



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 04:23 pm BST

PDB ID : 2A69  
Title : Crystal structure of the T. Thermophilus RNA polymerase holoenzyme in complex with antibiotic rifapentin  
Authors : Artsimovitch, I.; Vassilyeva, M.N.; Svetlov, D.; Svetlov, V.; Perederina, A.; Igarashi, N.; Matsugaki, N.; Wakatsuki, S.; Tahirov, T.H.; Vassilyev, D.G.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2005-07-02  
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

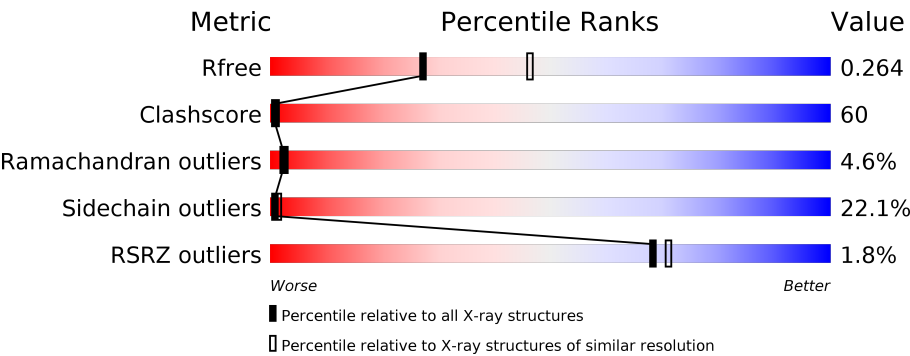
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	
1	B	315	
1	K	315	
1	L	315	
2	C	1119	
2	M	1119	

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Mol	Chain	Length	Quality of chain
3	D	1524	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>2%</div><div>23%</div><div>52%</div><div>16%</div><div>•</div><div>9%</div></div>
3	N	1524	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>2%</div><div>25%</div><div>51%</div><div>14%</div><div>•</div><div>9%</div></div>
4	E	99	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>5%</div><div>28%</div><div>49%</div><div>18%</div><div>•</div></div>
4	O	99	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>%</div><div>27%</div><div>49%</div><div>18%</div><div>•</div><div>•</div></div>
5	F	423	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>%</div><div>20%</div><div>46%</div><div>14%</div><div>•</div><div>18%</div></div>
5	P	423	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>%</div><div>20%</div><div>49%</div><div>11%</div><div>•</div><div>18%</div></div>

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 60572 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase alpha chain.

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

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

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

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

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

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

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

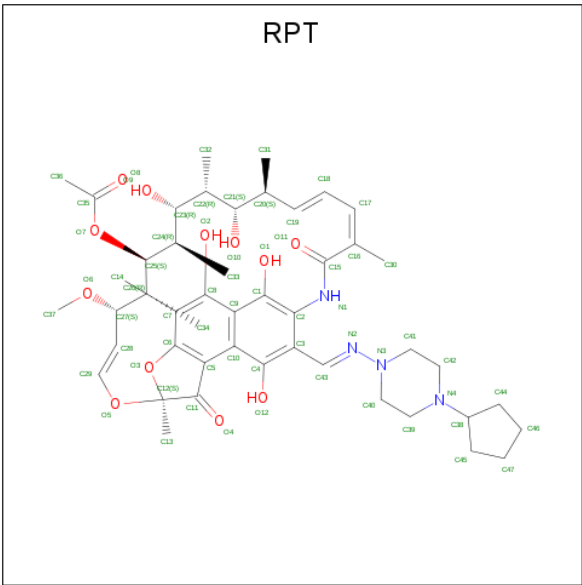
- Molecule 5 is a protein called RNA polymerase sigma factor rpoD.

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

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	P	20	Total	Mg	0	0
			20	20		
6	D	106	Total	Mg	0	0
			106	106		
6	K	19	Total	Mg	0	0
			19	19		
6	E	5	Total	Mg	0	0
			5	5		
6	B	21	Total	Mg	0	0
			21	21		
6	C	73	Total	Mg	0	0
			73	73		
6	A	33	Total	Mg	0	0
			33	33		
6	N	92	Total	Mg	0	0
			92	92		
6	O	8	Total	Mg	0	0
			8	8		
6	L	17	Total	Mg	0	0
			17	17		
6	F	28	Total	Mg	0	0
			28	28		
6	M	65	Total	Mg	0	0
			65	65		

- Molecule 7 is RIFAPENTINE (three-letter code: RPT) (formula: C<sub>47</sub>H<sub>64</sub>N<sub>4</sub>O<sub>12</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	N	O	0	0
			63	47	4	12		
7	M	1	Total	C	N	O	0	0
			63	47	4	12		

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	239	Total	O	0	0
			239	239		
9	B	258	Total	O	0	0
			258	258		
9	C	979	Total	O	0	0
			979	979		
9	D	1252	Total	O	0	0
			1252	1252		
9	E	117	Total	O	0	0
			117	117		

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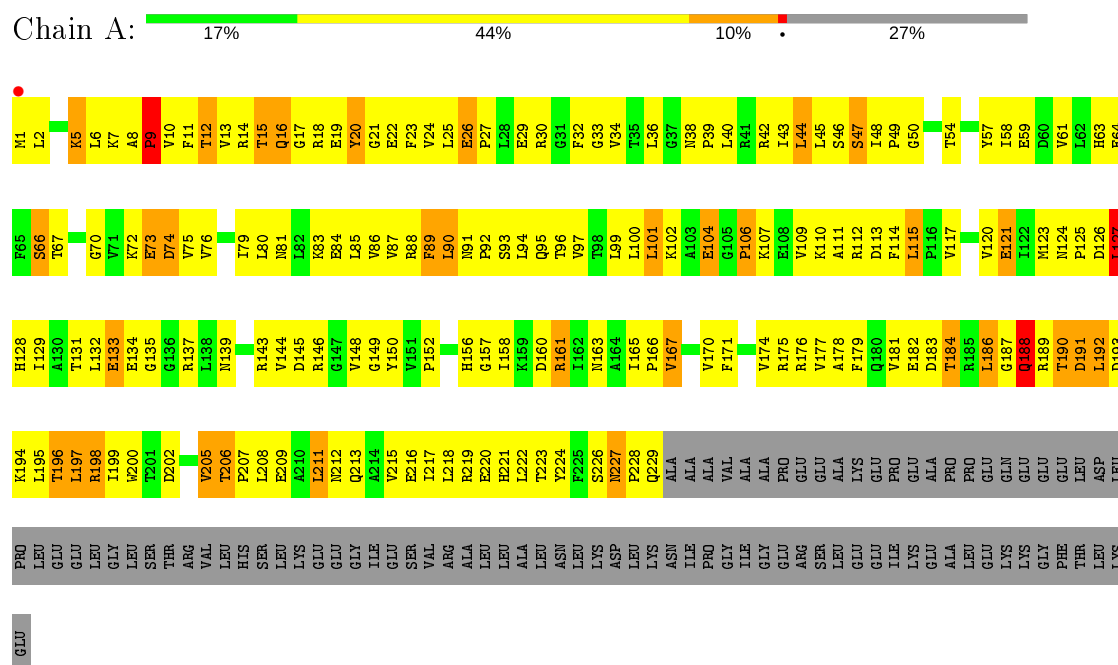
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	F	420	Total 420	O 420	0	0
9	K	183	Total 183	O 183	0	0
9	L	219	Total 219	O 219	0	0
9	M	998	Total 998	O 998	0	0
9	N	1265	Total 1265	O 1265	0	0
9	O	108	Total 108	O 108	0	0
9	P	361	Total 361	O 361	0	0

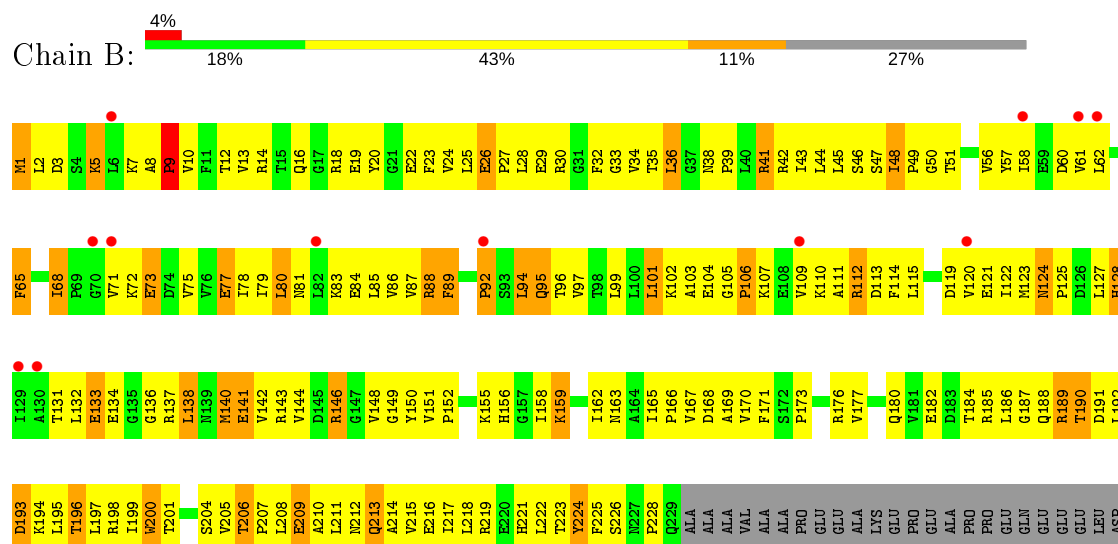
### 3 Residue-property plots

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

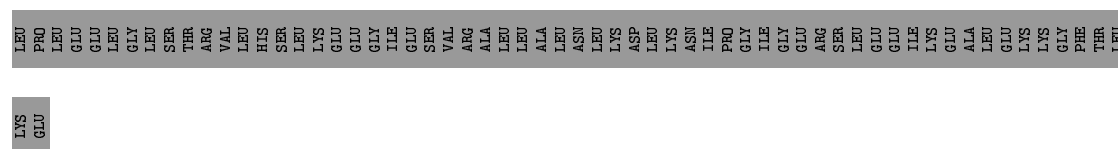
#### • Molecule 1: DNA-directed RNA polymerase alpha chain



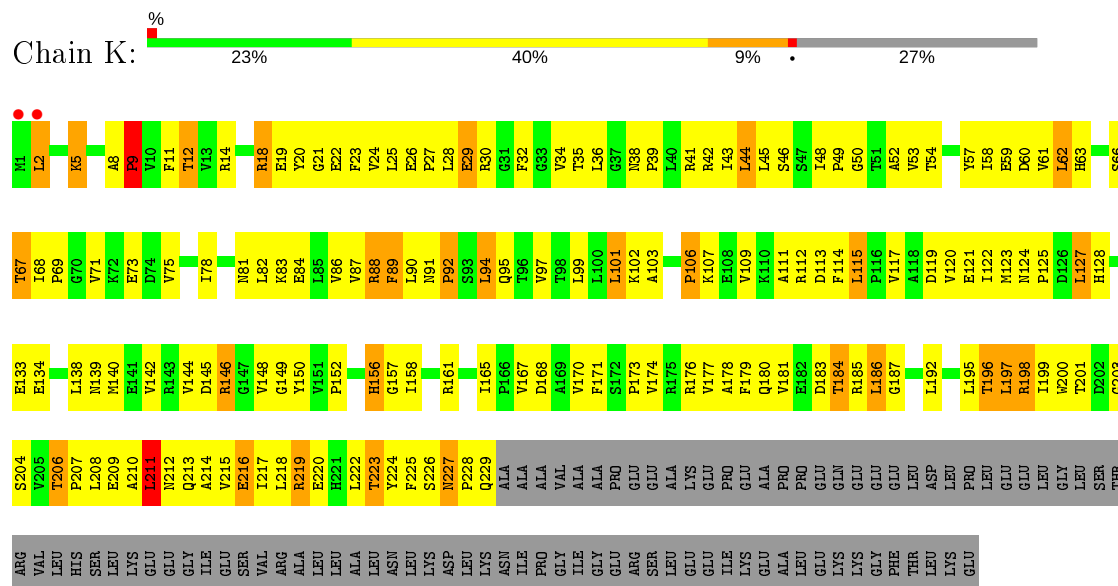
#### • Molecule 1: DNA-directed RNA polymerase alpha chain



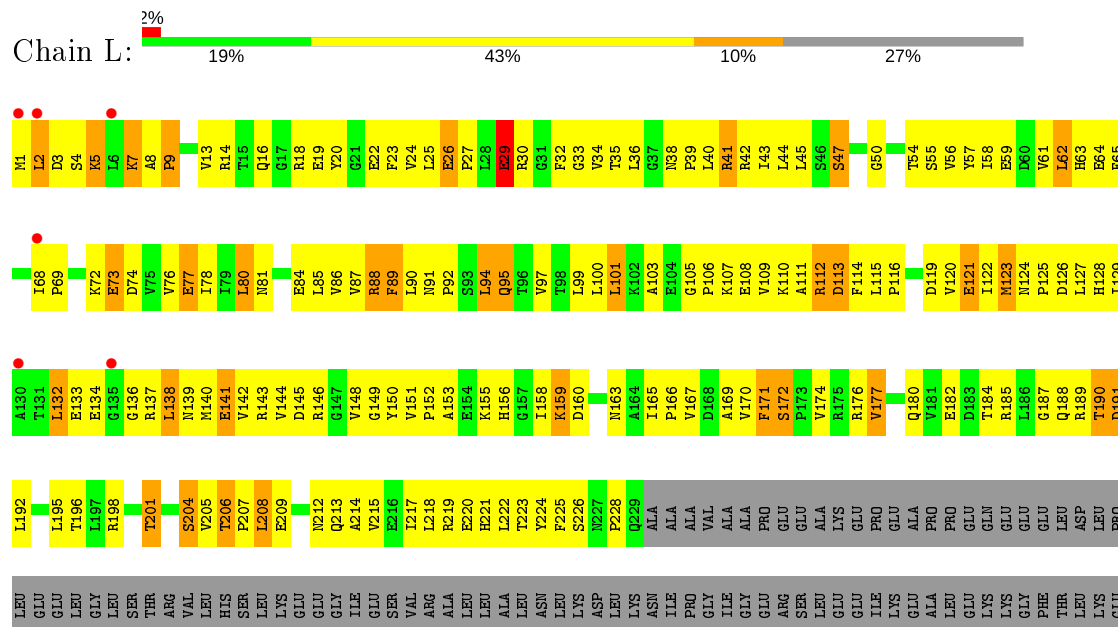




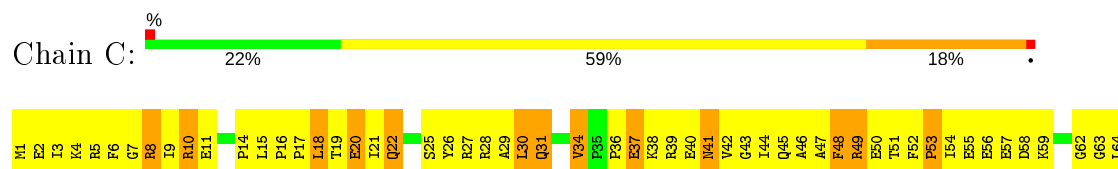
• Molecule 1: DNA-directed RNA polymerase alpha chain



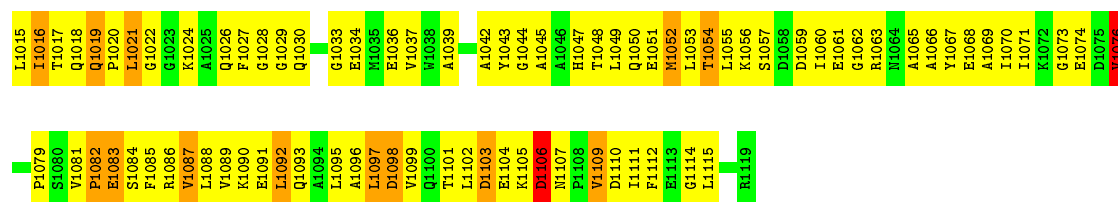
• Molecule 1: DNA-directed RNA polymerase alpha chain



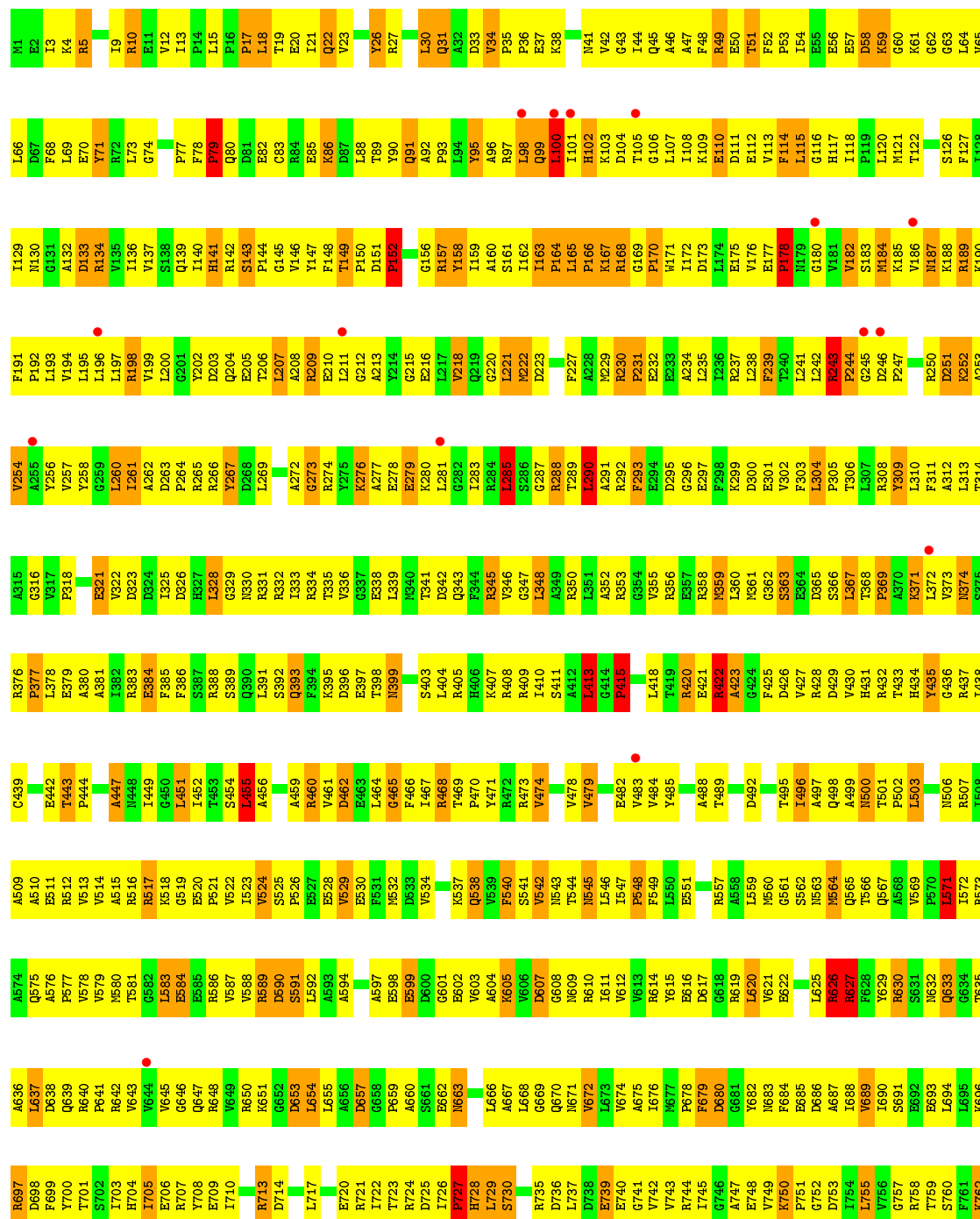
• Molecule 2: DNA-directed RNA polymerase beta chain

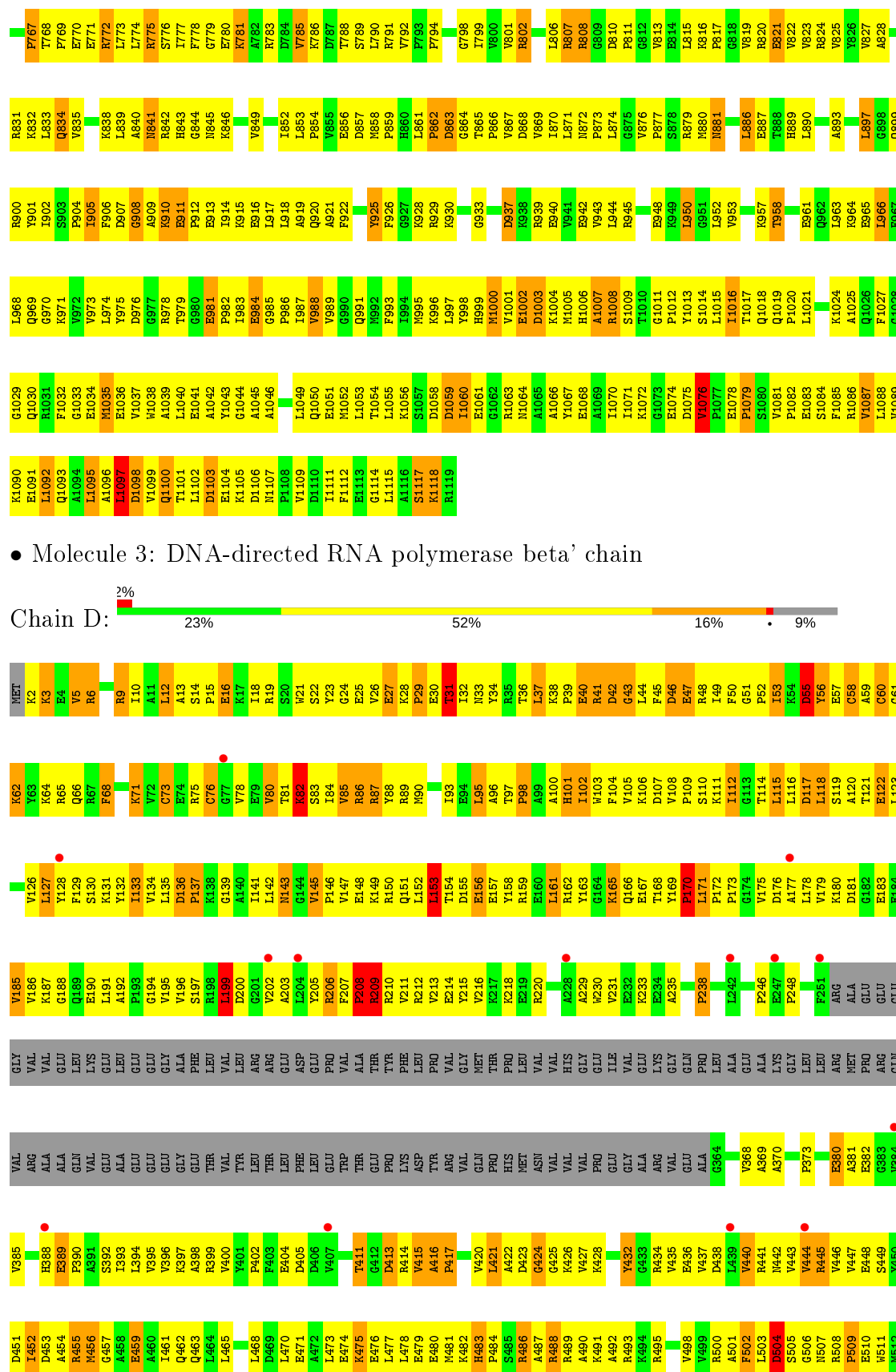




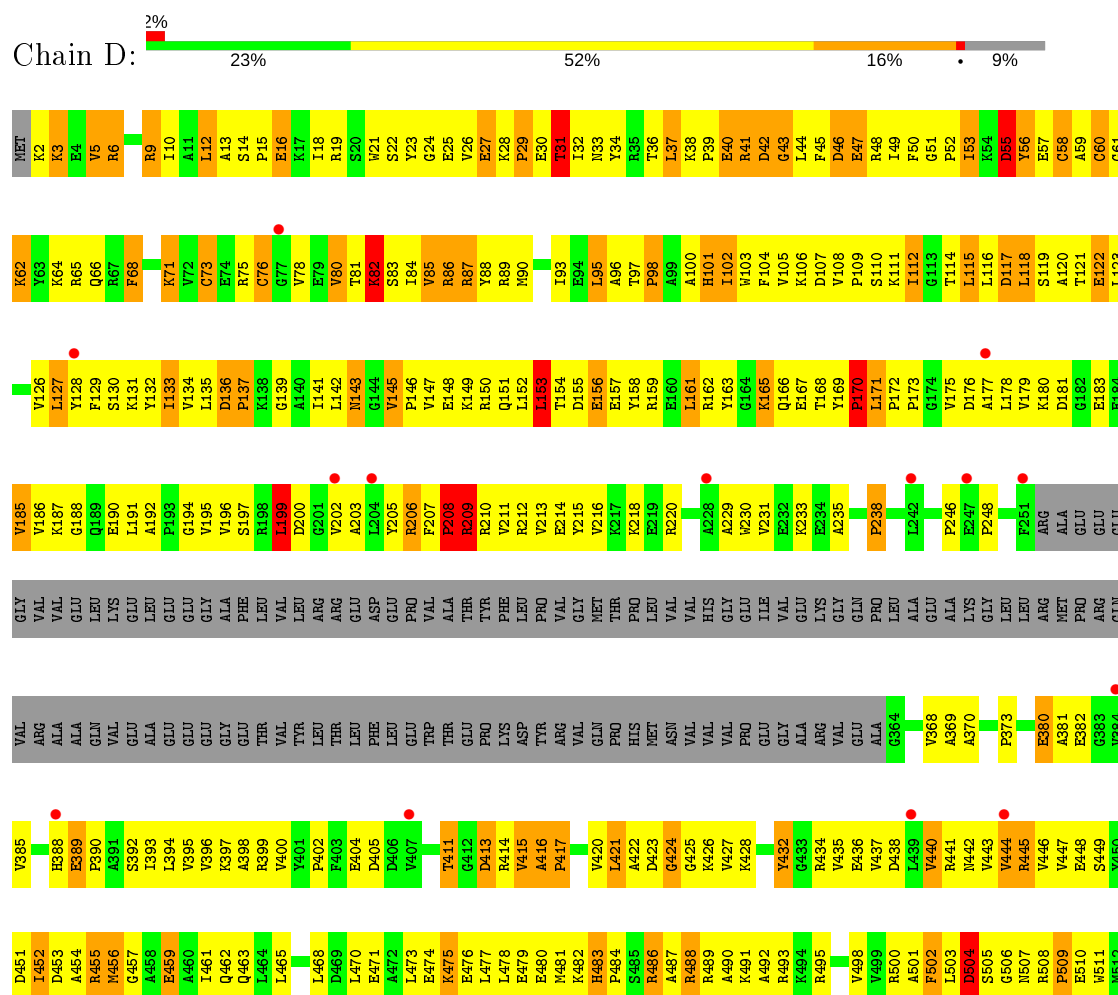


• Molecule 2: DNA-directed RNA polymerase beta chain

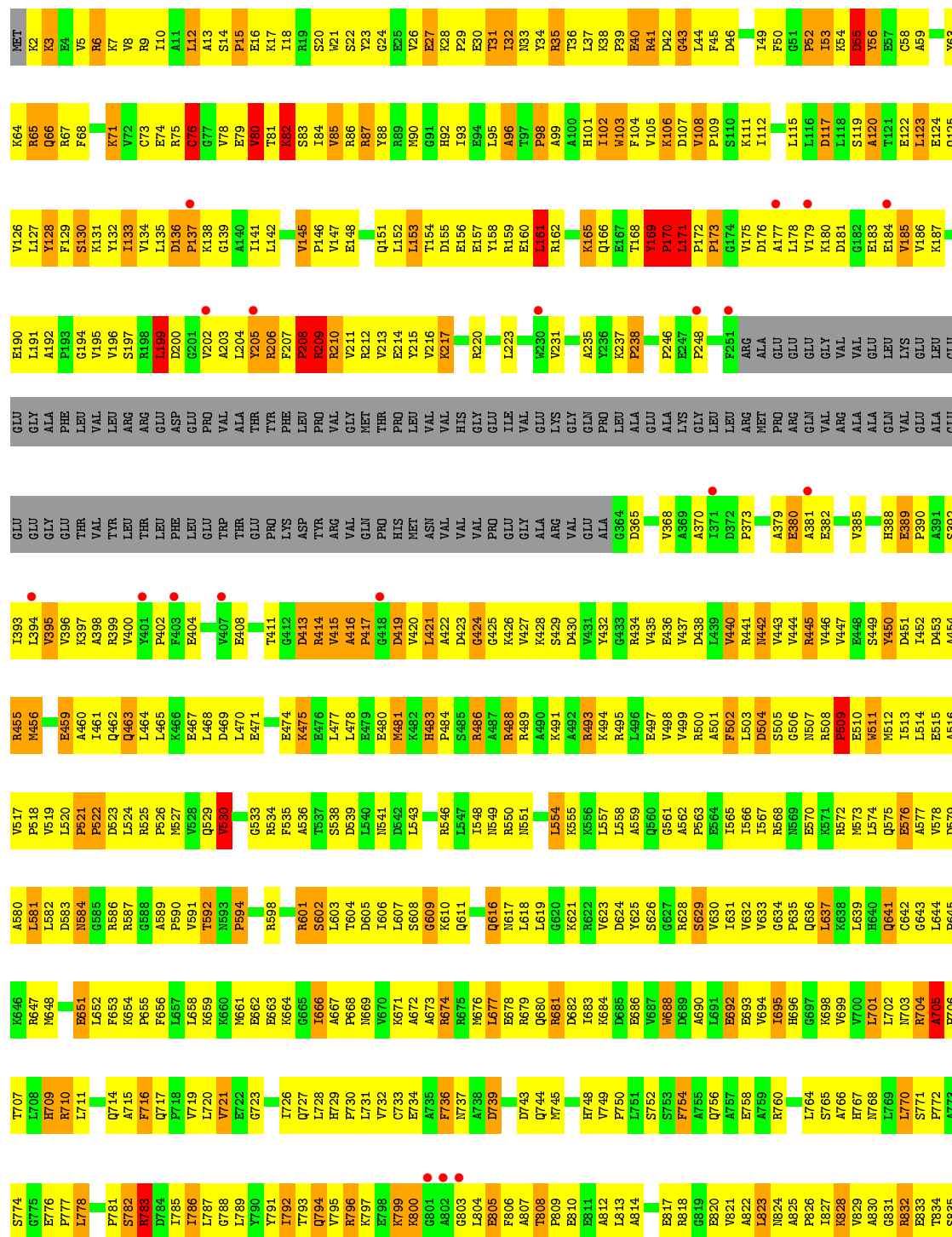


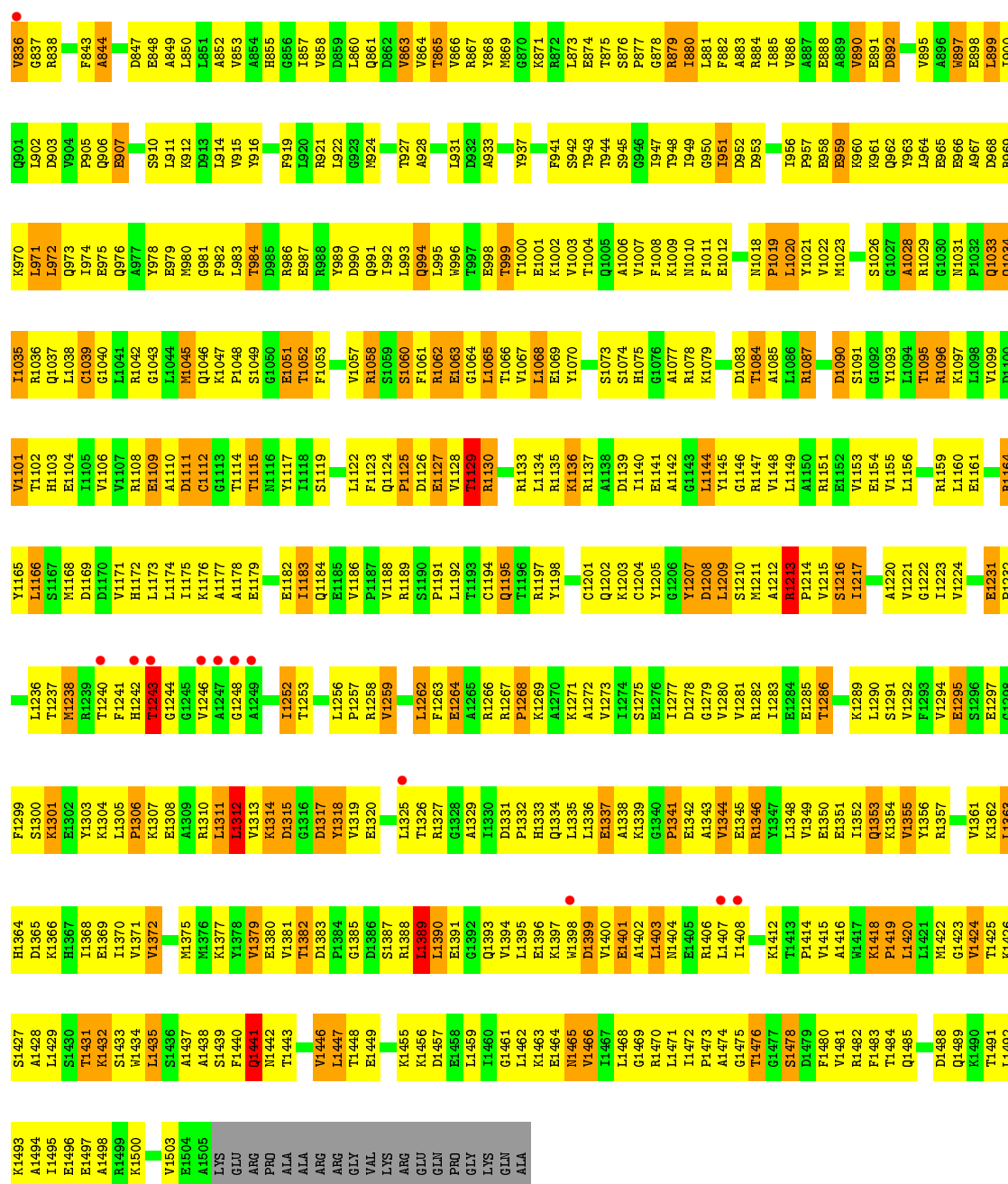


• Molecule 3: DNA-directed RNA polymerase beta' chain

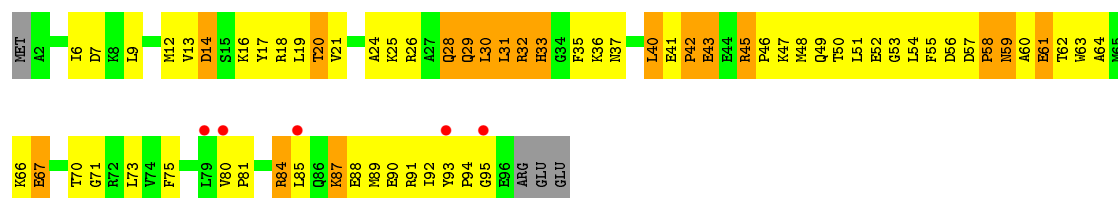


N1404	V1344	V1280	E1219	E1154	R1087	S1026	E959	V890	P826	Q762	L701	L574	E1513
E1405	E1345	V1281	V1221	L1156	D1090	G1027	K960	E891	L827	M763	L702	Q575	E515
R1406	R1346	E1282	E1223	L1157	S1091	A1028	Y963	E892	K828	L764	N703	E576	E514
L1407	I1347	I1283	G1222	E1284	G1092	R1029	L964	E893	V829	S765	R704	A577	A516
A1408	V1348	E1285	V1224	E1285	Y1093	G1090	E965	V895	A830	A766	A705	V578	V517
E1409	E1350	T1286	A1225	E1161	L1094	M1031	E966	A896	R832	L768	P706	D579	P518
E1410	E1351	E1287	E1226	E1162	T1095	P1032	E967	R897	E833	L769	L707	A580	V519
E1411	E1352	E1288	A1227	G1163	R1096	Q1033	D968	E898	7834	L770	R708	L581	L520
K1412	Q1353	R1289	Q1227	G1163	K1097	Q1034	R969	L899	S835	P845	R709	L582	P521
K1413	Q1353	L1269	E1228	L1165	L1098	L1035	K970	I900	V836	L771	K710	D583	P522
V1414	K1354	L1290	H1239	L1166	V1099	R1036	L971	Q901	E837	L772	L711	N584	D523
V1415	V1355	S1291	G1230	L1167	D1100	Q1037	L972	I902	R839	G774	G742	G585	L524
A1416	V1356	V1292	E1231	S1167	T1031	L1038	Q973	D903	E839	G775	I713	R596	R525
V1417	R1357	F1293	P1232	M1168	V1101	L1102	Q974	V904	L839	E776	Q714	R587	P526
K1418	A1358	L1294	G1233	T1169	T1102	C1039	L974	D904	K840	E833	A715	G588	M527
Q1359	Q1359	P1419	E1234	D1170	H1103	G1040	E975	R905	V841	P777	F716	A589	V528
Q1360	Q1360	E1295	Q1235	D1171	E1104	L1041	Q976	Q906	H842	L770	Q717	F653	Q529
L1420	V1361	F1299	L1236	H1172	T1105	R1042	A977	E907	F843	K780	F718	V591	V530
L1421	K1362	S1300	T1237	E1173	V1106	G1043	Y978	R908	A844	S782	L719	T592	D531
M1422	K1362	K1301	E1238	L1174	L1107	L1044	E979	R909	R845	R783	K720	N593	G532
E1423	L1363	E1423	T1237	L1175	K1047	R1044	M980	S910	P846	D784	V721	L557	G533
V1424	H1364	E1302	E1239	L1175	R1108	M1045	E981	L911	D847	L785	E722	L658	R534
T1425	D1365	Y1303	T1240	K1176	E1109	Q1046	F982	R912	E848	L786	G723	K659	F535
K1426	K1366	K1304	H1241	A1177	K1047	P1048	L983	D913	L849	L787	Q724	R598	A536
S1427	H1367	L1305	H1242	A1178	G1112	P1048	T984	I914	L850	G788	R725	M561	P599
A1428	L1368	P1306	T1243	E1179	G1113	E1051	D985	V915	L851	L789	L726	E263	R601
E1429	E1369	K1307	G1244	T1114	T1114	T1052	R986	Y916	A852	Y790	Q727	R601	D539
S1430	I1370	E1308	G1245	L1115	N1116	F1053	E987	Q917	V853	Y791	L728	K664	L540
T1431	V1371	A1309	E1246	V1186	Y1117	E1053	R988	A918	L792	G665	H729	G665	L540
K1432	R1372	L1310	A1247	V1187	E1118	P1056	Y989	F919	L857	L666	P730	L603	N541
S1433	A1373	L1311	G1248	P1187	T1118	P1056	Y989	F919	L857	L666	P730	L603	N541
V1434	Q1374	L1312	E1248	V1188	S1119	P1057	Y989	F919	L857	L666	P730	L603	N541
L1435	M1375	V1313	D1251	R1189	V1120	R1058	T992	I920	V859	L607	C733	L606	L543
S1436	M1376	K1314	I1252	S1190	P1121	R1058	T992	I920	V859	L607	C733	L606	L543
A1437	K1377	D1315	T1253	P1191	L1314	S1059	L995	G923	D861	R796	R669	S608	R545
V1438	Y1378	E1316	Q1254	L1192	Q1124	S1060	L996	G923	D862	K797	A735	G609	R546
S1439	V1379	D1317	G1255	L1193	Q1124	F1061	Y996	N924	D862	K671	F736	K610	L547
E1440	E1380	Y1318	L1256	T1193	E1127	R1062	T997	E925	V863	L799	N737	Q611	L548
N1441	V1381	V1319	P1257	K1195	T1128	E1063	E998	K926	V864	R800	A738	G612	N549
R1442	T1382	E1320	R1258	T1196	L1129	G1064	T999	T927	T865	R674	D739	R613	R550
T1443	D1383	A1321	V1259	L1197	R1130	L1065	T1000	A928	V866	A802	F740	F614	N551
	P1384	E1321	I1260	Y1198	R1130	T1066	E1001	R929	R867	G803	R675	R615	N552
	G1385	P1324	E1261		R1135	V1067	K1002	L930	V868	L804	G742	Q616	R553
	D1386	L1325	L1262	C1201	R1136	L1068	V1003	L931	R869	E805	D743	R617	L554
	R1387	T1326	F1263	Q1202	K1136	E1069	T1004		G870	F806	Q744	L618	K555
	L1388	R1327	E1264	K1203	R1137	Y1070	Q1005	T940	R871	Q807	Q680	L619	
	L1389		A1265	G1204	A1138	F1071	A1006	T943	R872	T808	R681	G620	L558
	L1390	I1330	R1266	E1205	D1139	I1072	V1007	T943	L873	P809	D682	K621	A559
	E1391	D1331	R1267	G1206	A1141	S1073	F1008	T944	E874	R810	I683	G820	A559
	E1392	P1332	P1268	I1207	E1141	S1074	K1009		R875	E811	L683	R622	Q560
	Q1393	K1456	K1269	D1208	A1142	H1075	L1010	T947	S876	A812	R748	R622	Q560
	V1394	Q1334	A1270	L1209	K1143	G1076	P877	T948	R877	L751	F750	R623	G561
	L1395	L1335	K1271	S1210	L1144	A1077	E1012	T949	G878	L813	P750	D624	A562
	E1396	L1336	K1272	S1211	Y1145	K1078	G950	R879	R879	E817	G753	R628	I565
	K1397	L1336	A1272	T1211	G1146	R1478	Y1015	I951	L880	R818	F754	S629	I566
	E1397	E1337	V1273	A1212	R1147	G1080	P1016	D952	L880	R818	F754	S629	I566
	V1398	L1338	E1274	E1213	L1148	E1081	P1016	D952	L880	R818	F754	S629	I566
	L1462	K1399	S1275	P1214	L1149	A1082	P1019	D953	R883	E820	A755	V630	I567
	K1463	V1400	E1276	E1214	L1149	A1082	P1019	D953	R883	E820	A755	V630	I567
	E1464	E1401	I1277	S1216	L1151	D1083	L1020	A954	R884	R821	F757	V632	R568
	N1465	E1401	I1277	S1216	L1151	D1083	L1020	A954	R884	R821	F757	V632	R568
	V1466	L1402	D1278	E1217	E1152	T1084	Y1021	V956	A887	L823	A759	G634	E570
	L1403	A1403	E1276	V1452	N1452	A1085	V1022	P957	E883	R760	V699	P635	E570





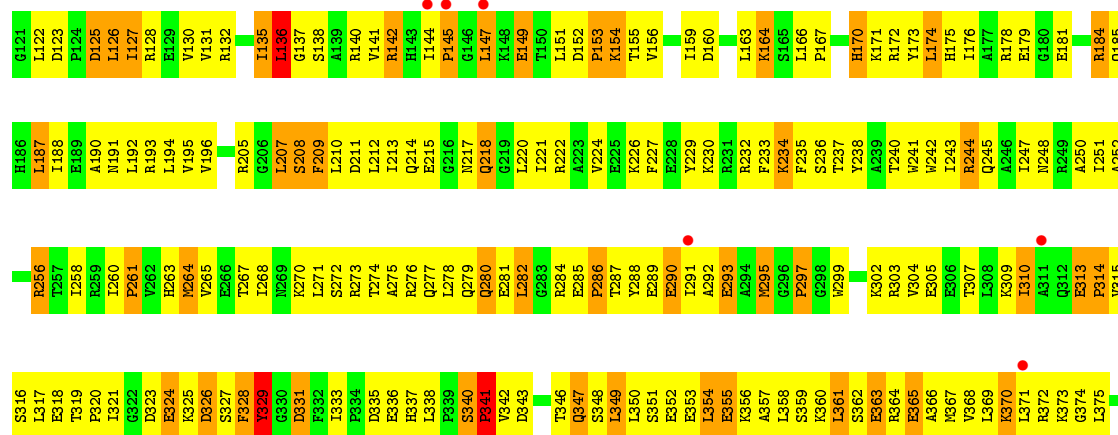
### • Molecule 4: RNA polymerase omega chain



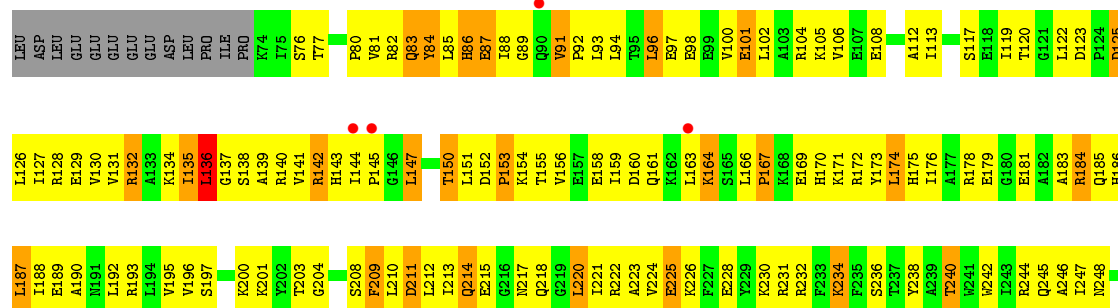
### • Molecule 4: RNA polymerase omega chain

A64	A65	A66	A67	A68	A69	A70	A71	A72	A73	A74	A75	A76	A77	A78	A79	A80	A81	A82	A83	A84	A85	A86	A87	A88	A89	A90	A91	A92	A93	A94	A95	A96	ARG	GLU	GLU
165	166	167	168	169	170	171	172	173	174	175	176	177	178	179	180	181	182	183	184	185	186	187	188	189	190	191	192	193	194	195	196	197	198	199	200
201	202	203	204	205	206	207	208	209	210	211	212	213	214	215	216	217	218	219	220	221	222	223	224	225	226	227	228	229	230	231	232	233	234	235	236
237	238	239	240	241	242	243	244	245	246	247	248	249	250	251	252	253	254	255	256	257	258	259	260	261	262	263	264	265	266	267	268	269	270	271	272
273	274	275	276	277	278	279	280	281	282	283	284	285	286	287	288	289	290	291	292	293	294	295	296	297	298	299	300	301	302	303	304	305	306	307	308
309	310	311	312	313	314	315	316	317	318	319	320	321	322	323	324	325	326	327	328	329	330	331	332	333	334	335	336	337	338	339	340	341	342	343	344
345	346	347	348	349	350	351	352	353	354	355	356	357	358	359	360	361	362	363	364	365	366	367	368	369	370	371	372	373	374	375	376	377	378	379	380
381	382	383	384	385	386	387	388	389	390	391	392	393	394	395	396	397	398	399	400	401	402	403	404	405	406	407	408	409	410	411	412	413	414	415	416
417	418	419	420	421	422	423	424	425	426	427	428	429	430	431	432	433	434	435	436	437	438	439	440	441	442	443	444	445	446	447	448	449	450	451	452
453	454	455	456	457	458	459	460	461	462	463	464	465	466	467	468	469	470	471	472	473	474	475	476	477	478	479	480	481	482	483	484	485	486	487	488
489	490	491	492	493	494	495	496	497	498	499	500	501	502	503	504	505	506	507	508	509	510	511	512	513	514	515	516	517	518	519	520	521	522	523	524
525	526	527	528	529	530	531	532	533	534	535	536	537	538	539	540	541	542	543	544	545	546	547	548	549	550	551	552	553	554	555	556	557	558	559	560
561	562	563	564	565	566	567	568	569	570	571	572	573	574	575	576	577	578	579	580	581	582	583	584	585	586	587	588	589	590	591	592	593	594	595	596
597	598	599	600	601	602	603	604	605	606	607	608	609	610	611	612	613	614	615	616	617	618	619	620	621	622	623	624	625	626	627	628	629	630	631	632
633	634	635	636	637																															

