23	2:M:699:PHE:O	2.09	0.53
2:M:584:GLU:CD	2:M:584:GLU:H	2.10	0.53
2:M:604:ALA:HB3	2:M:612:VAL:O	2.08	0.53
2:M:611:ILE:CD1	2:M:625:LEU:HD11	2.38	0.53
2:M:632:ASN:HB2	9:M:1672:HOH:O	2.09	0.53
3:N:1144:LEU:HA	3:N:1147:ARG:HG3	1.90	0.53
3:N:612:GLY:HA2	3:N:1441:GLN:HA	1.90	0.53
3:N:1466:VAL:HG11	7:N:1527:MXR:H20	1.90	0.53
3:N:17:LYS:HA	3:N:20:SER:HB3	1.91	0.53
3:N:527:MET:CE	5:P:258:ILE:HD11	2.39	0.53
5:P:130:VAL:HA	5:P:142:ARG:HH21	1.73	0.53
2:C:378:LEU:HG	2:C:382:ILE:HD11	1.90	0.53
2:C:385:PHE:O	2:C:389:SER:HB3	2.08	0.53
2:C:765:SER:O	2:C:767:PRO:HD3	2.09	0.53
2:C:897:LEU:HB3	2:C:899:GLN:HE21	1.73	0.53
2:C:4:LYS:O	2:C:901:TYR:HB3	2.08	0.53
3:D:1105:ILE:HD13	9:D:2099:HOH:O	2.09	0.53
3:D:1175:ILE:O	3:D:1179:GLU:HG3	2.08	0.53
3:D:1390:LEU:HA	9:D:2323:HOH:O	2.08	0.53
3:D:800:LYS:CE	3:D:804:LEU:HD13	2.39	0.53
5:F:130:VAL:HG11	5:F:159:ILE:HB	1.90	0.53
5:F:108:GLU:HG3	5:F:176:ILE:HG21	1.91	0.53
2:M:328:LEU:HD21	2:M:438:ILE:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:806:LEU:HD22	9:M:1891:HOH:O	2.07	0.53
2:M:877:PRO:HG2	3:N:1023:MET:CE	2.18	0.53
3:N:1047:LYS:HB3	3:N:1048:PRO:CD	2.38	0.53
3:N:1486:VAL:HG12	4:O:73:LEU:HD22	1.90	0.53
3:N:448:GLU:HG2	3:N:448:GLU:O	2.08	0.53
1:B:140:MET:HB2	9:B:514:HOH:O	2.08	0.53
2:C:1008:ARG:HH11	2:C:1028:GLY:CA	2.18	0.53
2:C:185:LYS:HB3	2:C:188:LYS:O	2.07	0.53
2:C:267:TYR:CD1	2:C:272:ALA:HB1	2.43	0.53
2:C:496:ILE:O	2:C:515:ALA:HB1	2.09	0.53
3:D:493:ARG:HA	3:D:1388:ARG:NH1	2.24	0.53
3:D:799:LYS:HB3	3:D:826:PRO:CG	2.37	0.53
3:D:1485:GLN:NE2	4:E:80:VAL:H	2.07	0.53
5:F:415:THR:HB	9:F:522:HOH:O	2.09	0.53
1:K:20:TYR:CD2	1:K:21:GLY:N	2.69	0.53
1:K:45:LEU:HD21	9:K:2558:HOH:O	2.08	0.53
3:N:1236:LEU:HA	3:N:1359:GLN:NE2	2.24	0.53
3:N:138:LYS:HD3	9:N:1530:HOH:O	2.08	0.53
3:N:169:TYR:CE1	3:N:197:SER:HB2	2.44	0.53
3:N:55:ASP:O	3:N:80:VAL:HG11	2.08	0.53
3:N:792:ILE:O	3:N:878:GLY:HA3	2.09	0.53
3:N:860:LEU:HD23	3:N:877:PRO:HB2	1.91	0.53
4:O:39:VAL:CG2	4:O:72:ARG:HD2	2.39	0.53
5:P:94:LEU:HD23	9:P:638:HOH:O	2.09	0.53
2:C:1054:THR:HG22	2:C:1059:ASP:CB	2.33	0.53
2:C:403:SER:O	2:C:407:LYS:HG3	2.09	0.53
3:D:1113:GLY:N	3:D:1195:GLN:HE22	2.07	0.53
3:D:113:GLY:HA3	3:D:120:ALA:HA	1.91	0.53
3:D:1274:ILE:HD12	9:D:1674:HOH:O	2.08	0.53
3:D:1274:ILE:HD11	3:D:1334:GLN:NE2	2.24	0.53
3:D:493:ARG:HB2	3:D:1388:ARG:CZ	2.39	0.53
3:D:591:VAL:HB	9:D:1809:HOH:O	2.08	0.53
3:D:615:ARG:O	3:D:616:GLN:C	2.44	0.53
3:D:996:TRP:HA	3:D:999:THR:HG22	1.89	0.53
9:C:1255:HOH:O	5:F:354:LEU:HD21	2.08	0.53
1:L:60:ASP:H	1:L:137:ARG:NH2	2.06	0.53
2:M:328:LEU:HD21	2:M:438:ILE:CD1	2.38	0.53
2:M:410:ILE:HD12	2:M:410:ILE:H	1.73	0.53
2:M:874:LEU:HD23	3:N:1023:MET:CE	2.37	0.53
2:M:915:LYS:HB3	9:M:2164:HOH:O	2.09	0.53
3:N:908:LYS:CB	3:N:1027:GLY:HA3	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1087:ARG:HD3	3:N:1238:MET:N	2.23	0.53
3:N:1141:GLU:CG	3:N:1168:MET:HE1	2.39	0.53
3:N:1323:GLN:HG3	3:N:1324:PRO:HD2	1.90	0.53
3:N:160:GLU:HG2	9:N:2310:HOH:O	2.09	0.53
3:N:46:ASP:HB3	3:N:49:ILE:HG13	1.89	0.53
3:N:55:ASP:HB3	3:N:82:LYS:HE2	1.90	0.53
3:N:785:ILE:HG22	3:N:789:LEU:HD12	1.91	0.53
3:N:860:LEU:O	3:N:877:PRO:HD2	2.07	0.53
3:N:996:TRP:HE3	3:N:999:THR:HG21	1.73	0.53
4:O:29:GLN:HB2	4:O:33:HIS:CD2	2.43	0.53
5:P:368:VAL:O	5:P:372:ARG:HB2	2.09	0.53
2:C:496:ILE:HD12	2:C:496:ILE:H	1.74	0.53
2:C:816:LYS:HB2	2:C:819:VAL:CG2	2.39	0.53
2:C:690:ILE:CG2	2:C:852:ILE:HG13	2.39	0.53
3:D:631:ILE:HG21	3:D:745:MET:SD	2.49	0.53
3:D:52:PRO:CB	3:D:80:VAL:HG13	2.39	0.53
4:E:31:LEU:HD23	4:E:35:PHE:HE1	1.73	0.53
2:M:54:ILE:HG23	2:M:54:ILE:O	2.09	0.53
3:N:1066:THR:HA	9:N:1984:HOH:O	2.09	0.53
3:N:1377:LYS:O	3:N:1395:LEU:N	2.37	0.53
3:N:1422:MET:HE3	3:N:1427:SER:HA	1.89	0.53
3:N:503:LEU:HD22	9:N:2051:HOH:O	2.09	0.53
3:N:550:ARG:NH1	3:N:573:MET:HB3	2.24	0.53
3:N:692:GLU:HG3	3:N:720:LEU:HD13	1.91	0.53
3:N:786:ILE:HD13	3:N:908:LYS:HB3	1.89	0.53
2:C:535:SER:HB2	2:C:537:LYS:HG3	1.91	0.53
3:D:1220:ALA:HB1	3:D:1223:ILE:CD1	2.36	0.53
3:D:1492:LEU:HD12	9:D:2354:HOH:O	2.09	0.53
3:D:53:ILE:HG22	9:D:1900:HOH:O	2.08	0.53
2:C:984:GLU:OE1	3:D:945:SER:HA	2.09	0.53
5:F:321:ILE:O	5:F:327:SER:HB3	2.08	0.53
1:K:133:GLU:HG2	1:K:134:GLU:H	1.72	0.53
1:L:65:PHE:HB2	9:L:1134:HOH:O	2.08	0.53
2:M:162:ILE:O	2:M:164:PRO:HD3	2.09	0.53
2:M:607:ASP:HB2	2:M:610:ARG:HG3	1.91	0.53
2:M:64:LEU:HD11	2:M:100:LEU:HD13	1.90	0.53
2:M:737:LEU:HD12	2:M:754:ILE:HB	1.91	0.53
2:M:753:ASP:O	2:M:792:VAL:HG23	2.09	0.53
3:N:1109:GLU:CD	3:N:1202:GLN:H	2.12	0.53
3:N:1114:THR:O	3:N:1114:THR:HG23	2.09	0.53
3:N:1462:LEU:N	3:N:1462:LEU:HD23	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:407:VAL:HG13	3:N:422:ALA:HB2	1.91	0.53
3:N:591:VAL:HG11	3:N:597:ASP:HA	1.91	0.53
2:C:1101:THR:OG1	2:C:1109:VAL:HG12	2.09	0.53
2:C:495:THR:HB	2:C:530:GLU:HG3	1.91	0.53
3:D:1310:ARG:NE	3:D:1327:ARG:HB3	2.24	0.53
3:D:1330:ILE:HB	3:D:1347:TYR:CZ	2.43	0.53
3:D:760:ARG:NH2	4:E:62:THR:N	2.57	0.53
1:K:23:PHE:O	1:K:196:THR:HA	2.09	0.53
1:L:80:LEU:HG	3:N:844:ALA:HB2	1.91	0.53
2:M:109:LYS:HE2	2:M:111:ASP:OD1	2.09	0.53
2:M:143:SER:HB2	2:M:276:LYS:HZ3	1.74	0.53
2:M:290:LEU:HD11	9:M:1886:HOH:O	2.09	0.53
2:M:413:LEU:N	2:M:413:LEU:HD12	2.21	0.53
2:M:549:PHE:HB3	2:M:552:HIS:CD2	2.42	0.53
3:N:1175:ILE:O	3:N:1179:GLU:HG3	2.09	0.53
3:N:81:THR:HG23	9:N:1885:HOH:O	2.09	0.53
5:P:127:ILE:HD11	9:P:595:HOH:O	2.08	0.53
1:A:181:VAL:HG11	9:A:337:HOH:O	2.10	0.52
1:B:57:TYR:CE1	1:B:163:ASN:HB2	2.44	0.52
1:B:218:LEU:O	1:B:222:LEU:HG	2.08	0.52
1:B:58:ILE:HD13	1:B:140:MET:HB3	1.91	0.52
2:C:162:ILE:HD11	2:C:306:THR:HG21	1.90	0.52
2:C:110:GLU:H	2:C:368:THR:HG21	1.74	0.52
2:C:52:PHE:O	2:C:54:ILE:N	2.42	0.52
3:D:407:VAL:HG13	3:D:421:LEU:O	2.09	0.52
3:D:570:GLU:HB2	5:F:214:GLN:OE1	2.08	0.52
4:E:8:LYS:HG3	9:E:100:HOH:O	2.09	0.52
5:F:282:LEU:HD13	9:F:621:HOH:O	2.08	0.52
2:C:818:GLY:HA2	5:F:309:LYS:HZ3	1.74	0.52
2:M:1115:LEU:HD12	2:M:1115:LEU:N	2.23	0.52
2:M:197:LEU:HB3	2:M:202:TYR:HB2	1.90	0.52
3:N:1176:LYS:O	3:N:1179:GLU:HB2	2.09	0.52
3:N:1243:THR:HG1	3:N:1253:THR:HB	1.73	0.52
3:N:104:PHE:CD2	3:N:1448:THR:HG23	2.44	0.52
3:N:49:ILE:HB	3:N:50:PHE:CD1	2.44	0.52
3:N:567:ILE:N	3:N:567:ILE:HD12	2.24	0.52
3:N:826:PRO:HB3	9:N:1811:HOH:O	2.08	0.52
3:N:984:THR:HG21	9:N:1536:HOH:O	2.09	0.52
4:O:33:HIS:HB2	4:O:37:ASN:ND2	2.24	0.52
5:P:369:LEU:O	5:P:373:LYS:HB2	2.09	0.52
1:A:211:LEU:O	1:A:214:ALA:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:LEU:HD21	1:B:199:ILE:HD11	1.91	0.52
1:B:23:PHE:CE2	1:B:199:ILE:HD12	2.44	0.52
2:C:166:PRO:HD3	2:C:265:ARG:HB2	1.91	0.52
2:C:260:LEU:HA	2:C:291:ALA:HB2	1.90	0.52
2:C:603:VAL:HG22	2:C:613:VAL:HG12	1.90	0.52
2:C:739:GLU:HA	9:C:1304:HOH:O	2.09	0.52
2:C:772:ARG:HB3	9:F:459:HOH:O	2.09	0.52
3:D:102:ILE:HG13	9:D:1613:HOH:O	2.09	0.52
3:D:62:LYS:HD2	9:D:1735:HOH:O	2.08	0.52
5:F:102:LEU:O	5:F:106:VAL:HG23	2.09	0.52
2:M:1005:MET:O	2:M:1005:MET:HG3	2.09	0.52
2:M:176:VAL:C	2:M:178:PRO:HD3	2.29	0.52
2:M:602:GLU:HA	2:M:647:GLN:O	2.09	0.52
2:M:577:PRO:HG3	2:M:993:PHE:CE2	2.43	0.52
3:N:141:ILE:HG13	3:N:142:LEU:N	2.24	0.52
3:N:104:PHE:HE2	3:N:1448:THR:HA	1.73	0.52
3:N:32:ILE:O	5:P:258:ILE:HG23	2.09	0.52
3:N:611:GLN:OE1	3:N:619:LEU:HD21	2.09	0.52
3:N:892:ASP:OD2	3:N:895:VAL:HG21	2.09	0.52
5:P:220:LEU:HD12	5:P:243:ILE:HD11	1.92	0.52
2:C:129:ILE:HG22	2:C:130:ASN:ND2	2.24	0.52
2:C:368:THR:HB	2:C:369:PRO:HD3	1.90	0.52
2:C:404:LEU:HA	2:C:407:LYS:HD2	1.91	0.52
2:C:6:PHE:N	2:C:6:PHE:CD1	2.77	0.52
5:F:371:LEU:HB2	5:F:372:ARG:HH11	1.74	0.52
5:F:393:THR:O	5:F:397:ILE:HG13	2.09	0.52
1:K:149:GLY:O	1:K:171:PHE:HB2	2.10	0.52
1:K:189:ARG:HD2	1:K:191:ASP:OD1	2.09	0.52
2:M:470:PRO:HB2	2:M:534:VAL:HG21	1.90	0.52
2:M:626:ARG:H	2:M:639:GLN:NE2	2.06	0.52
3:N:1305:LEU:HD22	3:N:1309:ALA:HB1	1.91	0.52
3:N:153:LEU:CD1	3:N:157:GLU:HB2	2.39	0.52
3:N:163:TYR:HB3	9:N:2151:HOH:O	2.10	0.52
3:N:179:VAL:HG13	3:N:183:GLU:HB3	1.92	0.52
3:N:498:VAL:HG23	3:N:499:VAL:N	2.24	0.52
3:N:584:ASN:HD21	3:N:590:PRO:HD2	1.72	0.52
3:N:408:GLU:HA	5:P:171:LYS:NZ	2.23	0.52
5:P:392:VAL:HG11	5:P:396:ARG:HD2	1.91	0.52
2:C:265:ARG:HB3	2:C:267:TYR:CD2	2.45	0.52
2:C:442:GLU:HB3	9:C:1185:HOH:O	2.08	0.52
2:C:643:VAL:HB	9:C:1145:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:114:THR:O	3:D:495:ARG:HG3	2.09	0.52
3:D:591:VAL:HG11	3:D:597:ASP:HA	1.92	0.52
3:D:710:ARG:HH21	3:D:1210:SER:CB	2.22	0.52
3:D:892:ASP:OD2	3:D:895:VAL:HG21	2.09	0.52
3:D:965:GLU:HA	3:D:968:ASP:HB2	1.91	0.52
1:K:127:LEU:HD12	1:K:127:LEU:C	2.30	0.52
1:L:45:LEU:HD21	1:L:177:VAL:HG13	1.91	0.52
2:M:289:THR:HG22	2:M:290:LEU:HD23	1.92	0.52
2:M:605:LYS:HG3	2:M:612:VAL:HB	1.92	0.52
3:N:1076:GLY:O	3:N:1079:LYS:HG2	2.09	0.52
3:N:1182:GLU:HG3	9:N:1552:HOH:O	2.08	0.52
3:N:1205:TYR:HE1	3:N:1221:VAL:HG13	1.73	0.52
3:N:408:GLU:HB3	9:N:1846:HOH:O	2.09	0.52
3:N:661:MET:O	3:N:664:LYS:O	2.26	0.52
5:P:115:LYS:O	5:P:119:ILE:HG13	2.08	0.52
5:P:141:VAL:O	5:P:145:PRO:HD2	2.09	0.52
3:N:534:ARG:HG3	5:P:312:GLN:NE2	2.24	0.52
1:B:198:ARG:HD2	9:B:489:HOH:O	2.09	0.52
2:C:142:ARG:HH21	2:C:325:ILE:HD11	1.72	0.52
2:C:212:GLY:HA3	2:C:218:VAL:HG23	1.90	0.52
2:C:208:ALA:HA	2:C:218:VAL:HG22	1.91	0.52
2:C:252:LYS:HD3	2:C:296:GLY:HA2	1.91	0.52
2:C:302:VAL:O	2:C:306:THR:HG23	2.09	0.52
2:C:480:THR:HG22	2:C:482:GLU:H	1.74	0.52
3:D:1189:ARG:NH1	3:D:1203:LYS:HB2	2.24	0.52
3:D:1284:GLU:HG3	9:D:1992:HOH:O	2.10	0.52
3:D:403:PHE:CZ	3:D:407:VAL:HG23	2.44	0.52
3:D:720:LEU:H	3:D:720:LEU:HD12	1.73	0.52
3:D:853:VAL:HA	3:D:858:VAL:O	2.10	0.52
4:E:54:LEU:O	4:E:54:LEU:HD23	2.09	0.52
5:F:181:GLU:O	5:F:184:ARG:HB3	2.10	0.52
5:F:338:LEU:HD12	9:F:562:HOH:O	2.09	0.52
1:K:206:THR:HG22	1:K:209:GLU:CG	2.36	0.52
1:L:101:LEU:HD11	1:L:113:ASP:HB2	1.91	0.52
2:M:131:GLY:N	9:M:1824:HOH:O	2.43	0.52
2:M:139:GLN:HE22	2:M:415:PRO:HD2	1.74	0.52
2:M:765:SER:O	2:M:767:PRO:HD3	2.10	0.52
3:N:1109:GLU:CG	3:N:1202:GLN:H	2.22	0.52
3:N:1277:ILE:CD1	3:N:1301:LYS:HB2	2.38	0.52
3:N:169:TYR:HB3	3:N:195:VAL:HG11	1.91	0.52
3:N:633:VAL:HG22	3:N:635:PRO:CD	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:63:TRP:O	4:O:67:GLU:HG3	2.09	0.52
5:P:152:ASP:HB3	5:P:153:PRO:HD3	1.92	0.52
5:P:306:GLU:HG3	9:P:674:HOH:O	2.10	0.52
5:P:363:GLU:HA	5:P:367:MET:HG3	1.91	0.52
1:B:71:VAL:HG22	1:B:132:LEU:CD1	2.39	0.52
1:B:156:HIS:CG	1:B:157:GLY:H	2.27	0.52
1:B:62:LEU:HD12	1:B:62:LEU:H	1.74	0.52
2:C:145:GLY:H	2:C:163:ILE:HG12	1.72	0.52
2:C:603:VAL:HG21	2:C:643:VAL:CG1	2.40	0.52
3:D:1363:LEU:HD12	3:D:1364:HIS:O	2.10	0.52
3:D:1394:VAL:HG21	9:D:2203:HOH:O	2.08	0.52
3:D:1503:VAL:HG13	9:D:1882:HOH:O	2.09	0.52
3:D:447:VAL:HA	9:D:2047:HOH:O	2.09	0.52
3:D:116:LEU:HD21	3:D:464:LEU:CB	2.38	0.52
3:D:567:ILE:HD12	3:D:567:ILE:N	2.24	0.52
3:D:715:ALA:O	3:D:764:LEU:HD12	2.08	0.52
3:D:774:SER:C	3:D:776:GLU:H	2.13	0.52
3:D:809:PRO:HB2	3:D:812:ALA:CB	2.40	0.52
4:E:94:PRO:HA	9:E:126:HOH:O	2.08	0.52
1:K:90:LEU:HD11	9:K:1139:HOH:O	2.09	0.52
2:M:670:GLN:O	2:M:672:VAL:HG12	2.10	0.52
3:N:1041:LEU:HD12	3:N:1058:ARG:CA	2.38	0.52
3:N:1097:LYS:O	3:N:1101:VAL:HG23	2.09	0.52
3:N:400:VAL:HG22	3:N:443:VAL:CG2	2.31	0.52
3:N:473:LEU:HD21	3:N:495:ARG:CZ	2.40	0.52
3:N:504:ASP:HB3	9:N:2286:HOH:O	2.08	0.52
3:N:710:ARG:NH2	3:N:1210:SER:OG	2.43	0.52
3:N:52:PRO:HB2	3:N:80:VAL:HG13	1.92	0.52
3:N:875:THR:HG22	3:N:879:ARG:HB2	1.92	0.52
5:P:393:THR:HG22	5:P:394:ARG:H	1.75	0.52
2:C:1059:ASP:OD1	2:C:1080:SER:HB3	2.10	0.52
2:C:195:LEU:HD12	2:C:234:ALA:HB1	1.91	0.52
2:C:64:LEU:HD22	2:C:359:MET:HG3	1.91	0.52
2:C:408:ARG:HH21	2:C:542:VAL:CG2	2.23	0.52
2:C:697:ARG:HD2	2:C:699:PHE:CD1	2.45	0.52
9:C:1344:HOH:O	3:D:603:LEU:HB3	2.09	0.52
3:D:916:TYR:CE2	3:D:920:LEU:HD13	2.45	0.52
2:M:926:PHE:O	2:M:930:LYS:HG3	2.10	0.52
3:N:1019:PRO:O	3:N:1023:MET:HG2	2.10	0.52
3:N:1272:ALA:CA	3:N:1326:THR:HB	2.40	0.52
3:N:637:LEU:CD1	3:N:641:GLN:HB2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:181:GLU:O	5:P:184:ARG:HB3	2.10	0.52
5:P:288:TYR:HA	5:P:291:ILE:HG22	1.91	0.52
1:B:5:LYS:O	1:B:8:ALA:HB2	2.09	0.52
2:C:196:LEU:O	2:C:199:VAL:HB	2.10	0.52
2:C:209:ARG:O	2:C:213:ALA:HB2	2.10	0.52
2:C:338:GLU:O	2:C:341:THR:HG22	2.10	0.52
2:C:367:LEU:HD13	9:C:1770:HOH:O	2.10	0.52
2:C:435:TYR:C	2:C:437:ARG:H	2.13	0.52
2:C:713:ARG:HH12	3:D:531:ASP:CG	2.14	0.52
2:C:722:ILE:HG13	2:C:757:GLY:O	2.10	0.52
2:C:966:LEU:HD11	2:C:986:PRO:HG2	1.91	0.52
2:C:878:SER:HB3	3:D:1029:ARG:HH11	1.74	0.52
3:D:1101:VAL:HG21	3:D:1424:VAL:CG2	2.31	0.52
3:D:1321:ALA:O	3:D:1339:LYS:HG3	2.10	0.52
3:D:989:TYR:CZ	3:D:993:LEU:HD11	2.45	0.52
4:E:54:LEU:HD23	4:E:58:PRO:HD2	1.91	0.52
5:F:151:LEU:HD21	9:F:675:HOH:O	2.08	0.52
2:M:165:LEU:O	2:M:265:ARG:HD2	2.10	0.52
2:M:166:PRO:HD3	2:M:265:ARG:CG	2.39	0.52
2:M:208:ALA:HA	2:M:218:VAL:HG22	1.91	0.52
2:M:402:SER:OG	2:M:566:THR:HG22	2.09	0.52
2:M:773:LEU:O	2:M:777:ILE:HG13	2.10	0.52
2:M:79:PRO:HA	9:M:2242:HOH:O	2.09	0.52
3:N:1283:ILE:HG22	3:N:1284:GLU:N	2.24	0.52
3:N:408:GLU:HG2	3:N:408:GLU:O	2.10	0.52
3:N:947:ILE:HD12	3:N:947:ILE:O	2.09	0.52
5:P:191:ASN:HB3	5:P:220:LEU:HD11	1.90	0.52
5:P:358:LEU:CD2	5:P:370:LYS:HZ2	2.23	0.52
1:A:107:LYS:HE3	1:A:113:ASP:OD2	2.10	0.52
1:A:55:SER:CB	1:A:158:ILE:HG21	2.40	0.52
1:B:19:GLU:O	1:B:200:TRP:HA	2.10	0.52
2:C:170:PRO:HD3	2:C:263:ASP:HB3	1.92	0.52
2:C:281:LEU:CD1	2:C:306:THR:HA	2.40	0.52
2:C:971:LYS:HE2	9:C:1494:HOH:O	2.09	0.52
3:D:1324:PRO:HG3	3:D:1330:ILE:HD11	1.91	0.52
3:D:1462:LEU:N	3:D:1462:LEU:HD23	2.24	0.52
3:D:551:ASN:O	3:D:555:LYS:HG3	2.09	0.52
3:D:697:GLY:C	9:D:1581:HOH:O	2.48	0.52
3:D:77:GLY:O	3:D:78:VAL:HG23	2.10	0.52
3:D:863:VAL:HG12	9:D:1596:HOH:O	2.10	0.52
5:F:88:ILE:CD1	5:F:193:ARG:HB2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:385:PHE:O	2:M:389:SER:HB3	2.10	0.52
2:M:54:ILE:HG22	2:M:66:LEU:HB3	1.92	0.52
2:M:807:ARG:HD3	9:M:1889:HOH:O	2.09	0.52
2:M:911:GLU:O	2:M:915:LYS:HG2	2.10	0.52
2:M:926:PHE:CD1	2:M:929:ARG:HD3	2.44	0.52
3:N:1487:VAL:HG13	3:N:1491:THR:HB	1.91	0.52
3:N:50:PHE:CB	3:N:522:PRO:HG2	2.40	0.52
2:M:770:GLU:CG	3:N:65:ARG:HH12	2.23	0.52
5:P:279:GLN:HA	9:P:477:HOH:O	2.10	0.52
1:A:128:HIS:CE1	1:A:131:THR:HG23	2.45	0.52
1:A:44:LEU:HB3	1:A:177:VAL:HG21	1.91	0.52
2:C:207:LEU:HD22	2:C:221:LEU:CD2	2.39	0.52
2:C:352:ALA:HA	2:C:355:VAL:HG12	1.91	0.52
2:C:70:GLU:HB3	9:C:1236:HOH:O	2.09	0.52
3:D:1481:VAL:CG1	4:E:18:ARG:HG3	2.40	0.52
3:D:162:ARG:HA	3:D:449:SER:HB3	1.91	0.52
3:D:567:ILE:H	3:D:567:ILE:HD12	1.75	0.52
3:D:675:ARG:O	3:D:678:GLU:HG2	2.10	0.52
3:D:864:VAL:HG12	3:D:865:THR:H	1.73	0.52
4:E:54:LEU:HA	4:E:58:PRO:HG2	1.91	0.52
5:F:163:LEU:HB3	5:F:174:LEU:HD13	1.92	0.52
1:K:146:ARG:HD2	9:K:2782:HOH:O	2.10	0.52
2:M:197:LEU:HD22	2:M:202:TYR:CD2	2.43	0.52
2:M:42:VAL:HG12	2:M:43:GLY:N	2.25	0.52
2:M:816:LYS:HE2	2:M:819:VAL:HG21	1.92	0.52
3:N:631:ILE:HG12	3:N:743:ASP:O	2.10	0.52
3:N:711:LEU:C	3:N:713:ILE:H	2.12	0.52
2:M:676:ILE:O	3:N:948:THR:HB	2.09	0.52
3:N:988:ARG:O	3:N:992:ILE:HG13	2.10	0.52
1:A:5:LYS:O	1:A:8:ALA:HB2	2.08	0.51
2:C:1060:ILE:CG2	2:C:1061:GLU:N	2.72	0.51
2:C:59:LYS:HB2	9:C:1378:HOH:O	2.08	0.51
2:C:815:LEU:HG	2:C:819:VAL:CG1	2.40	0.51
2:C:918:LEU:HD23	2:C:967:PHE:O	2.09	0.51
2:C:976:ASP:HB3	2:C:979:THR:HG22	1.92	0.51
3:D:105:VAL:HG13	3:D:124:GLU:OE1	2.10	0.51
3:D:1059:SER:OG	3:D:1065:LEU:HA	2.11	0.51
3:D:1280:VAL:O	3:D:1294:VAL:HA	2.10	0.51
3:D:1494:ALA:HB1	9:E:137:HOH:O	2.10	0.51
5:F:226:LYS:HD2	5:F:242:TRP:CZ2	2.45	0.51
5:F:88:ILE:CG1	5:F:193:ARG:HB2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:57:TYR:O	1:K:140:MET:HA	2.10	0.51
1:L:117:VAL:HA	9:L:1875:HOH:O	2.10	0.51
1:L:156:HIS:CG	1:L:157:GLY:H	2.28	0.51
1:L:9:PRO:HB3	1:L:25:LEU:HG	1.93	0.51
2:M:816:LYS:HB2	2:M:819:VAL:CG2	2.39	0.51
3:N:534:ARG:HG3	5:P:312:GLN:HE22	1.74	0.51
3:N:551:ASN:O	3:N:555:LYS:HG3	2.10	0.51
3:N:957:PRO:HD2	3:N:1007:VAL:HG12	1.91	0.51
4:O:51:LEU:HB2	9:O:1054:HOH:O	2.09	0.51
3:N:1485:GLN:NE2	4:O:80:VAL:H	2.08	0.51
5:P:336:GLU:HG3	9:P:629:HOH:O	2.09	0.51
3:D:1118:ILE:HG23	9:D:1773:HOH:O	2.09	0.51
3:D:127:LEU:HD11	3:D:461:ILE:HD11	1.92	0.51
3:D:1385:GLY:CA	3:D:1413:THR:HG21	2.39	0.51
3:D:126:VAL:HG11	3:D:152:LEU:HD12	1.92	0.51
3:D:133:ILE:HG22	3:D:455:ARG:C	2.31	0.51
3:D:661:MET:HE2	3:D:673:ALA:HB1	1.92	0.51
3:D:840:LYS:HB3	3:D:841:TYR:CD2	2.46	0.51
5:F:278:LEU:CB	5:F:286:PRO:HG2	2.40	0.51
9:D:2077:HOH:O	5:F:349:LEU:HD22	2.10	0.51
1:K:69:PRO:C	1:K:71:VAL:H	2.13	0.51
1:L:25:LEU:HD23	1:L:28:LEU:HD11	1.91	0.51
2:M:260:LEU:HD22	9:M:2052:HOH:O	2.10	0.51
2:M:464:LEU:HD12	2:M:465:GLY:N	2.25	0.51
2:M:498:GLN:HE21	2:M:498:GLN:HA	1.74	0.51
9:K:1749:HOH:O	2:M:929:ARG:HG3	2.08	0.51
3:N:192:ALA:HB2	3:N:393:ILE:HD11	1.92	0.51
3:N:428:LYS:HE2	9:N:1658:HOH:O	2.11	0.51
3:N:833:GLU:HG2	9:N:2184:HOH:O	2.08	0.51
5:P:189:GLU:HA	5:P:192:LEU:HD12	1.90	0.51
1:A:42:ARG:HH21	2:C:857:ASP:HB3	1.75	0.51
2:C:141:HIS:O	2:C:331:ARG:HA	2.10	0.51
2:C:631:SER:HB3	2:C:637:LEU:HD21	1.92	0.51
2:C:2:GLU:CG	2:C:899:GLN:HB3	2.28	0.51
3:D:1205:TYR:HE1	3:D:1221:VAL:HG13	1.75	0.51
3:D:10:ILE:HD11	3:D:1434:TRP:NE1	2.24	0.51
3:D:187:LYS:HG3	3:D:199:LEU:CD2	2.40	0.51
5:F:130:VAL:HA	5:F:142:ARG:NH2	2.26	0.51
5:F:361:LEU:HD21	5:F:404:ALA:HB1	1.92	0.51
1:L:196:THR:HG22	9:L:1676:HOH:O	2.10	0.51
1:L:57:TYR:CZ	1:L:161:ARG:HD3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:489:THR:HG21	9:M:2237:HOH:O	2.09	0.51
3:N:1342:GLU:HB3	9:N:2128:HOH:O	2.10	0.51
3:N:31:THR:HG23	3:N:45:PHE:HE2	1.75	0.51
3:N:398:ALA:HB1	3:N:446:VAL:O	2.10	0.51
3:N:39:PRO:HB3	3:N:45:PHE:C	2.31	0.51
3:N:861:GLN:HG2	9:N:2139:HOH:O	2.09	0.51
2:C:211:LEU:HD11	2:C:308:ARG:HA	1.93	0.51
2:C:512:ARG:HB3	2:C:523:ILE:HD11	1.92	0.51
2:C:633:GLN:HG3	9:C:1153:HOH:O	2.09	0.51
2:C:810:ASP:N	2:C:811:PRO:HD3	2.25	0.51
2:C:987:ILE:HG12	3:D:948:THR:HG21	1.91	0.51
3:D:10:ILE:HG13	3:D:1434:TRP:CE2	2.45	0.51
3:D:1115:THR:HG21	9:D:2063:HOH:O	2.10	0.51
3:D:1306:PRO:HG3	9:D:1723:HOH:O	2.10	0.51
3:D:1341:PRO:O	3:D:1345:GLU:HB2	2.10	0.51
3:D:18:ILE:HD12	3:D:518:PRO:CG	2.40	0.51
3:D:398:ALA:HB1	3:D:446:VAL:O	2.10	0.51
3:D:879:ARG:HD3	3:D:902:LEU:O	2.10	0.51
4:E:33:HIS:CB	4:E:37:ASN:HD21	2.21	0.51
4:E:60:ALA:O	4:E:63:TRP:HB2	2.10	0.51
2:M:191:PHE:CZ	2:M:238:LEU:HD11	2.45	0.51
2:M:218:VAL:HG12	9:M:1965:HOH:O	2.11	0.51
2:M:264:PRO:HB2	9:M:1685:HOH:O	2.11	0.51
2:M:141:HIS:CB	2:M:418:LEU:HG	2.40	0.51
2:M:561:GLY:HA3	2:M:842:ARG:O	2.11	0.51
2:M:897:LEU:HB3	2:M:899:GLN:HE21	1.76	0.51
3:N:1264:GLU:HG2	3:N:1425:THR:HG22	1.92	0.51
3:N:1485:GLN:O	4:O:75:PHE:HA	2.11	0.51
3:N:111:LYS:HE2	3:N:498:VAL:HG12	1.92	0.51
5:P:416:ARG:HD3	5:P:419:ARG:HD3	1.92	0.51
1:A:182:GLU:HG2	9:A:412:HOH:O	2.11	0.51
1:A:198:ARG:C	1:A:199:ILE:HD12	2.29	0.51
1:A:19:GLU:O	1:A:200:TRP:HA	2.10	0.51
2:C:1105:LYS:O	2:C:1105:LYS:HG3	2.10	0.51
2:C:1109:VAL:HG21	3:D:3:LYS:O	2.11	0.51
2:C:114:PHE:CD1	2:C:114:PHE:N	2.77	0.51
2:C:257:VAL:HG21	9:C:1517:HOH:O	2.11	0.51
2:C:278:GLU:HB2	9:C:1544:HOH:O	2.10	0.51
2:C:420:ARG:NH1	2:C:422:ARG:HH21	2.08	0.51
2:C:876:VAL:O	2:C:879:ARG:O	2.29	0.51
2:C:874:LEU:HD23	3:D:1023:MET:CE	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1258:ARG:NH2	3:D:1262:LEU:HD11	2.26	0.51
3:D:1277:ILE:CD1	3:D:1301:LYS:HB2	2.40	0.51
3:D:137:PRO:N	9:D:1592:HOH:O	2.43	0.51
3:D:26:VAL:HG23	9:D:2241:HOH:O	2.10	0.51
3:D:436:GLU:HB2	9:D:2406:HOH:O	2.10	0.51
3:D:480:GLU:O	3:D:480:GLU:HG3	2.10	0.51
5:F:410:TYR:O	5:F:413:SER:HB2	2.11	0.51
1:L:133:GLU:O	1:L:134:GLU:HG2	2.10	0.51
2:M:313:LEU:HD12	2:M:313:LEU:O	2.10	0.51
2:M:349:ALA:HB3	9:M:1970:HOH:O	2.10	0.51
2:M:398:THR:N	2:M:633:GLN:OE1	2.43	0.51
2:M:606:VAL:CG2	2:M:645:VAL:HG22	2.40	0.51
2:M:685:GLU:HG3	3:N:783:ARG:HD2	1.92	0.51
3:N:1145:TYR:CE2	3:N:1168:MET:HB2	2.44	0.51
3:N:145:VAL:HG13	3:N:146:PRO:N	2.26	0.51
3:N:65:ARG:CG	3:N:66:GLN:N	2.73	0.51
4:O:33:HIS:CB	4:O:37:ASN:HD21	2.24	0.51
5:P:350:LEU:HD12	5:P:422:LEU:HD12	1.92	0.51
2:C:334:ARG:HB2	9:C:1322:HOH:O	2.09	0.51
2:C:551:GLU:HB3	2:C:906:PHE:CD2	2.46	0.51
2:C:911:GLU:O	2:C:915:LYS:HG2	2.11	0.51
3:D:1372:VAL:HG13	3:D:1373:ARG:N	2.26	0.51
3:D:586:ARG:NH2	3:D:1444:THR:HG21	2.26	0.51
3:D:637:LEU:CD1	3:D:641:GLN:HB2	2.41	0.51
3:D:799:LYS:O	3:D:826:PRO:HD2	2.09	0.51
3:D:97:THR:HB	9:D:1781:HOH:O	2.10	0.51
5:F:273:ARG:HG2	9:F:688:HOH:O	2.10	0.51
1:K:49:PRO:HB3	1:K:148:VAL:HG22	1.92	0.51
1:K:19:GLU:HB3	9:K:2538:HOH:O	2.09	0.51
1:L:23:PHE:O	1:L:196:THR:HA	2.10	0.51
2:M:244:PRO:HD2	2:M:245:GLY:H	1.75	0.51
2:M:264:PRO:HB3	2:M:289:THR:HG21	1.93	0.51
2:M:411:SER:OG	2:M:452:ILE:HG23	2.11	0.51
2:M:477:GLY:O	2:M:508:ILE:HG12	2.11	0.51
2:M:976:ASP:HB3	2:M:979:THR:HG22	1.92	0.51
3:N:1113:GLY:N	3:N:1195:GLN:NE2	2.58	0.51
3:N:204:LEU:HD21	3:N:445:ARG:NH1	2.26	0.51
3:N:613:ARG:CZ	3:N:1097:LYS:HE2	2.40	0.51
3:N:34:TYR:OH	5:P:261:PRO:HD2	2.10	0.51
5:P:370:LYS:HD3	5:P:371:LEU:HG	1.93	0.51
2:C:165:LEU:HA	2:C:166:PRO:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:264:PRO:HB3	2:C:289:THR:HG21	1.91	0.51
2:C:551:GLU:OE2	2:C:552:HIS:NE2	2.43	0.51
3:D:1382:THR:HG21	3:D:1418:LYS:NZ	2.25	0.51
3:D:1441:GLN:HG3	3:D:1442:ASN:N	2.25	0.51
3:D:443:VAL:HG22	3:D:444:VAL:N	2.26	0.51
3:D:52:PRO:HD2	9:D:1552:HOH:O	2.10	0.51
3:D:820:GLU:HA	3:D:825:ALA:O	2.10	0.51
5:F:153:PRO:HD2	9:F:614:HOH:O	2.09	0.51
1:K:11:PHE:HB2	9:K:1022:HOH:O	2.10	0.51
2:M:516:ARG:HD2	9:M:1937:HOH:O	2.10	0.51
1:K:70:GLY:N	2:M:607:ASP:OD1	2.38	0.51
2:M:676:ILE:CG2	2:M:988:VAL:HG22	2.40	0.51
2:M:881:ASN:H	2:M:881:ASN:HD22	1.59	0.51
3:N:1382:THR:HG21	3:N:1418:LYS:HE3	1.92	0.51
3:N:26:VAL:HG11	3:N:44:LEU:HD23	1.91	0.51
3:N:141:ILE:HG21	3:N:449:SER:HA	1.92	0.51
2:M:1058:ASP:HB2	3:N:621:LYS:HE2	1.93	0.51
3:N:658:LEU:HD11	3:N:674:ARG:HH11	1.76	0.51
3:N:754:PHE:HE2	3:N:1476:THR:HG21	1.76	0.51
3:N:986:ARG:HG3	9:N:1540:HOH:O	2.11	0.51
3:N:996:TRP:O	3:N:999:THR:HG22	2.11	0.51
1:A:1:MET:HB3	9:A:440:HOH:O	2.10	0.51
1:A:49:PRO:O	1:A:173:PRO:HG2	2.10	0.51
2:C:334:ARG:NH1	2:C:415:PRO:HG2	2.25	0.51
3:D:1101:VAL:CA	3:D:1428:ALA:HB2	2.40	0.51
3:D:1120:VAL:HB	3:D:1144:LEU:HD21	1.92	0.51
3:D:1243:THR:HG22	3:D:1244:GLY:H	1.76	0.51
3:D:1305:LEU:HD22	3:D:1309:ALA:HB1	1.92	0.51
3:D:687:VAL:HG13	9:D:2185:HOH:O	2.11	0.51
4:E:17:TYR:CD2	4:E:17:TYR:N	2.78	0.51
5:F:339:PRO:HB3	5:F:343:ASP:HB2	1.92	0.51
2:M:1105:LYS:O	2:M:1107:ASN:N	2.44	0.51
2:M:208:ALA:HA	2:M:221:LEU:HD21	1.93	0.51
2:M:244:PRO:HG2	2:M:246:ASP:OD2	2.09	0.51
2:M:260:LEU:HA	2:M:291:ALA:HB2	1.91	0.51
2:M:333:ILE:HB	9:M:1750:HOH:O	2.10	0.51
1:K:180:GLN:HE22	2:M:929:ARG:HH21	1.59	0.51
2:M:98:LEU:HG	9:M:1826:HOH:O	2.10	0.51
3:N:1250:ALA:HB2	9:N:1888:HOH:O	2.09	0.51
7:N:1527:MXP:H11A	9:N:1557:HOH:O	2.11	0.51
3:N:14:SER:O	3:N:17:LYS:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:434:ARG:HB2	3:N:447:VAL:CG2	2.41	0.51
3:N:563:PRO:HG2	3:N:566:ILE:HD12	1.93	0.51
3:N:866:VAL:HG12	3:N:867:ARG:N	2.25	0.51
3:N:957:PRO:CD	3:N:1007:VAL:HG12	2.40	0.51
4:O:41:GLU:N	4:O:42:PRO:CD	2.74	0.51
5:P:103:ALA:HB3	9:P:455:HOH:O	2.11	0.51
2:C:275:TYR:HB2	9:C:1736:HOH:O	2.10	0.51
2:C:305:PRO:CA	2:C:308:ARG:HB2	2.41	0.51
2:C:129:ILE:CG1	2:C:386:PHE:HB3	2.41	0.51
2:C:676:ILE:O	2:C:676:ILE:CG2	2.56	0.51
2:C:6:PHE:CB	2:C:909:ALA:HA	2.40	0.51
2:C:742:VAL:HG12	2:C:743:VAL:N	2.26	0.51
3:D:1278:ASP:HA	3:D:1319:VAL:O	2.11	0.51
3:D:46:ASP:OD2	3:D:48:ARG:HG2	2.11	0.51
3:D:50:PHE:HB3	3:D:522:PRO:HG2	1.91	0.51
3:D:633:VAL:HG13	3:D:633:VAL:O	2.11	0.51
3:D:661:MET:O	3:D:664:LYS:O	2.28	0.51
4:E:41:GLU:N	4:E:42:PRO:CD	2.72	0.51
5:F:260:ILE:CG2	5:F:264:MET:HB2	2.40	0.51
1:K:25:LEU:HB2	9:K:1260:HOH:O	2.11	0.51
1:L:128:HIS:CE1	1:L:131:THR:HG23	2.46	0.51
2:M:267:TYR:HD1	9:M:2269:HOH:O	1.94	0.51
2:M:644:VAL:HG22	2:M:647:GLN:OE1	2.11	0.51
3:N:399:ARG:HD2	9:N:1669:HOH:O	2.09	0.51
5:P:163:LEU:HD22	5:P:174:LEU:HD12	1.91	0.51
3:N:569:ASN:HB3	5:P:214:GLN:NE2	2.25	0.51
1:A:9:PRO:HD2	1:B:224:TYR:CE1	2.46	0.51
1:B:68:ILE:HG23	1:B:137:ARG:NH1	2.25	0.51
2:C:18:LEU:HD21	2:C:542:VAL:CG1	2.41	0.51
2:C:498:GLN:NE2	2:C:498:GLN:HA	2.26	0.51
2:C:952:LEU:HD22	9:C:1205:HOH:O	2.10	0.51
3:D:1145:TYR:CE2	3:D:1168:MET:HB2	2.45	0.51
3:D:134:VAL:HG12	3:D:152:LEU:HB3	1.93	0.51
3:D:1393:GLN:HB2	3:D:1398:TRP:CE2	2.46	0.51
3:D:141:ILE:CG2	3:D:450:TYR:H	2.24	0.51
3:D:162:ARG:HD2	3:D:434:ARG:CZ	2.41	0.51
3:D:407:VAL:HG13	3:D:422:ALA:HB2	1.92	0.51
3:D:537:THR:C	5:F:317:LEU:HB2	2.32	0.51
3:D:581:LEU:O	3:D:603:LEU:HG	2.11	0.51
3:D:761:ILE:HG21	9:E:116:HOH:O	2.11	0.51
1:K:89:PHE:HB3	1:K:94:LEU:CD2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:50:GLY:HA3	1:L:171:PHE:O	2.11	0.51
2:M:437:ARG:HH22	2:M:491:GLU:CB	2.24	0.51
2:M:603:VAL:HG21	2:M:643:VAL:CG1	2.35	0.51
2:M:979:THR:HG23	2:M:981:GLU:N	2.24	0.51
3:N:1280:VAL:O	3:N:1294:VAL:HA	2.11	0.51
3:N:569:ASN:HD21	5:P:210:LEU:CD2	2.22	0.51
3:N:615:ARG:O	3:N:617:ASN:N	2.44	0.51
3:N:820:GLU:HA	3:N:825:ALA:O	2.11	0.51
9:N:2109:HOH:O	5:P:164:LYS:HE3	2.10	0.51
1:A:57:TYR:O	1:A:140:MET:HA	2.11	0.50
1:A:16:GLN:HG2	1:A:16:GLN:O	2.10	0.50
1:A:216:GLU:HG2	9:A:422:HOH:O	2.10	0.50
2:C:42:VAL:HG23	9:C:1299:HOH:O	2.10	0.50
2:C:890:LEU:HD12	2:C:914:ILE:HD13	1.93	0.50
2:C:861:LEU:HD21	2:C:925:TYR:HE2	1.76	0.50
2:C:942:GLU:O	2:C:945:ARG:HB3	2.11	0.50
3:D:1147:ARG:HD2	3:D:1188:VAL:HG21	1.92	0.50
3:D:448:GLU:HA	9:D:2218:HOH:O	2.11	0.50
3:D:6:ARG:HD3	9:D:1692:HOH:O	2.11	0.50
5:F:209:PHE:CE2	5:F:213:ILE:HD11	2.45	0.50
2:M:139:GLN:HE21	2:M:334:ARG:HD2	1.77	0.50
2:M:157:ARG:NH2	2:M:314:THR:O	2.44	0.50
2:M:275:TYR:HD2	9:M:1681:HOH:O	1.94	0.50
2:M:289:THR:O	2:M:291:ALA:N	2.44	0.50
2:M:358:ARG:HD3	2:M:371:LYS:O	2.11	0.50
2:M:463:GLU:HB3	9:M:1990:HOH:O	2.09	0.50
2:M:502:PRO:HB2	2:M:509:ALA:HB3	1.93	0.50
2:M:68:PHE:HE1	2:M:96:ALA:HB1	1.76	0.50
2:M:736:ASP:C	2:M:738:ASP:H	2.13	0.50
2:M:755:LEU:HD12	9:M:1781:HOH:O	2.10	0.50
3:N:955:VAL:O	3:N:1039:CYS:HB3	2.11	0.50
3:N:137:PRO:HD2	3:N:453:ASP:OD2	2.11	0.50
5:P:372:ARG:HD3	9:P:506:HOH:O	2.11	0.50
2:C:290:LEU:HB3	2:C:302:VAL:CG1	2.41	0.50
3:D:1018:ASN:HB3	3:D:1021:TYR:HB3	1.92	0.50
3:D:421:LEU:CG	3:D:429:SER:HB3	2.42	0.50
3:D:627:GLY:O	3:D:747:VAL:HG12	2.12	0.50
4:E:45:ARG:HH21	4:E:55:PHE:HB3	1.75	0.50
5:F:287:THR:HG23	5:F:289:GLU:HB3	1.92	0.50
5:F:88:ILE:HD13	5:F:193:ARG:HB2	1.93	0.50
1:L:69:PRO:C	1:L:71:VAL:H	2.13	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:573:ARG:HH12	2:M:697:ARG:HB3	1.75	0.50
2:M:671:ASN:H	2:M:671:ASN:ND2	2.08	0.50
2:M:710:ILE:CD1	2:M:790:LEU:HB2	2.41	0.50
2:M:930:LYS:HA	9:M:1678:HOH:O	2.11	0.50
1:K:179:PHE:HZ	2:M:939:ARG:HH22	1.57	0.50
3:N:9:ARG:HE	3:N:11:ALA:HB2	1.75	0.50
1:A:50:GLY:O	1:A:146:ARG:HA	2.11	0.50
2:C:1051:GLU:HG2	2:C:1056:LYS:HD2	1.93	0.50
2:C:1115:LEU:HD23	3:D:85:VAL:HG13	1.94	0.50
2:C:181:VAL:HG11	9:C:1754:HOH:O	2.10	0.50
2:C:185:LYS:CE	2:C:190:LYS:HE2	2.40	0.50
2:C:41:ASN:ND2	2:C:41:ASN:H	1.97	0.50
2:C:480:THR:HG22	2:C:481:ASP:H	1.76	0.50
2:C:756:VAL:HG21	2:C:823:VAL:HG11	1.92	0.50
2:C:877:PRO:CG	3:D:1023:MET:HE2	2.36	0.50
3:D:800:LYS:NZ	3:D:804:LEU:HD13	2.26	0.50
5:F:361:LEU:HD13	5:F:366:ALA:CB	2.42	0.50
2:M:136:ILE:CG2	2:M:336:VAL:HG22	2.41	0.50
2:M:253:ALA:O	2:M:256:TYR:HB2	2.11	0.50
2:M:274:ARG:HG2	9:M:1662:HOH:O	2.10	0.50
2:M:334:ARG:NH2	2:M:418:LEU:HD11	2.26	0.50
2:M:470:PRO:HD3	2:M:485:TYR:CE2	2.46	0.50
3:N:1299:PHE:N	3:N:1299:PHE:CD2	2.79	0.50
3:N:1495:ILE:HA	4:O:88:GLU:OE2	2.11	0.50
3:N:414:ARG:HB3	9:N:2299:HOH:O	2.11	0.50
3:N:52:PRO:CG	3:N:80:VAL:HG13	2.41	0.50
4:O:49:GLN:HB3	9:O:1772:HOH:O	2.11	0.50
1:A:183:ASP:HB3	9:A:322:HOH:O	2.11	0.50
2:C:42:VAL:HG12	2:C:43:GLY:N	2.23	0.50
2:C:759:THR:HB	2:C:785:VAL:CG2	2.41	0.50
2:C:578:VAL:HG11	2:C:991:GLN:HB3	1.93	0.50
3:D:1276:GLU:HG3	3:D:1303:TYR:OH	2.12	0.50
3:D:1466:VAL:CG2	3:D:1472:ILE:HD11	2.36	0.50
3:D:543:LEU:HB2	9:D:1714:HOH:O	2.10	0.50
3:D:1495:ILE:HD12	4:E:88:GLU:OE2	2.11	0.50
5:F:141:VAL:O	5:F:145:PRO:HD2	2.12	0.50
5:F:363:GLU:HA	5:F:367:MET:HG3	1.93	0.50
5:F:85:LEU:HD11	9:F:543:HOH:O	2.11	0.50
1:K:9:PRO:HB3	1:K:25:LEU:CD2	2.41	0.50
2:M:274:ARG:O	2:M:274:ARG:HG2	2.10	0.50
2:M:837:ASP:O	2:M:848:VAL:HG13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:877:PRO:HG3	3:N:1020:LEU:CD1	2.41	0.50
3:N:1189:ARG:HD3	9:N:1595:HOH:O	2.10	0.50
3:N:561:GLY:CA	5:P:184:ARG:HH12	2.23	0.50
2:M:1019:GLN:NE2	3:N:621:LYS:HA	2.22	0.50
2:C:1005:MET:HE2	3:D:648:MET:HB2	1.94	0.50
2:C:604:ALA:HB3	2:C:612:VAL:O	2.12	0.50
2:C:73:LEU:HD23	2:C:94:LEU:HD13	1.93	0.50
2:C:93:PRO:HG3	2:C:117:HIS:HE1	1.76	0.50
3:D:1223:ILE:CD1	3:D:1223:ILE:H	2.22	0.50
3:D:1192:LEU:HD13	3:D:1345:GLU:HG2	1.94	0.50
3:D:145:VAL:HG22	3:D:146:PRO:CD	2.41	0.50
3:D:610:LYS:CG	7:D:1527:MXR:C15	2.90	0.50
4:E:9:LEU:HD22	4:E:19:LEU:HD11	1.94	0.50
5:F:288:TYR:HA	5:F:291:ILE:HG22	1.92	0.50
2:M:186:VAL:HG23	2:M:187:ASN:H	1.75	0.50
2:M:227:PHE:HA	2:M:237:ARG:HH12	1.75	0.50
2:M:290:LEU:H	2:M:290:LEU:HD23	1.76	0.50
2:M:545:ASN:O	2:M:581:THR:HG21	2.11	0.50
2:M:78:PHE:CG	2:M:88:LEU:HD21	2.46	0.50
2:M:96:ALA:HB3	9:M:1826:HOH:O	2.10	0.50
2:M:565:GLN:HG2	2:M:995:MET:HE2	1.93	0.50
3:N:1128:VAL:HG13	9:N:2137:HOH:O	2.12	0.50
3:N:34:TYR:OH	5:P:264:MET:HG3	2.11	0.50
3:N:627:GLY:O	3:N:747:VAL:HG12	2.12	0.50
3:N:728:LEU:HD22	3:N:745:MET:SD	2.52	0.50
3:N:970:LYS:HD3	9:N:2041:HOH:O	2.12	0.50
3:N:1481:VAL:HG13	4:O:18:ARG:HG3	1.93	0.50
5:P:214:GLN:O	5:P:217:ASN:HB2	2.12	0.50
1:A:150:TYR:CE1	2:C:696:LYS:HA	2.47	0.50
2:C:6:PHE:HB2	2:C:908:GLY:C	2.32	0.50
2:C:897:LEU:HB3	2:C:899:GLN:HG2	1.93	0.50
3:D:11:ALA:HB1	3:D:507:ASN:OD1	2.12	0.50
3:D:641:GLN:HG2	9:D:1610:HOH:O	2.10	0.50
4:E:64:ALA:HA	4:E:67:GLU:OE1	2.12	0.50
5:F:88:ILE:CG2	5:F:193:ARG:HH11	2.24	0.50
1:K:18:ARG:HH11	1:K:123:MET:CE	2.21	0.50
1:K:19:GLU:O	1:K:200:TRP:HA	2.12	0.50
2:M:795:GLY:HA3	2:M:1004:LYS:HE2	1.93	0.50
2:M:110:GLU:HB3	9:M:2230:HOH:O	2.10	0.50
2:M:153:ALA:O	2:M:155:PRO:HD3	2.12	0.50
2:M:269:LEU:HB3	9:M:2007:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:496:ILE:HD12	2:M:496:ILE:H	1.77	0.50
2:M:517:ARG:HB2	9:M:2072:HOH:O	2.12	0.50
2:M:762:LYS:HG2	2:M:763:GLY:H	1.76	0.50
3:N:1128:VAL:HG11	9:N:1633:HOH:O	2.10	0.50
3:N:1408:ILE:O	3:N:1409:ALA:C	2.47	0.50
3:N:403:PHE:HE2	3:N:443:VAL:N	2.10	0.50
3:N:567:ILE:H	3:N:567:ILE:HD12	1.77	0.50
3:N:699:VAL:HG12	3:N:717:GLN:HA	1.93	0.50
5:P:392:VAL:HG11	5:P:396:ARG:CD	2.41	0.50
1:A:106:PRO:HG3	1:A:134:GLU:HG3	1.93	0.50
2:C:1004:LYS:HA	9:C:1776:HOH:O	2.11	0.50
2:C:197:LEU:HB3	2:C:202:TYR:HB2	1.92	0.50
2:C:244:PRO:CD	2:C:245:GLY:H	2.24	0.50
2:C:64:LEU:HD13	2:C:359:MET:CG	2.41	0.50
2:C:811:PRO:HD2	2:C:813:VAL:HG22	1.93	0.50
2:C:808:ARG:HA	2:C:815:LEU:HD22	1.92	0.50
2:C:689:VAL:HB	2:C:870:ILE:HG13	1.93	0.50
3:D:1216:SER:HB3	9:D:2106:HOH:O	2.11	0.50
3:D:418:GLY:N	3:D:429:SER:O	2.35	0.50
3:D:630:VAL:CA	3:D:744:GLN:HG2	2.38	0.50
3:D:753:SER:HB3	9:E:134:HOH:O	2.11	0.50
3:D:800:LYS:HE2	3:D:804:LEU:HD13	1.94	0.50
3:D:862:ASP:O	3:D:876:SER:HB2	2.12	0.50
4:E:38:THR:HG22	9:E:103:HOH:O	2.12	0.50
5:F:196:VAL:HG13	5:F:213:ILE:HD11	1.94	0.50
5:F:282:LEU:HD12	9:F:487:HOH:O	2.11	0.50
1:K:186:LEU:CB	1:K:192:LEU:HD11	2.40	0.50
1:L:19:GLU:O	1:L:200:TRP:HA	2.12	0.50
1:L:4:SER:HA	1:L:7:LYS:HG2	1.93	0.50
2:M:878:SER:HB3	3:N:1029:ARG:HH11	1.75	0.50
3:N:1310:ARG:HG3	3:N:1327:ARG:HB3	1.94	0.50
3:N:716:PHE:CE2	3:N:765:SER:HB3	2.47	0.50
3:N:630:VAL:CA	3:N:744:GLN:HG2	2.39	0.50
3:N:806:PHE:HE1	3:N:813:LEU:HB3	1.74	0.50
5:P:163:LEU:HB3	5:P:174:LEU:HD13	1.93	0.50
2:C:1096:ALA:O	3:D:13:ALA:CB	2.60	0.50
2:C:650:ARG:HB2	2:C:653:ASP:HB2	1.93	0.50
3:D:999:THR:O	3:D:1003:VAL:HG13	2.12	0.50
3:D:1281:VAL:HG21	3:D:1313:VAL:CG2	2.42	0.50
3:D:1295:GLU:HB3	3:D:1300:SER:OG	2.12	0.50
5:F:406:ARG:O	5:F:409:LYS:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:216:GLU:O	1:K:220:GLU:HG3	2.11	0.50
2:M:145:GLY:H	2:M:163:ILE:HG12	1.76	0.50
2:M:618:GLY:HA2	9:M:1827:HOH:O	2.10	0.50
2:M:57:GLU:O	2:M:62:GLY:HA3	2.11	0.50
2:M:876:VAL:O	2:M:879:ARG:O	2.29	0.50
4:O:89:MET:HA	9:O:1936:HOH:O	2.12	0.50
1:A:85:LEU:HB2	1:A:127:LEU:HD21	1.94	0.50
1:A:73:GLU:HG3	9:A:363:HOH:O	2.11	0.50
2:C:1034:GLU:CA	2:C:1037:VAL:HG23	2.42	0.50
2:C:165:LEU:HD12	2:C:166:PRO:C	2.32	0.50
2:C:262:ALA:O	2:C:264:PRO:O	2.30	0.50
2:C:32:ALA:HB2	2:C:73:LEU:HD11	1.93	0.50
2:C:584:GLU:H	2:C:584:GLU:CD	2.14	0.50
2:C:605:LYS:HB2	9:C:1120:HOH:O	2.11	0.50
2:C:70:GLU:HA	9:C:1632:HOH:O	2.12	0.50
3:D:1214:PRO:HB2	9:D:2327:HOH:O	2.11	0.50
3:D:520:LEU:O	3:D:525:ARG:NH1	2.45	0.50
3:D:614:PHE:HB3	3:D:617:ASN:HB3	1.94	0.50
4:E:40:LEU:HD22	9:E:124:HOH:O	2.11	0.50
4:E:45:ARG:HB2	4:E:46:PRO:CD	2.42	0.50
4:E:70:THR:HG22	4:E:71:GLY:N	2.27	0.50
5:F:167:PRO:HB2	5:F:169:GLU:OE1	2.12	0.50
1:K:211:LEU:O	1:K:211:LEU:HD12	2.11	0.50
1:K:34:VAL:HG22	2:M:939:ARG:NH2	2.27	0.50
2:M:1116:ALA:HA	9:M:2070:HOH:O	2.12	0.50
2:M:580:MET:HB3	2:M:584:GLU:CD	2.32	0.50
3:N:1209:LEU:HD13	9:N:1985:HOH:O	2.12	0.50
3:N:129:PHE:O	3:N:572:ARG:HG2	2.11	0.50
3:N:1310:ARG:NE	3:N:1327:ARG:HB3	2.27	0.50
3:N:19:ARG:HG2	9:N:2118:HOH:O	2.11	0.50
3:N:394:LEU:HD11	9:N:1920:HOH:O	2.11	0.50
2:M:713:ARG:NH2	3:N:531:ASP:HB3	2.27	0.50
3:N:131:LYS:HE3	3:N:568:ARG:HB2	1.94	0.50
2:M:729:LEU:HD13	3:N:675:ARG:CZ	2.42	0.50
5:P:278:LEU:CB	5:P:286:PRO:HG2	2.42	0.50
5:P:358:LEU:HD21	5:P:367:MET:CE	2.42	0.50
5:P:358:LEU:HD13	5:P:370:LYS:CG	2.42	0.50
2:C:461:VAL:HG12	2:C:462:ASP:O	2.12	0.49
3:D:1147:ARG:HB3	3:D:1188:VAL:HG23	1.93	0.49
3:D:1383:ASP:HB2	3:D:1416:ALA:CB	2.34	0.49
3:D:696:HIS:HB2	4:E:48:MET:CE	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:74:VAL:HA	9:E:163:HOH:O	2.12	0.49
5:F:113:ILE:HG23	5:F:127:ILE:CG2	2.42	0.49
5:F:189:GLU:HA	5:F:192:LEU:HD12	1.94	0.49
1:L:211:LEU:O	1:L:214:ALA:HB3	2.12	0.49
2:M:1034:GLU:CA	2:M:1037:VAL:HG23	2.42	0.49
2:M:196:LEU:O	2:M:199:VAL:HB	2.12	0.49
2:M:36:PRO:HG2	2:M:70:GLU:HB3	1.94	0.49
2:M:498:GLN:HB2	9:M:2088:HOH:O	2.11	0.49
3:N:1003:VAL:O	3:N:1006:ALA:HB3	2.12	0.49
3:N:1353:GLN:NE2	3:N:1363:LEU:O	2.43	0.49
3:N:1389:LEU:HD12	3:N:1390:LEU:HG	1.94	0.49
3:N:148:GLU:HG2	3:N:151:GLN:HE21	1.77	0.49
3:N:409:VAL:HB	3:N:421:LEU:HA	1.93	0.49
3:N:516:ALA:O	3:N:518:PRO:HD3	2.12	0.49
3:N:675:ARG:O	3:N:678:GLU:HG2	2.12	0.49
5:P:115:LYS:HD2	5:P:173:TYR:CE2	2.47	0.49
5:P:187:LEU:O	5:P:187:LEU:HD23	2.11	0.49
1:A:91:ASN:CG	1:A:92:PRO:HD2	2.32	0.49
1:B:25:LEU:HD23	1:B:28:LEU:HD11	1.94	0.49
1:B:85:LEU:HG	9:B:527:HOH:O	2.10	0.49
2:C:252:LYS:HB3	2:C:298:PHE:HZ	1.77	0.49
2:C:358:ARG:HG3	9:C:1597:HOH:O	2.11	0.49
2:C:523:ILE:HG22	9:C:1356:HOH:O	2.12	0.49
2:C:626:ARG:HB2	2:C:639:GLN:HE21	1.77	0.49
2:C:684:PHE:HE2	3:D:733:CYS:SG	2.35	0.49
2:C:789:SER:O	2:C:791:ARG:HG3	2.12	0.49
3:D:119:SER:HB2	3:D:123:LEU:CB	2.36	0.49
3:D:17:LYS:HB2	9:D:1656:HOH:O	2.12	0.49
3:D:39:PRO:HB3	3:D:45:PHE:C	2.33	0.49
2:C:1087:VAL:HG12	3:D:610:LYS:NZ	2.27	0.49
3:D:99:ALA:HB1	3:D:575:GLN:OE1	2.11	0.49
5:F:151:LEU:HD22	9:F:737:HOH:O	2.12	0.49
1:K:57:TYR:CE2	1:K:59:GLU:HA	2.46	0.49
2:M:305:PRO:CA	2:M:308:ARG:HB2	2.42	0.49
2:M:403:SER:O	2:M:407:LYS:HG3	2.12	0.49
1:A:189:ARG:HG3	9:A:334:HOH:O	2.12	0.49
2:C:435:TYR:OH	2:C:498:GLN:NE2	2.44	0.49
2:C:607:ASP:HB2	2:C:610:ARG:HG3	1.95	0.49
2:C:722:ILE:HG21	2:C:821:GLU:OE1	2.12	0.49
2:C:926:PHE:CD1	2:C:929:ARG:HD3	2.46	0.49
3:D:1281:VAL:HG23	3:D:1317:ASP:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1291:SER:HB2	3:D:1293:PHE:CE1	2.45	0.49
3:D:1307:LYS:HE3	9:D:2288:HOH:O	2.12	0.49
3:D:1388:ARG:HG3	3:D:1389:LEU:N	2.26	0.49
3:D:1420:LEU:HD12	3:D:1421:LEU:N	2.26	0.49
3:D:27:GLU:HA	9:D:2102:HOH:O	2.11	0.49
3:D:465:LEU:HD22	3:D:509:PRO:O	2.12	0.49
3:D:540:LEU:HA	3:D:543:LEU:HD12	1.94	0.49
3:D:656:PHE:HB3	3:D:694:VAL:HG11	1.93	0.49
3:D:65:ARG:HB2	5:F:375:LEU:O	2.11	0.49
3:D:984:THR:CG2	3:D:987:GLU:H	2.25	0.49
5:F:259:ARG:HA	9:F:658:HOH:O	2.12	0.49
1:K:134:GLU:HG2	9:K:1422:HOH:O	2.11	0.49
1:L:12:THR:OG1	1:L:24:VAL:HB	2.12	0.49
2:M:191:PHE:CD2	2:M:195:LEU:HD23	2.48	0.49
2:M:302:VAL:O	2:M:306:THR:HG23	2.11	0.49
2:M:338:GLU:O	2:M:341:THR:HG22	2.12	0.49
2:M:629:TYR:HB3	9:M:1712:HOH:O	2.11	0.49
2:M:679:PHE:C	3:N:943:THR:HG22	2.33	0.49
2:M:897:LEU:HB3	2:M:899:GLN:HG2	1.94	0.49
2:M:1115:LEU:CD2	3:N:85:VAL:HG13	2.40	0.49
3:N:862:ASP:O	3:N:877:PRO:HD3	2.13	0.49
3:N:928:ALA:O	3:N:931:LEU:HB2	2.12	0.49
4:O:72:ARG:HB2	9:O:4461:HOH:O	2.12	0.49
5:P:299:TRP:CE3	5:P:303:ARG:HD3	2.46	0.49
5:P:361:LEU:HD21	5:P:404:ALA:HB1	1.93	0.49
2:C:163:ILE:HG21	9:C:1347:HOH:O	2.11	0.49
2:C:21:ILE:O	2:C:25:SER:HB2	2.13	0.49
2:C:625:LEU:O	2:C:627:ARG:N	2.46	0.49
2:C:775:ARG:HG2	9:C:1674:HOH:O	2.12	0.49
2:C:810:ASP:N	2:C:811:PRO:CD	2.75	0.49
3:D:1396:GLU:O	3:D:1400:VAL:HG23	2.12	0.49
3:D:145:VAL:HG13	3:D:146:PRO:N	2.28	0.49
3:D:14:SER:O	3:D:17:LYS:N	2.46	0.49
3:D:787:LEU:HD21	3:D:947:ILE:CD1	2.43	0.49
3:D:957:PRO:HG3	3:D:1010:ASN:HD22	1.77	0.49
3:D:1209:LEU:HD21	4:E:16:LYS:HD2	1.94	0.49
2:M:1060:ILE:HB	9:M:1724:HOH:O	2.12	0.49
2:M:443:THR:CG2	2:M:449:ILE:HG13	2.42	0.49
2:M:810:ASP:N	2:M:811:PRO:CD	2.75	0.49
3:N:1066:THR:CG2	3:N:1069:GLU:HG3	2.42	0.49
3:N:1262:LEU:HD23	3:N:1352:ILE:HG12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1372:VAL:HA	3:N:1375:MET:SD	2.53	0.49
3:N:141:ILE:HG23	3:N:161:LEU:HD21	1.95	0.49
3:N:502:PHE:CE1	3:N:509:PRO:HB3	2.46	0.49
3:N:820:GLU:HG2	3:N:825:ALA:O	2.13	0.49
5:P:185:GLN:O	5:P:189:GLU:HG3	2.12	0.49
5:P:369:LEU:HD11	5:P:401:GLU:HB2	1.94	0.49
1:B:149:GLY:O	1:B:171:PHE:HB2	2.13	0.49
1:B:86:VAL:HG12	1:B:124:ASN:ND2	2.18	0.49
2:C:85:GLU:OE2	2:C:802:ARG:NH2	2.45	0.49
3:D:1159:ARG:HB3	3:D:1159:ARG:CZ	2.43	0.49
3:D:1463:LYS:HB2	7:D:1527:MXP:H23B	1.95	0.49
3:D:481:MET:HG3	3:D:1388:ARG:NH2	2.27	0.49
3:D:527:MET:HB3	9:D:1582:HOH:O	2.11	0.49