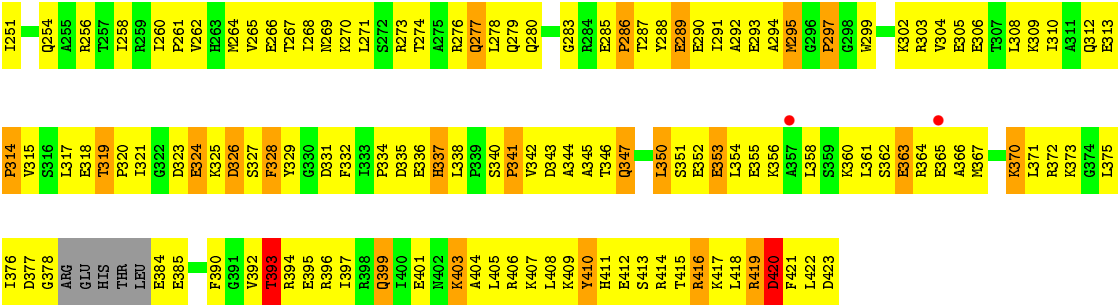
	MET	LYS	LYS	SER	LYS	ARG	LYS	ASN	ALA	GLN	ALA	GLN	GLU	VAL	THR	GLY	ALA	GLU	LEU	PRO	ASP	PHE	GLY	GLY	GLY	GLU	PRO	ASP	ASP	LEU	GLU	ASP	ASP	LEU	LEU	ASP	LEU	GLY	GLY	GLY	GLY	GLY	GLY															
	LEU	ASP	LEU	GLU	GLU	GLU	GLU	GLU	ASP	LEU	PRO	IIE	PRO	K74	I75	S76	T77	S78	R80	V81	R82	Q83	Y84	L85	H86	E87	I88	G89	Q90	V91	P92	L93	L94	T95	L96	E97	E99	V100	E101	L102	A103	R104	K105	V106	E107	E108	G109	M110	E111	A112	I113	K114	K115	L116	S117	E118	I119	T120



MET	LYS	LYS	SER	ARG	LYS	ASN	ALA	ALA	ALA	GLN	GLN	GLU	THR	GLU	VAL	LEU	VAL	GLN	GLU	GLU	ALA	GLU	GLU	LEU	PRO	GLU	PHE	PRO	GLY	GLY	GLU	PRO	ASP	ASP	LEU	ALA	LEU	LEU	GLU	ASP	ASP	ASP	LEU	LEU	ASP	LEU	PRO	GLU	GLY	GLY	GLY
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	239.50Å 239.50Å 253.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.50 24.85 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.50) 92.5 (24.85-2.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.13 (at 2.50Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.230 , 0.267 0.228 , 0.264	Depositor DCC
$R_{free}$ test set	29710 reflections (5.75%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.8	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 76.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.499 for -h,-k,l 0.076 for h,-h-k,-l 0.076 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	60572	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.81	1/1838 (0.1%)	0.88	4/2498 (0.2%)
1	B	0.74	0/1838	0.81	2/2498 (0.1%)
1	K	0.75	0/1838	0.86	3/2498 (0.1%)
1	L	0.73	1/1838 (0.1%)	0.80	2/2498 (0.1%)
2	C	0.83	2/8997 (0.0%)	0.89	7/12164 (0.1%)
2	M	0.81	0/8997	0.88	8/12164 (0.1%)
3	D	0.84	0/10975	0.94	20/14836 (0.1%)
3	N	0.82	0/10975	0.92	17/14836 (0.1%)
4	E	0.84	0/783	0.94	0/1054
4	O	0.82	0/783	0.96	2/1054 (0.2%)
5	F	0.74	0/2812	0.82	4/3781 (0.1%)
5	P	0.71	0/2812	0.80	1/3781 (0.0%)
All	All	0.81	4/54486 (0.0%)	0.89	70/73662 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	48	ILE	C-N	6.06	1.45	1.34
1	L	172	SER	N-CA	-5.43	1.35	1.46
2	C	792	VAL	CB-CG1	-5.28	1.41	1.52
2	C	393	GLN	CD-OE1	5.25	1.35	1.24

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1389	LEU	CA-CB-CG	8.13	133.99	115.30
1	K	211	LEU	CA-CB-CG	8.11	133.95	115.30
1	B	138	LEU	CA-CB-CG	7.70	133.00	115.30
1	A	192	LEU	CA-CB-CG	7.60	132.79	115.30
3	D	199	LEU	CA-CB-CG	-7.59	97.84	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	243	ARG	C-N-CD	-7.50	104.10	120.60
5	F	354	LEU	CA-CB-CG	7.15	131.75	115.30
3	N	705	ALA	C-N-CD	7.06	143.23	128.40
4	O	31	LEU	CA-CB-CG	7.06	131.53	115.30
3	D	1395	LEU	CA-CB-CG	6.81	130.96	115.30
1	A	90	LEU	CA-CB-CG	-6.79	99.68	115.30
3	N	199	LEU	CA-CB-CG	-6.78	99.71	115.30
3	N	1389	LEU	CA-CB-CG	6.77	130.87	115.30
2	M	571	LEU	CA-CB-CG	6.55	130.37	115.30
2	M	165	LEU	C-N-CD	-6.53	106.22	120.60
3	N	1312	LEU	CA-CB-CG	6.47	130.17	115.30
3	D	80	VAL	C-N-CA	6.43	137.77	121.70
5	P	136	LEU	CA-CB-CG	6.33	129.87	115.30
3	D	705	ALA	C-N-CD	6.30	141.63	128.40
1	K	115	LEU	CA-CB-CG	6.14	129.42	115.30
3	N	76	CYS	CA-CB-SG	6.09	124.96	114.00
3	D	73	CYS	CA-CB-SG	6.05	124.89	114.00
3	D	567	ILE	CG1-CB-CG2	-6.02	98.16	111.40
3	N	80	VAL	C-N-CA	5.96	136.59	121.70
3	N	82	LYS	C-N-CA	-5.91	106.93	121.70
2	C	620	LEU	CA-CB-CG	5.91	128.89	115.30
2	C	88	LEU	CA-CB-CG	5.89	128.85	115.30
3	N	209	ARG	N-CA-C	5.88	126.89	111.00
1	B	36	LEU	CA-CB-CG	5.79	128.60	115.30
3	N	1209	LEU	N-CA-C	-5.76	95.43	111.00
3	N	171	LEU	CA-CB-CG	5.76	128.55	115.30
1	K	2	LEU	CA-CB-CG	5.73	128.47	115.30
3	D	153	LEU	CA-CB-CG	5.72	128.45	115.30
3	D	1209	LEU	N-CA-C	-5.68	95.66	111.00
3	D	637	LEU	CA-CB-CG	5.65	128.30	115.30
1	A	127	LEU	CA-CB-CG	5.64	128.27	115.30
3	D	80	VAL	CA-C-N	-5.56	104.96	117.20
3	D	238	PRO	N-CA-CB	5.55	109.97	103.30
3	N	380	GLU	N-CA-C	-5.55	96.01	111.00
3	D	60	CYS	CA-CB-SG	5.53	123.95	114.00
2	M	100	LEU	CA-CB-CG	5.50	127.94	115.30
5	F	136	LEU	CA-CB-CG	5.49	127.92	115.30
3	D	208	PRO	CA-N-CD	-5.46	103.86	111.50
3	D	380	GLU	N-CA-C	-5.41	96.39	111.00
3	D	209	ARG	N-CA-C	5.41	125.59	111.00
3	N	80	VAL	CA-C-N	-5.38	105.36	117.20
2	M	728	HIS	N-CA-C	5.36	125.48	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	243	ARG	C-N-CD	-5.35	108.83	120.60
3	D	813	LEU	CA-CB-CG	5.33	127.57	115.30
1	L	132	LEU	CA-CB-CG	5.31	127.52	115.30
5	F	361	LEU	CA-CB-CG	5.30	127.48	115.30
1	L	171	PHE	C-N-CA	-5.27	108.53	121.70
3	D	248	PRO	N-CA-CB	5.25	109.60	103.30
3	D	708	LEU	CA-CB-CG	-5.25	103.23	115.30
3	D	1468	LEU	CA-CB-CG	5.22	127.31	115.30
2	M	207	LEU	CA-CB-CG	5.21	127.28	115.30
3	N	554	LEU	CA-CB-CG	5.20	127.27	115.30
2	C	165	LEU	C-N-CD	-5.20	109.16	120.60
2	C	737	LEU	CA-CB-CG	5.17	127.20	115.30
5	F	91	VAL	C-N-CD	5.12	139.15	128.40
4	O	49	GLN	N-CA-C	5.12	124.81	111.00
3	N	208	PRO	CA-N-CD	-5.11	104.34	111.50
2	C	728	HIS	N-CA-C	5.11	124.79	111.00
3	N	238	PRO	N-CA-CB	5.11	109.43	103.30
1	A	115	LEU	CA-CB-CG	5.08	127.00	115.30
2	M	58	ASP	C-N-CA	5.08	134.39	121.70
2	M	285	LEU	CA-CB-CG	5.08	126.98	115.30
2	C	917	LEU	CA-CB-CG	-5.04	103.70	115.30
3	N	248	PRO	N-CA-CB	5.04	109.35	103.30
3	N	637	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

There are no planarity outliers.

## 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	232	0
1	B	1806	0	1861	216	0
1	K	1806	0	1861	173	0
1	L	1806	0	1861	186	0
2	C	8829	0	8933	1215	0
2	M	8829	0	8933	1174	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	10797	0	10873	1490	0
3	N	10797	0	10873	1288	0
4	E	769	0	775	89	0
4	O	769	0	775	95	0
5	F	2771	0	2844	346	0
5	P	2771	0	2844	352	0
6	A	33	0	0	0	0
6	B	21	0	0	0	0
6	C	73	0	0	0	0
6	D	106	0	0	0	0
6	E	5	0	0	0	0
6	F	28	0	0	0	0
6	K	19	0	0	0	0
6	L	17	0	0	0	0
6	M	65	0	0	0	0
6	N	92	0	0	0	0
6	O	8	0	0	0	0
6	P	20	0	0	0	0
7	C	63	0	62	6	0
7	M	63	0	62	7	0
8	D	2	0	0	0	0
8	N	2	0	0	0	0
9	A	239	0	0	50	0
9	B	258	0	0	46	0
9	C	979	0	0	224	0
9	D	1252	0	0	277	0
9	E	117	0	0	28	0
9	F	420	0	0	94	0
9	K	183	0	0	39	0
9	L	219	0	0	46	0
9	M	998	0	0	249	0
9	N	1265	0	0	250	0
9	O	108	0	0	26	0
9	P	361	0	0	78	0
All	All	60572	0	54418	6470	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 60.

All (6470) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:GLN:HA	1:A:146:ARG:HH12	1.07	1.11
2:M:952:LEU:HD12	2:M:969:GLN:HE22	1.13	1.11
3:D:1087:ARG:HG2	3:D:1234:THR:HA	1.27	1.07
1:B:152:PRO:HD2	1:B:155:LYS:HD3	1.36	1.05
2:M:605:LYS:HB2	2:M:610:ARG:HH12	1.16	1.05
3:D:1481:VAL:HG11	4:E:18:ARG:HA	1.41	1.03
1:B:86:VAL:HG12	1:B:124:ASN:HD22	1.24	1.02
2:C:274:ARG:HD2	2:C:285:LEU:HD22	1.37	1.02
2:C:775:ARG:HH21	2:C:782:ALA:HB1	1.24	1.02
5:F:94:LEU:HD22	5:F:97:GLU:HG2	1.39	1.01
3:N:783:ARG:HH21	3:N:1029:ARG:HD3	1.26	1.01
2:C:110:GLU:HG2	2:C:369:PRO:HB3	1.42	1.00
3:N:197:SER:HB3	3:N:203:ALA:HB3	1.42	1.00
2:M:110:GLU:HG2	2:M:369:PRO:HG3	1.40	1.00
3:D:197:SER:HB3	3:D:203:ALA:HB3	1.43	1.00
3:N:210:ARG:HH11	3:N:398:ALA:HB3	1.26	0.99
3:N:1144:LEU:HD12	3:N:1171:VAL:HG13	1.43	0.99
3:N:52:PRO:HB2	3:N:80:VAL:HG13	1.45	0.99
3:N:1036:ARG:HH21	3:N:1042:ARG:HA	1.28	0.98
3:D:422:ALA:HB3	3:D:427:VAL:HG22	1.45	0.98
2:C:724:ARG:HG3	2:C:741:GLY:H	1.27	0.97
3:N:422:ALA:HB3	3:N:427:VAL:HG22	1.45	0.97
5:F:268:ILE:HA	5:F:271:LEU:HD12	1.45	0.97
2:M:1114:GLY:H	2:M:1115:LEU:HD12	1.26	0.97
2:M:1092:LEU:HD13	2:M:1099:VAL:HG21	1.47	0.97
1:L:88:ARG:HH11	1:L:88:ARG:HB3	1.29	0.96
3:N:423:ASP:HB2	5:P:178:ARG:HD2	1.45	0.96
2:M:905:ILE:HD12	2:M:905:ILE:H	1.31	0.95
2:M:169:GLY:HA2	2:M:263:ASP:HB3	1.48	0.95
2:M:404:LEU:HA	2:M:407:LYS:HD3	1.47	0.95
3:D:214:GLU:HB2	3:D:390:PRO:HD2	1.49	0.95
2:C:846:LYS:HD3	3:D:741:ASP:HB2	1.47	0.94
2:C:413:LEU:HD21	2:C:448:ASN:HD21	1.31	0.94
3:D:118:LEU:HB3	3:D:123:LEU:HD22	1.46	0.94
2:C:1114:GLY:H	2:C:1115:LEU:HD12	1.31	0.94
3:D:119:SER:HB2	3:D:123:LEU:H	1.32	0.94
3:D:1095:THR:HG23	3:D:1230:GLY:HA3	1.46	0.94
1:B:57:TYR:HB3	1:B:141:GLU:HG3	1.49	0.94
2:C:150:PRO:HA	2:C:158:TYR:HB3	1.50	0.94
3:D:191:LEU:HD12	3:D:211:VAL:HG21	1.47	0.94
3:N:1210:SER:HA	9:N:9537:HOH:O	1.68	0.94
3:D:1310:ARG:HE	3:D:1327:ARG:HB3	1.33	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:637:LEU:HD21	3:N:642:CYS:HA	1.50	0.94
3:N:928:ALA:HA	3:N:931:LEU:HD12	1.50	0.94
2:C:689:VAL:HB	2:C:870:ILE:HG13	1.50	0.94
2:M:1018:GLN:HE21	2:M:1060:ILE:HD11	1.28	0.94
3:N:1205:TYR:HD2	3:N:1215:VAL:HG21	1.32	0.93
2:C:329:GLY:HA3	2:C:489:THR:HG23	1.47	0.93
2:C:987:ILE:HG23	3:D:948:THR:HG21	1.48	0.93
3:N:1262:LEU:HD21	3:N:1351:GLU:HG3	1.51	0.93
3:N:1481:VAL:HG11	4:O:18:ARG:HA	1.48	0.93
3:D:1468:LEU:HD22	3:D:1470:ARG:HB2	1.51	0.92
5:P:371:LEU:HD22	5:P:375:LEU:HD22	1.52	0.92
3:N:1314:LYS:HZ2	3:N:1314:LYS:H	1.17	0.92
1:A:63:HIS:HB3	2:C:746:GLY:HA2	1.50	0.92
2:C:54:ILE:HD11	2:C:356:ARG:HG2	1.52	0.92
3:N:1101:VAL:HG21	3:N:1424:VAL:HG22	1.49	0.91
3:D:87:ARG:HB3	3:D:523:ASP:HB2	1.51	0.91
5:P:163:LEU:HD13	5:P:174:LEU:HD21	1.49	0.91
3:N:572:ARG:HH22	5:P:83:GLN:HG3	1.36	0.91
2:C:328:LEU:HD13	2:C:433:THR:HB	1.51	0.90
3:D:148:GLU:HB3	3:D:151:GLN:HB2	1.53	0.90
2:C:358:ARG:HH22	2:C:374:ASN:HB3	1.36	0.90
1:A:14:ARG:HH21	1:A:22:GLU:HB3	1.35	0.90
2:M:791:ARG:HB3	9:M:9759:HOH:O	1.71	0.90
3:D:145:VAL:HG22	3:D:146:PRO:HD2	1.53	0.90
4:E:67:GLU:HB2	4:E:73:LEU:HD11	1.52	0.90
2:M:289:THR:HG22	2:M:290:LEU:HD23	1.54	0.90
2:M:979:THR:HG23	2:M:981:GLU:H	1.37	0.90
3:D:41:ARG:HD3	3:D:42:ASP:H	1.37	0.89
1:L:57:TYR:HB3	1:L:141:GLU:HG3	1.53	0.89
2:C:93:PRO:HA	9:C:9729:HOH:O	1.71	0.89
3:D:1326:THR:HA	9:D:9756:HOH:O	1.71	0.89
3:D:871:LYS:HE3	3:D:873:LEU:HD21	1.54	0.89
2:C:479:VAL:HG21	2:C:503:LEU:HD11	1.55	0.89
2:C:211:LEU:HD11	2:C:308:ARG:HB2	1.54	0.88
3:D:1057:VAL:HG13	3:D:1069:GLU:HB3	1.55	0.88
2:C:860:HIS:HB2	9:C:9519:HOH:O	1.72	0.88
3:D:1096:ARG:HH11	3:D:1096:ARG:HB2	1.36	0.88
2:M:964:LYS:O	2:M:968:LEU:HG	1.72	0.88
5:P:394:ARG:HA	5:P:397:ILE:HD12	1.54	0.88
5:F:88:ILE:HD13	5:F:193:ARG:HB2	1.54	0.88
3:D:520:LEU:HD12	3:D:521:PRO:HD2	1.56	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:92:ALA:HB2	2:M:120:LEU:HD11	1.55	0.88
2:M:146:VAL:HG22	2:M:162:ILE:HA	1.56	0.88
2:C:671:ASN:ND2	2:C:671:ASN:H	1.70	0.88
2:C:979:THR:HG23	2:C:981:GLU:H	1.39	0.88
3:D:572:ARG:HH21	5:F:83:GLN:HE21	1.21	0.88
3:N:133:ILE:HG21	3:N:454:ALA:HB1	1.52	0.88
3:D:973:GLN:HA	3:D:976:GLN:HE21	1.34	0.88
3:N:18:ILE:HG23	3:N:518:PRO:HG3	1.56	0.87
3:N:978:TYR:HA	9:N:9888:HOH:O	1.72	0.87
5:P:88:ILE:HD13	5:P:193:ARG:HB2	1.55	0.87
3:D:906:GLN:HB3	3:D:911:LEU:HD11	1.54	0.87
2:C:945:ARG:HH11	2:C:945:ARG:HB3	1.37	0.87
3:N:566:ILE:HD11	5:P:192:LEU:HD21	1.54	0.87
5:F:125:ASP:HA	5:F:128:ARG:NH1	1.90	0.87
2:M:144:PRO:HA	2:M:163:ILE:HG12	1.57	0.87
2:C:724:ARG:HH12	2:C:734:LEU:HD23	1.37	0.87
2:C:671:ASN:HD22	2:C:671:ASN:N	1.71	0.86
1:K:186:LEU:HB2	1:K:192:LEU:HD11	1.55	0.86
5:P:260:ILE:HG23	5:P:264:MET:HB2	1.57	0.86
1:A:95:GLN:HA	1:A:146:ARG:NH1	1.88	0.86
2:C:66:LEU:HD22	2:C:372:LEU:HD23	1.57	0.86
3:D:18:ILE:HG23	3:D:518:PRO:HG3	1.58	0.86
2:C:1060:ILE:HD12	2:C:1063:ARG:HH12	1.38	0.86
2:C:671:ASN:H	2:C:671:ASN:HD22	0.91	0.86
3:D:57:GLU:HG3	3:D:64:LYS:HG2	1.57	0.86
1:L:112:ARG:HB3	1:L:112:ARG:HH11	1.38	0.86
2:M:165:LEU:O	2:M:265:ARG:HB2	1.76	0.86
2:M:129:ILE:HD13	2:M:134:ARG:HB2	1.55	0.85
3:N:119:SER:HB2	3:N:123:LEU:H	1.39	0.85
1:A:67:THR:HA	9:A:9598:HOH:O	1.75	0.85
2:C:579:VAL:HB	2:C:890:LEU:HD22	1.55	0.85
5:F:160:ASP:HA	5:F:163:LEU:HD12	1.58	0.85
1:A:186:LEU:HB2	1:A:192:LEU:HD11	1.58	0.85
1:B:87:VAL:HG21	1:B:144:VAL:HG11	1.57	0.85
3:D:1232:PRO:HB3	3:D:1361:VAL:HG21	1.58	0.85
3:D:560:GLN:HG2	5:F:218:GLN:HE22	1.39	0.85
2:C:135:VAL:HG11	2:C:407:LYS:HA	1.59	0.85
2:M:134:ARG:HH21	2:M:393:GLN:HA	1.41	0.85
2:C:49:ARG:HH11	2:C:49:ARG:HB2	1.41	0.85
2:C:874:LEU:HD21	3:D:787:LEU:HD22	1.59	0.84
4:E:85:LEU:HA	9:E:9594:HOH:O	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:433:THR:HG21	2:C:488:ALA:HB1	1.59	0.84
5:F:101:GLU:HA	9:F:9749:HOH:O	1.76	0.84
5:P:358:LEU:HD13	5:P:370:LYS:HG3	1.57	0.84
3:N:1380:GLU:HB3	3:N:1418:LYS:HG3	1.59	0.84
2:C:1005:MET:HB3	3:D:724:GLN:HE22	1.43	0.84
3:D:1223:ILE:HD12	3:D:1223:ILE:H	1.42	0.84
3:D:1160:LEU:HD11	3:D:1174:LEU:HD21	1.58	0.84
3:D:1466:VAL:HG23	3:D:1472:ILE:HD11	1.58	0.84
3:D:1209:LEU:HD21	4:E:16:LYS:NZ	1.92	0.84
3:D:44:LEU:HB3	3:D:525:ARG:HH21	1.43	0.84
2:M:1038:TRP:HE1	3:N:1463:LYS:HZ1	1.24	0.84
3:N:565:ILE:H	3:N:565:ILE:HD12	1.41	0.84
2:M:589:ARG:HB2	2:M:589:ARG:HH11	1.42	0.83
2:M:675:ALA:HA	2:M:989:VAL:HG12	1.58	0.83
3:D:86:ARG:O	3:D:522:PRO:HD2	1.77	0.83
2:C:953:VAL:HG13	2:C:966:LEU:HD13	1.59	0.83
2:C:656:ALA:HB3	9:C:2223:HOH:O	1.79	0.83
3:N:168:THR:HG22	3:N:170:PRO:HD2	1.61	0.83
3:N:785:ILE:HD12	3:N:785:ILE:H	1.42	0.83
2:C:232:GLU:HA	2:C:235:LEU:HD12	1.59	0.83
2:C:362:GLY:HA3	2:C:367:LEU:HD23	1.60	0.83
2:C:524:VAL:HG13	2:C:528:GLU:HB2	1.61	0.83
1:A:178:ALA:HB3	1:A:198:ARG:HG3	1.59	0.82
3:D:513:ILE:HG23	9:D:9966:HOH:O	1.77	0.82
2:C:943:VAL:HG23	2:C:985:GLY:H	1.43	0.82
5:F:191:ASN:HA	5:F:194:LEU:HD23	1.59	0.82
2:M:115:LEU:HD22	2:M:373:VAL:HG11	1.60	0.82
2:M:1096:ALA:O	3:N:13:ALA:HB2	1.79	0.82
2:C:47:ALA:HB1	2:C:345:ARG:HB3	1.61	0.82
3:D:209:ARG:HD2	3:D:210:ARG:HG2	1.62	0.82
3:N:214:GLU:HB2	3:N:390:PRO:HD2	1.60	0.82
3:N:704:ARG:HG3	3:N:736:PHE:HB3	1.60	0.82
2:M:51:THR:HG21	9:M:2064:HOH:O	1.80	0.82
3:N:186:VAL:HG21	3:N:213:VAL:HB	1.62	0.82
5:P:160:ASP:HA	5:P:163:LEU:HD12	1.62	0.82
5:P:166:LEU:HB3	5:P:170:HIS:HB2	1.59	0.82
3:N:55:ASP:HA	3:N:82:LYS:HG3	1.61	0.82
3:N:105:VAL:HG21	3:N:128:TYR:HE2	1.43	0.82
3:N:558:LEU:HD13	5:P:145:PRO:HB3	1.60	0.82
3:N:796:ARG:HH11	3:N:861:GLN:HB2	1.44	0.82
5:F:130:VAL:HG21	5:F:159:ILE:HG21	1.59	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:157:ARG:HD2	2:M:314:THR:HG22	1.62	0.82
2:M:447:ALA:HA	3:N:1085:ALA:HB1	1.62	0.81
1:A:87:VAL:HG21	1:A:144:VAL:HG11	1.62	0.81
3:D:699:VAL:H	3:D:756:GLN:NE2	1.77	0.81
3:N:165:LYS:HB3	3:N:395:VAL:HG11	1.60	0.81
1:A:133:GLU:HG2	1:A:134:GLU:H	1.46	0.81
5:F:291:ILE:HG21	5:F:304:VAL:HG11	1.62	0.81
3:D:1465:ASN:HD21	3:D:1470:ARG:HH11	1.25	0.81
1:K:35:THR:HG21	1:L:43:ILE:HD11	1.62	0.81
3:D:671:LYS:HG3	5:F:422:LEU:HA	1.60	0.81
2:M:436:GLY:HA2	2:M:538:GLN:O	1.78	0.81
2:C:672:VAL:HG23	2:C:868:ASP:HB2	1.62	0.81
2:C:457:ALA:HB3	2:C:538:GLN:HA	1.60	0.81
3:D:1101:VAL:HG21	3:D:1424:VAL:HG22	1.60	0.81
1:A:195:LEU:HD11	1:A:197:LEU:HD22	1.61	0.81
3:D:73:CYS:HB3	3:D:76:CYS:O	1.81	0.81
2:M:707:ARG:HH12	2:M:709:GLU:HB2	1.44	0.81
2:C:244:PRO:HD2	2:C:245:GLY:H	1.46	0.81
2:C:512:ARG:HB3	2:C:523:ILE:HD11	1.62	0.81
2:C:949:LYS:HD2	3:D:796:ARG:HH21	1.44	0.81
1:L:22:GLU:HG2	1:L:198:ARG:HG2	1.62	0.81
3:N:1123:PHE:HE2	3:N:1184:GLN:HA	1.46	0.81
3:D:530:VAL:HB	3:D:534:ARG:HB2	1.61	0.81
2:C:10:ARG:HA	2:C:10:ARG:HH11	1.45	0.80
2:M:462:ASP:HB3	2:M:468:ARG:HD2	1.62	0.80
2:M:904:PRO:HD2	2:M:908:GLY:HA2	1.63	0.80
3:N:148:GLU:HB3	3:N:151:GLN:HB2	1.61	0.80
2:C:675:ALA:HA	2:C:989:VAL:HG12	1.62	0.80
3:D:152:LEU:H	3:D:152:LEU:HD23	1.44	0.80
2:M:227:PHE:HA	2:M:230:ARG:HE	1.46	0.80
1:L:185:ARG:HG3	1:L:190:THR:HG22	1.62	0.80
2:M:890:LEU:HD12	2:M:914:ILE:HD13	1.61	0.80
3:N:1352:ILE:O	3:N:1355:VAL:HG23	1.81	0.80
3:D:1359:GLN:HB3	9:D:9531:HOH:O	1.81	0.80
3:D:487:ALA:HB3	9:D:9629:HOH:O	1.81	0.80
3:D:584:ASN:HD22	3:D:585:GLY:N	1.80	0.80
3:D:720:LEU:H	3:D:720:LEU:HD12	1.47	0.80
2:M:83:CYS:HA	2:M:88:LEU:HB3	1.64	0.80
1:A:206:THR:HG22	1:A:209:GLU:HG3	1.63	0.80
3:D:550:ARG:HA	9:D:9572:HOH:O	1.80	0.80
2:M:728:HIS:HB3	2:M:729:LEU:HD12	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:394:ARG:HA	5:F:397:ILE:HD12	1.62	0.80
1:K:24:VAL:HG22	1:K:196:THR:HB	1.64	0.80
3:D:153:LEU:HD12	3:D:154:THR:N	1.97	0.80
3:D:601:ARG:HD2	5:F:328:PHE:HE1	1.46	0.80
5:P:94:LEU:HB2	5:P:98:GLU:HG3	1.64	0.79
2:C:873:PRO:HG2	3:D:947:ILE:HD12	1.64	0.79
3:D:397:LYS:HG2	9:D:9991:HOH:O	1.82	0.79
1:L:214:ALA:HA	1:L:217:ILE:HD12	1.64	0.79
3:N:86:ARG:O	3:N:522:PRO:HD2	1.81	0.79
2:C:292:ARG:HD2	2:C:299:LYS:HE2	1.64	0.79
5:P:85:LEU:HA	5:P:88:ILE:HD12	1.65	0.79
2:C:36:PRO:HG2	2:C:70:GLU:HB3	1.63	0.79
3:N:1205:TYR:CD2	3:N:1215:VAL:HG21	2.17	0.79
1:B:176:ARG:HH22	3:D:884:ARG:HD3	1.47	0.79
2:C:773:LEU:HB2	5:F:373:LYS:HB3	1.64	0.79
3:D:704:ARG:HE	3:D:705:ALA:H	1.28	0.79
3:D:41:ARG:HH11	3:D:42:ASP:HB2	1.47	0.79
2:C:83:CYS:HA	2:C:88:LEU:HB3	1.64	0.79
1:K:227:ASN:HD22	1:K:227:ASN:H	1.30	0.79
2:M:676:ILE:HD12	2:M:871:LEU:HB2	1.63	0.79
3:N:1160:LEU:HD11	3:N:1174:LEU:HD21	1.64	0.79
3:D:697:GLY:HA2	9:D:2528:HOH:O	1.83	0.79
3:D:908:LYS:HB3	3:D:1027:GLY:HA3	1.65	0.78
3:D:400:VAL:HG21	3:D:441:ARG:HH11	1.49	0.78
2:M:333:ILE:HB	9:M:9987:HOH:O	1.84	0.78
3:N:1223:ILE:H	3:N:1223:ILE:HD12	1.47	0.78
3:D:9:ARG:HH12	3:D:506:GLY:HA2	1.48	0.78
3:N:26:VAL:HG11	3:N:44:LEU:HD23	1.64	0.78
2:C:690:ILE:HG23	2:C:852:ILE:HG23	1.64	0.78
2:M:326:ASP:HA	2:M:331:ARG:HD3	1.64	0.78
3:N:628:ARG:HD3	3:N:744:GLN:NE2	1.97	0.78
3:N:806:PHE:CE1	3:N:813:LEU:HB3	2.18	0.78
2:C:343:GLN:HG2	2:C:385:PHE:HB2	1.66	0.78
3:D:1045:MET:HG2	3:D:1073:SER:HA	1.65	0.78
3:N:1045:MET:HG2	3:N:1073:SER:HA	1.65	0.78
5:P:268:ILE:HA	5:P:271:LEU:HD12	1.65	0.78
2:C:462:ASP:HB3	2:C:468:ARG:HD2	1.66	0.78
1:K:42:ARG:HH12	2:M:857:ASP:HB3	1.49	0.78
3:D:1258:ARG:CZ	3:D:1262:LEU:HD11	2.13	0.78
1:L:13:VAL:HG11	1:L:208:LEU:HD11	1.65	0.78
2:C:455:LEU:HD12	2:C:459:ALA:HB3	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1381:VAL:HB	3:D:1389:LEU:O	1.84	0.78
2:M:329:GLY:HA3	2:M:489:THR:HG23	1.65	0.78
2:M:250:ARG:HG2	2:M:253:ALA:HB3	1.66	0.78
3:D:1109:GLU:HG2	3:D:1201:CYS:HA	1.65	0.78
1:K:123:MET:HG2	9:K:3485:HOH:O	1.82	0.78
2:M:724:ARG:HG3	2:M:741:GLY:H	1.49	0.78
2:M:707:ARG:HD2	2:M:824:ARG:HD3	1.65	0.78
2:C:144:PRO:HA	2:C:163:ILE:HG12	1.64	0.78
3:D:637:LEU:HD21	3:D:642:CYS:HA	1.66	0.77
2:M:833:LEU:HD11	2:M:849:VAL:HG21	1.65	0.77
2:C:41:ASN:HD22	2:C:41:ASN:H	1.29	0.77
5:F:117:SER:HA	9:F:9599:HOH:O	1.84	0.77
2:M:771:GLU:O	2:M:775:ARG:HG2	1.85	0.77
2:M:879:ARG:HH12	3:N:1029:ARG:NH2	1.83	0.77
1:A:198:ARG:HG2	9:A:9490:HOH:O	1.85	0.77
2:M:312:ALA:HB1	2:M:318:PRO:HG2	1.66	0.77
2:M:601:GLY:HA2	2:M:616:GLU:HG2	1.66	0.77
3:N:984:THR:HG22	3:N:987:GLU:HG3	1.66	0.77
1:A:133:GLU:HG2	1:A:134:GLU:N	2.00	0.77
2:C:405:ARG:HH12	2:C:563:ASN:ND2	1.83	0.77
1:K:54:THR:CG2	1:K:158:ILE:HG13	2.15	0.77
2:M:897:LEU:HB3	2:M:899:GLN:HE21	1.50	0.77
3:N:35:ARG:HD2	3:N:36:THR:H	1.47	0.77
3:N:53:ILE:HG23	3:N:54:LYS:H	1.48	0.77
1:A:126:ASP:HB2	9:A:9492:HOH:O	1.85	0.77
3:N:58:CYS:HA	3:N:78:VAL:HG11	1.66	0.77
2:C:1054:THR:HG21	2:C:1079:PRO:HB3	1.66	0.77
5:F:125:ASP:HA	5:F:128:ARG:HH12	1.48	0.77
5:P:132:ARG:HH11	5:P:136:LEU:HD21	1.50	0.77
3:N:396:VAL:HG21	3:N:447:VAL:HB	1.67	0.77
3:N:488:ARG:HB3	3:N:488:ARG:NH1	2.00	0.77
3:D:1194:CYS:HB3	3:D:1373:ARG:NH2	1.99	0.77
5:F:411:HIS:HA	5:F:414:ARG:HG3	1.67	0.77
3:N:1123:PHE:CE2	3:N:1184:GLN:HA	2.19	0.77
3:N:1277:ILE:HA	9:N:9881:HOH:O	1.84	0.77
3:N:906:GLN:HB3	3:N:911:LEU:HD11	1.66	0.77
3:D:631:ILE:HG21	3:D:745:MET:HG3	1.66	0.77
5:F:196:VAL:HG22	5:F:213:ILE:HD13	1.66	0.77
2:M:232:GLU:HA	2:M:235:LEU:HD12	1.65	0.77
3:D:1236:LEU:HD11	3:D:1356:TYR:HE1	1.49	0.77
1:K:198:ARG:HD3	1:K:200:TRP:HH2	1.50	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:67:ARG:HB2	5:P:375:LEU:HD11	1.66	0.76
3:D:1311:LEU:HA	9:D:9756:HOH:O	1.85	0.76
5:F:136:LEU:HD11	9:F:9565:HOH:O	1.84	0.76
2:C:903:SER:HA	9:C:2024:HOH:O	1.84	0.76
2:C:1098:ASP:HB2	3:D:21:TRP:HZ2	1.48	0.76
3:D:194:GLY:H	3:D:206:ARG:HA	1.50	0.76
1:L:206:THR:HG22	1:L:209:GLU:H	1.49	0.76
2:M:332:ARG:HD3	9:M:9675:HOH:O	1.86	0.76
2:M:997:LEU:HG	9:M:9828:HOH:O	1.83	0.76
3:N:1147:ARG:HB3	3:N:1188:VAL:HG21	1.65	0.76
3:N:217:LYS:HA	9:N:2156:HOH:O	1.85	0.76
1:A:110:LYS:HG3	9:A:9494:HOH:O	1.86	0.76
3:D:133:ILE:HG23	3:D:456:MET:SD	2.26	0.76
1:K:178:ALA:HB3	1:K:198:ARG:HG3	1.66	0.76
1:L:205:VAL:HG23	9:L:3448:HOH:O	1.85	0.76
3:N:141:ILE:HD13	3:N:450:TYR:HB2	1.67	0.76
1:B:206:THR:HG22	1:B:209:GLU:HB2	1.66	0.76
5:P:131:VAL:HG12	5:P:181:GLU:HG3	1.68	0.76
3:D:1175:ILE:O	3:D:1179:GLU:HG3	1.86	0.76
5:F:75:ILE:HG22	9:F:9601:HOH:O	1.85	0.76
3:N:1197:ARG:HG3	3:N:1198:TYR:H	1.49	0.76
2:M:420:ARG:HD2	2:M:420:ARG:H	1.50	0.76
3:N:1109:GLU:HG2	3:N:1201:CYS:HA	1.68	0.76
3:D:904:VAL:HG22	9:D:2047:HOH:O	1.84	0.76
1:L:152:PRO:HD2	1:L:155:LYS:HG3	1.66	0.76
3:N:1220:ALA:HB1	3:N:1223:ILE:HD13	1.67	0.76
3:N:422:ALA:H	3:N:427:VAL:HG11	1.51	0.76
3:N:6:ARG:HH11	3:N:6:ARG:HB3	1.51	0.76
1:L:56:VAL:HG13	1:L:142:VAL:HG12	1.68	0.76
3:N:119:SER:HB2	3:N:123:LEU:HB2	1.66	0.76
3:D:562:ALA:HB1	3:D:567:ILE:HD11	1.65	0.75
5:F:261:PRO:O	5:F:264:MET:HG2	1.86	0.75
2:C:710:ILE:HB	2:C:790:LEU:HD13	1.68	0.75
2:C:904:PRO:HD2	2:C:908:GLY:HA2	1.69	0.75
3:D:956:ILE:HG12	3:D:1039:CYS:O	1.85	0.75
9:M:2201:HOH:O	4:O:31:LEU:HB2	1.86	0.75
5:F:76:SER:O	5:F:80:PRO:HD2	1.86	0.75
2:M:396:ASP:HA	2:M:633:GLN:HE22	1.51	0.75
2:M:952:LEU:HD12	2:M:969:GLN:NE2	1.97	0.75
2:C:1056:LYS:HB3	3:D:624:ASP:H	1.52	0.75
2:C:157:ARG:HD2	2:C:314:THR:HG22	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:93:LEU:HG	5:F:190:ALA:CB	2.16	0.75
2:M:49:ARG:HA	9:M:9640:HOH:O	1.85	0.75
2:M:691:SER:HB2	2:M:858:MET:SD	2.27	0.75
3:N:192:ALA:O	3:N:195:VAL:HG23	1.85	0.75
2:M:1097:LEU:HD13	2:M:1097:LEU:H	1.51	0.75
3:N:1273:VAL:HG22	3:N:1326:THR:OG1	1.86	0.75
3:N:211:VAL:HG22	3:N:393:ILE:HG23	1.67	0.75
9:C:9697:HOH:O	4:E:28:GLN:HA	1.87	0.75
2:M:517:ARG:HE	2:M:522:VAL:HG11	1.50	0.75
3:D:422:ALA:H	3:D:427:VAL:HG11	1.52	0.75
2:M:598:GLU:O	2:M:651:LYS:HG3	1.87	0.75
3:D:65:ARG:HG3	3:D:66:GLN:H	1.49	0.75
5:F:120:THR:HB	9:F:9599:HOH:O	1.87	0.75
3:N:145:VAL:HG22	3:N:146:PRO:HD2	1.69	0.75
2:C:603:VAL:HG21	2:C:643:VAL:HG11	1.67	0.75
3:D:478:LEU:HD13	3:D:1388:ARG:HH22	1.52	0.75
1:L:24:VAL:HG12	9:L:3467:HOH:O	1.86	0.75
2:M:736:ASP:O	2:M:744:ARG:HG2	1.87	0.74
2:M:943:VAL:HG23	2:M:985:GLY:H	1.52	0.74
3:D:965:GLU:HG3	3:D:969:ARG:HH21	1.51	0.74
2:M:1038:TRP:HE1	3:N:1463:LYS:NZ	1.85	0.74
1:A:101:LEU:HG	1:A:114:PHE:HA	1.70	0.74
2:C:10:ARG:HA	2:C:10:ARG:NH1	2.03	0.74
2:C:186:VAL:HG23	2:C:187:ASN:H	1.51	0.74
3:D:890:VAL:HA	9:D:9911:HOH:O	1.87	0.74
1:L:156:HIS:ND1	1:L:158:ILE:HG12	2.02	0.74
3:N:468:LEU:HB3	9:N:9663:HOH:O	1.87	0.74
2:C:1056:LYS:HD3	3:D:623:VAL:HG13	1.69	0.74
3:D:1438:ALA:O	3:D:1443:THR:HG22	1.86	0.74
2:C:1054:THR:HG23	2:C:1082:PRO:HG3	1.70	0.74
2:C:132:ALA:HB1	2:C:632:ASN:HD21	1.53	0.74
3:D:55:ASP:HA	3:D:82:LYS:HG3	1.67	0.74
5:F:156:VAL:HA	5:F:159:ILE:HD12	1.68	0.74
5:F:248:ASN:HA	5:F:251:ILE:HD12	1.70	0.74
2:M:1111:ILE:HG13	2:M:1112:PHE:H	1.53	0.74
2:M:579:VAL:HG11	2:M:887:GLU:HG3	1.69	0.74
3:N:1290:LEU:HD23	3:N:1291:SER:H	1.52	0.74
1:K:117:VAL:HB	1:K:120:VAL:HG12	1.68	0.74
1:L:100:LEU:HB2	1:L:115:LEU:HD21	1.69	0.74
1:A:177:VAL:HG12	9:A:9593:HOH:O	1.88	0.74
2:C:144:PRO:HG2	2:C:265:ARG:HH12	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:282:GLY:HA2	2:C:308:ARG:HH12	1.53	0.74
3:N:1062:ARG:HG3	9:N:9910:HOH:O	1.87	0.74
3:N:136:ASP:HB2	3:N:137:PRO:HD3	1.70	0.74
3:N:1438:ALA:O	3:N:1443:THR:HG22	1.88	0.74
2:C:500:ASN:HD21	3:D:1067:VAL:HG23	1.52	0.74
2:C:72:ARG:HG2	9:C:9760:HOH:O	1.86	0.74
2:C:768:THR:HB	2:C:771:GLU:HB3	1.70	0.74
2:M:64:LEU:HA	9:M:9656:HOH:O	1.86	0.74
3:D:1109:GLU:OE1	3:D:1201:CYS:HB2	1.86	0.74
5:F:163:LEU:HD22	5:F:174:LEU:HG	1.69	0.74
5:P:92:PRO:HA	9:P:4361:HOH:O	1.87	0.74
1:B:20:TYR:HB3	9:B:9501:HOH:O	1.87	0.74
3:D:1087:ARG:HD3	3:D:1090:ASP:HB2	1.70	0.74
5:F:191:ASN:HB2	9:F:9537:HOH:O	1.87	0.74
2:M:786:LYS:HA	9:M:9505:HOH:O	1.87	0.74
3:N:1393:GLN:HB2	3:N:1398:TRP:HE1	1.53	0.74
3:N:644:LEU:HD12	3:N:645:PRO:HD2	1.70	0.74
5:P:142:ARG:HH11	5:P:142:ARG:HB3	1.53	0.74
1:B:16:GLN:HB2	9:B:9501:HOH:O	1.89	0.73
2:C:117:HIS:HA	9:C:9729:HOH:O	1.87	0.73
1:A:27:PRO:HG2	1:A:186:LEU:HD22	1.68	0.73
2:C:96:ALA:HA	9:C:9760:HOH:O	1.88	0.73
3:D:161:LEU:HD22	3:D:452:ILE:HG21	1.68	0.73
3:D:97:THR:HG21	3:D:571:LYS:HD3	1.70	0.73
1:K:87:VAL:HG21	1:K:144:VAL:HG11	1.70	0.73
3:D:1264:GLU:OE1	3:D:1425:THR:HB	1.88	0.73
3:N:12:LEU:HD23	3:N:13:ALA:H	1.53	0.73
3:N:194:GLY:H	3:N:206:ARG:HA	1.52	0.73
3:N:972:LEU:HD22	9:N:9844:HOH:O	1.88	0.73
2:C:1055:LEU:HD23	9:C:9632:HOH:O	1.87	0.73
2:C:136:ILE:HG21	2:C:336:VAL:HG13	1.70	0.73
3:D:1273:VAL:HG22	3:D:1326:THR:OG1	1.89	0.73
3:N:850:LEU:H	3:N:850:LEU:HD12	1.53	0.73
3:N:422:ALA:HB1	5:P:178:ARG:HH12	1.53	0.73
5:P:256:ARG:NH1	5:P:313:GLU:HG2	2.03	0.73
2:C:479:VAL:CG2	2:C:503:LEU:HD11	2.19	0.73
3:D:704:ARG:NE	3:D:705:ALA:H	1.86	0.73
3:N:399:ARG:HG3	9:N:2231:HOH:O	1.87	0.73
3:D:1221:VAL:HG13	9:D:9929:HOH:O	1.88	0.73
3:D:1277:ILE:HD12	3:D:1301:LYS:HB2	1.70	0.73
2:C:1091:GLU:OE1	3:D:613:ARG:HG2	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:1016:ILE:HG12	9:P:5990:HOH:O	1.88	0.73
2:C:233:GLU:OE1	2:C:237:ARG:HD3	1.89	0.73
3:D:633:VAL:HG22	3:D:635:PRO:HD3	1.71	0.73
2:M:1051:GLU:HG2	2:M:1056:LYS:HD2	1.70	0.73
3:N:783:ARG:NH2	3:N:1029:ARG:HD3	2.02	0.73
3:N:1465:ASN:HD21	3:N:1470:ARG:HD3	1.53	0.73
1:A:8:ALA:HB1	1:B:224:TYR:CE1	2.24	0.73
3:D:544:TYR:O	3:D:548:ILE:HG12	1.88	0.73
3:D:6:ARG:HH11	3:D:6:ARG:HB3	1.51	0.73
1:K:103:ALA:HB1	1:K:107:LYS:HD3	1.69	0.73
2:M:395:LYS:HE2	2:M:403:SER:HB2	1.69	0.73
2:M:603:VAL:HG21	2:M:643:VAL:HG11	1.70	0.73
3:N:807:ALA:HB2	3:N:833:GLU:OE1	1.89	0.73
1:A:222:LEU:HD12	1:B:215:VAL:HB	1.69	0.73
1:B:185:ARG:HG3	1:B:190:THR:HG23	1.71	0.73
1:A:42:ARG:NH2	1:B:34:VAL:HB	2.04	0.73
3:D:920:LEU:HB2	9:D:9488:HOH:O	1.88	0.73
2:C:1008:ARG:NH1	2:C:1020:PRO:HB3	2.04	0.73
3:D:1095:THR:O	3:D:1099:VAL:HG23	1.87	0.73
3:D:1412:LYS:O	3:D:1414:PRO:HD3	1.89	0.73
5:F:416:ARG:HB3	9:F:9582:HOH:O	1.89	0.73
1:L:57:TYR:HE1	1:L:163:ASN:HB2	1.53	0.73
2:M:362:GLY:HA3	2:M:367:LEU:HD23	1.71	0.73
2:M:710:ILE:HB	2:M:790:LEU:HD12	1.71	0.73
3:N:699:VAL:HG12	3:N:717:GLN:HA	1.69	0.73
5:P:234:LYS:HG3	9:P:3697:HOH:O	1.88	0.73
1:A:14:ARG:NH2	1:A:22:GLU:HB3	2.04	0.72
1:A:9:PRO:HD2	1:B:224:TYR:CZ	2.23	0.72
3:D:1310:ARG:NE	3:D:1327:ARG:HB3	2.04	0.72
2:M:264:PRO:HB3	2:M:289:THR:HG21	1.71	0.72
2:M:948:GLU:HA	9:M:9767:HOH:O	1.88	0.72
3:D:127:LEU:HD11	3:D:461:ILE:HD11	1.69	0.72
5:F:93:LEU:HD22	5:F:98:GLU:HB3	1.69	0.72
3:D:662:GLU:HB2	9:D:9514:HOH:O	1.89	0.72
2:M:626:ARG:NH1	2:M:637:LEU:HD12	2.04	0.72
2:M:651:LYS:HA	9:M:9639:HOH:O	1.89	0.72
3:N:1036:ARG:NH2	3:N:1042:ARG:HA	2.04	0.72
3:N:1112:CYS:HB2	3:N:1195:GLN:OE1	1.88	0.72
3:N:1381:VAL:HB	3:N:1389:LEU:O	1.87	0.72
3:N:44:LEU:HB3	3:N:525:ARG:HH21	1.54	0.72
3:N:87:ARG:HB3	3:N:523:ASP:HB2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ARG:NH2	1:A:202:ASP:HA	2.04	0.72
2:C:678:PRO:HG3	3:D:947:ILE:HD11	1.70	0.72
3:D:215:TYR:O	3:D:389:GLU:HB2	1.88	0.72
3:D:806:PHE:CE1	3:D:813:LEU:HB3	2.24	0.72
5:F:113:ILE:HA	5:F:116:LEU:HD12	1.70	0.72
1:K:222:LEU:HD11	1:L:218:LEU:HD23	1.72	0.72
2:M:71:TYR:HD2	2:M:71:TYR:H	1.36	0.72
3:N:108:VAL:HG23	3:N:109:PRO:HD3	1.71	0.72
3:N:1412:LYS:O	3:N:1414:PRO:HD3	1.89	0.72
3:N:885:ILE:HG13	9:N:9868:HOH:O	1.89	0.72
2:M:1082:PRO:HG2	3:N:1469:GLY:HA3	1.72	0.72
2:M:165:LEU:HB2	9:M:9535:HOH:O	1.89	0.72
3:N:1481:VAL:HG13	4:O:18:ARG:HE	1.54	0.72
3:N:475:LYS:HA	3:N:478:LEU:HD12	1.70	0.72
1:A:145:ASP:HB3	9:A:9484:HOH:O	1.90	0.72
2:C:478:VAL:HA	2:C:506:ASN:O	1.90	0.72
3:N:65:ARG:HG3	3:N:66:GLN:H	1.53	0.72
2:C:993:PHE:HE1	2:C:995:MET:HG2	1.53	0.72
3:D:842:VAL:HG23	9:D:2618:HOH:O	1.89	0.72
2:M:605:LYS:HB2	2:M:610:ARG:NH1	2.00	0.72
2:M:897:LEU:HG	2:M:920:GLN:NE2	2.04	0.72
3:N:1090:ASP:HA	3:N:1093:TYR:HB2	1.72	0.72
3:N:212:ARG:HA	9:N:2226:HOH:O	1.90	0.72
3:N:996:TRP:HA	3:N:999:THR:HG22	1.72	0.72
4:O:51:LEU:HD12	4:O:52:GLU:H	1.55	0.72
1:B:36:LEU:O	1:B:39:PRO:HD2	1.89	0.72
2:C:683:ASN:HA	2:C:687:ALA:HB3	1.71	0.72
2:C:8:ARG:HG2	9:C:9597:HOH:O	1.89	0.72
2:M:367:LEU:HD23	2:M:371:LYS:HZ2	1.55	0.72
2:M:679:PHE:HB3	9:M:9536:HOH:O	1.87	0.72
3:N:601:ARG:HG2	3:N:606:ILE:HD13	1.72	0.72
3:N:853:VAL:HG22	3:N:858:VAL:HG23	1.71	0.72
3:D:1292:VAL:HG23	3:D:1305:LEU:HD11	1.71	0.72
2:M:139:GLN:HB3	2:M:334:ARG:HD2	1.71	0.72
3:N:197:SER:HB2	3:N:205:TYR:CZ	2.25	0.72
1:A:8:ALA:HB1	1:B:224:TYR:HE1	1.54	0.72
2:C:833:LEU:HD12	2:C:834:GLN:H	1.54	0.72
1:A:42:ARG:HH11	2:C:978:ARG:HA	1.55	0.72
3:D:1166:LEU:HD23	3:D:1166:LEU:H	1.54	0.72
3:D:1209:LEU:HD21	4:E:16:LYS:HZ3	1.50	0.72
3:D:1272:ALA:HA	3:D:1326:THR:HB	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:187:LYS:HE2	3:D:213:VAL:HG12	1.72	0.72
3:D:41:ARG:HD3	3:D:42:ASP:N	2.05	0.72
3:D:723:GLY:HA3	9:D:9551:HOH:O	1.90	0.72
3:D:978:TYR:HA	9:D:9513:HOH:O	1.89	0.72
2:M:210:GLU:HA	9:M:2282:HOH:O	1.90	0.72
3:N:1382:THR:HG21	3:N:1418:LYS:NZ	2.05	0.72
2:C:728:HIS:HB3	2:C:729:LEU:HD12	1.72	0.71
2:M:512:ARG:HB3	2:M:523:ILE:HD11	1.72	0.71
3:N:119:SER:H	3:N:123:LEU:HD22	1.54	0.71
2:C:108:ILE:HB	2:C:368:THR:OG1	1.88	0.71
2:C:504:GLU:HG2	9:C:9601:HOH:O	1.89	0.71
3:D:12:LEU:HD13	3:D:511:TRP:HB2	1.70	0.71
3:D:654:LYS:HB3	3:D:655:PRO:HD3	1.72	0.71
2:M:546:LEU:HD11	2:M:666:LEU:HD23	1.71	0.71
5:P:178:ARG:HD3	9:P:3512:HOH:O	1.87	0.71
1:A:49:PRO:HB3	1:A:148:VAL:HG22	1.71	0.71
2:C:987:ILE:HG23	3:D:948:THR:CG2	2.21	0.71
5:F:80:PRO:HA	5:F:83:GLN:HB2	1.70	0.71
2:M:572:ILE:HD11	2:M:698:ASP:HB3	1.71	0.71
3:N:771:SER:HB2	3:N:778:LEU:HD13	1.72	0.71
2:C:64:LEU:HD22	2:C:359:MET:HG3	1.72	0.71
3:D:534:ARG:HD3	9:F:9549:HOH:O	1.90	0.71
3:D:564:GLU:HA	3:D:567:ILE:HD12	1.73	0.71
2:C:15:LEU:HD12	2:C:15:LEU:H	1.55	0.71
1:A:46:SER:HB3	2:C:856:GLU:HG2	1.73	0.71
3:D:178:LEU:HD11	9:D:9843:HOH:O	1.89	0.71
1:K:226:SER:O	1:K:228:PRO:HD3	1.90	0.71
2:M:1000:MET:O	2:M:1003:ASP:HB3	1.91	0.71
2:M:274:ARG:HD2	2:M:285:LEU:HB3	1.73	0.71
2:M:578:VAL:HG11	2:M:991:GLN:HB3	1.72	0.71
2:C:30:LEU:HB3	2:C:44:ILE:HD12	1.72	0.71
3:D:982:PHE:HB3	9:D:2466:HOH:O	1.89	0.71
1:K:39:PRO:O	1:K:43:ILE:HG12	1.90	0.71
3:N:1145:TYR:HE2	3:N:1168:MET:HB2	1.56	0.71
3:N:65:ARG:HA	9:N:2129:HOH:O	1.91	0.71
3:D:100:ALA:HB2	9:D:9966:HOH:O	1.90	0.71
3:D:1136:LYS:HE3	3:D:1139:ASP:OD2	1.90	0.71
1:L:24:VAL:HG13	1:L:196:THR:HB	1.73	0.71
2:M:772:ARG:HB2	2:M:772:ARG:HH11	1.54	0.71
2:M:948:GLU:HB2	9:M:9817:HOH:O	1.90	0.71
5:P:102:LEU:HD13	5:P:187:LEU:HG	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:561:GLY:HA3	5:F:184:ARG:HH12	1.55	0.71
3:D:825:ALA:HB1	9:D:9486:HOH:O	1.91	0.71
2:M:36:PRO:HG2	2:M:70:GLU:HB3	1.70	0.71
2:M:769:PRO:HD2	9:N:2324:HOH:O	1.91	0.71
3:N:1404:ASN:HD22	3:N:1408:ILE:HD12	1.56	0.71
3:N:1434:TRP:CZ3	3:N:1457:ASP:HB2	2.26	0.71
2:C:557:ARG:CZ	2:C:879:ARG:HD3	2.20	0.71
2:C:670:GLN:O	2:C:672:VAL:HG12	1.91	0.71
3:D:955:VAL:HB	3:D:1011:PHE:HE1	1.56	0.71
3:D:1129:THR:HG23	3:D:1130:ARG:H	1.56	0.71
3:D:165:LYS:HB3	3:D:395:VAL:HG11	1.71	0.71
9:K:3474:HOH:O	1:L:42:ARG:HB3	1.91	0.71
2:M:199:VAL:HG13	2:M:235:LEU:HG	1.71	0.71
1:B:97:VAL:HG11	1:B:120:VAL:HG21	1.72	0.71
2:C:127:PHE:HA	9:C:9502:HOH:O	1.89	0.71
2:C:352:ALA:O	2:C:356:ARG:HG3	1.91	0.71
3:D:1266:ARG:O	3:D:1268:PRO:HD3	1.91	0.71
4:E:30:LEU:O	4:E:35:PHE:HA	1.90	0.71
3:N:962:GLN:HA	9:N:2437:HOH:O	1.90	0.71
5:P:163:LEU:HB3	5:P:174:LEU:HG	1.73	0.71
1:B:94:LEU:HD21	1:B:119:ASP:HB2	1.73	0.70
3:D:1307:LYS:HD3	3:D:1307:LYS:H	1.56	0.70
3:D:1464:GLU:HG2	9:D:2152:HOH:O	1.89	0.70
3:D:177:ALA:HB1	3:D:199:LEU:HD22	1.73	0.70
5:F:88:ILE:HB	9:F:9492:HOH:O	1.90	0.70
2:M:409:ARG:HH22	7:M:8002:RPT:H18	1.55	0.70
1:A:10:VAL:HG12	1:A:12:THR:HG22	1.72	0.70
3:D:493:ARG:NE	3:D:1388:ARG:HB3	2.06	0.70
3:D:542:ASP:O	3:D:546:ARG:HG2	1.92	0.70
3:D:756:GLN:O	3:D:760:ARG:HG2	1.91	0.70
4:E:33:HIS:HB2	4:E:37:ASN:HD21	1.55	0.70
5:F:371:LEU:HD22	5:F:375:LEU:HD22	1.73	0.70
5:F:77:THR:O	5:F:81:VAL:HG23	1.90	0.70
2:M:150:PRO:HA	2:M:158:TYR:HB3	1.71	0.70
2:M:218:VAL:HA	2:M:221:LEU:HD23	1.71	0.70
2:M:704:HIS:HB2	2:M:831:ARG:HE	1.56	0.70
3:N:804:LEU:HB2	3:N:830:ALA:O	1.91	0.70
5:P:291:ILE:HG21	5:P:304:VAL:HG11	1.71	0.70
3:D:1220:ALA:HB1	3:D:1223:ILE:HD13	1.73	0.70
2:M:169:GLY:HA2	2:M:263:ASP:CB	2.20	0.70
1:B:99:LEU:HD21	1:B:122:ILE:HD11	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:611:ILE:HD11	2:C:641:PRO:HB3	1.73	0.70
3:D:233:LYS:HA	9:D:2088:HOH:O	1.90	0.70
5:F:398:ARG:HG2	5:F:402:ASN:HD22	1.56	0.70
1:K:19:GLU:HG3	9:K:4352:HOH:O	1.91	0.70
2:M:1014:SER:HB3	2:M:1017:THR:O	1.90	0.70
2:M:151:ASP:HB2	2:M:157:ARG:O	1.91	0.70
2:M:34:VAL:HB	2:M:38:LYS:HG3	1.73	0.70
3:N:884:ARG:HD2	9:N:9868:HOH:O	1.91	0.70
2:C:264:PRO:HB3	2:C:289:THR:HG21	1.74	0.70
3:D:161:LEU:HD23	3:D:449:SER:HB3	1.72	0.70
2:M:111:ASP:HA	9:M:2096:HOH:O	1.92	0.70
2:M:198:ARG:HH21	2:M:203:ASP:HB3	1.56	0.70
5:P:406:ARG:HA	5:P:409:LYS:HG2	1.72	0.70
2:C:554:ASP:OD2	2:C:556:ASN:HB3	1.91	0.70
3:D:1192:LEU:HD22	3:D:1345:GLU:HG2	1.73	0.70
3:N:153:LEU:HD11	3:N:158:TYR:N	2.06	0.70
2:C:1054:THR:HG22	2:C:1059:ASP:HB2	1.72	0.70
3:D:30:GLU:HB3	3:D:40:GLU:HB3	1.72	0.70
3:D:127:LEU:HD21	3:D:461:ILE:HD11	1.73	0.70
2:M:269:LEU:HD21	9:M:9709:HOH:O	1.90	0.70
2:M:767:PRO:HG2	9:M:2323:HOH:O	1.91	0.70
3:N:87:ARG:CB	3:N:523:ASP:HB2	2.21	0.70
2:C:773:LEU:HD13	9:F:9672:HOH:O	1.91	0.70
2:C:376:ARG:HH12	5:F:285:GLU:HG2	1.57	0.70
2:M:1095:LEU:HB2	2:M:1097:LEU:CD2	2.22	0.70
2:M:328:LEU:HD23	2:M:437:ARG:HD3	1.74	0.70
3:N:966:GLU:HA	3:N:969:ARG:NH1	2.07	0.70
5:P:156:VAL:HA	5:P:159:ILE:HD12	1.72	0.70
5:P:291:ILE:HG23	5:P:304:VAL:HG21	1.74	0.70
1:B:27:PRO:HB3	1:B:192:LEU:HD22	1.74	0.70
2:C:110:GLU:HG2	2:C:369:PRO:CB	2.20	0.70
2:C:269:LEU:HD12	2:C:288:ARG:H	1.57	0.70
2:C:791:ARG:HH11	2:C:791:ARG:HB3	1.57	0.70
2:M:136:ILE:HG21	2:M:336:VAL:HG13	1.73	0.70
2:M:139:GLN:OE1	2:M:415:PRO:HD2	1.92	0.70
3:D:131:LYS:HE2	5:F:83:GLN:HE22	1.55	0.70
3:D:1493:LYS:O	3:D:1497:GLU:HG2	1.91	0.70
3:N:1033:GLN:HE21	3:N:1036:ARG:HD3	1.57	0.70
1:B:156:HIS:ND1	1:B:158:ILE:HG12	2.06	0.69
2:C:84:ARG:HH21	2:C:128:ILE:HD11	1.57	0.69
2:C:42:VAL:HG12	2:C:43:GLY:H	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1109:VAL:HG23	3:D:3:LYS:HG2	1.73	0.69
4:E:9:LEU:HD13	4:E:19:LEU:HD11	1.73	0.69
5:P:112:ALA:HA	5:P:173:TYR:HD2	1.56	0.69
2:C:1000:MET:HB3	2:C:1002:GLU:HG3	1.74	0.69
3:D:1269:LYS:HB3	9:D:2348:HOH:O	1.92	0.69
3:D:566:ILE:HG23	5:F:214:GLN:OE1	1.92	0.69
2:M:182:VAL:HG12	2:M:193:LEU:HD13	1.73	0.69
3:N:1166:LEU:HD23	3:N:1166:LEU:H	1.56	0.69
3:N:704:ARG:HD2	3:N:705:ALA:H	1.57	0.69
1:A:117:VAL:HB	1:A:120:VAL:HG12	1.73	0.69
2:C:94:LEU:HD11	9:C:9738:HOH:O	1.91	0.69
2:M:157:ARG:HD2	2:M:314:THR:CG2	2.21	0.69
2:M:68:PHE:HE1	2:M:96:ALA:HB1	1.56	0.69
3:N:1393:GLN:HB2	3:N:1398:TRP:NE1	2.06	0.69
2:C:395:LYS:HE2	2:C:403:SER:HB2	1.74	0.69
2:C:420:ARG:HD3	2:C:422:ARG:HG3	1.73	0.69
5:F:358:LEU:HD21	5:F:370:LYS:HE3	1.74	0.69