5:F:364:ARG:HD2	9:F:435:HOH:O	2.12	0.49
2:M:678:PRO:O	3:N:943:THR:HA	2.11	0.49
2:M:985:GLY:C	9:N:1555:HOH:O	2.49	0.49
3:N:149:LYS:HA	9:N:2241:HOH:O	2.12	0.49
3:N:207:PHE:HA	9:N:1567:HOH:O	2.12	0.49
3:N:827:ILE:O	3:N:837:GLY:HA3	2.13	0.49
3:N:895:VAL:O	3:N:899:LEU:HG	2.12	0.49
5:P:299:TRP:HE3	9:P:492:HOH:O	1.94	0.49
2:M:818:GLY:N	5:P:309:LYS:HE2	2.26	0.49
1:A:133:GLU:HG2	1:A:134:GLU:H	1.77	0.49
2:C:1004:LYS:HG3	9:C:1776:HOH:O	2.12	0.49
2:C:113:VAL:HB	2:C:115:LEU:HD23	1.95	0.49
3:D:1283:ILE:HB	3:D:1315:ASP:OD2	2.13	0.49
3:D:409:VAL:HB	3:D:421:LEU:HA	1.94	0.49
3:D:674:ARG:HD3	9:D:1564:HOH:O	2.11	0.49
3:D:767:HIS:CD2	4:E:6:ILE:HG12	2.47	0.49
1:L:158:ILE:HG12	9:L:3428:HOH:O	2.13	0.49
2:M:101:ILE:HG23	2:M:107:LEU:CD2	2.41	0.49
2:M:209:ARG:O	2:M:213:ALA:HB2	2.12	0.49
2:M:364:GLU:O	2:M:367:LEU:HD21	2.12	0.49
2:M:139:GLN:CD	2:M:418:LEU:HD22	2.33	0.49
2:M:442:GLU:HG2	2:M:454:SER:OG	2.12	0.49
2:M:5:ARG:HB3	2:M:902:ILE:HB	1.93	0.49
3:N:1393:GLN:CB	3:N:1398:TRP:HE1	2.20	0.49
3:N:1435:LEU:HA	9:N:1677:HOH:O	2.13	0.49
3:N:185:VAL:HG22	3:N:203:ALA:HB2	1.95	0.49
3:N:527:MET:HE2	5:P:258:ILE:HD11	1.94	0.49
3:N:736:PHE:O	3:N:738:ALA:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:209:PHE:O	5:P:213:ILE:HG13	2.12	0.49
5:P:358:LEU:HD22	5:P:370:LYS:HE3	1.94	0.49
1:A:176:ARG:O	1:A:200:TRP:HE3	1.96	0.49
2:C:191:PHE:CD2	2:C:195:LEU:HD23	2.47	0.49
2:C:44:ILE:HG23	2:C:344:PHE:CE1	2.48	0.49
2:C:622:GLU:HB3	9:C:1635:HOH:O	2.12	0.49
2:C:722:ILE:O	2:C:722:ILE:HG23	2.13	0.49
2:C:816:LYS:O	2:C:819:VAL:HB	2.12	0.49
2:C:815:LEU:HD23	2:C:819:VAL:O	2.12	0.49
3:D:1114:THR:HG23	3:D:1116:ASN:HD21	1.78	0.49
3:D:1177:ALA:CB	3:D:1183:ILE:HD11	2.42	0.49
3:D:1189:ARG:HH11	3:D:1203:LYS:HB2	1.77	0.49
3:D:1272:ALA:CA	3:D:1326:THR:HB	2.41	0.49
3:D:521:PRO:O	3:D:525:ARG:HG2	2.13	0.49
3:D:530:VAL:HG13	9:D:2079:HOH:O	2.12	0.49
3:D:53:ILE:HG23	3:D:54:LYS:H	1.78	0.49
2:C:681:GLY:O	3:D:633:VAL:HG21	2.12	0.49
3:D:664:LYS:HA	9:D:1859:HOH:O	2.12	0.49
3:D:988:ARG:O	3:D:992:ILE:HG13	2.13	0.49
5:F:295:MET:HG2	5:F:299:TRP:CD2	2.47	0.49
1:L:2:LEU:HD12	1:L:3:ASP:HB2	1.95	0.49
2:M:1109:VAL:HA	3:N:3:LYS:HE3	1.93	0.49
2:M:185:LYS:HE2	2:M:190:LYS:HG2	1.95	0.49
2:M:136:ILE:HG21	2:M:336:VAL:HG13	1.93	0.49
2:M:358:ARG:HA	2:M:361:MET:HB2	1.95	0.49
2:M:923:GLU:O	2:M:927:GLY:HA3	2.12	0.49
2:M:93:PRO:HG3	2:M:117:HIS:HE1	1.76	0.49
3:N:1066:THR:HG22	3:N:1069:GLU:CG	2.42	0.49
3:N:1128:VAL:O	3:N:1129:THR:C	2.49	0.49
3:N:1246:VAL:HG13	3:N:1269:LYS:NZ	2.28	0.49
3:N:28:LYS:CG	3:N:41:ARG:HH11	2.25	0.49
3:N:443:VAL:HG22	3:N:444:VAL:H	1.77	0.49
5:P:287:THR:HG23	5:P:289:GLU:HB3	1.93	0.49
1:B:73:GLU:CD	1:B:130:ALA:HA	2.32	0.49
2:C:332:ARG:CZ	2:C:464:LEU:HD11	2.43	0.49
2:C:420:ARG:HG3	2:C:422:ARG:HG2	1.95	0.49
3:D:122:GLU:O	3:D:126:VAL:HG23	2.13	0.49
3:D:1382:THR:HG21	3:D:1418:LYS:HE3	1.95	0.49
3:D:507:ASN:HB2	9:D:1793:HOH:O	2.12	0.49
9:C:1813:HOH:O	3:D:532:GLY:HA3	2.13	0.49
3:D:584:ASN:CG	3:D:590:PRO:HD2	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:937:TYR:O	3:D:941:PHE:HD1	1.95	0.49
4:E:23:VAL:HG12	4:E:61:VAL:HG13	1.95	0.49
5:F:81:VAL:O	5:F:85:LEU:HB2	2.12	0.49
2:M:139:GLN:HE22	2:M:415:PRO:CD	2.26	0.49
2:M:331:ARG:NH1	2:M:427:VAL:HG12	2.27	0.49
2:M:352:ALA:HA	2:M:355:VAL:CG1	2.43	0.49
2:M:506:ASN:HB2	9:M:1906:HOH:O	2.12	0.49
2:M:967:PHE:CD1	2:M:972:VAL:HG12	2.47	0.49
3:N:1161:GLU:HG3	3:N:1164:ARG:CB	2.41	0.49
3:N:1363:LEU:HD12	3:N:1364:HIS:O	2.12	0.49
3:N:128:TYR:CE1	3:N:461:ILE:HG13	2.47	0.49
5:P:226:LYS:HD2	5:P:242:TRP:CZ2	2.48	0.49
2:C:1098:ASP:HB2	3:D:21:TRP:CZ2	2.46	0.49
2:C:341:THR:O	2:C:345:ARG:HG3	2.12	0.49
2:C:418:LEU:N	2:C:418:LEU:HD12	2.28	0.49
3:D:1051:GLU:HA	9:D:1601:HOH:O	2.12	0.49
3:D:1161:GLU:HG3	3:D:1164:ARG:CB	2.39	0.49
3:D:1379:VAL:HG11	3:D:1395:LEU:HD12	1.95	0.49
3:D:32:ILE:HD12	3:D:527:MET:HG2	1.94	0.49
2:C:1115:LEU:HD23	3:D:85:VAL:CA	2.43	0.49
3:D:527:MET:HE2	5:F:258:ILE:HD11	1.93	0.49
3:D:572:ARG:NH2	5:F:83:GLN:HE21	2.10	0.49
2:M:1096:ALA:O	3:N:13:ALA:CB	2.61	0.49
2:M:108:ILE:HB	2:M:368:THR:HG1	1.76	0.49
2:M:442:GLU:HG3	2:M:442:GLU:O	2.11	0.49
3:N:418:GLY:N	3:N:429:SER:O	2.34	0.49
3:N:141:ILE:HG21	3:N:450:TYR:H	1.78	0.49
3:N:528:VAL:O	3:N:535:PHE:HA	2.13	0.49
3:N:964:LEU:HD22	9:N:2037:HOH:O	2.13	0.49
5:P:191:ASN:OD1	5:P:194:LEU:HD13	2.13	0.49
3:N:34:TYR:HE2	5:P:260:ILE:HA	1.77	0.49
1:B:101:LEU:HD12	1:B:114:PHE:N	2.28	0.49
1:B:45:LEU:HB2	9:B:399:HOH:O	2.12	0.49
2:C:148:PHE:CZ	2:C:281:LEU:HD13	2.35	0.49
2:C:358:ARG:HA	2:C:361:MET:HB2	1.93	0.49
2:C:367:LEU:HA	2:C:371:LYS:CG	2.35	0.49
2:C:890:LEU:CA	2:C:914:ILE:HD11	2.33	0.49
3:D:1101:VAL:HG22	3:D:1428:ALA:HB2	1.94	0.49
3:D:116:LEU:HB3	3:D:118:LEU:HG	1.94	0.49
3:D:127:LEU:HD12	3:D:128:TYR:N	2.28	0.49
3:D:897:TRP:CH2	3:D:902:LEU:HD21	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:1162:HOH:O	3:D:943:THR:HG21	2.13	0.49
3:D:99:ALA:HA	3:D:575:GLN:HE22	1.77	0.49
3:D:1481:VAL:HG13	4:E:18:ARG:HG3	1.93	0.49
5:F:112:ALA:O	5:F:116:LEU:HG	2.13	0.49
2:M:254:VAL:HG13	2:M:258:TYR:HE1	1.77	0.49
2:M:770:GLU:O	2:M:773:LEU:HB3	2.13	0.49
2:M:987:ILE:HA	3:N:948:THR:HG21	1.95	0.49
2:M:564:MET:HG3	2:M:997:LEU:HD11	1.94	0.49
3:N:1141:GLU:HG2	3:N:1168:MET:HE1	1.95	0.49
3:N:1242:HIS:HE1	3:N:1266:ARG:HB3	1.78	0.49
3:N:709:HIS:CD2	3:N:711:LEU:HB2	2.48	0.49
3:N:804:LEU:HB3	9:N:1996:HOH:O	2.11	0.49
5:P:116:LEU:HB2	5:P:127:ILE:HD12	1.95	0.49
5:P:135:ILE:HD13	5:P:135:ILE:O	2.13	0.49
2:C:1033:GLY:O	2:C:1036:GLU:HG2	2.13	0.48
2:C:121:MET:HG3	9:C:1509:HOH:O	2.11	0.48
2:C:17:PRO:HG2	9:C:1758:HOH:O	2.12	0.48
2:C:208:ALA:HA	2:C:221:LEU:HD21	1.94	0.48
2:C:379:GLU:O	2:C:383:ARG:HB3	2.13	0.48
2:C:976:ASP:HB2	2:C:979:THR:HG22	1.94	0.48
3:D:1049:SER:OG	3:D:1051:GLU:HG3	2.13	0.48
3:D:1114:THR:O	3:D:1114:THR:HG23	2.13	0.48
3:D:1310:ARG:CZ	3:D:1327:ARG:HD3	2.43	0.48
3:D:186:VAL:HB	3:D:189:GLN:HB2	1.95	0.48
3:D:610:LYS:CG	7:D:1527:MXP:H15A	2.42	0.48
3:D:834:THR:HA	9:D:2405:HOH:O	2.13	0.48
4:E:28:GLN:HG3	9:E:134:HOH:O	2.12	0.48
1:K:7:LYS:HE2	1:K:186:LEU:CD1	2.29	0.48
2:M:242:LEU:HD22	9:M:1924:HOH:O	2.11	0.48
2:M:64:LEU:HD13	2:M:359:MET:CG	2.42	0.48
2:M:858:MET:HB2	2:M:859:PRO:CD	2.43	0.48
3:N:1116:ASN:N	3:N:1116:ASN:ND2	2.60	0.48
3:N:1128:VAL:HG12	9:N:1593:HOH:O	2.13	0.48
3:N:39:PRO:HB3	3:N:45:PHE:O	2.13	0.48
2:M:1101:THR:HB	3:N:5:VAL:HG13	1.94	0.48
3:N:984:THR:CG2	3:N:987:GLU:H	2.25	0.48
5:P:220:LEU:HB2	5:P:243:ILE:HD11	1.95	0.48
1:A:189:ARG:HD2	1:A:191:ASP:OD1	2.12	0.48
1:A:9:PRO:HB3	1:A:25:LEU:HG	1.94	0.48
2:C:18:LEU:HD23	2:C:404:LEU:HD21	1.95	0.48
2:C:367:LEU:O	2:C:371:LYS:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:139:GLN:NE2	2:C:418:LEU:HD22	2.28	0.48
3:D:14:SER:HB2	9:D:1656:HOH:O	2.13	0.48
3:D:128:TYR:CE1	3:D:461:ILE:HG13	2.45	0.48
3:D:614:PHE:O	3:D:615:ARG:C	2.51	0.48
3:D:741:ASP:N	3:D:741:ASP:OD2	2.41	0.48
9:D:1893:HOH:O	4:E:85:LEU:HG	2.13	0.48
5:F:277:GLN:O	5:F:280:GLN:HB3	2.13	0.48
1:K:150:TYR:CE2	1:K:152:PRO:HG3	2.44	0.48
1:K:55:SER:CB	1:K:158:ILE:HG21	2.43	0.48
2:M:200:LEU:HD13	2:M:300:ASP:OD2	2.12	0.48
2:M:439:CYS:SG	2:M:540:PHE:HB3	2.53	0.48
2:M:461:VAL:HG12	2:M:462:ASP:O	2.13	0.48
2:M:636:ALA:HB2	2:M:703:ILE:HG22	1.95	0.48
2:M:671:ASN:ND2	2:M:993:PHE:HD2	2.10	0.48
3:N:610:LYS:HG2	7:N:1527:MXR:C15	2.43	0.48
3:N:180:LYS:HG3	3:N:183:GLU:H	1.77	0.48
3:N:417:PRO:HD2	3:N:432:TYR:CE1	2.48	0.48
3:N:112:ILE:HD12	3:N:461:ILE:HG21	1.94	0.48
3:N:754:PHE:CE2	3:N:1476:THR:HG21	2.49	0.48
5:P:371:LEU:HD12	9:P:669:HOH:O	2.11	0.48
1:A:201:THR:HG22	1:A:203:GLY:H	1.78	0.48
1:A:5:LYS:HB2	9:A:440:HOH:O	2.12	0.48
2:C:1054:THR:HG23	2:C:1082:PRO:HG3	1.93	0.48
2:C:15:LEU:HD21	2:C:583:LEU:HD11	1.93	0.48
2:C:198:ARG:HD2	2:C:228:ALA:CB	2.44	0.48
2:C:468:ARG:NE	2:C:485:TYR:HB3	2.27	0.48
2:C:644:VAL:HG22	2:C:647:GLN:OE1	2.14	0.48
2:C:888:THR:HG22	9:C:1474:HOH:O	2.13	0.48
3:D:190:GLU:HB2	9:D:1738:HOH:O	2.14	0.48
3:D:760:ARG:HH22	4:E:62:THR:CA	2.26	0.48
3:D:881:LEU:O	3:D:885:ILE:HG13	2.13	0.48
5:F:109:GLY:O	5:F:113:ILE:HG13	2.13	0.48
5:F:247:ILE:HG22	5:F:251:ILE:HD11	1.95	0.48
5:F:312:GLN:HB2	9:F:706:HOH:O	2.12	0.48
2:M:139:GLN:HG2	2:M:140:ILE:H	1.77	0.48
2:M:601:GLY:HA2	2:M:616:GLU:HG3	1.95	0.48
2:M:615:TYR:HH	2:M:623:TYR:HH	1.60	0.48
1:K:34:VAL:HG22	2:M:939:ARG:HH21	1.79	0.48
3:N:1123:PHE:CE1	3:N:1134:LEU:HD12	2.48	0.48
3:N:161:LEU:O	3:N:449:SER:CB	2.59	0.48
3:N:524:LEU:C	3:N:526:PRO:HD3	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:93:LEU:HG	5:P:190:ALA:HB1	1.96	0.48
5:P:306:GLU:O	5:P:310:ILE:HG13	2.13	0.48
1:B:12:THR:OG1	1:B:24:VAL:HB	2.14	0.48
1:B:58:ILE:HG21	1:B:68:ILE:HD13	1.96	0.48
2:C:183:SER:CB	2:C:190:LYS:HD3	2.43	0.48
2:C:290:LEU:HB3	2:C:302:VAL:HG11	1.94	0.48
2:C:472:ARG:O	2:C:531:PHE:HD2	1.96	0.48
2:C:627:ARG:O	2:C:638:ASP:HA	2.13	0.48
2:C:809:GLY:HA2	9:C:1126:HOH:O	2.12	0.48
3:D:491:LYS:HE2	9:D:1851:HOH:O	2.12	0.48
5:F:369:LEU:HD11	5:F:401:GLU:HB2	1.94	0.48
1:L:22:GLU:HG2	1:L:198:ARG:HG2	1.94	0.48
2:M:1014:SER:O	2:M:1018:GLN:HG3	2.14	0.48
2:M:101:ILE:HG22	2:M:102:HIS:N	2.28	0.48
2:M:258:TYR:HB3	9:M:1886:HOH:O	2.13	0.48
2:M:412:ALA:HB1	2:M:419:THR:CG2	2.43	0.48
3:N:1312:LEU:HD12	9:N:2368:HOH:O	2.12	0.48
3:N:9:ARG:HH22	3:N:507:ASN:HD21	1.61	0.48
3:N:534:ARG:HG2	9:P:456:HOH:O	2.13	0.48
3:N:553:ARG:HH12	5:P:211:ASP:HA	1.78	0.48
5:P:339:PRO:HB3	5:P:343:ASP:HB2	1.94	0.48
3:N:572:ARG:NH1	5:P:79:ASP:OD1	2.39	0.48
1:B:107:LYS:HG3	1:B:108:GLU:H	1.78	0.48
2:C:1115:LEU:CB	3:D:85:VAL:HG13	2.43	0.48
2:C:281:LEU:HD12	2:C:305:PRO:O	2.13	0.48
2:C:140:ILE:HA	2:C:332:ARG:O	2.14	0.48
2:C:405:ARG:HA	9:C:1409:HOH:O	2.12	0.48
2:C:462:ASP:HB3	2:C:468:ARG:HD3	1.96	0.48
2:C:831:ARG:HD2	9:C:1303:HOH:O	2.14	0.48
3:D:32:ILE:HG12	9:D:1967:HOH:O	2.13	0.48
3:D:760:ARG:HB2	4:E:3:GLU:OE2	2.14	0.48
3:D:805:GLU:OE1	3:D:809:PRO:HG2	2.14	0.48
3:D:829:VAL:H	3:D:835:SER:CB	2.26	0.48
3:D:840:LYS:HB3	3:D:841:TYR:CE2	2.48	0.48
3:D:938:GLY:O	3:D:942:SER:HB3	2.14	0.48
5:F:369:LEU:HA	9:F:450:HOH:O	2.13	0.48
2:M:165:LEU:HB2	9:M:2226:HOH:O	2.14	0.48
2:M:212:GLY:HA3	2:M:218:VAL:CG2	2.44	0.48
2:M:305:PRO:HA	2:M:308:ARG:CD	2.44	0.48
2:M:380:ALA:O	2:M:384:GLU:HB2	2.14	0.48
2:M:968:LEU:HD22	9:M:2164:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1198:TYR:HE2	9:N:2318:HOH:O	1.96	0.48
3:N:1264:GLU:OE2	3:N:1425:THR:HB	2.14	0.48
3:N:57:GLU:HG3	3:N:64:LYS:HG2	1.95	0.48
5:P:136:LEU:HD23	5:P:181:GLU:OE2	2.13	0.48
5:P:80:PRO:HA	5:P:83:GLN:HB2	1.95	0.48
1:A:112:ARG:HA	9:A:397:HOH:O	2.13	0.48
1:A:16:GLN:CG	1:A:16:GLN:O	2.62	0.48
1:A:64:GLU:HG3	1:A:165:ILE:HD12	1.96	0.48
1:B:101:LEU:HB2	1:B:114:PHE:CD2	2.48	0.48
2:C:1065:ALA:CB	2:C:1077:PRO:HG2	2.43	0.48
2:C:672:VAL:CG2	2:C:868:ASP:HB2	2.44	0.48
3:D:1104:GLU:O	3:D:1106:VAL:HG23	2.14	0.48
3:D:1209:LEU:HD12	3:D:1219:GLU:OE1	2.14	0.48
3:D:1258:ARG:NH2	3:D:1351:GLU:OE2	2.46	0.48
3:D:1290:LEU:HD22	3:D:1291:SER:H	1.79	0.48
3:D:12:LEU:HD13	3:D:511:TRP:HB2	1.94	0.48
3:D:126:VAL:HG12	3:D:132:TYR:HB2	1.96	0.48
3:D:162:ARG:HH11	3:D:434:ARG:HH22	1.62	0.48
3:D:34:TYR:O	3:D:35:ARG:C	2.51	0.48
3:D:670:VAL:O	3:D:674:ARG:HG3	2.14	0.48
3:D:760:ARG:HH22	4:E:62:THR:N	2.11	0.48
3:D:947:ILE:O	3:D:947:ILE:HD12	2.14	0.48
4:E:4:PRO:HB2	9:E:109:HOH:O	2.13	0.48
5:F:134:LYS:HB2	5:F:178:ARG:NH2	2.28	0.48
5:F:80:PRO:HA	5:F:83:GLN:HB2	1.94	0.48
5:F:82:ARG:HD3	9:F:608:HOH:O	2.14	0.48
2:M:435:TYR:C	2:M:437:ARG:H	2.15	0.48
2:M:544:THR:O	2:M:547:ILE:HG13	2.14	0.48
2:M:958:THR:HG23	2:M:961:GLU:H	1.79	0.48
3:N:1110:ALA:O	3:N:1111:ASP:C	2.49	0.48
3:N:1147:ARG:HD2	3:N:1188:VAL:HG21	1.95	0.48
3:N:1282:ARG:HA	3:N:1315:ASP:OD1	2.14	0.48
3:N:1310:ARG:HE	3:N:1327:ARG:HB3	1.78	0.48
3:N:1351:GLU:HA	3:N:1354:LYS:HG3	1.95	0.48
3:N:417:PRO:HD2	3:N:432:TYR:CD1	2.48	0.48
3:N:409:VAL:O	3:N:437:VAL:HG21	2.13	0.48
3:N:443:VAL:HG11	3:N:445:ARG:HE	1.79	0.48
3:N:853:VAL:HA	3:N:858:VAL:O	2.14	0.48
1:A:23:PHE:O	1:A:196:THR:HA	2.13	0.48
1:A:222:LEU:HD11	1:B:218:LEU:HD23	1.95	0.48
1:B:156:HIS:CG	1:B:157:GLY:N	2.82	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:120:LEU:HA	9:C:1499:HOH:O	2.12	0.48
2:C:412:ALA:HB1	2:C:419:THR:CG2	2.44	0.48
3:D:1041:LEU:CD1	3:D:1058:ARG:HA	2.42	0.48
3:D:409:VAL:HG12	3:D:435:VAL:HG11	1.94	0.48
3:D:486:ARG:HB2	9:D:2292:HOH:O	2.12	0.48
3:D:565:ILE:HD12	5:F:192:LEU:CD1	2.42	0.48
1:K:197:LEU:N	1:K:197:LEU:HD23	2.29	0.48
1:K:206:THR:CG2	1:K:209:GLU:HG3	2.39	0.48
2:M:682:TYR:CE1	2:M:851:LYS:HD2	2.49	0.48
3:N:1197:ARG:N	9:N:1577:HOH:O	2.46	0.48
3:N:521:PRO:O	3:N:525:ARG:HG2	2.13	0.48
1:B:7:LYS:HG3	9:B:434:HOH:O	2.13	0.48
2:C:305:PRO:HA	2:C:308:ARG:CD	2.42	0.48
2:C:211:LEU:CD1	2:C:308:ARG:HA	2.44	0.48
2:C:724:ARG:HG2	2:C:734:LEU:CD2	2.43	0.48
2:C:719:PRO:HB3	2:C:820:ARG:CZ	2.43	0.48
3:D:204:LEU:O	3:D:393:ILE:HA	2.13	0.48
3:D:45:PHE:HB3	3:D:86:ARG:NH2	2.29	0.48
3:D:466:LYS:NZ	9:D:1668:HOH:O	2.47	0.48
3:D:705:ALA:HB3	3:D:706:PRO:CD	2.43	0.48
4:E:73:LEU:N	9:E:131:HOH:O	2.46	0.48
5:F:172:ARG:NH1	9:F:462:HOH:O	2.45	0.48
2:M:1088:LEU:HG	2:M:1092:LEU:HD12	1.95	0.48
2:M:431:HIS:H	2:M:434:HIS:CD2	2.30	0.48
2:M:625:LEU:O	2:M:627:ARG:N	2.47	0.48
3:N:1047:LYS:HB3	3:N:1048:PRO:HD2	1.94	0.48
3:N:1110:ALA:O	3:N:1112:CYS:N	2.46	0.48
3:N:1240:THR:O	3:N:1257:PRO:HB3	2.14	0.48
3:N:615:ARG:HH21	3:N:1089:ALA:CB	2.20	0.48
2:M:1056:LYS:HB3	3:N:623:VAL:HG13	1.94	0.48
3:N:820:GLU:HG3	3:N:836:VAL:HG11	1.95	0.48
1:A:206:THR:HG22	1:A:209:GLU:CG	2.40	0.48
1:A:7:LYS:NZ	1:A:186:LEU:HD21	2.29	0.48
2:C:11:GLU:HB2	9:C:1190:HOH:O	2.14	0.48
2:C:139:GLN:OE1	2:C:414:GLY:HA3	2.14	0.48
2:C:165:LEU:HD12	2:C:166:PRO:CA	2.43	0.48
2:C:611:ILE:CD1	2:C:625:LEU:HD11	2.44	0.48
2:C:851:LYS:HG3	9:C:1250:HOH:O	2.12	0.48
2:C:676:ILE:HG22	2:C:988:VAL:HG22	1.96	0.48
3:D:12:LEU:HD23	3:D:13:ALA:H	1.79	0.48
3:D:702:LEU:HD13	3:D:716:PHE:HD1	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:D:2077:HOH:O	5:F:349:LEU:HD13	2.13	0.48
5:F:358:LEU:HD13	5:F:370:LYS:HG3	1.96	0.48
1:K:101:LEU:HD12	1:K:114:PHE:CD1	2.49	0.48
1:K:9:PRO:HB3	1:K:25:LEU:HD21	1.96	0.48
1:L:50:GLY:O	1:L:146:ARG:HA	2.13	0.48
1:L:207:PRO:HD2	9:L:3232:HOH:O	2.13	0.48
3:N:1321:ALA:O	3:N:1339:LYS:HG3	2.13	0.48
3:N:421:LEU:CG	3:N:429:SER:HB3	2.43	0.48
3:N:73:CYS:SG	3:N:74:GLU:N	2.86	0.48
3:N:81:THR:HG22	3:N:82:LYS:N	2.29	0.48
4:O:54:LEU:HD23	4:O:58:PRO:HD2	1.96	0.48
5:P:292:ALA:O	5:P:299:TRP:HB2	2.14	0.48
1:B:39:PRO:O	1:B:43:ILE:HG12	2.14	0.48
2:C:19:THR:HG22	2:C:19:THR:O	2.14	0.48
2:C:143:SER:CB	2:C:276:LYS:HZ1	2.23	0.48
2:C:289:THR:O	2:C:291:ALA:N	2.46	0.48
2:C:410:ILE:HD12	2:C:410:ILE:H	1.78	0.48
2:C:410:ILE:HD12	2:C:410:ILE:N	2.29	0.48
2:C:762:LYS:HG3	2:C:786:LYS:HD2	1.95	0.48
2:C:879:ARG:HB3	9:C:1196:HOH:O	2.14	0.48
3:D:1238:MET:HG3	3:D:1257:PRO:HG3	1.95	0.48
3:D:550:ARG:NH1	3:D:573:MET:HB3	2.29	0.48
5:F:128:ARG:HB2	9:F:652:HOH:O	2.14	0.48
3:D:561:GLY:CA	5:F:184:ARG:HH12	2.21	0.48
2:M:1098:ASP:HB2	3:N:21:TRP:CZ2	2.47	0.48
2:M:369:PRO:HG2	9:M:2247:HOH:O	2.14	0.48
2:M:496:ILE:O	2:M:515:ALA:HB1	2.14	0.48
2:M:644:VAL:HG22	9:M:2151:HOH:O	2.13	0.48
3:N:116:LEU:HB3	3:N:118:LEU:HG	1.96	0.48
3:N:1177:ALA:CB	3:N:1183:ILE:HD11	2.44	0.48
3:N:127:LEU:HD12	3:N:128:TYR:N	2.29	0.48
3:N:126:VAL:O	3:N:132:TYR:CD1	2.67	0.48
3:N:1384:PRO:O	3:N:1413:THR:HG21	2.13	0.48
3:N:407:VAL:HA	3:N:422:ALA:CB	2.44	0.48
3:N:465:LEU:HB3	9:N:2360:HOH:O	2.14	0.48
3:N:47:GLU:HA	3:N:51:GLY:O	2.13	0.48
3:N:540:LEU:HD21	3:N:603:LEU:HD23	1.95	0.48
4:O:31:LEU:HD23	4:O:35:PHE:CE1	2.48	0.48
5:P:240:THR:O	5:P:244:ARG:HG3	2.13	0.48
1:A:162:ILE:HG13	1:A:163:ASN:N	2.28	0.47
1:B:50:GLY:O	1:B:146:ARG:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:43:GLY:HA2	2:C:341:THR:OG1	2.13	0.47
2:C:544:THR:O	2:C:547:ILE:HG13	2.13	0.47
2:C:556:ASN:HA	9:C:1448:HOH:O	2.12	0.47
2:C:571:LEU:CD2	2:C:700:TYR:HA	2.44	0.47
2:C:679:PHE:CE1	2:C:870:ILE:HD13	2.49	0.47
2:C:843:HIS:CD2	2:C:884:GLN:HA	2.49	0.47
2:C:896:PHE:CD2	2:C:925:TYR:HB2	2.49	0.47
2:C:930:LYS:HD3	9:C:1707:HOH:O	2.14	0.47
2:C:926:PHE:O	2:C:930:LYS:HG3	2.12	0.47
3:D:1128:VAL:O	3:D:1129:THR:C	2.51	0.47
3:D:1323:GLN:HG3	3:D:1324:PRO:HD2	1.95	0.47
3:D:133:ILE:HG22	3:D:455:ARG:CA	2.43	0.47
3:D:666:ILE:H	3:D:666:ILE:HG13	1.55	0.47
3:D:693:GLU:O	4:E:48:MET:HE1	2.14	0.47
1:K:155:LYS:HD3	9:K:3774:HOH:O	2.14	0.47
2:M:252:LYS:NZ	2:M:296:GLY:HA3	2.29	0.47
2:M:614:ARG:HD3	9:M:2272:HOH:O	2.14	0.47
2:M:650:ARG:HB2	2:M:653:ASP:HB2	1.94	0.47
2:M:879:ARG:H	2:M:879:ARG:HD2	1.79	0.47
1:K:180:GLN:NE2	2:M:929:ARG:HH21	2.11	0.47
3:N:1000:THR:HG23	3:N:1001:GLU:N	2.29	0.47
3:N:147:VAL:HG21	9:N:2101:HOH:O	2.13	0.47
3:N:87:ARG:HA	3:N:523:ASP:HB2	1.96	0.47
3:N:916:TYR:CE2	3:N:920:LEU:HD13	2.49	0.47
5:P:139:ALA:HB1	9:P:558:HOH:O	2.13	0.47
5:P:358:LEU:HD21	5:P:367:MET:HE1	1.96	0.47
1:A:49:PRO:CB	1:A:148:VAL:HG22	2.42	0.47
2:C:101:ILE:HG22	2:C:102:HIS:N	2.28	0.47
2:C:218:VAL:HA	2:C:221:LEU:HD23	1.95	0.47
2:C:333:ILE:N	2:C:333:ILE:HD12	2.28	0.47
2:C:378:LEU:HG	2:C:382:ILE:CD1	2.44	0.47
2:C:704:HIS:O	2:C:828:ALA:HA	2.14	0.47
3:D:1262:LEU:HD23	3:D:1352:ILE:CG1	2.38	0.47
3:D:1337:GLU:HB2	9:D:1785:HOH:O	2.14	0.47
3:D:62:LYS:HB2	9:D:1735:HOH:O	2.14	0.47
4:E:94:PRO:CG	9:E:180:HOH:O	2.56	0.47
5:F:138:SER:H	5:F:140:ARG:HE	1.62	0.47
5:F:187:LEU:HD23	5:F:187:LEU:C	2.34	0.47
2:M:1002:GLU:HG3	3:N:744:GLN:HE22	1.79	0.47
2:M:176:VAL:O	2:M:178:PRO:HD3	2.13	0.47
2:M:276:LYS:HG2	2:M:280:LYS:HZ2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:72:ARG:HB2	9:M:1985:HOH:O	2.13	0.47
3:N:133:ILE:HG22	3:N:455:ARG:CA	2.44	0.47
3:N:1467:ILE:HG12	7:N:1527:MXP:H16A	1.96	0.47
3:N:603:LEU:HA	3:N:606:ILE:HD12	1.96	0.47
3:N:633:VAL:C	3:N:635:PRO:HD3	2.35	0.47
5:P:119:ILE:HD13	5:P:170:HIS:ND1	2.29	0.47
5:P:277:GLN:O	5:P:280:GLN:HB3	2.13	0.47
1:B:120:VAL:HG11	9:B:416:HOH:O	2.15	0.47
1:B:69:PRO:C	1:B:71:VAL:H	2.18	0.47
2:C:115:LEU:HD22	2:C:373:VAL:CG1	2.41	0.47
2:C:207:LEU:O	2:C:211:LEU:HB3	2.14	0.47
2:C:281:LEU:O	2:C:282:GLY:O	2.32	0.47
2:C:837:ASP:O	2:C:848:VAL:HG13	2.14	0.47
3:D:1087:ARG:NH1	3:D:1234:THR:O	2.47	0.47
3:D:1408:ILE:O	3:D:1409:ALA:C	2.49	0.47
3:D:1463:LYS:O	3:D:1467:ILE:HG13	2.13	0.47
3:D:1476:THR:CG2	4:E:21:VAL:HG22	2.44	0.47
3:D:403:PHE:HE2	3:D:443:VAL:N	2.12	0.47
3:D:528:VAL:HG12	3:D:529:GLN:N	2.29	0.47
2:C:1006:HIS:O	3:D:648:MET:HE3	2.14	0.47
2:C:1106:ASP:OD1	3:D:7:LYS:HD2	2.14	0.47
4:E:4:PRO:HG2	9:E:175:HOH:O	2.12	0.47
4:E:82:GLU:HG3	4:E:83:ASP:H	1.78	0.47
1:K:9:PRO:HB3	1:K:25:LEU:CG	2.44	0.47
2:M:262:ALA:O	2:M:264:PRO:O	2.32	0.47
2:M:631:SER:HG	2:M:635:THR:H	1.59	0.47
3:N:1090:ASP:OD1	3:N:1241:PHE:CZ	2.68	0.47
3:N:1129:THR:HG23	3:N:1130:ARG:H	1.78	0.47
3:N:1238:MET:HG3	3:N:1257:PRO:HG3	1.96	0.47
3:N:1481:VAL:CG1	4:O:18:ARG:HG3	2.44	0.47
4:O:87:LYS:HD3	9:O:2559:HOH:O	2.15	0.47
5:P:321:ILE:O	5:P:327:SER:HB3	2.13	0.47
1:B:87:VAL:CG2	1:B:144:VAL:HG11	2.36	0.47
2:C:772:ARG:HD3	9:F:459:HOH:O	2.15	0.47
2:C:923:GLU:O	2:C:927:GLY:HA3	2.15	0.47
3:D:1372:VAL:O	3:D:1375:MET:HB2	2.13	0.47
3:D:432:TYR:O	3:D:448:GLU:HA	2.15	0.47
3:D:87:ARG:HB2	3:D:523:ASP:HB2	1.96	0.47
3:D:895:VAL:O	3:D:899:LEU:HG	2.14	0.47
4:E:67:GLU:OE1	4:E:73:LEU:HD11	2.15	0.47
5:F:358:LEU:CD2	5:F:370:LYS:HZ2	2.24	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:410:ILE:HD11	2:M:455:LEU:HB3	1.96	0.47
2:M:668:LEU:O	2:M:993:PHE:CZ	2.67	0.47
2:M:670:GLN:HE22	2:M:699:PHE:C	2.18	0.47
2:M:975:TYR:HA	2:M:982:PRO:HA	1.95	0.47
3:N:1440:PHE:N	3:N:1440:PHE:CD2	2.82	0.47
9:M:1815:HOH:O	3:N:1456:LYS:HD3	2.13	0.47
3:N:162:ARG:HA	3:N:449:SER:CB	2.44	0.47
3:N:807:ALA:HB2	9:N:1559:HOH:O	2.15	0.47
3:N:81:THR:HB	3:N:85:VAL:CG2	2.43	0.47
3:N:87:ARG:HD2	9:N:1572:HOH:O	2.14	0.47
3:N:787:LEU:HD21	3:N:947:ILE:HD11	1.96	0.47
3:N:957:PRO:HB3	3:N:959:GLU:HG3	1.95	0.47
1:A:184:THR:HG23	1:A:192:LEU:CB	2.42	0.47
1:B:102:LYS:HA	1:B:138:LEU:O	2.15	0.47
2:C:1058:ASP:OD1	2:C:1084:SER:HB3	2.14	0.47
2:C:157:ARG:N	9:C:1172:HOH:O	2.46	0.47
2:C:21:ILE:HG12	2:C:455:LEU:HD21	1.96	0.47
3:D:109:PRO:HB2	9:D:2000:HOH:O	2.13	0.47
3:D:119:SER:CB	3:D:123:LEU:HD13	2.44	0.47
3:D:1500:LYS:HE3	9:D:2173:HOH:O	2.13	0.47
3:D:589:ALA:HA	9:D:1703:HOH:O	2.12	0.47
5:F:365:GLU:HG2	5:F:397:ILE:HA	1.96	0.47
2:M:164:PRO:HB3	9:M:1703:HOH:O	2.14	0.47
2:M:160:ALA:O	2:M:173:ASP:HA	2.14	0.47
2:M:378:LEU:HG	2:M:382:ILE:CD1	2.44	0.47
2:M:965:GLU:HG3	9:M:2274:HOH:O	2.15	0.47
3:N:1236:LEU:HD11	3:N:1356:TYR:CE1	2.48	0.47
3:N:1448:THR:O	3:N:1451:ALA:HB3	2.14	0.47
3:N:100:ALA:CB	3:N:513:ILE:HD13	2.29	0.47
9:M:2079:HOH:O	3:N:606:ILE:HG21	2.15	0.47
3:N:611:GLN:CG	3:N:619:LEU:HD11	2.42	0.47
3:N:752:SER:HB2	9:N:1905:HOH:O	2.14	0.47
3:N:795:VAL:HA	3:N:861:GLN:O	2.15	0.47
2:M:817:PRO:HG3	5:P:288:TYR:OH	2.14	0.47
5:P:353:GLU:HG2	9:P:485:HOH:O	2.13	0.47
1:A:59:GLU:HG3	1:A:139:ASN:CG	2.35	0.47
1:A:5:LYS:HD2	9:A:440:HOH:O	2.14	0.47
1:B:27:PRO:HB3	1:B:192:LEU:CD2	2.45	0.47
2:C:129:ILE:HG22	2:C:130:ASN:N	2.29	0.47
2:C:313:LEU:HA	9:C:1596:HOH:O	2.15	0.47
2:C:422:ARG:HG3	2:C:423:ALA:H	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:479:VAL:HG21	2:C:503:LEU:HD11	1.96	0.47
2:C:726:ILE:O	2:C:726:ILE:HG22	2.14	0.47
3:D:1109:GLU:HG2	3:D:1202:GLN:N	2.29	0.47
3:D:133:ILE:HG12	3:D:133:ILE:H	1.35	0.47
3:D:17:LYS:HA	3:D:20:SER:HB3	1.95	0.47
3:D:180:LYS:HG3	3:D:183:GLU:H	1.79	0.47
3:D:524:LEU:C	3:D:526:PRO:HD3	2.35	0.47
3:D:75:ARG:HB2	9:D:1539:HOH:O	2.15	0.47
3:D:80:VAL:HG12	3:D:81:THR:N	2.29	0.47
5:F:350:LEU:O	5:F:354:LEU:HB2	2.14	0.47
1:L:195:LEU:C	9:L:1676:HOH:O	2.53	0.47
2:M:421:GLU:O	2:M:421:GLU:HG2	2.15	0.47
2:M:328:LEU:HD22	2:M:437:ARG:CB	2.44	0.47
2:M:497:ALA:HA	2:M:515:ALA:HA	1.96	0.47
3:N:34:TYR:O	3:N:35:ARG:C	2.52	0.47
3:N:137:PRO:HD2	3:N:453:ASP:CB	2.45	0.47
3:N:486:ARG:HH12	3:N:1389:LEU:HD11	1.78	0.47
3:N:844:ALA:O	3:N:867:ARG:HB3	2.14	0.47
3:N:900:ILE:HG13	3:N:900:ILE:O	2.15	0.47
5:P:280:GLN:HG2	5:P:280:GLN:O	2.14	0.47
1:A:133:GLU:N	9:A:320:HOH:O	2.46	0.47
2:C:129:ILE:HG23	9:C:1478:HOH:O	2.14	0.47
2:C:274:ARG:O	2:C:274:ARG:HG2	2.15	0.47
2:C:279:GLU:HG3	2:C:280:LYS:N	2.30	0.47
2:C:726:ILE:HG22	9:C:1346:HOH:O	2.14	0.47
2:C:865:THR:C	9:C:1269:HOH:O	2.52	0.47
2:C:958:THR:HG23	2:C:961:GLU:H	1.78	0.47
3:D:1066:THR:HG22	3:D:1069:GLU:HG3	1.96	0.47
3:D:1403:LEU:HD12	9:D:1814:HOH:O	2.15	0.47
3:D:18:ILE:HG21	3:D:516:ALA:O	2.14	0.47
3:D:455:ARG:HH11	3:D:463:GLN:HG3	1.78	0.47
3:D:520:LEU:HD23	3:D:540:LEU:CD2	2.45	0.47
3:D:637:LEU:HD11	3:D:642:CYS:CA	2.45	0.47
5:F:140:ARG:HG3	5:F:141:VAL:N	2.29	0.47
1:K:209:GLU:O	1:K:213:GLN:HG3	2.15	0.47
2:M:1050:GLN:NE2	9:M:2160:HOH:O	2.48	0.47
2:M:1067:TYR:O	2:M:1071:ILE:HG12	2.14	0.47
2:M:175:GLU:HB3	2:M:183:SER:OG	2.14	0.47
2:M:332:ARG:HH21	2:M:338:GLU:CD	2.17	0.47
2:M:362:GLY:HA3	2:M:367:LEU:HD23	1.95	0.47
3:N:1394:VAL:HG21	9:N:1598:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1490:LYS:HB2	9:O:3444:HOH:O	2.14	0.47
3:N:540:LEU:HA	3:N:543:LEU:HD12	1.97	0.47
3:N:543:LEU:HA	3:N:546:ARG:HG3	1.96	0.47
5:P:109:GLY:O	5:P:113:ILE:HG13	2.15	0.47
5:P:160:ASP:OD1	5:P:178:ARG:NH2	2.48	0.47
5:P:361:LEU:HD23	5:P:362:SER:N	2.29	0.47
5:P:81:VAL:O	5:P:85:LEU:HB2	2.14	0.47
1:A:182:GLU:O	1:A:194:LYS:HB3	2.14	0.47
1:B:185:ARG:HB3	9:D:1701:HOH:O	2.14	0.47
2:C:165:LEU:HG	2:C:265:ARG:HH12	1.79	0.47
2:C:289:THR:HG22	2:C:290:LEU:HD23	1.97	0.47
2:C:5:ARG:HB3	2:C:902:ILE:HB	1.97	0.47
2:C:875:GLY:HA2	2:C:879:ARG:NH1	2.30	0.47
3:D:1236:LEU:HA	3:D:1359:GLN:NE2	2.30	0.47
3:D:397:LYS:CE	3:D:448:GLU:HB3	2.45	0.47
2:M:1015:LEU:N	9:M:1708:HOH:O	2.47	0.47
2:M:165:LEU:HD12	2:M:166:PRO:HA	1.95	0.47
2:M:267:TYR:HB2	2:M:272:ALA:CB	2.44	0.47
2:M:448:ASN:HB3	2:M:452:ILE:HD11	1.97	0.47
2:M:472:ARG:O	2:M:531:PHE:HD2	1.97	0.47
2:M:839:LEU:HD21	2:M:849:VAL:CG2	2.45	0.47
3:N:1045:MET:HG3	3:N:1073:SER:HA	1.97	0.47
3:N:1111:ASP:HB3	3:N:1203:LYS:HG3	1.96	0.47
3:N:171:LEU:HD22	3:N:175:VAL:HB	1.96	0.47
3:N:685:ASP:HB3	9:N:1697:HOH:O	2.14	0.47
3:N:827:ILE:HG23	3:N:837:GLY:HA2	1.97	0.47
3:N:84:ILE:O	3:N:87:ARG:HB3	2.15	0.47
4:O:39:VAL:HG21	4:O:72:ARG:HD2	1.97	0.47
2:C:290:LEU:H	2:C:290:LEU:HD23	1.78	0.47
2:C:535:SER:CB	2:C:537:LYS:HG3	2.45	0.47
2:C:627:ARG:HG3	2:C:628:PHE:N	2.29	0.47
3:D:1003:VAL:O	3:D:1006:ALA:HB3	2.15	0.47
3:D:1212:ALA:HB3	9:D:1618:HOH:O	2.15	0.47
3:D:205:TYR:HB2	3:D:393:ILE:HG12	1.95	0.47
3:D:443:VAL:HG11	3:D:445:ARG:HE	1.80	0.47
3:D:525:ARG:N	3:D:526:PRO:HD3	2.29	0.47
3:D:827:ILE:O	3:D:837:GLY:HA3	2.15	0.47
3:D:907:GLU:O	3:D:911:LEU:HD13	2.15	0.47
5:F:261:PRO:O	5:F:265:VAL:HG23	2.14	0.47
1:L:15:THR:C	1:L:16:GLN:HG2	2.35	0.47
2:M:1034:GLU:O	2:M:1037:VAL:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:405:ARG:CZ	9:M:1857:HOH:O	2.63	0.47
2:M:648:ARG:HG3	2:M:648:ARG:O	2.14	0.47
2:M:798:GLY:H	2:M:827:VAL:CG1	2.27	0.47
3:N:1341:PRO:O	3:N:1343:ALA:N	2.48	0.47
3:N:582:LEU:HA	3:N:603:LEU:HD12	1.96	0.47
3:N:874:GLU:HG3	9:N:1713:HOH:O	2.14	0.47
3:N:933:ALA:O	3:N:937:TYR:HD1	1.98	0.47
5:P:234:LYS:HE2	9:P:430:HOH:O	2.14	0.47
5:P:358:LEU:HD22	5:P:370:LYS:CE	2.45	0.47
1:A:89:PHE:HB3	1:A:94:LEU:HD22	1.97	0.47
1:B:165:ILE:HG22	9:B:502:HOH:O	2.14	0.47
2:C:301:GLU:O	2:C:305:PRO:HG2	2.15	0.47
2:C:497:ALA:HA	2:C:515:ALA:HA	1.96	0.47
3:D:421:LEU:HB2	3:D:427:VAL:HG12	1.95	0.47
3:D:65:ARG:CG	3:D:66:GLN:N	2.77	0.47
3:D:844:ALA:O	3:D:867:ARG:HB3	2.15	0.47
3:D:983:LEU:HD13	3:D:991:GLN:OE1	2.15	0.47
5:F:309:LYS:O	5:F:312:GLN:HB2	2.15	0.47
2:M:113:VAL:O	2:M:115:LEU:HD23	2.15	0.47
2:M:551:GLU:O	3:N:1065:LEU:HB3	2.15	0.47
3:N:204:LEU:HG	3:N:441:ARG:HH12	1.80	0.47
3:N:18:ILE:HD12	3:N:518:PRO:HD3	1.97	0.47
3:N:85:VAL:HG12	3:N:89:ARG:NE	2.30	0.47
2:M:983:ILE:HG23	3:N:944:THR:O	2.15	0.47
3:N:593:ASN:HD21	5:P:206:GLY:HA2	1.80	0.47
5:P:410:TYR:O	5:P:413:SER:HB2	2.15	0.47
5:P:95:THR:HG22	5:P:96:LEU:HD23	1.97	0.47
1:B:141:GLU:HG3	9:B:405:HOH:O	2.14	0.47
1:B:15:THR:C	1:B:16:GLN:HG2	2.35	0.47
1:B:46:SER:HB2	9:B:503:HOH:O	2.14	0.47
2:C:1025:ALA:C	2:C:1026:GLN:HG3	2.35	0.47
2:C:1071:ILE:O	3:D:659:LYS:HB2	2.15	0.47
2:C:176:VAL:O	2:C:178:PRO:HD3	2.15	0.47
2:C:732:ALA:O	2:C:735:ARG:HG3	2.15	0.47
3:D:1051:GLU:H	3:D:1051:GLU:HG3	1.46	0.47
3:D:1240:THR:O	3:D:1257:PRO:HB3	2.15	0.47
3:D:1478:SER:HG	3:D:1481:VAL:HG23	1.80	0.47
3:D:407:VAL:HA	3:D:422:ALA:CB	2.45	0.47
2:C:1035:MET:HG2	3:D:707:THR:O	2.14	0.47
3:D:699:VAL:HG21	3:D:760:ARG:HB3	1.97	0.47
3:D:810:GLU:HG2	9:D:2253:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:843:PHE:CD2	3:D:849:ALA:HA	2.49	0.47
1:K:89:PHE:HD1	1:K:120:VAL:HG23	1.80	0.47
1:K:45:LEU:HD23	9:K:1231:HOH:O	2.14	0.47
2:M:1060:ILE:HG22	2:M:1061:GLU:H	1.78	0.47
2:M:172:ILE:HD12	2:M:172:ILE:H	1.78	0.47
2:M:224:GLU:HG3	9:M:2180:HOH:O	2.14	0.47
5:P:372:ARG:HB3	9:P:615:HOH:O	2.14	0.47
5:P:371:LEU:HD22	5:P:375:LEU:HD22	1.95	0.47
2:C:1030:GLN:CD	3:D:628:ARG:HB3	2.35	0.46
2:C:122:THR:HG22	2:C:123:GLU:N	2.31	0.46
2:C:166:PRO:HD3	2:C:265:ARG:HG3	1.97	0.46
2:C:183:SER:HB3	2:C:190:LYS:HD3	1.97	0.46
2:C:36:PRO:HB2	2:C:70:GLU:HG2	1.97	0.46
2:C:54:ILE:HG22	2:C:66:LEU:HB3	1.96	0.46
3:D:1106:VAL:HG12	3:D:1107:VAL:N	2.30	0.46
3:D:481:MET:HB2	3:D:1388:ARG:NH1	2.30	0.46
3:D:204:LEU:HG	3:D:441:ARG:NH1	2.30	0.46
3:D:39:PRO:HD2	3:D:47:GLU:OE1	2.15	0.46
2:C:1115:LEU:HB3	3:D:85:VAL:CG1	2.44	0.46
4:E:42:PRO:HD3	9:E:101:HOH:O	2.16	0.46
5:F:292:ALA:O	5:F:299:TRP:HB2	2.15	0.46
1:K:106:PRO:HG3	1:K:134:GLU:CG	2.45	0.46
1:L:162:ILE:HA	9:L:1885:HOH:O	2.15	0.46
2:M:379:GLU:O	2:M:383:ARG:HB3	2.15	0.46
2:M:439:CYS:SG	2:M:541:SER:N	2.87	0.46
2:M:627:ARG:O	2:M:638:ASP:HA	2.15	0.46
2:M:751:PRO:HG3	2:M:796:GLU:HG2	1.98	0.46
2:M:815:LEU:HD23	2:M:819:VAL:O	2.15	0.46
2:M:851:LYS:NZ	9:M:2027:HOH:O	2.48	0.46
3:N:1112:CYS:HB2	3:N:1195:GLN:CG	2.45	0.46
3:N:153:LEU:HD12	3:N:157:GLU:HB2	1.97	0.46
3:N:421:LEU:HB2	3:N:427:VAL:HG12	1.96	0.46
3:N:133:ILE:HG22	3:N:455:ARG:C	2.35	0.46
3:N:702:LEU:HD23	3:N:745:MET:HE1	1.97	0.46
4:O:45:ARG:HB3	9:O:1014:HOH:O	2.14	0.46
4:O:70:THR:HG21	4:O:72:ARG:HE	1.80	0.46
5:P:288:TYR:HA	5:P:291:ILE:CG2	2.45	0.46
1:A:227:ASN:H	1:A:227:ASN:HD22	1.61	0.46
1:B:217:ILE:O	1:B:221:HIS:ND1	2.43	0.46
2:C:1050:GLN:HG2	2:C:1079:PRO:HG2	1.97	0.46
2:C:204:GLN:NE2	2:C:222:MET:HA	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:267:TYR:HB2	2:C:272:ALA:CB	2.45	0.46
2:C:328:LEU:CD1	2:C:433:THR:HB	2.44	0.46
2:C:557:ARG:NE	2:C:560:MET:SD	2.88	0.46
2:C:672:VAL:HG23	2:C:868:ASP:HB2	1.96	0.46
3:D:1097:LYS:O	3:D:1101:VAL:HG23	2.16	0.46
3:D:204:LEU:HA	3:D:441:ARG:NH2	2.18	0.46
3:D:204:LEU:HD21	3:D:445:ARG:NH1	2.30	0.46
3:D:422:ALA:O	3:D:427:VAL:HB	2.16	0.46
3:D:39:PRO:HB3	3:D:45:PHE:O	2.15	0.46
3:D:543:LEU:HA	3:D:546:ARG:HG3	1.96	0.46
3:D:702:LEU:HD13	3:D:716:PHE:CD1	2.50	0.46
3:D:863:VAL:HA	9:D:1596:HOH:O	2.14	0.46
5:F:396:ARG:HA	5:F:399:GLN:HB2	1.97	0.46
2:M:18:LEU:HB2	2:M:590:ASP:CB	2.44	0.46
2:M:279:GLU:HG3	2:M:280:LYS:N	2.29	0.46
2:M:400:PRO:HG2	9:M:1638:HOH:O	2.15	0.46
3:N:1108:ARG:NE	3:N:1198:TYR:O	2.47	0.46
3:N:850:LEU:O	3:N:853:VAL:HB	2.14	0.46
4:O:59:ASN:N	9:O:4171:HOH:O	2.48	0.46
5:P:398:ARG:HG3	5:P:402:ASN:ND2	2.29	0.46
2:C:648:ARG:HG3	2:C:648:ARG:O	2.14	0.46
3:D:1037:GLN:OE1	3:D:1042:ARG:HD3	2.15	0.46
3:D:112:ILE:HD12	3:D:461:ILE:HG21	1.96	0.46
3:D:26:VAL:HG11	3:D:44:LEU:HD23	1.96	0.46
3:D:527:MET:HE1	5:F:258:ILE:HD11	1.97	0.46
3:D:537:THR:O	5:F:317:LEU:HB2	2.15	0.46
3:D:730:PRO:HA	3:D:733:CYS:SG	2.55	0.46
3:D:795:VAL:HG22	3:D:876:SER:HB3	1.96	0.46
5:F:319:THR:O	5:F:321:ILE:HG12	2.15	0.46
2:M:1078:GLU:HA	2:M:1079:PRO:HD3	1.86	0.46
2:M:62:GLY:HA2	2:M:359:MET:CE	2.45	0.46
3:N:1217:ILE:HD12	3:N:1480:PHE:CE2	2.51	0.46
3:N:187:LYS:HG3	3:N:199:LEU:CD2	2.44	0.46
4:O:33:HIS:CD2	4:O:89:MET:HG2	2.49	0.46
1:A:161:ARG:HB2	1:A:161:ARG:HH11	1.79	0.46
1:B:23:PHE:O	1:B:196:THR:HA	2.14	0.46
2:C:147:TYR:HE1	9:C:1347:HOH:O	1.98	0.46
2:C:160:ALA:O	2:C:173:ASP:HA	2.15	0.46
2:C:271:GLU:HA	2:C:275:TYR:CD1	2.51	0.46
2:C:328:LEU:HB2	2:C:433:THR:CG2	2.46	0.46
2:C:139:GLN:HA	2:C:411:SER:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:64:LEU:HB2	2:C:359:MET:CE	2.45	0.46
1:A:65:PHE:CE1	2:C:799:ILE:HD11	2.51	0.46
3:D:951:ILE:CD1	3:D:1062:ARG:HG3	2.45	0.46
3:D:1382:THR:OG1	3:D:1418:LYS:HE3	2.16	0.46
3:D:677:LEU:HD21	9:D:2185:HOH:O	2.14	0.46
3:D:928:ALA:O	3:D:931:LEU:HB2	2.16	0.46
1:K:42:ARG:HE	2:M:857:ASP:HB3	1.79	0.46
1:L:102:LYS:HA	1:L:138:LEU:O	2.16	0.46
1:L:200:TRP:HZ3	9:N:2120:HOH:O	1.98	0.46
2:M:426:ASP:OD1	2:M:427:VAL:HG22	2.14	0.46
2:M:459:ALA:HB1	2:M:467:ILE:CG2	2.46	0.46
2:M:760:SER:O	2:M:786:LYS:N	2.40	0.46
3:N:1195:GLN:CG	3:N:1196:THR:N	2.78	0.46
3:N:1281:VAL:HG21	3:N:1313:VAL:HG21	1.96	0.46
3:N:1476:THR:CG2	4:O:21:VAL:HG22	2.42	0.46
3:N:562:ALA:HB1	3:N:567:ILE:CD1	2.45	0.46
3:N:705:ALA:HB2	9:N:1965:HOH:O	2.16	0.46
3:N:705:ALA:HB3	3:N:706:PRO:CD	2.45	0.46
5:P:123:ASP:HB2	5:P:126:LEU:HD13	1.96	0.46
5:P:420:ASP:O	5:P:422:LEU:HD23	2.16	0.46
1:B:128:HIS:HE1	1:B:131:THR:HG23	1.81	0.46
1:B:85:LEU:HD13	1:B:127:LEU:HD23	1.98	0.46
2:C:31:GLN:NE2	2:C:71:TYR:OH	2.49	0.46
2:C:479:VAL:HG11	2:C:532:MET:HE2	1.97	0.46
2:C:588:VAL:HG21	9:C:1718:HOH:O	2.15	0.46
2:C:798:GLY:H	2:C:827:VAL:CG1	2.29	0.46
2:C:89:THR:HA	2:C:129:ILE:O	2.15	0.46
3:D:952:ASP:HA	3:D:1062:ARG:NH2	2.31	0.46
3:D:23:TYR:O	3:D:49:ILE:HG23	2.16	0.46
3:D:795:VAL:HG12	3:D:796:ARG:N	2.31	0.46
3:D:860:LEU:O	3:D:877:PRO:HD2	2.14	0.46
5:F:116:LEU:CB	5:F:127:ILE:HD12	2.46	0.46
5:F:151:LEU:HD11	9:F:626:HOH:O	2.14	0.46
5:F:171:LYS:HA	9:F:473:HOH:O	2.16	0.46
1:K:58:ILE:HG21	1:K:68:ILE:HD11	1.97	0.46
1:L:89:PHE:HB3	1:L:94:LEU:HD22	1.98	0.46
2:M:1077:PRO:HG3	9:M:2203:HOH:O	2.15	0.46
2:M:468:ARG:HB3	2:M:487:THR:HA	1.97	0.46
2:M:718:GLY:HA3	2:M:761:PHE:CE1	2.51	0.46
2:M:843:HIS:CD2	2:M:884:GLN:HA	2.50	0.46
3:N:403:PHE:CD1	3:N:405:ASP:O	2.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:18:ILE:HD12	3:N:518:PRO:CD	2.45	0.46
4:O:82:GLU:HG3	4:O:83:ASP:H	1.80	0.46
5:P:209:PHE:HE2	5:P:213:ILE:HD11	1.79	0.46
1:B:57:TYR:O	1:B:140:MET:HA	2.15	0.46
1:B:60:ASP:HB2	1:B:137:ARG:NH1	2.31	0.46
2:C:575:GLN:O	2:C:667:ALA:HB1	2.15	0.46
2:C:6:PHE:CD1	2:C:909:ALA:HB2	2.50	0.46
2:C:762:LYS:C	2:C:763:GLY:O	2.52	0.46
2:C:939:ARG:HD3	2:C:975:TYR:CE2	2.51	0.46
2:C:975:TYR:HA	2:C:982:PRO:HA	1.97	0.46
3:D:1076:GLY:O	3:D:1079:LYS:HG2	2.16	0.46
3:D:191:LEU:HD13	3:D:393:ILE:HG21	1.97	0.46
3:D:421:LEU:HD11	3:D:446:VAL:CG2	2.45	0.46
3:D:455:ARG:NH1	3:D:463:GLN:HG3	2.31	0.46
4:E:13:VAL:HG23	9:E:151:HOH:O	2.14	0.46
1:K:132:LEU:HD12	1:K:132:LEU:N	2.30	0.46
1:K:35:THR:HG21	1:L:43:ILE:HD11	1.98	0.46
1:L:69:PRO:O	1:L:71:VAL:HG23	2.15	0.46
1:L:73:GLU:CD	1:L:130:ALA:HA	2.34	0.46
2:M:491:GLU:OE1	2:M:516:ARG:NH2	2.48	0.46
2:M:810:ASP:N	2:M:811:PRO:HD3	2.30	0.46
3:N:1115:THR:HG21	3:N:1151:ARG:HH21	1.80	0.46
3:N:1266:ARG:O	3:N:1268:PRO:HD3	2.15	0.46
3:N:145:VAL:HG22	3:N:146:PRO:CD	2.46	0.46
5:P:396:ARG:HA	5:P:399:GLN:HB2	1.98	0.46
1:B:179:PHE:HZ	9:B:437:HOH:O	1.99	0.46
2:C:140:ILE:HD13	2:C:331:ARG:HH21	1.80	0.46
2:C:674:VAL:HB	2:C:869:VAL:HG13	1.98	0.46
2:C:875:GLY:HA2	2:C:879:ARG:HH11	1.80	0.46
2:C:89:THR:HB	2:C:129:ILE:O	2.16	0.46
2:C:929:ARG:HH12	2:C:940:GLU:CD	2.19	0.46
3:D:1377:LYS:NZ	9:D:1537:HOH:O	2.45	0.46
3:D:1389:LEU:HD12	3:D:1390:LEU:HG	1.98	0.46
3:D:1472:ILE:O	3:D:1477:GLY:HA3	2.14	0.46
3:D:421:LEU:HD11	3:D:446:VAL:HG21	1.97	0.46
3:D:443:VAL:HG22	3:D:444:VAL:H	1.81	0.46
3:D:53:ILE:HG23	3:D:54:LYS:N	2.30	0.46
3:D:73:CYS:HB2	9:D:2023:HOH:O	2.14	0.46
1:B:176:ARG:NH2	3:D:847:ASP:HA	2.31	0.46
1:L:27:PRO:HB3	1:L:192:LEU:HD22	1.98	0.46
2:M:333:ILE:N	2:M:333:ILE:HD12	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:119:SER:HB3	9:N:1620:HOH:O	2.15	0.46
3:N:1311:LEU:H	3:N:1311:LEU:HD23	1.81	0.46
3:N:1410:GLU:OE2	3:N:1414:PRO:HG3	2.16	0.46
3:N:1382:THR:HG21	3:N:1418:LYS:NZ	2.31	0.46
3:N:407:VAL:HG22	3:N:422:ALA:HB2	1.98	0.46
3:N:522:PRO:HA	3:N:525:ARG:NH1	2.31	0.46
3:N:644:LEU:HD23	3:N:718:PRO:HB3	1.98	0.46
3:N:937:TYR:O	3:N:941:PHE:HD1	1.99	0.46
1:B:205:VAL:HB	9:B:448:HOH:O	2.15	0.46
1:B:22:GLU:HG2	1:B:198:ARG:HG2	1.97	0.46
2:C:101:ILE:HG23	2:C:107:LEU:CD2	2.43	0.46
2:C:799:ILE:N	2:C:799:ILE:HD13	2.30	0.46
3:D:1335:LEU:CD2	3:D:1344:VAL:HA	2.29	0.46
3:D:409:VAL:O	3:D:437:VAL:HG21	2.16	0.46
3:D:498:VAL:CG2	3:D:499:VAL:N	2.79	0.46
3:D:562:ALA:HB1	3:D:567:ILE:CD1	2.45	0.46
3:D:131:LYS:HG3	3:D:572:ARG:HH21	1.81	0.46
3:D:693:GLU:HG3	4:E:48:MET:CE	2.46	0.46
3:D:643:GLY:CA	3:D:727:GLN:HB2	2.46	0.46
3:D:783:ARG:NH1	3:D:1029:ARG:HG3	2.30	0.46
3:D:800:LYS:HE3	3:D:830:ALA:HB3	1.98	0.46
4:E:26:ARG:HH11	4:E:29:GLN:CD	2.18	0.46
5:F:241:TRP:HB2	9:F:438:HOH:O	2.15	0.46
5:F:398:ARG:HG3	5:F:402:ASN:ND2	2.31	0.46
2:M:1097:LEU:HD21	3:N:103:TRP:HZ3	1.81	0.46
2:M:122:THR:HG22	2:M:123:GLU:N	2.30	0.46
2:M:352:ALA:C	2:M:355:VAL:HG12	2.36	0.46
2:M:518:LYS:HG3	9:M:1841:HOH:O	2.16	0.46
2:M:82:GLU:OE2	2:M:86:LYS:HE3	2.16	0.46
2:M:988:VAL:HG11	3:N:949:ILE:O	2.16	0.46
3:N:1344:VAL:HG12	3:N:1348:LEU:HD22	1.97	0.46
3:N:1385:GLY:CA	3:N:1413:THR:HG21	2.46	0.46
3:N:1426:LYS:HA	9:N:1705:HOH:O	2.15	0.46
3:N:137:PRO:HD2	3:N:453:ASP:CG	2.36	0.46
3:N:795:VAL:HG22	3:N:876:SER:HB3	1.97	0.46
1:A:9:PRO:HD2	1:B:224:TYR:CD1	2.51	0.46
2:C:437:ARG:NH2	2:C:488:ALA:HA	2.31	0.46
3:D:1083:ASP:O	3:D:1087:ARG:HG3	2.15	0.46
3:D:48:ARG:NH2	9:D:1710:HOH:O	2.48	0.46
3:D:525:ARG:HA	3:D:538:SER:OG	2.15	0.46
2:C:1067:TYR:CE1	3:D:655:PRO:HG3	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:866:VAL:HG12	3:D:867:ARG:N	2.30	0.46
5:F:214:GLN:O	5:F:217:ASN:HB2	2.16	0.46
1:K:36:LEU:O	1:K:39:PRO:HD2	2.16	0.46
2:M:103:LYS:HB3	9:M:2059:HOH:O	2.15	0.46
2:M:115:LEU:HD22	2:M:373:VAL:CG1	2.41	0.46
2:M:211:LEU:HD11	2:M:308:ARG:HA	1.98	0.46
2:M:540:PHE:HE1	2:M:906:PHE:HE1	1.64	0.46
2:M:612:VAL:HG22	2:M:622:GLU:HA	1.97	0.46
2:M:9:ILE:HG12	2:M:907:ASP:OD2	2.15	0.46
3:N:1197:ARG:HG3	3:N:1198:TYR:H	1.80	0.46
3:N:560:GLN:O	5:P:184:ARG:NH2	2.48	0.46
5:P:113:ILE:HG23	5:P:127:ILE:CG2	2.46	0.46
5:P:266:GLU:O	5:P:270:LYS:HG3	2.16	0.46
5:P:358:LEU:HD13	5:P:370:LYS:HG3	1.97	0.46
5:P:400:ILE:HA	9:P:540:HOH:O	2.15	0.46
5:P:406:ARG:HA	5:P:409:LYS:HG2	1.97	0.46
1:A:198:ARG:HD2	1:A:200:TRP:CH2	2.51	0.46
1:A:212:ASN:O	1:A:215:VAL:HG22	2.16	0.46
2:C:199:VAL:HG13	2:C:235:LEU:CD2	2.46	0.46
2:C:292:ARG:HH11	2:C:299:LYS:HD3	1.81	0.46
2:C:564:MET:SD	2:C:846:LYS:HE3	2.55	0.46
2:C:841:ASN:C	2:C:841:ASN:HD22	2.19	0.46
3:D:1295:GLU:HB3	3:D:1300:SER:HB3	1.97	0.46
3:D:1326:THR:HG22	3:D:1327:ARG:N	2.31	0.46
3:D:27:GLU:O	3:D:28:LYS:HG2	2.16	0.46
3:D:539:ASP:OD2	5:F:318:GLU:HB2	2.15	0.46
3:D:704:ARG:CG	3:D:705:ALA:H	2.24	0.46
3:D:45:PHE:HD1	3:D:86:ARG:HH22	1.64	0.46
3:D:911:LEU:O	3:D:915:VAL:HG23	2.15	0.46
3:D:1485:GLN:HE21	4:E:80:VAL:H	1.63	0.46
5:F:176:ILE:HA	9:F:463:HOH:O	2.16	0.46
5:F:368:VAL:O	5:F:372:ARG:HB2	2.16	0.46
1:K:46:SER:HB3	2:M:856:GLU:CG	2.45	0.46
1:K:51:THR:HA	1:K:145:ASP:O	2.16	0.46
2:M:1097:LEU:N	2:M:1097:LEU:HD12	2.30	0.46
2:M:1109:VAL:HG11	3:N:5:VAL:HG13	1.97	0.46
2:M:143:SER:C	2:M:163:ILE:HD11	2.37	0.46
2:M:110:GLU:HB2	2:M:369:PRO:HG3	1.97	0.46
2:M:538:GLN:CD	9:M:1660:HOH:O	2.54	0.46
2:M:976:ASP:HB2	2:M:979:THR:HG22	1.96	0.46
3:N:18:ILE:HG21	3:N:516:ALA:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:1115:LEU:CB	3:N:85:VAL:HG13	2.42	0.46
3:N:884:ARG:O	3:N:888:GLU:HB2	2.16	0.46
4:O:53:GLY:C	4:O:55:PHE:N	2.67	0.46
5:P:138:SER:H	5:P:140:ARG:HE	1.64	0.46
3:N:131:LYS:HD2	5:P:83:GLN:OE1	2.15	0.46
5:P:88:ILE:HD13	5:P:193:ARG:CB	2.46	0.46
1:A:69:PRO:C	1:A:71:VAL:H	2.18	0.45
1:B:9:PRO:HD3	9:B:452:HOH:O	2.17	0.45
2:C:437:ARG:HG2	2:C:467:ILE:HG22	1.97	0.45
2:C:411:SER:OG	2:C:452:ILE:HG23	2.16	0.45
2:C:791:ARG:HD3	9:C:1572:HOH:O	2.15	0.45
2:C:86:LYS:HD2	9:C:1425:HOH:O	2.16	0.45
2:C:6:PHE:HB2	2:C:908:GLY:O	2.16	0.45
3:D:1144:LEU:HB3	3:D:1166:LEU:HD11	1.97	0.45
3:D:1267:ARG:HG2	3:D:1267:ARG:O	2.16	0.45
3:D:1455:LYS:NZ	9:D:2342:HOH:O	2.48	0.45
2:C:1087:VAL:HG12	3:D:610:LYS:HZ3	1.81	0.45
3:D:803:GLY:CA	9:D:1726:HOH:O	2.64	0.45
5:F:148:LYS:HE3	9:F:489:HOH:O	2.16	0.45
1:L:124:ASN:OD1	1:L:127:LEU:HB2	2.17	0.45
2:M:1114:GLY:HA2	9:M:1820:HOH:O	2.15	0.45
2:M:265:ARG:NH2	9:M:2236:HOH:O	2.48	0.45
2:M:217:LEU:HB2	2:M:311:PHE:CE1	2.50	0.45
2:M:9:ILE:HD11	2:M:537:LYS:CE	2.45	0.45
2:M:612:VAL:HG22	2:M:622:GLU:HG3	1.99	0.45
2:M:675:ALA:CA	2:M:989:VAL:HG12	2.41	0.45
3:N:102:ILE:HD12	3:N:579:ASP:CG	2.36	0.45
3:N:1258:ARG:NE	3:N:1262:LEU:HD11	2.31	0.45
3:N:1283:ILE:CG2	3:N:1290:LEU:HD21	2.46	0.45
3:N:10:ILE:HD11	3:N:1434:TRP:NE1	2.31	0.45
3:N:625:TYR:O	3:N:749:VAL:HG23	2.16	0.45
4:O:45:ARG:HB2	4:O:46:PRO:CD	2.45	0.45
4:O:70:THR:HG22	4:O:71:GLY:N	2.31	0.45
4:O:87:LYS:HB3	9:O:2559:HOH:O	2.15	0.45
3:N:573:MET:SD	5:P:210:LEU:HB3	2.56	0.45
2:C:146:VAL:HG22	2:C:162:ILE:HG23	1.97	0.45
2:C:137:VAL:CG2	2:C:391:LEU:HG	2.46	0.45
2:C:425:PHE:O	2:C:429:ASP:OD2	2.35	0.45
2:C:536:PRO:HB2	9:C:1738:HOH:O	2.16	0.45
2:C:18:LEU:CD2	2:C:542:VAL:HG11	2.45	0.45
2:C:916:GLU:O	2:C:919:ALA:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1031:ASN:O	3:D:1034:GLN:HB2	2.16	0.45
3:D:195:VAL:HG12	3:D:196:VAL:N	2.31	0.45
3:D:66:GLN:O	3:D:67:ARG:C	2.53	0.45
3:D:736:PHE:O	3:D:738:ALA:N	2.50	0.45
3:D:907:GLU:HG2	3:D:908:LYS:H	1.81	0.45
2:C:1044:GLY:CA	4:E:17:TYR:HE1	2.21	0.45
5:F:288:TYR:HA	5:F:291:ILE:CG2	2.46	0.45
5:F:80:PRO:O	5:F:83:GLN:HB2	2.16	0.45
5:F:94:LEU:HD12	5:F:98:GLU:OE2	2.16	0.45
1:K:158:ILE:HG23	1:K:158:ILE:HD12	1.88	0.45
1:K:55:SER:HB2	1:K:158:ILE:HG21	1.98	0.45
1:K:162:ILE:HG13	1:K:163:ASN:N	2.32	0.45
2:M:165:LEU:HA	2:M:166:PRO:O	2.15	0.45
2:M:367:LEU:O	2:M:371:LYS:HB2	2.17	0.45
2:M:49:ARG:HG2	2:M:266:ARG:HH12	1.82	0.45
2:M:914:ILE:HA	2:M:914:ILE:HD12	1.75	0.45
3:N:1203:LYS:HG2	9:N:1955:HOH:O	2.15	0.45
3:N:1264:GLU:HG2	3:N:1425:THR:H	1.81	0.45
3:N:23:TYR:O	3:N:24:GLY:O	2.35	0.45
3:N:204:LEU:O	3:N:393:ILE:HA	2.15	0.45
3:N:570:GLU:CA	5:P:214:GLN:HE22	2.29	0.45
5:P:142:ARG:NH1	5:P:150:THR:OG1	2.49	0.45
5:P:157:GLU:HG2	9:P:498:HOH:O	2.16	0.45
1:A:158:ILE:HG22	1:A:160:ASP:H	1.81	0.45
2:C:1002:GLU:HA	9:C:1756:HOH:O	2.15	0.45
2:C:271:GLU:HA	2:C:275:TYR:HD1	1.81	0.45
2:C:460:ARG:NE	2:C:485:TYR:CZ	2.84	0.45
2:C:612:VAL:HG22	2:C:622:GLU:HA	1.99	0.45
2:C:905:ILE:H	2:C:905:ILE:CD1	2.13	0.45
2:C:551:GLU:HA	2:C:906:PHE:CE2	2.51	0.45
3:D:1116:ASN:ND2	3:D:1116:ASN:N	2.63	0.45
3:D:1350:GLU:OE2	3:D:1357:ARG:NH1	2.48	0.45
3:D:421:LEU:HB3	3:D:444:VAL:HG11	1.98	0.45
3:D:667:ALA:HB2	3:D:676:MET:SD	2.56	0.45
3:D:699:VAL:H	3:D:756:GLN:NE2	2.15	0.45
3:D:710:ARG:NH2	3:D:1210:SER:HB2	2.31	0.45
3:D:814:ALA:O	3:D:818:ARG:HG3	2.17	0.45
3:D:754:PHE:HA	4:E:24:ALA:HB1	1.98	0.45
5:F:82:ARG:O	5:F:86:HIS:HB2	2.15	0.45
2:M:1044:GLY:HA3	4:O:17:TYR:HE1	1.80	0.45
2:M:19:THR:HG22	2:M:19:THR:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:51:THR:HB	2:M:348:LEU:HD23	1.98	0.45
2:M:838:LYS:HZ2	2:M:846:LYS:HE2	1.81	0.45
3:N:999:THR:O	3:N:1003:VAL:HG13	2.16	0.45
3:N:102:ILE:HD12	3:N:579:ASP:CB	2.45	0.45
3:N:1378:TYR:HA	3:N:1394:VAL:HA	1.98	0.45
3:N:157:GLU:HA	3:N:160:GLU:OE1	2.16	0.45
3:N:455:ARG:NH2	9:N:2369:HOH:O	2.49	0.45
3:N:584:ASN:HD21	3:N:590:PRO:CD	2.29	0.45
3:N:684:LYS:HD2	9:N:2165:HOH:O	2.16	0.45
4:O:16:LYS:HB2	9:O:3818:HOH:O	2.14	0.45
5:P:300:ASP:HB3	9:P:433:HOH:O	2.16	0.45
5:P:419:ARG:O	5:P:421:PHE:N	2.49	0.45
1:B:169:ALA:HB1	1:B:171:PHE:HD2	1.80	0.45
2:C:212:GLY:HA3	2:C:218:VAL:CG2	2.45	0.45
2:C:352:ALA:HA	2:C:355:VAL:CG1	2.46	0.45
2:C:110:GLU:HB2	2:C:369:PRO:HG3	1.98	0.45
2:C:64:LEU:HB2	2:C:359:MET:SD	2.56	0.45
3:D:1110:ALA:O	3:D:1111:ASP:C	2.52	0.45
3:D:1299:PHE:N	3:D:1299:PHE:CD2	2.84	0.45
3:D:9:ARG:HA	3:D:1434:TRP:CH2	2.50	0.45
3:D:1492:LEU:HA	9:D:2354:HOH:O	2.16	0.45
3:D:473:LEU:HD21	3:D:495:ARG:CZ	2.46	0.45
3:D:87:ARG:HA	3:D:523:ASP:HB2	1.98	0.45
3:D:684:LYS:HD3	3:D:686:GLU:OE1	2.17	0.45
4:E:44:GLU:HG2	9:E:142:HOH:O	2.16	0.45
2:C:114:PHE:CE2	5:F:283:GLY:HA3	2.51	0.45
5:F:336:GLU:N	9:F:562:HOH:O	2.48	0.45
5:F:371:LEU:HB2	5:F:372:ARG:NH1	2.32	0.45
5:F:392:VAL:HG11	5:F:396:ARG:CD	2.46	0.45
1:L:156:HIS:CG	1:L:157:GLY:N	2.84	0.45
1:L:165:ILE:HG13	1:L:165:ILE:O	2.16	0.45
2:M:285:LEU:HD22	9:M:1655:HOH:O	2.15	0.45
2:M:329:GLY:HA3	2:M:489:THR:HG23	1.98	0.45
2:M:418:LEU:N	2:M:418:LEU:CD1	2.80	0.45
2:M:752:GLY:H	2:M:792:VAL:HB	1.82	0.45
3:N:104:PHE:CE2	3:N:1448:THR:HG23	2.51	0.45
3:N:1369:GLU:O	3:N:1372:VAL:HG12	2.17	0.45
3:N:1505:ALA:HB1	9:N:2193:HOH:O	2.17	0.45
3:N:93:ILE:HD13	3:N:548:ILE:HD11	1.98	0.45
4:O:75:PHE:HE1	9:O:3411:HOH:O	1.98	0.45
4:O:76:GLY:HA3	4:O:79:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1060:ILE:HG22	2:C:1061:GLU:H	1.81	0.45
2:C:265:ARG:HD3	2:C:267:TYR:HB3	1.99	0.45
2:C:443:THR:HA	2:C:444:PRO:HD3	1.79	0.45
2:C:474:VAL:HA	2:C:478:VAL:O	2.17	0.45
2:C:54:ILE:HG23	2:C:54:ILE:O	2.16	0.45
2:C:565:GLN:OE1	2:C:842:ARG:HG2	2.17	0.45
3:D:1000:THR:HG23	3:D:1001:GLU:N	2.31	0.45
3:D:1047:LYS:HG2	3:D:1053:PHE:CE2	2.51	0.45
3:D:540:LEU:HD21	3:D:603:LEU:HD23	1.98	0.45
3:D:72:VAL:CG2	3:D:78:VAL:H	2.29	0.45
4:E:31:LEU:HD23	4:E:35:PHE:CE1	2.52	0.45
3:D:760:ARG:HD2	4:E:3:GLU:OE1	2.17	0.45
3:D:563:PRO:HG2	5:F:188:ILE:HG21	1.99	0.45
5:F:340:SER:O	5:F:342:VAL:N	2.50	0.45
5:F:394:ARG:NE	5:F:398:ARG:HB2	2.31	0.45
2:M:118:ILE:HD12	2:M:118:ILE:O	2.16	0.45
2:M:807:ARG:HA	2:M:821:GLU:HB2	1.99	0.45
3:N:1299:PHE:HD2	3:N:1299:PHE:N	2.15	0.45
3:N:126:VAL:CG1	3:N:132:TYR:HB2	2.47	0.45
3:N:1420:LEU:HD23	9:N:1853:HOH:O	2.15	0.45
3:N:45:PHE:HD1	3:N:86:ARG:NH2	2.15	0.45
3:N:675:ARG:HH22	5:P:421:PHE:HE2	1.63	0.45
3:N:700:VAL:HG22	3:N:718:PRO:HG3	1.98	0.45
3:N:779:ALA:HA	9:N:1773:HOH:O	2.16	0.45
3:N:796:ARG:NH1	3:N:861:GLN:HE21	2.14	0.45
3:N:939:PHE:O	3:N:943:THR:HG23	2.17	0.45
5:P:360:LYS:HG2	9:P:511:HOH:O	2.17	0.45
5:P:91:VAL:HG21	9:P:550:HOH:O	2.17	0.45
1:A:151:VAL:H	1:A:169:ALA:HB3	1.81	0.45
1:A:28:LEU:HD23	1:A:28:LEU:HA	1.75	0.45
2:C:418:LEU:CD1	2:C:418:LEU:N	2.79	0.45
2:C:598:GLU:HG3	2:C:623:TYR:OH	2.17	0.45
2:C:68:PHE:HE1	2:C:96:ALA:HB1	1.82	0.45
3:D:892:ASP:O	3:D:895:VAL:N	2.49	0.45
3:D:95:LEU:HD23	3:D:574:LEU:HD11	1.98	0.45
2:M:455:LEU:HD12	2:M:456:ALA:N	2.32	0.45
3:N:1084:THR:HG21	9:N:2214:HOH:O	2.16	0.45
3:N:409:VAL:HG12	3:N:435:VAL:HG11	1.98	0.45
3:N:28:LYS:HG3	3:N:41:ARG:CD	2.47	0.45
3:N:403:PHE:CE2	3:N:443:VAL:N	2.85	0.45
3:N:704:ARG:CG	3:N:705:ALA:H	2.27	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:728:LEU:HD12	9:N:1892:HOH:O	2.17	0.45
3:N:861:GLN:HG2	3:N:861:GLN:H	1.55	0.45
3:N:560:GLN:NE2	5:P:221:ILE:HB	2.31	0.45
5:P:351:SER:O	5:P:355:GLU:HB2	2.15	0.45
5:P:361:LEU:HD21	5:P:404:ALA:CB	2.46	0.45
1:A:58:ILE:HG21	1:A:68:ILE:CD1	2.45	0.45
1:B:61:VAL:H	1:B:137:ARG:HH22	1.65	0.45
2:C:1009:SER:CB	3:D:651:GLU:HG2	2.47	0.45
2:C:342:ASP:O	2:C:346:VAL:HG23	2.16	0.45
2:C:469:THR:OG1	2:C:470:PRO:HD2	2.16	0.45
2:C:739:GLU:CD	2:C:742:VAL:HB	2.37	0.45
2:C:837:ASP:OD1	2:C:999:HIS:NE2	2.49	0.45
2:C:876:VAL:HB	2:C:877:PRO:HD3	1.98	0.45
3:D:1108:ARG:HB2	9:D:2164:HOH:O	2.15	0.45
3:D:1173:LEU:HD23	3:D:1174:LEU:HD23	1.98	0.45
3:D:1242:HIS:NE2	3:D:1266:ARG:HD3	2.31	0.45
3:D:1285:GLU:HG2	3:D:1285:GLU:O	2.17	0.45
3:D:1487:VAL:HG13	3:D:1491:THR:HB	1.97	0.45
3:D:584:ASN:HD21	3:D:590:PRO:HB2	1.82	0.45
3:D:617:ASN:C	3:D:618:LEU:HD12	2.37	0.45
3:D:640:HIS:HE1	4:E:3:GLU:HG2	1.80	0.45
5:F:284:ARG:HB2	9:F:621:HOH:O	2.17	0.45
5:F:393:THR:HG22	5:F:394:ARG:H	1.82	0.45
2:M:1059:ASP:CG	2:M:1062:GLY:HA3	2.37	0.45
2:M:551:GLU:HB3	2:M:906:PHE:CD2	2.51	0.45
2:M:92:ALA:HB2	2:M:120:LEU:CD1	2.45	0.45
3:N:105:VAL:HG21	3:N:128:TYR:HE2	1.75	0.45
3:N:1335:LEU:O	3:N:1335:LEU:HG	2.16	0.45
3:N:1350:GLU:HG3	3:N:1350:GLU:O	2.16	0.45
3:N:16:GLU:HG3	9:N:1701:HOH:O	2.16	0.45
3:N:486:ARG:HG2	9:N:1964:HOH:O	2.15	0.45
3:N:586:ARG:HG2	9:N:2201:HOH:O	2.16	0.45
3:N:770:LEU:HB2	3:N:1210:SER:O	2.17	0.45
3:N:838:ARG:HB3	9:N:2366:HOH:O	2.17	0.45
5:P:125:ASP:HA	9:P:579:HOH:O	2.16	0.45
9:N:1980:HOH:O	5:P:210:LEU:HD12	2.17	0.45
3:N:569:ASN:ND2	5:P:210:LEU:HD22	2.29	0.45
2:C:266:ARG:HA	2:C:288:ARG:HD3	1.97	0.45
2:C:475:VAL:HG12	2:C:475:VAL:O	2.17	0.45
2:C:471:TYR:CD2	2:C:496:ILE:HG21	2.51	0.45
2:C:810:ASP:H	2:C:811:PRO:HD3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:971:LYS:HG2	9:C:1494:HOH:O	2.17	0.45
3:D:1047:LYS:HB3	3:D:1048:PRO:CD	2.46	0.45
3:D:137:PRO:HD2	3:D:453:ASP:CB	2.46	0.45
4:E:37:ASN:HA	4:E:93:TYR:CE2	2.52	0.45
5:F:361:LEU:HD13	5:F:366:ALA:HB2	1.98	0.45
2:M:1048:THR:O	2:M:1052:MET:HG2	2.17	0.45
2:M:18:LEU:HD13	2:M:590:ASP:OD2	2.16	0.45
2:M:715:THR:CG2	2:M:717:LEU:HG	2.45	0.45
2:M:694:LEU:CD1	2:M:868:ASP:HB3	2.47	0.45
3:N:1107:VAL:HA	3:N:1200:VAL:O	2.17	0.45
3:N:119:SER:CB	3:N:123:LEU:HD13	2.46	0.45
3:N:1372:VAL:HG13	3:N:1373:ARG:N	2.32	0.45
3:N:44:LEU:HB3	3:N:525:ARG:HH21	1.82	0.45
3:N:809:PRO:HB2	3:N:812:ALA:CB	2.45	0.45
3:N:896:ALA:O	3:N:900:ILE:HG23	2.17	0.45
1:A:158:ILE:HG22	1:A:159:LYS:N	2.32	0.45
1:A:64:GLU:O	1:A:64:GLU:HG2	2.14	0.45
2:C:13:ILE:HG12	2:C:534:VAL:HG13	1.98	0.45
2:C:185:LYS:NZ	2:C:190:LYS:HE2	2.32	0.45
2:C:36:PRO:HG2	2:C:70:GLU:HB3	1.97	0.45
2:C:670:GLN:HE22	2:C:699:PHE:C	2.21	0.45
2:C:841:ASN:HD21	2:C:845:ASN:N	2.15	0.45
2:C:926:PHE:HE1	2:C:929:ARG:NH1	2.15	0.45
3:D:1124:GLN:HA	3:D:1125:PRO:HD3	1.79	0.45
3:D:141:ILE:HG13	3:D:142:LEU:N	2.31	0.45
3:D:72:VAL:HG23	3:D:78:VAL:N	2.32	0.45
3:D:850:LEU:O	3:D:853:VAL:HB	2.16	0.45
4:E:46:PRO:CB	4:E:54:LEU:HD22	2.46	0.45
5:F:248:ASN:HA	5:F:251:ILE:HD12	1.98	0.45
2:M:9:ILE:HD11	2:M:537:LYS:HE2	1.98	0.45
2:M:537:LYS:HG2	2:M:537:LYS:H	1.44	0.45
2:M:854:PRO:C	2:M:856:GLU:N	2.70	0.45
2:M:987:ILE:HG22	2:M:988:VAL:O	2.17	0.45
3:N:1045:MET:HG3	3:N:1073:SER:OG	2.17	0.45
3:N:1120:VAL:HB	3:N:1144:LEU:HD21	1.99	0.45
3:N:28:LYS:HA	3:N:29:PRO:HD3	1.72	0.45
3:N:863:VAL:HG11	9:N:2345:HOH:O	2.17	0.45
5:P:132:ARG:HB3	5:P:136:LEU:HD21	1.99	0.45
1:B:55:SER:HB2	1:B:158:ILE:HD13	1.96	0.45
2:C:338:GLU:HA	2:C:341:THR:HG22	1.99	0.45
2:C:358:ARG:HD3	2:C:371:LYS:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:9:ILE:HG12	2:C:907:ASP:CG	2.38	0.45
2:C:889:HIS:HD2	2:C:970:GLY:HA3	1.81	0.45
2:C:939:ARG:HB3	2:C:982:PRO:HG3	1.98	0.45
3:D:1087:ARG:CD	3:D:1236:LEU:O	2.65	0.45
3:D:1254:GLN:HB2	9:D:1984:HOH:O	2.17	0.45
3:D:1368:ILE:HG13	3:D:1368:ILE:H	1.57	0.45
3:D:1448:THR:O	3:D:1451:ALA:HB3	2.16	0.45
3:D:31:THR:HG23	3:D:45:PHE:HE2	1.80	0.45
2:C:1109:VAL:CG1	3:D:5:VAL:HG13	2.46	0.45
3:D:637:LEU:HD12	3:D:641:GLN:HB2	1.99	0.45
3:D:76:CYS:N	9:D:1539:HOH:O	2.49	0.45
1:K:198:ARG:C	1:K:199:ILE:HD12	2.37	0.45
2:M:165:LEU:O	2:M:265:ARG:HB2	2.17	0.45
2:M:572:ILE:HD11	2:M:701:THR:HB	1.99	0.45
2:M:673:LEU:CD2	2:M:867:VAL:HG12	2.46	0.45
2:M:90:TYR:HE1	9:M:2242:HOH:O	2.00	0.45
3:N:1376:MET:HG2	3:N:1421:LEU:HD12	1.98	0.45
3:N:103:TRP:NE1	3:N:1444:THR:HG23	2.31	0.45
3:N:477:LEU:HD22	3:N:492:ALA:HB1	1.99	0.45
3:N:500:ARG:HG3	3:N:500:ARG:HH11	1.82	0.45
3:N:50:PHE:HB3	3:N:522:PRO:CG	2.46	0.45
3:N:54:LYS:O	3:N:55:ASP:O	2.34	0.45
3:N:656:PHE:HB3	3:N:694:VAL:HG11	1.98	0.45
2:C:102:HIS:CE1	2:C:365:ASP:HA	2.52	0.44
2:C:221:LEU:HD11	9:C:1633:HOH:O	2.17	0.44
2:C:410:ILE:CD1	2:C:455:LEU:HB3	2.46	0.44
2:C:750:LYS:HG3	3:D:681:ARG:NH2	2.24	0.44
3:D:1465:ASN:HA	3:D:1465:ASN:HD22	1.50	0.44
3:D:169:TYR:HA	3:D:170:PRO:HD3	1.82	0.44
3:D:514:LEU:HA	9:D:1709:HOH:O	2.15	0.44
3:D:609:GLY:O	3:D:610:LYS:O	2.35	0.44
3:D:820:GLU:HB2	3:D:836:VAL:HG11	1.99	0.44
5:F:420:ASP:O	5:F:422:LEU:HD23	2.16	0.44
2:M:1058:ASP:OD1	2:M:1084:SER:HB3	2.16	0.44
2:M:1115:LEU:HD12	2:M:1115:LEU:H	1.81	0.44
2:M:281:LEU:O	2:M:282:GLY:O	2.35	0.44
2:M:690:ILE:HG12	2:M:694:LEU:HD12	1.99	0.44
2:M:863:ASP:OD1	2:M:865:THR:HG22	2.16	0.44
3:N:486:ARG:N	9:N:1964:HOH:O	2.49	0.44
3:N:644:LEU:HD12	3:N:645:PRO:CD	2.46	0.44
3:N:860:LEU:HB2	9:N:2139:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:988:VAL:HG13	3:N:948:THR:OG1	2.17	0.44
4:O:32:ARG:HD2	9:O:4200:HOH:O	2.16	0.44
5:P:195:VAL:HG11	5:P:217:ASN:OD1	2.17	0.44
5:P:340:SER:OG	5:P:342:VAL:HG23	2.17	0.44
2:C:158:TYR:CE1	2:C:313:LEU:HG	2.52	0.44
2:C:598:GLU:O	2:C:651:LYS:HG3	2.16	0.44
3:D:1161:GLU:CG	3:D:1164:ARG:HD2	2.46	0.44
3:D:625:TYR:O	3:D:749:VAL:HG23	2.16	0.44
3:D:810:GLU:HA	3:D:813:LEU:HD23	1.98	0.44
3:D:960:LYS:HG2	3:D:964:LEU:HD12	1.99	0.44
5:F:191:ASN:OD1	5:F:194:LEU:HD13	2.17	0.44
5:F:256:ARG:HH12	5:F:311:ALA:HA	1.82	0.44
1:L:228:PRO:O	1:L:229:GLN:HG3	2.17	0.44
2:M:355:VAL:CG2	2:M:372:LEU:HG	2.48	0.44
2:M:861:LEU:HD21	2:M:925:TYR:HE2	1.81	0.44
3:N:1010:ASN:HA	9:N:1747:HOH:O	2.17	0.44
3:N:1109:GLU:HG2	3:N:1202:GLN:N	2.30	0.44
3:N:1263:PHE:O	3:N:1375:MET:HE2	2.18	0.44
3:N:169:TYR:HA	3:N:170:PRO:HD3	1.83	0.44
3:N:455:ARG:HA	9:N:2093:HOH:O	2.17	0.44
3:N:611:GLN:OE1	3:N:619:LEU:HD11	2.17	0.44
3:N:708:LEU:HD23	3:N:708:LEU:HA	1.80	0.44
3:N:72:VAL:HG23	3:N:78:VAL:N	2.30	0.44
5:P:226:LYS:HD2	5:P:242:TRP:HZ2	1.82	0.44
1:A:86:VAL:CG1	1:A:124:ASN:HB2	2.48	0.44
2:C:208:ALA:CA	2:C:221:LEU:HD21	2.48	0.44
2:C:258:TYR:HB3	9:C:1773:HOH:O	2.17	0.44
2:C:265:ARG:CG	2:C:266:ARG:N	2.80	0.44
2:C:380:ALA:O	2:C:384:GLU:HB2	2.18	0.44
2:C:402:SER:OG	2:C:566:THR:O	2.36	0.44
2:C:601:GLY:O	2:C:649:VAL:HG22	2.18	0.44
2:C:684:PHE:HD2	3:D:740:PHE:HE1	1.65	0.44
2:C:690:ILE:HG12	2:C:694:LEU:HD12	1.99	0.44
3:D:1310:ARG:HE	3:D:1327:ARG:HB3	1.80	0.44
3:D:136:ASP:CB	3:D:137:PRO:HD3	2.20	0.44
3:D:28:LYS:CG	3:D:41:ARG:HH11	2.24	0.44
2:C:1058:ASP:HB2	3:D:621:LYS:HE2	1.99	0.44
3:D:814:ALA:HB2	9:D:1889:HOH:O	2.18	0.44
3:D:560:GLN:OE1	5:F:218:GLN:HG3	2.18	0.44
5:F:94:LEU:HB2	5:F:98:GLU:CD	2.37	0.44
2:M:1021:LEU:HD13	5:P:331:ASP:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:12:VAL:HG13	2:M:13:ILE:HG23	1.98	0.44
2:M:36:PRO:HG3	2:M:71:TYR:CE2	2.53	0.44
2:M:762:LYS:C	2:M:763:GLY:O	2.53	0.44
2:M:78:PHE:HB3	2:M:79:PRO:HD2	1.99	0.44
2:M:850:ALA:HA	3:N:632:VAL:CG1	2.47	0.44
2:M:926:PHE:CE2	2:M:960:GLU:HG3	2.52	0.44
3:N:1159:ARG:CZ	3:N:1159:ARG:HB3	2.47	0.44
3:N:1207:TYR:H	3:N:1366:LYS:HZ1	1.65	0.44
3:N:1326:THR:HG22	3:N:1327:ARG:N	2.33	0.44
3:N:666:ILE:HG13	3:N:666:ILE:H	1.61	0.44
2:M:729:LEU:HD13	3:N:675:ARG:NH2	2.33	0.44
3:N:826:PRO:HD2	3:N:829:VAL:HG22	1.99	0.44
1:L:152:PRO:HG2	3:N:857:ILE:HD12	2.00	0.44
5:P:318:GLU:HG2	9:P:448:HOH:O	2.16	0.44
1:B:10:VAL:HG12	1:B:12:THR:HG23	1.98	0.44
2:C:113:VAL:O	2:C:115:LEU:HD23	2.17	0.44
2:C:529:VAL:HG21	9:C:1134:HOH:O	2.18	0.44
2:C:598:GLU:HG2	9:C:1352:HOH:O	2.18	0.44
2:C:674:VAL:HB	2:C:869:VAL:CG1	2.47	0.44
2:C:759:THR:HB	2:C:785:VAL:HG21	1.99	0.44
2:C:863:ASP:OD1	2:C:865:THR:HG22	2.16	0.44
3:D:1376:MET:HA	9:D:2082:HOH:O	2.17	0.44
3:D:1380:GLU:HB2	3:D:1420:LEU:CD2	2.47	0.44
3:D:614:PHE:CB	3:D:617:ASN:HB3	2.47	0.44
3:D:624:ASP:HB3	3:D:625:TYR:CD1	2.53	0.44
3:D:63:TYR:HB2	9:D:2023:HOH:O	2.17	0.44
3:D:85:VAL:HG11	3:D:89:ARG:CZ	2.48	0.44
4:E:40:LEU:C	4:E:42:PRO:HD2	2.37	0.44
1:K:227:ASN:HD22	1:K:227:ASN:H	1.65	0.44
1:K:229:GLN:HE21	1:K:229:GLN:HB2	1.56	0.44
1:L:45:LEU:HD11	1:L:177:VAL:CG2	2.48	0.44
1:L:45:LEU:HD21	1:L:177:VAL:HG22	1.99	0.44
2:M:211:LEU:CD1	2:M:308:ARG:HA	2.47	0.44
2:M:810:ASP:H	2:M:811:PRO:HD3	1.82	0.44
2:M:968:LEU:CB	9:M:2164:HOH:O	2.58	0.44
2:M:862:PRO:HD3	2:M:973:VAL:O	2.18	0.44
3:N:1182:GLU:HB3	9:N:2331:HOH:O	2.17	0.44
3:N:165:LYS:HE2	9:N:2305:HOH:O	2.17	0.44
3:N:420:VAL:HG13	9:N:2303:HOH:O	2.17	0.44
2:M:1030:GLN:NE2	3:N:628:ARG:HB3	2.32	0.44
4:O:45:ARG:HH21	4:O:55:PHE:HB3	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:276:ARG:HA	9:P:451:HOH:O	2.17	0.44
2:M:114:PHE:CD2	5:P:283:GLY:HA3	2.52	0.44
1:A:127:LEU:HD11	1:A:129:ILE:CD1	2.47	0.44
1:A:88:ARG:O	1:A:88:ARG:HG3	2.16	0.44
1:B:27:PRO:HB3	1:B:192:LEU:HD22	1.99	0.44
1:B:23:PHE:HE2	1:B:199:ILE:HD12	1.81	0.44
2:C:139:GLN:HG2	2:C:140:ILE:N	2.33	0.44
2:C:278:GLU:HG3	2:C:283:ILE:HG23	2.00	0.44
2:C:443:THR:CG2	2:C:449:ILE:HG13	2.48	0.44
2:C:474:VAL:HG13	2:C:529:VAL:O	2.17	0.44
3:D:28:LYS:HA	3:D:29:PRO:HD3	1.69	0.44
2:C:1043:TYR:HE1	3:D:710:ARG:O	2.00	0.44
3:D:880:ILE:O	3:D:883:ALA:HB3	2.17	0.44
5:F:351:SER:O	5:F:355:GLU:HB2	2.17	0.44
1:K:132:LEU:HD21	1:K:138:LEU:HB2	2.00	0.44
1:K:212:ASN:O	1:K:215:VAL:HG22	2.18	0.44
1:L:191:ASP:O	1:L:192:LEU:HG	2.18	0.44
2:M:227:PHE:HD2	2:M:237:ARG:CZ	2.30	0.44
2:M:247:PRO:HB2	9:M:2082:HOH:O	2.16	0.44
2:M:474:VAL:HA	2:M:478:VAL:O	2.17	0.44
3:N:1002:LYS:HA	9:N:1776:HOH:O	2.17	0.44
3:N:1217:ILE:H	3:N:1217:ILE:HG13	1.68	0.44
3:N:1326:THR:HG22	3:N:1327:ARG:H	1.81	0.44
3:N:1426:LYS:HG2	9:N:1735:HOH:O	2.18	0.44
3:N:204:LEU:HA	3:N:441:ARG:NH2	2.20	0.44
3:N:204:LEU:O	3:N:393:ILE:HG23	2.17	0.44
3:N:421:LEU:HD11	3:N:446:VAL:CG2	2.48	0.44
3:N:66:GLN:O	3:N:67:ARG:C	2.55	0.44
3:N:953:ASP:O	3:N:955:VAL:HG23	2.17	0.44
1:A:229:GLN:HB2	1:A:229:GLN:HE21	1.57	0.44
1:A:39:PRO:HG3	1:B:39:PRO:CG	2.44	0.44
1:B:59:GLU:HG3	1:B:139:ASN:HB3	2.00	0.44
2:C:217:LEU:HB2	2:C:311:PHE:CE1	2.53	0.44
2:C:48:PHE:CE1	2:C:348:LEU:HD11	2.53	0.44
3:D:1155:VAL:CG1	3:D:1177:ALA:HB1	2.47	0.44
3:D:631:ILE:O	3:D:632:VAL:HG23	2.18	0.44
3:D:660:LYS:HE3	3:D:663:GLU:CD	2.38	0.44
2:C:873:PRO:HB3	3:D:949:ILE:HG12	2.00	0.44
4:E:85:LEU:HD23	4:E:86:GLN:N	2.32	0.44
4:E:88:GLU:HB3	9:E:137:HOH:O	2.18	0.44
5:F:240:THR:O	5:F:244:ARG:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:300:ASP:CG	5:F:301:ALA:N	2.71	0.44
5:F:299:TRP:CE3	5:F:303:ARG:HD3	2.52	0.44
5:F:419:ARG:O	5:F:421:PHE:N	2.50	0.44
1:K:92:PRO:HB3	9:K:3732:HOH:O	2.17	0.44
2:M:1010:THR:HG22	2:M:1011:GLY:N	2.32	0.44
2:M:1105:LYS:HB3	9:M:1845:HOH:O	2.16	0.44
2:M:118:ILE:HA	2:M:119:PRO:HD3	1.88	0.44
2:M:264:PRO:HA	9:M:1703:HOH:O	2.17	0.44
2:M:281:LEU:HD12	2:M:305:PRO:O	2.17	0.44
2:M:319:GLY:HA2	9:M:1910:HOH:O	2.18	0.44
2:M:405:ARG:NH1	2:M:566:THR:HG21	2.32	0.44
3:N:1167:SER:O	3:N:1171:VAL:HG23	2.18	0.44
3:N:122:GLU:O	3:N:126:VAL:HG23	2.18	0.44
3:N:1247:ALA:HB3	9:N:1888:HOH:O	2.16	0.44
3:N:1412:LYS:O	3:N:1414:PRO:HD3	2.18	0.44
5:P:141:VAL:HG22	9:P:496:HOH:O	2.18	0.44
2:C:265:ARG:HG2	2:C:267:TYR:N	2.31	0.44
2:C:267:TYR:H	2:C:267:TYR:HD2	1.64	0.44
2:C:278:GLU:HA	2:C:283:ILE:HA	2.00	0.44
2:C:398:THR:O	2:C:635:THR:HG21	2.17	0.44
2:C:588:VAL:HG21	2:C:664:GLY:O	2.18	0.44
2:C:92:ALA:HB2	2:C:120:LEU:HD11	1.99	0.44
3:D:1209:LEU:C	3:D:1211:MET:N	2.71	0.44
3:D:1326:THR:HA	9:D:2026:HOH:O	2.17	0.44
3:D:52:PRO:CG	3:D:78:VAL:HG13	2.47	0.44
1:K:64:GLU:HG2	1:K:64:GLU:O	2.17	0.44
1:K:8:ALA:HB2	9:K:1466:HOH:O	2.18	0.44
2:M:1034:GLU:O	2:M:1037:VAL:HG23	2.17	0.44
2:M:207:LEU:HD22	2:M:221:LEU:HD22	1.99	0.44
2:M:340:MET:SD	2:M:344:PHE:HB2	2.58	0.44
2:M:573:ARG:HB3	2:M:670:GLN:OE1	2.17	0.44
2:M:599:GLU:HB2	9:M:1699:HOH:O	2.18	0.44
2:M:732:ALA:O	2:M:735:ARG:HG3	2.18	0.44
2:M:751:PRO:CG	2:M:796:GLU:HG2	2.48	0.44
2:M:873:PRO:HB3	3:N:949:ILE:HG12	1.99	0.44
3:N:118:LEU:O	3:N:119:SER:C	2.56	0.44
3:N:1231:GLU:HG2	3:N:1232:PRO:N	2.33	0.44
3:N:172:PRO:O	3:N:174:GLY:N	2.51	0.44
3:N:421:LEU:HB3	3:N:444:VAL:HG11	2.00	0.44
3:N:52:PRO:CB	3:N:80:VAL:HG13	2.47	0.44
3:N:643:GLY:CA	3:N:727:GLN:HB2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:699:VAL:H	3:N:756:GLN:HE21	1.59	0.44
3:N:795:VAL:HG12	3:N:796:ARG:N	2.32	0.44
3:N:799:LYS:HE2	3:N:801:GLY:HA3	2.00	0.44
4:O:33:HIS:HB3	9:O:1494:HOH:O	2.18	0.44
4:O:29:GLN:HE22	4:O:89:MET:HE1	1.83	0.44
5:P:385:GLU:O	5:P:397:ILE:HD13	2.18	0.44
1:A:106:PRO:HG3	1:A:133:GLU:O	2.17	0.44
1:A:158:ILE:C	1:A:159:LYS:HG3	2.38	0.44
1:A:33:GLY:O	1:A:195:LEU:HD22	2.18	0.44
1:A:67:THR:O	1:A:67:THR:HG23	2.17	0.44
1:B:158:ILE:HD11	1:B:166:PRO:N	2.33	0.44
2:C:1118:LYS:O	2:C:1119:ARG:OXT	2.36	0.44
2:C:146:VAL:N	9:C:1337:HOH:O	2.50	0.44
2:C:191:PHE:CZ	2:C:238:LEU:HD11	2.52	0.44
2:C:212:GLY:C	2:C:215:GLY:H	2.21	0.44
3:D:1074:SER:O	3:D:1077:ALA:HB3	2.18	0.44
3:D:1123:PHE:HB3	3:D:1132:LEU:HG	1.98	0.44
3:D:1478:SER:HG	3:D:1481:VAL:H	1.66	0.44
3:D:204:LEU:HD11	3:D:445:ARG:HH12	1.81	0.44
3:D:508:ARG:CG	3:D:509:PRO:HD2	2.36	0.44
3:D:798:GLU:HB2	3:D:828:LYS:CE	2.40	0.44
5:F:392:VAL:HG11	5:F:396:ARG:HD2	2.00	0.44
2:M:176:VAL:HB	9:M:2210:HOH:O	2.18	0.44
2:M:207:LEU:O	2:M:211:LEU:HB3	2.18	0.44
2:M:64:LEU:HB2	2:M:359:MET:SD	2.57	0.44
2:M:564:MET:SD	2:M:846:LYS:HE3	2.58	0.44
2:M:942:GLU:O	2:M:945:ARG:HB3	2.17	0.44
3:N:36:THR:O	3:N:38:LYS:N	2.51	0.44
3:N:44:LEU:O	3:N:50:PHE:CE1	2.70	0.44
3:N:528:VAL:HG12	3:N:529:GLN:N	2.33	0.44
1:L:80:LEU:HD23	3:N:867:ARG:HD2	1.99	0.44
5:P:226:LYS:HE3	9:P:445:HOH:O	2.18	0.44
5:P:205:ARG:CD	5:P:251:ILE:HG21	2.48	0.44
2:C:264:PRO:HB3	2:C:289:THR:CB	2.47	0.44
2:C:146:VAL:HG11	2:C:306:THR:HG22	1.99	0.44
2:C:545:ASN:O	2:C:581:THR:HG21	2.17	0.44
3:D:1008:PHE:HB3	9:D:1941:HOH:O	2.17	0.44
3:D:1276:GLU:OE2	3:D:1303:TYR:HE2	2.00	0.44
3:D:162:ARG:HA	3:D:449:SER:OG	2.17	0.44
3:D:569:ASN:HD21	5:F:210:LEU:HD22	1.82	0.44
3:D:554:LEU:HD23	3:D:570:GLU:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1052:MET:SD	3:D:623:VAL:HG21	2.57	0.44
3:D:937:TYR:HD2	3:D:941:PHE:HE1	1.66	0.44
5:F:151:LEU:HD23	9:F:489:HOH:O	2.17	0.44
5:F:306:GLU:HG3	9:F:582:HOH:O	2.18	0.44
1:L:101:LEU:CD1	9:L:1850:HOH:O	2.64	0.44
2:M:64:LEU:CD1	2:M:100:LEU:HD13	2.48	0.44
2:M:198:ARG:NE	2:M:228:ALA:HA	2.33	0.44
2:M:207:LEU:HD13	2:M:221:LEU:HD13	2.00	0.44
2:M:564:MET:SD	2:M:846:LYS:HG3	2.58	0.44
2:M:7:GLY:O	2:M:907:ASP:OD1	2.36	0.44
3:N:155:ASP:HA	3:N:158:TYR:HB3	2.00	0.44
3:N:195:VAL:HG12	3:N:196:VAL:N	2.32	0.44
3:N:638:LYS:C	3:N:729:HIS:HD2	2.21	0.44
3:N:987:GLU:HA	9:N:2147:HOH:O	2.18	0.44
3:N:996:TRP:HA	3:N:999:THR:CG2	2.46	0.44
4:O:57:ASP:N	4:O:58:PRO:HD3	2.32	0.44
5:P:140:ARG:HG3	5:P:141:VAL:N	2.33	0.44
5:P:396:ARG:HG2	9:P:513:HOH:O	2.18	0.44
1:A:42:ARG:HH12	1:B:34:VAL:CG1	2.28	0.43
2:C:257:VAL:HG12	2:C:263:ASP:OD1	2.17	0.43
2:C:516:ARG:N	9:C:1381:HOH:O	2.50	0.43
2:C:663:ASN:C	2:C:665:PHE:H	2.22	0.43
2:C:813:VAL:HB	9:C:1471:HOH:O	2.18	0.43
2:C:73:LEU:CD2	2:C:94:LEU:HB2	2.47	0.43
2:C:979:THR:HG23	2:C:981:GLU:HB2	2.00	0.43
2:C:874:LEU:HA	3:D:1023:MET:HE1	1.99	0.43
3:D:951:ILE:HD12	3:D:1062:ARG:HG3	1.99	0.43
3:D:1251:ASP:O	3:D:1270:ALA:HB3	2.18	0.43
3:D:1393:GLN:HG3	3:D:1398:TRP:HZ2	1.83	0.43
3:D:158:TYR:CE1	3:D:454:ALA:HB3	2.53	0.43
3:D:481:MET:CE	3:D:1389:LEU:HG	2.48	0.43
5:F:115:LYS:HD2	5:F:173:TYR:HE2	1.82	0.43
5:F:185:GLN:O	5:F:189:GLU:HG3	2.17	0.43
5:F:205:ARG:HD3	5:F:251:ILE:HG21	2.00	0.43
1:K:224:TYR:CD1	1:L:9:PRO:HD2	2.53	0.43
1:L:125:PRO:HD2	9:L:3251:HOH:O	2.18	0.43
1:L:7:LYS:HE3	9:L:1689:HOH:O	2.18	0.43
2:M:757:GLY:HA2	2:M:789:SER:CB	2.35	0.43
3:N:1025:GLN:HE21	3:N:1025:GLN:HB3	1.62	0.43
3:N:615:ARG:NH2	3:N:1089:ALA:HB2	2.23	0.43
3:N:15:PRO:HG3	9:N:2008:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:37:LEU:HD13	3:N:535:PHE:HZ	1.83	0.43
3:N:93:ILE:CD1	3:N:548:ILE:HD11	2.48	0.43
3:N:800:LYS:CE	3:N:804:LEU:HD13	2.48	0.43
4:O:67:GLU:H	4:O:67:GLU:HG3	1.68	0.43
5:P:101:GLU:O	5:P:105:LYS:HG3	2.17	0.43
5:P:403:LYS:HB2	9:P:540:HOH:O	2.17	0.43
5:P:82:ARG:O	5:P:86:HIS:HB2	2.18	0.43
1:A:218:LEU:HD23	1:B:222:LEU:HD21	1.99	0.43
2:C:1088:LEU:HG	2:C:1092:LEU:HD12	2.00	0.43
2:C:20:GLU:HB2	9:C:1289:HOH:O	2.18	0.43
2:C:191:PHE:CE2	2:C:238:LEU:HD11	2.54	0.43
2:C:292:ARG:HD2	2:C:299:LYS:CG	2.47	0.43
2:C:352:ALA:C	2:C:355:VAL:HG12	2.39	0.43
2:C:454:SER:HB3	9:C:1409:HOH:O	2.18	0.43
2:C:599:GLU:CG	2:C:600:ASP:H	2.29	0.43
2:C:720:GLU:HA	9:C:1430:HOH:O	2.18	0.43
2:C:32:ALA:HB2	2:C:73:LEU:CD1	2.47	0.43
2:C:564:MET:CE	2:C:846:LYS:HE3	2.49	0.43
2:C:958:THR:HG23	2:C:961:GLU:HB2	2.00	0.43
3:D:1147:ARG:HD2	3:D:1188:VAL:CG2	2.48	0.43
3:D:1220:ALA:O	3:D:1224:VAL:HG23	2.18	0.43
3:D:143:ASN:HD21	3:D:145:VAL:HG12	1.81	0.43
3:D:31:THR:HG22	3:D:32:ILE:HB	2.00	0.43
5:F:152:ASP:HB3	9:F:665:HOH:O	2.17	0.43
1:K:61:VAL:HG11	1:K:75:VAL:HG21	1.99	0.43
1:K:91:ASN:N	9:K:1900:HOH:O	2.51	0.43
1:L:33:GLY:O	1:L:195:LEU:HD22	2.19	0.43
1:L:77:GLU:O	1:L:77:GLU:HG3	2.15	0.43
2:M:1082:PRO:C	2:M:1084:SER:N	2.71	0.43
2:M:11:GLU:HB3	9:M:2054:HOH:O	2.18	0.43
2:M:133:ASP:OD2	2:M:133:ASP:N	2.51	0.43
2:M:610:ARG:NE	9:M:1664:HOH:O	2.49	0.43
3:N:131:LYS:HE3	3:N:568:ARG:HB3	1.99	0.43
3:N:1325:LEU:C	9:N:2368:HOH:O	2.57	0.43
3:N:761:ILE:CD1	4:O:20:THR:HA	2.49	0.43
3:N:938:GLY:O	3:N:942:SER:HB3	2.18	0.43
4:O:57:ASP:H	4:O:58:PRO:HD3	1.83	0.43
5:P:271:LEU:HD23	5:P:291:ILE:HD11	2.00	0.43
1:A:158:ILE:HD13	1:A:158:ILE:HA	1.88	0.43
2:C:1033:GLY:H	2:C:1036:GLU:HG3	1.83	0.43
2:C:208:ALA:HA	2:C:218:VAL:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:230:ARG:HG2	9:C:1514:HOH:O	2.17	0.43
2:C:345:ARG:HD2	9:C:1463:HOH:O	2.18	0.43
2:C:561:GLY:HA3	2:C:842:ARG:O	2.19	0.43
2:C:569:VAL:HG12	2:C:996:LYS:O	2.18	0.43
2:C:601:GLY:HA3	2:C:615:TYR:HA	2.01	0.43
2:C:575:GLN:C	2:C:667:ALA:HB1	2.38	0.43
2:C:670:GLN:HE22	2:C:699:PHE:HA	1.81	0.43
2:C:911:GLU:HG2	2:C:915:LYS:NZ	2.33	0.43
3:D:1047:LYS:HB3	3:D:1048:PRO:HD2	2.00	0.43
3:D:1095:THR:HG22	9:D:1551:HOH:O	2.16	0.43
3:D:1110:ALA:O	3:D:1112:CYS:N	2.50	0.43
3:D:610:LYS:HG2	7:D:1527:MXP:H15A	1.99	0.43
3:D:678:GLU:HB2	9:D:1759:HOH:O	2.18	0.43
3:D:704:ARG:HG2	3:D:705:ALA:N	2.30	0.43
3:D:848:GLU:N	9:D:1677:HOH:O	2.51	0.43
3:D:844:ALA:HB3	3:D:848:GLU:OE2	2.19	0.43
3:D:888:GLU:HB3	9:D:1740:HOH:O	2.18	0.43
5:F:93:LEU:HA	5:F:93:LEU:HD23	1.81	0.43
1:K:138:LEU:HA	9:K:2460:HOH:O	2.19	0.43
1:K:102:LYS:HA	1:K:138:LEU:O	2.18	0.43
9:K:1685:HOH:O	1:L:219:ARG:HD2	2.18	0.43
2:M:1063:ARG:O	2:M:1066:ALA:HB3	2.18	0.43
2:M:208:ALA:CA	2:M:221:LEU:HD21	2.47	0.43
2:M:278:GLU:HG3	2:M:283:ILE:HA	1.99	0.43
2:M:422:ARG:HG2	9:M:1926:HOH:O	2.18	0.43
2:M:462:ASP:O	2:M:463:GLU:C	2.57	0.43
2:M:537:LYS:HD3	2:M:905:ILE:HD11	2.01	0.43
3:N:1066:THR:O	3:N:1070:TYR:HB2	2.18	0.43
3:N:961:LYS:HE3	9:N:2153:HOH:O	2.17	0.43
9:N:2374:HOH:O	4:O:51:LEU:HD23	2.18	0.43
1:A:227:ASN:HD22	1:A:227:ASN:N	2.15	0.43
2:C:22:GLN:HE22	2:C:135:VAL:CG1	2.30	0.43
2:C:263:ASP:CB	2:C:264:PRO:HD3	2.48	0.43
2:C:313:LEU:HD13	2:C:321:GLU:HB2	1.99	0.43
2:C:413:LEU:HD12	2:C:413:LEU:N	2.24	0.43
2:C:49:ARG:HG2	2:C:266:ARG:HH12	1.83	0.43
2:C:517:ARG:HB2	9:C:1698:HOH:O	2.17	0.43
2:C:610:ARG:NE	9:C:1120:HOH:O	2.52	0.43
2:C:631:SER:HG	2:C:635:THR:H	1.66	0.43
2:C:690:ILE:HD12	2:C:833:LEU:HD21	2.01	0.43
2:C:896:PHE:CE2	2:C:925:TYR:HB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1281:VAL:HG21	3:D:1313:VAL:HG21	1.99	0.43
3:D:1304:LYS:HB3	9:D:1723:HOH:O	2.18	0.43
3:D:1354:LYS:HE2	9:D:2358:HOH:O	2.19	0.43
3:D:1395:LEU:HD23	3:D:1396:GLU:N	2.33	0.43
3:D:1426:LYS:HD2	9:D:2086:HOH:O	2.17	0.43
3:D:420:VAL:HA	9:D:2307:HOH:O	2.19	0.43
3:D:584:ASN:HD21	3:D:590:PRO:HD2	1.81	0.43
3:D:649:ALA:HB3	3:D:691:LEU:HD21	1.98	0.43
2:C:1009:SER:HB2	3:D:651:GLU:HG2	2.01	0.43
3:D:688:TRP:HA	3:D:688:TRP:CE3	2.53	0.43
3:D:84:ILE:HG13	3:D:85:VAL:N	2.34	0.43
3:D:86:ARG:HB3	3:D:523:ASP:OD2	2.18	0.43
4:E:53:GLY:C	4:E:55:PHE:N	2.70	0.43
5:F:418:LEU:N	5:F:418:LEU:HD12	2.33	0.43
1:L:115:LEU:HD12	1:L:115:LEU:O	2.18	0.43
1:L:55:SER:HB2	1:L:158:ILE:HD13	1.96	0.43
2:M:199:VAL:HG13	2:M:235:LEU:CG	2.42	0.43
2:M:65:VAL:HB	2:M:101:ILE:HB	2.00	0.43
2:M:679:PHE:O	2:M:680:ASP:C	2.56	0.43
2:M:876:VAL:HB	2:M:877:PRO:HD3	2.01	0.43
2:M:881:ASN:N	2:M:881:ASN:ND2	2.66	0.43
2:M:964:LYS:O	2:M:968:LEU:HG	2.18	0.43
3:N:1004:THR:HG21	9:N:2039:HOH:O	2.17	0.43
3:N:1031:ASN:O	3:N:1035:ILE:HG12	2.18	0.43
3:N:1147:ARG:HB3	3:N:1188:VAL:HG23	1.99	0.43
3:N:9:ARG:HA	3:N:1434:TRP:CH2	2.52	0.43
2:M:1013:TYR:OH	3:N:624:ASP:OD2	2.33	0.43
3:N:637:LEU:HD11	3:N:641:GLN:HB2	2.00	0.43
5:P:137:GLY:HA2	9:P:480:HOH:O	2.19	0.43
5:P:163:LEU:HD22	5:P:174:LEU:HB2	2.01	0.43
1:A:63:HIS:HB3	2:C:746:GLY:HA2	1.99	0.43
1:B:72:LYS:HB3	1:B:131:THR:OG1	2.19	0.43
2:C:139:GLN:N	9:C:1322:HOH:O	2.52	0.43
2:C:207:LEU:HD13	2:C:221:LEU:CD1	2.48	0.43
2:C:679:PHE:CE1	2:C:859:PRO:HD3	2.53	0.43
2:C:798:GLY:H	2:C:827:VAL:HG11	1.82	0.43
2:C:971:LYS:HB3	2:C:987:ILE:C	2.39	0.43
2:C:987:ILE:HG12	3:D:948:THR:CG2	2.48	0.43
3:D:1109:GLU:CD	3:D:1202:GLN:HB2	2.39	0.43
3:D:1186:VAL:HA	3:D:1187:PRO:HD3	1.90	0.43
3:D:1195:GLN:CG	3:D:1196:THR:N	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1197:ARG:HG3	3:D:1198:TYR:H	1.82	0.43
3:D:126:VAL:O	3:D:132:TYR:CD1	2.70	0.43
3:D:128:TYR:HB3	3:D:129:PHE:HD1	1.84	0.43
3:D:111:LYS:NZ	3:D:1449:GLU:HG2	2.34	0.43
3:D:843:PHE:CE1	3:D:864:VAL:HG11	2.47	0.43
3:D:871:LYS:O	3:D:873:LEU:HG	2.18	0.43
3:D:875:THR:HG22	3:D:879:ARG:HB2	1.99	0.43
5:F:209:PHE:O	5:F:213:ILE:HG13	2.18	0.43
1:K:123:MET:HB3	9:K:2581:HOH:O	2.17	0.43
2:M:182:VAL:HB	2:M:193:LEU:HD13	2.00	0.43
2:M:260:LEU:HG	2:M:261:ILE:HG13	2.00	0.43
2:M:437:ARG:HH22	2:M:491:GLU:HB2	1.82	0.43
2:M:687:ALA:C	2:M:688:ILE:HD12	2.38	0.43
3:N:1171:VAL:HG12	3:N:1171:VAL:O	2.18	0.43
3:N:206:ARG:HG2	9:N:2269:HOH:O	2.18	0.43
3:N:45:PHE:HB3	3:N:86:ARG:NH2	2.33	0.43
3:N:561:GLY:HA3	5:P:184:ARG:CZ	2.48	0.43
3:N:715:ALA:O	3:N:764:LEU:HD12	2.17	0.43
3:N:853:VAL:HG22	3:N:858:VAL:HG23	2.00	0.43
3:N:879:ARG:HD3	3:N:902:LEU:O	2.17	0.43
5:P:375:LEU:HB3	9:P:476:HOH:O	2.18	0.43
2:C:232:GLU:O	2:C:235:LEU:HB2	2.18	0.43
2:C:280:LYS:HB3	9:C:1547:HOH:O	2.18	0.43
2:C:396:ASP:O	2:C:402:SER:HB3	2.18	0.43
2:C:462:ASP:O	2:C:463:GLU:C	2.56	0.43
2:C:572:ILE:CG2	2:C:703:ILE:HD13	2.48	0.43
1:A:67:THR:HG21	2:C:609:ASN:HD21	1.82	0.43
2:C:64:LEU:HD11	2:C:100:LEU:HD13	2.00	0.43
2:C:78:PHE:HB2	2:C:88:LEU:HD21	2.01	0.43
3:D:1139:ASP:O	3:D:1142:ALA:HB3	2.18	0.43
3:D:1112:CYS:CB	3:D:1195:GLN:HG2	2.42	0.43
3:D:192:ALA:HB2	3:D:393:ILE:CD1	2.48	0.43
3:D:400:VAL:HG21	9:D:2433:HOH:O	2.19	0.43
3:D:417:PRO:HD2	3:D:432:TYR:CE1	2.54	0.43
3:D:614:PHE:O	3:D:615:ARG:O	2.36	0.43
3:D:633:VAL:C	3:D:635:PRO:HD3	2.39	0.43
5:F:196:VAL:HG13	5:F:213:ILE:CD1	2.48	0.43
5:F:226:LYS:HB2	5:F:238:TYR:OH	2.19	0.43
5:F:271:LEU:HD23	5:F:291:ILE:HD11	2.00	0.43
5:F:338:LEU:HA	5:F:339:PRO:HD3	1.85	0.43
5:F:412:GLU:OE1	5:F:418:LEU:HD13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:415:THR:HG22	5:F:417:LYS:HG3	2.00	0.43
5:F:79:ASP:CG	5:F:80:PRO:HD3	2.39	0.43
1:L:107:LYS:HG3	1:L:108:GLU:N	2.34	0.43
1:L:44:LEU:CD2	1:L:199:ILE:HD13	2.48	0.43
2:M:244:PRO:CD	2:M:245:GLY:H	2.31	0.43
2:M:288:ARG:HB3	9:M:1852:HOH:O	2.17	0.43
2:M:816:LYS:O	2:M:819:VAL:HB	2.18	0.43
2:M:897:LEU:HD23	2:M:899:GLN:NE2	2.33	0.43
2:M:969:GLN:HE21	2:M:969:GLN:HB3	1.71	0.43
3:N:1285:GLU:O	3:N:1285:GLU:HG2	2.19	0.43
3:N:1393:GLN:HB2	3:N:1398:TRP:CE2	2.53	0.43
3:N:403:PHE:CZ	3:N:407:VAL:HG23	2.53	0.43
3:N:611:GLN:NE2	7:N:1527:MXR:C16	2.80	0.43
4:O:53:GLY:C	4:O:55:PHE:H	2.22	0.43
5:P:215:GLU:OE2	5:P:254:GLN:NE2	2.49	0.43
2:C:511:GLU:HG3	9:C:1690:HOH:O	2.17	0.43
2:C:762:LYS:HB2	2:C:786:LYS:HD2	2.01	0.43
3:D:1036:ARG:HH21	3:D:1042:ARG:HA	1.84	0.43
3:D:1065:LEU:CD1	3:D:1069:GLU:HB2	2.48	0.43
3:D:1119:SER:HA	3:D:1186:VAL:O	2.19	0.43
3:D:1115:THR:HG21	3:D:1151:ARG:HH21	1.83	0.43
3:D:724:GLN:N	9:D:1680:HOH:O	2.46	0.43
3:D:799:LYS:O	3:D:829:VAL:HG13	2.19	0.43
4:E:39:VAL:HG21	4:E:72:ARG:HD2	2.00	0.43
5:F:225:GLU:HG3	5:F:226:LYS:N	2.32	0.43
5:F:348:SER:OG	5:F:349:LEU:N	2.51	0.43
1:L:86:VAL:HG12	1:L:124:ASN:HB2	2.00	0.43
1:L:57:TYR:HB3	1:L:141:GLU:HG3	2.01	0.43
2:M:17:PRO:O	2:M:20:GLU:HB2	2.18	0.43
2:M:232:GLU:O	2:M:235:LEU:HB2	2.18	0.43
2:M:495:THR:HB	2:M:530:GLU:HG3	2.00	0.43
2:M:532:MET:HG3	2:M:533:ASP:N	2.33	0.43
2:M:551:GLU:HB3	2:M:906:PHE:HD2	1.84	0.43
2:M:601:GLY:O	2:M:649:VAL:HG22	2.18	0.43
3:N:1035:ILE:CA	3:N:1038:LEU:HD12	2.49	0.43
3:N:1281:VAL:HG21	3:N:1313:VAL:HG22	2.00	0.43
3:N:448:GLU:HG3	9:N:1563:HOH:O	2.17	0.43
3:N:44:LEU:O	3:N:525:ARG:NH2	2.51	0.43
3:N:133:ILE:HG23	3:N:456:MET:SD	2.58	0.43
3:N:47:GLU:HG2	3:N:53:ILE:HG22	2.00	0.43
2:M:1044:GLY:HA3	4:O:17:TYR:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:94:LEU:HB3	9:P:503:HOH:O	2.18	0.43
1:B:4:SER:HA	1:B:7:LYS:HG2	2.00	0.43
2:C:175:GLU:HB3	2:C:183:SER:OG	2.18	0.43
2:C:174:LEU:HB2	2:C:310:LEU:HD22	2.01	0.43
2:C:419:THR:N	9:C:1152:HOH:O	2.50	0.43
2:C:937:ASP:OD2	2:C:939:ARG:HD2	2.18	0.43
3:D:1082:ALA:O	3:D:1086:LEU:HG	2.18	0.43
3:D:1107:VAL:HA	3:D:1200:VAL:O	2.19	0.43
3:D:1154:GLU:HG2	9:D:2105:HOH:O	2.19	0.43
3:D:1166:LEU:HD23	3:D:1166:LEU:H	1.84	0.43
3:D:1495:ILE:HA	4:E:88:GLU:OE2	2.19	0.43
3:D:644:LEU:HD12	3:D:645:PRO:CD	2.48	0.43
3:D:806:PHE:CD1	3:D:813:LEU:HB3	2.53	0.43
4:E:19:LEU:O	4:E:23:VAL:HG23	2.19	0.43
4:E:54:LEU:HG	4:E:58:PRO:CB	2.49	0.43
1:K:161:ARG:HG2	9:K:1051:HOH:O	2.18	0.43
1:K:176:ARG:HA	9:K:2558:HOH:O	2.18	0.43
1:L:42:ARG:HH11	1:L:42:ARG:HG2	1.83	0.43
2:M:1033:GLY:HA3	9:N:1659:HOH:O	2.18	0.43
2:M:32:ALA:HB2	2:M:73:LEU:HD11	2.00	0.43
3:N:1031:ASN:O	3:N:1034:GLN:HB2	2.19	0.43
3:N:1209:LEU:C	3:N:1211:MET:N	2.72	0.43
3:N:1352:ILE:CG2	3:N:1368:ILE:HD13	2.49	0.43
3:N:489:ARG:HG3	3:N:1388:ARG:NH2	2.27	0.43
3:N:554:LEU:HD23	3:N:570:GLU:HG2	2.01	0.43
1:L:176:ARG:HD3	3:N:884:ARG:CZ	2.48	0.43
5:P:356:LYS:O	5:P:360:LYS:HG3	2.19	0.43
1:B:44:LEU:HD11	1:B:199:ILE:HD11	2.00	0.43
2:C:1034:GLU:O	2:C:1037:VAL:N	2.52	0.43
2:C:1070:ILE:HG23	3:D:656:PHE:CE2	2.53	0.43
2:C:118:ILE:HG22	2:C:382:ILE:HD13	2.00	0.43
2:C:144:PRO:CG	2:C:165:LEU:HB3	2.48	0.43
2:C:455:LEU:HD12	2:C:456:ALA:N	2.34	0.43
2:C:487:THR:HG22	2:C:488:ALA:N	2.34	0.43
2:C:458:TYR:HB2	2:C:538:GLN:HB2	2.01	0.43
2:C:832:LYS:HG2	9:C:1178:HOH:O	2.17	0.43
3:D:1041:LEU:HD12	3:D:1058:ARG:CA	2.48	0.43
3:D:1147:ARG:NH1	3:D:1190:SER:HB2	2.34	0.43
7:D:1527:MXP:H15	7:D:1527:MXP:H9	1.89	0.43
3:D:185:VAL:HG22	3:D:203:ALA:HB2	2.00	0.43
3:D:116:LEU:CD1	3:D:465:LEU:HG	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:829:VAL:O	3:D:831:GLY:N	2.52	0.43
5:F:361:LEU:HG	5:F:408:LEU:HD21	2.01	0.43
1:K:101:LEU:HG	1:K:113:ASP:C	2.40	0.43
1:K:161:ARG:HH11	1:K:161:ARG:HB2	1.84	0.43
1:L:81:ASN:ND2	1:L:128:HIS:O	2.52	0.43
2:M:209:ARG:HB2	9:M:2284:HOH:O	2.19	0.43
2:M:309:TYR:HA	2:M:312:ALA:HB3	2.00	0.43
2:M:342:ASP:O	2:M:346:VAL:HG23	2.18	0.43
2:M:350:ARG:HG2	9:M:1970:HOH:O	2.18	0.43
2:M:432:ARG:HD2	9:M:1743:HOH:O	2.19	0.43
2:M:520:GLU:HA	2:M:521:PRO:HD3	1.84	0.43
2:M:457:ALA:HB3	2:M:538:GLN:HA	2.00	0.43
2:M:540:PHE:CE1	2:M:906:PHE:HE1	2.36	0.43
2:M:620:LEU:HD12	2:M:620:LEU:O	2.19	0.43
2:M:640:ARG:HA	2:M:641:PRO:HD3	1.93	0.43
2:M:836:GLY:HA2	3:N:725:SER:OG	2.19	0.43
2:M:837:ASP:OD1	2:M:999:HIS:NE2	2.51	0.43
3:N:1243:THR:CB	3:N:1253:THR:HB	2.49	0.43
3:N:126:VAL:HG11	3:N:152:LEU:CD1	2.49	0.43
3:N:131:LYS:HD2	5:P:83:GLN:CD	2.39	0.43
3:N:1467:ILE:HG13	3:N:1467:ILE:H	1.58	0.43
3:N:191:LEU:HD23	3:N:191:LEU:HA	1.75	0.43
3:N:565:ILE:CD1	5:P:84:TYR:HB3	2.49	0.43
4:O:41:GLU:HB2	4:O:45:ARG:NH1	2.34	0.43
1:A:220:GLU:HG2	9:A:339:HOH:O	2.18	0.43
1:A:95:GLN:HA	9:A:395:HOH:O	2.17	0.43
2:C:144:PRO:HA	2:C:163:ILE:HG13	2.01	0.43
2:C:267:TYR:N	2:C:267:TYR:HD2	2.16	0.43
2:C:313:LEU:HD13	2:C:321:GLU:O	2.19	0.43
2:C:317:VAL:HG12	2:C:317:VAL:O	2.19	0.43
2:C:464:LEU:HD12	2:C:465:GLY:H	1.83	0.43
3:D:1045:MET:HG3	3:D:1073:SER:CA	2.46	0.43
3:D:1292:VAL:HB	9:D:2010:HOH:O	2.19	0.43
3:D:145:VAL:HG22	3:D:146:PRO:HD2	2.01	0.43
3:D:1491:THR:HG22	3:D:1495:ILE:HD13	2.01	0.43
3:D:478:LEU:HD21	3:D:500:ARG:HH22	1.83	0.43
3:D:522:PRO:N	9:D:1713:HOH:O	2.51	0.43
3:D:583:ASP:C	3:D:583:ASP:OD1	2.57	0.43
3:D:809:PRO:O	3:D:812:ALA:HB3	2.19	0.43
5:F:172:ARG:HG3	9:F:453:HOH:O	2.19	0.43
5:F:201:LYS:HE2	9:F:724:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:32:ILE:HG22	5:F:258:ILE:CD1	2.47	0.43
1:K:106:PRO:HG3	1:K:133:GLU:O	2.19	0.43
1:K:158:ILE:O	1:K:159:LYS:HG3	2.19	0.43
1:K:70:GLY:H	2:M:607:ASP:CG	2.19	0.43
1:K:78:ILE:HG13	1:K:78:ILE:H	1.65	0.43
2:M:193:LEU:HD21	9:M:1951:HOH:O	2.18	0.43
2:M:405:ARG:HH11	2:M:566:THR:HG21	1.84	0.43
2:M:495:THR:H	2:M:530:GLU:CD	2.22	0.43
2:M:82:GLU:HG2	2:M:86:LYS:HD2	2.00	0.43
2:M:905:ILE:HD11	9:M:1895:HOH:O	2.19	0.43
3:N:1383:ASP:HB2	3:N:1416:ALA:CB	2.37	0.43
3:N:519:VAL:HG13	3:N:544:TYR:CE1	2.54	0.43
4:O:91:ARG:CZ	9:O:1090:HOH:O	2.67	0.43
1:B:60:ASP:N	1:B:137:ARG:NH2	2.65	0.42
1:B:208:LEU:HD12	1:B:212:ASN:OD1	2.19	0.42
2:C:1082:PRO:C	2:C:1084:SER:N	2.71	0.42
2:C:1085:PHE:CD2	3:D:1468:LEU:HA	2.54	0.42
2:C:1091:GLU:O	2:C:1094:ALA:HB3	2.19	0.42
2:C:203:ASP:OD1	2:C:206:THR:HG22	2.19	0.42
2:C:212:GLY:O	2:C:215:GLY:O	2.37	0.42
2:C:271:GLU:HG2	2:C:275:TYR:HE1	1.84	0.42
2:C:286:SER:C	2:C:287:GLY:O	2.56	0.42
2:C:355:VAL:CG2	2:C:372:LEU:HG	2.49	0.42
2:C:431:HIS:HD2	2:C:433:THR:H	1.61	0.42
2:C:408:ARG:NH2	2:C:542:VAL:HG22	2.33	0.42
2:C:585:GLU:HB2	9:C:1331:HOH:O	2.18	0.42
3:D:1109:GLU:HG2	3:D:1201:CYS:CA	2.47	0.42
3:D:1155:VAL:HG11	3:D:1177:ALA:CB	2.49	0.42
3:D:1242:HIS:HE1	3:D:1266:ARG:HB3	1.84	0.42
3:D:732:VAL:HG12	9:D:1673:HOH:O	2.19	0.42
1:K:128:HIS:CE1	1:K:131:THR:HG23	2.54	0.42
1:K:206:THR:HG22	1:K:209:GLU:CB	2.48	0.42
1:L:13:VAL:HG13	1:L:23:PHE:CD1	2.54	0.42
2:M:16:PRO:HB3	2:M:460:ARG:NH1	2.34	0.42
2:M:622:GLU:O	2:M:624:PRO:HD3	2.18	0.42
2:M:874:LEU:HD23	3:N:1023:MET:HE3	2.00	0.42
2:M:98:LEU:HB2	9:M:1972:HOH:O	2.17	0.42
3:N:1023:MET:HG2	3:N:1023:MET:H	1.46	0.42
3:N:1124:GLN:HA	3:N:1125:PRO:HD3	1.72	0.42
3:N:1114:THR:HG22	3:N:1195:GLN:HB3	1.99	0.42
3:N:18:ILE:HG23	3:N:518:PRO:CG	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:393:ILE:HG13	9:N:1934:HOH:O	2.19	0.42
3:N:661:MET:CE	3:N:673:ALA:HB1	2.49	0.42
3:N:679:ARG:HB2	3:N:682:ASP:CG	2.39	0.42
4:O:41:GLU:CA	4:O:45:ARG:HD3	2.40	0.42
3:N:573:MET:CE	5:P:210:LEU:HB3	2.48	0.42