2:M:385:PHE:HA	9:M:9823:HOH:O	1.92	0.69
3:N:643:GLY:HA3	3:N:727:GLN:HB2	1.72	0.69
3:D:100:ALA:HA	9:D:9738:HOH:O	1.91	0.69
1:K:101:LEU:HG	1:K:114:PHE:HA	1.72	0.69
1:L:97:VAL:HG11	1:L:120:VAL:HG21	1.72	0.69
2:M:1042:ALA:HB1	3:N:710:ARG:HE	1.58	0.69
2:M:197:LEU:HB3	2:M:202:TYR:HB2	1.75	0.69
1:B:89:PHE:HB3	1:B:94:LEU:HD13	1.75	0.69
2:C:706:GLU:HB3	2:C:708:TYR:CE1	2.26	0.69
3:D:1420:LEU:HD12	3:D:1421:LEU:N	2.07	0.69
3:D:153:LEU:CD1	3:D:157:GLU:HB2	2.23	0.69
5:F:131:VAL:HG12	5:F:181:GLU:HG3	1.74	0.69
1:K:206:THR:HG23	1:K:209:GLU:HB2	1.75	0.69
2:M:983:ILE:HG21	2:M:987:ILE:HD11	1.73	0.69
3:N:1238:MET:HG2	3:N:1256:LEU:HD23	1.74	0.69
3:N:152:LEU:HD23	3:N:152:LEU:H	1.58	0.69
3:N:397:LYS:HG2	9:N:2231:HOH:O	1.91	0.69
5:P:274:THR:O	5:P:278:LEU:HG	1.92	0.69
1:B:184:THR:HB	1:B:194:LYS:HZ3	1.55	0.69
2:C:41:ASN:H	2:C:41:ASN:ND2	1.90	0.69
3:D:1324:PRO:HA	9:D:9544:HOH:O	1.92	0.69
5:F:144:ILE:HB	5:F:145:PRO:HD3	1.75	0.69
1:L:63:HIS:HB2	9:L:3319:HOH:O	1.91	0.69
2:M:881:ASN:H	2:M:881:ASN:HD22	1.39	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1033:GLN:HE21	3:N:1036:ARG:HH11	1.40	0.69
3:N:1057:VAL:HG23	9:N:2261:HOH:O	1.92	0.69
3:N:1357:ARG:HG3	9:N:9798:HOH:O	1.93	0.69
2:C:1008:ARG:NH2	2:C:1028:GLY:HA2	2.08	0.69
3:D:908:LYS:CB	3:D:1027:GLY:HA3	2.23	0.69
3:D:427:VAL:CG2	3:D:435:VAL:HB	2.22	0.69
3:D:477:LEU:HD22	3:D:492:ALA:HB1	1.73	0.69
2:C:889:HIS:HE1	3:D:951:ILE:H	1.40	0.69
4:E:48:MET:HB2	4:E:54:LEU:HD12	1.75	0.69
2:M:768:THR:HB	2:M:771:GLU:HB3	1.75	0.69
4:O:10:PHE:HE2	4:O:16:LYS:HG3	1.58	0.69
2:C:1008:ARG:HH21	2:C:1028:GLY:HA2	1.58	0.69
2:M:678:PRO:HD2	9:N:9516:HOH:O	1.93	0.69
2:M:857:ASP:HB2	2:M:978:ARG:HG2	1.73	0.69
3:N:63:TYR:HB3	3:N:68:PHE:CE1	2.28	0.69
3:N:905:PRO:HD3	9:N:2419:HOH:O	1.91	0.69
2:C:1111:ILE:HG13	2:C:1112:PHE:H	1.57	0.69
3:D:1139:ASP:HB3	3:D:1357:ARG:NH2	2.08	0.69
1:K:49:PRO:HB3	1:K:148:VAL:HG22	1.75	0.69
1:L:112:ARG:HB3	1:L:112:ARG:NH1	2.07	0.69
2:C:367:LEU:HB3	2:C:371:LYS:HG2	1.75	0.69
3:D:1361:VAL:HG23	9:D:9531:HOH:O	1.93	0.69
3:D:625:TYR:O	3:D:749:VAL:HG23	1.92	0.69
3:D:709:HIS:NE2	3:D:711:LEU:HB2	2.07	0.69
5:P:361:LEU:HG	5:P:408:LEU:HD21	1.75	0.69
2:C:199:VAL:HG21	9:C:2083:HOH:O	1.92	0.68
3:D:1476:THR:HG23	4:E:21:VAL:HG22	1.76	0.68
3:D:561:GLY:HA3	5:F:184:ARG:HH22	1.58	0.68
2:M:670:GLN:O	2:M:672:VAL:HG12	1.93	0.68
3:N:793:THR:HB	3:N:879:ARG:HD3	1.74	0.68
2:C:775:ARG:NH2	2:C:782:ALA:HB1	2.02	0.68
2:C:96:ALA:HB2	9:C:9738:HOH:O	1.93	0.68
3:D:1118:ILE:HG21	3:D:1346:ARG:NH2	2.09	0.68
3:D:119:SER:HB2	3:D:123:LEU:N	2.06	0.68
3:D:699:VAL:HG12	3:D:717:GLN:HA	1.76	0.68
2:M:518:LYS:HA	9:M:9720:HOH:O	1.93	0.68
2:M:833:LEU:HD12	2:M:834:GLN:N	2.08	0.68
3:N:507:ASN:HB2	9:N:9590:HOH:O	1.92	0.68
2:C:305:PRO:HA	2:C:308:ARG:HB3	1.74	0.68
2:C:455:LEU:H	2:C:455:LEU:HD23	1.57	0.68
3:D:1404:ASN:ND2	3:D:1408:ILE:HD12	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:820:GLU:HB2	3:D:836:VAL:HG11	1.76	0.68
5:F:372:ARG:HB2	9:F:9526:HOH:O	1.93	0.68
5:P:144:ILE:HB	5:P:145:PRO:HD3	1.74	0.68
5:P:315:VAL:HA	9:P:4529:HOH:O	1.93	0.68
1:A:14:ARG:HH22	1:A:24:VAL:HG23	1.58	0.68
2:C:597:ALA:HB2	2:C:655:LEU:HD21	1.74	0.68
3:D:1452:ILE:HG12	9:D:9759:HOH:O	1.93	0.68
1:K:61:VAL:HA	9:K:3552:HOH:O	1.94	0.68
3:N:551:ASN:HA	9:N:9830:HOH:O	1.91	0.68
5:P:185:GLN:HA	5:P:188:ILE:HD12	1.75	0.68
2:C:1096:ALA:O	3:D:13:ALA:HB2	1.93	0.68
2:M:598:GLU:HB3	9:M:9583:HOH:O	1.93	0.68
3:N:1115:THR:HG22	9:N:2569:HOH:O	1.93	0.68
1:B:115:LEU:HB2	9:B:9609:HOH:O	1.93	0.68
1:B:58:ILE:HB	1:B:61:VAL:HB	1.74	0.68
3:D:153:LEU:HD12	3:D:154:THR:H	1.57	0.68
3:D:520:LEU:HD23	3:D:540:LEU:HD22	1.75	0.68
3:D:528:VAL:O	3:D:535:PHE:HA	1.92	0.68
1:B:80:LEU:HD23	3:D:867:ARG:HH12	1.59	0.68
3:D:877:PRO:HA	9:D:9580:HOH:O	1.91	0.68
3:D:996:TRP:CE3	3:D:999:THR:HG21	2.29	0.68
1:K:18:ARG:O	1:K:207:PRO:HD3	1.93	0.68
1:L:27:PRO:HB3	1:L:192:LEU:HD22	1.75	0.68
5:P:248:ASN:HA	5:P:251:ILE:HD12	1.76	0.68
2:C:292:ARG:HB2	2:C:299:LYS:HE2	1.74	0.68
3:D:209:ARG:NH2	3:D:397:LYS:HG3	2.09	0.68
3:D:628:ARG:HD3	3:D:744:GLN:NE2	2.08	0.68
5:F:166:LEU:HB3	5:F:170:HIS:HB2	1.76	0.68
2:M:915:LYS:HE2	9:M:9698:HOH:O	1.93	0.68
3:N:30:GLU:HG3	3:N:41:ARG:HG2	1.76	0.68
3:D:1236:LEU:HD11	3:D:1356:TYR:CE1	2.29	0.68
3:D:538:SER:HB3	9:F:9546:HOH:O	1.92	0.68
3:D:584:ASN:HD21	3:D:589:ALA:HA	1.59	0.68
5:F:152:ASP:HA	9:F:9491:HOH:O	1.94	0.68
5:F:93:LEU:HG	5:F:190:ALA:HB1	1.76	0.68
2:M:326:ASP:HB2	2:M:431:HIS:ND1	2.09	0.68
2:M:683:ASN:HA	2:M:687:ALA:HB3	1.76	0.68
3:N:808:THR:HB	3:N:809:PRO:HD3	1.76	0.68
3:D:475:LYS:HG3	9:D:9989:HOH:O	1.92	0.68
3:D:988:ARG:HD2	3:D:989:TYR:N	2.09	0.68
2:C:432:ARG:HA	9:C:9669:HOH:O	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:755:LEU:HD22	2:C:825:VAL:HG11	1.76	0.68
3:D:86:ARG:HH11	3:D:86:ARG:HG2	1.58	0.68
1:K:95:GLN:HG2	1:K:146:ARG:NH1	2.08	0.68
2:M:773:LEU:HG	9:M:2483:HOH:O	1.93	0.68
4:O:30:LEU:O	4:O:35:PHE:HA	1.93	0.68
1:A:14:ARG:NH2	1:A:24:VAL:HG23	2.10	0.67
1:B:156:HIS:CE1	1:B:166:PRO:HB3	2.29	0.67
2:C:1042:ALA:HB3	3:D:710:ARG:HB3	1.76	0.67
3:D:490:ALA:HA	9:D:9583:HOH:O	1.93	0.67
3:D:611:GLN:HB3	3:D:616:GLN:NE2	2.09	0.67
5:F:212:LEU:HD11	9:F:9654:HOH:O	1.94	0.67
5:F:395:GLU:O	5:F:399:GLN:HB2	1.94	0.67
1:L:101:LEU:HD11	1:L:113:ASP:HB2	1.76	0.67
2:M:630:ARG:HA	2:M:705:ILE:HD11	1.75	0.67
3:N:119:SER:HB2	3:N:123:LEU:N	2.09	0.67
5:P:228:GLU:HB3	9:P:4672:HOH:O	1.94	0.67
2:C:732:ALA:HA	2:C:735:ARG:NH1	2.09	0.67
2:C:833:LEU:HD12	2:C:834:GLN:N	2.08	0.67
3:D:483:HIS:HB2	3:D:484:PRO:HD3	1.76	0.67
3:D:708:LEU:O	3:D:1227:GLN:HG2	1.94	0.67
3:D:715:ALA:HB3	3:D:764:LEU:HA	1.73	0.67
2:M:422:ARG:HA	9:M:9874:HOH:O	1.91	0.67
2:M:575:GLN:HE21	2:M:671:ASN:HB2	1.59	0.67
2:M:672:VAL:HG23	2:M:868:ASP:HB2	1.76	0.67
3:N:1040:GLY:O	3:N:1060:SER:HB3	1.94	0.67
3:N:187:LYS:HE2	3:N:213:VAL:HG12	1.76	0.67
5:P:384:GLU:HA	9:P:4435:HOH:O	1.94	0.67
2:C:312:ALA:HB1	2:C:318:PRO:HG2	1.75	0.67
2:C:724:ARG:HH22	2:C:734:LEU:HB3	1.60	0.67
1:L:116:PRO:HD2	9:L:4090:HOH:O	1.94	0.67
2:M:141:HIS:HB3	2:M:418:LEU:HD23	1.75	0.67
2:M:22:GLN:NE2	2:M:336:VAL:HG21	2.09	0.67
3:N:1271:LYS:HG2	3:N:1272:ALA:N	2.09	0.67
5:P:260:ILE:HD11	5:P:310:ILE:HG22	1.76	0.67
1:A:95:GLN:HG2	1:A:146:ARG:HH22	1.58	0.67
1:B:46:SER:O	1:B:148:VAL:HB	1.94	0.67
2:C:534:VAL:HB	2:C:538:GLN:OE1	1.93	0.67
3:D:1045:MET:CG	3:D:1073:SER:HA	2.24	0.67
3:D:1330:ILE:HA	9:D:2043:HOH:O	1.94	0.67
9:D:9593:HOH:O	5:F:222:ARG:HA	1.93	0.67
2:M:958:THR:OG1	2:M:961:GLU:HG2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1277:ILE:HD12	3:N:1301:LYS:HB2	1.76	0.67
3:N:754:PHE:HZ	4:O:21:VAL:HG13	1.59	0.67
5:P:76:SER:O	5:P:80:PRO:HD2	1.95	0.67
2:C:95:TYR:HA	9:C:2013:HOH:O	1.94	0.67
3:D:422:ALA:HB3	3:D:427:VAL:CG2	2.21	0.67
3:D:661:MET:HE3	3:D:673:ALA:HB1	1.74	0.67
5:F:361:LEU:HD23	5:F:362:SER:H	1.59	0.67
2:M:45:GLN:HB2	2:M:71:TYR:CE1	2.30	0.67
3:N:810:GLU:O	3:N:813:LEU:HG	1.94	0.67
3:N:898:GLU:HB2	3:N:921:ARG:HH22	1.59	0.67
2:M:1021:LEU:HD21	5:P:332:PHE:HA	1.75	0.67
3:D:754:PHE:HZ	4:E:21:VAL:HG13	1.60	0.67
2:M:23:VAL:HG12	9:M:9741:HOH:O	1.93	0.67
2:M:140:ILE:HA	2:M:332:ARG:O	1.95	0.67
2:M:478:VAL:HA	2:M:506:ASN:O	1.95	0.67
2:M:815:LEU:HD23	9:M:9901:HOH:O	1.95	0.67
2:M:92:ALA:HB1	9:M:2197:HOH:O	1.94	0.67
3:N:119:SER:OG	3:N:123:LEU:HD13	1.95	0.67
3:N:216:VAL:HG13	9:N:9526:HOH:O	1.94	0.67
3:N:529:GLN:HB2	9:N:9903:HOH:O	1.94	0.67
3:N:830:ALA:HA	9:N:9638:HOH:O	1.95	0.67
2:C:882:LEU:HD23	2:C:885:ILE:HB	1.76	0.67
2:C:72:ARG:HE	2:C:97:ARG:HH12	1.42	0.67
3:D:1280:VAL:HB	9:D:9793:HOH:O	1.95	0.67
1:K:43:ILE:HD11	1:L:35:THR:HG21	1.76	0.67
2:M:724:ARG:HG3	2:M:740:GLU:HA	1.75	0.67
3:N:1311:LEU:H	3:N:1311:LEU:HD23	1.60	0.67
4:O:51:LEU:HG	4:O:53:GLY:H	1.60	0.67
4:O:54:LEU:HD11	9:O:3983:HOH:O	1.93	0.67
9:N:9768:HOH:O	5:P:254:GLN:HG2	1.95	0.67
3:D:186:VAL:HG21	3:D:213:VAL:HB	1.76	0.67
2:C:1109:VAL:HG11	3:D:5:VAL:HG13	1.77	0.67
3:D:834:THR:HG22	3:D:838:ARG:HD2	1.77	0.67
2:M:689:VAL:HG23	2:M:870:ILE:HB	1.77	0.67
2:M:758:ARG:HB3	2:M:788:THR:O	1.95	0.67
3:N:1194:CYS:HB2	9:N:9589:HOH:O	1.93	0.67
3:N:796:ARG:NH1	3:N:861:GLN:HB2	2.10	0.67
1:B:226:SER:HB3	9:B:9483:HOH:O	1.95	0.67
3:D:207:PHE:HB3	3:D:208:PRO:HD2	1.77	0.67
3:D:393:ILE:HG22	9:D:9798:HOH:O	1.95	0.67
5:F:275:ALA:HA	5:F:278:LEU:HD12	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:189:ARG:HG2	9:L:4538:HOH:O	1.94	0.67
2:M:346:VAL:HG12	2:M:350:ARG:HE	1.60	0.67
3:N:1149:LEU:HD12	3:N:1161:GLU:O	1.93	0.67
3:N:1271:LYS:HG2	3:N:1272:ALA:H	1.59	0.67
1:B:78:ILE:HA	9:B:9525:HOH:O	1.94	0.67
2:C:1115:LEU:H	2:C:1115:LEU:HD12	1.60	0.67
3:D:1076:GLY:O	3:D:1079:LYS:HG3	1.95	0.67
3:D:1314:LYS:HD3	9:D:9730:HOH:O	1.94	0.67
3:N:1484:THR:HG21	9:O:5601:HOH:O	1.95	0.67
3:N:207:PHE:HB3	3:N:208:PRO:HD2	1.76	0.67
3:N:464:LEU:HD11	9:N:9679:HOH:O	1.95	0.67
3:N:661:MET:HA	3:N:666:ILE:HD12	1.77	0.67
2:C:881:ASN:HD22	2:C:881:ASN:H	1.44	0.66
3:D:1147:ARG:HB3	3:D:1188:VAL:HG21	1.77	0.66
5:F:321:ILE:HB	5:F:327:SER:OG	1.94	0.66
1:K:197:LEU:H	1:K:197:LEU:HD23	1.60	0.66
3:N:1337:GLU:HB3	9:N:9525:HOH:O	1.94	0.66
2:C:660:ALA:HB1	2:C:667:ALA:O	1.94	0.66
4:E:33:HIS:HB2	4:E:37:ASN:ND2	2.11	0.66
2:M:1000:MET:HB3	2:M:1002:GLU:HG3	1.75	0.66
2:M:186:VAL:HG23	2:M:187:ASN:H	1.60	0.66
2:M:686:ASP:HB2	9:N:2186:HOH:O	1.94	0.66
3:N:135:LEU:HD13	3:N:147:VAL:HG23	1.75	0.66
3:N:426:LYS:HG3	3:N:434:ARG:NH1	2.10	0.66
3:N:559:ALA:HA	9:P:4212:HOH:O	1.94	0.66
1:B:132:LEU:HD21	1:B:136:GLY:O	1.96	0.66
1:B:51:THR:HB	9:B:9600:HOH:O	1.95	0.66
3:D:795:VAL:HG23	3:D:879:ARG:NH1	2.09	0.66
1:K:54:THR:HG21	9:K:3856:HOH:O	1.95	0.66
2:M:961:GLU:HG3	9:M:9678:HOH:O	1.94	0.66
3:N:41:ARG:HD3	3:N:42:ASP:H	1.60	0.66
4:O:78:ASN:HB3	9:O:3563:HOH:O	1.94	0.66
2:C:373:VAL:HG12	9:C:9971:HOH:O	1.95	0.66
2:C:708:TYR:HE2	2:C:793:PRO:HD2	1.60	0.66
3:D:1112:CYS:HA	9:D:2465:HOH:O	1.93	0.66
3:D:1399:ASP:O	3:D:1403:LEU:HB2	1.95	0.66
1:K:89:PHE:HB2	1:K:94:LEU:HD13	1.77	0.66
1:L:88:ARG:NH1	1:L:88:ARG:HB3	2.09	0.66
2:M:905:ILE:H	2:M:905:ILE:CD1	2.06	0.66
3:N:1091:SER:HA	9:N:9756:HOH:O	1.96	0.66
3:N:185:VAL:HG13	9:N:9966:HOH:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:35:ARG:HD2	3:N:36:THR:N	2.09	0.66
3:N:459:GLU:HA	9:N:9521:HOH:O	1.95	0.66
3:N:656:PHE:HB3	3:N:694:VAL:HG11	1.77	0.66
2:C:101:ILE:HG23	2:C:107:LEU:HD22	1.76	0.66
2:C:197:LEU:HB3	2:C:202:TYR:HB2	1.77	0.66
2:C:503:LEU:HD12	2:C:505:GLY:H	1.60	0.66
2:C:52:PHE:CG	2:C:68:PHE:HB2	2.31	0.66
3:D:846:PRO:HB3	9:D:2128:HOH:O	1.94	0.66
3:D:850:LEU:HD12	3:D:850:LEU:H	1.59	0.66
3:D:770:LEU:HG	3:D:919:PHE:CE1	2.30	0.66
1:A:86:VAL:HG21	1:A:202:ASP:O	1.96	0.66
3:D:924:MET:HG2	9:D:9500:HOH:O	1.94	0.66
4:E:36:LYS:HB3	9:E:9557:HOH:O	1.95	0.66
2:M:660:ALA:HB1	2:M:667:ALA:O	1.94	0.66
3:N:907:GLU:O	3:N:911:LEU:HD13	1.96	0.66
2:C:420:ARG:HD2	2:C:420:ARG:H	1.59	0.66
3:D:1066:THR:HG22	3:D:1069:GLU:HG3	1.75	0.66
3:D:1097:LYS:HA	9:D:9591:HOH:O	1.94	0.66
3:D:1124:GLN:NE2	3:D:1135:ARG:HA	2.11	0.66
3:D:1432:LYS:NZ	3:D:1460:ILE:HG13	2.10	0.66
3:D:875:THR:HB	9:D:9975:HOH:O	1.96	0.66
4:E:43:GLU:CD	4:E:43:GLU:H	1.99	0.66
5:F:108:GLU:HG3	5:F:176:ILE:HG21	1.78	0.66
2:M:292:ARG:HB2	2:M:299:LYS:HE2	1.78	0.66
3:N:953:ASP:OD1	3:N:1019:PRO:HG2	1.96	0.66
3:N:1129:THR:HA	9:N:2005:HOH:O	1.95	0.66
3:N:1301:LYS:HE3	3:N:1301:LYS:HA	1.75	0.66
5:P:88:ILE:HG23	9:P:4361:HOH:O	1.96	0.66
3:D:1031:ASN:HB3	3:D:1034:GLN:HG3	1.77	0.66
3:D:611:GLN:HG3	5:F:326:ASP:HB2	1.78	0.66
3:D:796:ARG:HH11	3:D:861:GLN:HB2	1.59	0.66
3:D:906:GLN:HB3	3:D:911:LEU:CD1	2.25	0.66
5:F:406:ARG:HA	5:F:409:LYS:HG2	1.78	0.66
2:M:347:GLY:HA2	2:M:350:ARG:HD2	1.76	0.66
3:N:1145:TYR:CE2	3:N:1168:MET:HB2	2.30	0.66
3:N:1209:LEU:HD23	3:N:1210:SER:N	2.11	0.66
1:B:38:ASN:O	1:B:41:ARG:HG2	1.96	0.66
2:C:182:VAL:HG12	2:C:193:LEU:HD13	1.78	0.66
2:C:405:ARG:HD2	2:C:442:GLU:OE1	1.96	0.66
2:C:703:ILE:HD11	2:C:830:LYS:HG2	1.78	0.66
2:C:724:ARG:HH11	2:C:724:ARG:HB3	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1262:LEU:HD23	3:D:1352:ILE:HG13	1.78	0.66
3:D:176:ASP:HA	9:D:2419:HOH:O	1.96	0.66
3:D:462:GLN:HA	3:D:513:ILE:HD13	1.78	0.66
5:F:335:ASP:OD1	5:F:338:LEU:HB2	1.94	0.66
1:K:91:ASN:HB2	9:K:5800:HOH:O	1.94	0.66
2:M:939:ARG:HD3	2:M:982:PRO:HD3	1.77	0.66
3:N:1399:ASP:O	3:N:1403:LEU:HB2	1.95	0.66
3:N:535:PHE:HB3	5:P:314:PRO:HB3	1.78	0.66
1:B:180:GLN:HA	9:B:9698:HOH:O	1.94	0.66
2:C:1014:SER:HB3	2:C:1017:THR:O	1.95	0.66
2:C:256:TYR:CE1	2:C:293:PHE:HB2	2.30	0.66
3:D:1096:ARG:CB	3:D:1096:ARG:HH11	2.08	0.66
3:D:1462:LEU:HD22	3:D:1472:ILE:HG23	1.78	0.66
3:D:924:MET:HB3	4:E:7:ASP:OD1	1.96	0.66
3:N:1166:LEU:HD12	3:N:1171:VAL:HG22	1.78	0.66
3:N:984:THR:HG22	3:N:987:GLU:H	1.61	0.66
2:C:328:LEU:HB2	2:C:488:ALA:HB2	1.77	0.65
2:C:610:ARG:HB2	9:C:9703:HOH:O	1.96	0.65
3:D:1197:ARG:HG3	3:D:1198:TYR:H	1.61	0.65
3:D:1462:LEU:HD22	3:D:1473:PRO:HD2	1.76	0.65
3:D:699:VAL:CG1	3:D:717:GLN:HG3	2.26	0.65
3:D:928:ALA:HA	3:D:931:LEU:HD12	1.78	0.65
2:M:1018:GLN:NE2	2:M:1060:ILE:HD11	2.07	0.65
2:M:820:ARG:HB2	9:M:2167:HOH:O	1.95	0.65
2:C:146:VAL:HG22	2:C:162:ILE:HA	1.78	0.65
5:F:235:PHE:HA	9:F:9701:HOH:O	1.95	0.65
1:L:78:ILE:HG12	9:L:4728:HOH:O	1.97	0.65
2:M:1084:SER:O	2:M:1087:VAL:HG12	1.95	0.65
2:M:89:THR:O	2:M:91:GLN:HG3	1.96	0.65
2:M:966:LEU:HD21	2:M:986:PRO:HG2	1.78	0.65
3:N:1036:ARG:HH21	3:N:1042:ARG:CA	2.05	0.65
3:N:1471:LEU:HD12	3:N:1472:ILE:H	1.61	0.65
3:N:28:LYS:HG3	3:N:29:PRO:HD2	1.78	0.65
5:P:320:PRO:HB2	5:P:324:GLU:HG2	1.78	0.65
2:C:137:VAL:HG23	2:C:391:LEU:HG	1.77	0.65
2:C:478:VAL:HG13	2:C:506:ASN:HB3	1.78	0.65
1:K:41:ARG:O	1:K:45:LEU:HD12	1.96	0.65
3:N:1258:ARG:HH21	3:N:1351:GLU:HG2	1.62	0.65
5:P:404:ALA:HB2	9:P:3792:HOH:O	1.97	0.65
5:P:419:ARG:HD3	9:P:6175:HOH:O	1.95	0.65
1:B:73:GLU:HB3	1:B:77:GLU:CG	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:252:LYS:HE3	9:C:9859:HOH:O	1.95	0.65
2:C:328:LEU:HD22	2:C:433:THR:HG22	1.78	0.65
3:D:1031:ASN:HA	9:D:2225:HOH:O	1.97	0.65
3:D:572:ARG:HD2	9:F:9689:HOH:O	1.95	0.65
2:M:300:ASP:HB2	9:M:9603:HOH:O	1.95	0.65
2:M:305:PRO:HG3	2:M:308:ARG:HH21	1.61	0.65
2:M:451:LEU:HD12	2:M:451:LEU:H	1.58	0.65
2:M:454:SER:HB3	9:M:2089:HOH:O	1.95	0.65
2:M:479:VAL:HG21	2:M:503:LEU:HD11	1.78	0.65
3:N:1272:ALA:HA	3:N:1326:THR:HB	1.78	0.65
3:N:875:THR:HG23	9:N:2072:HOH:O	1.95	0.65
2:C:1060:ILE:HA	2:C:1063:ARG:NH1	2.12	0.65
3:D:1491:THR:O	3:D:1495:ILE:HD13	1.96	0.65
2:M:573:ARG:HG3	2:M:698:ASP:O	1.94	0.65
2:M:576:ALA:HB3	9:M:2073:HOH:O	1.96	0.65
3:N:1191:PRO:HA	9:N:9589:HOH:O	1.96	0.65
3:N:1462:LEU:HD22	3:N:1472:ILE:HG23	1.78	0.65
3:N:480:GLU:OE2	3:N:484:PRO:HG2	1.97	0.65
5:P:393:THR:HG22	5:P:394:ARG:H	1.61	0.65
1:A:11:PHE:CD1	1:B:225:PHE:HA	2.31	0.65
1:A:150:TYR:CE1	2:C:696:LYS:HA	2.32	0.65
3:D:190:GLU:HG3	3:D:210:ARG:NE	2.12	0.65
2:M:794:PRO:HB2	2:M:1027:PHE:CZ	2.31	0.65
2:M:231:PRO:HG2	9:M:2420:HOH:O	1.95	0.65
2:M:310:LEU:HD13	9:M:9990:HOH:O	1.97	0.65
2:M:597:ALA:HB2	2:M:655:LEU:HD21	1.77	0.65
3:N:105:VAL:HG12	3:N:106:LYS:NZ	2.11	0.65
3:N:1147:ARG:HB3	3:N:1188:VAL:CG2	2.27	0.65
3:N:137:PRO:HD2	3:N:453:ASP:CB	2.27	0.65
3:N:117:ASP:HB2	3:N:495:ARG:NH2	2.12	0.65
3:N:566:ILE:HG12	5:P:217:ASN:HD22	1.61	0.65
3:N:728:LEU:HD12	3:N:729:HIS:H	1.62	0.65
3:N:906:GLN:HB3	3:N:911:LEU:CD1	2.25	0.65
4:O:74:VAL:HG12	4:O:79:LEU:HD21	1.78	0.65
5:P:266:GLU:HA	5:P:269:ASN:HD22	1.60	0.65
1:B:77:GLU:HB2	3:D:872:ARG:HH21	1.62	0.65
2:C:1067:TYR:O	2:C:1071:ILE:HG12	1.97	0.65
2:C:798:GLY:H	2:C:827:VAL:HG11	1.62	0.65
3:D:1187:PRO:HG3	9:D:9606:HOH:O	1.96	0.65
3:D:630:VAL:HA	3:D:744:GLN:HG2	1.78	0.65
3:D:980:MET:HG3	9:D:2017:HOH:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:314:PRO:HB2	9:F:9527:HOH:O	1.96	0.65
2:M:162:ILE:HB	2:M:172:ILE:HB	1.78	0.65
2:M:498:GLN:O	2:M:501:THR:HG23	1.96	0.65
2:M:833:LEU:HD12	2:M:834:GLN:H	1.62	0.65
3:N:536:ALA:HA	5:P:315:VAL:H	1.61	0.65
3:N:654:LYS:HB3	3:N:655:PRO:HD3	1.78	0.65
5:P:220:LEU:O	5:P:224:VAL:HG23	1.96	0.65
5:P:262:VAL:HG12	5:P:266:GLU:OE1	1.95	0.65
1:B:150:TYR:CD2	3:D:857:ILE:HG13	2.32	0.65
2:C:350:ARG:HB3	2:C:350:ARG:HH11	1.59	0.65
2:C:524:VAL:CG1	2:C:528:GLU:HB2	2.26	0.65
2:C:860:HIS:CD2	2:C:975:TYR:HB2	2.32	0.65
3:D:478:LEU:HD13	3:D:1388:ARG:NH2	2.12	0.65
5:F:351:SER:O	5:F:355:GLU:HB2	1.96	0.65
1:K:223:THR:HA	9:K:5661:HOH:O	1.95	0.65
3:N:1213:ARG:HE	3:N:1213:ARG:N	1.95	0.65
3:N:1243:THR:OG1	3:N:1253:THR:HB	1.97	0.65
3:N:127:LEU:HD12	3:N:128:TYR:N	2.11	0.65
3:N:171:LEU:HD22	3:N:390:PRO:HG3	1.79	0.65
3:N:427:VAL:CG2	3:N:435:VAL:HB	2.27	0.65
5:P:208:SER:HB2	5:P:211:ASP:OD1	1.96	0.65
5:P:222:ARG:HA	9:P:3420:HOH:O	1.96	0.65
1:B:68:ILE:HD12	1:B:71:VAL:HG21	1.78	0.65
2:C:115:LEU:HB3	9:C:9971:HOH:O	1.97	0.65
3:D:1285:GLU:H	3:D:1285:GLU:CD	2.00	0.65
1:L:58:ILE:HB	1:L:61:VAL:HB	1.78	0.65
2:M:1072:LYS:HA	9:M:9641:HOH:O	1.97	0.65
3:N:136:ASP:CB	3:N:137:PRO:HD3	2.27	0.65
3:N:1466:VAL:HG23	3:N:1472:ILE:HD11	1.79	0.65
3:N:971:LEU:HA	3:N:974:ILE:HD12	1.79	0.65
1:B:101:LEU:HD21	1:B:113:ASP:HB3	1.78	0.65
2:C:181:VAL:HG11	9:C:2145:HOH:O	1.97	0.65
2:C:394:PHE:HB3	7:C:8001:RPT:H321	1.79	0.65
2:C:701:THR:HG23	2:C:832:LYS:HG3	1.79	0.65
2:C:910:LYS:HB2	2:C:913:GLU:OE1	1.97	0.65
3:D:546:ARG:O	3:D:550:ARG:HG2	1.97	0.65
2:M:583:LEU:O	2:M:587:VAL:HG23	1.96	0.65
2:M:739:GLU:HG3	9:M:9543:HOH:O	1.96	0.65
3:N:101:HIS:HD2	3:N:582:LEU:HD13	1.62	0.65
3:N:992:ILE:HB	9:N:9914:HOH:O	1.97	0.65
2:C:433:THR:HA	9:C:9591:HOH:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1437:ALA:HA	3:D:1440:PHE:CE1	2.32	0.64
3:D:190:GLU:HG3	3:D:210:ARG:HE	1.62	0.64
3:D:172:PRO:HD2	3:D:389:GLU:O	1.97	0.64
4:E:49:GLN:HB2	9:E:9593:HOH:O	1.96	0.64
2:M:95:TYR:CD2	2:M:114:PHE:HB3	2.32	0.64
3:N:756:GLN:O	3:N:760:ARG:HG2	1.95	0.64
5:P:361:LEU:HD22	5:P:366:ALA:HB2	1.79	0.64
2:C:971:LYS:HA	2:C:988:VAL:HA	1.79	0.64
3:D:396:VAL:HG21	3:D:447:VAL:HB	1.77	0.64
3:D:800:LYS:HE3	3:D:830:ALA:HB3	1.78	0.64
1:L:87:VAL:HG21	1:L:144:VAL:HG11	1.78	0.64
2:M:1034:GLU:HA	2:M:1037:VAL:HG23	1.78	0.64
2:M:10:ARG:HA	2:M:10:ARG:HH11	1.62	0.64
2:M:409:ARG:HA	2:M:454:SER:HA	1.78	0.64
3:N:434:ARG:HB2	3:N:447:VAL:HG22	1.79	0.64
3:N:715:ALA:O	3:N:764:LEU:HD12	1.97	0.64
2:C:676:ILE:HG23	3:D:948:THR:HB	1.80	0.64
3:D:122:GLU:O	3:D:126:VAL:HG23	1.98	0.64
3:D:1254:GLN:HG3	9:D:2555:HOH:O	1.96	0.64
1:L:80:LEU:HB3	3:N:867:ARG:NH2	2.13	0.64
2:M:198:ARG:HH12	2:M:231:PRO:HG3	1.62	0.64
3:N:543:LEU:HD22	3:N:580:ALA:HB1	1.78	0.64
1:A:20:TYR:HD2	1:A:21:GLY:N	1.95	0.64
2:C:162:ILE:O	2:C:164:PRO:HD3	1.96	0.64
2:C:650:ARG:HG3	2:C:653:ASP:HB2	1.78	0.64
2:C:71:TYR:HB2	9:C:9517:HOH:O	1.97	0.64
3:D:1046:GLN:HA	3:D:1052:THR:HA	1.80	0.64
2:C:432:ARG:HD3	3:D:1048:PRO:HG2	1.79	0.64
3:D:208:PRO:HB2	3:D:395:VAL:HG13	1.78	0.64
3:D:996:TRP:HE3	3:D:999:THR:HG21	1.60	0.64
5:F:163:LEU:HB3	5:F:174:LEU:HG	1.80	0.64
2:M:726:ILE:HG22	9:M:2191:HOH:O	1.98	0.64
3:N:428:LYS:HE3	3:N:434:ARG:HH12	1.63	0.64
1:B:85:LEU:HD12	1:B:124:ASN:HB3	1.78	0.64
2:C:197:LEU:HA	2:C:200:LEU:HD12	1.80	0.64
2:C:580:MET:HA	9:C:9544:HOH:O	1.97	0.64
2:C:678:PRO:O	3:D:943:THR:HA	1.97	0.64
3:D:804:LEU:HB2	3:D:830:ALA:O	1.98	0.64
1:L:33:GLY:O	1:L:195:LEU:HD22	1.97	0.64
3:N:13:ALA:HA	9:N:9515:HOH:O	1.98	0.64
3:N:672:ALA:HB2	5:P:420:ASP:OD1	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:975:GLU:O	3:N:979:GLU:HG3	1.97	0.64
5:P:80:PRO:HA	5:P:83:GLN:HB2	1.80	0.64
1:B:186:LEU:HD23	9:B:9707:HOH:O	1.96	0.64
3:D:1377:LYS:O	3:D:1394:VAL:HA	1.97	0.64
3:D:795:VAL:HG23	3:D:879:ARG:HH12	1.63	0.64
5:F:291:ILE:HG23	5:F:304:VAL:HG21	1.79	0.64
2:M:52:PHE:CD2	2:M:68:PHE:HB2	2.33	0.64
3:N:191:LEU:HD22	3:N:195:VAL:HG21	1.78	0.64
5:P:226:LYS:HB2	9:P:6226:HOH:O	1.96	0.64
5:P:279:GLN:HA	9:P:4921:HOH:O	1.97	0.64
2:C:720:GLU:HG2	2:C:760:SER:HB3	1.80	0.64
2:C:76:PRO:HG3	9:C:2288:HOH:O	1.98	0.64
3:D:178:LEU:HG	3:D:200:ASP:H	1.62	0.64
1:K:20:TYR:HD2	1:K:21:GLY:H	1.46	0.64
1:L:81:ASN:HB3	9:L:4066:HOH:O	1.97	0.64
1:L:89:PHE:HB2	1:L:94:LEU:HD13	1.78	0.64
3:N:1282:ARG:HD3	3:N:1295:GLU:OE2	1.98	0.64
3:N:817:GLU:O	3:N:821:VAL:HG23	1.98	0.64
1:B:180:GLN:HG3	9:B:9530:HOH:O	1.97	0.64
1:A:177:VAL:O	2:C:864:GLY:HA3	1.97	0.64
2:C:889:HIS:CE1	3:D:951:ILE:H	2.15	0.64
3:D:214:GLU:HG3	3:D:390:PRO:HB2	1.80	0.64
4:E:47:LYS:HA	4:E:54:LEU:HB3	1.80	0.64
1:L:32:PHE:HB2	9:L:5175:HOH:O	1.98	0.64
1:A:193:ASP:HA	9:A:9491:HOH:O	1.96	0.64
1:B:214:ALA:HA	1:B:217:ILE:HD12	1.79	0.64
2:C:1008:ARG:HE	2:C:1028:GLY:N	1.96	0.64
2:C:1098:ASP:HB2	3:D:21:TRP:CZ2	2.33	0.64
2:C:595:LEU:HB3	9:C:9812:HOH:O	1.98	0.64
2:C:673:LEU:HD22	2:C:867:VAL:HA	1.79	0.64
3:D:590:PRO:HA	9:D:9578:HOH:O	1.96	0.64
2:M:455:LEU:HD12	2:M:456:ALA:O	1.98	0.64
2:M:987:ILE:HG12	3:N:948:THR:HG21	1.80	0.64
2:M:1046:ALA:HB1	3:N:1471:LEU:HD11	1.80	0.64
3:N:795:VAL:HG11	3:N:863:VAL:HG13	1.79	0.64
5:P:305:GLU:HG2	9:P:3554:HOH:O	1.98	0.64
2:C:1021:LEU:HD22	9:F:9484:HOH:O	1.98	0.64
2:C:413:LEU:HD12	2:C:413:LEU:H	1.63	0.64
2:C:716:LYS:HD3	9:C:2019:HOH:O	1.96	0.64
2:C:926:PHE:O	2:C:930:LYS:HG3	1.97	0.64
3:D:395:VAL:HG12	9:D:2245:HOH:O	1.99	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:817:GLU:HG3	3:D:839:LEU:HD13	1.78	0.64
1:L:62:LEU:HD12	9:L:4737:HOH:O	1.97	0.64
2:M:511:GLU:O	2:M:526:PRO:HD3	1.98	0.64
4:O:41:GLU:O	4:O:45:ARG:HG2	1.98	0.64
5:P:163:LEU:HB3	5:P:174:LEU:CG	2.28	0.64
2:C:250:ARG:HG2	2:C:253:ALA:HB3	1.79	0.63
2:C:379:GLU:O	2:C:383:ARG:HB3	1.97	0.63
2:C:605:LYS:HD3	2:C:610:ARG:NH1	2.13	0.63
2:C:730:SER:O	2:C:734:LEU:HD13	1.98	0.63
3:D:1124:GLN:NE2	3:D:1135:ARG:HG2	2.13	0.63
3:D:860:LEU:HD23	3:D:877:PRO:HB2	1.79	0.63
2:M:612:VAL:HG22	2:M:622:GLU:HG3	1.80	0.63
2:M:694:LEU:HD11	2:M:868:ASP:HB3	1.80	0.63
3:N:1093:TYR:HA	9:N:2053:HOH:O	1.98	0.63
3:N:185:VAL:CG1	3:N:191:LEU:HD21	2.28	0.63
5:P:123:ASP:HB3	5:P:125:ASP:OD1	1.98	0.63
1:B:103:ALA:O	1:B:138:LEU:HD23	1.97	0.63
2:C:156:GLY:HA3	9:C:2245:HOH:O	1.97	0.63
2:C:399:ASN:HD22	2:C:399:ASN:N	1.96	0.63
2:C:404:LEU:HD22	2:C:591:SER:HB3	1.80	0.63
3:D:1465:ASN:HD21	3:D:1470:ARG:NH1	1.95	0.63
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.80	0.63
3:D:808:THR:HB	3:D:809:PRO:HD3	1.80	0.63
3:D:907:GLU:O	3:D:911:LEU:HD13	1.97	0.63
2:M:575:GLN:HA	2:M:662:GLU:OE2	1.98	0.63
2:M:68:PHE:HZ	2:M:71:TYR:HB3	1.63	0.63
2:C:816:LYS:HE2	2:C:819:VAL:HG21	1.78	0.63
3:D:396:VAL:HG11	9:D:9781:HOH:O	1.98	0.63
3:N:119:SER:H	3:N:123:LEU:HB2	1.63	0.63
3:N:1192:LEU:HD12	3:N:1346:ARG:HH21	1.63	0.63
1:A:42:ARG:NH1	2:C:978:ARG:HA	2.12	0.63
2:C:1067:TYR:CG	5:F:341:PRO:HB3	2.34	0.63
2:C:724:ARG:HB2	2:C:740:GLU:HG3	1.79	0.63
9:C:9697:HOH:O	4:E:31:LEU:HD11	1.99	0.63
1:K:109:VAL:HG23	9:K:3900:HOH:O	1.98	0.63
1:L:172:SER:HB3	9:L:4444:HOH:O	1.97	0.63
2:M:1095:LEU:HD11	3:N:607:LEU:HD11	1.80	0.63
3:N:1046:GLN:HA	3:N:1052:THR:HA	1.80	0.63
3:N:52:PRO:CG	3:N:78:VAL:HG13	2.27	0.63
3:N:535:PHE:O	5:P:315:VAL:N	2.30	0.63
3:N:125:GLN:HE22	3:N:587:ARG:HH21	1.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:1056:LYS:O	3:N:624:ASP:HB2	1.98	0.63
3:N:95:LEU:HD12	3:N:515:GLU:C	2.18	0.63
1:A:181:VAL:HG12	9:A:9491:HOH:O	1.97	0.63
2:C:355:VAL:CG2	2:C:372:LEU:HG	2.28	0.63
2:C:771:GLU:O	2:C:775:ARG:HG2	1.98	0.63
3:D:1272:ALA:HB2	9:D:2257:HOH:O	1.97	0.63
3:D:829:VAL:HA	9:D:2030:HOH:O	1.97	0.63
1:K:99:LEU:HB3	1:K:114:PHE:CD2	2.34	0.63
3:N:584:ASN:ND2	3:N:590:PRO:HD2	2.14	0.63
3:N:628:ARG:HD3	3:N:744:GLN:HE22	1.63	0.63
4:O:31:LEU:HD23	4:O:35:PHE:CE1	2.33	0.63
4:O:84:ARG:HH11	4:O:84:ARG:HB2	1.64	0.63
5:P:130:VAL:HG21	5:P:159:ILE:HG21	1.80	0.63
1:A:198:ARG:HD3	1:A:200:TRP:HH2	1.62	0.63
2:C:1066:ALA:O	2:C:1070:ILE:HG13	1.99	0.63
2:C:95:TYR:CD2	2:C:114:PHE:HB3	2.34	0.63
5:F:112:ALA:HA	5:F:173:TYR:HD2	1.63	0.63
2:M:191:PHE:HZ	2:M:196:LEU:HB2	1.64	0.63
2:M:19:THR:HG22	2:M:22:GLN:HB2	1.79	0.63
2:M:516:ARG:NE	3:N:1068:LEU:HD13	2.13	0.63
2:M:943:VAL:HA	9:M:2224:HOH:O	1.99	0.63
3:N:1465:ASN:ND2	3:N:1470:ARG:HD3	2.12	0.63
2:C:1034:GLU:HA	2:C:1037:VAL:HG23	1.81	0.63
2:C:1084:SER:O	2:C:1087:VAL:HG12	1.98	0.63
2:C:145:GLY:H	2:C:163:ILE:HG23	1.63	0.63
2:C:516:ARG:HD3	2:C:521:PRO:HA	1.81	0.63
2:C:595:LEU:HD23	2:C:655:LEU:HD12	1.81	0.63
2:C:724:ARG:HG3	2:C:741:GLY:N	2.07	0.63
3:D:111:LYS:HD3	9:D:9759:HOH:O	1.97	0.63
3:D:1147:ARG:HB2	3:D:1166:LEU:HD21	1.80	0.63
3:D:135:LEU:HD13	3:D:147:VAL:HG23	1.80	0.63
3:D:551:ASN:O	3:D:555:LYS:HG3	1.98	0.63
3:D:705:ALA:HB3	3:D:706:PRO:HD3	1.79	0.63
2:C:949:LYS:CD	3:D:796:ARG:HH21	2.12	0.63
2:M:443:THR:O	2:M:559:LEU:HD11	1.99	0.63
2:M:816:LYS:HB2	2:M:819:VAL:HG21	1.81	0.63
3:N:1095:THR:O	3:N:1099:VAL:HG23	1.99	0.63
3:N:1147:ARG:O	3:N:1165:TYR:HA	1.99	0.63
3:N:393:ILE:H	3:N:393:ILE:HD12	1.64	0.63
4:O:72:ARG:HD2	9:O:5366:HOH:O	1.98	0.63
2:C:25:SER:HB2	2:C:335:THR:HB	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1290:LEU:HD13	3:D:1305:LEU:HD12	1.80	0.63
3:D:699:VAL:HG21	3:D:760:ARG:HB3	1.81	0.63
3:D:787:LEU:HD21	3:D:947:ILE:HD13	1.80	0.63
2:M:1115:LEU:HD12	2:M:1115:LEU:H	1.64	0.63
2:M:428:ARG:HG2	2:M:451:LEU:HG	1.81	0.63
2:M:863:ASP:OD2	2:M:865:THR:HG22	1.99	0.63
3:N:1159:ARG:HD3	9:N:9583:HOH:O	1.98	0.63
1:A:97:VAL:HG23	9:A:9486:HOH:O	1.98	0.63
3:D:393:ILE:HD12	3:D:393:ILE:H	1.64	0.63
5:F:347:GLN:HG2	9:F:9631:HOH:O	1.98	0.63
1:K:78:ILE:HA	1:K:81:ASN:ND2	2.14	0.63
2:M:367:LEU:HB3	2:M:371:LYS:HG2	1.81	0.63
2:M:431:HIS:H	2:M:434:HIS:CE1	2.17	0.63
3:N:1329:ALA:HA	9:N:9884:HOH:O	1.98	0.63
3:N:1500:LYS:HA	9:N:2479:HOH:O	1.99	0.63
3:N:589:ALA:HB3	9:N:9549:HOH:O	1.98	0.63
3:N:800:LYS:HE3	3:N:830:ALA:HB3	1.80	0.63
2:C:1034:GLU:HG3	9:C:9762:HOH:O	1.98	0.62
2:C:151:ASP:HB2	2:C:157:ARG:O	1.98	0.62
2:C:305:PRO:HG3	2:C:308:ARG:NH2	2.14	0.62
2:C:721:ARG:HH21	2:C:783:ARG:HH21	1.47	0.62
3:D:1063:GLU:HG2	3:D:1064:GLY:N	2.14	0.62
3:D:126:VAL:HG22	9:D:2697:HOH:O	1.98	0.62
3:D:531:ASP:C	3:D:533:GLY:H	2.00	0.62
3:D:584:ASN:ND2	3:D:590:PRO:HD2	2.14	0.62
3:D:810:GLU:O	3:D:813:LEU:HG	1.98	0.62
5:F:273:ARG:HB3	9:F:9511:HOH:O	1.97	0.62
3:N:423:ASP:OD2	5:P:174:LEU:HD22	1.98	0.62
2:C:244:PRO:HB3	9:C:9757:HOH:O	1.99	0.62
2:C:557:ARG:HB2	9:C:9570:HOH:O	1.98	0.62
3:D:101:HIS:HD1	3:D:103:TRP:HB2	1.63	0.62
3:D:1495:ILE:HD11	9:E:9594:HOH:O	1.97	0.62
3:D:434:ARG:HB2	3:D:447:VAL:HG13	1.80	0.62
5:F:347:GLN:HG3	9:F:9808:HOH:O	1.99	0.62
2:M:603:VAL:HG21	2:M:643:VAL:CG1	2.28	0.62
2:M:802:ARG:HB3	9:M:9780:HOH:O	1.98	0.62
3:N:177:ALA:HB3	9:N:2388:HOH:O	1.99	0.62
5:P:87:GLU:O	5:P:91:VAL:HG23	1.99	0.62
1:B:151:VAL:HG23	9:B:9528:HOH:O	1.99	0.62
2:C:503:LEU:HD13	2:C:507:ARG:O	1.99	0.62
2:C:606:VAL:HG22	2:C:645:VAL:HG22	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:672:VAL:CG2	2:C:868:ASP:HB2	2.30	0.62
2:C:675:ALA:HB2	2:C:867:VAL:HG11	1.81	0.62
2:M:222:MET:HB3	9:M:9807:HOH:O	1.98	0.62
1:K:67:THR:HG23	2:M:627:ARG:NH2	2.14	0.62
3:N:674:ARG:HG2	3:N:674:ARG:HH11	1.64	0.62
5:P:154:LYS:O	5:P:158:GLU:HG3	1.98	0.62
1:B:132:LEU:HG	1:B:136:GLY:HA3	1.80	0.62
2:C:313:LEU:HA	9:C:2113:HOH:O	1.98	0.62
1:A:42:ARG:NH1	2:C:857:ASP:HB3	2.15	0.62
2:C:554:ASP:HB2	2:C:880:MET:HB2	1.80	0.62
2:C:579:VAL:HB	2:C:890:LEU:CD2	2.28	0.62
3:D:1436:SER:HB3	9:D:9596:HOH:O	1.98	0.62
3:D:26:VAL:HG11	3:D:44:LEU:HD23	1.82	0.62
3:D:471:GLU:O	3:D:475:LYS:HD2	1.99	0.62
2:M:15:LEU:H	2:M:15:LEU:HD12	1.64	0.62
2:M:308:ARG:HB3	9:M:9658:HOH:O	1.99	0.62
2:M:310:LEU:O	2:M:314:THR:HG23	1.99	0.62
5:P:395:GLU:O	5:P:399:GLN:HB2	1.98	0.62
1:A:189:ARG:HB3	9:A:9613:HOH:O	1.99	0.62
9:A:9505:HOH:O	1:B:43:ILE:HD11	1.98	0.62
3:D:478:LEU:HD22	3:D:1388:ARG:CZ	2.28	0.62
3:D:1399:ASP:HA	9:D:2529:HOH:O	1.99	0.62
3:D:146:PRO:HG2	9:D:9964:HOH:O	1.99	0.62
3:D:679:ARG:HB2	3:D:682:ASP:OD2	2.00	0.62
3:D:860:LEU:HA	3:D:877:PRO:HB2	1.81	0.62
3:D:972:LEU:HD23	3:D:973:GLN:N	2.14	0.62
1:K:62:LEU:HD12	9:K:3552:HOH:O	1.98	0.62
1:K:88:ARG:HD2	1:K:88:ARG:O	1.99	0.62
2:M:1105:LYS:HG2	9:M:2030:HOH:O	1.99	0.62
2:M:276:LYS:HB3	9:M:9769:HOH:O	1.99	0.62
2:M:42:VAL:HG12	2:M:43:GLY:H	1.65	0.62
1:A:120:VAL:HG13	9:A:9516:HOH:O	1.99	0.62
1:A:74:ASP:HA	9:A:9598:HOH:O	1.99	0.62
1:B:184:THR:HB	1:B:194:LYS:NZ	2.15	0.62
2:C:580:MET:HB3	2:C:584:GLU:OE2	2.00	0.62
2:C:724:ARG:NE	2:C:737:LEU:O	2.32	0.62
3:D:128:TYR:CE1	3:D:461:ILE:HG13	2.34	0.62
3:D:1342:GLU:HB3	9:D:9499:HOH:O	2.00	0.62
3:D:117:ASP:HB2	3:D:495:ARG:NH2	2.13	0.62
5:F:316:SER:HB3	5:F:318:GLU:O	2.00	0.62
1:L:26:GLU:HB3	9:L:3467:HOH:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:139:GLN:O	2:M:333:ILE:HA	2.00	0.62