2:M:1013:TYR:O	5:P:334:PRO:HA	2.19	0.42
1:B:51:THR:HA	1:B:145:ASP:O	2.20	0.42
1:B:91:ASN:O	1:B:94:LEU:HD12	2.18	0.42
2:C:1048:THR:O	2:C:1052:MET:HG2	2.19	0.42
2:C:1103:ASP:HB2	9:C:1226:HOH:O	2.19	0.42
2:C:311:PHE:HB3	9:C:1209:HOH:O	2.18	0.42
1:A:67:THR:OG1	2:C:609:ASN:ND2	2.52	0.42
3:D:1129:THR:HG23	3:D:1130:ARG:H	1.83	0.42
3:D:12:LEU:HD11	3:D:512:MET:HG2	2.01	0.42
3:D:660:LYS:HE2	9:D:1780:HOH:O	2.19	0.42
3:D:853:VAL:HG22	3:D:858:VAL:HG23	2.01	0.42
3:D:795:VAL:CG1	3:D:863:VAL:HG13	2.45	0.42
3:D:996:TRP:O	3:D:999:THR:HG22	2.19	0.42
3:D:560:GLN:HG2	5:F:221:ILE:HG21	2.01	0.42
2:M:446:GLY:O	2:M:447:ALA:C	2.57	0.42
2:M:443:THR:CG2	2:M:450:GLY:H	2.33	0.42
2:M:52:PHE:HB3	2:M:53:PRO:HD3	2.00	0.42
2:M:724:ARG:HD2	2:M:740:GLU:HG2	2.02	0.42
2:M:722:ILE:HG13	2:M:757:GLY:O	2.19	0.42
2:M:943:VAL:HG11	2:M:973:VAL:HG13	2.01	0.42
2:M:952:LEU:CD1	2:M:969:GLN:HE22	2.23	0.42
3:N:1274:ILE:H	3:N:1274:ILE:HD12	1.82	0.42
3:N:1394:VAL:HB	3:N:1397:LYS:HD2	2.02	0.42
3:N:168:THR:HA	3:N:394:LEU:HA	2.02	0.42
3:N:455:ARG:HH11	3:N:463:GLN:HG3	1.84	0.42
3:N:633:VAL:HG13	3:N:633:VAL:O	2.18	0.42
4:O:85:LEU:HD23	4:O:86:GLN:N	2.34	0.42
5:P:172:ARG:NH1	9:P:483:HOH:O	2.50	0.42
5:P:217:ASN:O	5:P:221:ILE:HG13	2.20	0.42
5:P:309:LYS:O	5:P:312:GLN:HB2	2.19	0.42
5:P:321:ILE:HD11	5:P:329:TYR:HB2	2.00	0.42
1:A:101:LEU:HD23	1:A:102:LYS:N	2.34	0.42
1:A:206:THR:HG23	1:A:209:GLU:H	1.84	0.42
2:C:1084:SER:O	2:C:1087:VAL:HG12	2.19	0.42
2:C:144:PRO:HG2	2:C:165:LEU:HB3	2.01	0.42
2:C:267:TYR:N	2:C:267:TYR:CD2	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:370:ALA:HB1	9:C:1667:HOH:O	2.18	0.42
2:C:52:PHE:HB3	2:C:53:PRO:HD3	1.99	0.42
2:C:560:MET:O	2:C:564:MET:HE3	2.19	0.42
2:C:627:ARG:HG2	9:C:1753:HOH:O	2.19	0.42
2:C:674:VAL:HG11	2:C:992:MET:HB3	2.02	0.42
2:C:78:PHE:HB3	2:C:79:PRO:HD2	2.00	0.42
2:C:707:ARG:NH2	2:C:824:ARG:CZ	2.82	0.42
2:C:946:ARG:HD2	2:C:984:GLU:HB3	1.99	0.42
3:D:1107:VAL:HG12	3:D:1217:ILE:HA	2.01	0.42
3:D:1428:ALA:O	3:D:1431:THR:CG2	2.66	0.42
3:D:153:LEU:HD12	3:D:154:THR:N	2.34	0.42
3:D:15:PRO:HA	3:D:18:ILE:HG12	2.00	0.42
3:D:754:PHE:CG	4:E:24:ALA:HB1	2.55	0.42
3:D:795:VAL:HA	3:D:861:GLN:O	2.19	0.42
3:D:729:HIS:CE1	3:D:935:LYS:HD3	2.54	0.42
3:D:98:PRO:HG3	3:D:515:GLU:HB3	2.01	0.42
5:F:271:LEU:HD22	5:F:304:VAL:HG13	1.99	0.42
1:K:16:GLN:HA	9:K:3198:HOH:O	2.18	0.42
2:M:129:ILE:HG22	2:M:130:ASN:ND2	2.33	0.42
2:M:161:SER:HB3	9:M:2298:HOH:O	2.19	0.42
2:M:173:ASP:O	2:M:184:MET:HA	2.19	0.42
2:M:232:GLU:HG3	2:M:235:LEU:CD1	2.49	0.42
2:M:300:ASP:HA	9:M:1862:HOH:O	2.19	0.42
2:M:412:ALA:HB1	2:M:419:THR:HG23	2.00	0.42
2:M:514:VAL:HG23	9:M:1623:HOH:O	2.18	0.42
2:M:627:ARG:HG3	2:M:628:PHE:N	2.33	0.42
2:M:808:ARG:HA	2:M:815:LEU:HD22	2.00	0.42
2:M:564:MET:CE	2:M:846:LYS:HE3	2.50	0.42
2:M:897:LEU:HD23	9:M:1930:HOH:O	2.19	0.42
2:M:674:VAL:HG11	2:M:992:MET:HB3	2.01	0.42
3:N:1167:SER:HB3	9:N:1789:HOH:O	2.19	0.42
3:N:1182:GLU:CG	9:N:1552:HOH:O	2.66	0.42
3:N:1462:LEU:HD22	3:N:1472:ILE:CG2	2.47	0.42
3:N:399:ARG:NE	9:N:2195:HOH:O	2.52	0.42
3:N:1216:SER:HB3	4:O:16:LYS:H	1.84	0.42
5:P:247:ILE:O	5:P:251:ILE:HG13	2.20	0.42
1:B:99:LEU:HD21	1:B:122:ILE:HD11	2.00	0.42
1:B:24:VAL:HG13	1:B:196:THR:HB	2.01	0.42
2:C:260:LEU:CB	2:C:291:ALA:HB1	2.45	0.42
2:C:549:PHE:HB3	2:C:552:HIS:CD2	2.49	0.42
2:C:840:ALA:HB2	2:C:846:LYS:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:897:LEU:HB3	2:C:899:GLN:NE2	2.33	0.42
3:D:1019:PRO:O	3:D:1023:MET:HG2	2.19	0.42
3:D:1047:LYS:HA	3:D:1053:PHE:CE1	2.54	0.42
3:D:1129:THR:HA	9:D:1695:HOH:O	2.18	0.42
3:D:1144:LEU:HA	3:D:1147:ARG:HG3	2.01	0.42
3:D:1108:ARG:NH2	3:D:1198:TYR:HB2	2.34	0.42
3:D:1382:THR:HG21	3:D:1418:LYS:CE	2.50	0.42
3:D:133:ILE:HG23	3:D:456:MET:SD	2.60	0.42
3:D:568:ARG:HG3	3:D:572:ARG:HE	1.85	0.42
3:D:820:GLU:HB3	3:D:836:VAL:HG21	2.02	0.42
4:E:85:LEU:HD23	4:E:85:LEU:C	2.39	0.42
5:F:363:GLU:CA	5:F:367:MET:HG3	2.49	0.42
1:K:158:ILE:C	1:K:159:LYS:HG3	2.40	0.42
2:M:165:LEU:HD12	2:M:166:PRO:C	2.40	0.42
2:M:612:VAL:HG22	2:M:622:GLU:CB	2.48	0.42
2:M:684:PHE:HD2	3:N:740:PHE:HE1	1.67	0.42
2:M:850:ALA:HA	3:N:632:VAL:HG11	2.01	0.42
3:N:9:ARG:HA	3:N:1434:TRP:HH2	1.83	0.42
3:N:111:LYS:NZ	3:N:1452:ILE:HG21	2.34	0.42
3:N:139:GLY:O	3:N:147:VAL:HB	2.20	0.42
3:N:434:ARG:H	3:N:447:VAL:HG23	1.84	0.42
3:N:799:LYS:CB	3:N:826:PRO:HG2	2.48	0.42
3:N:834:THR:HA	3:N:838:ARG:HD2	2.01	0.42
3:N:892:ASP:O	3:N:895:VAL:N	2.51	0.42
5:P:286:PRO:HD3	9:P:477:HOH:O	2.19	0.42
1:A:55:SER:HB2	1:A:158:ILE:HG13	2.01	0.42
1:B:133:GLU:O	1:B:134:GLU:HG2	2.19	0.42
1:B:58:ILE:CG2	1:B:137:ARG:NH2	2.80	0.42
1:B:90:LEU:HG	1:B:90:LEU:O	2.19	0.42
2:C:1016:ILE:HG23	3:D:526:PRO:HG2	2.01	0.42
2:C:1033:GLY:O	2:C:1037:VAL:HG23	2.18	0.42
2:C:1109:VAL:HA	3:D:3:LYS:HE3	2.00	0.42
2:C:91:GLN:HA	2:C:119:PRO:HA	2.01	0.42
2:C:173:ASP:O	2:C:184:MET:HA	2.20	0.42
2:C:263:ASP:HB2	2:C:264:PRO:CD	2.48	0.42
2:C:679:PHE:O	2:C:680:ASP:C	2.57	0.42
2:C:724:ARG:HA	2:C:737:LEU:CD2	2.49	0.42
2:C:833:LEU:HD12	2:C:834:GLN:N	2.34	0.42
2:C:889:HIS:CD2	9:C:1474:HOH:O	2.72	0.42
2:C:950:LEU:HB3	2:C:952:LEU:HD23	2.01	0.42
3:D:1023:MET:HG2	3:D:1023:MET:H	1.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1311:LEU:HB3	9:D:1836:HOH:O	2.20	0.42
3:D:1314:LYS:HA	9:D:1812:HOH:O	2.19	0.42
3:D:1407:LEU:HD11	9:D:2177:HOH:O	2.19	0.42
3:D:671:LYS:N	9:D:1660:HOH:O	2.38	0.42
3:D:796:ARG:NH1	3:D:861:GLN:HE21	2.17	0.42
5:F:111:GLU:O	5:F:115:LYS:HG3	2.20	0.42
5:F:260:ILE:HD12	9:F:458:HOH:O	2.19	0.42
2:C:769:PRO:HB3	5:F:373:LYS:O	2.19	0.42
1:L:63:HIS:HB3	9:L:3750:HOH:O	2.20	0.42
1:L:63:HIS:HD2	9:L:3508:HOH:O	2.03	0.42
2:M:212:GLY:C	2:M:215:GLY:H	2.22	0.42
2:M:286:SER:C	2:M:287:GLY:O	2.57	0.42
2:M:742:VAL:HG12	2:M:743:VAL:H	1.85	0.42
2:M:814:GLU:HB2	9:M:1921:HOH:O	2.18	0.42
3:N:1223:ILE:N	3:N:1223:ILE:HD12	2.27	0.42
3:N:152:LEU:CD2	3:N:152:LEU:H	2.24	0.42
3:N:407:VAL:HG22	3:N:422:ALA:CB	2.50	0.42
3:N:829:VAL:H	3:N:835:SER:CB	2.32	0.42
5:P:200:LYS:HD3	9:P:559:HOH:O	2.20	0.42
5:P:416:ARG:HB2	9:P:461:HOH:O	2.18	0.42
1:A:86:VAL:HG13	1:A:124:ASN:HB2	2.01	0.42
2:C:1118:LYS:H	2:C:1118:LYS:HG3	1.77	0.42
2:C:176:VAL:O	2:C:176:VAL:HG23	2.20	0.42
2:C:253:ALA:O	2:C:256:TYR:HB2	2.19	0.42
2:C:115:LEU:HA	2:C:375:SER:HB3	2.01	0.42
2:C:878:SER:OG	3:D:1029:ARG:HD3	2.20	0.42
2:C:953:VAL:HG13	2:C:966:LEU:HD13	2.01	0.42
2:C:971:LYS:HB3	2:C:988:VAL:N	2.35	0.42
3:D:118:LEU:O	3:D:119:SER:C	2.58	0.42
3:D:1231:GLU:CB	3:D:1232:PRO:HD3	2.49	0.42
3:D:1481:VAL:HG13	4:E:18:ARG:HE	1.84	0.42
3:D:1503:VAL:HB	9:D:2384:HOH:O	2.18	0.42
3:D:38:LYS:N	9:D:1967:HOH:O	2.44	0.42
2:C:1090:LYS:HD2	3:D:90:MET:CE	2.50	0.42
5:F:358:LEU:HD22	5:F:370:LYS:HE3	2.02	0.42
1:K:106:PRO:HG3	1:K:134:GLU:HG2	2.01	0.42
1:K:184:THR:HG23	1:K:192:LEU:CD1	2.49	0.42
1:K:227:ASN:N	1:K:227:ASN:HD22	2.16	0.42
1:L:48:ILE:HD13	1:L:210:ALA:HB1	2.02	0.42
1:L:89:PHE:HE2	1:L:146:ARG:HB3	1.83	0.42
2:M:263:ASP:C	2:M:264:PRO:O	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:670:GLN:HE22	2:M:699:PHE:HA	1.84	0.42
2:M:630:ARG:HB2	2:M:705:ILE:HG21	2.02	0.42
2:M:798:GLY:H	2:M:827:VAL:HG11	1.83	0.42
3:N:1290:LEU:HD23	3:N:1291:SER:H	1.82	0.42
3:N:1425:THR:HG23	3:N:1426:LYS:N	2.35	0.42
3:N:23:TYR:O	3:N:49:ILE:HG23	2.20	0.42
3:N:500:ARG:HG3	3:N:500:ARG:NH1	2.35	0.42
3:N:610:LYS:CD	7:N:1527:MXP:H15B	2.31	0.42
4:O:35:PHE:HZ	4:O:60:ALA:HA	1.85	0.42
4:O:54:LEU:HD11	9:O:1151:HOH:O	2.20	0.42
1:B:173:PRO:HB3	1:B:204:SER:HB3	2.02	0.42
1:B:89:PHE:HE2	1:B:146:ARG:HB3	1.84	0.42
2:C:1100:GLN:HB2	2:C:1100:GLN:HE21	1.60	0.42
2:C:264:PRO:HB3	2:C:289:THR:CG2	2.49	0.42
2:C:265:ARG:HB3	2:C:267:TYR:CE2	2.55	0.42
2:C:136:ILE:CG2	2:C:336:VAL:HG22	2.49	0.42
2:C:411:SER:HA	2:C:452:ILE:HA	2.00	0.42
2:C:446:GLY:O	2:C:447:ALA:C	2.58	0.42
2:C:479:VAL:HG21	2:C:503:LEU:CD1	2.50	0.42
2:C:710:ILE:HB	2:C:790:LEU:HD13	2.00	0.42
3:D:131:LYS:HG3	3:D:572:ARG:NH2	2.34	0.42
3:D:1382:THR:CG2	3:D:1418:LYS:HE3	2.49	0.42
3:D:185:VAL:HG21	3:D:191:LEU:HD11	2.01	0.42
3:D:462:GLN:HB2	3:D:513:ILE:HG21	2.02	0.42
5:F:152:ASP:O	5:F:156:VAL:HB	2.19	0.42
5:F:249:ARG:HD2	9:F:655:HOH:O	2.19	0.42
1:L:54:THR:O	1:L:54:THR:HG22	2.20	0.42
2:M:1003:ASP:O	2:M:1005:MET:N	2.53	0.42
2:M:146:VAL:HG22	2:M:162:ILE:HG23	2.01	0.42
2:M:254:VAL:HA	2:M:257:VAL:HG23	2.01	0.42
2:M:265:ARG:CG	2:M:266:ARG:N	2.82	0.42
2:M:352:ALA:CA	2:M:355:VAL:HG12	2.48	0.42
2:M:62:GLY:HA2	2:M:359:MET:HE1	2.01	0.42
2:M:599:GLU:CG	2:M:600:ASP:N	2.82	0.42
2:M:916:GLU:O	2:M:919:ALA:HB3	2.19	0.42
3:N:1119:SER:HA	3:N:1186:VAL:O	2.20	0.42
3:N:1242:HIS:CE1	3:N:1266:ARG:HB3	2.54	0.42
3:N:1272:ALA:CB	3:N:1326:THR:HB	2.50	0.42
3:N:1373:ARG:HD3	9:N:1685:HOH:O	2.18	0.42
3:N:1466:VAL:CG2	3:N:1472:ILE:HD11	2.39	0.42
3:N:497:GLU:HB2	9:N:1731:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:670:VAL:O	3:N:674:ARG:HG3	2.19	0.42
5:P:114:LYS:HD2	9:P:618:HOH:O	2.20	0.42
1:A:101:LEU:HD12	1:A:114:PHE:CE1	2.55	0.42
1:A:156:HIS:CD2	1:A:157:GLY:H	2.38	0.42
1:B:28:LEU:HA	9:B:395:HOH:O	2.19	0.42
1:B:86:VAL:HG12	1:B:124:ASN:HB2	2.00	0.42
2:C:1081:VAL:HA	2:C:1082:PRO:HD3	1.86	0.42
2:C:1109:VAL:HG11	3:D:5:VAL:HG22	2.01	0.42
2:C:1115:LEU:HD12	2:C:1115:LEU:H	1.83	0.42
2:C:715:THR:HG22	2:C:717:LEU:H	1.85	0.42
2:C:671:ASN:ND2	2:C:993:PHE:HD2	2.16	0.42
3:D:1495:ILE:O	3:D:1498:ALA:HB3	2.20	0.42
3:D:168:THR:HA	3:D:394:LEU:HA	2.02	0.42
3:D:403:PHE:CE2	3:D:443:VAL:N	2.88	0.42
3:D:481:MET:HE3	3:D:1389:LEU:HG	2.00	0.42
3:D:55:ASP:O	3:D:80:VAL:CG1	2.67	0.42
3:D:612:GLY:H	3:D:617:ASN:HD21	1.68	0.42
3:D:749:VAL:HA	3:D:750:PRO:HD3	1.90	0.42
3:D:862:ASP:O	3:D:877:PRO:HD3	2.20	0.42
3:D:932:ASP:O	3:D:935:LYS:HB3	2.20	0.42
5:F:167:PRO:HD2	5:F:170:HIS:HD2	1.84	0.42
5:F:394:ARG:HB3	9:F:575:HOH:O	2.19	0.42
1:L:183:ASP:HA	1:L:192:LEU:O	2.20	0.42
1:L:60:ASP:HB2	1:L:137:ARG:NH1	2.34	0.42
2:M:129:ILE:HG22	2:M:130:ASN:N	2.35	0.42
2:M:171:TRP:HZ3	9:M:2226:HOH:O	2.02	0.42
2:M:267:TYR:CD1	2:M:272:ALA:HB1	2.54	0.42
2:M:443:THR:HG21	2:M:449:ILE:HG13	2.02	0.42
2:M:560:MET:O	2:M:564:MET:HE3	2.19	0.42
3:N:1074:SER:O	3:N:1077:ALA:HB3	2.20	0.42
3:N:1082:ALA:O	3:N:1086:LEU:HG	2.19	0.42
3:N:1109:GLU:HG2	3:N:1201:CYS:CA	2.48	0.42
3:N:145:VAL:HG22	3:N:146:PRO:HD2	2.02	0.42
3:N:185:VAL:HG21	3:N:191:LEU:HD11	2.00	0.42
3:N:667:ALA:HB1	9:N:1656:HOH:O	2.19	0.42
3:N:820:GLU:HB3	3:N:836:VAL:HG21	2.01	0.42
4:O:77:GLU:HG3	9:O:3449:HOH:O	2.20	0.42
4:O:6:ILE:HG23	4:O:7:ASP:N	2.34	0.42
5:P:284:ARG:O	5:P:286:PRO:N	2.53	0.42
1:A:79:ILE:O	1:A:83:LYS:HG3	2.19	0.42
1:B:158:ILE:HD11	1:B:165:ILE:C	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1034:GLU:HA	2:C:1037:VAL:CG2	2.47	0.42
2:C:142:ARG:HG2	9:C:1315:HOH:O	2.20	0.42
2:C:839:LEU:HD21	2:C:849:VAL:CG2	2.50	0.42
2:C:911:GLU:HB3	2:C:912:PRO:HD3	2.02	0.42
2:C:967:PHE:CD1	2:C:972:VAL:HG12	2.55	0.42
3:D:957:PRO:HD2	3:D:1007:VAL:HG12	2.00	0.42
3:D:1258:ARG:NE	3:D:1262:LEU:HD11	2.35	0.42
3:D:1311:LEU:CD2	3:D:1311:LEU:H	2.32	0.42
3:D:133:ILE:HD11	3:D:155:ASP:OD1	2.19	0.42
3:D:141:ILE:HG21	3:D:450:TYR:H	1.85	0.42
3:D:544:TYR:N	9:D:1714:HOH:O	2.52	0.42
3:D:729:HIS:ND1	3:D:730:PRO:HD2	2.34	0.42
3:D:84:ILE:O	3:D:87:ARG:HB3	2.19	0.42
1:K:181:VAL:HG12	9:K:2597:HOH:O	2.20	0.42
2:M:178:PRO:HB3	9:M:1853:HOH:O	2.19	0.42
2:M:183:SER:CB	2:M:190:LYS:HD3	2.50	0.42
2:M:259:GLY:O	2:M:290:LEU:O	2.38	0.42
2:M:289:THR:HG22	2:M:290:LEU:H	1.84	0.42
2:M:461:VAL:HG12	9:M:1945:HOH:O	2.19	0.42
2:M:487:THR:HG22	2:M:488:ALA:N	2.35	0.42
2:M:498:GLN:NE2	2:M:498:GLN:HA	2.34	0.42
2:M:580:MET:HB3	2:M:584:GLU:OE1	2.20	0.42
2:M:676:ILE:O	2:M:676:ILE:CG2	2.68	0.42
2:M:722:ILE:HG23	2:M:805:ARG:HH21	1.85	0.42
3:N:1153:VAL:HG12	3:N:1155:VAL:CG2	2.50	0.42
3:N:1205:TYR:CE2	3:N:1366:LYS:HD3	2.54	0.42
3:N:1264:GLU:CG	3:N:1425:THR:H	2.32	0.42
3:N:1382:THR:HG21	3:N:1418:LYS:CE	2.50	0.42
3:N:421:LEU:HD13	3:N:444:VAL:CG1	2.50	0.42
3:N:48:ARG:HB2	9:N:2213:HOH:O	2.18	0.42
3:N:500:ARG:O	3:N:504:ASP:HB2	2.20	0.42
3:N:526:PRO:HB2	5:P:317:LEU:HD11	2.02	0.42
3:N:704:ARG:HB2	3:N:736:PHE:HB3	2.01	0.42
3:N:633:VAL:HB	3:N:740:PHE:CE1	2.55	0.42
1:A:143:ARG:HB2	9:A:331:HOH:O	2.19	0.42
1:A:55:SER:HB2	1:A:158:ILE:HG21	2.01	0.42
2:C:139:GLN:HE22	2:C:415:PRO:HG2	1.85	0.42
2:C:247:PRO:HB2	9:C:1179:HOH:O	2.20	0.42
2:C:254:VAL:HA	2:C:257:VAL:HG23	2.02	0.42
2:C:299:LYS:O	2:C:299:LYS:HG3	2.20	0.42
2:C:443:THR:HG23	2:C:449:ILE:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:460:ARG:HG2	2:C:485:TYR:CE2	2.55	0.42
2:C:12:VAL:HB	2:C:472:ARG:CZ	2.50	0.42
2:C:634:GLY:HA2	9:C:1287:HOH:O	2.20	0.42
2:C:6:PHE:CE1	2:C:909:ALA:HB2	2.54	0.42
3:D:1066:THR:CG2	3:D:1069:GLU:HG3	2.49	0.42
3:D:1134:LEU:HD22	9:D:1694:HOH:O	2.20	0.42
3:D:119:SER:CB	3:D:123:LEU:HB2	2.40	0.42
3:D:1263:PHE:CE2	3:D:1371:VAL:HG11	2.55	0.42
3:D:126:VAL:CG1	3:D:132:TYR:HB2	2.49	0.42
3:D:1467:ILE:HG12	7:D:1527:MXP:H16A	2.02	0.42
3:D:42:ASP:HA	3:D:46:ASP:OD1	2.19	0.42
3:D:162:ARG:O	3:D:449:SER:OG	2.38	0.42
3:D:112:ILE:CD1	3:D:461:ILE:HG21	2.50	0.42
3:D:897:TRP:HB2	9:D:1776:HOH:O	2.20	0.42
4:E:48:MET:N	4:E:54:LEU:HB2	2.34	0.42
5:F:93:LEU:HG	5:F:190:ALA:HB1	2.02	0.42
5:F:192:LEU:O	5:F:196:VAL:HG23	2.19	0.42
5:F:88:ILE:HB	5:F:193:ARG:HD2	2.01	0.42
5:F:88:ILE:HD13	5:F:193:ARG:CB	2.50	0.42
1:K:177:VAL:O	2:M:864:GLY:HA3	2.19	0.42
1:K:48:ILE:HG22	1:K:173:PRO:CD	2.49	0.42
1:L:108:GLU:HG2	9:L:1515:HOH:O	2.19	0.42
1:L:133:GLU:HB3	9:L:1918:HOH:O	2.20	0.42
1:L:27:PRO:HB3	1:L:192:LEU:CD2	2.50	0.42
2:M:146:VAL:HG11	2:M:306:THR:CG2	2.47	0.42
2:M:411:SER:CB	2:M:452:ILE:HG23	2.50	0.42
2:M:479:VAL:CG1	2:M:532:MET:HE2	2.50	0.42
2:M:601:GLY:HA3	2:M:615:TYR:HA	2.02	0.42
3:N:1066:THR:OG1	3:N:1067:VAL:N	2.51	0.42
3:N:1465:ASN:ND2	3:N:1470:ARG:HD3	2.15	0.42
3:N:563:PRO:HG2	5:P:188:ILE:HG21	2.00	0.42
2:M:1067:TYR:CE1	3:N:655:PRO:HG3	2.50	0.42
3:N:76:CYS:HA	9:N:1714:HOH:O	2.20	0.42
3:N:959:GLU:H	3:N:959:GLU:HG2	1.24	0.42
3:N:959:GLU:O	3:N:963:TYR:HD1	2.03	0.42
2:C:124:ASP:HB2	2:C:407:LYS:NZ	2.35	0.41
2:C:204:GLN:NE2	9:C:1386:HOH:O	2.53	0.41
2:C:426:ASP:OD1	2:C:427:VAL:HG22	2.19	0.41
2:C:752:GLY:H	2:C:792:VAL:HB	1.85	0.41
2:C:854:PRO:C	2:C:856:GLU:N	2.72	0.41
2:C:950:LEU:HD12	9:C:1205:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1065:LEU:HD11	3:D:1070:TYR:N	2.35	0.41
3:D:587:ARG:O	3:D:588:GLY:O	2.38	0.41
3:D:614:PHE:CG	3:D:617:ASN:HB3	2.55	0.41
3:D:661:MET:CE	3:D:673:ALA:HB1	2.50	0.41
3:D:804:LEU:O	3:D:831:GLY:HA2	2.20	0.41
5:F:88:ILE:HD13	5:F:193:ARG:CD	2.47	0.41
1:K:156:HIS:CD2	1:K:157:GLY:H	2.38	0.41
1:K:41:ARG:HD2	9:K:1774:HOH:O	2.19	0.41
1:K:54:THR:O	1:K:54:THR:HG22	2.19	0.41
2:M:170:PRO:HG2	2:M:258:TYR:HD2	1.82	0.41
2:M:301:GLU:O	2:M:305:PRO:HG2	2.20	0.41
2:M:202:TYR:OH	2:M:304:LEU:HD22	2.20	0.41
2:M:756:VAL:HG12	2:M:757:GLY:N	2.35	0.41
3:N:1195:GLN:HG3	3:N:1196:THR:N	2.34	0.41
3:N:1274:ILE:HD11	3:N:1334:GLN:HE21	1.82	0.41
3:N:1283:ILE:HD12	3:N:1315:ASP:CG	2.40	0.41
3:N:584:ASN:OD1	3:N:590:PRO:HD2	2.20	0.41
2:M:1043:TYR:HE1	3:N:710:ARG:O	2.03	0.41
3:N:840:LYS:HB3	3:N:841:TYR:CE2	2.55	0.41
3:N:984:THR:HG23	3:N:986:ARG:H	1.85	0.41
4:O:40:LEU:C	4:O:42:PRO:HD2	2.41	0.41
5:P:271:LEU:CG	5:P:295:MET:HE1	2.50	0.41
5:P:348:SER:OG	5:P:349:LEU:N	2.53	0.41
1:A:124:ASN:OD1	1:A:127:LEU:HB3	2.18	0.41
2:C:274:ARG:CZ	2:C:285:LEU:H	2.33	0.41
2:C:290:LEU:N	2:C:290:LEU:HD23	2.36	0.41
2:C:328:LEU:HD13	2:C:433:THR:CB	2.47	0.41
2:C:86:LYS:CD	9:C:1425:HOH:O	2.69	0.41
2:C:952:LEU:N	2:C:952:LEU:HD22	2.35	0.41
2:C:969:GLN:HG3	9:C:1350:HOH:O	2.20	0.41
2:C:862:PRO:HD3	2:C:973:VAL:O	2.19	0.41
3:D:1134:LEU:HD21	3:D:1175:ILE:HG23	2.01	0.41
3:D:172:PRO:O	3:D:174:GLY:N	2.52	0.41
2:C:1094:ALA:CB	3:D:603:LEU:HD22	2.51	0.41
3:D:608:SER:C	3:D:610:LYS:N	2.72	0.41
2:C:1039:ALA:HB3	3:D:713:ILE:HD12	2.02	0.41
3:D:804:LEU:N	9:D:1726:HOH:O	2.53	0.41
5:F:104:ARG:NH1	9:F:673:HOH:O	2.53	0.41
5:F:116:LEU:HB2	5:F:127:ILE:HD12	2.01	0.41
5:F:222:ARG:HG2	9:F:631:HOH:O	2.19	0.41
5:F:85:LEU:HA	5:F:88:ILE:CD1	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:124:ASN:OD1	1:K:127:LEU:HB3	2.20	0.41
1:L:44:LEU:HD23	1:L:48:ILE:CD1	2.50	0.41
2:M:260:LEU:CB	2:M:291:ALA:HB1	2.42	0.41
2:M:22:GLN:OE1	2:M:336:VAL:HG21	2.20	0.41
2:M:724:ARG:HA	2:M:737:LEU:CD2	2.50	0.41
2:M:926:PHE:O	2:M:929:ARG:HB3	2.20	0.41
3:N:1135:ARG:HH21	3:N:1350:GLU:CD	2.23	0.41
3:N:122:GLU:N	9:N:1620:HOH:O	2.52	0.41
3:N:1323:GLN:HG3	3:N:1324:PRO:CD	2.50	0.41
3:N:186:VAL:HB	3:N:189:GLN:HB2	2.02	0.41
3:N:432:TYR:O	3:N:448:GLU:HA	2.20	0.41
3:N:633:VAL:O	3:N:635:PRO:HD3	2.20	0.41
3:N:1486:VAL:CG1	4:O:73:LEU:HD22	2.50	0.41
5:P:147:LEU:HD23	5:P:147:LEU:HA	1.80	0.41
5:P:220:LEU:O	5:P:223:ALA:HB3	2.20	0.41
1:A:180:GLN:HE21	1:A:180:GLN:HB3	1.62	0.41
1:A:211:LEU:HD12	1:A:211:LEU:O	2.21	0.41
2:C:118:ILE:CG2	2:C:382:ILE:HD13	2.50	0.41
2:C:394:PHE:HB2	9:C:1403:HOH:O	2.19	0.41
2:C:412:ALA:HB1	2:C:419:THR:HG21	2.01	0.41
2:C:709:GLU:HG3	2:C:824:ARG:CG	2.50	0.41
2:C:853:LEU:HG	9:C:1271:HOH:O	2.20	0.41
3:D:103:TRP:HE1	3:D:604:THR:CG2	2.33	0.41
3:D:116:LEU:HD23	3:D:118:LEU:HD21	2.01	0.41
3:D:1283:ILE:HG22	3:D:1284:GLU:N	2.35	0.41
3:D:1350:GLU:O	3:D:1350:GLU:HG3	2.21	0.41
3:D:835:SER:O	3:D:837:GLY:N	2.53	0.41
3:D:874:GLU:HG3	9:D:1855:HOH:O	2.20	0.41
5:F:76:SER:O	5:F:80:PRO:HG2	2.20	0.41
3:D:131:LYS:HD2	5:F:83:GLN:CD	2.40	0.41
1:K:18:ARG:HH12	1:K:88:ARG:CD	2.33	0.41
1:K:79:ILE:O	1:K:83:LYS:HG3	2.19	0.41
2:M:557:ARG:CZ	2:M:879:ARG:HG2	2.50	0.41
3:N:119:SER:CB	3:N:123:LEU:HB2	2.40	0.41
3:N:131:LYS:O	3:N:133:ILE:HD13	2.21	0.41
3:N:405:ASP:HB3	9:N:1860:HOH:O	2.20	0.41
3:N:688:TRP:HA	3:N:688:TRP:CE3	2.56	0.41
2:C:64:LEU:HG	2:C:65:VAL:N	2.34	0.41
2:C:815:LEU:HD12	9:C:1534:HOH:O	2.20	0.41
2:C:540:PHE:HE1	2:C:906:PHE:HE1	1.68	0.41
3:D:1057:VAL:HG22	3:D:1069:GLU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1217:ILE:N	9:D:2106:HOH:O	2.52	0.41
3:D:1490:LYS:HG2	9:D:2098:HOH:O	2.19	0.41
3:D:501:ALA:HB2	9:D:2147:HOH:O	2.20	0.41
3:D:560:GLN:O	5:F:132:ARG:NH1	2.47	0.41
3:D:633:VAL:O	3:D:635:PRO:HD3	2.20	0.41
5:F:117:SER:HB3	5:F:122:LEU:O	2.19	0.41
1:K:115:LEU:HA	1:K:116:PRO:HD3	1.90	0.41
1:K:159:LYS:HA	9:K:1082:HOH:O	2.19	0.41
2:M:1100:GLN:HB2	2:M:1100:GLN:HE21	1.65	0.41
2:M:597:ALA:O	2:M:652:GLY:N	2.53	0.41
2:M:875:GLY:HA2	2:M:879:ARG:HH11	1.85	0.41
3:N:686:GLU:HA	3:N:689:ASP:OD2	2.21	0.41
3:N:696:HIS:HB3	9:N:1565:HOH:O	2.19	0.41
5:P:172:ARG:HD3	9:P:483:HOH:O	2.21	0.41
5:P:315:VAL:HG11	9:P:467:HOH:O	2.20	0.41
1:A:11:PHE:CD1	1:B:225:PHE:HA	2.55	0.41
1:A:47:SER:OG	1:B:32:PHE:HZ	2.03	0.41
1:B:23:PHE:CD2	1:B:211:LEU:HD22	2.56	0.41
2:C:1034:GLU:O	2:C:1037:VAL:HG23	2.21	0.41
2:C:127:PHE:O	2:C:133:ASP:HA	2.21	0.41
2:C:396:ASP:HA	2:C:633:GLN:CD	2.40	0.41
3:D:1171:VAL:HG12	3:D:1171:VAL:O	2.21	0.41
3:D:1191:PRO:HD3	3:D:1204:CYS:O	2.21	0.41
3:D:1192:LEU:HD22	3:D:1345:GLU:HG2	2.02	0.41
3:D:196:VAL:HG13	9:D:1768:HOH:O	2.20	0.41
3:D:90:MET:HE2	3:D:521:PRO:HD3	2.01	0.41
3:D:688:TRP:HE3	3:D:688:TRP:HA	1.86	0.41
3:D:693:GLU:HG2	9:D:1780:HOH:O	2.21	0.41
3:D:699:VAL:HG12	3:D:717:GLN:CA	2.51	0.41
3:D:767:HIS:NE2	4:E:6:ILE:HG12	2.36	0.41
3:D:850:LEU:CD1	3:D:850:LEU:H	2.24	0.41
1:L:147:GLY:N	1:L:171:PHE:CE1	2.88	0.41
2:M:113:VAL:HB	2:M:115:LEU:HD23	2.02	0.41
2:M:22:GLN:HE22	2:M:135:VAL:CG1	2.33	0.41
2:M:475:VAL:O	2:M:478:VAL:HB	2.20	0.41
3:N:1364:HIS:ND1	3:N:1366:LYS:HB2	2.36	0.41
3:N:50:PHE:CD2	3:N:522:PRO:HG3	2.56	0.41
3:N:87:ARG:HB2	3:N:523:ASP:HB2	2.03	0.41
3:N:570:GLU:HB2	5:P:214:GLN:NE2	2.35	0.41
3:N:852:ALA:HB1	3:N:857:ILE:HB	2.02	0.41
5:P:163:LEU:HD13	5:P:174:LEU:CD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:118:ILE:H	2:C:118:ILE:HG13	1.64	0.41
2:C:24:GLU:HG2	2:C:27:ARG:CD	2.50	0.41
2:C:462:ASP:HB3	2:C:468:ARG:CD	2.50	0.41
2:C:479:VAL:HG13	2:C:508:ILE:HD12	2.03	0.41
2:C:592:LEU:HA	2:C:592:LEU:HD23	1.90	0.41
2:C:620:LEU:O	2:C:620:LEU:HD12	2.21	0.41
2:C:742:VAL:HG21	9:C:1160:HOH:O	2.19	0.41
3:D:1122:LEU:O	3:D:1134:LEU:HA	2.20	0.41
3:D:1209:LEU:HD12	3:D:1219:GLU:CD	2.41	0.41
3:D:204:LEU:HD21	3:D:445:ARG:HH12	1.86	0.41
3:D:29:PRO:HG2	3:D:549:ASN:HD21	1.84	0.41
3:D:766:ALA:O	3:D:769:LEU:HD21	2.19	0.41
3:D:832:ARG:HB2	9:D:1797:HOH:O	2.19	0.41
3:D:889:ALA:HB1	3:D:930:LEU:HA	2.02	0.41
4:E:41:GLU:HB2	4:E:45:ARG:NH1	2.36	0.41
5:F:196:VAL:HG22	5:F:213:ILE:HD13	2.01	0.41
5:F:215:GLU:OE2	5:F:254:GLN:NE2	2.50	0.41
5:F:75:ILE:HG13	9:F:645:HOH:O	2.20	0.41
1:L:127:LEU:HD12	9:L:1125:HOH:O	2.20	0.41
2:M:1034:GLU:HA	2:M:1037:VAL:CG2	2.49	0.41
2:M:292:ARG:NH1	2:M:299:LYS:HD3	2.35	0.41
2:M:327:HIS:O	2:M:330:ASN:HB2	2.21	0.41
2:M:374:ASN:O	2:M:377:PRO:HD2	2.20	0.41
2:M:663:ASN:C	2:M:665:PHE:H	2.24	0.41
3:N:1276:GLU:OE2	3:N:1303:TYR:HE2	2.04	0.41
3:N:1389:LEU:HD12	3:N:1390:LEU:N	2.32	0.41
3:N:637:LEU:HD12	3:N:641:GLN:HB2	2.02	0.41
3:N:775:GLY:C	9:N:1689:HOH:O	2.58	0.41
3:N:806:PHE:O	3:N:808:THR:N	2.53	0.41
5:P:169:GLU:HG3	5:P:169:GLU:H	1.67	0.41
3:N:570:GLU:HB2	5:P:214:GLN:HE22	1.85	0.41
5:P:305:GLU:HG2	5:P:309:LYS:HE3	2.01	0.41
1:B:57:TYR:CE2	1:B:59:GLU:HA	2.55	0.41
2:C:1002:GLU:O	2:C:1003:ASP:C	2.58	0.41
2:C:274:ARG:HB2	2:C:285:LEU:HB3	2.02	0.41
2:C:162:ILE:CD1	2:C:306:THR:HG21	2.50	0.41
2:C:437:ARG:HG2	2:C:467:ILE:O	2.21	0.41
9:A:432:HOH:O	2:C:832:LYS:HE3	2.20	0.41
2:C:914:ILE:HA	2:C:914:ILE:HD12	1.74	0.41
9:C:1734:HOH:O	3:D:1471:LEU:HD12	2.20	0.41
3:D:165:LYS:HG2	9:D:1699:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:596:SER:C	3:D:598:ARG:H	2.24	0.41
3:D:601:ARG:HG3	9:D:2091:HOH:O	2.21	0.41
2:C:1013:TYR:OH	3:D:624:ASP:OD2	2.37	0.41
3:D:771:SER:HA	3:D:772:PRO:HD3	1.91	0.41
5:F:321:ILE:HG13	5:F:329:TYR:HA	2.01	0.41
1:K:101:LEU:HD23	1:K:102:LYS:N	2.35	0.41
1:K:158:ILE:HG22	1:K:159:LYS:N	2.35	0.41
1:L:172:SER:OG	1:L:174:VAL:HB	2.21	0.41
2:M:22:GLN:HE22	2:M:135:VAL:HG12	1.85	0.41
2:M:264:PRO:HB3	2:M:289:THR:CB	2.50	0.41
2:M:299:LYS:O	2:M:299:LYS:HG3	2.21	0.41
2:M:663:ASN:HD22	2:M:663:ASN:HA	1.52	0.41
2:M:724:ARG:HB2	2:M:740:GLU:HA	2.01	0.41
2:M:968:LEU:HD13	9:M:2164:HOH:O	2.21	0.41
3:N:1007:VAL:CG2	3:N:1008:PHE:N	2.84	0.41
3:N:1333:HIS:O	3:N:1336:LEU:HB3	2.19	0.41
3:N:611:GLN:N	9:N:1557:HOH:O	2.54	0.41
3:N:637:LEU:HD11	3:N:642:CYS:CA	2.51	0.41
3:N:818:ARG:O	3:N:821:VAL:HB	2.20	0.41
3:N:911:LEU:O	3:N:915:VAL:HG23	2.20	0.41
4:O:49:GLN:C	4:O:51:LEU:N	2.74	0.41
1:A:46:SER:HB3	2:C:856:GLU:CD	2.41	0.41
2:C:172:ILE:HD12	2:C:172:ILE:N	2.34	0.41
2:C:313:LEU:HD12	2:C:313:LEU:O	2.21	0.41
2:C:414:GLY:O	2:C:416:GLY:N	2.54	0.41
2:C:469:THR:HG23	2:C:471:TYR:CE1	2.56	0.41
2:C:511:GLU:N	9:C:1690:HOH:O	2.53	0.41
2:C:952:LEU:CD1	2:C:969:GLN:HE22	2.19	0.41
2:C:96:ALA:HB2	9:C:1545:HOH:O	2.20	0.41
3:D:1326:THR:HG22	3:D:1327:ARG:H	1.85	0.41
3:D:1339:LYS:HB3	3:D:1343:ALA:HB2	2.02	0.41
3:D:1459:LEU:HB2	3:D:1470:ARG:NH1	2.35	0.41
3:D:415:VAL:HG13	3:D:419:ASP:HB2	2.01	0.41
3:D:925:GLU:OE1	4:E:6:ILE:HG22	2.20	0.41
3:D:998:GLU:HB3	9:D:2202:HOH:O	2.20	0.41
4:E:50:THR:HA	9:E:107:HOH:O	2.20	0.41
5:F:280:GLN:NE2	9:F:601:HOH:O	2.54	0.41
5:F:284:ARG:O	5:F:286:PRO:N	2.53	0.41
1:K:16:GLN:HB2	9:K:3198:HOH:O	2.20	0.41
1:L:101:LEU:HD12	1:L:114:PHE:CA	2.50	0.41
1:L:117:VAL:HB	1:L:120:VAL:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:142:VAL:HG23	1:L:142:VAL:O	2.21	0.41
2:M:1008:ARG:CZ	2:M:1020:PRO:HB3	2.51	0.41
2:M:1054:THR:HB	2:M:1055:LEU:H	1.61	0.41
2:M:140:ILE:H	2:M:140:ILE:HD12	1.86	0.41
2:M:278:GLU:HA	2:M:283:ILE:HA	2.03	0.41
2:M:676:ILE:HG21	2:M:988:VAL:HG22	2.01	0.41
3:N:1051:GLU:HG3	3:N:1051:GLU:H	1.53	0.41
3:N:105:VAL:HG12	3:N:106:LYS:HG3	2.02	0.41
3:N:1147:ARG:NH1	9:N:2122:HOH:O	2.52	0.41
3:N:1223:ILE:O	3:N:1224:VAL:C	2.59	0.41
3:N:1341:PRO:HB2	9:N:1945:HOH:O	2.19	0.41
3:N:206:ARG:HA	9:N:2058:HOH:O	2.20	0.41
3:N:165:LYS:CG	3:N:397:LYS:HD3	2.50	0.41
3:N:489:ARG:HD3	9:N:1694:HOH:O	2.20	0.41
3:N:804:LEU:O	3:N:831:GLY:HA2	2.21	0.41
3:N:899:LEU:HD12	3:N:900:ILE:HG23	2.02	0.41
5:P:350:LEU:O	5:P:354:LEU:HB2	2.21	0.41
5:P:371:LEU:HB2	5:P:372:ARG:HH11	1.86	0.41
1:A:170:VAL:HA	9:A:399:HOH:O	2.21	0.41
1:A:18:ARG:HH12	1:A:88:ARG:HD3	1.86	0.41
1:A:227:ASN:N	1:A:227:ASN:ND2	2.65	0.41
2:C:1067:TYR:CE1	2:C:1071:ILE:HD11	2.56	0.41
2:C:45:GLN:NE2	9:C:1426:HOH:O	2.52	0.41
2:C:612:VAL:HG22	2:C:622:GLU:CB	2.51	0.41
2:C:612:VAL:HG22	2:C:622:GLU:HG3	2.02	0.41
2:C:724:ARG:HB2	2:C:740:GLU:HA	2.02	0.41
2:C:7:GLY:O	2:C:907:ASP:OD1	2.38	0.41
2:C:807:ARG:HA	2:C:821:GLU:HB2	2.02	0.41
2:C:818:GLY:N	5:F:309:LYS:CE	2.82	0.41
2:C:969:GLN:HE21	2:C:969:GLN:HB3	1.72	0.41
3:D:1361:VAL:HG23	9:D:1625:HOH:O	2.21	0.41
3:D:33:ASN:HB3	9:D:2304:HOH:O	2.21	0.41
3:D:482:LYS:HB2	9:D:1744:HOH:O	2.20	0.41
3:D:647:ARG:HB2	9:D:1878:HOH:O	2.21	0.41
3:D:704:ARG:HB2	3:D:736:PHE:HB3	2.03	0.41
3:D:85:VAL:HG11	3:D:89:ARG:NH2	2.35	0.41
3:D:899:LEU:HD12	3:D:900:ILE:HG23	2.03	0.41
4:E:53:GLY:C	4:E:55:PHE:H	2.24	0.41
1:K:49:PRO:HB3	1:K:148:VAL:CG2	2.51	0.41
1:L:75:VAL:O	1:L:79:ILE:HG23	2.20	0.41
2:M:190:LYS:H	2:M:190:LYS:HG3	1.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:280:LYS:HA	9:M:1935:HOH:O	2.20	0.41
2:M:56:GLU:OE2	2:M:356:ARG:HG2	2.20	0.41
2:M:34:VAL:CG2	2:M:38:LYS:HD3	2.49	0.41
2:M:911:GLU:HB3	2:M:912:PRO:HD3	2.03	0.41
2:M:958:THR:HG23	2:M:961:GLU:HB2	2.03	0.41
3:N:1148:VAL:HG21	3:N:1203:LYS:HA	2.03	0.41
3:N:1369:GLU:HA	3:N:1372:VAL:HG12	2.02	0.41
3:N:1264:GLU:HA	3:N:1423:GLY:CA	2.51	0.41
3:N:1442:ASN:N	9:N:1579:HOH:O	2.53	0.41
3:N:192:ALA:HB2	3:N:393:ILE:CD1	2.51	0.41
3:N:611:GLN:CG	3:N:619:LEU:CG	2.91	0.41
3:N:705:ALA:CB	3:N:706:PRO:CD	2.94	0.41
3:N:711:LEU:C	3:N:713:ILE:N	2.74	0.41
3:N:60:CYS:N	3:N:76:CYS:SG	2.91	0.41
3:N:771:SER:HA	3:N:772:PRO:HD3	1.86	0.41
4:O:16:LYS:HD3	4:O:17:TYR:CE2	2.56	0.41
5:P:207:LEU:HD23	5:P:207:LEU:HA	1.95	0.41
1:B:111:ALA:HB3	1:B:124:ASN:O	2.21	0.41
2:C:1063:ARG:O	2:C:1066:ALA:HB3	2.21	0.41
2:C:149:THR:HA	2:C:150:PRO:HD3	1.92	0.41
2:C:317:VAL:HB	9:C:1324:HOH:O	2.20	0.41
2:C:35:PRO:HB3	9:C:1537:HOH:O	2.21	0.41
2:C:36:PRO:CB	2:C:70:GLU:HG2	2.51	0.41
2:C:815:LEU:HG	2:C:819:VAL:HG11	2.00	0.41
3:D:119:SER:N	3:D:123:LEU:HD22	2.26	0.41
3:D:44:LEU:HD21	3:D:544:TYR:HB3	2.03	0.41
3:D:29:PRO:CB	3:D:545:ARG:HG2	2.49	0.41
3:D:93:ILE:HD13	3:D:547:LEU:HD23	2.03	0.41
1:K:198:ARG:NH2	9:K:1749:HOH:O	2.54	0.41
1:K:48:ILE:HD11	1:K:210:ALA:O	2.21	0.41
2:M:1090:LYS:HD2	3:N:90:MET:CE	2.51	0.41
2:M:131:GLY:HA2	9:M:1651:HOH:O	2.20	0.41
2:M:218:VAL:CA	2:M:221:LEU:HD23	2.50	0.41
2:M:255:ALA:HB3	2:M:298:PHE:CZ	2.56	0.41
2:M:129:ILE:CD1	2:M:386:PHE:HB3	2.51	0.41
2:M:408:ARG:HD2	2:M:408:ARG:HH11	1.74	0.41
2:M:535:SER:HB2	2:M:537:LYS:HG3	2.03	0.41
2:M:971:LYS:HB3	2:M:988:VAL:N	2.36	0.41
3:N:1000:THR:CG2	3:N:1001:GLU:N	2.84	0.41
3:N:1075:HIS:CE1	9:N:1553:HOH:O	2.74	0.41
3:N:1155:VAL:CG1	3:N:1177:ALA:HB1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1441:GLN:N	9:N:1579:HOH:O	2.54	0.41
3:N:398:ALA:HB2	9:N:1561:HOH:O	2.21	0.41
3:N:417:PRO:HG3	3:N:430:ASP:O	2.21	0.41
3:N:562:ALA:HB3	9:P:599:HOH:O	2.20	0.41
3:N:572:ARG:HD3	3:N:572:ARG:HH11	1.63	0.41
3:N:591:VAL:CG1	3:N:597:ASP:HA	2.50	0.41
3:N:889:ALA:HB1	3:N:930:LEU:HA	2.03	0.41
4:O:36:LYS:HG2	9:O:3235:HOH:O	2.20	0.41
4:O:54:LEU:HA	4:O:58:PRO:CG	2.50	0.41
5:P:277:GLN:HA	9:P:458:HOH:O	2.21	0.41
1:B:158:ILE:CG2	1:B:159:LYS:N	2.83	0.41
2:C:1097:LEU:N	2:C:1097:LEU:CD1	2.84	0.41
2:C:162:ILE:HD12	2:C:172:ILE:HB	2.03	0.41
2:C:166:PRO:HD3	2:C:265:ARG:CB	2.51	0.41
2:C:663:ASN:HD22	2:C:663:ASN:HA	1.51	0.41
2:C:707:ARG:CZ	2:C:824:ARG:CZ	2.98	0.41
3:D:1035:ILE:CA	3:D:1038:LEU:HD12	2.50	0.41
3:D:1116:ASN:HB3	9:D:2418:HOH:O	2.20	0.41
3:D:1243:THR:CB	3:D:1253:THR:HB	2.50	0.41
3:D:1384:PRO:HB3	3:D:1387:SER:O	2.20	0.41
3:D:155:ASP:HA	3:D:158:TYR:HB3	2.03	0.41
3:D:687:VAL:CG1	9:D:2185:HOH:O	2.67	0.41
3:D:729:HIS:ND1	3:D:730:PRO:CD	2.84	0.41
4:E:49:GLN:C	4:E:51:LEU:N	2.73	0.41
2:C:818:GLY:CA	5:F:309:LYS:NZ	2.83	0.41
1:K:85:LEU:HB2	1:K:127:LEU:HD21	2.03	0.41
1:K:198:ARG:HB2	1:K:200:TRP:CH2	2.55	0.41
1:L:41:ARG:NH1	1:L:177:VAL:HG23	2.36	0.41
2:M:182:VAL:HG12	2:M:193:LEU:HD13	2.02	0.41
2:M:271:GLU:HA	2:M:275:TYR:CD1	2.56	0.41
2:M:474:VAL:HG23	2:M:478:VAL:O	2.21	0.41
3:N:1404:ASN:HA	9:N:1794:HOH:O	2.19	0.41
3:N:601:ARG:HG2	3:N:605:ASP:OD1	2.21	0.41
3:N:712:GLY:O	3:N:713:ILE:HG13	2.21	0.41
3:N:907:GLU:HG2	3:N:908:LYS:H	1.85	0.41
3:N:937:TYR:HD2	3:N:941:PHE:HE1	1.69	0.41
5:P:132:ARG:NH2	5:P:184:ARG:NH1	2.69	0.41
2:C:91:GLN:HG2	2:C:119:PRO:HG3	2.03	0.40
2:C:234:ALA:HA	2:C:237:ARG:HB2	2.02	0.40
2:C:269:LEU:O	2:C:269:LEU:HD23	2.22	0.40
2:C:292:ARG:NH1	9:C:1267:HOH:O	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:442:GLU:O	2:C:442:GLU:HG3	2.21	0.40
2:C:518:LYS:N	9:C:1698:HOH:O	2.52	0.40
2:C:495:THR:HG21	2:C:524:VAL:HG21	2.02	0.40
2:C:874:LEU:HD23	3:D:1023:MET:HE1	2.03	0.40
2:C:966:LEU:HD21	2:C:986:PRO:CG	2.51	0.40
3:D:1412:LYS:O	3:D:1414:PRO:HD3	2.21	0.40
3:D:1447:LEU:O	3:D:1448:THR:C	2.60	0.40
3:D:674:ARG:HG2	3:D:674:ARG:HH11	1.86	0.40
3:D:684:LYS:HG2	9:D:2411:HOH:O	2.20	0.40
3:D:717:GLN:CG	9:D:1581:HOH:O	2.68	0.40
2:C:836:GLY:HA3	3:D:724:GLN:OE1	2.20	0.40
3:D:760:ARG:HD2	4:E:3:GLU:CD	2.41	0.40
3:D:820:GLU:CB	3:D:836:VAL:HG21	2.51	0.40
5:F:90:GLN:HE21	5:F:90:GLN:HB3	1.73	0.40
1:L:101:LEU:HD12	1:L:113:ASP:C	2.40	0.40
1:L:71:VAL:HG22	1:L:132:LEU:CD1	2.50	0.40
2:M:242:LEU:HD23	2:M:242:LEU:HA	1.78	0.40
2:M:414:GLY:O	2:M:416:GLY:N	2.54	0.40
2:M:437:ARG:NH1	2:M:488:ALA:HA	2.35	0.40
2:M:471:TYR:CD2	2:M:496:ILE:HG21	2.55	0.40
2:M:512:ARG:HB3	2:M:523:ILE:HD11	2.03	0.40
2:M:840:ALA:HB2	2:M:846:LYS:HA	2.02	0.40
2:M:861:LEU:CD2	2:M:925:TYR:HE2	2.33	0.40
2:M:929:ARG:HH22	2:M:940:GLU:CD	2.24	0.40
3:N:1047:LYS:HG2	3:N:1053:PHE:CZ	2.56	0.40
3:N:1223:ILE:O	3:N:1227:GLN:HG3	2.22	0.40
3:N:1396:GLU:HG2	3:N:1396:GLU:O	2.22	0.40
3:N:515:GLU:HG3	9:N:1827:HOH:O	2.20	0.40
3:N:516:ALA:HB1	9:N:2118:HOH:O	2.21	0.40
3:N:106:LYS:HZ2	3:N:587:ARG:HH11	1.69	0.40
3:N:729:HIS:CE1	3:N:935:LYS:HD3	2.56	0.40
3:N:850:LEU:H	3:N:850:LEU:CD1	2.24	0.40
5:P:256:ARG:HA	9:P:486:HOH:O	2.21	0.40
5:P:321:ILE:HB	5:P:327:SER:OG	2.21	0.40
2:C:15:LEU:HA	2:C:16:PRO:HD3	1.95	0.40
2:C:181:VAL:HG12	2:C:182:VAL:N	2.36	0.40
2:C:464:LEU:HD12	2:C:465:GLY:N	2.36	0.40
2:C:468:ARG:NH1	9:C:1743:HOH:O	2.54	0.40
2:C:708:TYR:N	2:C:708:TYR:CD1	2.89	0.40
2:C:858:MET:HB2	2:C:859:PRO:CD	2.51	0.40
2:C:958:THR:HA	9:C:1402:HOH:O	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1007:VAL:CG2	3:D:1008:PHE:N	2.84	0.40
3:D:1114:THR:HG23	3:D:1116:ASN:ND2	2.36	0.40
3:D:1310:ARG:HG3	3:D:1327:ARG:CB	2.48	0.40
3:D:1394:VAL:HG23	9:D:2328:HOH:O	2.21	0.40
3:D:152:LEU:HD23	3:D:152:LEU:N	2.27	0.40
3:D:400:VAL:HG13	3:D:402:PRO:CD	2.51	0.40
3:D:610:LYS:HB3	7:D:1527:MXF:H15	2.03	0.40
3:D:709:HIS:CD2	3:D:711:LEU:HB2	2.56	0.40
3:D:840:LYS:NZ	9:D:2398:HOH:O	2.55	0.40
5:F:270:LYS:N	9:F:511:HOH:O	2.54	0.40
5:F:364:ARG:HH12	5:F:396:ARG:CZ	2.34	0.40
5:F:94:LEU:HB2	5:F:98:GLU:CG	2.52	0.40
1:K:107:LYS:HE3	1:K:113:ASP:OD2	2.19	0.40
1:K:176:ARG:HG3	1:K:200:TRP:CE3	2.57	0.40
1:K:201:THR:HG21	1:K:205:VAL:O	2.20	0.40
1:L:158:ILE:CG2	1:L:159:LYS:N	2.84	0.40
1:L:197:LEU:HD21	1:L:199:ILE:CD1	2.47	0.40
2:M:1060:ILE:O	2:M:1063:ARG:HG2	2.20	0.40
2:M:143:SER:HB2	2:M:276:LYS:HZ1	1.83	0.40
2:M:308:ARG:HG2	9:M:1753:HOH:O	2.21	0.40
2:M:361:MET:HE2	9:M:2183:HOH:O	2.20	0.40
2:M:400:PRO:O	2:M:401:LEU:C	2.58	0.40
2:M:443:THR:HA	2:M:444:PRO:HD3	1.80	0.40
2:M:606:VAL:HG21	2:M:645:VAL:HG22	2.03	0.40
2:M:674:VAL:O	2:M:989:VAL:HA	2.20	0.40
2:M:75:GLU:HA	2:M:76:PRO:HD3	1.97	0.40
2:M:929:ARG:HH12	2:M:940:GLU:CD	2.24	0.40
3:N:1087:ARG:HD3	3:N:1238:MET:H	1.86	0.40
3:N:1161:GLU:H	3:N:1161:GLU:HG2	1.37	0.40
3:N:489:ARG:NH2	3:N:1389:LEU:HD11	2.32	0.40
3:N:530:VAL:HG23	3:N:534:ARG:O	2.21	0.40
3:N:596:SER:C	3:N:598:ARG:H	2.24	0.40
3:N:951:ILE:HD12	3:N:1062:ARG:HG3	2.02	0.40
1:B:61:VAL:N	1:B:137:ARG:NH2	2.67	0.40
2:C:1010:THR:HG22	2:C:1011:GLY:N	2.36	0.40
2:C:263:ASP:C	2:C:264:PRO:O	2.59	0.40
2:C:491:GLU:HG2	9:C:1297:HOH:O	2.21	0.40
2:C:721:ARG:NE	9:C:1244:HOH:O	2.55	0.40
2:C:773:LEU:HG	2:C:777:ILE:HD11	2.03	0.40
2:C:865:THR:HG23	2:C:865:THR:O	2.21	0.40
3:D:1066:THR:OG1	3:D:1067:VAL:N	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1335:LEU:HD23	3:D:1344:VAL:CA	2.28	0.40
3:D:1353:GLN:OE1	3:D:1365:ASP:OD2	2.39	0.40
3:D:1372:VAL:CG1	3:D:1373:ARG:N	2.84	0.40
3:D:521:PRO:O	3:D:525:ARG:NH1	2.52	0.40
3:D:93:ILE:HD13	3:D:548:ILE:HD11	2.03	0.40
3:D:638:LYS:C	3:D:729:HIS:HD2	2.25	0.40
3:D:797:LYS:HA	3:D:828:LYS:HB2	2.04	0.40
5:F:205:ARG:NH1	5:F:248:ASN:OD1	2.54	0.40
5:F:272:SER:O	5:F:276:ARG:HG3	2.22	0.40
1:K:28:LEU:HD23	1:K:28:LEU:HA	1.77	0.40
1:L:10:VAL:HG12	1:L:12:THR:HG23	2.02	0.40
2:M:1017:THR:OG1	2:M:1019:GLN:HG3	2.22	0.40
2:M:118:ILE:HG13	2:M:118:ILE:H	1.63	0.40
2:M:221:LEU:HG	2:M:222:MET:N	2.37	0.40
2:M:234:ALA:HA	2:M:237:ARG:HB2	2.02	0.40
2:M:110:GLU:HB3	2:M:369:PRO:HG3	2.02	0.40
2:M:420:ARG:HG2	2:M:420:ARG:H	1.44	0.40
2:M:424:GLY:N	9:M:1722:HOH:O	2.54	0.40
2:M:480:THR:CG2	2:M:481:ASP:H	2.34	0.40
2:M:586:ARG:NE	2:M:590:ASP:OD2	2.53	0.40
2:M:742:VAL:CG1	2:M:743:VAL:N	2.83	0.40
2:M:950:LEU:HB3	2:M:952:LEU:HD23	2.02	0.40
3:N:1366:LYS:O	3:N:1369:GLU:HB2	2.22	0.40
3:N:1435:LEU:HD23	3:N:1467:ILE:HD12	2.02	0.40
3:N:46:ASP:O	3:N:48:ARG:N	2.54	0.40
3:N:793:THR:HG22	3:N:879:ARG:HA	2.03	0.40
3:N:862:ASP:O	3:N:876:SER:HB2	2.21	0.40
3:N:776:GLU:HB3	3:N:912:LYS:HE2	2.03	0.40
3:N:932:ASP:O	3:N:935:LYS:HB3	2.22	0.40
4:O:26:ARG:HG2	4:O:67:GLU:OE1	2.22	0.40
1:A:13:VAL:CG1	1:A:15:THR:HG22	2.49	0.40
1:A:95:GLN:HG2	9:A:325:HOH:O	2.21	0.40
1:A:96:THR:N	9:A:349:HOH:O	2.54	0.40
2:C:166:PRO:HG2	9:C:1175:HOH:O	2.21	0.40
2:C:378:LEU:O	2:C:382:ILE:HG13	2.22	0.40
2:C:400:PRO:O	2:C:401:LEU:C	2.58	0.40
2:C:410:ILE:N	2:C:453:THR:O	2.53	0.40
2:C:54:ILE:HD13	9:C:1578:HOH:O	2.21	0.40
2:C:686:ASP:N	9:C:1222:HOH:O	2.54	0.40
2:C:549:PHE:HE2	2:C:887:GLU:N	2.20	0.40
2:C:897:LEU:CD1	2:C:921:ALA:HA	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1106:VAL:HG21	3:D:1474:ALA:HB2	2.03	0.40
3:D:1256:LEU:N	3:D:1257:PRO:CD	2.85	0.40
3:D:1305:LEU:HD22	3:D:1309:ALA:CB	2.52	0.40
3:D:46:ASP:O	3:D:48:ARG:N	2.54	0.40
3:D:500:ARG:O	3:D:504:ASP:HB2	2.21	0.40
3:D:521:PRO:HA	3:D:522:PRO:HD3	1.91	0.40
3:D:778:LEU:HD11	9:D:1940:HOH:O	2.21	0.40
3:D:898:GLU:OE2	3:D:921:ARG:NH1	2.54	0.40
3:D:97:THR:O	3:D:98:PRO:O	2.40	0.40
5:F:280:GLN:O	5:F:280:GLN:HG2	2.22	0.40
1:K:180:GLN:HE21	1:K:180:GLN:HB3	1.65	0.40
1:K:42:ARG:NH1	1:L:34:VAL:HB	2.14	0.40
2:M:1008:ARG:HD2	2:M:1028:GLY:H	1.85	0.40
2:M:172:ILE:HG22	2:M:173:ASP:N	2.36	0.40
2:M:176:VAL:HG23	2:M:176:VAL:O	2.22	0.40
2:M:284:ARG:HD2	9:M:2219:HOH:O	2.21	0.40
2:M:443:THR:HG21	2:M:450:GLY:H	1.85	0.40
2:M:713:ARG:HB2	2:M:720:GLU:OE1	2.21	0.40
3:N:1109:GLU:CD	3:N:1202:GLN:HB2	2.42	0.40
3:N:1144:LEU:HD12	3:N:1171:VAL:HG13	2.04	0.40
3:N:1161:GLU:CG	3:N:1164:ARG:HD2	2.52	0.40
3:N:1384:PRO:C	3:N:1413:THR:HG21	2.42	0.40
3:N:1399:ASP:O	3:N:1403:LEU:HB2	2.21	0.40
3:N:610:LYS:CG	7:N:1527:MXP:H15A	2.47	0.40
3:N:565:ILE:HD12	5:P:192:LEU:CD1	2.50	0.40
3:N:935:LYS:HE2	3:N:935:LYS:HB3	1.94	0.40
3:N:982:PHE:HA	9:N:1762:HOH:O	2.21	0.40
5:P:363:GLU:CA	5:P:367:MET:HG3	2.51	0.40
5:P:399:GLN:O	5:P:403:LYS:HB2	2.21	0.40
1:A:43:ILE:HG21	1:A:214:ALA:HA	2.04	0.40
1:A:44:LEU:O	1:A:174:VAL:HG21	2.21	0.40
1:A:42:ARG:HD3	1:B:35:THR:OG1	2.21	0.40
2:C:1005:MET:HB2	3:D:629:SER:HB2	2.02	0.40
2:C:1059:ASP:CG	2:C:1062:GLY:HA3	2.42	0.40
2:C:1097:LEU:HD12	2:C:1097:LEU:H	1.86	0.40
2:C:207:LEU:HD13	2:C:221:LEU:HD13	2.03	0.40
2:C:861:LEU:CD2	2:C:925:TYR:HE2	2.34	0.40
3:D:1209:LEU:HD23	3:D:1211:MET:CG	2.50	0.40
3:D:1364:HIS:ND1	3:D:1366:LYS:HB2	2.36	0.40
3:D:1476:THR:C	3:D:1478:SER:H	2.24	0.40
3:D:659:LYS:O	3:D:659:LYS:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:758:GLU:O	3:D:762:GLN:HG3	2.20	0.40
3:D:99:ALA:HA	3:D:575:GLN:NE2	2.37	0.40
5:F:220:LEU:HB2	5:F:243:ILE:HD11	2.02	0.40
5:F:364:ARG:HD3	9:F:425:HOH:O	2.21	0.40
1:K:20:TYR:HE2	1:K:22:GLU:HG3	1.85	0.40
1:K:41:ARG:NH2	2:M:860:HIS:HB3	2.37	0.40
1:L:145:ASP:O	1:L:171:PHE:HE1	2.04	0.40
2:M:174:LEU:CD2	2:M:184:MET:HG3	2.52	0.40
2:M:183:SER:HB3	2:M:190:LYS:HD3	2.03	0.40
2:M:351:LEU:HD11	2:M:373:VAL:HG13	2.03	0.40
2:M:73:LEU:HD23	2:M:94:LEU:HD13	2.04	0.40
2:M:890:LEU:HD12	2:M:914:ILE:CD1	2.46	0.40
3:N:1095:THR:O	3:N:1096:ARG:C	2.60	0.40
3:N:1148:VAL:HG13	3:N:1163:GLY:O	2.21	0.40
3:N:1500:LYS:O	3:N:1503:VAL:HG23	2.22	0.40
3:N:153:LEU:HB3	9:N:1717:HOH:O	2.20	0.40
3:N:199:LEU:H	3:N:199:LEU:HG	1.60	0.40
3:N:397:LYS:HE3	3:N:448:GLU:HB3	2.04	0.40
3:N:447:VAL:HG11	9:N:1573:HOH:O	2.21	0.40
3:N:478:LEU:HD21	3:N:500:ARG:HH21	1.84	0.40
3:N:489:ARG:HG2	3:N:490:ALA:N	2.37	0.40
3:N:733:CYS:HG	3:N:740:PHE:HZ	1.66	0.40
3:N:835:SER:O	3:N:837:GLY:N	2.54	0.40
4:O:85:LEU:HD23	4:O:85:LEU:C	2.42	0.40
5:P:295:MET:HB3	5:P:299:TRP:CG	2.57	0.40
5:P:368:VAL:HA	9:P:506:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	227/315 (72%)	200 (88%)	24 (11%)	3 (1%)	12	30
1	B	227/315 (72%)	195 (86%)	29 (13%)	3 (1%)	12	30
1	K	227/315 (72%)	201 (88%)	22 (10%)	4 (2%)	8	21
1	L	227/315 (72%)	199 (88%)	25 (11%)	3 (1%)	12	30
2	C	1117/1119 (100%)	905 (81%)	154 (14%)	58 (5%)	2	3
2	M	1117/1119 (100%)	904 (81%)	153 (14%)	60 (5%)	2	3
3	D	1317/1524 (86%)	1098 (83%)	170 (13%)	49 (4%)	3	7
3	N	1317/1524 (86%)	1089 (83%)	176 (13%)	52 (4%)	3	6
4	E	93/99 (94%)	77 (83%)	12 (13%)	4 (4%)	2	5
4	O	93/99 (94%)	77 (83%)	10 (11%)	6 (6%)	1	2
5	F	341/423 (81%)	285 (84%)	37 (11%)	19 (6%)	2	3
5	P	341/423 (81%)	287 (84%)	36 (11%)	18 (5%)	2	3
All	All	6644/7590 (88%)	5517 (83%)	848 (13%)	279 (4%)	3	5

All (279) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	B	29	GLU
2	C	7	GLY
2	C	178	PRO
2	C	231	PRO
2	C	244	PRO
2	C	262	ALA
2	C	290	LEU
2	C	363	SER
2	C	369	PRO
2	C	465	GLY
2	C	517	ARG
2	C	548	PRO
2	C	598	GLU
2	C	627	ARG
2	C	767	PRO
2	C	864	GLY
2	C	908	GLY
2	C	1079	PRO
2	C	1106	ASP
3	D	55	ASP
3	D	82	LYS

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Mol	Chain	Res	Type
3	D	136	ASP
3	D	199	LEU
3	D	610	LYS
3	D	822	ALA
3	D	1129	THR
3	D	1208	ASP
3	D	1243	THR
3	D	1441	GLN
4	E	42	PRO
4	E	58	PRO
5	F	76	SER
5	F	95	THR
5	F	147	LEU
5	F	232	ARG
5	F	325	LYS
5	F	390	PHE
1	K	29	GLU
1	L	29	GLU
2	M	7	GLY
2	M	178	PRO
2	M	231	PRO
2	M	244	PRO
2	M	262	ALA
2	M	290	LEU
2	M	369	PRO
2	M	465	GLY
2	M	548	PRO
2	M	598	GLU
2	M	627	ARG
2	M	767	PRO
2	M	864	GLY
2	M	908	GLY
2	M	1079	PRO
2	M	1106	ASP
3	N	55	ASP
3	N	82	LYS
3	N	136	ASP
3	N	199	LEU
3	N	705	ALA
3	N	822	ALA
3	N	1129	THR
3	N	1208	ASP