2:M:433:THR:HG21	2:M:488:ALA:HB1	1.81	0.62
2:M:640:ARG:HB3	9:M:2138:HOH:O	1.99	0.62
2:M:971:LYS:HA	2:M:988:VAL:HA	1.81	0.62
3:N:1127:GLU:HB2	9:N:9636:HOH:O	1.99	0.62
2:M:770:GLU:HG2	3:N:65:ARG:NH2	2.15	0.62
5:P:321:ILE:HD11	5:P:329:TYR:HB2	1.81	0.62
2:C:376:ARG:NH1	5:F:285:GLU:HG2	2.15	0.62
3:D:179:VAL:HB	9:D:2419:HOH:O	1.99	0.62
1:L:5:LYS:HA	1:L:5:LYS:NZ	2.15	0.62
3:N:450:TYR:HB3	9:N:9938:HOH:O	1.99	0.62
3:N:633:VAL:HG22	3:N:635:PRO:HD3	1.82	0.62
2:C:398:THR:OG1	2:C:633:GLN:HG3	2.00	0.62
3:D:562:ALA:HB1	3:D:567:ILE:CD1	2.29	0.62
3:D:572:ARG:HH22	5:F:83:GLN:HG3	1.65	0.62
1:L:64:GLU:HG3	9:L:4182:HOH:O	1.99	0.62
2:M:97:ARG:HD2	9:M:9731:HOH:O	2.00	0.62
3:N:1493:LYS:O	3:N:1497:GLU:HG2	1.99	0.62
2:C:333:ILE:CD1	2:C:467:ILE:HG13	2.29	0.62
2:C:543:ASN:HD22	2:C:562:SER:HB3	1.64	0.62
2:C:569:VAL:HG23	2:C:635:THR:HG22	1.81	0.62
2:C:702:SER:HB2	9:C:9792:HOH:O	1.99	0.62
3:D:1318:TYR:HB3	9:D:2293:HOH:O	1.99	0.62
3:D:502:PHE:CE2	3:D:1452:ILE:HG13	2.35	0.62
3:D:473:LEU:HD21	3:D:495:ARG:CZ	2.30	0.62
3:D:675:ARG:O	3:D:678:GLU:HG2	1.99	0.62
4:E:41:GLU:HG2	9:E:9566:HOH:O	1.99	0.62
2:M:207:LEU:HD23	2:M:211:LEU:HD23	1.81	0.62
2:M:276:LYS:H	2:M:276:LYS:HD2	1.64	0.62
3:N:1057:VAL:HG13	3:N:1069:GLU:HB3	1.81	0.62
3:N:972:LEU:HD13	9:N:2036:HOH:O	2.00	0.62
3:D:500:ARG:HH22	3:D:1388:ARG:NH1	1.97	0.62
3:D:1432:LYS:HG3	3:D:1433:SER:H	1.65	0.62
3:D:197:SER:CB	3:D:203:ALA:HB3	2.25	0.62
5:F:398:ARG:HG2	5:F:402:ASN:ND2	2.14	0.62
2:M:1095:LEU:HB2	2:M:1097:LEU:HD21	1.81	0.62
2:M:37:GLU:HA	9:M:2385:HOH:O	1.98	0.62
2:M:468:ARG:HD3	2:M:485:TYR:HB3	1.81	0.62
3:N:139:GLY:O	3:N:147:VAL:HB	2.00	0.62
3:N:692:GLU:HG2	3:N:720:LEU:HD12	1.81	0.62
2:C:178:PRO:HA	9:C:2061:HOH:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:298:PHE:HB3	9:C:2271:HOH:O	2.01	0.61
3:D:109:PRO:HD3	9:D:9821:HOH:O	2.00	0.61
3:D:1251:ASP:O	3:D:1270:ALA:HB3	1.99	0.61
3:D:41:ARG:NH1	3:D:42:ASP:HB2	2.13	0.61
3:D:402:PRO:HG2	3:D:444:VAL:HG11	1.80	0.61
3:D:877:PRO:O	3:D:880:ILE:HG22	1.99	0.61
3:D:9:ARG:HA	3:D:1434:TRP:HH2	1.64	0.61
2:M:157:ARG:HD3	2:M:158:TYR:N	2.15	0.61
2:M:630:ARG:HA	9:M:9812:HOH:O	2.00	0.61
2:M:939:ARG:HG3	9:M:9643:HOH:O	2.00	0.61
3:N:662:GLU:HB2	9:N:2066:HOH:O	2.00	0.61
3:N:728:LEU:HD22	3:N:745:MET:SD	2.40	0.61
4:O:47:LYS:HA	4:O:54:LEU:HB3	1.81	0.61
5:P:342:VAL:HB	9:P:5304:HOH:O	2.00	0.61
1:B:33:GLY:O	1:B:195:LEU:HD22	2.00	0.61
2:C:640:ARG:NH1	2:C:642:ARG:HH22	1.98	0.61
3:D:611:GLN:HB2	9:F:9660:HOH:O	2.00	0.61
2:M:162:ILE:O	2:M:164:PRO:HD3	2.00	0.61
9:M:2401:HOH:O	5:P:409:LYS:HD2	1.98	0.61
2:C:84:ARG:NH2	2:C:128:ILE:HD11	2.15	0.61
3:D:1304:LYS:HA	9:D:2093:HOH:O	2.00	0.61
3:D:141:ILE:HG21	3:D:161:LEU:HD21	1.82	0.61
3:N:421:LEU:HD12	3:N:435:VAL:HG11	1.81	0.61
3:N:705:ALA:HB3	3:N:706:PRO:HD3	1.82	0.61
2:C:480:THR:HG22	2:C:482:GLU:H	1.66	0.61
3:D:1137:ARG:O	3:D:1141:GLU:HG3	2.00	0.61
3:D:1183:ILE:HG22	9:D:9811:HOH:O	2.00	0.61
2:M:149:THR:HG22	9:M:2395:HOH:O	2.00	0.61
2:M:178:PRO:HB3	9:M:9661:HOH:O	2.01	0.61
2:M:198:ARG:NH1	2:M:231:PRO:HG3	2.16	0.61
2:M:468:ARG:HD2	9:M:2017:HOH:O	1.98	0.61
2:M:720:GLU:HG2	2:M:760:SER:HB3	1.83	0.61
2:M:745:ILE:HG13	9:M:9989:HOH:O	2.00	0.61
3:N:1236:LEU:HA	9:N:2360:HOH:O	1.98	0.61
3:N:957:PRO:HB3	3:N:959:GLU:OE1	2.00	0.61
1:B:110:LYS:HG3	9:B:9511:HOH:O	1.99	0.61
3:D:1154:GLU:HG2	9:D:9504:HOH:O	2.00	0.61
3:D:1299:PHE:HB2	9:D:9955:HOH:O	1.98	0.61
5:F:100:VAL:HG21	9:F:9680:HOH:O	2.00	0.61
1:L:54:THR:HG22	1:L:158:ILE:HG13	1.82	0.61
2:M:437:ARG:CZ	2:M:488:ALA:HA	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:428:LYS:HE3	3:N:434:ARG:NH1	2.15	0.61
5:P:120:THR:HB	9:P:4895:HOH:O	2.00	0.61
5:P:166:LEU:O	5:P:171:LYS:HB2	2.00	0.61
2:C:197:LEU:HD12	2:C:207:LEU:HD11	1.81	0.61
2:C:218:VAL:HA	2:C:221:LEU:HD23	1.82	0.61
2:C:511:GLU:O	2:C:526:PRO:HD3	1.99	0.61
2:C:62:GLY:O	2:C:103:LYS:HG3	2.00	0.61
2:C:769:PRO:HG3	9:F:9763:HOH:O	1.99	0.61
3:D:1135:ARG:HD3	9:D:2109:HOH:O	2.01	0.61
3:D:501:ALA:HB2	9:D:9860:HOH:O	1.99	0.61
5:F:278:LEU:O	5:F:282:LEU:HG	2.00	0.61
2:M:431:HIS:CD2	2:M:433:THR:H	2.19	0.61
2:M:569:VAL:HG12	2:M:996:LYS:O	2.01	0.61
3:N:1425:THR:HG23	3:N:1426:LYS:N	2.16	0.61
3:N:422:ALA:HB3	3:N:427:VAL:CG2	2.25	0.61
3:N:863:VAL:HG23	9:N:9553:HOH:O	2.01	0.61
1:A:184:THR:HG23	1:A:192:LEU:HB2	1.83	0.61
1:B:26:GLU:HG2	1:B:27:PRO:HA	1.82	0.61
2:C:108:ILE:H	2:C:108:ILE:HD12	1.65	0.61
2:C:543:ASN:ND2	2:C:562:SER:HB3	2.16	0.61
3:D:1403:LEU:O	3:D:1407:LEU:HB2	2.00	0.61
3:D:668:PRO:HB2	9:F:9602:HOH:O	2.00	0.61
2:M:139:GLN:HE21	2:M:334:ARG:HD2	1.64	0.61
2:M:707:ARG:NH1	2:M:709:GLU:HB2	2.15	0.61
3:N:208:PRO:HB2	3:N:395:VAL:HG22	1.81	0.61
3:N:618:LEU:HD22	9:N:2165:HOH:O	2.00	0.61
2:M:1115:LEU:HD23	3:N:85:VAL:HG13	1.82	0.61
3:N:860:LEU:HA	3:N:877:PRO:HB2	1.82	0.61
3:N:983:LEU:HA	3:N:987:GLU:OE2	2.01	0.61
5:P:291:ILE:HB	9:P:3811:HOH:O	1.99	0.61
2:C:318:PRO:HD2	9:C:2113:HOH:O	2.00	0.61
2:C:625:LEU:HD11	2:C:641:PRO:HG3	1.82	0.61
3:D:1412:LYS:HE3	9:D:2567:HOH:O	2.00	0.61
3:D:760:ARG:HB2	9:E:9559:HOH:O	2.00	0.61
3:D:807:ALA:HB2	3:D:833:GLU:OE1	2.01	0.61
5:F:131:VAL:HG13	5:F:178:ARG:HD3	1.81	0.61
5:F:361:LEU:HD23	5:F:362:SER:N	2.14	0.61
2:M:1017:THR:HG23	9:P:5990:HOH:O	2.01	0.61
2:M:140:ILE:HG22	2:M:333:ILE:HG13	1.83	0.61
2:M:148:PHE:HB3	9:M:9990:HOH:O	2.00	0.61
3:N:1137:ARG:HA	3:N:1140:ILE:HD12	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:15:PRO:HA	3:N:18:ILE:HG12	1.83	0.61
3:N:535:PHE:HB2	9:P:5489:HOH:O	1.99	0.61
3:N:950:GLY:H	3:N:953:ASP:HB2	1.66	0.61
3:N:984:THR:HB	3:N:987:GLU:OE1	2.01	0.61
4:O:82:GLU:HG2	9:O:5722:HOH:O	2.01	0.61
5:P:372:ARG:HD2	9:P:5354:HOH:O	2.01	0.61
1:B:57:TYR:HB3	1:B:141:GLU:CG	2.29	0.61
2:C:498:GLN:O	2:C:501:THR:HG23	2.00	0.61
3:D:1394:VAL:HB	3:D:1397:LYS:HD2	1.83	0.61
3:D:163:TYR:HB3	9:D:2435:HOH:O	2.01	0.61
3:D:28:LYS:HD3	3:D:41:ARG:CZ	2.30	0.61
3:D:964:LEU:HD22	9:D:9566:HOH:O	2.01	0.61
2:M:510:ALA:HB3	2:M:513:VAL:HG23	1.81	0.61
2:M:439:CYS:HB2	2:M:541:SER:HB3	1.82	0.61
2:M:773:LEU:O	2:M:777:ILE:HG13	2.01	0.61
3:N:45:PHE:HD1	3:N:86:ARG:HH22	1.48	0.61
3:N:584:ASN:HB2	3:N:602:SER:OG	2.00	0.61
3:N:715:ALA:HB3	3:N:764:LEU:HA	1.82	0.61
3:N:82:LYS:HD3	9:N:2443:HOH:O	2.01	0.61
1:A:58:ILE:HB	1:A:61:VAL:HB	1.83	0.61
2:C:342:ASP:O	2:C:346:VAL:HG23	2.00	0.61
2:C:377:PRO:HA	9:C:2397:HOH:O	1.99	0.61
3:D:601:ARG:HD2	5:F:328:PHE:CE1	2.33	0.61
2:M:611:ILE:HD11	2:M:641:PRO:HG3	1.82	0.61
2:M:806:LEU:HB2	9:M:9775:HOH:O	2.01	0.61
3:N:171:LEU:HB2	3:N:390:PRO:HA	1.82	0.61
3:N:543:LEU:HD23	9:N:9696:HOH:O	2.01	0.61
3:N:770:LEU:HB2	9:N:9545:HOH:O	2.01	0.61
1:A:20:TYR:HD2	1:A:21:GLY:H	1.48	0.60
2:C:260:LEU:HB2	2:C:291:ALA:HB1	1.83	0.60
2:C:789:SER:O	2:C:791:ARG:HG2	2.01	0.60
3:D:438:ASP:HB2	9:D:9897:HOH:O	2.01	0.60
1:L:101:LEU:HG	1:L:114:PHE:HA	1.81	0.60
2:M:321:GLU:HB3	9:M:9537:HOH:O	2.00	0.60
3:N:185:VAL:HG12	3:N:191:LEU:HD21	1.83	0.60
3:N:659:LYS:HE3	3:N:663:GLU:OE1	2.00	0.60
3:N:838:ARG:HB2	9:N:9806:HOH:O	2.01	0.60
4:O:21:VAL:O	4:O:25:LYS:HG3	1.99	0.60
2:C:470:PRO:HB3	2:C:485:TYR:CZ	2.36	0.60
3:D:1147:ARG:O	3:D:1165:TYR:HA	2.01	0.60
3:D:119:SER:HB2	3:D:123:LEU:HB2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:183:GLU:HA	3:D:186:VAL:HG12	1.82	0.60
3:D:61:GLY:CA	3:D:64:LYS:HE3	2.31	0.60
1:L:103:ALA:HB1	1:L:107:LYS:HD2	1.83	0.60
1:L:36:LEU:O	1:L:39:PRO:HD2	2.01	0.60
2:M:772:ARG:HG3	2:M:773:LEU:N	2.15	0.60
2:M:841:ASN:ND2	2:M:844:GLY:H	1.99	0.60
3:N:481:MET:SD	3:N:1388:ARG:HG2	2.40	0.60
3:N:584:ASN:HD21	3:N:590:PRO:HB2	1.66	0.60
4:O:50:THR:HB	9:O:3763:HOH:O	2.00	0.60
5:P:117:SER:HA	9:P:4895:HOH:O	2.01	0.60
5:P:225:GLU:HB3	9:P:3420:HOH:O	2.00	0.60
2:C:424:GLY:HA3	9:C:2382:HOH:O	2.02	0.60
3:D:1084:THR:HG21	9:D:2388:HOH:O	2.02	0.60
3:D:728:LEU:HD13	3:D:745:MET:HE1	1.83	0.60
3:D:817:GLU:HG2	3:D:840:LYS:HZ2	1.66	0.60
5:F:403:LYS:HA	5:F:403:LYS:NZ	2.16	0.60
1:L:101:LEU:HD21	1:L:113:ASP:HB3	1.83	0.60
1:L:110:LYS:HG3	9:L:5936:HOH:O	2.00	0.60
3:N:139:GLY:H	3:N:147:VAL:HG21	1.65	0.60
4:O:60:ALA:O	4:O:63:TRP:HB2	2.01	0.60
5:P:209:PHE:O	5:P:213:ILE:HG13	2.00	0.60
1:A:5:LYS:O	1:A:8:ALA:HB2	2.01	0.60
2:C:29:ALA:HB2	2:C:337:GLY:CA	2.30	0.60
2:C:575:GLN:H	2:C:667:ALA:HB1	1.65	0.60
2:C:603:VAL:HG21	2:C:643:VAL:CG1	2.30	0.60
3:D:28:LYS:HB2	3:D:41:ARG:HD2	1.83	0.60
3:D:455:ARG:HH11	3:D:455:ARG:HG2	1.65	0.60
5:F:417:LYS:HA	9:F:9602:HOH:O	2.01	0.60
1:L:45:LEU:HD21	1:L:177:VAL:HG22	1.81	0.60
2:M:358:ARG:HH22	2:M:374:ASN:HB3	1.66	0.60
2:M:137:VAL:HG11	2:M:393:GLN:NE2	2.15	0.60
3:N:829:VAL:HG23	9:N:2131:HOH:O	2.01	0.60
1:A:221:HIS:HA	1:A:224:TYR:CD2	2.36	0.60
1:B:212:ASN:O	1:B:215:VAL:HG22	2.01	0.60
2:C:122:THR:HA	9:C:9789:HOH:O	2.00	0.60
2:C:244:PRO:HG2	2:C:246:ASP:OD2	2.01	0.60
2:C:332:ARG:HA	2:C:465:GLY:O	2.02	0.60
2:C:431:HIS:H	2:C:434:HIS:CE1	2.19	0.60
3:D:105:VAL:HG21	3:D:128:TYR:HE2	1.66	0.60
1:L:184:THR:HG23	1:L:192:LEU:HB3	1.83	0.60
2:M:1016:ILE:HG23	3:N:526:PRO:HG2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:643:VAL:HG22	2:M:647:GLN:HE22	1.65	0.60
2:M:679:PHE:HD2	2:M:680:ASP:H	1.49	0.60
2:M:887:GLU:HB3	9:M:9573:HOH:O	2.01	0.60
2:M:944:LEU:HD21	2:M:963:LEU:HD22	1.84	0.60
3:N:1220:ALA:O	3:N:1224:VAL:HG23	2.00	0.60
3:N:130:SER:HB3	3:N:132:TYR:CE1	2.36	0.60
3:N:141:ILE:HG12	3:N:449:SER:HA	1.84	0.60
2:M:1109:VAL:HG11	3:N:5:VAL:HG22	1.84	0.60
1:B:80:LEU:HD23	3:D:867:ARG:NH1	2.17	0.60
2:C:513:VAL:HG13	9:C:9526:HOH:O	2.02	0.60
3:D:1336:LEU:HA	3:D:1344:VAL:HG22	1.83	0.60
9:C:9676:HOH:O	3:D:621:LYS:HE2	2.02	0.60
3:D:87:ARG:HB3	3:D:523:ASP:CB	2.28	0.60
5:F:317:LEU:O	5:F:329:TYR:HB3	2.01	0.60
2:M:212:GLY:HA3	2:M:218:VAL:HG23	1.82	0.60
2:M:571:LEU:HG	2:M:700:TYR:HA	1.83	0.60
2:M:752:GLY:H	2:M:792:VAL:HB	1.65	0.60
2:M:674:VAL:HG23	2:M:869:VAL:O	2.01	0.60
3:N:1212:ALA:HB3	3:N:1213:ARG:HH21	1.66	0.60
3:N:1428:ALA:O	3:N:1431:THR:HG22	2.02	0.60
3:N:1459:LEU:HD22	3:N:1465:ASN:HD22	1.66	0.60
3:N:210:ARG:NH1	3:N:398:ALA:HB3	2.07	0.60
3:N:402:PRO:HG2	3:N:444:VAL:HG11	1.83	0.60
3:N:65:ARG:HB3	9:N:9605:HOH:O	2.01	0.60
3:N:704:ARG:CG	3:N:736:PHE:HB3	2.30	0.60
3:N:73:CYS:HB3	3:N:76:CYS:O	2.02	0.60
3:N:782:SER:O	3:N:786:ILE:HG13	2.02	0.60
2:C:571:LEU:HD21	2:C:700:TYR:HD2	1.67	0.60
2:C:798:GLY:H	2:C:827:VAL:CG1	2.14	0.60
3:D:136:ASP:CB	3:D:137:PRO:HD3	2.31	0.60
2:C:882:LEU:HD22	3:D:951:ILE:CD1	2.32	0.60
1:L:41:ARG:HG2	1:L:177:VAL:HG21	1.84	0.60
1:L:212:ASN:O	1:L:215:VAL:HG22	2.01	0.60
2:M:1115:LEU:HD12	2:M:1115:LEU:N	2.17	0.60
2:M:256:TYR:CE1	2:M:293:PHE:HB2	2.37	0.60
2:M:609:ASN:HB2	9:M:9673:HOH:O	2.02	0.60
2:M:900:ARG:HD2	9:M:9963:HOH:O	2.02	0.60
3:N:964:LEU:HD22	3:N:1058:ARG:NH1	2.16	0.60
4:O:36:LYS:HB2	9:O:6252:HOH:O	2.01	0.60
4:O:76:GLY:N	4:O:79:LEU:HD22	2.16	0.60
2:C:1086:ARG:HB3	2:C:1112:PHE:HE2	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:269:LEU:HD12	2:C:288:ARG:N	2.16	0.60
2:C:740:GLU:HB2	9:C:2377:HOH:O	2.01	0.60
3:D:1082:ALA:O	3:D:1086:LEU:HD13	2.00	0.60
3:D:136:ASP:HB3	3:D:137:PRO:HD3	1.84	0.60
3:D:486:ARG:HH21	3:D:489:ARG:NH2	1.99	0.60
3:D:903:ASP:HA	9:D:9918:HOH:O	2.01	0.60
3:D:972:LEU:O	3:D:976:GLN:HG3	2.01	0.60
3:N:1491:THR:O	3:N:1495:ILE:HD13	2.00	0.60
3:N:831:GLY:HA3	9:N:9512:HOH:O	2.02	0.60
2:M:1115:LEU:HB3	3:N:85:VAL:HG12	1.83	0.60
1:A:213:GLN:O	1:A:217:ILE:HG13	2.02	0.60
1:B:123:MET:C	1:B:125:PRO:HD3	2.22	0.60
2:C:395:LYS:HE3	2:C:407:LYS:HD2	1.83	0.60
2:C:470:PRO:HG2	2:C:538:GLN:OE1	2.02	0.60
1:B:38:ASN:OD1	2:C:979:THR:HA	2.02	0.60
9:C:9634:HOH:O	3:D:630:VAL:HG23	2.01	0.60
3:D:810:GLU:HA	3:D:813:LEU:HD23	1.84	0.60
1:K:149:GLY:O	1:K:171:PHE:HB2	2.02	0.60
2:M:776:SER:HB2	9:M:9826:HOH:O	2.01	0.60
3:N:183:GLU:HA	3:N:186:VAL:HG12	1.83	0.60
3:N:191:LEU:HD13	3:N:195:VAL:HG11	1.83	0.60
3:N:215:TYR:HB2	3:N:389:GLU:HA	1.84	0.60
3:N:631:ILE:O	3:N:632:VAL:HG23	2.02	0.60
5:P:415:THR:HB	9:P:3726:HOH:O	2.01	0.60
2:C:1090:LYS:HE2	2:C:1112:PHE:CE1	2.37	0.60
2:C:124:ASP:HB3	2:C:592:LEU:HD12	1.82	0.60
2:C:858:MET:SD	2:C:867:VAL:HG23	2.42	0.60
2:C:874:LEU:HD23	3:D:1023:MET:SD	2.42	0.60
3:D:1468:LEU:HD13	3:D:1470:ARG:HD3	1.83	0.60
3:D:569:ASN:OD1	5:F:80:PRO:HB3	2.02	0.60
3:D:965:GLU:HA	3:D:968:ASP:HB2	1.84	0.60
3:N:1128:VAL:HG22	9:N:9749:HOH:O	2.00	0.60
3:N:440:VAL:HG13	9:N:2153:HOH:O	2.01	0.60
3:N:502:PHE:CE1	3:N:509:PRO:HB3	2.37	0.60
1:A:36:LEU:O	1:A:39:PRO:HD2	2.02	0.59
2:C:1000:MET:SD	2:C:1001:VAL:HG22	2.42	0.59
2:C:1043:TYR:HE2	3:D:768:ASN:OD1	1.85	0.59
2:C:1060:ILE:HD12	2:C:1063:ARG:NH1	2.15	0.59
2:C:329:GLY:N	2:C:488:ALA:HB3	2.17	0.59
1:A:150:TYR:HE1	2:C:696:LYS:HA	1.67	0.59
3:D:1077:ALA:HB2	9:D:9550:HOH:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1087:ARG:O	3:D:1091:SER:HB3	2.02	0.59
3:D:131:LYS:HB3	3:D:456:MET:HE3	1.83	0.59
3:D:61:GLY:HA3	3:D:64:LYS:HE3	1.84	0.59
3:D:844:ALA:O	3:D:867:ARG:HB3	2.01	0.59
5:F:352:GLU:O	5:F:356:LYS:HG3	2.02	0.59
1:K:213:GLN:O	1:K:217:ILE:HG13	2.02	0.59
1:L:14:ARG:HB2	9:L:5263:HOH:O	2.02	0.59
2:M:1024:LYS:HE2	9:M:9718:HOH:O	2.02	0.59
2:M:66:LEU:HD22	2:M:372:LEU:HD23	1.83	0.59
2:M:880:MET:HG2	3:N:1038:LEU:HD21	1.84	0.59
2:M:500:ASN:HD21	3:N:1067:VAL:CG2	2.15	0.59
3:N:1389:LEU:HD12	3:N:1390:LEU:H	1.67	0.59
3:N:536:ALA:HA	5:P:315:VAL:O	2.02	0.59
3:N:543:LEU:O	3:N:546:ARG:HB2	2.02	0.59
3:N:898:GLU:HB2	3:N:921:ARG:NH2	2.16	0.59
4:O:25:LYS:HA	4:O:28:GLN:NE2	2.17	0.59
1:B:101:LEU:HD12	1:B:114:PHE:CE1	2.37	0.59
1:B:38:ASN:HB3	1:B:39:PRO:HD3	1.84	0.59
2:C:312:ALA:HB1	9:C:2264:HOH:O	2.03	0.59
3:D:1428:ALA:O	3:D:1431:THR:HG23	2.02	0.59
3:D:703:ASN:ND2	3:D:704:ARG:H	2.00	0.59
4:E:33:HIS:CD2	4:E:89:MET:HG2	2.37	0.59
1:K:218:LEU:O	1:K:222:LEU:HD23	2.02	0.59
3:N:1000:THR:O	3:N:1003:VAL:HG22	2.02	0.59
1:B:58:ILE:HD13	1:B:140:MET:HB3	1.83	0.59
2:C:1015:LEU:HD12	9:C:9604:HOH:O	2.01	0.59
2:C:200:LEU:HB2	9:C:9888:HOH:O	2.02	0.59
3:D:108:VAL:HB	3:D:109:PRO:HD3	1.83	0.59
3:D:1243:THR:HB	3:D:1253:THR:HG22	1.83	0.59
3:D:9:ARG:HA	3:D:1434:TRP:CH2	2.38	0.59
3:D:75:ARG:HA	9:D:9977:HOH:O	2.02	0.59
3:D:863:VAL:HA	9:D:9541:HOH:O	2.02	0.59
3:D:98:PRO:HD3	9:D:9723:HOH:O	2.03	0.59
3:D:998:GLU:HA	9:D:9510:HOH:O	2.00	0.59
1:L:74:ASP:O	1:L:78:ILE:HG13	2.03	0.59
9:K:3920:HOH:O	2:M:608:GLY:HA3	2.02	0.59
2:M:621:VAL:HG13	9:M:9824:HOH:O	2.02	0.59
3:N:1146:GLY:HA3	3:N:1207:TYR:HB2	1.84	0.59
3:N:133:ILE:HG21	3:N:454:ALA:CB	2.30	0.59
5:P:358:LEU:HD11	5:P:370:LYS:HZ2	1.66	0.59
1:A:161:ARG:HB2	1:A:161:ARG:NH1	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:GLU:HG2	1:B:127:LEU:HD11	1.84	0.59
1:B:140:MET:HG2	9:B:9655:HOH:O	2.02	0.59
2:C:583:LEU:O	2:C:587:VAL:HG23	2.01	0.59
2:C:744:ARG:HG3	2:C:747:ALA:HB2	1.83	0.59
2:C:549:PHE:CD2	2:C:886:LEU:HB3	2.38	0.59
3:D:1152:GLU:CD	3:D:1159:ARG:HH12	2.06	0.59
3:D:813:LEU:O	3:D:817:GLU:HB2	2.02	0.59
5:F:402:ASN:O	5:F:406:ARG:HG3	2.01	0.59
1:K:11:PHE:CD1	1:L:225:PHE:HA	2.37	0.59
1:L:123:MET:C	1:L:125:PRO:HD3	2.22	0.59
2:M:840:ALA:HB1	9:M:9563:HOH:O	2.01	0.59
3:N:1211:MET:SD	3:N:1213:ARG:HD2	2.41	0.59
3:N:1221:VAL:HB	9:N:9633:HOH:O	2.01	0.59
2:C:102:HIS:HB2	2:C:106:GLY:O	2.02	0.59
2:C:18:LEU:HD21	2:C:542:VAL:HG11	1.82	0.59
2:C:274:ARG:HB2	2:C:285:LEU:HD13	1.84	0.59
2:C:595:LEU:HD11	9:C:9740:HOH:O	2.02	0.59
3:D:1119:SER:HA	3:D:1186:VAL:O	2.02	0.59
3:D:51:GLY:HA3	9:D:9784:HOH:O	2.02	0.59
3:D:530:VAL:HG11	9:F:9549:HOH:O	2.01	0.59
1:L:90:LEU:HB3	9:L:4208:HOH:O	2.02	0.59
2:M:89:THR:HA	2:M:129:ILE:O	2.03	0.59
2:M:499:ALA:HA	9:M:2087:HOH:O	2.01	0.59
2:M:605:LYS:CB	2:M:610:ARG:HH12	2.03	0.59
3:N:1176:LYS:HD3	3:N:1176:LYS:O	2.02	0.59
3:N:1403:LEU:HD23	3:N:1407:LEU:HD22	1.83	0.59
3:N:729:HIS:HE1	3:N:731:LEU:HG	1.66	0.59
3:N:8:VAL:HG11	9:N:9848:HOH:O	2.01	0.59
3:N:950:GLY:O	3:N:953:ASP:N	2.31	0.59
3:N:975:GLU:HA	9:N:9710:HOH:O	2.03	0.59
1:A:226:SER:O	1:A:228:PRO:HD3	2.01	0.59
2:C:284:ARG:HG2	2:C:285:LEU:H	1.68	0.59
3:D:1420:LEU:HD12	3:D:1421:LEU:H	1.67	0.59
3:D:528:VAL:HG23	3:D:536:ALA:O	2.03	0.59
2:M:141:HIS:CE1	2:M:334:ARG:HE	2.20	0.59
2:M:333:ILE:HD13	2:M:467:ILE:HG13	1.85	0.59
2:M:617:ASP:HB2	9:M:2181:HOH:O	2.03	0.59
2:M:1042:ALA:HB3	3:N:710:ARG:HB3	1.84	0.59
2:C:383:ARG:HB2	2:C:383:ARG:CZ	2.31	0.59
3:D:793:THR:HG22	3:D:879:ARG:HA	1.84	0.59
4:E:48:MET:N	4:E:54:LEU:HB2	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:148:VAL:HG22	9:L:4917:HOH:O	2.02	0.59
1:L:5:LYS:O	1:L:8:ALA:HB2	2.02	0.59
2:M:689:VAL:CG2	2:M:870:ILE:HB	2.32	0.59
2:M:757:GLY:HA2	2:M:789:SER:HB3	1.85	0.59
3:N:546:ARG:HA	9:N:9543:HOH:O	2.01	0.59
3:N:573:MET:HG2	9:N:9529:HOH:O	2.01	0.59
2:C:276:LYS:O	2:C:280:LYS:HB2	2.02	0.59
2:C:8:ARG:NH1	2:C:8:ARG:HB2	2.18	0.59
3:D:1124:GLN:HE21	3:D:1135:ARG:HA	1.67	0.59
3:D:1147:ARG:O	3:D:1166:LEU:HD23	2.02	0.59
3:D:1147:ARG:HB3	3:D:1188:VAL:CG2	2.32	0.59
3:D:139:GLY:O	3:D:147:VAL:HB	2.02	0.59
1:L:94:LEU:HD21	1:L:119:ASP:HB2	1.84	0.59
1:K:9:PRO:HD2	1:L:224:TYR:CE1	2.38	0.59
2:M:260:LEU:HB2	2:M:291:ALA:HB1	1.85	0.59
2:M:541:SER:HB2	9:M:9944:HOH:O	2.03	0.59
3:N:884:ARG:HB2	9:N:2140:HOH:O	2.02	0.59
2:C:6:PHE:HB2	9:C:2024:HOH:O	2.01	0.59
3:D:857:ILE:HA	9:D:2193:HOH:O	2.02	0.59
4:E:87:LYS:HB2	9:E:9519:HOH:O	2.01	0.59
5:F:256:ARG:CZ	5:F:260:ILE:HD12	2.32	0.59
1:K:36:LEU:O	1:K:39:PRO:HD2	2.03	0.59
2:M:56:GLU:CG	2:M:64:LEU:HD23	2.33	0.59
3:N:1110:ALA:HB3	9:N:9637:HOH:O	2.01	0.59
3:N:172:PRO:HD2	3:N:389:GLU:O	2.03	0.59
3:N:441:ARG:O	3:N:443:VAL:HG23	2.02	0.59
3:N:59:ALA:HA	9:N:9941:HOH:O	2.02	0.59
3:N:820:GLU:HG2	3:N:825:ALA:O	2.03	0.59
4:O:48:MET:N	4:O:54:LEU:HB2	2.17	0.59
5:P:350:LEU:HA	9:P:3715:HOH:O	2.02	0.59
1:B:216:GLU:HB2	9:B:9598:HOH:O	2.03	0.59
2:C:376:ARG:HH22	5:F:285:GLU:HB3	1.67	0.59
2:C:708:TYR:H	2:C:708:TYR:HD1	1.49	0.59
2:C:874:LEU:HD21	3:D:787:LEU:CD2	2.32	0.59
3:D:817:GLU:HG2	3:D:840:LYS:NZ	2.17	0.59
5:F:85:LEU:HA	5:F:88:ILE:HD12	1.84	0.59
1:K:2:LEU:HD22	9:K:5005:HOH:O	2.03	0.59
1:K:94:LEU:HD11	1:K:119:ASP:HB3	1.84	0.59
1:L:137:ARG:NH1	1:L:137:ARG:HB3	2.18	0.59
2:M:129:ILE:HA	9:M:9795:HOH:O	2.02	0.59
2:M:139:GLN:HE22	2:M:415:PRO:HG2	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:437:ARG:NH1	2:M:488:ALA:HA	2.17	0.59
2:M:549:PHE:CD2	2:M:886:LEU:HB3	2.38	0.59
4:O:45:ARG:O	4:O:47:LYS:HE3	2.03	0.59
2:C:1063:ARG:O	2:C:1066:ALA:HB3	2.02	0.58
2:C:29:ALA:HB2	2:C:337:GLY:HA3	1.83	0.58
2:C:536:PRO:HD2	2:C:537:LYS:HD2	1.85	0.58
2:C:750:LYS:HD2	9:C:9787:HOH:O	2.02	0.58
3:D:208:PRO:HB2	3:D:395:VAL:HG22	1.84	0.58
3:D:116:LEU:HD23	3:D:468:LEU:HD11	1.85	0.58
3:D:493:ARG:NH1	3:D:1390:LEU:HB2	2.17	0.58
3:N:1364:HIS:ND1	3:N:1366:LYS:HB2	2.18	0.58
5:P:385:GLU:O	5:P:397:ILE:HD13	2.03	0.58
2:C:1054:THR:HG22	2:C:1059:ASP:OD2	2.03	0.58
2:C:655:LEU:HB2	9:C:9812:HOH:O	2.02	0.58
2:C:975:TYR:HA	2:C:982:PRO:HA	1.84	0.58
2:C:993:PHE:CE1	2:C:995:MET:HG2	2.37	0.58
3:D:908:LYS:CG	3:D:1027:GLY:HA3	2.33	0.58
3:D:1288:GLU:OE2	3:D:1289:LYS:HE3	2.03	0.58
3:D:187:LYS:HD3	9:D:9662:HOH:O	2.01	0.58
5:F:404:ALA:HB3	9:F:9613:HOH:O	2.01	0.58
1:L:16:GLN:HB2	9:L:4742:HOH:O	2.01	0.58
3:N:1122:LEU:HD11	3:N:1186:VAL:HG23	1.84	0.58
3:N:1492:LEU:HD12	3:N:1493:LYS:NZ	2.18	0.58
3:N:422:ALA:H	3:N:427:VAL:CG1	2.16	0.58
5:P:88:ILE:CD1	5:P:193:ARG:HB2	2.31	0.58
5:P:419:ARG:HG3	5:P:420:ASP:H	1.68	0.58
5:P:96:LEU:HB2	9:P:5295:HOH:O	2.03	0.58
1:B:22:GLU:HG2	1:B:198:ARG:HG2	1.85	0.58
1:B:65:PHE:CD1	3:D:813:LEU:HD22	2.38	0.58
2:C:142:ARG:NH1	2:C:325:ILE:HG12	2.18	0.58
2:C:203:ASP:HB2	9:C:2302:HOH:O	2.03	0.58
2:C:431:HIS:CD2	2:C:433:THR:H	2.21	0.58
2:C:698:ASP:HA	9:C:9547:HOH:O	2.04	0.58
2:C:732:ALA:HB3	9:C:9678:HOH:O	2.04	0.58
3:D:101:HIS:CE1	3:D:582:LEU:HD22	2.38	0.58
3:D:601:ARG:NH2	3:D:612:GLY:HA2	2.19	0.58
3:D:671:LYS:HG2	9:F:9580:HOH:O	2.03	0.58
3:D:834:THR:HB	3:D:838:ARG:HB3	1.85	0.58
5:F:247:ILE:HG22	5:F:251:ILE:HD11	1.85	0.58
1:K:101:LEU:HD21	1:K:113:ASP:HB3	1.85	0.58
2:M:242:LEU:HD23	2:M:244:PRO:HD3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:500:ASN:HB3	9:M:9721:HOH:O	2.03	0.58
2:M:86:LYS:HE3	2:M:813:VAL:HG12	1.85	0.58
9:M:9760:HOH:O	3:N:1047:LYS:HD3	2.03	0.58
3:N:177:ALA:HB1	3:N:199:LEU:HD22	1.84	0.58
3:N:440:VAL:HG23	9:N:9588:HOH:O	2.04	0.58
3:N:984:THR:H	3:N:987:GLU:CD	2.06	0.58
2:C:630:ARG:HA	2:C:705:ILE:HD11	1.85	0.58
3:D:1129:THR:HA	9:D:9663:HOH:O	2.03	0.58
3:D:1129:THR:HG22	9:D:2414:HOH:O	2.02	0.58
3:D:1136:LYS:HA	9:D:2534:HOH:O	2.03	0.58
3:D:1379:VAL:HG11	3:D:1395:LEU:HD23	1.85	0.58
3:D:148:GLU:HA	9:D:2669:HOH:O	2.03	0.58
3:D:704:ARG:NH1	3:D:738:ALA:HA	2.17	0.58
9:D:2680:HOH:O	5:F:375:LEU:HD21	2.02	0.58
2:M:182:VAL:CG1	2:M:193:LEU:HD13	2.32	0.58
2:M:204:GLN:HB3	9:M:9981:HOH:O	2.03	0.58
2:M:263:ASP:HB2	2:M:264:PRO:HD3	1.85	0.58
3:N:1262:LEU:CD2	3:N:1351:GLU:HG3	2.31	0.58
3:N:211:VAL:HG13	3:N:393:ILE:HA	1.85	0.58
4:O:43:GLU:HG2	4:O:44:GLU:H	1.67	0.58
5:P:269:ASN:HB3	5:P:273:ARG:HH21	1.68	0.58
1:B:5:LYS:O	1:B:8:ALA:HB2	2.04	0.58
2:C:104:ASP:HB2	9:C:9663:HOH:O	2.03	0.58
2:C:145:GLY:HA3	9:C:2408:HOH:O	2.04	0.58
2:C:816:LYS:HB2	2:C:819:VAL:HG21	1.84	0.58
5:F:205:ARG:HD2	5:F:251:ILE:HD13	1.85	0.58
5:F:393:THR:HG22	5:F:394:ARG:H	1.69	0.58
5:F:410:TYR:HD2	5:F:414:ARG:HH22	1.50	0.58
2:M:890:LEU:HA	2:M:914:ILE:CD1	2.33	0.58
2:M:973:VAL:O	2:M:974:LEU:HD12	2.03	0.58
3:N:111:LYS:HZ1	3:N:498:VAL:HG12	1.67	0.58
3:N:422:ALA:HB1	5:P:178:ARG:NH1	2.17	0.58
1:B:86:VAL:HA	9:B:9563:HOH:O	2.03	0.58
2:C:244:PRO:CD	2:C:245:GLY:H	2.15	0.58
2:C:838:LYS:HG3	2:C:997:LEU:HB2	1.85	0.58
3:D:1087:ARG:HA	3:D:1090:ASP:HB2	1.86	0.58
3:D:1146:GLY:HA3	3:D:1207:TYR:HB2	1.84	0.58
3:D:1279:GLY:O	3:D:1318:TYR:HA	2.03	0.58
3:D:380:GLU:O	3:D:382:GLU:N	2.36	0.58
3:D:574:LEU:O	3:D:578:VAL:HG23	2.03	0.58
3:D:788:GLY:O	3:D:792:ILE:HG22	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:804:LEU:HD23	3:D:804:LEU:H	1.68	0.58
2:M:525:SER:OG	2:M:528:GLU:HG3	2.04	0.58
2:M:672:VAL:CG2	2:M:868:ASP:HB2	2.33	0.58
3:N:1441:GLN:NE2	3:N:1442:ASN:H	2.00	0.58
3:N:104:PHE:CD2	3:N:1448:THR:HG23	2.38	0.58
3:N:470:LEU:HD23	9:N:9663:HOH:O	2.02	0.58
5:P:155:THR:HA	5:P:158:GLU:OE2	2.04	0.58
5:P:291:ILE:O	5:P:295:MET:HB2	2.04	0.58
1:A:2:LEU:HB2	9:A:9681:HOH:O	2.03	0.58
2:C:15:LEU:HD13	2:C:583:LEU:HD11	1.85	0.58
2:C:469:THR:HG23	2:C:470:PRO:HD2	1.84	0.58
2:C:826:TYR:HD1	9:C:9672:HOH:O	1.85	0.58
3:D:996:TRP:CD2	3:D:1056:PRO:HG2	2.39	0.58
3:D:1109:GLU:CD	3:D:1202:GLN:H	2.07	0.58
3:D:584:ASN:HD22	3:D:584:ASN:C	2.07	0.58
2:M:1055:LEU:HD22	2:M:1066:ALA:HB2	1.84	0.58
2:M:244:PRO:HG2	2:M:246:ASP:OD2	2.04	0.58
2:M:49:ARG:HH11	2:M:49:ARG:HB2	1.68	0.58
2:M:705:ILE:HD11	9:M:9812:HOH:O	2.03	0.58
2:M:838:LYS:HD2	2:M:846:LYS:HZ3	1.69	0.58
3:N:1102:THR:HG22	3:N:1222:GLY:HA2	1.84	0.58
3:N:616:GLN:OE1	3:N:619:LEU:HB3	2.03	0.58
3:N:805:GLU:HB3	9:N:9995:HOH:O	2.02	0.58
5:P:294:ALA:HB2	9:P:3431:HOH:O	2.02	0.58
5:P:260:ILE:HD11	5:P:310:ILE:CG2	2.32	0.58
1:B:92:PRO:HA	1:B:146:ARG:NH1	2.18	0.58
2:C:1110:ASP:HA	9:C:9781:HOH:O	2.04	0.58
2:C:497:ALA:HA	2:C:515:ALA:HA	1.86	0.58
2:C:526:PRO:HB2	9:C:9595:HOH:O	2.02	0.58
2:C:945:ARG:NH1	2:C:945:ARG:HB3	2.16	0.58
2:C:981:GLU:HG3	9:C:9552:HOH:O	2.04	0.58
3:D:1372:VAL:HA	3:D:1375:MET:SD	2.44	0.58
3:D:178:LEU:CD2	3:D:199:LEU:H	2.17	0.58
1:L:81:ASN:O	1:L:84:GLU:HB3	2.04	0.58
2:M:1050:GLN:HG2	2:M:1079:PRO:HG2	1.85	0.58
2:M:145:GLY:HA3	9:M:9769:HOH:O	2.02	0.58
2:M:27:ARG:HD3	9:M:9741:HOH:O	2.03	0.58
2:M:49:ARG:HD3	9:M:9640:HOH:O	2.01	0.58
2:M:772:ARG:HB2	2:M:772:ARG:NH1	2.19	0.58
3:N:1124:GLN:N	3:N:1133:ARG:O	2.36	0.58
3:N:1119:SER:HA	3:N:1186:VAL:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:119:SER:CB	3:N:123:LEU:HB2	2.34	0.58
3:N:462:GLN:HA	3:N:513:ILE:HD13	1.84	0.58
3:N:969:ARG:O	3:N:972:LEU:HB3	2.04	0.58
9:N:9535:HOH:O	5:P:326:ASP:HB2	2.03	0.58
1:B:14:ARG:HD2	9:B:9709:HOH:O	2.04	0.58
2:C:1003:ASP:HA	9:C:9634:HOH:O	2.04	0.58
2:C:158:TYR:CE1	2:C:313:LEU:HG	2.38	0.58
3:D:1135:ARG:NH1	3:D:1357:ARG:HH22	2.02	0.58
3:D:139:GLY:H	3:D:147:VAL:HG21	1.69	0.58
3:D:211:VAL:HG22	3:D:393:ILE:HG23	1.85	0.58
5:F:102:LEU:O	5:F:106:VAL:HG23	2.04	0.58
5:F:138:SER:O	5:F:141:VAL:HG12	2.04	0.58
2:M:841:ASN:OD1	2:M:845:ASN:HB3	2.04	0.58
9:M:2376:HOH:O	3:N:1079:LYS:HB2	2.04	0.58
3:N:535:PHE:CB	5:P:314:PRO:HB3	2.34	0.58
1:A:54:THR:HG22	1:A:158:ILE:HG13	1.85	0.58
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.86	0.58
1:B:47:SER:O	1:B:49:PRO:N	2.36	0.58
2:C:122:THR:HB	2:C:124:ASP:OD1	2.03	0.58
3:D:1198:TYR:OH	3:D:1432:LYS:HG2	2.04	0.58
3:D:131:LYS:HA	3:D:456:MET:HG3	1.85	0.58
3:D:476:GLU:HG2	9:D:9483:HOH:O	2.02	0.58
2:C:1115:LEU:HB3	3:D:85:VAL:HG13	1.85	0.58
1:K:117:VAL:HB	1:K:120:VAL:CG1	2.34	0.58
2:M:1037:VAL:HG13	2:M:1049:LEU:HD11	1.85	0.58
2:M:700:TYR:HB3	9:M:9662:HOH:O	2.04	0.58
2:M:755:LEU:HB2	2:M:790:LEU:HD22	1.85	0.58
2:M:846:LYS:HE3	9:M:9651:HOH:O	2.03	0.58
2:M:913:GLU:HG3	9:M:9616:HOH:O	2.04	0.58
2:M:862:PRO:HA	2:M:975:TYR:CE1	2.38	0.58
3:N:1031:ASN:HB3	3:N:1034:GLN:CD	2.24	0.58
3:N:1213:ARG:HB2	3:N:1214:PRO:CD	2.33	0.58
3:N:421:LEU:HD11	3:N:437:VAL:HG22	1.85	0.58
3:N:129:PHE:CE2	3:N:587:ARG:HD3	2.38	0.58
3:N:701:LEU:HD23	3:N:748:HIS:HB2	1.85	0.58
3:N:760:ARG:HH21	4:O:3:GLU:CD	2.07	0.58
2:C:601:GLY:HA2	2:C:616:GLU:HG2	1.85	0.57
2:C:802:ARG:HB2	9:C:9893:HOH:O	2.04	0.57
2:C:694:LEU:HD11	2:C:868:ASP:HB3	1.85	0.57
3:D:36:THR:C	3:D:38:LYS:H	2.08	0.57
3:D:483:HIS:ND1	3:D:483:HIS:N	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:493:ARG:HH12	3:D:1390:LEU:H	1.51	0.57
4:E:26:ARG:HG2	4:E:67:GLU:OE1	2.03	0.57
5:F:136:LEU:HD12	5:F:137:GLY:N	2.19	0.57
5:F:366:ALA:HB3	5:F:367:MET:HE2	1.86	0.57
1:L:226:SER:O	1:L:228:PRO:HD3	2.03	0.57
2:M:191:PHE:CZ	2:M:196:LEU:HB2	2.39	0.57
2:M:629:TYR:HB2	2:M:637:LEU:HG	1.86	0.57
3:N:105:VAL:HG13	3:N:124:GLU:OE1	2.03	0.57
3:N:1280:VAL:HG22	9:N:9926:HOH:O	2.04	0.57
3:N:1475:GLY:O	3:N:1478:SER:HB3	2.04	0.57
4:O:70:THR:HG21	4:O:72:ARG:HH21	1.69	0.57
1:A:133:GLU:HB2	9:C:2067:HOH:O	2.04	0.57
1:A:158:ILE:HD13	9:A:9582:HOH:O	2.04	0.57
1:A:79:ILE:HD11	9:A:9511:HOH:O	2.04	0.57
1:A:80:LEU:HD22	9:A:9571:HOH:O	2.02	0.57
1:B:86:VAL:CG1	1:B:124:ASN:HD22	2.10	0.57
2:C:108:ILE:HD11	2:C:365:ASP:OD2	2.04	0.57
2:C:662:GLU:HG3	9:C:2147:HOH:O	2.04	0.57
2:C:720:GLU:HA	2:C:759:THR:O	2.04	0.57
3:D:1293:PHE:CD2	3:D:1302:GLU:HA	2.38	0.57
3:D:1376:MET:SD	3:D:1421:LEU:HD12	2.44	0.57
1:K:67:THR:HG21	2:M:609:ASN:HD21	1.69	0.57
3:N:1109:GLU:OE1	3:N:1201:CYS:HB2	2.03	0.57
3:N:181:ASP:OD2	3:N:199:LEU:HB2	2.05	0.57
3:N:408:GLU:HG3	9:N:9853:HOH:O	2.04	0.57
3:N:480:GLU:O	3:N:484:PRO:HD2	2.04	0.57
3:N:625:TYR:O	3:N:749:VAL:HG23	2.05	0.57
3:N:972:LEU:HD23	3:N:973:GLN:N	2.18	0.57
5:P:373:LYS:HD3	5:P:378:GLY:C	2.25	0.57
1:A:222:LEU:HD11	1:B:218:LEU:HD23	1.85	0.57
1:B:132:LEU:HD13	1:B:138:LEU:HD22	1.87	0.57
2:C:252:LYS:NZ	2:C:296:GLY:HA3	2.19	0.57
2:C:799:ILE:HB	9:C:9767:HOH:O	2.03	0.57
2:C:92:ALA:HB1	9:C:9550:HOH:O	2.03	0.57
2:C:99:GLN:HB2	9:C:2236:HOH:O	2.04	0.57
3:D:137:PRO:HD2	3:D:453:ASP:CB	2.34	0.57
3:D:477:LEU:HD23	9:D:9483:HOH:O	2.03	0.57
2:C:1005:MET:HB2	3:D:629:SER:HB2	1.85	0.57
3:D:704:ARG:HG2	3:D:736:PHE:HB3	1.84	0.57
4:E:17:TYR:N	4:E:17:TYR:CD2	2.71	0.57
5:F:207:LEU:HB3	5:F:212:LEU:HG	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:369:LEU:HD23	9:F:9483:HOH:O	2.02	0.57
1:K:156:HIS:HD2	1:K:157:GLY:H	1.50	0.57
2:M:130:ASN:HB3	9:M:9727:HOH:O	2.04	0.57
2:M:56:GLU:HG2	2:M:64:LEU:HD23	1.85	0.57
2:M:798:GLY:H	2:M:827:VAL:HG11	1.68	0.57
3:N:787:LEU:HD11	3:N:947:ILE:HG12	1.86	0.57
3:N:804:LEU:HG	9:N:9546:HOH:O	2.04	0.57
5:P:408:LEU:O	5:P:412:GLU:HG2	2.03	0.57
3:N:572:ARG:NH2	5:P:83:GLN:HG3	2.13	0.57
1:A:72:LYS:HD2	1:A:73:GLU:OE2	2.05	0.57
2:C:101:ILE:HD12	2:C:107:LEU:HD13	1.86	0.57
2:C:897:LEU:HD23	2:C:899:GLN:NE2	2.19	0.57
3:D:369:ALA:HB3	9:D:2237:HOH:O	2.03	0.57
3:D:603:LEU:O	3:D:607:LEU:HD12	2.04	0.57
3:D:929:ARG:HD3	9:D:2352:HOH:O	2.04	0.57
1:K:20:TYR:CD2	1:K:21:GLY:N	2.73	0.57
1:L:36:LEU:HB3	9:L:4428:HOH:O	2.04	0.57
2:M:269:LEU:HG	2:M:285:LEU:HD21	1.87	0.57
2:M:52:PHE:CG	2:M:68:PHE:HB2	2.39	0.57
2:M:710:ILE:HD12	2:M:790:LEU:HB2	1.86	0.57
2:M:679:PHE:CD1	2:M:870:ILE:HD13	2.40	0.57
2:M:976:ASP:CB	2:M:979:THR:HG22	2.35	0.57
3:N:1437:ALA:O	3:N:1446:VAL:HG21	2.04	0.57
3:N:212:ARG:HD2	9:N:9862:HOH:O	2.03	0.57
5:P:208:SER:HB2	5:P:211:ASP:CG	2.25	0.57
5:P:419:ARG:HG3	5:P:420:ASP:N	2.20	0.57
1:A:114:PHE:HB3	9:A:9585:HOH:O	2.04	0.57
1:A:123:MET:O	1:A:125:PRO:HD3	2.04	0.57
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.86	0.57