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Mol	Chain	Res	Type
3	N	1243	THR
4	O	42	PRO
4	O	58	PRO
5	P	76	SER
5	P	95	THR
5	P	147	LEU
5	P	232	ARG
5	P	325	LYS
5	P	390	PHE
1	A	187	GLY
1	B	187	GLY
2	C	59	LYS
2	C	156	GLY
2	C	251	ASP
2	C	282	GLY
2	C	626	ARG
2	C	680	ASP
2	C	738	ASP
2	C	777	ILE
2	C	807	ARG
2	C	809	GLY
2	C	811	PRO
2	C	1004	LYS
3	D	24	GLY
3	D	98	PRO
3	D	137	PRO
3	D	504	ASP
3	D	588	GLY
3	D	616	GLN
3	D	705	ALA
3	D	803	GLY
3	D	1064	GLY
3	D	1196	THR
3	D	1265	ALA
4	E	4	PRO
5	F	153	PRO
5	F	255	ALA
5	F	416	ARG
1	K	187	GLY
1	L	187	GLY
2	M	59	LYS
2	M	156	GLY

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Mol	Chain	Res	Type
2	M	251	ASP
2	M	282	GLY
2	M	363	SER
2	M	517	ARG
2	M	626	ARG
2	M	680	ASP
2	M	738	ASP
2	M	777	ILE
2	M	807	ARG
2	M	809	GLY
2	M	811	PRO
2	M	1004	LYS
3	N	24	GLY
3	N	137	PRO
3	N	504	ASP
3	N	588	GLY
3	N	803	GLY
3	N	1064	GLY
3	N	1125	PRO
3	N	1197	ARG
3	N	1265	ALA
3	N	1342	GLU
3	N	1441	GLN
4	O	4	PRO
5	P	153	PRO
5	P	255	ALA
5	P	416	ARG
2	C	40	GLU
2	C	74	GLY
2	C	164	PRO
2	C	727	PRO
2	C	812	GLY
2	C	874	LEU
2	C	911	GLU
3	D	31	THR
3	D	47	GLU
3	D	96	ALA
3	D	119	SER
3	D	592	THR
3	D	594	PRO
3	D	807	ALA
3	D	844	ALA

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Mol	Chain	Res	Type
3	D	1125	PRO
3	D	1197	ARG
3	D	1241	PHE
3	D	1388	ARG
4	E	82	GLU
5	F	167	PRO
5	F	203	THR
5	F	286	PRO
5	F	297	PRO
5	F	341	PRO
5	F	393	THR
2	M	40	GLU
2	M	74	GLY
2	M	164	PRO
2	M	699	PHE
2	M	727	PRO
2	M	911	GLU
2	M	1045	ALA
3	N	31	THR
3	N	96	ALA
3	N	98	PRO
3	N	119	SER
3	N	592	THR
3	N	594	PRO
3	N	807	ALA
3	N	844	ALA
3	N	1111	ASP
3	N	1196	THR
3	N	1241	PHE
3	N	1388	ARG
4	O	82	GLU
5	P	167	PRO
5	P	203	THR
5	P	286	PRO
5	P	297	PRO
5	P	364	ARG
5	P	393	THR
1	A	26	GLU
2	C	111	ASP
2	C	170	PRO
2	C	250	ARG
2	C	699	PHE

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Mol	Chain	Res	Type
2	C	1045	ALA
3	D	484	PRO
3	D	1111	ASP
3	D	1432	LYS
5	F	421	PHE
2	M	111	ASP
2	M	170	PRO
2	M	188	LYS
2	M	250	ARG
2	M	268	ASP
2	M	812	GLY
3	N	484	PRO
3	N	526	PRO
3	N	617	ASN
3	N	892	ASP
3	N	1066	THR
3	N	1341	PRO
3	N	1432	LYS
5	P	421	PHE
2	C	53	PRO
2	C	188	LYS
2	C	268	ASP
2	C	400	PRO
2	C	1113	GLU
3	D	173	PRO
3	D	483	HIS
3	D	522	PRO
3	D	530	VAL
3	D	533	GLY
3	D	808	THR
3	D	892	ASP
3	D	1306	PRO
5	F	138	SER
1	K	26	GLU
2	M	10	ARG
2	M	53	PRO
2	M	90	TYR
2	M	292	ARG
2	M	984	GLU
2	M	1113	GLU
3	N	47	GLU
3	N	173	PRO

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Mol	Chain	Res	Type
3	N	483	HIS
3	N	522	PRO
3	N	766	ALA
3	N	808	THR
3	N	1306	PRO
5	P	341	PRO
2	C	10	ARG
2	C	90	TYR
2	C	180	GLY
2	C	377	PRO
2	C	1059	ASP
5	F	293	GLU
5	F	375	LEU
2	M	180	GLY
2	M	377	PRO
2	M	874	LEU
2	M	1005	MET
3	N	530	VAL
3	N	787	LEU
5	P	138	SER
2	C	336	VAL
3	D	526	PRO
3	D	1385	GLY
3	N	1385	GLY
2	C	264	PRO
2	C	415	PRO
1	K	9	PRO
2	M	261	ILE
2	M	336	VAL
2	M	415	PRO
2	M	505	GLY
3	N	1248	GLY
2	C	261	ILE
2	C	505	GLY
3	D	1248	GLY
1	L	9	PRO
2	M	264	PRO
2	M	529	VAL
3	N	1349	VAL
2	C	450	GLY
3	D	108	VAL
3	D	1267	ARG

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Mol	Chain	Res	Type
2	M	905	ILE
3	N	108	VAL
4	O	5	GLY
4	O	57	ASP
1	B	9	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%)	161 (80%)	41 (20%)	1	3
1	B	202/273 (74%)	163 (81%)	39 (19%)	1	3
1	K	202/273 (74%)	159 (79%)	43 (21%)	1	3
1	L	202/273 (74%)	166 (82%)	36 (18%)	2	4
2	C	941/941 (100%)	755 (80%)	186 (20%)	1	3
2	M	941/941 (100%)	757 (80%)	184 (20%)	1	3
3	D	1112/1279 (87%)	935 (84%)	177 (16%)	2	6
3	N	1112/1279 (87%)	934 (84%)	178 (16%)	2	6
4	E	84/88 (96%)	68 (81%)	16 (19%)	1	4
4	O	84/88 (96%)	68 (81%)	16 (19%)	1	4
5	F	295/370 (80%)	252 (85%)	43 (15%)	3	7
5	P	295/370 (80%)	254 (86%)	41 (14%)	3	8
All	All	5672/6448 (88%)	4672 (82%)	1000 (18%)	2	4

All (1000) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASP
1	A	9	PRO
1	A	12	THR
1	A	15	THR
1	A	16	GLN

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Mol	Chain	Res	Type
1	A	20	TYR
1	A	44	LEU
1	A	45	LEU
1	A	47	SER
1	A	67	THR
1	A	73	GLU
1	A	74	ASP
1	A	77	GLU
1	A	84	GLU
1	A	88	ARG
1	A	89	PHE
1	A	92	PRO
1	A	96	THR
1	A	101	LEU
1	A	115	LEU
1	A	120	VAL
1	A	121	GLU
1	A	127	LEU
1	A	133	GLU
1	A	142	VAL
1	A	145	ASP
1	A	154	GLU
1	A	167	VAL
1	A	170	VAL
1	A	180	GLN
1	A	184	THR
1	A	190	THR
1	A	196	THR
1	A	197	LEU
1	A	198	ARG
1	A	205	VAL
1	A	211	LEU
1	A	216	GLU
1	A	223	THR
1	A	227	ASN
1	A	229	GLN
1	B	1	MET
1	B	3	ASP
1	B	25	LEU
1	B	26	GLU
1	B	27	PRO
1	B	38	ASN

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Mol	Chain	Res	Type
1	B	47	SER
1	B	62	LEU
1	B	67	THR
1	B	69	PRO
1	B	73	GLU
1	B	74	ASP
1	B	77	GLU
1	B	82	LEU
1	B	89	PHE
1	B	96	THR
1	B	112	ARG
1	B	119	ASP
1	B	123	MET
1	B	124	ASN
1	B	126	ASP
1	B	137	ARG
1	B	140	MET
1	B	154	GLU
1	B	162	ILE
1	B	170	VAL
1	B	184	THR
1	B	188	GLN
1	B	190	THR
1	B	192	LEU
1	B	196	THR
1	B	197	LEU
1	B	200	TRP
1	B	206	THR
1	B	208	LEU
1	B	209	GLU
1	B	213	GLN
1	B	220	GLU
1	B	227	ASN
2	C	6	PHE
2	C	11	GLU
2	C	15	LEU
2	C	24	GLU
2	C	26	TYR
2	C	30	LEU
2	C	34	VAL
2	C	35	PRO
2	C	36	PRO

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Mol	Chain	Res	Type
2	C	37	GLU
2	C	41	ASN
2	C	44	ILE
2	C	48	PHE
2	C	52	PHE
2	C	58	ASP
2	C	73	LEU
2	C	81	ASP
2	C	89	THR
2	C	94	LEU
2	C	95	TYR
2	C	98	LEU
2	C	100	LEU
2	C	104	ASP
2	C	108	ILE
2	C	112	GLU
2	C	114	PHE
2	C	115	LEU
2	C	117	HIS
2	C	129	ILE
2	C	133	ASP
2	C	140	ILE
2	C	141	HIS
2	C	149	THR
2	C	151	ASP
2	C	158	TYR
2	C	163	ILE
2	C	178	PRO
2	C	182	VAL
2	C	186	VAL
2	C	194	VAL
2	C	196	LEU
2	C	205	GLU
2	C	209	ARG
2	C	221	LEU
2	C	223	ASP
2	C	229	MET
2	C	238	LEU
2	C	239	PHE
2	C	241	LEU
2	C	254	VAL
2	C	257	VAL

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Mol	Chain	Res	Type
2	C	260	LEU
2	C	264	PRO
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	297	GLU
2	C	303	PHE
2	C	304	LEU
2	C	309	TYR
2	C	321	GLU
2	C	332	ARG
2	C	339	LEU
2	C	343	GLN
2	C	359	MET
2	C	360	LEU
2	C	365	ASP
2	C	366	SER
2	C	367	LEU
2	C	392	SER
2	C	393	GLN
2	C	394	PHE
2	C	396	ASP
2	C	398	THR
2	C	402	SER
2	C	413	LEU
2	C	415	PRO
2	C	420	ARG
2	C	425	PHE
2	C	426	ASP
2	C	427	VAL
2	C	443	THR
2	C	448	ASN
2	C	451	LEU
2	C	452	ILE
2	C	454	SER
2	C	463	GLU
2	C	469	THR
2	C	479	VAL
2	C	486	MET

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Mol	Chain	Res	Type
2	C	508	ILE
2	C	516	ARG
2	C	528	GLU
2	C	533	ASP
2	C	542	VAL
2	C	543	ASN
2	C	557	ARG
2	C	559	LEU
2	C	564	MET
2	C	566	THR
2	C	578	VAL
2	C	583	LEU
2	C	584	GLU
2	C	605	LYS
2	C	607	ASP
2	C	614	ARG
2	C	619	ARG
2	C	633	GLN
2	C	645	VAL
2	C	657	ASP
2	C	661	SER
2	C	663	ASN
2	C	668	LEU
2	C	671	ASN
2	C	672	VAL
2	C	674	VAL
2	C	679	PHE
2	C	685	GLU
2	C	690	ILE
2	C	693	GLU
2	C	698	ASP
2	C	699	PHE
2	C	701	THR
2	C	725	ASP
2	C	727	PRO
2	C	729	LEU
2	C	734	LEU
2	C	737	LEU
2	C	758	ARG
2	C	760	SER
2	C	765	SER
2	C	769	PRO

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Mol	Chain	Res	Type
2	C	775	ARG
2	C	780	GLU
2	C	785	VAL
2	C	799	ILE
2	C	821	GLU
2	C	839	LEU
2	C	841	ASN
2	C	853	LEU
2	C	861	LEU
2	C	862	PRO
2	C	863	ASP
2	C	868	ASP
2	C	870	ILE
2	C	881	ASN
2	C	890	LEU
2	C	901	TYR
2	C	904	PRO
2	C	905	ILE
2	C	907	ASP
2	C	916	GLU
2	C	923	GLU
2	C	925	TYR
2	C	937	ASP
2	C	950	LEU
2	C	953	VAL
2	C	959	PRO
2	C	971	LYS
2	C	981	GLU
2	C	984	GLU
2	C	995	MET
2	C	1002	GLU
2	C	1016	ILE
2	C	1017	THR
2	C	1018	GLN
2	C	1030	GLN
2	C	1034	GLU
2	C	1035	MET
2	C	1036	GLU
2	C	1054	THR
2	C	1060	ILE
2	C	1079	PRO
2	C	1087	VAL

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Mol	Chain	Res	Type
2	C	1092	LEU
2	C	1095	LEU
2	C	1098	ASP
2	C	1100	GLN
2	C	1109	VAL
2	C	1110	ASP
2	C	1117	SER
2	C	1118	LYS
2	C	1119	ARG
3	D	12	LEU
3	D	14	SER
3	D	15	PRO
3	D	32	ILE
3	D	40	GLU
3	D	56	TYR
3	D	80	VAL
3	D	85	VAL
3	D	101	HIS
3	D	102	ILE
3	D	112	ILE
3	D	115	LEU
3	D	116	LEU
3	D	117	ASP
3	D	128	TYR
3	D	133	ILE
3	D	135	LEU
3	D	136	ASP
3	D	141	ILE
3	D	145	VAL
3	D	153	LEU
3	D	155	ASP
3	D	160	GLU
3	D	166	GLN
3	D	171	LEU
3	D	187	LYS
3	D	189	GLN
3	D	190	GLU
3	D	197	SER
3	D	205	TYR
3	D	394	LEU
3	D	400	VAL
3	D	402	PRO