1:A:222:LEU:HD12	1:B:215:VAL:CB	2.34	0.57
2:C:214:TYR:HD2	9:C:9769:HOH:O	1.87	0.57
2:C:598:GLU:O	2:C:651:LYS:HG3	2.04	0.57
2:C:841:ASN:HD21	2:C:845:ASN:N	2.03	0.57
3:D:1102:THR:HG22	3:D:1222:GLY:HA2	1.85	0.57
3:D:1431:THR:HG21	9:D:9888:HOH:O	2.04	0.57
3:D:817:GLU:O	3:D:821:VAL:HG23	2.04	0.57
4:E:60:ALA:O	4:E:63:TRP:HB2	2.05	0.57
2:M:1114:GLY:N	2:M:1115:LEU:HD12	2.09	0.57
2:M:575:GLN:H	2:M:667:ALA:HB1	1.69	0.57
3:N:127:LEU:HD11	3:N:461:ILE:HD11	1.86	0.57
3:N:1281:VAL:HG23	3:N:1317:ASP:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:520:LEU:HD12	3:N:521:PRO:HD2	1.85	0.57
5:P:160:ASP:HB2	9:P:4343:HOH:O	2.03	0.57
1:A:107:LYS:HA	9:A:9530:HOH:O	2.03	0.57
2:C:643:VAL:HG13	2:C:647:GLN:OE1	2.04	0.57
2:C:580:MET:O	2:C:902:ILE:HA	2.04	0.57
3:D:1289:LYS:HD2	9:D:9996:HOH:O	2.04	0.57
3:D:422:ALA:H	3:D:427:VAL:CG1	2.16	0.57
3:D:540:LEU:HD21	3:D:603:LEU:HD21	1.87	0.57
5:F:350:LEU:HD12	5:F:422:LEU:HD12	1.85	0.57
1:L:2:LEU:HD13	1:L:3:ASP:OD1	2.04	0.57
2:M:1082:PRO:HA	9:M:9532:HOH:O	2.04	0.57
2:M:274:ARG:HB2	2:M:285:LEU:HD13	1.87	0.57
2:M:45:GLN:HG2	9:M:2429:HOH:O	2.03	0.57
2:M:838:LYS:HG3	2:M:997:LEU:HB2	1.87	0.57
4:O:85:LEU:HD23	4:O:86:GLN:H	1.70	0.57
1:A:182:GLU:HG2	9:A:9502:HOH:O	2.03	0.57
2:C:208:ALA:O	2:C:218:VAL:HG21	2.05	0.57
3:D:1094:LEU:HB3	9:D:9776:HOH:O	2.04	0.57
5:F:205:ARG:HG2	9:F:9829:HOH:O	2.05	0.57
1:L:41:ARG:CZ	1:L:177:VAL:HG23	2.35	0.57
2:M:112:GLU:HG3	9:M:9726:HOH:O	2.03	0.57
2:M:292:ARG:HD2	2:M:299:LYS:HG2	1.85	0.57
2:M:143:SER:HB3	2:M:330:ASN:O	2.03	0.57
2:M:510:ALA:HB3	2:M:513:VAL:CG2	2.34	0.57
3:N:1103:HIS:HD2	3:N:1462:LEU:H	1.53	0.57
3:N:119:SER:H	3:N:123:LEU:CD2	2.18	0.57
3:N:178:LEU:HD11	3:N:203:ALA:HB2	1.86	0.57
3:N:380:GLU:O	3:N:382:GLU:N	2.37	0.57
2:M:1104:GLU:HA	3:N:6:ARG:CD	2.35	0.57
4:O:4:PRO:HG2	9:O:6061:HOH:O	2.05	0.57
5:P:223:ALA:HA	9:P:6226:HOH:O	2.05	0.57
2:C:1005:MET:HE2	3:D:648:MET:HB2	1.87	0.57
2:C:599:GLU:HG2	2:C:600:ASP:N	2.20	0.57
2:C:837:ASP:OD1	2:C:996:LYS:HE3	2.04	0.57
3:D:658:LEU:HD11	3:D:674:ARG:HH11	1.69	0.57
2:C:882:LEU:HD22	3:D:951:ILE:HD13	1.86	0.57
5:F:361:LEU:HD12	5:F:408:LEU:HD11	1.87	0.57
1:K:227:ASN:N	1:K:227:ASN:HD22	2.01	0.57
2:M:49:ARG:NH1	2:M:49:ARG:HB2	2.20	0.57
3:N:820:GLU:HB2	3:N:836:VAL:HG11	1.87	0.57
4:O:48:MET:HB2	4:O:54:LEU:CD1	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:131:VAL:CG1	5:P:181:GLU:HG3	2.33	0.57
1:A:89:PHE:HE2	1:A:146:ARG:HD3	1.69	0.57
1:A:224:TYR:CD2	1:B:9:PRO:HG2	2.40	0.57
1:B:226:SER:O	1:B:228:PRO:HD3	2.04	0.57
2:C:148:PHE:HZ	2:C:281:LEU:HD13	1.70	0.57
2:C:383:ARG:HB2	2:C:383:ARG:NH1	2.20	0.57
3:D:1243:THR:OG1	3:D:1253:THR:HB	2.05	0.57
3:D:1304:LYS:HD2	9:D:2299:HOH:O	2.04	0.57
3:D:1350:GLU:O	3:D:1354:LYS:HG2	2.05	0.57
3:D:1353:GLN:HG3	9:D:2099:HOH:O	2.05	0.57
3:D:1236:LEU:HA	3:D:1359:GLN:OE1	2.04	0.57
3:D:1393:GLN:HB2	3:D:1398:TRP:CZ2	2.39	0.57
3:D:1455:LYS:HD3	3:D:1456:LYS:N	2.19	0.57
3:D:486:ARG:HA	3:D:489:ARG:HG2	1.87	0.57
3:D:572:ARG:NH2	5:F:83:GLN:HG3	2.20	0.57
3:D:650:LEU:HD13	3:D:688:TRP:HZ3	1.70	0.57
3:D:730:PRO:HA	3:D:733:CYS:SG	2.44	0.57
1:L:209:GLU:HB3	9:L:3774:HOH:O	2.05	0.57
2:M:147:TYR:HB3	2:M:323:ASP:OD2	2.05	0.57
3:N:1090:ASP:O	3:N:1093:TYR:HB3	2.05	0.57
9:L:5963:HOH:O	3:N:721:VAL:HG12	2.05	0.57
3:N:875:THR:HG21	3:N:902:LEU:HD13	1.86	0.57
2:C:64:LEU:HD13	2:C:359:MET:HG3	1.86	0.57
2:C:1071:ILE:HD13	3:D:655:PRO:HB3	1.87	0.57
2:M:1006:HIS:O	3:N:648:MET:HE2	2.04	0.57
2:M:736:ASP:HA	2:M:744:ARG:HD3	1.87	0.57
3:N:1049:SER:HB3	3:N:1051:GLU:OE2	2.04	0.57
3:N:22:SER:HB3	9:N:9776:HOH:O	2.04	0.57
5:P:256:ARG:HH12	5:P:313:GLU:HG2	1.70	0.57
2:C:513:VAL:HG23	9:C:2376:HOH:O	2.04	0.56
2:C:614:ARG:HG2	9:C:2116:HOH:O	2.04	0.56
3:D:191:LEU:HD22	3:D:195:VAL:HG21	1.87	0.56
3:D:399:ARG:HB2	3:D:444:VAL:HG13	1.86	0.56
5:F:166:LEU:O	5:F:171:LYS:HB2	2.04	0.56
2:M:439:CYS:SG	2:M:540:PHE:HB3	2.45	0.56
2:M:721:ARG:HG2	9:M:9686:HOH:O	2.05	0.56
4:O:66:LYS:HE3	9:O:4471:HOH:O	2.05	0.56
5:P:309:LYS:HA	5:P:312:GLN:HE21	1.70	0.56
5:P:403:LYS:NZ	5:P:403:LYS:HA	2.20	0.56
2:C:1076:VAL:HG23	3:D:752:SER:HA	1.87	0.56
3:D:133:ILE:HG22	3:D:455:ARG:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:148:GLU:HG2	3:D:151:GLN:NE2	2.20	0.56
3:D:470:LEU:HB2	3:D:503:LEU:HD11	1.87	0.56
3:D:510:GLU:O	3:D:513:ILE:HD12	2.05	0.56
3:D:695:ILE:HG21	3:D:720:LEU:HD11	1.87	0.56
3:D:81:THR:O	3:D:82:LYS:O	2.22	0.56
3:D:89:ARG:HA	9:D:9567:HOH:O	2.05	0.56
3:D:967:ALA:O	3:D:995:LEU:HD21	2.04	0.56
5:F:142:ARG:HB2	9:F:9491:HOH:O	2.05	0.56
5:F:208:SER:HA	9:F:9790:HOH:O	2.05	0.56
5:F:260:ILE:HG23	5:F:264:MET:HB2	1.85	0.56
1:K:20:TYR:HD2	1:K:21:GLY:N	2.03	0.56
2:M:1079:PRO:HA	9:M:9805:HOH:O	2.05	0.56
2:M:231:PRO:HB2	9:M:9876:HOH:O	2.05	0.56
2:M:750:LYS:HG3	3:N:680:GLN:OE1	2.05	0.56
3:N:1147:ARG:HB2	3:N:1166:LEU:HD21	1.86	0.56
3:N:1336:LEU:HD23	9:N:2315:HOH:O	2.04	0.56
3:N:1350:GLU:O	3:N:1354:LYS:HG2	2.04	0.56
3:N:395:VAL:HG23	9:N:2392:HOH:O	2.06	0.56
3:N:488:ARG:HH11	3:N:488:ARG:HB3	1.70	0.56
3:N:734:GLU:HB3	9:N:2085:HOH:O	2.04	0.56
3:N:699:VAL:N	3:N:756:GLN:HE22	2.02	0.56
5:P:299:TRP:HE3	9:P:3308:HOH:O	1.87	0.56
5:P:404:ALA:O	5:P:408:LEU:HD23	2.05	0.56
1:B:206:THR:CG2	1:B:209:GLU:H	2.19	0.56
2:C:666:LEU:HD21	2:C:668:LEU:HD11	1.87	0.56
3:D:1031:ASN:HB3	3:D:1034:GLN:CG	2.35	0.56
3:D:1087:ARG:HD3	3:D:1090:ASP:CB	2.34	0.56
3:D:486:ARG:HH21	3:D:489:ARG:CZ	2.18	0.56
5:F:401:GLU:O	5:F:405:LEU:HB2	2.05	0.56
1:K:5:LYS:O	1:K:8:ALA:HB2	2.06	0.56
2:M:1008:ARG:NH1	2:M:1011:GLY:HA3	2.21	0.56
2:M:578:VAL:HG23	2:M:579:VAL:HG12	1.88	0.56
2:M:605:LYS:HD3	2:M:610:ARG:CZ	2.35	0.56
2:M:516:ARG:NH1	3:N:1068:LEU:HD22	2.20	0.56
2:M:1085:PHE:CD2	3:N:1468:LEU:HA	2.40	0.56
3:N:411:THR:HG23	3:N:429:SER:HB3	1.87	0.56
3:N:80:VAL:HG12	3:N:81:THR:N	2.20	0.56
5:P:289:GLU:O	5:P:293:GLU:HG3	2.05	0.56
5:P:355:GLU:HA	9:P:3471:HOH:O	2.05	0.56
5:P:401:GLU:O	5:P:405:LEU:HB2	2.05	0.56
1:A:101:LEU:HD21	1:A:113:ASP:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:172:ILE:H	2:C:172:ILE:HD12	1.70	0.56
2:C:332:ARG:NE	2:C:464:LEU:HD11	2.19	0.56
2:C:585:GLU:O	2:C:588:VAL:HG22	2.04	0.56
2:C:640:ARG:HH11	2:C:642:ARG:HH22	1.52	0.56
3:D:1191:PRO:HB3	3:D:1370:ILE:HD13	1.87	0.56
3:D:1272:ALA:CA	3:D:1326:THR:HB	2.34	0.56
3:D:58:CYS:SG	3:D:59:ALA:N	2.78	0.56
3:D:607:LEU:HB3	3:D:614:PHE:HE2	1.70	0.56
2:C:684:PHE:HE2	3:D:733:CYS:HG	1.52	0.56
5:F:120:THR:HG22	5:F:122:LEU:HD13	1.87	0.56
9:C:9961:HOH:O	5:F:354:LEU:HD11	2.05	0.56
2:M:1063:ARG:O	2:M:1066:ALA:HB3	2.05	0.56
2:M:145:GLY:O	2:M:163:ILE:HG23	2.04	0.56
3:N:1018:ASN:HB3	3:N:1021:TYR:HB3	1.87	0.56
3:N:1209:LEU:HD23	3:N:1210:SER:H	1.69	0.56
3:N:1279:GLY:O	3:N:1318:TYR:HA	2.05	0.56
3:N:138:LYS:HA	9:N:9563:HOH:O	2.04	0.56
3:N:1394:VAL:HG11	9:N:9728:HOH:O	2.04	0.56
3:N:683:ILE:HG21	3:N:688:TRP:CZ3	2.41	0.56
3:N:865:THR:HG23	3:N:874:GLU:HG2	1.86	0.56
3:N:882:PHE:CE1	3:N:906:GLN:HG3	2.40	0.56
3:N:969:ARG:HB2	9:N:9844:HOH:O	2.05	0.56
1:B:150:TYR:CE2	3:D:857:ILE:HG13	2.40	0.56
1:B:57:TYR:HE1	1:B:163:ASN:HB2	1.69	0.56
2:C:275:TYR:CD2	2:C:276:LYS:HG3	2.41	0.56
3:D:1087:ARG:NH2	3:D:1238:MET:HB2	2.21	0.56
3:D:424:GLY:HA2	3:D:435:VAL:O	2.05	0.56
3:D:774:SER:C	3:D:776:GLU:H	2.08	0.56
1:K:150:TYR:CE2	1:K:152:PRO:HG3	2.39	0.56
2:M:173:ASP:O	2:M:184:MET:HA	2.04	0.56
3:N:530:VAL:HG23	3:N:534:ARG:O	2.05	0.56
3:N:53:ILE:HG23	3:N:54:LYS:N	2.18	0.56
3:N:844:ALA:O	3:N:867:ARG:HB3	2.05	0.56
4:O:81:PRO:HB2	9:O:4797:HOH:O	2.05	0.56
5:P:230:LYS:HB2	9:P:4672:HOH:O	2.04	0.56
5:P:264:MET:O	5:P:267:THR:HB	2.05	0.56
2:C:227:PHE:HD2	2:C:230:ARG:HH21	1.54	0.56
2:C:338:GLU:HA	2:C:341:THR:HG22	1.88	0.56
2:C:498:GLN:NE2	3:D:1068:LEU:HD12	2.21	0.56
3:D:179:VAL:HG13	3:D:389:GLU:HG3	1.86	0.56
5:F:196:VAL:HG13	5:F:213:ILE:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:220:LEU:HD12	5:F:243:ILE:HD11	1.87	0.56
1:L:156:HIS:CE1	1:L:166:PRO:HB3	2.41	0.56
2:M:1071:ILE:HG13	9:M:9978:HOH:O	2.03	0.56
2:M:116:GLY:HA3	2:M:378:LEU:HD23	1.88	0.56
2:M:742:VAL:HG12	2:M:743:VAL:N	2.21	0.56
3:N:1122:LEU:O	3:N:1134:LEU:HD12	2.05	0.56
2:M:685:GLU:HG2	3:N:739:ASP:HB2	1.87	0.56
3:N:788:GLY:O	3:N:792:ILE:HG22	2.05	0.56
3:N:804:LEU:HD23	3:N:804:LEU:H	1.71	0.56
4:O:94:PRO:HA	9:O:5690:HOH:O	2.05	0.56
5:P:407:LYS:HA	9:P:3848:HOH:O	2.05	0.56
1:A:81:ASN:HA	1:A:84:GLU:OE2	2.06	0.56
2:C:1050:GLN:HG2	2:C:1079:PRO:HG2	1.88	0.56
2:C:114:PHE:HD1	2:C:114:PHE:H	1.53	0.56
2:C:648:ARG:HB3	9:C:2219:HOH:O	2.06	0.56
2:C:89:THR:HA	2:C:129:ILE:O	2.06	0.56
2:C:837:ASP:HA	2:C:999:HIS:HE1	1.71	0.56
3:D:1091:SER:HA	9:D:2229:HOH:O	2.06	0.56
3:D:10:ILE:HG13	3:D:1434:TRP:CE2	2.40	0.56
3:D:171:LEU:HB2	3:D:390:PRO:HA	1.86	0.56
3:D:901:GLN:HB2	9:D:2047:HOH:O	2.06	0.56
5:F:291:ILE:O	5:F:295:MET:HB2	2.06	0.56
2:M:139:GLN:HG2	2:M:140:ILE:H	1.70	0.56
2:M:257:VAL:HG13	9:M:9572:HOH:O	2.06	0.56
2:M:41:ASN:HB2	9:M:2429:HOH:O	2.04	0.56
3:N:949:ILE:HD11	3:N:1023:MET:HE1	1.87	0.56
3:N:1147:ARG:O	3:N:1166:LEU:HD23	2.05	0.56
3:N:661:MET:HG2	3:N:666:ILE:HD12	1.87	0.56
3:N:699:VAL:H	3:N:756:GLN:HE22	1.52	0.56
3:N:864:VAL:HG12	3:N:865:THR:H	1.68	0.56
3:N:570:GLU:OE2	5:P:214:GLN:HG3	2.05	0.56
5:P:226:LYS:HE3	9:P:4530:HOH:O	2.05	0.56
1:B:2:LEU:HD12	1:B:3:ASP:N	2.20	0.56
2:C:251:ASP:HB3	2:C:252:LYS:HD2	1.87	0.56
2:C:257:VAL:HG21	9:C:2339:HOH:O	2.05	0.56
3:D:1366:LYS:O	3:D:1369:GLU:HB2	2.06	0.56
3:D:68:PHE:HE2	9:D:2680:HOH:O	1.88	0.56
3:D:699:VAL:HG12	3:D:717:GLN:HG3	1.86	0.56
3:D:842:VAL:HG22	9:D:2270:HOH:O	2.05	0.56
3:D:963:TYR:CE2	3:D:1002:LYS:HB3	2.41	0.56
4:E:95:GLY:HA3	9:E:9521:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:58:ILE:HG21	1:K:68:ILE:HD11	1.88	0.56
2:M:276:LYS:O	2:M:280:LYS:HB2	2.05	0.56
2:M:484:VAL:HA	9:M:9777:HOH:O	2.06	0.56
2:M:589:ARG:CB	2:M:589:ARG:HH11	2.17	0.56
2:M:789:SER:O	2:M:791:ARG:HG2	2.06	0.56
3:N:1429:LEU:HG	3:N:1441:GLN:HG3	1.88	0.56
3:N:1495:ILE:HG23	9:N:9711:HOH:O	2.06	0.56
3:N:148:GLU:CB	3:N:151:GLN:HB2	2.34	0.56
3:N:714:GLN:HB2	3:N:736:PHE:HZ	1.71	0.56
3:N:814:ALA:HB2	9:N:9921:HOH:O	2.06	0.56
1:A:128:HIS:HB2	9:A:9508:HOH:O	2.06	0.56
2:C:1003:ASP:O	2:C:1005:MET:N	2.38	0.56
2:C:100:LEU:HD12	2:C:101:ILE:O	2.06	0.56
2:C:606:VAL:CG2	2:C:645:VAL:HG22	2.35	0.56
2:C:630:ARG:HH22	2:C:707:ARG:N	2.04	0.56
2:C:965:GLU:HG2	9:C:2373:HOH:O	2.06	0.56
3:D:132:TYR:HA	9:D:9863:HOH:O	2.06	0.56
3:D:135:LEU:HD11	3:D:139:GLY:HA3	1.86	0.56
3:D:488:ARG:HG2	9:D:9629:HOH:O	2.06	0.56
3:D:799:LYS:H	3:D:826:PRO:HG2	1.71	0.56
3:D:971:LEU:O	3:D:975:GLU:HG3	2.06	0.56
5:F:234:LYS:CD	5:F:236:SER:HB3	2.35	0.56
5:F:385:GLU:O	5:F:397:ILE:HD13	2.05	0.56
5:F:418:LEU:HB2	9:F:9856:HOH:O	2.06	0.56
1:K:106:PRO:HD3	9:K:4154:HOH:O	2.06	0.56
3:N:1301:LYS:HD2	9:N:2174:HOH:O	2.05	0.56
1:A:7:LYS:HG3	9:A:9524:HOH:O	2.05	0.56
1:B:25:LEU:HD23	1:B:28:LEU:HD21	1.87	0.56
2:C:265:ARG:HA	9:C:9902:HOH:O	2.04	0.56
2:C:36:PRO:HB2	2:C:70:GLU:HG2	1.88	0.56
2:C:54:ILE:HB	9:C:9495:HOH:O	2.05	0.56
2:C:57:GLU:HB3	9:C:9973:HOH:O	2.05	0.56
3:D:1289:LYS:HB3	9:D:2542:HOH:O	2.06	0.56
3:D:1334:GLN:HA	9:D:9693:HOH:O	2.05	0.56
3:D:1335:LEU:HD21	9:D:9614:HOH:O	2.05	0.56
3:D:142:LEU:HA	9:D:9874:HOH:O	2.05	0.56
3:D:33:ASN:HA	9:F:9729:HOH:O	2.05	0.56
3:D:790:TYR:HD2	3:D:906:GLN:O	1.89	0.56
5:F:191:ASN:CA	5:F:194:LEU:HD23	2.34	0.56
1:L:137:ARG:HH11	1:L:137:ARG:HB3	1.71	0.56
2:M:442:GLU:HG3	9:M:9719:HOH:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:551:GLU:HA	2:M:906:PHE:CE2	2.41	0.56
3:N:1003:VAL:O	3:N:1007:VAL:HG13	2.06	0.56
3:N:1204:CYS:HB3	9:N:9589:HOH:O	2.05	0.56
3:N:161:LEU:HD22	3:N:452:ILE:HG21	1.88	0.56
3:N:574:LEU:O	3:N:578:VAL:HG23	2.05	0.56
3:N:68:PHE:O	3:N:71:LYS:HG2	2.05	0.56
2:C:358:ARG:NH2	2:C:374:ASN:HB3	2.15	0.56
2:C:838:LYS:HD2	2:C:997:LEU:HD12	1.86	0.56
2:C:879:ARG:HB2	9:C:9557:HOH:O	2.06	0.56
3:D:1311:LEU:HD23	3:D:1311:LEU:H	1.71	0.56
3:D:126:VAL:HG12	3:D:132:TYR:HB2	1.88	0.56
3:D:192:ALA:O	3:D:195:VAL:HG23	2.05	0.56
3:D:524:LEU:C	3:D:526:PRO:HD3	2.26	0.56
3:D:806:PHE:CZ	3:D:813:LEU:HB3	2.40	0.56
4:E:26:ARG:O	4:E:29:GLN:HG3	2.06	0.56
5:F:234:LYS:HD3	5:F:236:SER:HB3	1.88	0.56
9:K:6004:HOH:O	1:L:43:ILE:HD13	2.05	0.56
2:M:584:GLU:CD	2:M:584:GLU:H	2.08	0.56
3:N:949:ILE:HD11	3:N:1023:MET:CE	2.36	0.56
3:N:1280:VAL:O	3:N:1294:VAL:HA	2.06	0.56
2:M:1008:ARG:HD2	3:N:624:ASP:O	2.06	0.56
3:N:783:ARG:HE	3:N:1029:ARG:CD	2.18	0.56
2:C:236:ILE:HG13	9:C:9904:HOH:O	2.05	0.55
2:C:426:ASP:OD1	2:C:427:VAL:HG23	2.05	0.55
3:D:1209:LEU:HD22	3:D:1211:MET:CE	2.36	0.55
3:D:1369:GLU:O	3:D:1372:VAL:HG12	2.05	0.55
3:D:502:PHE:CE1	3:D:509:PRO:HB3	2.40	0.55
3:D:584:ASN:CG	3:D:590:PRO:HD2	2.25	0.55
3:D:704:ARG:HD3	3:D:738:ALA:HB2	1.88	0.55
3:D:98:PRO:HG3	3:D:515:GLU:HB3	1.88	0.55
3:D:999:THR:O	3:D:1002:LYS:HB2	2.06	0.55
5:F:81:VAL:O	5:F:85:LEU:HG	2.06	0.55
1:L:103:ALA:HA	9:L:4911:HOH:O	2.06	0.55
1:L:206:THR:HG22	1:L:209:GLU:HG3	1.88	0.55
2:M:206:THR:O	2:M:210:GLU:HG3	2.05	0.55
2:M:61:LYS:HD2	9:M:9929:HOH:O	2.06	0.55
2:M:911:GLU:O	2:M:915:LYS:HG2	2.06	0.55
3:N:1278:ASP:HB2	3:N:1318:TYR:HE1	1.70	0.55
3:N:1273:VAL:O	3:N:1325:LEU:HB2	2.06	0.55
3:N:1342:GLU:CD	3:N:1342:GLU:H	2.09	0.55
3:N:1103:HIS:CD2	3:N:1463:LYS:H	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:36:THR:C	3:N:38:LYS:H	2.09	0.55
3:N:399:ARG:HB3	3:N:402:PRO:HG3	1.88	0.55
3:N:434:ARG:HB2	3:N:447:VAL:HG13	1.88	0.55
3:N:787:LEU:HD21	3:N:947:ILE:HD11	1.87	0.55
5:P:195:VAL:HG11	5:P:217:ASN:OD1	2.06	0.55
1:B:73:GLU:HB3	1:B:77:GLU:HG2	1.86	0.55
2:C:269:LEU:O	2:C:269:LEU:HD23	2.06	0.55
2:C:292:ARG:HD2	2:C:299:LYS:CE	2.35	0.55
2:C:389:SER:C	2:C:391:LEU:H	2.08	0.55
2:C:724:ARG:NH2	2:C:734:LEU:HB3	2.20	0.55
3:D:709:HIS:HE2	3:D:711:LEU:HB2	1.71	0.55
3:D:737:ASN:HA	9:D:9487:HOH:O	2.05	0.55
1:K:181:VAL:HG11	9:K:3503:HOH:O	2.05	0.55
1:K:227:ASN:HB2	9:K:5811:HOH:O	2.05	0.55
2:M:1090:LYS:HE2	2:M:1112:PHE:HE1	1.71	0.55
2:M:208:ALA:O	2:M:218:VAL:HG21	2.06	0.55
2:M:471:TYR:CE2	2:M:496:ILE:HG21	2.41	0.55
2:M:577:PRO:HA	2:M:993:PHE:HD2	1.72	0.55
2:M:748:GLU:HG3	9:M:2069:HOH:O	2.05	0.55
2:M:957:LYS:HG2	9:M:9678:HOH:O	2.05	0.55
3:N:1401:GLU:OE1	3:N:1415:VAL:HG11	2.06	0.55
3:N:1459:LEU:HD22	3:N:1465:ASN:ND2	2.20	0.55
3:N:390:PRO:HG2	9:N:2717:HOH:O	2.06	0.55
5:P:167:PRO:HB2	5:P:169:GLU:OE2	2.05	0.55
5:P:304:VAL:HG22	9:P:3308:HOH:O	2.06	0.55
2:M:772:ARG:HE	5:P:373:LYS:HD2	1.70	0.55
2:M:772:ARG:NE	5:P:373:LYS:HD2	2.21	0.55
5:P:82:ARG:HG3	5:P:86:HIS:CE1	2.41	0.55
2:C:1086:ARG:HH11	3:D:88:TYR:HE1	1.54	0.55
2:C:115:LEU:HD22	2:C:373:VAL:HG11	1.88	0.55
2:C:758:ARG:HB3	2:C:788:THR:O	2.07	0.55
2:C:811:PRO:HD3	9:C:9578:HOH:O	2.05	0.55
2:C:976:ASP:CB	2:C:979:THR:HG22	2.37	0.55
3:D:1004:THR:O	3:D:1007:VAL:HG22	2.06	0.55
3:D:1066:THR:CG2	3:D:1069:GLU:H	2.19	0.55
3:D:1097:LYS:HD3	9:D:9906:HOH:O	2.07	0.55
3:D:121:THR:HG23	9:D:2262:HOH:O	2.06	0.55
3:D:1364:HIS:NE2	3:D:1366:LYS:HE3	2.22	0.55
3:D:966:GLU:O	3:D:969:ARG:HG2	2.06	0.55
5:F:278:LEU:HD22	5:F:290:GLU:HB3	1.88	0.55
1:K:122:ILE:HD12	9:K:4736:HOH:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:1027:PHE:HA	9:M:9907:HOH:O	2.05	0.55
2:M:18:LEU:HB2	2:M:590:ASP:HB3	1.87	0.55
3:N:1341:PRO:O	3:N:1344:VAL:HG23	2.06	0.55
3:N:397:LYS:HB2	9:N:2381:HOH:O	2.05	0.55
1:A:212:ASN:O	1:A:215:VAL:HG22	2.06	0.55
1:A:75:VAL:N	9:A:9598:HOH:O	2.39	0.55
2:C:1015:LEU:HD22	5:F:333:ILE:HG21	1.88	0.55
2:C:479:VAL:HG23	2:C:506:ASN:HA	1.88	0.55
2:C:555:ALA:HA	3:D:1070:TYR:OH	2.07	0.55
3:D:1094:LEU:HD23	3:D:1230:GLY:HA2	1.87	0.55
3:D:698:LYS:HA	9:E:9480:HOH:O	2.06	0.55
5:F:247:ILE:O	5:F:251:ILE:HG13	2.06	0.55
2:M:12:VAL:HG13	2:M:13:ILE:HG23	1.89	0.55
2:M:239:PHE:CZ	2:M:254:VAL:HB	2.40	0.55
2:M:252:LYS:NZ	2:M:296:GLY:HA3	2.22	0.55
2:M:41:ASN:O	2:M:46:ALA:HB2	2.06	0.55
2:M:52:PHE:CE1	2:M:66:LEU:HG	2.42	0.55
1:K:42:ARG:NH1	2:M:857:ASP:HB3	2.17	0.55
3:N:208:PRO:HB2	3:N:395:VAL:HG13	1.87	0.55
4:O:76:GLY:HA3	4:O:79:LEU:HD13	1.89	0.55
1:B:10:VAL:HG12	1:B:12:THR:HG23	1.87	0.55
2:C:198:ARG:NH2	2:C:203:ASP:HB3	2.22	0.55
2:C:460:ARG:HD2	2:C:485:TYR:CE2	2.41	0.55
2:C:544:THR:O	2:C:547:ILE:HG13	2.06	0.55
2:C:808:ARG:HG2	9:C:9965:HOH:O	2.05	0.55
3:D:119:SER:CB	3:D:123:LEU:HB2	2.37	0.55
3:D:536:ALA:HA	9:F:9527:HOH:O	2.07	0.55
3:D:764:LEU:HB3	9:D:9549:HOH:O	2.07	0.55
5:F:195:VAL:HG11	5:F:217:ASN:OD1	2.07	0.55
5:F:357:ALA:HA	9:F:9770:HOH:O	2.07	0.55
1:K:42:ARG:HG2	1:K:42:ARG:HH11	1.70	0.55
1:L:59:GLU:HG3	1:L:139:ASN:HB3	1.88	0.55
2:M:197:LEU:HD12	2:M:207:LEU:HD11	1.89	0.55
2:M:567:GLN:HB2	2:M:997:LEU:HD22	1.88	0.55
2:M:953:VAL:HG13	2:M:966:LEU:HD22	1.89	0.55
2:M:975:TYR:HA	2:M:982:PRO:HA	1.88	0.55
9:N:9664:HOH:O	4:O:5:GLY:HA2	2.06	0.55
5:P:278:LEU:HB2	5:P:286:PRO:HG2	1.88	0.55
1:B:95:GLN:HA	1:B:146:ARG:HD2	1.87	0.55
2:C:41:ASN:O	2:C:46:ALA:HB2	2.07	0.55
2:C:704:HIS:CD2	2:C:831:ARG:HH21	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1412:LYS:HG2	3:D:1414:PRO:HG3	1.89	0.55
3:D:135:LEU:CD1	3:D:147:VAL:HG23	2.37	0.55
3:D:18:ILE:HG21	3:D:516:ALA:O	2.07	0.55
3:D:462:GLN:HB3	9:D:9482:HOH:O	2.06	0.55
2:C:885:ILE:HD12	3:D:949:ILE:HB	1.87	0.55
5:F:363:GLU:HA	5:F:367:MET:CE	2.37	0.55
3:D:572:ARG:NH2	5:F:83:GLN:HE21	1.97	0.55
2:M:1104:GLU:HG3	3:N:6:ARG:HD2	1.88	0.55
3:N:104:PHE:CE2	3:N:1448:THR:HG23	2.41	0.55
3:N:434:ARG:HB2	3:N:447:VAL:CG2	2.35	0.55
2:M:769:PRO:HB2	3:N:65:ARG:NH2	2.21	0.55
3:N:679:ARG:HD3	3:N:682:ASP:OD2	2.06	0.55
3:N:774:SER:C	3:N:776:GLU:H	2.09	0.55
5:P:135:ILE:O	5:P:135:ILE:HD13	2.06	0.55
1:A:191:ASP:O	1:A:192:LEU:HD23	2.07	0.55
1:B:132:LEU:HD22	9:B:9571:HOH:O	2.05	0.55
1:B:65:PHE:HD1	3:D:813:LEU:HD22	1.72	0.55
2:C:264:PRO:HB2	9:C:9939:HOH:O	2.07	0.55
3:D:785:ILE:HD12	3:D:785:ILE:H	1.72	0.55
3:D:823:LEU:HG	9:D:9683:HOH:O	2.07	0.55
2:M:26:TYR:O	2:M:30:LEU:HD12	2.06	0.55
2:M:462:ASP:HB3	2:M:468:ARG:CD	2.33	0.55
2:M:9:ILE:HG13	2:M:9:ILE:O	2.07	0.55
3:N:46:ASP:HB3	3:N:49:ILE:HG13	1.88	0.55
3:N:75:ARG:HH11	3:N:75:ARG:HG3	1.72	0.55
3:N:911:LEU:O	3:N:915:VAL:HG23	2.07	0.55
5:P:172:ARG:O	5:P:176:ILE:HD13	2.07	0.55
1:A:156:HIS:CD2	1:A:158:ILE:HG12	2.42	0.55
1:B:73:GLU:HB3	1:B:77:GLU:HG3	1.88	0.55
1:B:81:ASN:O	1:B:84:GLU:HB3	2.06	0.55
1:B:94:LEU:HD11	1:B:119:ASP:HB3	1.88	0.55
2:C:529:VAL:HG21	9:C:9927:HOH:O	2.05	0.55
2:C:396:ASP:HA	2:C:633:GLN:HE22	1.72	0.55
2:C:674:VAL:HG23	2:C:869:VAL:O	2.06	0.55
2:C:724:ARG:CD	2:C:740:GLU:HA	2.37	0.55
3:D:1206:GLY:HA3	3:D:1366:LYS:NZ	2.22	0.55
3:D:1271:LYS:HG2	9:D:2043:HOH:O	2.06	0.55
3:D:145:VAL:HB	9:D:9524:HOH:O	2.05	0.55
3:D:156:GLU:CD	3:D:156:GLU:H	2.10	0.55
3:D:28:LYS:CB	3:D:41:ARG:HD2	2.37	0.55
3:D:9:ARG:NH1	3:D:506:GLY:HA2	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:1097:LEU:HD13	2:M:1097:LEU:N	2.22	0.55
2:M:549:PHE:CE2	2:M:886:LEU:HB3	2.42	0.55
3:N:1220:ALA:HB1	3:N:1223:ILE:CD1	2.36	0.55
3:N:28:LYS:HB2	3:N:41:ARG:HD2	1.89	0.55
3:N:630:VAL:HA	3:N:744:GLN:HG2	1.88	0.55
5:P:164:LYS:HA	5:P:171:LYS:HE3	1.88	0.55
5:P:234:LYS:HD3	5:P:236:SER:H	1.72	0.55
5:P:247:ILE:HG22	5:P:251:ILE:HD11	1.89	0.55
5:P:412:GLU:HG3	5:P:418:LEU:HD22	1.88	0.55
2:C:575:GLN:HB2	2:C:670:GLN:HG2	1.87	0.55
2:C:575:GLN:N	2:C:667:ALA:HB1	2.20	0.55
2:C:874:LEU:HD12	3:D:784:ASP:OD2	2.06	0.55
2:C:860:HIS:NE2	2:C:975:TYR:HB2	2.22	0.55
2:C:976:ASP:OD1	2:C:978:ARG:HD3	2.07	0.55
3:D:1101:VAL:HG22	3:D:1428:ALA:HB2	1.88	0.55
3:D:1115:THR:HG23	9:D:2006:HOH:O	2.06	0.55
3:D:1382:THR:HG21	3:D:1418:LYS:HE3	1.88	0.55
3:D:421:LEU:HD12	3:D:435:VAL:HG11	1.88	0.55
3:D:537:THR:C	5:F:317:LEU:HB2	2.28	0.55
5:F:136:LEU:HB3	5:F:185:GLN:HE22	1.71	0.55
5:F:416:ARG:HB2	9:F:9697:HOH:O	2.06	0.55
1:L:41:ARG:HG3	9:L:4703:HOH:O	2.06	0.55
2:M:1117:SER:HB2	9:M:2359:HOH:O	2.07	0.55
2:M:251:ASP:HB3	2:M:252:LYS:HD2	1.89	0.55
2:M:411:SER:OG	2:M:452:ILE:HG23	2.06	0.55
3:N:424:GLY:HA3	9:N:2149:HOH:O	2.07	0.55
3:N:709:HIS:ND1	3:N:709:HIS:N	2.55	0.55
5:P:184:ARG:O	5:P:188:ILE:HG13	2.07	0.55
5:P:217:ASN:O	5:P:221:ILE:HG13	2.07	0.55
5:P:416:ARG:NH1	5:P:419:ARG:HB3	2.22	0.55
2:C:626:ARG:HB2	2:C:626:ARG:HH11	1.71	0.55
2:C:64:LEU:HA	9:C:9791:HOH:O	2.07	0.55
2:C:817:PRO:HB3	5:F:305:GLU:OE2	2.07	0.55
2:C:831:ARG:HA	9:C:9771:HOH:O	2.06	0.55
3:D:1206:GLY:HA3	3:D:1366:LYS:HZ3	1.72	0.55
3:D:668:PRO:HD2	3:D:672:ALA:CB	2.37	0.55
2:M:157:ARG:HD3	2:M:158:TYR:H	1.72	0.55
2:M:232:GLU:HG2	9:M:2023:HOH:O	2.07	0.55
2:M:244:PRO:HD2	2:M:245:GLY:H	1.72	0.55
2:M:363:SER:HB3	9:M:9637:HOH:O	2.06	0.55
2:M:64:LEU:HD12	2:M:65:VAL:N	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:78:PHE:HB2	2:M:88:LEU:HD21	1.87	0.55
3:N:119:SER:N	3:N:123:LEU:HB2	2.21	0.55
3:N:1281:VAL:HG21	3:N:1313:VAL:HG21	1.88	0.55
3:N:865:THR:CG2	3:N:874:GLU:HG2	2.36	0.55
5:P:136:LEU:HB3	5:P:185:GLN:HE22	1.71	0.55
5:P:222:ARG:HH12	5:P:246:ALA:HB2	1.71	0.55
1:B:27:PRO:O	1:B:28:LEU:HD23	2.07	0.54
2:C:1115:LEU:HD12	2:C:1115:LEU:N	2.22	0.54
2:C:209:ARG:N	2:C:209:ARG:HD2	2.22	0.54
2:C:432:ARG:HG2	9:C:9920:HOH:O	2.06	0.54
3:D:148:GLU:CB	3:D:151:GLN:HB2	2.33	0.54
3:D:675:ARG:HD3	9:D:2158:HOH:O	2.06	0.54
4:E:92:ILE:HG21	9:E:9509:HOH:O	2.07	0.54
1:L:39:PRO:O	1:L:43:ILE:HG12	2.08	0.54
2:M:144:PRO:HG3	9:M:9535:HOH:O	2.07	0.54
2:M:165:LEU:HD11	9:M:2143:HOH:O	2.07	0.54
3:N:1011:PHE:HB3	3:N:1021:TYR:CD1	2.42	0.54
3:N:12:LEU:HD22	3:N:511:TRP:HB2	1.89	0.54
3:N:483:HIS:HB2	3:N:484:PRO:HD3	1.88	0.54
3:N:71:LYS:HE3	9:N:9778:HOH:O	2.06	0.54
5:P:152:ASP:HB2	5:P:153:PRO:HD3	1.88	0.54
5:P:185:GLN:O	5:P:189:GLU:HG3	2.07	0.54
2:C:290:LEU:HB3	2:C:302:VAL:HG11	1.89	0.54
2:C:522:VAL:HG12	2:C:524:VAL:HG23	1.88	0.54
2:C:612:VAL:HG22	2:C:622:GLU:HA	1.89	0.54
2:C:72:ARG:HG3	2:C:72:ARG:HH11	1.71	0.54
3:D:996:TRP:HB2	3:D:1044:LEU:HD11	1.89	0.54
3:D:119:SER:H	3:D:123:LEU:HD13	1.72	0.54
3:D:1258:ARG:O	3:D:1262:LEU:HD13	2.08	0.54
3:D:1321:ALA:O	3:D:1339:LYS:HD3	2.07	0.54
3:D:1432:LYS:HZ1	3:D:1460:ILE:HG13	1.71	0.54
3:D:207:PHE:CB	3:D:208:PRO:HD2	2.34	0.54
3:D:519:VAL:HG13	3:D:544:TYR:CZ	2.42	0.54
3:D:775:GLY:HA2	9:D:2120:HOH:O	2.07	0.54
3:D:809:PRO:HB2	3:D:812:ALA:HB2	1.88	0.54
3:D:929:ARG:HH11	3:D:929:ARG:HG3	1.72	0.54
2:M:313:LEU:HD12	2:M:313:LEU:O	2.07	0.54
2:M:405:ARG:HG2	9:M:2089:HOH:O	2.06	0.54
2:M:428:ARG:CZ	2:M:451:LEU:HD11	2.37	0.54
3:N:1242:HIS:CE1	3:N:1266:ARG:HD3	2.42	0.54
3:N:546:ARG:HG3	9:N:9696:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:550:ARG:NH1	3:N:573:MET:HB3	2.21	0.54
3:N:586:ARG:HD2	9:N:2319:HOH:O	2.07	0.54
3:N:996:TRP:O	3:N:999:THR:HG22	2.07	0.54
4:O:48:MET:HB2	4:O:54:LEU:HD12	1.89	0.54
2:C:1062:GLY:HA2	9:C:9628:HOH:O	2.06	0.54
2:C:206:THR:HG21	9:C:2105:HOH:O	2.07	0.54
2:C:212:GLY:HA3	2:C:218:VAL:HG23	1.89	0.54
2:C:715:THR:HG22	2:C:717:LEU:HG	1.90	0.54
3:D:1307:LYS:HG2	3:D:1308:GLU:OE1	2.08	0.54
2:C:1043:TYR:HE1	3:D:710:ARG:O	1.90	0.54
3:D:957:PRO:HG2	3:D:1007:VAL:HA	1.88	0.54
3:D:965:GLU:O	3:D:968:ASP:HB2	2.08	0.54
5:F:125:ASP:HA	5:F:128:ARG:CZ	2.37	0.54
5:F:102:LEU:HD12	5:F:187:LEU:HG	1.89	0.54
2:M:148:PHE:HZ	2:M:281:LEU:HD13	1.72	0.54
2:M:157:ARG:CD	2:M:314:THR:HG22	2.35	0.54
2:M:368:THR:HB	2:M:369:PRO:HD3	1.89	0.54
2:M:500:ASN:HD21	3:N:1067:VAL:HG23	1.73	0.54
2:M:584:GLU:O	2:M:588:VAL:HG13	2.07	0.54
2:M:675:ALA:HB2	2:M:867:VAL:HG11	1.88	0.54
2:M:721:ARG:NH2	2:M:785:VAL:HG21	2.22	0.54
2:M:862:PRO:HA	2:M:975:TYR:HE1	1.72	0.54
3:N:131:LYS:HG2	3:N:568:ARG:HG2	1.89	0.54
5:P:308:LEU:O	5:P:312:GLN:HG3	2.07	0.54
1:A:94:LEU:HB2	9:A:9536:HOH:O	2.06	0.54
1:B:105:GLY:O	1:B:132:LEU:HD23	2.06	0.54
1:B:184:THR:O	1:B:192:LEU:HB2	2.08	0.54
2:C:73:LEU:HB3	2:C:94:LEU:HD13	1.89	0.54
3:D:1104:GLU:HA	3:D:1461:GLY:HA2	1.88	0.54
3:D:1318:TYR:HD1	3:D:1319:VAL:H	1.55	0.54
3:D:1413:THR:HA	9:D:2122:HOH:O	2.07	0.54
3:D:493:ARG:HG2	3:D:493:ARG:HH11	1.71	0.54
3:D:628:ARG:HD3	3:D:744:GLN:HE22	1.71	0.54
3:D:868:TYR:CG	3:D:869:MET:N	2.75	0.54
1:K:224:TYR:CD2	1:L:9:PRO:HG2	2.42	0.54
1:K:58:ILE:HB	1:K:61:VAL:HB	1.89	0.54
1:K:67:THR:CG2	2:M:609:ASN:HD21	2.20	0.54
2:M:1034:GLU:HA	2:M:1037:VAL:CG2	2.37	0.54
2:M:152:PRO:HG2	9:M:9934:HOH:O	2.06	0.54
2:M:17:PRO:O	2:M:20:GLU:HB3	2.07	0.54
2:M:455:LEU:CD1	2:M:459:ALA:HB3	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:988:VAL:HG13	9:M:9722:HOH:O	2.07	0.54
3:N:1035:ILE:HG22	3:N:1039:CYS:SG	2.47	0.54
3:N:1404:ASN:ND2	3:N:1408:ILE:HD12	2.20	0.54
3:N:1478:SER:O	3:N:1482:ARG:HG3	2.07	0.54
3:N:42:ASP:O	3:N:43:GLY:O	2.26	0.54
3:N:514:LEU:HD23	9:N:9923:HOH:O	2.08	0.54
3:N:644:LEU:HD12	3:N:645:PRO:CD	2.35	0.54
3:N:639:LEU:HD11	3:N:731:LEU:HD12	1.89	0.54
2:M:1076:VAL:CG2	3:N:752:SER:HB3	2.37	0.54
3:N:829:VAL:HA	9:N:2355:HOH:O	2.06	0.54
5:P:154:LYS:HD2	9:P:3317:HOH:O	2.07	0.54
5:P:332:PHE:HB2	9:P:5627:HOH:O	2.07	0.54
1:B:97:VAL:HG13	9:B:9502:HOH:O	2.07	0.54
2:C:200:LEU:HD13	2:C:300:ASP:CG	2.28	0.54
2:C:437:ARG:O	2:C:467:ILE:HD13	2.08	0.54
2:C:736:ASP:O	2:C:744:ARG:HG2	2.07	0.54
2:C:859:PRO:O	2:C:867:VAL:HG22	2.08	0.54
3:D:1080:GLY:O	3:D:1084:THR:HG23	2.07	0.54
3:D:116:LEU:O	3:D:118:LEU:HG	2.07	0.54
3:D:1412:LYS:HE2	3:D:1414:PRO:HG3	1.88	0.54
3:D:1478:SER:OG	3:D:1481:VAL:HG23	2.08	0.54
3:D:152:LEU:HD23	3:D:152:LEU:N	2.20	0.54
3:D:186:VAL:HG11	3:D:213:VAL:HB	1.89	0.54
5:F:264:MET:O	5:F:267:THR:HB	2.07	0.54
1:K:54:THR:HG22	1:K:158:ILE:HG13	1.88	0.54
1:L:110:LYS:HB2	1:L:110:LYS:HZ2	1.71	0.54
2:M:159:ILE:HG22	9:M:9660:HOH:O	2.06	0.54
2:M:198:ARG:NH2	2:M:203:ASP:HB3	2.21	0.54
2:M:335:THR:HG21	2:M:461:VAL:HG11	1.89	0.54
2:M:642:ARG:HG3	2:M:657:ASP:OD2	2.06	0.54
2:M:690:ILE:HG23	2:M:852:ILE:HA	1.90	0.54
2:M:704:HIS:CB	2:M:831:ARG:HE	2.19	0.54
2:M:83:CYS:HA	2:M:88:LEU:HD23	1.90	0.54
3:N:1148:VAL:O	3:N:1189:ARG:HG2	2.06	0.54
3:N:1232:PRO:HB3	3:N:1361:VAL:HG21	1.88	0.54
3:N:1236:LEU:HD11	3:N:1356:TYR:CE1	2.43	0.54
3:N:423:ASP:OD1	5:P:174:LEU:HD13	2.08	0.54
3:N:704:ARG:HG3	3:N:736:PHE:CB	2.33	0.54
2:M:1043:TYR:HE1	3:N:710:ARG:O	1.91	0.54
3:N:565:ILE:HD13	5:P:189:GLU:HG2	1.88	0.54
5:P:201:LYS:HB2	9:P:4870:HOH:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:269:ASN:O	5:P:273:ARG:HG3	2.07	0.54
5:P:419:ARG:NH1	5:P:419:ARG:HB2	2.22	0.54
1:A:123:MET:C	1:A:125:PRO:HD3	2.28	0.54
1:A:91:ASN:CG	1:A:92:PRO:HD2	2.27	0.54
2:C:304:LEU:HD23	2:C:305:PRO:HD3	1.90	0.54
2:C:593:ALA:HA	9:C:9558:HOH:O	2.07	0.54
2:C:841:ASN:HD21	2:C:845:ASN:H	1.55	0.54
2:C:862:PRO:HG3	2:C:975:TYR:HE1	1.72	0.54
3:D:1008:PHE:HZ	3:D:1032:PRO:HA	1.73	0.54
3:D:664:LYS:HD3	9:D:2194:HOH:O	2.07	0.54
3:D:709:HIS:HA	3:D:1227:GLN:HG2	1.90	0.54
5:F:108:GLU:HG3	5:F:176:ILE:CG2	2.37	0.54
5:F:279:GLN:HB2	9:F:9647:HOH:O	2.07	0.54
2:M:260:LEU:HG	2:M:261:ILE:HG13	1.89	0.54
2:M:273:GLY:HA2	2:M:276:LYS:HD3	1.89	0.54
2:M:637:LEU:HD23	2:M:637:LEU:N	2.23	0.54
3:N:1117:TYR:HB3	9:N:2569:HOH:O	2.07	0.54
3:N:1350:GLU:HG3	3:N:1354:LYS:HE3	1.88	0.54
3:N:178:LEU:HG	3:N:200:ASP:H	1.71	0.54
3:N:427:VAL:HG21	3:N:435:VAL:HB	1.87	0.54
3:N:486:ARG:HA	3:N:489:ARG:HD3	1.89	0.54
3:N:799:LYS:O	3:N:799:LYS:HD3	2.07	0.54
5:P:264:MET:HB3	9:P:3779:HOH:O	2.07	0.54
1:B:101:LEU:HG	1:B:114:PHE:HA	1.89	0.54
1:B:86:VAL:HG12	1:B:124:ASN:ND2	2.08	0.54
2:C:123:GLU:HB2	9:C:2092:HOH:O	2.07	0.54
2:C:139:GLN:HG3	2:C:411:SER:O	2.07	0.54
2:C:405:ARG:NH2	2:C:566:THR:HG21	2.23	0.54
2:C:577:PRO:HG3	2:C:993:PHE:CD2	2.42	0.54
3:D:1118:ILE:HG23	9:D:9597:HOH:O	2.08	0.54
3:D:1246:VAL:HG21	9:D:2550:HOH:O	2.06	0.54
3:D:1487:VAL:HA	9:D:9715:HOH:O	2.06	0.54
3:D:178:LEU:HD21	3:D:199:LEU:H	1.73	0.54
3:D:427:VAL:HG21	3:D:435:VAL:HB	1.89	0.54
3:D:470:LEU:HD12	9:D:2635:HOH:O	2.07	0.54
3:D:852:ALA:O	3:D:857:ILE:HG12	2.07	0.54
2:C:1090:LYS:HE3	3:D:88:TYR:O	2.06	0.54
3:D:899:LEU:HD12	3:D:900:ILE:HG23	1.89	0.54
2:M:1085:PHE:HE1	2:M:1111:ILE:HG21	1.73	0.54
2:M:497:ALA:HA	2:M:515:ALA:HA	1.88	0.54
2:M:545:ASN:O	2:M:581:THR:HG21	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:730:SER:HB3	9:M:2237:HOH:O	2.07	0.54
2:M:798:GLY:H	2:M:827:VAL:CG1	2.20	0.54
3:N:1252:ILE:HD13	9:N:9977:HOH:O	2.08	0.54
3:N:1266:ARG:O	3:N:1268:PRO:HD3	2.08	0.54
3:N:690:ALA:O	3:N:694:VAL:HG23	2.08	0.54
5:P:159:ILE:O	5:P:163:LEU:HG	2.07	0.54
5:P:192:LEU:O	5:P:196:VAL:HG23	2.08	0.54
5:P:287:THR:N	5:P:290:GLU:OE1	2.41	0.54
2:C:124:ASP:CB	2:C:592:LEU:HD12	2.37	0.54
2:C:567:GLN:HB2	2:C:997:LEU:HD22	1.90	0.54
2:C:666:LEU:CD2	2:C:668:LEU:HD11	2.38	0.54
2:C:724:ARG:HD2	2:C:740:GLU:HA	1.89	0.54
3:D:1065:LEU:HD11	3:D:1070:TYR:N	2.23	0.54
3:D:1396:GLU:O	3:D:1400:VAL:HG23	2.08	0.54
3:D:465:LEU:HD13	9:D:2007:HOH:O	2.08	0.54