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Mol	Chain	Res	Type
3	D	405	ASP
3	D	406	ASP
3	D	438	ASP
3	D	456	MET
3	D	465	LEU
3	D	489	ARG
3	D	493	ARG
3	D	504	ASP
3	D	505	SER
3	D	508	ARG
3	D	521	PRO
3	D	554	LEU
3	D	565	ILE
3	D	569	ASN
3	D	573	MET
3	D	581	LEU
3	D	591	VAL
3	D	594	PRO
3	D	605	ASP
3	D	608	SER
3	D	615	ARG
3	D	617	ASN
3	D	619	LEU
3	D	624	ASP
3	D	625	TYR
3	D	636	GLN
3	D	641	GLN
3	D	660	LYS
3	D	695	ILE
3	D	704	ARG
3	D	719	VAL
3	D	724	GLN
3	D	726	ILE
3	D	736	PHE
3	D	739	ASP
3	D	741	ASP
3	D	749	VAL
3	D	754	PHE
3	D	756	GLN
3	D	781	PRO
3	D	783	ARG
3	D	792	ILE

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Mol	Chain	Res	Type
3	D	810	GLU
3	D	824	ASN
3	D	832	ARG
3	D	839	LEU
3	D	845	ASN
3	D	847	ASP
3	D	861	GLN
3	D	863	VAL
3	D	864	VAL
3	D	865	THR
3	D	868	TYR
3	D	876	SER
3	D	880	ILE
3	D	888	GLU
3	D	892	ASP
3	D	899	LEU
3	D	901	GLN
3	D	914	LEU
3	D	915	VAL
3	D	942	SER
3	D	944	THR
3	D	948	THR
3	D	951	ILE
3	D	958	GLU
3	D	959	GLU
3	D	968	ASP
3	D	972	LEU
3	D	975	GLU
3	D	984	THR
3	D	985	ASP
3	D	999	THR
3	D	1001	GLU
3	D	1003	VAL
3	D	1023	MET
3	D	1025	GLN
3	D	1032	PRO
3	D	1033	GLN
3	D	1038	LEU
3	D	1041	LEU
3	D	1051	GLU
3	D	1052	THR
3	D	1065	LEU

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Mol	Chain	Res	Type
3	D	1068	LEU
3	D	1074	SER
3	D	1083	ASP
3	D	1090	ASP
3	D	1093	TYR
3	D	1095	THR
3	D	1109	GLU
3	D	1111	ASP
3	D	1112	CYS
3	D	1115	THR
3	D	1116	ASN
3	D	1129	THR
3	D	1132	LEU
3	D	1134	LEU
3	D	1151	ARG
3	D	1166	LEU
3	D	1173	LEU
3	D	1183	ILE
3	D	1198	TYR
3	D	1207	TYR
3	D	1228	SER
3	D	1234	THR
3	D	1243	THR
3	D	1251	ASP
3	D	1252	ILE
3	D	1258	ARG
3	D	1260	ILE
3	D	1274	ILE
3	D	1280	VAL
3	D	1290	LEU
3	D	1299	PHE
3	D	1302	GLU
3	D	1305	LEU
3	D	1315	ASP
3	D	1320	GLU
3	D	1344	VAL
3	D	1345	GLU
3	D	1348	LEU
3	D	1359	GLN
3	D	1363	LEU
3	D	1382	THR
3	D	1383	ASP

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Mol	Chain	Res	Type
3	D	1387	SER
3	D	1407	LEU
3	D	1415	VAL
3	D	1420	LEU
3	D	1431	THR
3	D	1433	SER
3	D	1439	SER
3	D	1440	PHE
3	D	1441	GLN
3	D	1460	ILE
3	D	1465	ASN
3	D	1466	VAL
3	D	1468	LEU
3	D	1478	SER
3	D	1485	GLN
3	D	1488	ASP
3	D	1491	THR
3	D	1496	GLU
4	E	4	PRO
4	E	20	THR
4	E	30	LEU
4	E	41	GLU
4	E	42	PRO
4	E	43	GLU
4	E	46	PRO
4	E	51	LEU
4	E	56	ASP
4	E	57	ASP
4	E	62	THR
4	E	67	GLU
4	E	72	ARG
4	E	79	LEU
4	E	81	PRO
4	E	94	PRO
5	F	79	ASP
5	F	83	GLN
5	F	84	TYR
5	F	86	HIS
5	F	91	VAL
5	F	94	LEU
5	F	117	SER
5	F	122	LEU

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Mol	Chain	Res	Type
5	F	123	ASP
5	F	125	ASP
5	F	127	ILE
5	F	135	ILE
5	F	145	PRO
5	F	149	GLU
5	F	150	THR
5	F	169	GLU
5	F	174	LEU
5	F	178	ARG
5	F	192	LEU
5	F	194	LEU
5	F	225	GLU
5	F	240	THR
5	F	245	GLN
5	F	249	ARG
5	F	262	VAL
5	F	281	GLU
5	F	282	LEU
5	F	291	ILE
5	F	297	PRO
5	F	317	LEU
5	F	335	ASP
5	F	336	GLU
5	F	341	PRO
5	F	348	SER
5	F	351	SER
5	F	353	GLU
5	F	362	SER
5	F	372	ARG
5	F	393	THR
5	F	399	GLN
5	F	408	LEU
5	F	410	TYR
5	F	420	ASP
1	K	3	ASP
1	K	9	PRO
1	K	12	THR
1	K	15	THR
1	K	16	GLN
1	K	20	TYR
1	K	44	LEU

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Mol	Chain	Res	Type
1	K	45	LEU
1	K	47	SER
1	K	67	THR
1	K	73	GLU
1	K	74	ASP
1	K	80	LEU
1	K	82	LEU
1	K	84	GLU
1	K	86	VAL
1	K	88	ARG
1	K	89	PHE
1	K	92	PRO
1	K	96	THR
1	K	101	LEU
1	K	115	LEU
1	K	120	VAL
1	K	121	GLU
1	K	127	LEU
1	K	133	GLU
1	K	142	VAL
1	K	154	GLU
1	K	167	VAL
1	K	170	VAL
1	K	180	GLN
1	K	184	THR
1	K	190	THR
1	K	196	THR
1	K	197	LEU
1	K	198	ARG
1	K	206	THR
1	K	211	LEU
1	K	216	GLU
1	K	222	LEU
1	K	223	THR
1	K	227	ASN
1	K	229	GLN
1	L	1	MET
1	L	9	PRO
1	L	25	LEU
1	L	26	GLU
1	L	27	PRO
1	L	38	ASN

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Mol	Chain	Res	Type
1	L	62	LEU
1	L	67	THR
1	L	69	PRO
1	L	73	GLU
1	L	74	ASP
1	L	77	GLU
1	L	89	PHE
1	L	96	THR
1	L	112	ARG
1	L	119	ASP
1	L	124	ASN
1	L	126	ASP
1	L	137	ARG
1	L	140	MET
1	L	154	GLU
1	L	162	ILE
1	L	173	PRO
1	L	184	THR
1	L	188	GLN
1	L	190	THR
1	L	192	LEU
1	L	193	ASP
1	L	196	THR
1	L	197	LEU
1	L	200	TRP
1	L	206	THR
1	L	207	PRO
1	L	208	LEU
1	L	209	GLU
1	L	227	ASN
2	M	11	GLU
2	M	24	GLU
2	M	26	TYR
2	M	30	LEU
2	M	34	VAL
2	M	35	PRO
2	M	37	GLU
2	M	41	ASN
2	M	44	ILE
2	M	48	PHE
2	M	52	PHE
2	M	73	LEU

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Mol	Chain	Res	Type
2	M	79	PRO
2	M	81	ASP
2	M	89	THR
2	M	94	LEU
2	M	95	TYR
2	M	98	LEU
2	M	100	LEU
2	M	104	ASP
2	M	108	ILE
2	M	112	GLU
2	M	114	PHE
2	M	115	LEU
2	M	117	HIS
2	M	133	ASP
2	M	140	ILE
2	M	141	HIS
2	M	149	THR
2	M	150	PRO
2	M	151	ASP
2	M	158	TYR
2	M	163	ILE
2	M	182	VAL
2	M	186	VAL
2	M	191	PHE
2	M	194	VAL
2	M	205	GLU
2	M	209	ARG
2	M	219	GLN
2	M	221	LEU
2	M	222	MET
2	M	229	MET
2	M	235	LEU
2	M	238	LEU
2	M	239	PHE
2	M	241	LEU
2	M	254	VAL
2	M	256	TYR
2	M	257	VAL
2	M	260	LEU
2	M	264	PRO
2	M	267	TYR
2	M	275	TYR

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Mol	Chain	Res	Type
2	M	279	GLU
2	M	281	LEU
2	M	285	LEU
2	M	286	SER
2	M	290	LEU
2	M	297	GLU
2	M	303	PHE
2	M	304	LEU
2	M	309	TYR
2	M	321	GLU
2	M	332	ARG
2	M	339	LEU
2	M	343	GLN
2	M	359	MET
2	M	360	LEU
2	M	365	ASP
2	M	366	SER
2	M	367	LEU
2	M	384	GLU
2	M	392	SER
2	M	393	GLN
2	M	394	PHE
2	M	396	ASP
2	M	402	SER
2	M	413	LEU
2	M	415	PRO
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	452	ILE
2	M	454	SER
2	M	463	GLU
2	M	469	THR
2	M	474	VAL
2	M	479	VAL
2	M	502	PRO
2	M	508	ILE
2	M	516	ARG

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Mol	Chain	Res	Type
2	M	524	VAL
2	M	527	GLU
2	M	528	GLU
2	M	533	ASP
2	M	537	LYS
2	M	542	VAL
2	M	543	ASN
2	M	559	LEU
2	M	564	MET
2	M	566	THR
2	M	583	LEU
2	M	588	VAL
2	M	605	LYS
2	M	607	ASP
2	M	614	ARG
2	M	619	ARG
2	M	633	GLN
2	M	645	VAL
2	M	657	ASP
2	M	661	SER
2	M	663	ASN
2	M	668	LEU
2	M	671	ASN
2	M	672	VAL
2	M	674	VAL
2	M	679	PHE
2	M	684	PHE
2	M	690	ILE
2	M	693	GLU
2	M	697	ARG
2	M	698	ASP
2	M	699	PHE
2	M	701	THR
2	M	725	ASP
2	M	727	PRO
2	M	729	LEU
2	M	734	LEU
2	M	737	LEU
2	M	758	ARG
2	M	760	SER
2	M	765	SER
2	M	775	ARG

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Mol	Chain	Res	Type
2	M	785	VAL
2	M	794	PRO
2	M	799	ILE
2	M	821	GLU
2	M	822	VAL
2	M	839	LEU
2	M	841	ASN
2	M	853	LEU
2	M	861	LEU
2	M	862	PRO
2	M	863	ASP
2	M	870	ILE
2	M	881	ASN
2	M	890	LEU
2	M	901	TYR
2	M	904	PRO
2	M	905	ILE
2	M	907	ASP
2	M	916	GLU
2	M	917	LEU
2	M	923	GLU
2	M	937	ASP
2	M	950	LEU
2	M	953	VAL
2	M	959	PRO
2	M	981	GLU
2	M	984	GLU
2	M	995	MET
2	M	1002	GLU
2	M	1016	ILE
2	M	1017	THR
2	M	1018	GLN
2	M	1030	GLN
2	M	1035	MET
2	M	1036	GLU
2	M	1054	THR
2	M	1060	ILE
2	M	1075	ASP
2	M	1079	PRO
2	M	1087	VAL
2	M	1092	LEU
2	M	1098	ASP

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Mol	Chain	Res	Type
2	M	1109	VAL
2	M	1110	ASP
2	M	1117	SER
2	M	1118	LYS
3	N	3	LYS
3	N	12	LEU
3	N	14	SER
3	N	15	PRO
3	N	20	SER
3	N	32	ILE
3	N	40	GLU
3	N	80	VAL
3	N	82	LYS
3	N	85	VAL
3	N	102	ILE
3	N	115	LEU
3	N	116	LEU
3	N	117	ASP
3	N	128	TYR
3	N	133	ILE
3	N	135	LEU
3	N	136	ASP
3	N	141	ILE
3	N	145	VAL
3	N	153	LEU
3	N	155	ASP
3	N	160	GLU
3	N	166	GLN
3	N	171	LEU
3	N	181	ASP
3	N	187	LYS
3	N	189	GLN
3	N	190	GLU
3	N	193	PRO
3	N	197	SER
3	N	205	TYR
3	N	394	LEU
3	N	400	VAL
3	N	402	PRO
3	N	405	ASP
3	N	406	ASP
3	N	431	VAL

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Mol	Chain	Res	Type
3	N	438	ASP
3	N	449	SER
3	N	456	MET
3	N	461	ILE
3	N	465	LEU
3	N	489	ARG
3	N	493	ARG
3	N	504	ASP
3	N	505	SER
3	N	521	PRO
3	N	565	ILE
3	N	569	ASN
3	N	581	LEU
3	N	590	PRO
3	N	591	VAL
3	N	594	PRO
3	N	605	ASP
3	N	614	PHE
3	N	615	ARG
3	N	617	ASN
3	N	619	LEU
3	N	624	ASP
3	N	636	GLN
3	N	639	LEU
3	N	641	GLN
3	N	642	CYS
3	N	660	LYS
3	N	682	ASP
3	N	688	TRP
3	N	704	ARG
3	N	719	VAL
3	N	724	GLN
3	N	726	ILE
3	N	736	PHE
3	N	739	ASP
3	N	741	ASP
3	N	749	VAL
3	N	754	PHE
3	N	781	PRO
3	N	783	ARG
3	N	792	ILE
3	N	810	GLU

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Mol	Chain	Res	Type
3	N	824	ASN
3	N	832	ARG
3	N	839	LEU
3	N	847	ASP
3	N	863	VAL
3	N	864	VAL
3	N	865	THR
3	N	880	ILE
3	N	888	GLU
3	N	892	ASP
3	N	899	LEU
3	N	901	GLN
3	N	910	SER
3	N	915	VAL
3	N	942	SER
3	N	944	THR
3	N	948	THR
3	N	951	ILE
3	N	958	GLU
3	N	959	GLU
3	N	968	ASP
3	N	972	LEU
3	N	975	GLU
3	N	985	ASP
3	N	1001	GLU
3	N	1003	VAL
3	N	1023	MET
3	N	1025	GLN
3	N	1032	PRO
3	N	1033	GLN
3	N	1038	LEU
3	N	1041	LEU
3	N	1051	GLU
3	N	1052	THR
3	N	1065	LEU
3	N	1068	LEU
3	N	1083	ASP
3	N	1090	ASP
3	N	1095	THR
3	N	1109	GLU
3	N	1112	CYS
3	N	1115	THR

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Mol	Chain	Res	Type
3	N	1116	ASN
3	N	1129	THR
3	N	1133	ARG
3	N	1134	LEU
3	N	1151	ARG
3	N	1166	LEU
3	N	1173	LEU
3	N	1183	ILE
3	N	1198	TYR
3	N	1207	TYR
3	N	1210	SER
3	N	1228	SER
3	N	1243	THR
3	N	1251	ASP
3	N	1252	ILE
3	N	1258	ARG
3	N	1260	ILE
3	N	1274	ILE
3	N	1280	VAL
3	N	1290	LEU
3	N	1299	PHE
3	N	1300	SER
3	N	1302	GLU
3	N	1305	LEU
3	N	1306	PRO
3	N	1311	LEU
3	N	1315	ASP
3	N	1320	GLU
3	N	1344	VAL
3	N	1345	GLU
3	N	1348	LEU
3	N	1350	GLU
3	N	1363	LEU
3	N	1382	THR
3	N	1383	ASP
3	N	1403	LEU
3	N	1407	LEU
3	N	1415	VAL
3	N	1419	PRO
3	N	1420	LEU
3	N	1424	VAL
3	N	1431	THR

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Mol	Chain	Res	Type
3	N	1433	SER
3	N	1440	PHE
3	N	1441	GLN
3	N	1460	ILE
3	N	1462	LEU
3	N	1465	ASN
3	N	1466	VAL
3	N	1468	LEU
3	N	1478	SER
3	N	1481	VAL
3	N	1485	GLN
3	N	1488	ASP
3	N	1491	THR
3	N	1496	GLU
4	O	4	PRO
4	O	15	SER
4	O	20	THR
4	O	30	LEU
4	O	41	GLU
4	O	42	PRO
4	O	43	GLU
4	O	46	PRO
4	O	51	LEU
4	O	56	ASP
4	O	57	ASP
4	O	62	THR
4	O	67	GLU
4	O	79	LEU
4	O	81	PRO
4	O	94	PRO
5	P	80	PRO
5	P	83	GLN
5	P	84	TYR
5	P	86	HIS
5	P	91	VAL
5	P	94	LEU
5	P	117	SER
5	P	122	LEU
5	P	123	ASP
5	P	125	ASP
5	P	127	ILE
5	P	135	ILE

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Mol	Chain	Res	Type
5	P	149	GLU
5	P	174	LEU
5	P	178	ARG
5	P	194	LEU
5	P	225	GLU
5	P	240	THR
5	P	245	GLN
5	P	249	ARG
5	P	259	ARG
5	P	261	PRO
5	P	262	VAL
5	P	281	GLU
5	P	282	LEU
5	P	297	PRO
5	P	317	LEU
5	P	335	ASP
5	P	336	GLU
5	P	338	LEU
5	P	341	PRO
5	P	342	VAL
5	P	348	SER
5	P	350	LEU
5	P	351	SER
5	P	353	GLU
5	P	362	SER
5	P	393	THR
5	P	408	LEU
5	P	410	TYR
5	P	420	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (159) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	63	HIS
1	A	81	ASN
1	A	124	ASN
1	A	139	ASN
1	A	156	HIS
1	A	180	GLN
1	A	221	HIS
1	A	227	ASN

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Mol	Chain	Res	Type
1	A	229	GLN
1	B	38	ASN
1	B	95	GLN
1	B	124	ASN
1	B	128	HIS
1	B	163	ASN
1	B	180	GLN
1	B	227	ASN
2	C	31	GLN
2	C	41	ASN
2	C	117	HIS
2	C	130	ASN
2	C	139	GLN
2	C	204	GLN
2	C	343	GLN
2	C	393	GLN
2	C	431	HIS
2	C	434	HIS
2	C	498	GLN
2	C	609	ASN
2	C	632	ASN
2	C	639	GLN
2	C	663	ASN
2	C	670	GLN
2	C	671	ASN
2	C	834	GLN
2	C	841	ASN
2	C	881	ASN
2	C	889	HIS
2	C	899	GLN
2	C	969	GLN
2	C	1018	GLN
2	C	1019	GLN
2	C	1047	HIS
2	C	1107	ASN
3	D	66	GLN
3	D	143	ASN
3	D	151	GLN
3	D	166	GLN
3	D	507	ASN
3	D	549	ASN
3	D	611	GLN

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Mol	Chain	Res	Type
3	D	727	GLN
3	D	756	GLN
3	D	816	HIS
3	D	824	ASN
3	D	861	GLN
3	D	1005	GLN
3	D	1025	GLN
3	D	1116	ASN
3	D	1195	GLN
3	D	1202	GLN
3	D	1323	GLN
3	D	1441	GLN
3	D	1465	ASN
3	D	1485	GLN
4	E	28	GLN
4	E	29	GLN
4	E	37	ASN
4	E	59	ASN
4	E	86	GLN
5	F	83	GLN
5	F	86	HIS
5	F	90	GLN
5	F	245	GLN
5	F	312	GLN
5	F	337	HIS
5	F	402	ASN
1	K	63	HIS
1	K	124	ASN
1	K	128	HIS
1	K	139	ASN
1	K	156	HIS
1	K	163	ASN
1	K	180	GLN
1	K	227	ASN
1	K	229	GLN
1	L	38	ASN
1	L	95	GLN
1	L	124	ASN
1	L	128	HIS
1	L	163	ASN
1	L	180	GLN
1	L	227	ASN

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Mol	Chain	Res	Type
2	M	22	GLN
2	M	31	GLN
2	M	41	ASN
2	M	117	HIS
2	M	130	ASN
2	M	139	GLN
2	M	204	GLN
2	M	343	GLN
2	M	374	ASN
2	M	393	GLN
2	M	431	HIS
2	M	434	HIS
2	M	498	GLN
2	M	609	ASN
2	M	632	ASN
2	M	639	GLN
2	M	663	ASN
2	M	670	GLN
2	M	671	ASN
2	M	834	GLN
2	M	841	ASN
2	M	881	ASN
2	M	889	HIS
2	M	969	GLN
2	M	1019	GLN
2	M	1100	GLN
3	N	143	ASN
3	N	151	GLN
3	N	166	GLN
3	N	507	ASN
3	N	549	ASN
3	N	611	GLN
3	N	640	HIS
3	N	696	HIS
3	N	703	ASN
3	N	709	HIS
3	N	727	GLN
3	N	744	GLN
3	N	756	GLN
3	N	768	ASN
3	N	824	ASN
3	N	861	GLN

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Mol	Chain	Res	Type
3	N	994	GLN
3	N	1025	GLN
3	N	1046	GLN
3	N	1116	ASN
3	N	1195	GLN
3	N	1202	GLN
3	N	1323	GLN
3	N	1333	HIS
3	N	1334	GLN
3	N	1359	GLN
3	N	1404	ASN
3	N	1465	ASN
3	N	1485	GLN
4	O	28	GLN
4	O	29	GLN
4	O	37	ASN
4	O	59	ASN
4	O	86	GLN
5	P	83	GLN
5	P	86	HIS
5	P	90	GLN
5	P	214	GLN
5	P	312	GLN
5	P	402	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MXP	D	1527	-	25,30,30	2.87	11 (44%)	27,38,38	3.35	8 (29%)
7	MXP	N	1527	-	25,30,30	3.15	12 (48%)	27,38,38	3.56	11 (40%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MXP	D	1527	-	-	7/27/28/28	0/1/1/1
7	MXP	N	1527	-	-	7/27/28/28	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	N	1527	MXP	C9-C10	7.23	1.41	1.34
7	D	1527	MXP	C9-C10	6.34	1.40	1.34
7	D	1527	MXP	O1-C5	6.19	1.43	1.35
7	N	1527	MXP	O1-C5	6.18	1.43	1.35
7	N	1527	MXP	C1-C5	5.45	1.45	1.35
7	D	1527	MXP	C3-C6	4.81	1.59	1.50
7	N	1527	MXP	C3-C6	4.41	1.58	1.50
7	N	1527	MXP	C21-C20	4.32	1.38	1.32
7	D	1527	MXP	O6-C22	4.26	1.29	1.21
7	N	1527	MXP	O5-C22	-4.05	1.27	1.34
7	D	1527	MXP	C21-C20	3.96	1.38	1.32
7	D	1527	MXP	C9-C8	3.90	1.56	1.42
7	N	1527	MXP	C9-C8	3.82	1.56	1.42
7	N	1527	MXP	O6-C22	3.52	1.28	1.21
7	N	1527	MXP	O2-C2	3.50	1.43	1.36
7	D	1527	MXP	O5-C22	-3.38	1.28	1.34
7	D	1527	MXP	C1-C5	3.08	1.41	1.35
7	N	1527	MXP	C8-C7	3.03	1.43	1.34
7	D	1527	MXP	O5-C23	-3.02	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	N	1527	MXP	C7-C6	2.88	1.55	1.48
7	D	1527	MXP	C8-C7	2.65	1.42	1.34
7	N	1527	MXP	O5-C23	-2.63	1.39	1.45
7	D	1527	MXP	C7-C6	2.17	1.53	1.48

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	1527	MXP	O4-C6-C7	12.36	138.42	120.83
7	D	1527	MXP	O4-C6-C7	11.53	137.24	120.83
7	D	1527	MXP	C8-C9-C10	-6.76	116.93	127.30
7	N	1527	MXP	C8-C9-C10	-6.57	117.22	127.30
7	D	1527	MXP	C23-O5-C22	6.10	122.86	115.66
7	N	1527	MXP	C23-O5-C22	5.90	122.63	115.66
7	N	1527	MXP	O5-C22-N1	5.55	115.04	109.16
7	D	1527	MXP	O5-C22-N1	5.12	114.59	109.16
7	N	1527	MXP	C15-C7-C6	4.92	124.54	115.53
7	D	1527	MXP	C15-C7-C6	4.53	123.84	115.53
7	N	1527	MXP	O6-C22-N1	-3.84	120.10	125.41
7	D	1527	MXP	O6-C22-N1	-3.71	120.27	125.41
7	N	1527	MXP	O2-C2-C3	-3.04	118.35	121.76
7	N	1527	MXP	O1-C5-C1	-2.62	117.16	119.70
7	N	1527	MXP	O4-C6-C3	-2.56	113.92	119.91
7	D	1527	MXP	O4-C6-C3	-2.50	114.06	119.91
7	N	1527	MXP	C17-C5-C1	2.38	124.37	121.22
7	D	1527	MXP	C12-C11-C10	2.29	119.46	113.45
7	N	1527	MXP	C12-C11-C10	2.27	119.42	113.45

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	N	1527	MXP	C5-C17-C18-C19
7	D	1527	MXP	C5-C17-C18-C19
7	D	1527	MXP	C10-C11-C12-C13
7	D	1527	MXP	C2-C3-C6-O4
7	N	1527	MXP	C10-C11-C12-C13
7	N	1527	MXP	C18-C17-C5-C1
7	N	1527	MXP	C18-C19-C20-C21
7	D	1527	MXP	C18-C19-C20-C21
7	D	1527	MXP	C18-C17-C5-C1
7	N	1527	MXP	C2-C3-C6-O4

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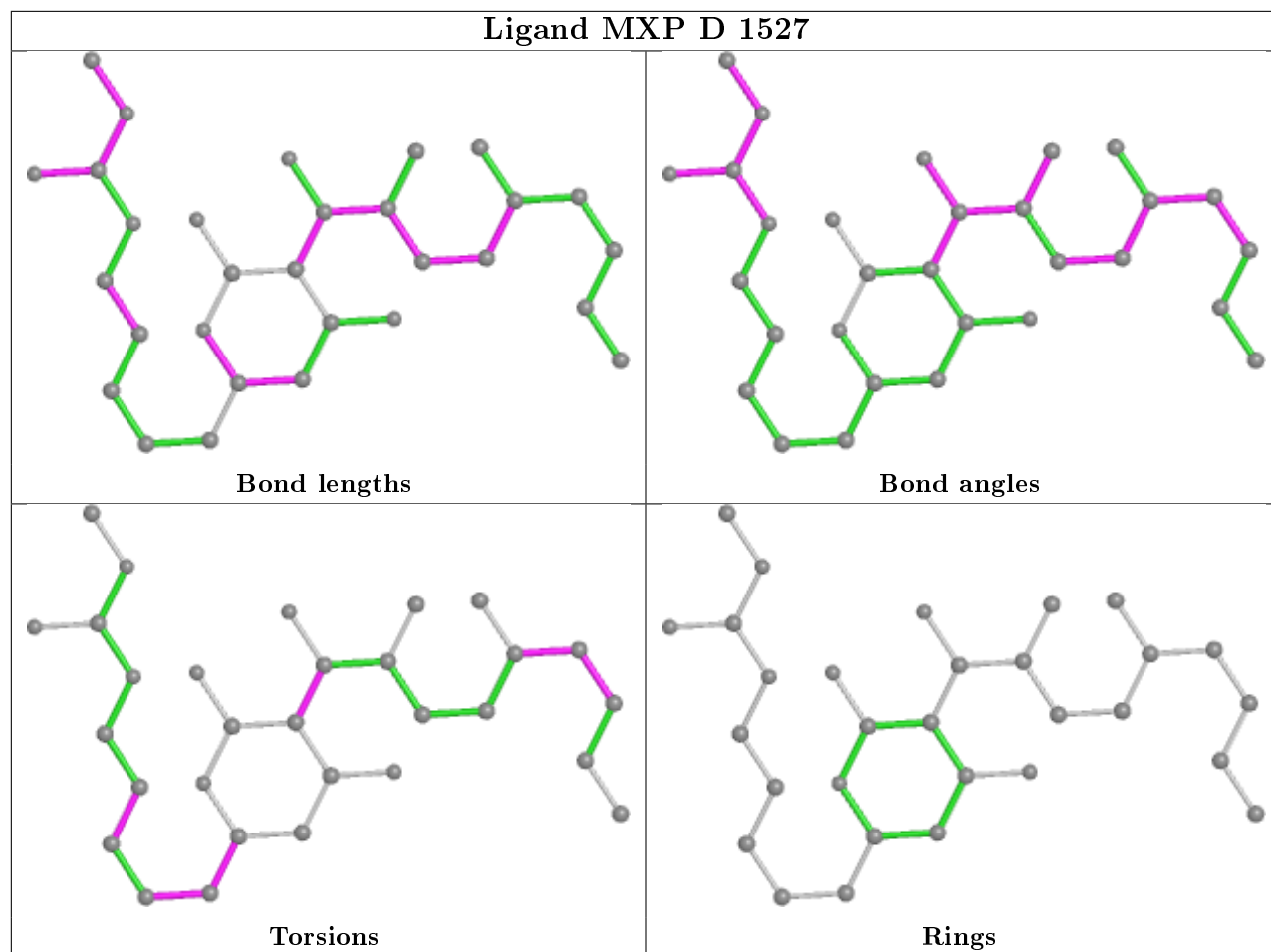
Mol	Chain	Res	Type	Atoms
7	D	1527	MXP	C16-C10-C11-C12
7	N	1527	MXP	C16-C10-C11-C12
7	N	1527	MXP	C9-C10-C11-C12
7	D	1527	MXP	C9-C10-C11-C12

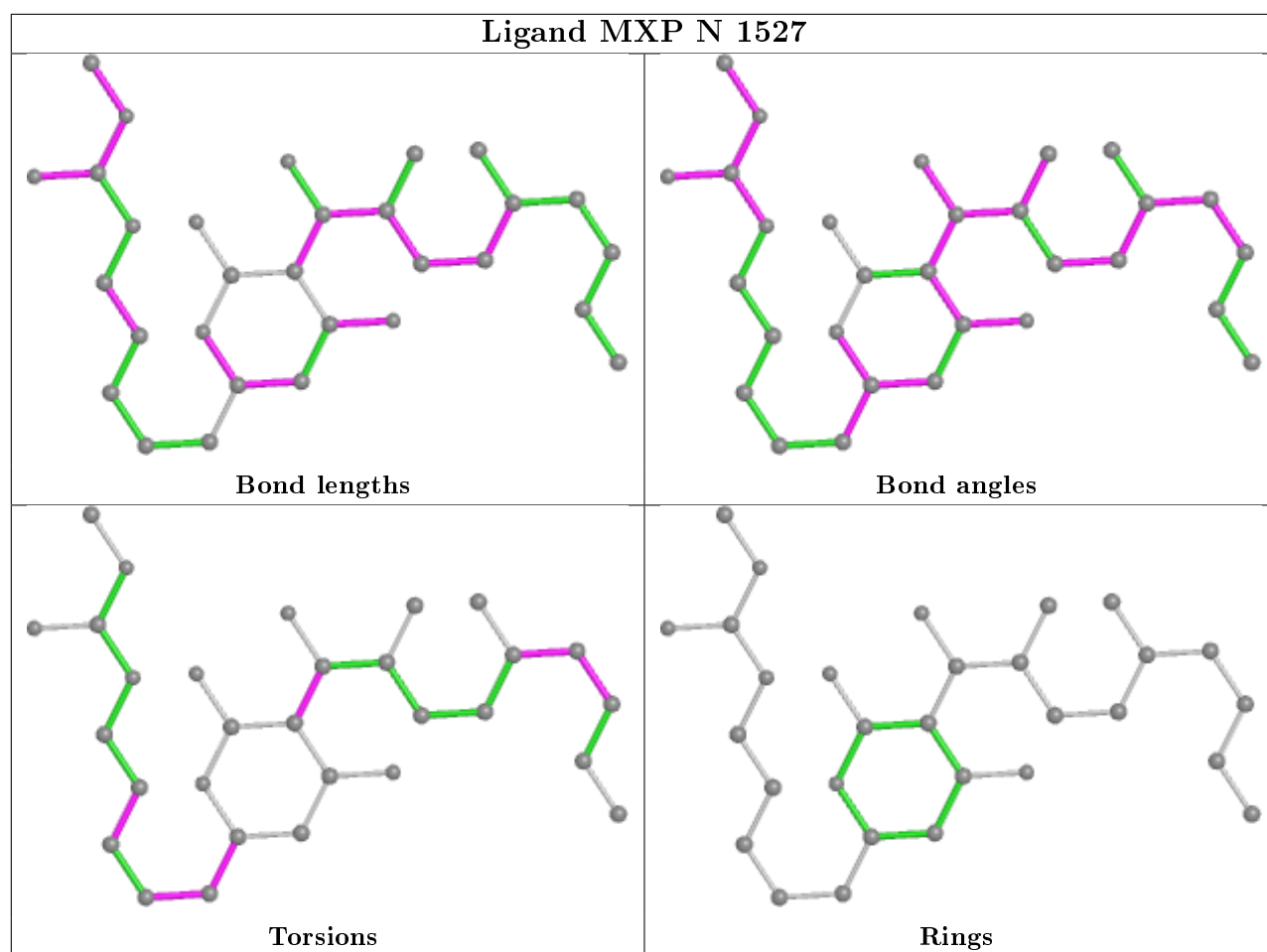
There are no ring outliers.

2 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	1527	MXP	18	0
7	N	1527	MXP	18	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	229/315 (72%)	-0.06	3 (1%) 77 78	28, 50, 78, 101	0
1	B	229/315 (72%)	-0.06	8 (3%) 44 44	36, 71, 86, 104	0
1	K	229/315 (72%)	-0.08	2 (0%) 84 85	25, 52, 81, 93	0
1	L	229/315 (72%)	-0.05	6 (2%) 56 57	47, 73, 86, 104	0
2	C	1119/1119 (100%)	-0.06	27 (2%) 59 60	14, 62, 88, 96	0
2	M	1119/1119 (100%)	-0.09	14 (1%) 77 78	11, 60, 86, 101	0
3	D	1321/1524 (86%)	-0.08	20 (1%) 73 76	10, 53, 85, 107	0
3	N	1321/1524 (86%)	-0.10	21 (1%) 72 74	11, 54, 85, 109	0
4	E	95/99 (95%)	-0.13	2 (2%) 63 65	30, 64, 90, 95	0
4	O	95/99 (95%)	-0.19	2 (2%) 63 65	29, 61, 83, 100	0
5	F	345/423 (81%)	-0.10	5 (1%) 75 77	27, 68, 89, 100	0
5	P	345/423 (81%)	-0.07	9 (2%) 56 57	23, 68, 91, 103	0
All	All	6676/7590 (87%)	-0.09	119 (1%) 68 70	10, 59, 87, 109	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	1241	PHE	8.6
3	N	1240	THR	6.2
3	N	1243	THR	6.1
2	C	186	VAL	6.0
2	M	186	VAL	5.8
3	D	1240	THR	5.7
3	D	1248	GLY	4.8
3	D	407	VAL	4.5
5	P	145	PRO	4.4
2	C	207	LEU	4.4
5	P	90	GLN	4.3

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Mol	Chain	Res	Type	RSRZ
2	C	307	LEU	4.2
3	N	1247	ALA	4.2
2	M	372	LEU	4.2
3	N	191	LEU	4.0
4	E	95	VAL	4.0
2	C	164	PRO	3.8
3	D	1245	GLY	3.8
1	L	1	MET	3.7
2	C	372	LEU	3.6
4	O	95	VAL	3.6
3	N	1398	TRP	3.6
2	M	418	LEU	3.6
3	N	1248	GLY	3.6
3	D	409	VAL	3.5
5	P	405	LEU	3.4
3	D	1398	TRP	3.4
3	D	1242	HIS	3.4
3	D	1246	VAL	3.4
3	N	802	ALA	3.4
3	D	1247	ALA	3.4
2	C	211	LEU	3.4
3	D	43	GLY	3.4
1	A	158	ILE	3.4
3	D	1243	THR	3.3
4	E	56	ASP	3.3
2	C	260	LEU	3.3
2	C	226	VAL	3.3
3	N	1238	MET	3.3
1	A	1	MET	3.2
3	N	1242	HIS	3.2
3	N	839	LEU	3.2
1	B	6	LEU	3.1
3	N	611	GLN	3.1
3	N	1246	VAL	3.1
5	P	88	ILE	3.1
2	C	306	THR	3.1
5	F	142	ARG	3.0
1	B	1	MET	3.0
1	K	5	LYS	2.9
1	K	6	LEU	2.8
2	M	615	TYR	2.8
2	M	269	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
3	N	1241	PHE	2.8
3	D	422	ALA	2.7
5	F	150	THR	2.7
1	L	2	LEU	2.7
3	N	203	ALA	2.7
1	B	71	VAL	2.7
1	B	138	LEU	2.6
2	C	208	ALA	2.5
5	P	354	LEU	2.5
2	C	65	VAL	2.5
2	M	417	GLY	2.4
3	N	119	SER	2.4
2	M	105	THR	2.4
2	C	333	ILE	2.4
3	D	395	VAL	2.4
2	M	207	LEU	2.4
3	N	816	HIS	2.4
3	D	801	GLY	2.4
3	N	450	TYR	2.4
2	C	170	PRO	2.4
1	L	82	LEU	2.3
2	C	475	VAL	2.3
2	C	529	VAL	2.3
1	B	117	VAL	2.3
2	C	303	PHE	2.3
1	B	5	LYS	2.3
1	A	93	SER	2.3
3	D	1249	ALA	2.3
5	P	369	LEU	2.3
4	O	94	PRO	2.3
2	M	307	LEU	2.3
1	B	68	ILE	2.3
2	C	726	ILE	2.3
3	D	802	ALA	2.3
2	C	417	GLY	2.2
3	D	1407	LEU	2.2
2	C	373	VAL	2.2
5	P	144	ILE	2.2
2	C	183	SER	2.2
5	F	90	GLN	2.2
5	P	357	ALA	2.2
5	F	397	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	2	LEU	2.2
2	M	280	LYS	2.2
2	M	208	ALA	2.2
2	C	344	PHE	2.2
3	N	185	VAL	2.2
1	L	131	THR	2.2
1	L	5	LYS	2.1
3	D	1244	GLY	2.1
2	C	116	GLY	2.1
1	L	144	VAL	2.1
2	C	479	VAL	2.1
2	C	155	PRO	2.1
3	N	501	ALA	2.1
2	C	513	VAL	2.1
2	C	125	GLY	2.1
2	M	313	LEU	2.1
5	F	139	ALA	2.0
5	P	384	GLU	2.0
2	C	99	GLN	2.0
2	M	115	LEU	2.0
2	M	243	ARG	2.0
3	D	1401	GLU	2.0
3	N	806	PHE	2.0
3	N	489	ARG	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](#)

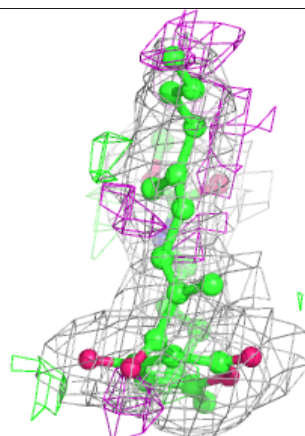
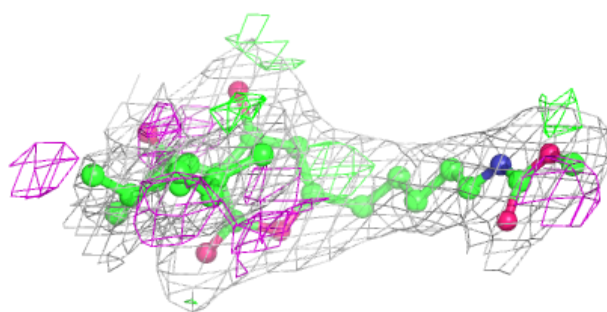
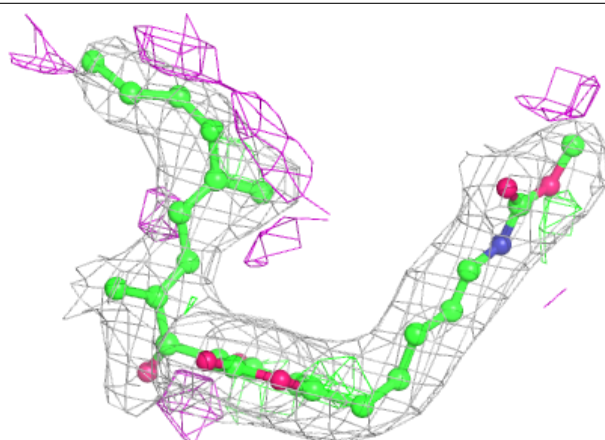
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	MXP	D	1527	30/30	0.96	0.19	13,20,27,34	0
7	MXP	N	1527	30/30	0.96	0.17	17,30,38,40	0
6	ZN	N	1526	1/1	0.97	0.18	66,66,66,66	0
8	MG	N	1528	1/1	0.97	0.07	41,41,41,41	0
6	ZN	D	1525	1/1	0.97	0.14	62,62,62,62	0
8	MG	D	1528	1/1	0.98	0.09	35,35,35,35	0
6	ZN	D	1526	1/1	0.99	0.21	48,48,48,48	0
6	ZN	N	1525	1/1	0.99	0.17	58,58,58,58	0

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

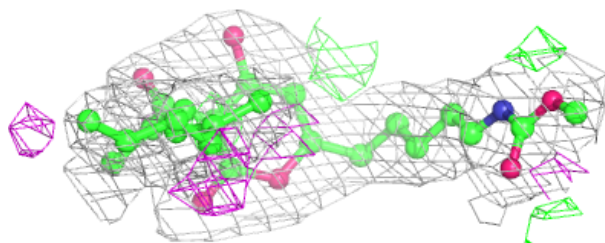
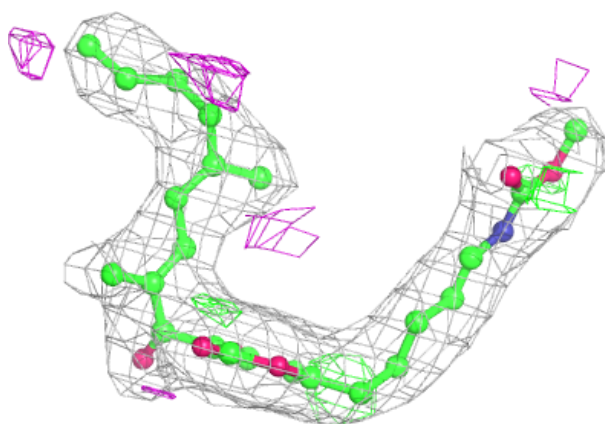
Electron density around MXP D 1527:

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



Electron density around MXP N 1527:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.