4:E:25:LYS:O	4:E:29:GLN:HG2	2.08	0.54
5:F:132:ARG:O	5:F:136:LEU:HG	2.07	0.54
1:L:115:LEU:O	1:L:115:LEU:HD12	2.08	0.54
1:L:84:GLU:HG3	1:L:127:LEU:HD22	1.88	0.54
2:M:253:ALA:HB3	9:M:2207:HOH:O	2.08	0.54
2:M:432:ARG:CZ	2:M:519:GLY:HA3	2.38	0.54
2:M:63:GLY:HA3	2:M:103:LYS:HE2	1.89	0.54
2:M:759:THR:HB	2:M:785:VAL:HG21	1.88	0.54
2:M:897:LEU:HB3	2:M:899:GLN:NE2	2.19	0.54
3:N:1372:VAL:HA	3:N:1375:MET:HG3	1.90	0.54
3:N:1103:HIS:HD2	3:N:1462:LEU:N	2.06	0.54
3:N:661:MET:CE	3:N:677:LEU:HD11	2.38	0.54
3:N:962:GLN:O	3:N:966:GLU:HG3	2.08	0.54
5:P:93:LEU:HA	5:P:98:GLU:OE1	2.08	0.54
2:C:176:VAL:HG12	2:C:182:VAL:HG13	1.89	0.54
2:C:877:PRO:HG3	3:D:1020:LEU:HD12	1.89	0.54
3:D:510:GLU:HB3	9:D:9600:HOH:O	2.08	0.54
3:D:84:ILE:O	3:D:87:ARG:HG3	2.07	0.54
3:D:850:LEU:O	3:D:853:VAL:HB	2.08	0.54
4:E:13:VAL:HG23	9:E:9552:HOH:O	2.06	0.54
4:E:48:MET:CB	4:E:54:LEU:HB2	2.38	0.54
3:D:561:GLY:HA3	5:F:184:ARG:NH1	2.23	0.54
5:F:356:LYS:O	5:F:360:LYS:HG2	2.07	0.54
2:M:1016:ILE:HD13	2:M:1016:ILE:H	1.71	0.54
2:M:1115:LEU:HD11	9:M:9579:HOH:O	2.07	0.54
2:M:537:LYS:HA	2:M:545:ASN:HD21	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:650:ARG:HD2	2:M:653:ASP:OD2	2.08	0.54
2:M:577:PRO:HG3	2:M:993:PHE:CE2	2.43	0.54
3:N:1058:ARG:HH11	3:N:1058:ARG:HG3	1.73	0.54
3:N:871:LYS:HE2	9:N:9777:HOH:O	2.07	0.54
4:O:94:PRO:HG3	9:O:5923:HOH:O	2.06	0.54
1:A:93:SER:HB2	9:A:9533:HOH:O	2.06	0.54
2:C:794:PRO:HB3	9:C:9647:HOH:O	2.07	0.54
3:D:399:ARG:NH2	3:D:432:TYR:HE2	2.06	0.54
3:D:400:VAL:CG1	3:D:441:ARG:HD3	2.38	0.54
3:D:404:GLU:HB3	3:D:414:ARG:CD	2.38	0.54
3:D:42:ASP:O	3:D:43:GLY:O	2.25	0.54
3:D:471:GLU:HG2	9:D:9659:HOH:O	2.07	0.54
3:D:502:PHE:CZ	3:D:509:PRO:HB3	2.42	0.54
2:C:983:ILE:HG23	3:D:944:THR:O	2.08	0.54
1:K:198:ARG:HB2	1:K:200:TRP:CZ3	2.43	0.54
1:K:216:GLU:O	1:K:220:GLU:HG3	2.07	0.54
1:K:27:PRO:HG2	1:K:186:LEU:HD22	1.90	0.54
1:L:40:LEU:HD11	9:L:4428:HOH:O	2.08	0.54
2:M:580:MET:HB3	2:M:584:GLU:OE1	2.08	0.54
2:M:724:ARG:CG	2:M:740:GLU:HA	2.38	0.54
3:N:999:THR:O	3:N:1002:LYS:HB2	2.08	0.54
3:N:1252:ILE:HD12	3:N:1252:ILE:H	1.72	0.54
3:N:1503:VAL:HG12	9:N:9617:HOH:O	2.08	0.54
3:N:32:ILE:HG12	3:N:38:LYS:O	2.08	0.54
3:N:699:VAL:HG21	3:N:760:ARG:HB3	1.90	0.54
3:N:799:LYS:H	3:N:826:PRO:HG2	1.72	0.54
3:N:981:GLY:HA3	9:N:2378:HOH:O	2.07	0.54
4:O:85:LEU:HD23	4:O:86:GLN:N	2.23	0.54
5:P:102:LEU:O	5:P:106:VAL:HG23	2.08	0.54
5:P:184:ARG:HD3	5:P:188:ILE:HD11	1.90	0.54
1:A:50:GLY:O	1:A:146:ARG:HA	2.07	0.53
1:A:160:ASP:HB2	9:A:9521:HOH:O	2.08	0.53
1:B:137:ARG:HB2	9:B:9548:HOH:O	2.07	0.53
2:C:1008:ARG:HE	2:C:1028:GLY:H	1.56	0.53
2:C:1070:ILE:HA	9:C:9807:HOH:O	2.07	0.53
2:C:536:PRO:HB2	2:C:905:ILE:HD13	1.89	0.53
2:C:436:GLY:HA2	2:C:538:GLN:O	2.08	0.53
2:C:9:ILE:HG12	2:C:907:ASP:CG	2.29	0.53
3:D:1087:ARG:HD2	3:D:1256:LEU:HD22	1.90	0.53
3:D:1472:ILE:HG22	3:D:1474:ALA:H	1.73	0.53
3:D:149:LYS:HE3	9:D:2297:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:560:GLN:HG3	5:F:221:ILE:HG21	1.89	0.53
4:E:88:GLU:HB2	9:E:9594:HOH:O	2.07	0.53
1:K:198:ARG:HD3	1:K:200:TRP:CH2	2.37	0.53
1:L:180:GLN:HG2	9:N:9580:HOH:O	2.07	0.53
2:M:200:LEU:HD13	2:M:300:ASP:CG	2.28	0.53
2:M:208:ALA:HB1	2:M:218:VAL:HG13	1.90	0.53
2:M:460:ARG:O	2:M:468:ARG:HG3	2.08	0.53
2:M:604:ALA:HB3	2:M:612:VAL:O	2.08	0.53
2:M:714:ASP:HB2	9:M:2167:HOH:O	2.07	0.53
3:N:1379:VAL:HA	3:N:1420:LEU:HB2	1.91	0.53
3:N:455:ARG:HH21	5:P:140:ARG:HD3	1.73	0.53
2:C:242:LEU:HD23	9:C:9503:HOH:O	2.08	0.53
2:C:358:ARG:HB3	2:C:371:LYS:O	2.09	0.53
2:C:437:ARG:HG3	2:C:469:THR:OG1	2.07	0.53
2:C:464:LEU:O	2:C:466:PHE:N	2.40	0.53
2:C:553:ASP:HA	2:C:881:ASN:HA	1.89	0.53
2:C:926:PHE:CD2	2:C:930:LYS:HE2	2.43	0.53
2:C:937:ASP:HB2	2:C:940:GLU:HG3	1.89	0.53
3:D:1278:ASP:HB2	3:D:1318:TYR:HE1	1.72	0.53
3:D:1379:VAL:HG12	3:D:1419:PRO:HA	1.89	0.53
3:D:424:GLY:HA2	3:D:436:GLU:HA	1.90	0.53
3:D:516:ALA:O	3:D:518:PRO:HD3	2.09	0.53
3:D:667:ALA:HB2	3:D:676:MET:CE	2.38	0.53
3:D:844:ALA:HA	3:D:867:ARG:NH1	2.22	0.53
1:K:170:VAL:HG12	9:K:5166:HOH:O	2.07	0.53
2:M:163:ILE:HB	9:M:2375:HOH:O	2.08	0.53
2:M:254:VAL:HG13	2:M:258:TYR:HE1	1.73	0.53
2:M:460:ARG:HD3	9:M:2017:HOH:O	2.07	0.53
2:M:961:GLU:HA	9:M:9902:HOH:O	2.07	0.53
3:N:1264:GLU:OE2	3:N:1424:VAL:HG12	2.08	0.53
3:N:756:GLN:HE21	3:N:760:ARG:HD2	1.72	0.53
3:N:792:ILE:O	3:N:878:GLY:HA3	2.08	0.53
2:M:1093:GLN:HB3	3:N:90:MET:CE	2.38	0.53
3:N:984:THR:HG23	3:N:986:ARG:H	1.73	0.53
4:O:90:GLU:HA	9:O:4524:HOH:O	2.08	0.53
5:P:291:ILE:CG2	5:P:304:VAL:HG21	2.38	0.53
1:A:34:VAL:HG21	2:C:939:ARG:HD2	1.90	0.53
2:C:173:ASP:O	2:C:184:MET:HA	2.08	0.53
2:C:176:VAL:C	2:C:178:PRO:HD3	2.28	0.53
2:C:350:ARG:HG2	2:C:353:ARG:NH2	2.24	0.53
2:C:516:ARG:NH2	3:D:1068:LEU:HB3	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:625:LEU:CD1	2:C:641:PRO:HG3	2.38	0.53
2:C:927:GLY:HA2	2:C:930:LYS:HE3	1.90	0.53
2:C:72:ARG:HE	2:C:97:ARG:NH1	2.06	0.53
3:D:1264:GLU:OE2	3:D:1424:VAL:N	2.41	0.53
3:D:1434:TRP:CZ3	3:D:1457:ASP:HB2	2.44	0.53
3:D:15:PRO:HA	3:D:18:ILE:HG12	1.90	0.53
3:D:647:ARG:NH1	3:D:650:LEU:HD23	2.24	0.53
3:D:769:LEU:H	3:D:769:LEU:HD12	1.74	0.53
3:D:789:LEU:O	3:D:792:ILE:HG23	2.08	0.53
3:D:89:ARG:O	3:D:521:PRO:HG3	2.08	0.53
9:C:9784:HOH:O	3:D:943:THR:HG21	2.08	0.53
1:K:150:TYR:HE2	1:K:152:PRO:HG3	1.72	0.53
1:K:14:ARG:HH12	1:K:24:VAL:HG23	1.73	0.53
2:M:358:ARG:HB3	2:M:371:LYS:O	2.08	0.53
2:M:514:VAL:HG11	2:M:516:ARG:NH1	2.23	0.53
2:M:810:ASP:HB3	2:M:813:VAL:HG22	1.90	0.53
3:N:957:PRO:HG2	3:N:1007:VAL:HG12	1.91	0.53
3:N:1406:ARG:HG3	3:N:1406:ARG:HH11	1.73	0.53
3:N:30:GLU:HB3	3:N:40:GLU:HB3	1.90	0.53
5:P:363:GLU:HA	5:P:367:MET:CE	2.37	0.53
1:A:30:ARG:NH2	1:A:191:ASP:HB2	2.24	0.53
1:B:83:LYS:HE2	1:B:168:ASP:HB2	1.89	0.53
2:C:41:ASN:N	2:C:41:ASN:ND2	2.55	0.53
2:C:741:GLY:HA3	9:C:9522:HOH:O	2.07	0.53
3:D:130:SER:HB3	3:D:132:TYR:CE1	2.43	0.53
3:D:526:PRO:O	3:D:537:THR:HA	2.08	0.53
5:F:307:THR:O	5:F:310:ILE:HG13	2.08	0.53
2:M:379:GLU:HG2	9:M:2388:HOH:O	2.07	0.53
2:M:343:GLN:HG2	2:M:385:PHE:HB2	1.91	0.53
2:M:642:ARG:HG3	2:M:654:LEU:HD21	1.91	0.53
2:M:662:GLU:HB3	9:M:9635:HOH:O	2.07	0.53
3:N:1294:VAL:HB	9:N:2223:HOH:O	2.09	0.53
3:N:436:GLU:HB2	3:N:445:ARG:HB2	1.89	0.53
3:N:524:LEU:C	3:N:526:PRO:HD3	2.28	0.53
3:N:583:ASP:OD2	3:N:604:THR:HG21	2.09	0.53
3:N:699:VAL:HG22	3:N:756:GLN:NE2	2.23	0.53
3:N:772:PRO:HA	9:N:9537:HOH:O	2.08	0.53
3:N:829:VAL:H	3:N:835:SER:HB2	1.73	0.53
9:M:9722:HOH:O	3:N:948:THR:HB	2.08	0.53
5:P:278:LEU:CB	5:P:286:PRO:HG2	2.38	0.53
1:A:156:HIS:CD2	1:A:157:GLY:N	2.76	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:126:VAL:O	3:D:132:TYR:HD1	1.91	0.53
3:D:1267:ARG:HH21	3:D:1331:ASP:CG	2.12	0.53
3:D:171:LEU:HD22	3:D:390:PRO:HG3	1.90	0.53
3:D:800:LYS:HD3	3:D:804:LEU:HD13	1.90	0.53
3:D:955:VAL:HG11	3:D:1015:TYR:HE2	1.73	0.53
3:D:992:ILE:HD13	9:D:2530:HOH:O	2.08	0.53
1:K:83:LYS:HE2	1:K:168:ASP:H	1.73	0.53
1:K:44:LEU:O	1:K:174:VAL:HG21	2.08	0.53
1:L:218:LEU:O	1:L:222:LEU:HG	2.08	0.53
2:M:1012:PRO:HD2	2:M:1021:LEU:O	2.09	0.53
2:M:1050:GLN:HG3	9:N:2259:HOH:O	2.07	0.53
2:M:247:PRO:HB3	9:M:2135:HOH:O	2.08	0.53
2:M:549:PHE:CZ	2:M:886:LEU:HD12	2.44	0.53
3:N:103:TRP:HH2	3:N:1447:LEU:HD23	1.73	0.53
3:N:1289:LYS:HE2	9:N:9835:HOH:O	2.09	0.53
3:N:9:ARG:HA	3:N:1455:LYS:O	2.07	0.53
3:N:102:ILE:HD13	3:N:586:ARG:HB2	1.88	0.53
3:N:631:ILE:HG21	3:N:745:MET:SD	2.48	0.53
5:P:89:GLY:HA2	9:P:4587:HOH:O	2.08	0.53
1:A:26:GLU:HB3	1:A:194:LYS:HG3	1.91	0.53
1:A:7:LYS:HD3	9:A:9619:HOH:O	2.08	0.53
2:C:1092:LEU:HD13	2:C:1099:VAL:HG21	1.91	0.53
2:C:202:TYR:OH	2:C:304:LEU:HD22	2.09	0.53
2:C:302:VAL:C	2:C:305:PRO:HD2	2.29	0.53
2:C:517:ARG:NH1	2:C:522:VAL:HG11	2.24	0.53
2:C:64:LEU:CD1	2:C:100:LEU:HD13	2.39	0.53
2:C:679:PHE:C	3:D:943:THR:HG22	2.28	0.53
2:C:722:ILE:HG12	2:C:757:GLY:O	2.09	0.53
2:C:853:LEU:HD23	2:C:858:MET:HB2	1.91	0.53
2:C:876:VAL:HB	3:D:949:ILE:HG13	1.91	0.53
3:D:1066:THR:CG2	3:D:1069:GLU:HG3	2.38	0.53
3:D:1382:THR:HA	3:D:1389:LEU:HD13	1.91	0.53
3:D:153:LEU:HD11	3:D:158:TYR:N	2.23	0.53
3:D:445:ARG:HG2	3:D:445:ARG:HH11	1.74	0.53
3:D:554:LEU:O	3:D:558:LEU:HG	2.09	0.53
3:D:85:VAL:HB	9:D:9784:HOH:O	2.07	0.53
3:D:963:TYR:CD2	3:D:1002:LYS:HB3	2.43	0.53
9:C:9697:HOH:O	4:E:28:GLN:HG3	2.08	0.53
4:E:31:LEU:HD12	4:E:32:ARG:HD3	1.89	0.53
4:E:41:GLU:HG3	9:E:9492:HOH:O	2.07	0.53
2:M:129:ILE:HG12	2:M:386:PHE:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1135:ARG:HG2	3:N:1136:LYS:HE3	1.90	0.53
3:N:169:TYR:HA	3:N:392:SER:HA	1.91	0.53
3:N:52:PRO:HG3	3:N:78:VAL:HG22	1.90	0.53
3:N:906:GLN:HE22	3:N:910:SER:HB2	1.72	0.53
5:P:234:LYS:HD2	5:P:236:SER:HB2	1.89	0.53
1:A:18:ARG:O	1:A:207:PRO:HD3	2.07	0.53
1:B:219:ARG:O	1:B:223:THR:HG23	2.09	0.53
3:D:633:VAL:HG22	3:D:635:PRO:CD	2.37	0.53
1:K:38:ASN:HB3	1:K:39:PRO:HD3	1.90	0.53
1:L:92:PRO:HD3	9:L:6230:HOH:O	2.08	0.53
2:M:1018:GLN:NE2	2:M:1063:ARG:HH22	2.07	0.53
2:M:195:LEU:HD12	2:M:234:ALA:HB1	1.90	0.53
2:M:710:ILE:HD11	2:M:758:ARG:CZ	2.39	0.53
2:M:79:PRO:HG2	2:M:82:GLU:HB2	1.90	0.53
2:M:838:LYS:HE2	2:M:997:LEU:HD12	1.90	0.53
2:M:876:VAL:HA	9:M:9508:HOH:O	2.08	0.53
3:N:809:PRO:HB2	3:N:812:ALA:HB2	1.90	0.53
3:N:950:GLY:C	3:N:952:ASP:N	2.58	0.53
2:M:772:ARG:HD2	5:P:373:LYS:HD2	1.91	0.53
2:C:739:GLU:HB3	9:C:9747:HOH:O	2.08	0.53
3:D:95:LEU:HD21	3:D:574:LEU:HD11	1.90	0.53
5:F:408:LEU:HA	5:F:411:HIS:CE1	2.43	0.53
1:L:149:GLY:O	1:L:171:PHE:HB2	2.08	0.53
2:M:338:GLU:O	2:M:341:THR:HG22	2.08	0.53
2:M:42:VAL:HA	9:M:2303:HOH:O	2.09	0.53
2:M:73:LEU:HD22	2:M:118:ILE:HD11	1.90	0.53
2:M:987:ILE:HG23	9:M:9722:HOH:O	2.08	0.53
3:N:1173:LEU:HD23	3:N:1174:LEU:HD23	1.90	0.53
3:N:1494:ALA:HB1	4:O:88:GLU:OE2	2.09	0.53
3:N:493:ARG:HG3	3:N:494:LYS:N	2.23	0.53
3:N:115:LEU:HD12	3:N:498:VAL:HG23	1.91	0.53
3:N:863:VAL:HG21	9:N:9770:HOH:O	2.07	0.53
2:M:1093:GLN:HB3	3:N:90:MET:HE1	1.89	0.53
1:B:14:ARG:HG2	9:B:9567:HOH:O	2.08	0.53
2:C:409:ARG:HH12	7:C:8001:RPT:H18	1.74	0.53
2:C:496:ILE:HD12	2:C:496:ILE:H	1.74	0.53
2:C:405:ARG:HH12	2:C:563:ASN:HD22	1.53	0.53
2:C:625:LEU:HD13	2:C:639:GLN:O	2.08	0.53
2:C:6:PHE:CE2	2:C:913:GLU:HB3	2.44	0.53
3:D:1395:LEU:HB3	9:D:9895:HOH:O	2.08	0.53
3:D:178:LEU:HD22	9:D:9887:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:154:LYS:HZ2	5:F:154:LYS:HB2	1.73	0.53
5:F:215:GLU:HG2	9:F:9503:HOH:O	2.08	0.53
5:F:282:LEU:HD12	5:F:284:ARG:O	2.09	0.53
2:M:166:PRO:HD3	2:M:265:ARG:HB2	1.90	0.53
2:M:610:ARG:HG2	9:M:9673:HOH:O	2.09	0.53
2:M:625:LEU:HD13	2:M:639:GLN:O	2.09	0.53
2:M:54:ILE:HG22	2:M:66:LEU:HB3	1.90	0.53
3:N:584:ASN:CG	3:N:590:PRO:HD2	2.28	0.53
3:N:636:GLN:HB2	9:N:2002:HOH:O	2.09	0.53
3:N:681:ARG:HH11	3:N:681:ARG:HB3	1.74	0.53
5:P:138:SER:O	5:P:141:VAL:HG12	2.09	0.53
5:P:277:GLN:O	5:P:280:GLN:HB3	2.09	0.53
1:B:149:GLY:O	1:B:171:PHE:HB2	2.09	0.53
2:C:1002:GLU:HA	2:C:1006:HIS:HE1	1.73	0.53
2:C:162:ILE:HD12	2:C:172:ILE:HB	1.91	0.53
2:C:405:ARG:HH21	2:C:566:THR:HG21	1.73	0.53
2:C:721:ARG:HA	9:C:9648:HOH:O	2.09	0.53
1:A:63:HIS:CD2	2:C:801:VAL:HG12	2.44	0.53
2:C:902:ILE:O	2:C:904:PRO:HD3	2.09	0.53
3:D:143:ASN:HD21	3:D:145:VAL:HG12	1.74	0.53
3:D:576:GLU:HA	3:D:579:ASP:OD2	2.09	0.53
3:D:613:ARG:O	3:D:617:ASN:HB2	2.08	0.53
5:F:373:LYS:HB2	9:F:9672:HOH:O	2.08	0.53
1:K:123:MET:O	1:K:125:PRO:HD3	2.08	0.53
1:L:72:LYS:HE2	9:L:5229:HOH:O	2.09	0.53
2:M:254:VAL:HG21	9:M:9516:HOH:O	2.08	0.53
2:M:907:ASP:HA	9:M:2423:HOH:O	2.09	0.53
3:N:1189:ARG:HB3	3:N:1189:ARG:HH11	1.73	0.53
3:N:1459:LEU:HD13	3:N:1465:ASN:HD21	1.73	0.53
3:N:14:SER:HB2	3:N:16:GLU:HG2	1.91	0.53
3:N:204:LEU:HD21	9:N:9631:HOH:O	2.08	0.53
3:N:404:GLU:HB3	3:N:414:ARG:CZ	2.39	0.53
3:N:566:ILE:HG12	5:P:217:ASN:ND2	2.23	0.53
3:N:969:ARG:HA	9:N:2036:HOH:O	2.09	0.53
1:A:44:LEU:O	1:A:174:VAL:HG21	2.09	0.52
2:C:601:GLY:O	2:C:648:ARG:HA	2.10	0.52
2:C:918:LEU:HB3	2:C:968:LEU:HD23	1.90	0.52
3:D:1105:ILE:HG13	9:D:9769:HOH:O	2.08	0.52
3:D:133:ILE:HG21	3:D:454:ALA:HB1	1.91	0.52
3:D:57:GLU:CD	3:D:64:LYS:HE2	2.29	0.52
3:D:863:VAL:HG21	9:D:2215:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:17:TYR:O	4:E:21:VAL:HG23	2.10	0.52
5:F:107:GLU:HG2	9:F:9515:HOH:O	2.08	0.52
1:K:52:ALA:HA	9:K:3524:HOH:O	2.09	0.52
2:M:1060:ILE:HG22	2:M:1061:GLU:N	2.25	0.52
2:M:333:ILE:CD1	2:M:467:ILE:HG13	2.39	0.52
2:M:380:ALA:O	2:M:384:GLU:HB2	2.09	0.52
2:M:910:LYS:HG2	9:M:2099:HOH:O	2.08	0.52
3:N:1047:LYS:HB3	3:N:1048:PRO:CD	2.40	0.52
3:N:1097:LYS:O	3:N:1101:VAL:HG23	2.08	0.52
3:N:1312:LEU:HB2	9:N:9707:HOH:O	2.10	0.52
3:N:1402:ALA:HB2	3:N:1415:VAL:CG2	2.39	0.52
3:N:1503:VAL:HG11	9:N:9596:HOH:O	2.09	0.52
3:N:699:VAL:HG12	3:N:717:GLN:CA	2.37	0.52
4:O:79:LEU:HD11	9:O:4245:HOH:O	2.08	0.52
5:P:347:GLN:HG3	9:P:3973:HOH:O	2.09	0.52
1:A:91:ASN:HB3	9:A:9551:HOH:O	2.10	0.52
2:C:708:TYR:N	2:C:708:TYR:CD1	2.77	0.52
2:C:732:ALA:HB1	2:C:735:ARG:NH2	2.24	0.52
2:C:811:PRO:HD2	2:C:813:VAL:HG22	1.91	0.52
3:D:1068:LEU:HD23	3:D:1072:ILE:HG12	1.89	0.52
3:D:131:LYS:O	3:D:133:ILE:HD13	2.09	0.52
3:D:1274:ILE:HD11	3:D:1334:GLN:HB3	1.91	0.52
3:D:95:LEU:HD12	3:D:517:VAL:HG23	1.90	0.52
3:D:957:PRO:CG	3:D:1007:VAL:HA	2.40	0.52
5:F:184:ARG:HE	5:F:188:ILE:HD11	1.74	0.52
5:F:368:VAL:HG12	9:F:9483:HOH:O	2.08	0.52
2:M:170:PRO:HG2	2:M:258:TYR:HD2	1.74	0.52
2:M:460:ARG:HB3	2:M:460:ARG:HH11	1.74	0.52
2:M:626:ARG:HA	9:M:9546:HOH:O	2.08	0.52
2:M:841:ASN:HD22	2:M:841:ASN:C	2.12	0.52
3:N:215:TYR:HA	9:N:9773:HOH:O	2.09	0.52
2:M:1101:THR:HB	3:N:5:VAL:HG13	1.92	0.52
3:N:800:LYS:HD2	9:N:2127:HOH:O	2.08	0.52
3:N:781:PRO:HB2	3:N:911:LEU:HD23	1.91	0.52
3:N:916:TYR:O	3:N:919:PHE:HB3	2.09	0.52
4:O:33:HIS:CG	4:O:89:MET:HG2	2.43	0.52
2:C:1055:LEU:HD21	2:C:1079:PRO:HG3	1.91	0.52
2:C:346:VAL:HG12	9:C:9903:HOH:O	2.08	0.52
2:C:516:ARG:CZ	3:D:1068:LEU:HB3	2.39	0.52
2:C:778:PHE:HB3	9:C:2430:HOH:O	2.10	0.52
9:A:9609:HOH:O	2:C:856:GLU:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1231:GLU:HG2	3:D:1232:PRO:N	2.25	0.52
3:D:1192:LEU:HD21	3:D:1372:VAL:HG13	1.91	0.52
3:D:1496:GLU:HA	3:D:1499:ARG:HD2	1.90	0.52
3:D:86:ARG:NH1	3:D:86:ARG:HG2	2.21	0.52
5:F:127:ILE:HD11	9:F:9599:HOH:O	2.08	0.52
5:F:278:LEU:CB	5:F:286:PRO:HG2	2.39	0.52
1:K:30:ARG:HG3	1:K:30:ARG:HH11	1.74	0.52
1:L:7:LYS:HG3	9:L:5022:HOH:O	2.09	0.52
1:K:224:TYR:HB3	1:L:9:PRO:HB2	1.91	0.52
2:M:1104:GLU:HA	3:N:6:ARG:HD2	1.92	0.52
2:M:376:ARG:HG2	9:M:2218:HOH:O	2.08	0.52
2:M:464:LEU:O	2:M:466:PHE:N	2.43	0.52
2:M:643:VAL:HG13	2:M:647:GLN:OE1	2.09	0.52
2:M:73:LEU:HD11	9:M:2198:HOH:O	2.08	0.52
2:M:783:ARG:HB3	9:M:2452:HOH:O	2.08	0.52
2:M:801:VAL:O	2:M:802:ARG:HG3	2.10	0.52
2:M:937:ASP:HB3	2:M:940:GLU:H	1.73	0.52
3:N:1004:THR:O	3:N:1007:VAL:HG22	2.10	0.52
3:N:1104:GLU:O	3:N:1106:VAL:HG23	2.09	0.52
3:N:1382:THR:HG21	3:N:1418:LYS:HZ1	1.74	0.52
3:N:1493:LYS:HA	3:N:1496:GLU:CG	2.39	0.52
3:N:462:GLN:HA	3:N:513:ILE:CD1	2.40	0.52
3:N:732:VAL:HG13	9:N:9614:HOH:O	2.09	0.52
5:P:113:ILE:HG23	5:P:127:ILE:CG2	2.39	0.52
5:P:266:GLU:HA	5:P:269:ASN:ND2	2.24	0.52
5:P:403:LYS:HD2	9:P:3729:HOH:O	2.09	0.52
1:A:149:GLY:O	1:A:171:PHE:HB2	2.09	0.52
1:A:161:ARG:HB2	1:A:161:ARG:HH11	1.72	0.52
1:A:57:TYR:CE2	1:A:59:GLU:HA	2.45	0.52
2:C:165:LEU:HD13	9:C:9966:HOH:O	2.10	0.52
2:C:199:VAL:HG13	2:C:235:LEU:HG	1.91	0.52
2:C:693:GLU:HG3	9:C:9813:HOH:O	2.10	0.52
2:C:732:ALA:O	2:C:735:ARG:HG3	2.09	0.52
3:D:104:PHE:CD2	3:D:1448:THR:HG23	2.44	0.52
3:D:420:VAL:HG13	5:F:164:LYS:HE2	1.91	0.52
3:D:584:ASN:ND2	3:D:589:ALA:HA	2.23	0.52
2:C:1033:GLY:HA2	3:D:619:LEU:O	2.09	0.52
3:D:893:GLU:HA	9:D:9543:HOH:O	2.08	0.52
1:L:14:ARG:HG2	9:L:5424:HOH:O	2.08	0.52
2:M:998:TYR:CZ	2:M:1000:MET:HA	2.45	0.52
2:M:902:ILE:O	2:M:904:PRO:HD3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:207:PHE:CB	3:N:208:PRO:HD2	2.37	0.52
3:N:424:GLY:HA2	3:N:436:GLU:HA	1.91	0.52
3:N:52:PRO:HB2	9:N:9523:HOH:O	2.08	0.52
5:P:264:MET:O	5:P:268:ILE:HG13	2.08	0.52
2:C:182:VAL:CG1	2:C:193:LEU:HD13	2.39	0.52
2:C:195:LEU:HD23	2:C:238:LEU:HG	1.91	0.52
2:C:328:LEU:HB2	2:C:488:ALA:CB	2.39	0.52
2:C:129:ILE:CG1	2:C:386:PHE:HB3	2.40	0.52
2:C:52:PHE:HB3	2:C:53:PRO:HD3	1.89	0.52
2:C:918:LEU:HD23	2:C:967:PHE:O	2.09	0.52
3:D:1144:LEU:HA	3:D:1147:ARG:HG3	1.90	0.52
3:D:572:ARG:HB3	9:F:9505:HOH:O	2.09	0.52
2:C:1042:ALA:CB	3:D:710:ARG:HB3	2.39	0.52
2:M:366:SER:HB2	9:M:9558:HOH:O	2.09	0.52
2:M:669:GLY:HA3	2:M:995:MET:HA	1.91	0.52
2:M:807:ARG:HB2	2:M:807:ARG:NH1	2.24	0.52
2:M:881:ASN:ND2	2:M:881:ASN:H	2.08	0.52
3:N:1009:LYS:HG3	9:N:9751:HOH:O	2.08	0.52
3:N:1243:THR:HG22	3:N:1244:GLY:H	1.74	0.52
3:N:35:ARG:HG2	3:N:35:ARG:HH11	1.74	0.52
5:P:269:ASN:CB	5:P:273:ARG:HH21	2.23	0.52
5:P:336:GLU:CD	5:P:336:GLU:H	2.12	0.52
1:A:46:SER:HB3	2:C:856:GLU:CG	2.38	0.52
1:B:123:MET:O	1:B:125:PRO:HD3	2.10	0.52
2:C:708:TYR:CE2	2:C:793:PRO:HD2	2.41	0.52
3:D:1341:PRO:HA	3:D:1344:VAL:HG23	1.91	0.52
3:D:36:THR:HB	3:D:38:LYS:HG3	1.91	0.52
3:D:641:GLN:HB3	3:D:717:GLN:O	2.10	0.52
3:D:721:VAL:HA	9:D:9665:HOH:O	2.08	0.52
3:D:838:ARG:HH11	3:D:874:GLU:HB3	1.73	0.52
3:D:890:VAL:HG23	9:D:2176:HOH:O	2.08	0.52
3:D:926:LYS:HE2	9:D:9484:HOH:O	2.08	0.52
5:F:166:LEU:HD13	5:F:170:HIS:HB2	1.92	0.52
1:L:50:GLY:O	1:L:146:ARG:HA	2.10	0.52
1:L:176:ARG:HB2	9:N:9671:HOH:O	2.08	0.52
2:M:1092:LEU:HD23	2:M:1097:LEU:HD23	1.92	0.52
2:M:176:VAL:HG12	2:M:182:VAL:HG13	1.91	0.52
3:N:972:LEU:HD11	9:N:9509:HOH:O	2.10	0.52
1:A:150:TYR:HE2	1:A:152:PRO:HG3	1.74	0.52
1:A:176:ARG:HB3	9:A:9641:HOH:O	2.10	0.52
2:C:1081:VAL:HG21	2:C:1111:ILE:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:682:TYR:HB3	2:C:689:VAL:HG22	1.92	0.52
2:C:813:VAL:HG13	9:C:9732:HOH:O	2.08	0.52
2:C:839:LEU:HD21	2:C:849:VAL:CG2	2.40	0.52
2:C:852:ILE:H	2:C:852:ILE:HD12	1.75	0.52
3:D:1047:LYS:HA	3:D:1053:PHE:CE1	2.45	0.52
3:D:126:VAL:O	3:D:132:TYR:CD1	2.62	0.52
3:D:1432:LYS:CG	3:D:1433:SER:H	2.22	0.52
3:D:724:GLN:C	3:D:724:GLN:HE21	2.13	0.52
3:D:62:LYS:HE2	3:D:75:ARG:NH1	2.25	0.52
3:D:897:TRP:CH2	3:D:902:LEU:HD21	2.45	0.52
4:E:29:GLN:HB3	9:E:9534:HOH:O	2.09	0.52
1:L:101:LEU:HB2	1:L:114:PHE:CD2	2.44	0.52
1:K:32:PHE:HZ	1:L:47:SER:HG	1.56	0.52
2:M:146:VAL:HG13	2:M:161:SER:O	2.09	0.52
2:M:177:GLU:HB2	9:M:9838:HOH:O	2.09	0.52
2:M:290:LEU:HB3	2:M:302:VAL:CG1	2.40	0.52
2:M:601:GLY:O	2:M:648:ARG:HA	2.10	0.52
2:M:694:LEU:CD1	2:M:868:ASP:HB3	2.39	0.52
3:N:1018:ASN:O	3:N:1022:VAL:HG23	2.10	0.52
2:M:1038:TRP:HH2	3:N:1096:ARG:HD2	1.74	0.52
3:N:1109:GLU:HG2	3:N:1201:CYS:CA	2.38	0.52
3:N:122:GLU:HG2	9:N:2158:HOH:O	2.09	0.52
3:N:516:ALA:O	3:N:518:PRO:HD3	2.10	0.52
1:A:198:ARG:C	1:A:199:ILE:HD12	2.31	0.52
2:C:1005:MET:CE	3:D:648:MET:HB2	2.40	0.52
2:C:281:LEU:CD1	2:C:306:THR:HA	2.39	0.52
2:C:4:LYS:HG2	9:C:9667:HOH:O	2.10	0.52
2:C:470:PRO:HB2	2:C:534:VAL:HG21	1.91	0.52
2:C:586:ARG:HD2	2:C:590:ASP:OD2	2.10	0.52
2:C:961:GLU:HA	9:C:2350:HOH:O	2.10	0.52
3:D:1011:PHE:HZ	3:D:1039:CYS:HG	1.56	0.52
3:D:10:ILE:HG13	3:D:1434:TRP:CZ2	2.44	0.52
3:D:1342:GLU:H	3:D:1342:GLU:CD	2.13	0.52
3:D:1482:ARG:HB2	3:D:1483:PHE:CE1	2.44	0.52
3:D:455:ARG:HG2	3:D:455:ARG:NH1	2.25	0.52
3:D:45:PHE:HD1	3:D:86:ARG:HH21	1.56	0.52
3:D:925:GLU:HG2	3:D:926:LYS:N	2.24	0.52
3:D:787:LEU:HD21	3:D:947:ILE:CD1	2.40	0.52
4:E:48:MET:HB3	4:E:54:LEU:HB2	1.92	0.52
9:D:2311:HOH:O	5:F:147:LEU:HD21	2.10	0.52
2:M:1038:TRP:HA	2:M:1041:GLU:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:1091:GLU:HA	3:N:520:LEU:HD13	1.91	0.52
2:M:578:VAL:CG2	2:M:579:VAL:HG12	2.40	0.52
2:M:636:ALA:HB3	9:M:9891:HOH:O	2.09	0.52
2:M:69:LEU:HD21	2:M:99:GLN:NE2	2.25	0.52
3:N:1177:ALA:HB3	3:N:1183:ILE:HD11	1.91	0.52
1:B:50:GLY:O	1:B:146:ARG:HA	2.10	0.52
2:C:1101:THR:C	2:C:1102:LEU:HD12	2.30	0.52
2:C:198:ARG:HD3	9:C:9933:HOH:O	2.09	0.52
2:C:34:VAL:CG1	2:C:38:LYS:HG3	2.40	0.52
2:C:551:GLU:HB3	2:C:906:PHE:HD2	1.75	0.52
2:C:685:GLU:OE1	3:D:739:ASP:HA	2.10	0.52
2:C:721:ARG:HH21	2:C:783:ARG:NH2	2.07	0.52
3:D:1003:VAL:O	3:D:1006:ALA:HB3	2.10	0.52
3:D:1379:VAL:O	3:D:1420:LEU:HD23	2.10	0.52
3:D:213:VAL:HG11	9:D:9853:HOH:O	2.09	0.52
3:D:653:PHE:CE2	3:D:695:ILE:HG13	2.44	0.52
1:K:2:LEU:HD11	9:K:4002:HOH:O	2.09	0.52
2:M:1016:ILE:HD13	2:M:1016:ILE:N	2.24	0.52
2:M:142:ARG:NH1	2:M:325:ILE:HG12	2.25	0.52
2:M:137:VAL:HG22	2:M:391:LEU:O	2.10	0.52
2:M:413:LEU:HD12	2:M:413:LEU:N	2.25	0.52
2:M:752:GLY:O	3:N:679:ARG:HG2	2.10	0.52
2:M:840:ALA:HB2	2:M:846:LYS:HA	1.92	0.52
3:N:183:GLU:HA	3:N:186:VAL:CG1	2.40	0.52
3:N:75:ARG:HB2	9:N:9539:HOH:O	2.10	0.52
5:P:128:ARG:HD3	9:P:3878:HOH:O	2.08	0.52
1:A:9:PRO:HB3	1:A:25:LEU:HD21	1.92	0.52
1:B:19:GLU:HG3	1:B:201:THR:O	2.09	0.52
2:C:461:VAL:HG23	9:C:9546:HOH:O	2.10	0.52
2:C:773:LEU:HB2	5:F:373:LYS:CB	2.39	0.52
2:C:694:LEU:CD1	2:C:868:ASP:HB3	2.40	0.52
3:D:1166:LEU:HD12	3:D:1171:VAL:HG22	1.92	0.52
3:D:1280:VAL:O	3:D:1294:VAL:HA	2.10	0.52
3:D:149:LYS:HA	9:D:9512:HOH:O	2.09	0.52
3:D:30:GLU:HB3	3:D:40:GLU:CB	2.40	0.52
3:D:434:ARG:HB2	3:D:447:VAL:CG1	2.39	0.52
3:D:566:ILE:HD13	5:F:217:ASN:HB3	1.91	0.52
5:F:358:LEU:CD2	5:F:370:LYS:HE3	2.40	0.52
5:F:408:LEU:O	5:F:412:GLU:HG2	2.10	0.52
1:L:125:PRO:HD2	9:L:4231:HOH:O	2.10	0.52
2:M:332:ARG:NH2	2:M:464:LEU:HD11	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:334:ARG:CZ	2:M:418:LEU:HD21	2.40	0.52
2:M:18:LEU:HD23	2:M:404:LEU:HD21	1.92	0.52
2:M:724:ARG:HG3	2:M:741:GLY:N	2.24	0.52
3:N:135:LEU:HD11	3:N:452:ILE:HG13	1.91	0.52
3:N:1443:THR:HG23	9:N:2462:HOH:O	2.10	0.52
3:N:459:GLU:HG3	3:N:460:ALA:N	2.24	0.52
3:N:658:LEU:O	3:N:661:MET:HB2	2.09	0.52
2:M:1035:MET:HG2	3:N:707:THR:O	2.09	0.52
3:N:731:LEU:HB2	9:N:9614:HOH:O	2.10	0.52
5:P:337:HIS:H	5:P:337:HIS:CD2	2.28	0.52
2:C:742:VAL:HG12	2:C:743:VAL:N	2.25	0.51
3:D:134:VAL:HG12	3:D:152:LEU:HB3	1.93	0.51
3:D:97:THR:CG2	3:D:571:LYS:HD3	2.40	0.51
3:D:592:THR:N	3:D:600:LEU:HD21	2.24	0.51
5:F:128:ARG:O	5:F:132:ARG:HG3	2.10	0.51
5:F:171:LYS:HE3	5:F:175:HIS:NE2	2.25	0.51
5:F:323:ASP:O	5:F:325:LYS:N	2.43	0.51
1:L:170:VAL:HG23	9:L:5477:HOH:O	2.10	0.51
1:L:19:GLU:O	1:L:201:THR:HG23	2.09	0.51
2:M:998:TYR:OH	2:M:1000:MET:HA	2.10	0.51
3:N:1366:LYS:O	3:N:1369:GLU:HB2	2.10	0.51
3:N:206:ARG:O	3:N:206:ARG:HD3	2.10	0.51
3:N:789:LEU:O	3:N:792:ILE:HG23	2.09	0.51
5:P:129:GLU:HB3	5:P:142:ARG:HH21	1.75	0.51
1:A:18:ARG:HH11	1:A:123:MET:HE1	1.75	0.51
2:C:101:ILE:HG22	2:C:102:HIS:N	2.25	0.51
2:C:1057:SER:HB2	3:D:622:ARG:O	2.09	0.51
2:C:333:ILE:HD13	2:C:467:ILE:HG13	1.92	0.51
2:C:333:ILE:HD12	2:C:333:ILE:N	2.25	0.51
2:C:595:LEU:O	2:C:655:LEU:HG	2.10	0.51
2:C:710:ILE:HD11	2:C:758:ARG:NH2	2.26	0.51
3:D:1240:THR:HA	9:D:2338:HOH:O	2.09	0.51
3:D:1290:LEU:HD22	3:D:1291:SER:H	1.75	0.51
3:D:1417:TRP:HE1	3:D:1419:PRO:HG3	1.75	0.51
3:D:416:ALA:H	3:D:417:PRO:CD	2.23	0.51
3:D:478:LEU:HD21	3:D:500:ARG:HH21	1.75	0.51
3:D:480:GLU:O	3:D:484:PRO:HD2	2.10	0.51
3:D:491:LYS:HD3	3:D:492:ALA:N	2.26	0.51
3:D:505:SER:HB3	9:D:9680:HOH:O	2.09	0.51
3:D:553:ARG:HH12	5:F:211:ASP:HA	1.75	0.51
5:F:132:ARG:NH2	5:F:184:ARG:NH1	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:209:PHE:CE2	5:F:213:ILE:HD11	2.45	0.51
5:F:420:ASP:O	5:F:422:LEU:HD23	2.11	0.51
2:M:101:ILE:HG22	2:M:102:HIS:N	2.26	0.51
2:M:148:PHE:CZ	2:M:281:LEU:HD13	2.45	0.51
2:M:461:VAL:HG22	9:M:9987:HOH:O	2.10	0.51
3:N:123:LEU:HG	3:N:152:LEU:HD13	1.92	0.51
9:M:2035:HOH:O	3:N:1456:LYS:HE2	2.10	0.51
1:A:26:GLU:CB	1:A:194:LYS:HG3	2.41	0.51
2:C:65:VAL:HB	2:C:101:ILE:HB	1.92	0.51
2:C:1030:GLN:HE22	3:D:628:ARG:NH2	2.08	0.51
2:C:209:ARG:O	2:C:213:ALA:HB2	2.11	0.51
2:C:208:ALA:HB1	2:C:218:VAL:HG13	1.92	0.51
2:C:254:VAL:HG22	9:C:2339:HOH:O	2.10	0.51
2:C:436:GLY:HA3	2:C:469:THR:HG21	1.92	0.51
2:C:791:ARG:HB3	2:C:791:ARG:NH1	2.25	0.51
2:C:89:THR:O	2:C:91:GLN:HG3	2.09	0.51
3:D:701:LEU:HD21	3:D:763:MET:HE1	1.93	0.51
3:D:974:ILE:HG22	9:D:9555:HOH:O	2.11	0.51
2:M:1090:LYS:HG2	2:M:1112:PHE:CZ	2.44	0.51
2:M:176:VAL:C	2:M:178:PRO:HD3	2.31	0.51
2:M:182:VAL:HB	2:M:192:PRO:HA	1.92	0.51
2:M:197:LEU:HD22	2:M:202:TYR:CD2	2.45	0.51
2:M:498:GLN:HG3	2:M:516:ARG:HH21	1.75	0.51
2:M:739:GLU:HA	9:M:2220:HOH:O	2.09	0.51
2:M:679:PHE:HD1	2:M:870:ILE:HD13	1.74	0.51
2:M:890:LEU:HA	2:M:914:ILE:HD11	1.91	0.51
3:N:1066:THR:HG22	3:N:1069:GLU:HB2	1.90	0.51
3:N:1380:GLU:HG3	3:N:1381:VAL:H	1.75	0.51
3:N:196:VAL:HG13	3:N:202:VAL:CG1	2.40	0.51
3:N:404:GLU:OE1	3:N:414:ARG:HD3	2.10	0.51
3:N:423:ASP:HB2	5:P:178:ARG:CD	2.30	0.51
1:A:227:ASN:H	1:A:227:ASN:ND2	2.09	0.51
1:B:106:PRO:HB3	9:B:9545:HOH:O	2.10	0.51
1:B:182:GLU:O	1:B:194:LYS:HB3	2.11	0.51
2:C:101:ILE:HG23	2:C:107:LEU:CD2	2.38	0.51
3:D:1149:LEU:HD12	3:D:1161:GLU:O	2.11	0.51
3:D:1235:GLN:HB3	3:D:1359:GLN:HE22	1.75	0.51
3:D:603:LEU:O	3:D:606:ILE:HB	2.10	0.51
3:D:794:GLN:HG2	3:D:905:PRO:HB3	1.91	0.51
1:K:150:TYR:CE1	2:M:696:LYS:HA	2.44	0.51
1:L:91:ASN:O	1:L:94:LEU:HD12	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:137:VAL:HG23	2:M:391:LEU:HG	1.91	0.51
2:M:257:VAL:HG22	9:M:9998:HOH:O	2.10	0.51
2:M:26:TYR:CE2	2:M:30:LEU:HD11	2.46	0.51
2:M:722:ILE:CD1	2:M:823:VAL:HG21	2.39	0.51
5:P:142:ARG:HH11	5:P:142:ARG:CB	2.22	0.51
5:P:306:GLU:O	5:P:310:ILE:HG13	2.10	0.51
5:P:323:ASP:O	5:P:325:LYS:N	2.43	0.51
1:A:24:VAL:HG22	1:A:196:THR:HB	1.92	0.51
2:C:129:ILE:HD13	2:C:134:ARG:HB2	1.93	0.51
2:C:83:CYS:HA	2:C:88:LEU:HD23	1.92	0.51
3:D:1066:THR:HG23	3:D:1068:LEU:H	1.75	0.51
3:D:1057:VAL:HA	3:D:1069:GLU:OE2	2.10	0.51
3:D:1318:TYR:HD1	3:D:1319:VAL:N	2.09	0.51
3:D:44:LEU:O	3:D:525:ARG:NH2	2.43	0.51
3:D:540:LEU:HA	3:D:543:LEU:HD12	1.92	0.51
3:D:807:ALA:HA	9:D:9904:HOH:O	2.10	0.51
3:D:887:ALA:HA	9:D:9543:HOH:O	2.09	0.51
5:F:132:ARG:HG2	5:F:181:GLU:OE1	2.10	0.51
1:K:94:LEU:HD21	1:K:119:ASP:HB2	1.93	0.51
1:L:121:GLU:HG3	9:L:3921:HOH:O	2.10	0.51
1:L:184:THR:O	1:L:192:LEU:HB2	2.10	0.51
2:M:269:LEU:HD12	2:M:288:ARG:H	1.76	0.51
2:M:52:PHE:HE1	2:M:66:LEU:HG	1.75	0.51
3:N:1380:GLU:HG3	3:N:1381:VAL:N	2.25	0.51
3:N:493:ARG:HH22	3:N:1388:ARG:HB3	1.76	0.51
3:N:637:LEU:HD11	3:N:642:CYS:N	2.26	0.51
4:O:70:THR:HB	4:O:72:ARG:HE	1.75	0.51
5:P:93:LEU:HG	5:P:190:ALA:CB	2.40	0.51
5:P:323:ASP:C	5:P:325:LYS:H	2.14	0.51
5:P:416:ARG:HD2	5:P:419:ARG:HB3	1.91	0.51
1:B:18:ARG:O	1:B:207:PRO:HD3	2.11	0.51
1:A:219:ARG:CZ	1:B:219:ARG:HG2	2.41	0.51
1:B:23:PHE:HE2	1:B:199:ILE:HD12	1.76	0.51
2:C:1014:SER:HA	9:F:9484:HOH:O	2.11	0.51
2:C:1014:SER:OG	5:F:331:ASP:HA	2.11	0.51
2:C:132:ALA:HB1	2:C:632:ASN:ND2	2.23	0.51
2:C:208:ALA:HA	2:C:218:VAL:HG22	1.93	0.51
2:C:565:GLN:OE1	2:C:842:ARG:HG2	2.11	0.51
2:C:886:LEU:HD23	3:D:951:ILE:HG13	1.91	0.51
2:C:958:THR:HG23	2:C:961:GLU:H	1.74	0.51
3:D:1109:GLU:HG2	3:D:1201:CYS:CA	2.37	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1209:LEU:HD21	4:E:16:LYS:HZ2	1.73	0.51
3:D:704:ARG:HB2	3:D:736:PHE:CD2	2.46	0.51
3:D:890:VAL:HG11	3:D:922:LEU:HD13	1.93	0.51
2:M:1086:ARG:HB3	2:M:1112:PHE:CE2	2.45	0.51
2:M:166:PRO:HG3	2:M:265:ARG:HE	1.74	0.51
2:M:879:ARG:HH12	3:N:1029:ARG:HH22	1.58	0.51
3:N:1112:CYS:HB2	3:N:1195:GLN:CD	2.30	0.51
3:N:119:SER:HB2	3:N:123:LEU:CB	2.40	0.51
3:N:52:PRO:HG3	3:N:78:VAL:HG13	1.92	0.51
3:N:937:TYR:O	3:N:941:PHE:HD1	1.93	0.51
1:A:146:ARG:HD2	9:A:9500:HOH:O	2.10	0.51
2:C:332:ARG:HE	2:C:464:LEU:HD11	1.75	0.51
2:C:437:ARG:HA	2:C:467:ILE:HG21	1.91	0.51
2:C:495:THR:HB	2:C:530:GLU:HG3	1.93	0.51
2:C:663:ASN:HB2	9:C:2433:HOH:O	2.11	0.51
3:D:1104:GLU:O	3:D:1106:VAL:HG23	2.10	0.51
3:D:1333:HIS:O	3:D:1336:LEU:HB3	2.10	0.51
3:D:154:THR:HA	9:D:9863:HOH:O	2.10	0.51
3:D:36:THR:O	3:D:38:LYS:N	2.44	0.51
3:D:519:VAL:HG13	3:D:544:TYR:CE1	2.46	0.51
3:D:864:VAL:HG12	3:D:865:THR:H	1.75	0.51
3:D:970:LYS:HB2	3:D:970:LYS:NZ	2.25	0.51
4:E:64:ALA:HA	4:E:67:GLU:CD	2.31	0.51
1:K:95:GLN:HG2	1:K:146:ARG:HH12	1.74	0.51
1:K:9:PRO:HB2	1:L:224:TYR:HB3	1.93	0.51
2:M:122:THR:HG21	9:M:2321:HOH:O	2.11	0.51
2:M:182:VAL:HG13	9:M:9636:HOH:O	2.08	0.51
2:M:232:GLU:O	2:M:235:LEU:HB2	2.10	0.51
1:K:133:GLU:OE1	2:M:605:LYS:HB3	2.11	0.51
2:M:759:THR:HB	2:M:785:VAL:CG2	2.41	0.51
2:M:877:PRO:HB3	3:N:1020:LEU:HD13	1.93	0.51
3:N:1492:LEU:O	3:N:1496:GLU:HG2	2.11	0.51
3:N:191:LEU:HB3	3:N:195:VAL:HG21	1.93	0.51
3:N:421:LEU:HD12	3:N:435:VAL:CG1	2.41	0.51
3:N:539:ASP:HB3	9:N:9742:HOH:O	2.11	0.51
3:N:565:ILE:CD1	5:P:189:GLU:HG2	2.41	0.51
9:M:9978:HOH:O	5:P:345:ALA:HB1	2.09	0.51
1:A:11:PHE:HD1	1:A:25:LEU:HD12	1.76	0.51
2:C:238:LEU:HB2	9:C:2083:HOH:O	2.11	0.51
2:C:549:PHE:CE2	2:C:886:LEU:HB3	2.46	0.51
2:C:876:VAL:HB	2:C:877:PRO:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:901:TYR:CE2	2:C:917:LEU:HD13	2.46	0.51
3:D:797:LYS:NZ	3:D:1016:PRO:HB3	2.26	0.51
3:D:908:LYS:HG2	3:D:1027:GLY:HA3	1.91	0.51
3:D:1292:VAL:H	3:D:1305:LEU:HD21	1.76	0.51
3:D:530:VAL:HB	3:D:534:ARG:CB	2.38	0.51
3:D:829:VAL:HG21	9:D:9486:HOH:O	2.10	0.51
3:D:959:GLU:CD	3:D:959:GLU:H	2.12	0.51
2:M:676:ILE:HG23	9:M:9722:HOH:O	2.10	0.51
2:M:783:ARG:HG2	2:M:785:VAL:HG12	1.92	0.51
2:M:392:SER:O	7:M:8002:RPT:H371	2.11	0.51
2:M:958:THR:HG23	9:M:9678:HOH:O	2.10	0.51
2:M:976:ASP:OD1	2:M:978:ARG:HG3	2.11	0.51
3:N:1020:LEU:HA	3:N:1023:MET:CE	2.41	0.51
3:N:546:ARG:CZ	3:N:550:ARG:HH22	2.22	0.51
3:N:823:LEU:H	3:N:823:LEU:HD23	1.76	0.51
1:A:70:GLY:HA2	1:A:133:GLU:OE2	2.09	0.51
2:C:1027:PHE:HA	9:C:9777:HOH:O	2.10	0.51
2:C:292:ARG:HG2	9:C:2101:HOH:O	2.11	0.51
2:C:328:LEU:HD23	2:C:437:ARG:HD3	1.93	0.51
3:D:1333:HIS:CE1	3:D:1421:LEU:HD23	2.45	0.51
3:D:704:ARG:HH11	3:D:738:ALA:HA	1.75	0.51
3:D:770:LEU:HG	3:D:919:PHE:HE1	1.75	0.51
4:E:91:ARG:HD2	9:E:9516:HOH:O	2.11	0.51
5:F:152:ASP:HB2	5:F:153:PRO:HD3	1.92	0.51
5:F:260:ILE:HG23	5:F:264:MET:CG	2.40	0.51
5:F:365:GLU:OE1	5:F:400:ILE:HD12	2.11	0.51
1:K:117:VAL:HG22	9:K:3709:HOH:O	2.10	0.51
2:M:744:ARG:HG3	2:M:747:ALA:HB2	1.93	0.51
2:M:777:ILE:HG22	2:M:778:PHE:CD1	2.45	0.51
3:N:180:LYS:O	3:N:184:GLU:HG3	2.11	0.51
3:N:183:GLU:O	3:N:186:VAL:HG12	2.11	0.51
3:N:423:ASP:HB3	5:P:175:HIS:HA	1.93	0.51
1:B:184:THR:HG23	1:B:192:LEU:HB3	1.93	0.51
2:C:1083:GLU:HG2	9:C:9596:HOH:O	2.11	0.51
2:C:1097:LEU:HD22	2:C:1097:LEU:H	1.76	0.51
2:C:28:ARG:HG3	2:C:40:GLU:OE1	2.10	0.51
2:C:520:GLU:HB2	9:C:2128:HOH:O	2.11	0.51
2:C:760:SER:O	2:C:785:VAL:HG22	2.10	0.51
3:D:1410:GLU:HG2	9:D:2012:HOH:O	2.10	0.51
3:D:49:ILE:HB	3:D:50:PHE:CD1	2.45	0.51
3:D:750:PRO:HB2	3:D:756:GLN:OE1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:805:GLU:OE1	3:D:809:PRO:HD2	2.11	0.51
5:F:352:GLU:HG3	9:F:9610:HOH:O	2.11	0.51
1:L:109:VAL:HG21	1:L:138:LEU:HD21	1.92	0.51
1:L:215:VAL:HG21	9:L:5732:HOH:O	2.10	0.51
2:M:132:ALA:HB1	2:M:632:ASN:ND2	2.26	0.51
2:M:145:GLY:C	2:M:163:ILE:HG23	2.31	0.51
2:M:257:VAL:HA	9:M:2289:HOH:O	2.11	0.51
2:M:405:ARG:NH2	2:M:566:THR:HG21	2.26	0.51
2:M:774:LEU:HA	2:M:777:ILE:HD12	1.93	0.51
3:N:105:VAL:HG21	3:N:128:TYR:CE2	2.35	0.51
1:B:75:VAL:O	1:B:79:ILE:HG23	2.11	0.50
2:C:1081:VAL:HG12	2:C:1086:ARG:HE	1.76	0.50
2:C:54:ILE:HG22	2:C:66:LEU:HB3	1.93	0.50
3:D:1150:ALA:HA	9:D:2006:HOH:O	2.10	0.50
3:D:1478:SER:O	3:D:1482:ARG:HG3	2.10	0.50
2:C:1052:MET:HG3	3:D:623:VAL:CG2	2.41	0.50
3:D:566:ILE:HG23	5:F:217:ASN:HD22	1.77	0.50
2:M:420:ARG:CD	2:M:420:ARG:H	2.22	0.50
2:M:872:ASN:ND2	2:M:874:LEU:HB2	2.26	0.50
3:N:209:ARG:HG3	9:N:2381:HOH:O	2.09	0.50
5:P:101:GLU:HA	5:P:104:ARG:NH1	2.26	0.50
5:P:366:ALA:HB3	5:P:367:MET:HE2	1.94	0.50
5:P:416:ARG:HB3	5:P:419:ARG:HG2	1.93	0.50
5:P:419:ARG:O	5:P:421:PHE:N	2.44	0.50
1:A:211:LEU:O	1:A:215:VAL:HG13	2.11	0.50
2:C:162:ILE:HB	2:C:172:ILE:HD13	1.93	0.50
2:C:21:ILE:HD12	2:C:21:ILE:H	1.76	0.50
2:C:263:ASP:HB2	2:C:264:PRO:HD3	1.92	0.50
2:C:338:GLU:O	2:C:341:THR:HG22	2.11	0.50
2:C:523:ILE:HG21	9:D:2662:HOH:O	2.12	0.50
2:C:572:ILE:HG21	2:C:703:ILE:HD13	1.93	0.50
2:C:971:LYS:HD2	2:C:986:PRO:HB2	1.92	0.50
3:D:1063:GLU:HG2	3:D:1064:GLY:H	1.76	0.50
3:D:1136:LYS:HB2	3:D:1139:ASP:OD2	2.11	0.50
3:D:161:LEU:HD13	3:D:452:ILE:HD12	1.94	0.50
3:D:965:GLU:HG3	3:D:969:ARG:NH2	2.23	0.50
5:F:362:SER:HB2	9:F:9725:HOH:O	2.10	0.50
1:K:68:ILE:HA	9:K:4093:HOH:O	2.11	0.50
2:M:265:ARG:HB3	2:M:267:TYR:CE2	2.46	0.50
2:M:682:TYR:N	9:M:9536:HOH:O	2.44	0.50
2:M:841:ASN:HB2	9:M:9839:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1281:VAL:HG21	3:N:1313:VAL:CG2	2.40	0.50
3:N:12:LEU:HB2	9:N:9590:HOH:O	2.11	0.50
3:N:603:LEU:O	3:N:606:ILE:HB	2.11	0.50
3:N:737:ASN:HA	9:N:9612:HOH:O	2.10	0.50
1:A:156:HIS:NE2	1:A:166:PRO:HB3	2.26	0.50
1:B:72:LYS:HE2	1:B:131:THR:OG1	2.11	0.50
2:C:625:LEU:O	2:C:627:ARG:N	2.45	0.50
2:C:80:GLN:HG2	2:C:90:TYR:CE2	2.47	0.50
3:D:1324:PRO:HG3	3:D:1330:ILE:HD11	1.92	0.50
3:D:132:TYR:HD2	9:D:9863:HOH:O	1.93	0.50
3:D:656:PHE:HB3	3:D:694:VAL:HG11	1.93	0.50
5:F:126:LEU:O	5:F:130:VAL:HG23	2.11	0.50
5:F:258:ILE:HB	9:F:9558:HOH:O	2.12	0.50
1:K:97:VAL:HG23	9:K:3291:HOH:O	2.11	0.50
2:M:1051:GLU:HG3	2:M:1055:LEU:HB2	1.92	0.50
2:M:132:ALA:HB1	2:M:632:ASN:HD21	1.77	0.50
2:M:333:ILE:HD12	2:M:465:GLY:O	2.11	0.50
2:M:666:LEU:HD12	2:M:667:ALA:H	1.76	0.50
2:M:676:ILE:HG23	2:M:676:ILE:O	2.10	0.50
2:M:721:ARG:HH22	2:M:785:VAL:HG21	1.76	0.50
2:M:996:LYS:HD2	9:M:9662:HOH:O	2.11	0.50
3:N:1156:LEU:CD1	3:N:1176:LYS:HD2	2.41	0.50
3:N:1493:LYS:HD3	3:N:1496:GLU:OE2	2.12	0.50
3:N:14:SER:OG	3:N:17:LYS:HB2	2.11	0.50
3:N:39:PRO:HD2	9:N:2247:HOH:O	2.11	0.50
3:N:434:ARG:HB2	3:N:447:VAL:CG1	2.41	0.50
3:N:574:LEU:O	3:N:577:ALA:HB3	2.11	0.50
3:N:101:HIS:CD2	3:N:582:LEU:HD13	2.45	0.50
3:N:814:ALA:HB3	9:N:2003:HOH:O	2.11	0.50
4:O:51:LEU:HG	4:O:53:GLY:N	2.26	0.50
1:A:14:ARG:NH1	1:A:24:VAL:HG23	2.26	0.50
1:A:183:ASP:HB3	9:A:9649:HOH:O	2.10	0.50
1:B:189:ARG:HH11	1:B:189:ARG:HG3	1.75	0.50
1:B:13:VAL:HG13	1:B:23:PHE:CD1	2.46	0.50
2:C:425:PHE:HB2	9:C:9673:HOH:O	2.11	0.50
3:D:1262:LEU:HD23	3:D:1352:ILE:CG1	2.40	0.50
3:D:519:VAL:HA	3:D:544:TYR:OH	2.12	0.50
3:D:762:GLN:NE2	4:E:20:THR:HG21	2.26	0.50
4:E:64:ALA:O	4:E:67:GLU:HG3	2.12	0.50
5:F:112:ALA:HA	5:F:173:TYR:CD2	2.46	0.50
1:K:19:GLU:HB3	9:K:4176:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:462:ASP:HA	9:M:2351:HOH:O	2.12	0.50
3:N:108:VAL:CG2	3:N:109:PRO:HD3	2.40	0.50
3:N:119:SER:N	3:N:123:LEU:HD22	2.22	0.50
2:C:1091:GLU:HG2	3:D:606:ILE:HG21	1.94	0.50
2:C:230:ARG:HG3	9:C:9560:HOH:O	2.11	0.50
2:C:436:GLY:O	2:C:459:ALA:HB2	2.12	0.50
3:D:493:ARG:NH1	3:D:1390:LEU:H	2.08	0.50
3:D:826:PRO:HB3	3:D:828:LYS:NZ	2.27	0.50
5:F:111:GLU:O	5:F:115:LYS:HG2	2.11	0.50
1:L:180:GLN:HG3	9:L:3887:HOH:O	2.10	0.50
2:M:304:LEU:HD23	2:M:305:PRO:HD3	1.92	0.50
2:M:964:LYS:HB3	9:M:9902:HOH:O	2.11	0.50
3:N:963:TYR:CD2	3:N:1002:LYS:HB3	2.46	0.50
3:N:1136:LYS:H	3:N:1136:LYS:HE3	1.76	0.50
3:N:131:LYS:HB3	9:N:2083:HOH:O	2.11	0.50
5:P:366:ALA:HB3	5:P:367:MET:CE	2.42	0.50
1:B:38:ASN:HB2	9:B:9725:HOH:O	2.10	0.50
2:C:302:VAL:O	2:C:305:PRO:HD2	2.12	0.50
2:C:462:ASP:HA	9:C:9665:HOH:O	2.11	0.50
3:D:1192:LEU:CD2	3:D:1345:GLU:HG2	2.39	0.50
3:D:500:ARG:HH22	3:D:1388:ARG:HH11	1.60	0.50
3:D:699:VAL:HG12	3:D:717:GLN:CA	2.40	0.50
2:C:886:LEU:HG	3:D:951:ILE:HG13	1.93	0.50
5:F:109:GLY:O	5:F:113:ILE:HG13	2.12	0.50
2:M:160:ALA:O	2:M:173:ASP:HA	2.12	0.50
2:M:197:LEU:HD22	2:M:202:TYR:HD2	1.75	0.50
2:M:260:LEU:HA	2:M:291:ALA:CB	2.42	0.50
2:M:768:THR:CB	2:M:771:GLU:HB3	2.41	0.50
2:M:841:ASN:HD21	2:M:845:ASN:H	1.59	0.50
2:M:984:GLU:HA	9:M:2224:HOH:O	2.10	0.50
3:N:960:LYS:HB3	9:N:9922:HOH:O	2.12	0.50
4:O:32:ARG:HB3	9:O:5813:HOH:O	2.11	0.50
3:N:420:VAL:O	5:P:164:LYS:HD3	2.12	0.50
5:P:261:PRO:O	5:P:265:VAL:HG23	2.11	0.50
1:A:16:GLN:NE2	1:A:17:GLY:N	2.60	0.50
1:A:197:LEU:HD23	1:A:197:LEU:N	2.26	0.50
2:C:1008:ARG:HE	2:C:1028:GLY:CA	2.24	0.50
2:C:161:SER:HB3	9:C:2166:HOH:O	2.11	0.50
2:C:413:LEU:HD12	2:C:413:LEU:N	2.27	0.50
2:C:432:ARG:HD3	3:D:1048:PRO:CG	2.42	0.50
2:C:508:ILE:HG21	9:C:9927:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:408:ARG:NH1	2:C:542:VAL:HG23	2.27	0.50
2:C:561:GLY:HA3	2:C:842:ARG:O	2.11	0.50
2:C:724:ARG:CG	2:C:740:GLU:HA	2.42	0.50
3:D:1336:LEU:HD21	3:D:1419:PRO:O	2.12	0.50
3:D:1103:HIS:CD2	3:D:1463:LYS:H	2.30	0.50
3:D:18:ILE:HD12	3:D:518:PRO:CG	2.42	0.50
3:D:677:LEU:HD21	3:D:687:VAL:HG21	1.94	0.50
3:D:872:ARG:HB3	9:D:9540:HOH:O	2.11	0.50
5:F:220:LEU:HD21	9:F:9537:HOH:O	2.12	0.50
5:F:237:THR:HB	9:F:9628:HOH:O	2.11	0.50
1:K:123:MET:C	1:K:125:PRO:HD3	2.32	0.50
1:K:184:THR:O	1:K:192:LEU:HD12	2.12	0.50
2:M:143:SER:HB2	2:M:332:ARG:HB2	1.93	0.50
2:M:580:MET:HB3	2:M:584:GLU:CD	2.30	0.50
2:M:637:LEU:HA	2:M:659:PRO:HG3	1.94	0.50
2:M:721:ARG:O	2:M:758:ARG:HA	2.11	0.50
2:M:821:GLU:HA	9:M:9975:HOH:O	2.12	0.50
2:M:872:ASN:HD21	2:M:874:LEU:HB2	1.76	0.50
2:M:939:ARG:HB3	2:M:982:PRO:HG3	1.94	0.50
3:N:957:PRO:CG	3:N:1007:VAL:HA	2.42	0.50
3:N:546:ARG:NH1	3:N:550:ARG:HH22	2.09	0.50
3:N:559:ALA:O	5:P:132:ARG:NH2	2.44	0.50
5:P:358:LEU:HD21	5:P:370:LYS:HE3	1.94	0.50
1:A:101:LEU:HD11	1:A:113:ASP:HB2	1.94	0.50
1:B:42:ARG:HH11	1:B:42:ARG:HG2	1.76	0.50
2:C:137:VAL:HG21	2:C:393:GLN:HE21	1.76	0.50
2:C:404:LEU:HD13	9:C:9579:HOH:O	2.12	0.50
2:C:630:ARG:HH22	2:C:707:ARG:HB2	1.76	0.50
7:C:8001:RPT:H422	9:C:9511:HOH:O	2.11	0.50
3:D:1047:LYS:HB3	3:D:1048:PRO:CD	2.42	0.50
3:D:1047:LYS:HG2	3:D:1053:PHE:CE2	2.46	0.50
3:D:1283:ILE:N	3:D:1315:ASP:OD1	2.43	0.50
3:D:1440:PHE:HD1	3:D:1441:GLN:H	1.59	0.50
3:D:183:GLU:HA	3:D:186:VAL:CG1	2.42	0.50
3:D:211:VAL:HG13	3:D:393:ILE:HA	1.93	0.50
3:D:465:LEU:HD22	3:D:509:PRO:O	2.12	0.50
3:D:32:ILE:HD12	3:D:527:MET:HG2	1.94	0.50
5:F:323:ASP:C	5:F:325:LYS:H	2.15	0.50
1:K:133:GLU:CD	2:M:605:LYS:HB3	2.33	0.50
2:M:413:LEU:H	2:M:413:LEU:HD12	1.77	0.50
2:M:693:GLU:HA	2:M:696:LYS:HG3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:808:ARG:HG2	2:M:808:ARG:HH11	1.75	0.50
3:N:959:GLU:HG3	3:N:1006:ALA:HB1	1.94	0.50
3:N:1045:MET:HA	9:N:2418:HOH:O	2.12	0.50
3:N:1169:ASP:HB2	9:N:2387:HOH:O	2.12	0.50
3:N:1462:LEU:HD22	3:N:1472:ILE:CG2	2.42	0.50
3:N:28:LYS:CB	3:N:41:ARG:HD2	2.42	0.50
3:N:12:LEU:HD11	3:N:512:MET:HG2	1.93	0.50
2:M:1019:GLN:HE22	3:N:621:LYS:HA	1.76	0.50
5:P:225:GLU:HG3	5:P:226:LYS:HG2	1.94	0.50
5:P:419:ARG:HH11	5:P:419:ARG:HB2	1.77	0.50
2:C:25:SER:CB	2:C:335:THR:HB	2.42	0.50
2:C:952:LEU:HB3	2:C:966:LEU:CD1	2.42	0.50
3:D:1108:ARG:HH12	3:D:1460:ILE:HG22	1.77	0.50
3:D:1120:VAL:HB	3:D:1144:LEU:HD21	1.94	0.50
3:D:521:PRO:O	3:D:525:ARG:HG2	2.12	0.50
3:D:607:LEU:HB3	3:D:614:PHE:CE2	2.47	0.50
3:D:637:LEU:HD12	3:D:641:GLN:OE1	2.12	0.50
3:D:58:CYS:HA	3:D:78:VAL:HG11	1.93	0.50
3:D:796:ARG:NH1	3:D:861:GLN:HB2	2.25	0.50
4:E:9:LEU:HD22	4:E:19:LEU:HD13	1.94	0.50
3:D:561:GLY:HA3	5:F:184:ARG:NH2	2.25	0.50
2:M:289:THR:HG22	2:M:290:LEU:H	1.76	0.50
2:M:352:ALA:HA	2:M:355:VAL:HG12	1.92	0.50
2:M:367:LEU:O	2:M:372:LEU:HD13	2.12	0.50
2:M:479:VAL:CG2	2:M:503:LEU:HD11	2.41	0.50
2:M:57:GLU:HG3	2:M:58:ASP:OD2	2.12	0.50
2:M:594:ALA:HB1	2:M:654:LEU:HD12	1.92	0.50
2:M:605:LYS:HD3	2:M:610:ARG:NH2	2.26	0.50
3:N:1047:LYS:HA	3:N:1053:PHE:CE1	2.47	0.50
3:N:1077:ALA:HA	9:N:9982:HOH:O	2.11	0.50
3:N:126:VAL:O	3:N:132:TYR:HD1	1.94	0.50
3:N:10:ILE:HD11	3:N:1434:TRP:NE1	2.26	0.50
3:N:493:ARG:O	3:N:497:GLU:HG3	2.11	0.50
3:N:573:MET:SD	5:P:210:LEU:HD22	2.51	0.50
3:N:818:ARG:HG3	9:N:2703:HOH:O	2.11	0.50
3:N:879:ARG:HH21	3:N:903:ASP:C	2.14	0.50
3:N:966:GLU:HG2	9:N:9886:HOH:O	2.11	0.50
4:O:84:ARG:NH1	9:O:4797:HOH:O	2.44	0.50
2:M:1016:ILE:CD1	5:P:317:LEU:HD21	2.42	0.50
1:A:209:GLU:O	1:A:213:GLN:HG3	2.11	0.49
1:B:204:SER:HB2	9:B:9508:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:LEU:O	1:B:215:VAL:HG13	2.12	0.49
2:C:1012:PRO:HD2	2:C:1021:LEU:O	2.12	0.49
2:C:1015:LEU:HA	9:C:9604:HOH:O	2.12	0.49
2:C:339:LEU:HD22	2:C:391:LEU:HD13	1.94	0.49
2:C:505:GLY:HA3	9:C:9890:HOH:O	2.11	0.49
2:C:52:PHE:CD2	2:C:68:PHE:HB2	2.47	0.49
2:C:557:ARG:NH1	2:C:879:ARG:HD3	2.26	0.49
2:C:976:ASP:HB2	2:C:979:THR:HG22	1.93	0.49
3:D:1009:LYS:HA	3:D:1012:GLU:OE2	2.12	0.49
3:D:1209:LEU:HD22	3:D:1211:MET:HE1	1.94	0.49
3:D:818:ARG:HB3	9:D:9509:HOH:O	2.12	0.49
5:F:142:ARG:HB3	5:F:142:ARG:HH11	1.76	0.49
1:K:184:THR:HG23	1:K:192:LEU:HB3	1.94	0.49
1:L:29:GLU:N	9:L:5175:HOH:O	2.45	0.49
2:M:170:PRO:HG2	2:M:258:TYR:CD2	2.47	0.49
2:M:176:VAL:HG12	2:M:182:VAL:CG1	2.42	0.49
2:M:345:ARG:HH11	2:M:345:ARG:HB3	1.77	0.49
2:M:687:ALA:C	2:M:688:ILE:HD12	2.33	0.49
2:M:68:PHE:HB3	9:M:9640:HOH:O	2.11	0.49
2:M:781:LYS:HG2	9:M:2296:HOH:O	2.11	0.49
2:M:807:ARG:HB2	2:M:807:ARG:CZ	2.40	0.49
3:N:1172:HIS:HE1	9:N:2297:HOH:O	1.95	0.49
3:N:1278:ASP:HA	3:N:1319:VAL:O	2.12	0.49
3:N:191:LEU:HD12	3:N:211:VAL:HG21	1.92	0.49
3:N:550:ARG:HG3	3:N:550:ARG:NH1	2.26	0.49
3:N:619:LEU:HD13	9:N:9535:HOH:O	2.10	0.49
2:C:1090:LYS:HG2	2:C:1112:PHE:CZ	2.47	0.49
2:C:54:ILE:CD1	2:C:356:ARG:HG2	2.35	0.49
2:C:367:LEU:O	2:C:371:LYS:HB3	2.12	0.49
2:C:441:VAL:HG12	2:C:559:LEU:HA	1.93	0.49
2:C:498:GLN:HG3	9:C:9731:HOH:O	2.12	0.49
2:C:569:VAL:HG12	2:C:996:LYS:O	2.12	0.49
2:C:580:MET:HB3	2:C:584:GLU:CD	2.31	0.49
2:C:745:ILE:HD11	9:C:9745:HOH:O	2.12	0.49
2:C:690:ILE:CG2	2:C:852:ILE:HG23	2.39	0.49
2:C:978:ARG:HD3	9:C:9846:HOH:O	2.11	0.49
3:D:1072:ILE:O	3:D:1075:HIS:HD2	1.96	0.49
3:D:608:SER:HB3	3:D:1443:THR:OG1	2.12	0.49
3:D:841:TYR:HB3	3:D:843:PHE:CE2	2.47	0.49
3:D:880:ILE:O	3:D:883:ALA:HB3	2.12	0.49
5:F:323:ASP:HB3	5:F:325:LYS:HE3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:411:HIS:HB2	9:F:9615:HOH:O	2.11	0.49
5:F:79:ASP:HB3	5:F:80:PRO:CD	2.41	0.49
1:K:69:PRO:O	1:K:71:VAL:HG23	2.11	0.49
2:M:1040:LEU:HG	2:M:1045:ALA:CB	2.42	0.49
2:M:114:PHE:H	2:M:114:PHE:HD1	1.60	0.49
2:M:166:PRO:HD3	2:M:265:ARG:CB	2.42	0.49
2:M:376:ARG:HB3	2:M:377:PRO:HD3	1.95	0.49
2:M:671:ASN:HD21	2:M:993:PHE:HD2	1.60	0.49
2:M:820:ARG:HG2	2:M:820:ARG:HH11	1.76	0.49
3:N:1068:LEU:C	3:N:1070:TYR:N	2.65	0.49
3:N:602:SER:O	3:N:606:ILE:HG12	2.12	0.49
3:N:644:LEU:HB3	9:N:9610:HOH:O	2.11	0.49
3:N:924:MET:O	3:N:927:THR:HB	2.12	0.49
1:A:64:GLU:OE2	1:A:76:VAL:HG13	2.11	0.49
1:B:206:THR:HG22	1:B:209:GLU:H	1.77	0.49
2:C:1054:THR:HG22	2:C:1059:ASP:CB	2.41	0.49
2:C:197:LEU:HD22	2:C:202:TYR:HD2	1.77	0.49
2:C:768:THR:CB	2:C:771:GLU:HB3	2.42	0.49
2:C:983:ILE:HG22	2:C:987:ILE:HD11	1.94	0.49
2:C:669:GLY:HA3	2:C:995:MET:HA	1.93	0.49
3:D:1225:ALA:HA	3:D:1367:HIS:ND1	2.28	0.49
3:D:154:THR:HG23	3:D:157:GLU:H	1.77	0.49
3:D:175:VAL:HG12	3:D:176:ASP:OD1	2.11	0.49
3:D:474:GLU:HG3	3:D:500:ARG:HE	1.77	0.49
5:F:394:ARG:HG2	9:F:9632:HOH:O	2.12	0.49
5:F:82:ARG:HA	9:F:9663:HOH:O	2.12	0.49
1:K:9:PRO:HB3	1:K:25:LEU:HG	1.94	0.49
2:M:95:TYR:CD1	2:M:95:TYR:N	2.81	0.49
3:N:1011:PHE:CD2	3:N:1021:TYR:HB2	2.47	0.49
3:N:1106:VAL:HG21	3:N:1474:ALA:HB2	1.93	0.49
3:N:399:ARG:HB2	3:N:444:VAL:HG13	1.94	0.49
3:N:93:ILE:CD1	3:N:548:ILE:HD11	2.42	0.49
3:N:795:VAL:CG1	3:N:863:VAL:HG13	2.42	0.49
4:O:47:LYS:N	4:O:54:LEU:HD22	2.27	0.49
5:P:132:ARG:O	5:P:136:LEU:HG	2.12	0.49
1:B:26:GLU:HG2	1:B:27:PRO:CA	2.42	0.49
2:C:1013:TYR:HE1	2:C:1020:PRO:HG3	1.76	0.49
2:C:207:LEU:HD22	2:C:221:LEU:HD22	1.94	0.49
2:C:328:LEU:CD2	2:C:437:ARG:HD3	2.43	0.49
2:C:51:THR:HB	2:C:348:LEU:HD23	1.94	0.49
2:C:584:GLU:HG2	9:C:9657:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1061:PHE:HE1	3:D:1065:LEU:HD23	1.78	0.49
2:C:516:ARG:NE	3:D:1068:LEU:HD13	2.27	0.49
3:D:116:LEU:CD2	3:D:468:LEU:HD11	2.42	0.49
3:D:1192:LEU:HD13	3:D:1345:GLU:HG2	1.94	0.49
3:D:1192:LEU:HD21	3:D:1372:VAL:CG1	2.42	0.49
3:D:1403:LEU:HD11	9:D:9892:HOH:O	2.11	0.49
3:D:462:GLN:HG2	9:D:9936:HOH:O	2.12	0.49
3:D:678:GLU:HG3	3:D:679:ARG:HG3	1.94	0.49
3:D:901:GLN:HG2	9:D:9763:HOH:O	2.12	0.49
5:F:272:SER:HB2	9:F:9540:HOH:O	2.11	0.49
2:M:121:MET:HB3	9:M:9714:HOH:O	2.12	0.49
2:M:209:ARG:O	2:M:213:ALA:HB2	2.12	0.49
2:M:54:ILE:HG23	2:M:54:ILE:O	2.13	0.49
2:M:571:LEU:HA	2:M:701:THR:O	2.13	0.49
2:M:627:ARG:O	2:M:638:ASP:HB3	2.13	0.49
2:M:640:ARG:HD3	2:M:642:ARG:HH22	1.76	0.49
2:M:56:GLU:HB2	2:M:64:LEU:HB3	1.94	0.49
3:N:1124:GLN:CG	3:N:1133:ARG:HD2	2.42	0.49
3:N:1333:HIS:O	3:N:1336:LEU:HB3	2.12	0.49
3:N:421:LEU:HD11	3:N:437:VAL:CG2	2.42	0.49
3:N:576:GLU:HA	3:N:579:ASP:OD2	2.12	0.49
2:M:752:GLY:HA3	3:N:679:ARG:HA	1.93	0.49
3:N:561:GLY:HA2	5:P:132:ARG:CZ	2.43	0.49
5:P:297:PRO:HB2	9:P:4687:HOH:O	2.13	0.49
5:P:328:PHE:O	5:P:331:ASP:N	2.35	0.49
5:P:403:LYS:HA	5:P:403:LYS:HZ3	1.76	0.49
2:C:146:VAL:HG13	2:C:161:SER:O	2.12	0.49
2:C:184:MET:HB2	2:C:193:LEU:HD12	1.95	0.49
2:C:260:LEU:HA	2:C:291:ALA:CB	2.42	0.49
2:C:301:GLU:O	2:C:305:PRO:HG2	2.13	0.49
3:D:212:ARG:HA	9:D:9662:HOH:O	2.11	0.49
3:D:434:ARG:HB2	3:D:447:VAL:HG22	1.94	0.49
3:D:860:LEU:HD23	3:D:877:PRO:CB	2.43	0.49
3:D:947:ILE:O	3:D:947:ILE:HD12	2.12	0.49
5:F:217:ASN:O	5:F:221:ILE:HG13	2.12	0.49
5:F:252:ALA:HB1	5:F:265:VAL:HG21	1.93	0.49
5:F:419:ARG:O	5:F:421:PHE:N	2.46	0.49
2:M:1079:PRO:HD3	9:M:2202:HOH:O	2.11	0.49
2:M:64:LEU:HD22	2:M:359:MET:HG3	1.95	0.49
2:M:388:ARG:HG3	9:M:9960:HOH:O	2.12	0.49
2:M:34:VAL:CB	2:M:38:LYS:HG3	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:643:VAL:HG22	2:M:647:GLN:NE2	2.26	0.49
2:M:762:LYS:HD3	2:M:771:GLU:OE1	2.12	0.49
2:M:98:LEU:HG	9:M:9996:HOH:O	2.12	0.49
3:N:1216:SER:OG	4:O:15:SER:HA	2.12	0.49
3:N:131:LYS:CG	3:N:568:ARG:HG2	2.42	0.49
2:M:1005:MET:HB2	3:N:648:MET:HE3	1.93	0.49
3:N:976:GLN:HA	3:N:979:GLU:OE1	2.12	0.49
1:A:190:THR:HG22	9:A:9695:HOH:O	2.12	0.49
1:A:42:ARG:HB3	9:B:9613:HOH:O	2.11	0.49
1:B:192:LEU:HB3	9:B:9480:HOH:O	2.12	0.49
1:B:94:LEU:HD11	1:B:119:ASP:CB	2.42	0.49
2:C:1034:GLU:HA	2:C:1037:VAL:CG2	2.41	0.49
2:C:286:SER:HB3	2:C:299:LYS:CE	2.43	0.49
2:C:352:ALA:HA	2:C:355:VAL:HG12	1.94	0.49
2:C:332:ARG:HB2	2:C:466:PHE:CE1	2.47	0.49
2:C:620:LEU:O	2:C:620:LEU:HD22	2.13	0.49
2:C:783:ARG:HD3	9:C:9806:HOH:O	2.11	0.49
2:C:703:ILE:CD1	2:C:830:LYS:HG2	2.43	0.49
3:D:1156:LEU:HG	3:D:1177:ALA:HB2	1.94	0.49
3:D:1295:GLU:HB3	3:D:1300:SER:CB	2.43	0.49
3:D:131:LYS:HG3	9:D:9749:HOH:O	2.12	0.49
3:D:400:VAL:HG13	3:D:441:ARG:HD3	1.94	0.49
3:D:530:VAL:N	3:D:534:ARG:O	2.37	0.49
3:D:704:ARG:HB2	3:D:736:PHE:HD2	1.77	0.49
3:D:765:SER:O	3:D:767:HIS:N	2.46	0.49
3:D:770:LEU:HD22	3:D:777:PRO:HA	1.93	0.49
4:E:36:LYS:HD2	9:E:9566:HOH:O	2.11	0.49
5:F:115:LYS:HG3	5:F:173:TYR:CE2	2.48	0.49
5:F:335:ASP:CG	5:F:338:LEU:HD12	2.33	0.49
1:K:19:GLU:CD	1:K:19:GLU:H	2.16	0.49
1:L:123:MET:HE2	1:L:204:SER:HA	1.94	0.49
1:L:65:PHE:HB2	9:L:5784:HOH:O	2.12	0.49
2:M:1000:MET:SD	2:M:1001:VAL:HG22	2.52	0.49
2:M:470:PRO:HB2	2:M:483:VAL:HG11	1.94	0.49
2:M:876:VAL:O	2:M:879:ARG:O	2.31	0.49
2:M:577:PRO:HA	2:M:993:PHE:CD2	2.48	0.49
3:N:1139:ASP:O	3:N:1142:ALA:HB3	2.12	0.49
3:N:1243:THR:HB	3:N:1253:THR:HG22	1.94	0.49
3:N:131:LYS:HD2	5:P:83:GLN:NE2	2.27	0.49
3:N:1353:GLN:O	3:N:1357:ARG:HD2	2.12	0.49
3:N:396:VAL:HA	9:N:9955:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:550:ARG:HH11	3:N:550:ARG:HG3	1.76	0.49
3:N:699:VAL:HG22	3:N:756:GLN:HE22	1.77	0.49
3:N:81:THR:O	3:N:82:LYS:C	2.51	0.49
5:P:163:LEU:HB3	5:P:174:LEU:CD1	2.43	0.49
5:P:292:ALA:HB1	5:P:299:TRP:O	2.13	0.49
5:P:356:LYS:NZ	5:P:417:LYS:HE2	2.26	0.49
1:B:159:LYS:N	1:B:159:LYS:HD3	2.27	0.49
2:C:127:PHE:CE1	2:C:386:PHE:HE2	2.31	0.49
2:C:218:VAL:HG22	2:C:221:LEU:CD2	2.43	0.49
2:C:712:ALA:O	2:C:820:ARG:HB2	2.12	0.49
3:D:447:VAL:HG12	9:D:9781:HOH:O	2.12	0.49
3:D:1495:ILE:HG12	4:E:80:VAL:HG11	1.93	0.49
5:F:366:ALA:HB3	5:F:367:MET:CE	2.42	0.49
1:L:13:VAL:HG13	1:L:23:PHE:CD1	2.48	0.49
2:M:1070:ILE:HD13	9:N:2071:HOH:O	2.12	0.49
2:M:1118:LYS:HD2	9:N:9587:HOH:O	2.13	0.49
2:M:353:ARG:HG2	9:M:9825:HOH:O	2.12	0.49
2:M:976:ASP:HB3	2:M:979:THR:HG22	1.94	0.49
3:N:1007:VAL:HG23	3:N:1008:PHE:N	2.28	0.49
3:N:169:TYR:N	3:N:170:PRO:CD	2.76	0.49
5:P:247:ILE:O	5:P:251:ILE:HG13	2.12	0.49
5:P:82:ARG:HB2	9:P:5834:HOH:O	2.13	0.49
5:P:85:LEU:HD22	5:P:193:ARG:HD3	1.94	0.49
1:A:102:LYS:HG3	1:A:139:ASN:HB2	1.93	0.49
1:A:218:LEU:O	1:A:222:LEU:HD23	2.12	0.49
2:C:1065:ALA:HB1	9:C:9619:HOH:O	2.12	0.49
2:C:175:GLU:HB3	2:C:183:SER:OG	2.13	0.49
2:C:537:LYS:CD	2:C:537:LYS:H	2.26	0.49
2:C:676:ILE:O	2:C:676:ILE:HG23	2.12	0.49
2:C:722:ILE:HD12	2:C:805:ARG:CZ	2.43	0.49
2:C:769:PRO:HD2	9:D:2497:HOH:O	2.13	0.49
2:C:390:GLN:O	7:C:8001:RPT:H142	2.11	0.49
2:C:969:GLN:HB3	9:D:2069:HOH:O	2.13	0.49
4:E:13:VAL:HG12	4:E:75:PHE:CE1	2.48	0.49
1:L:129:ILE:HD13	9:L:4066:HOH:O	2.11	0.49
2:M:1068:GLU:OE1	5:P:345:ALA:HA	2.13	0.49
2:M:56:GLU:HB3	9:M:9605:HOH:O	2.12	0.49
2:M:881:ASN:N	2:M:881:ASN:HD22	2.04	0.49
2:M:671:ASN:HD22	2:M:993:PHE:HA	1.76	0.49
3:N:1066:THR:HG23	3:N:1069:GLU:H	1.78	0.49
5:P:350:LEU:O	5:P:354:LEU:HG	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:358:LEU:CD2	5:P:370:LYS:HE3	2.42	0.49
1:A:109:VAL:HG23	1:A:132:LEU:HD13	1.94	0.49
2:C:444:PRO:HB3	7:C:8001:RPT:H302	1.95	0.49
2:C:57:GLU:HG3	2:C:58:ASP:OD2	2.13	0.49
2:C:726:ILE:HG22	9:C:2076:HOH:O	2.12	0.49
2:C:777:ILE:HD12	9:C:9524:HOH:O	2.12	0.49
2:C:8:ARG:HB2	9:C:9660:HOH:O	2.13	0.49
2:C:862:PRO:HA	2:C:975:TYR:CE1	2.48	0.49
3:D:1114:THR:HG23	3:D:1116:ASN:ND2	2.28	0.49
3:D:149:LYS:HA	9:D:9954:HOH:O	2.12	0.49
3:D:230:TRP:HA	9:D:2088:HOH:O	2.13	0.49
3:D:478:LEU:HD21	3:D:500:ARG:NH2	2.28	0.49
3:D:462:GLN:HG3	3:D:513:ILE:HD13	1.94	0.49
3:D:928:ALA:O	3:D:931:LEU:HB2	2.13	0.49
2:M:21:ILE:HD12	2:M:21:ILE:H	1.77	0.49
2:M:474:VAL:HG11	2:M:529:VAL:HG12	1.95	0.49
2:M:546:LEU:O	2:M:546:LEU:HD23	2.13	0.49
3:N:1182:GLU:HG2	9:N:9579:HOH:O	2.11	0.49
3:N:1258:ARG:HH21	3:N:1351:GLU:CG	2.25	0.49
3:N:18:ILE:HG23	3:N:518:PRO:CG	2.36	0.49
3:N:424:GLY:HA2	3:N:435:VAL:O	2.12	0.49
3:N:428:LYS:HB3	3:N:450:TYR:HE1	1.78	0.49
3:N:488:ARG:CZ	3:N:488:ARG:HB3	2.42	0.49
3:N:578:VAL:O	3:N:582:LEU:HD12	2.13	0.49
3:N:634:GLY:O	3:N:637:LEU:HB3	2.13	0.49
3:N:850:LEU:O	3:N:853:VAL:HB	2.13	0.49
3:N:880:ILE:O	3:N:883:ALA:HB3	2.13	0.49
1:A:14:ARG:CZ	1:A:24:VAL:HG23	2.43	0.49
1:B:103:ALA:HB1	1:B:107:LYS:HD2	1.95	0.49
2:C:365:ASP:O	2:C:367:LEU:HD12	2.13	0.49
2:C:37:GLU:HA	9:C:9707:HOH:O	2.12	0.49
2:C:862:PRO:HG3	2:C:975:TYR:CE1	2.48	0.49
2:C:893:ALA:O	2:C:897:LEU:HB2	2.13	0.49
3:D:1087:ARG:HH21	3:D:1238:MET:HB2	1.77	0.49
3:D:1267:ARG:HH22	3:D:1333:HIS:CD2	2.31	0.49
3:D:462:GLN:HA	3:D:513:ILE:CD1	2.41	0.49
3:D:702:LEU:HG	3:D:745:MET:HE3	1.94	0.49
3:D:809:PRO:O	3:D:812:ALA:HB3	2.13	0.49
4:E:45:ARG:HB2	4:E:46:PRO:CD	2.43	0.49
5:F:117:SER:HB3	9:F:9892:HOH:O	2.13	0.49
1:K:68:ILE:HD13	1:K:138:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:281:LEU:CD1	2:M:306:THR:HA	2.43	0.49
2:M:338:GLU:HA	2:M:341:THR:HG22	1.94	0.49
2:M:543:ASN:HD22	2:M:562:SER:HB3	1.77	0.49
2:M:409:ARG:NH2	7:M:8002:RPT:H18	2.24	0.49
2:M:928:LYS:HA	9:M:2129:HOH:O	2.12	0.49
3:N:1007:VAL:O	3:N:1010:ASN:HB3	2.12	0.49
3:N:1112:CYS:HA	3:N:1195:GLN:HE22	1.78	0.49
3:N:1489:GLN:O	3:N:1493:LYS:HG2	2.12	0.49
3:N:463:GLN:O	3:N:467:GLU:HG3	2.13	0.49
3:N:843:PHE:CE1	3:N:864:VAL:HG11	2.48	0.49
3:N:996:TRP:HA	3:N:999:THR:CG2	2.40	0.49
4:O:33:HIS:HB3	9:O:4524:HOH:O	2.10	0.49
5:P:356:LYS:O	5:P:360:LYS:HG2	2.12	0.49
5:P:361:LEU:HD13	5:P:366:ALA:CB	2.43	0.49
1:A:89:PHE:CZ	1:A:146:ARG:HB2	2.48	0.48
1:B:101:LEU:HD12	1:B:114:PHE:CD1	2.48	0.48
1:B:89:PHE:HB2	9:B:9688:HOH:O	2.13	0.48
2:C:396:ASP:HA	2:C:633:GLN:NE2	2.27	0.48
3:D:116:LEU:HB3	3:D:118:LEU:HD21	1.94	0.48
3:D:186:VAL:HG23	3:D:211:VAL:CG1	2.43	0.48
3:D:669:ASN:O	3:D:672:ALA:HB3	2.12	0.48
3:D:896:ALA:HB2	9:D:9543:HOH:O	2.13	0.48
3:D:423:ASP:OD2	5:F:174:LEU:HD22	2.13	0.48
1:K:32:PHE:N	9:K:4346:HOH:O	2.40	0.48
2:M:720:GLU:HA	2:M:759:THR:O	2.13	0.48
3:N:1318:TYR:HD1	3:N:1319:VAL:N	2.11	0.48
3:N:1382:THR:HG22	9:N:9550:HOH:O	2.13	0.48
3:N:237:LYS:HA	9:N:2400:HOH:O	2.13	0.48
3:N:958:GLU:O	3:N:961:LYS:HG2	2.13	0.48
3:N:998:GLU:HG2	9:N:9574:HOH:O	2.12	0.48
1:A:81:ASN:HA	1:A:84:GLU:CD	2.33	0.48
2:C:231:PRO:HB3	9:C:9728:HOH:O	2.13	0.48
2:C:461:VAL:HG13	2:C:465:GLY:HA2	1.95	0.48
2:C:470:PRO:HB2	2:C:483:VAL:HG11	1.94	0.48
2:C:502:PRO:HB2	2:C:509:ALA:HB3	1.95	0.48
2:C:535:SER:O	2:C:538:GLN:HG2	2.13	0.48
2:C:570:PRO:CD	2:C:635:THR:HB	2.43	0.48
2:C:840:ALA:HB2	2:C:846:LYS:HA	1.94	0.48
3:D:105:VAL:HG12	3:D:106:LYS:NZ	2.28	0.48
3:D:1144:LEU:HB3	3:D:1166:LEU:HD11	1.95	0.48
3:D:633:VAL:C	3:D:635:PRO:HD3	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:666:ILE:HG22	3:D:676:MET:HE1	1.96	0.48
3:D:86:ARG:HG3	3:D:86:ARG:O	2.12	0.48
4:E:26:ARG:HH11	4:E:29:GLN:NE2	2.10	0.48
5:F:123:ASP:H	5:F:126:LEU:HD22	1.79	0.48
5:F:192:LEU:O	5:F:192:LEU:HD23	2.13	0.48
5:F:282:LEU:HD11	5:F:286:PRO:HG3	1.96	0.48
5:F:369:LEU:HD11	5:F:401:GLU:HB2	1.96	0.48
1:L:74:ASP:OD2	1:L:76:VAL:HG23	2.13	0.48
2:M:1111:ILE:HG13	2:M:1112:PHE:N	2.25	0.48
2:M:242:LEU:HD13	9:M:2044:HOH:O	2.13	0.48
2:M:302:VAL:HB	9:M:9592:HOH:O	2.13	0.48
2:M:502:PRO:HB2	2:M:509:ALA:HB3	1.94	0.48
2:M:728:HIS:NE2	2:M:775:ARG:NH2	2.60	0.48
2:M:889:HIS:CD2	2:M:970:GLY:HA3	2.48	0.48
3:N:1275:SER:HB3	3:N:1325:LEU:CD1	2.43	0.48
3:N:671:LYS:HE2	9:N:2679:HOH:O	2.12	0.48
2:M:1015:LEU:HB2	5:P:334:PRO:O	2.13	0.48
2:C:56:GLU:HB3	9:C:9504:HOH:O	2.13	0.48
2:C:580:MET:O	2:C:903:SER:N	2.45	0.48
2:C:604:ALA:HB3	2:C:612:VAL:O	2.13	0.48
3:D:1097:LYS:O	3:D:1101:VAL:HG23	2.13	0.48
3:D:1159:ARG:CZ	3:D:1159:ARG:HB3	2.42	0.48
3:D:1188:VAL:HG22	3:D:1189:ARG:O	2.14	0.48
3:D:1281:VAL:HG21	3:D:1313:VAL:CG2	2.43	0.48
3:D:1281:VAL:HG21	3:D:1313:VAL:HG21	1.95	0.48
3:D:169:TYR:N	3:D:170:PRO:CD	2.77	0.48
3:D:170:PRO:HG2	9:D:2240:HOH:O	2.13	0.48
3:D:181:ASP:O	3:D:185:VAL:HG23	2.13	0.48
3:D:428:LYS:HD3	9:D:2416:HOH:O	2.12	0.48
3:D:631:ILE:O	3:D:632:VAL:HG23	2.13	0.48
3:D:847:ASP:HA	3:D:850:LEU:CD1	2.44	0.48
5:F:361:LEU:HD22	5:F:366:ALA:HB2	1.95	0.48
1:K:54:THR:HG23	1:K:156:HIS:CE1	2.47	0.48
1:K:91:ASN:O	1:K:94:LEU:HD12	2.12	0.48
1:L:100:LEU:O	1:L:115:LEU:HG	2.13	0.48
2:M:910:LYS:HD3	9:M:9697:HOH:O	2.13	0.48
3:N:1356:TYR:CD2	3:N:1363:LEU:HD23	2.49	0.48
3:N:1406:ARG:HA	9:N:2372:HOH:O	2.13	0.48
3:N:1425:THR:HG23	3:N:1426:LYS:H	1.78	0.48
3:N:1198:TYR:HE2	3:N:1432:LYS:HE2	1.79	0.48
3:N:438:ASP:HB2	9:N:9821:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:12:LEU:HD22	3:N:511:TRP:CB	2.43	0.48
3:N:52:PRO:HD2	3:N:79:GLU:O	2.12	0.48
3:N:777:PRO:HG2	3:N:915:VAL:HB	1.96	0.48
5:P:119:ILE:HD13	5:P:170:HIS:ND1	2.27	0.48
3:N:563:PRO:HG3	5:P:188:ILE:HG21	1.96	0.48
1:A:195:LEU:HD12	1:A:196:THR:N	2.27	0.48
2:C:56:GLU:HG2	2:C:64:LEU:HD23	1.94	0.48
2:C:704:HIS:HB2	2:C:831:ARG:NE	2.27	0.48
2:C:724:ARG:HG3	2:C:740:GLU:HA	1.95	0.48
2:C:775:ARG:HE	2:C:782:ALA:CB	2.25	0.48
2:C:954:THR:OG1	2:C:957:LYS:HG3	2.12	0.48
3:D:105:VAL:HG12	3:D:106:LYS:HZ2	1.77	0.48
3:D:122:GLU:HA	3:D:122:GLU:OE1	2.13	0.48
3:D:1278:ASP:HA	3:D:1319:VAL:O	2.13	0.48
3:D:754:PHE:HE2	3:D:1476:THR:HG21	1.79	0.48
3:D:525:ARG:HA	3:D:538:SER:HB2	1.94	0.48
5:F:273:ARG:HA	5:F:276:ARG:HD2	1.94	0.48
1:L:23:PHE:O	1:L:196:THR:HA	2.14	0.48
2:M:1097:LEU:HD22	2:M:1097:LEU:N	2.29	0.48
2:M:45:GLN:CG	2:M:49:ARG:HH22	2.27	0.48
2:M:514:VAL:HG22	9:M:9787:HOH:O	2.13	0.48
2:M:683:ASN:HB2	9:M:9667:HOH:O	2.13	0.48
2:M:71:TYR:CD2	2:M:71:TYR:N	2.81	0.48
2:M:909:ALA:C	2:M:910:LYS:HD2	2.34	0.48
3:N:1304:LYS:HG2	9:N:2548:HOH:O	2.13	0.48
3:N:95:LEU:HD11	3:N:517:VAL:HG23	1.96	0.48
3:N:581:LEU:H	3:N:581:LEU:HD23	1.78	0.48
3:N:884:ARG:HD3	9:N:9544:HOH:O	2.13	0.48
4:O:18:ARG:O	4:O:22:VAL:HG23	2.13	0.48
5:P:122:LEU:HD11	5:P:126:LEU:HD23	1.95	0.48
5:P:353:GLU:OE1	5:P:356:LYS:HE2	2.13	0.48
2:C:1073:GLY:HA3	9:C:9551:HOH:O	2.13	0.48
2:C:160:ALA:O	2:C:173:ASP:HA	2.13	0.48
2:C:470:PRO:HD3	2:C:485:TYR:CE2	2.49	0.48
2:C:820:ARG:HD3	9:C:2168:HOH:O	2.12	0.48
3:D:1107:VAL:HG12	3:D:1217:ILE:HA	1.95	0.48
3:D:911:LEU:O	3:D:915:VAL:HG23	2.14	0.48
4:E:16:LYS:HA	9:E:9481:HOH:O	2.12	0.48
4:E:50:THR:HG22	9:E:9491:HOH:O	2.12	0.48
2:M:165:LEU:HA	2:M:166:PRO:O	2.14	0.48
2:M:625:LEU:O	2:M:627:ARG:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1136:LYS:HB2	3:N:1139:ASP:OD2	2.13	0.48
3:N:415:VAL:HG23	9:N:2389:HOH:O	2.13	0.48
3:N:546:ARG:NH2	3:N:550:ARG:HH12	2.12	0.48
3:N:714:GLN:OE1	3:N:765:SER:HA	2.13	0.48
1:B:170:VAL:HG23	1:B:170:VAL:O	2.13	0.48
2:C:426:ASP:HB2	9:C:2334:HOH:O	2.13	0.48
2:C:588:VAL:HG21	2:C:664:GLY:O	2.13	0.48
2:C:722:ILE:HG23	2:C:722:ILE:O	2.14	0.48
3:D:1112:CYS:HB2	3:D:1195:GLN:OE1	2.14	0.48
3:D:1302:GLU:HG3	9:D:9628:HOH:O	2.14	0.48
3:D:1307:LYS:CD	3:D:1307:LYS:H	2.23	0.48
3:D:142:LEU:HB3	9:D:9718:HOH:O	2.13	0.48
3:D:790:TYR:CD1	3:D:1022:VAL:HG13	2.48	0.48
3:D:829:VAL:H	3:D:835:SER:HB2	1.78	0.48
4:E:17:TYR:HD2	4:E:17:TYR:H	1.62	0.48
5:F:151:LEU:HB2	5:F:155:THR:H	1.79	0.48
5:F:278:LEU:HB2	5:F:286:PRO:HG2	1.95	0.48
1:L:170:VAL:C	1:L:172:SER:H	2.16	0.48
1:L:206:THR:HG23	1:L:208:LEU:H	1.78	0.48
1:L:219:ARG:O	1:L:223:THR:HG23	2.13	0.48
2:M:102:HIS:HB2	2:M:106:GLY:O	2.14	0.48
2:M:1081:VAL:HB	2:M:1086:ARG:NE	2.29	0.48
2:M:205:GLU:OE2	2:M:206:THR:HB	2.14	0.48
2:M:274:ARG:HB2	2:M:285:LEU:CD1	2.43	0.48
2:M:260:LEU:HA	2:M:291:ALA:HB2	1.95	0.48
2:M:609:ASN:ND2	2:M:627:ARG:HE	2.12	0.48
3:N:1045:MET:HE1	9:N:9654:HOH:O	2.14	0.48
3:N:1303:TYR:HD2	9:N:2651:HOH:O	1.96	0.48
3:N:1459:LEU:HD13	3:N:1465:ASN:ND2	2.28	0.48
3:N:152:LEU:HD21	9:N:9735:HOH:O	2.13	0.48
3:N:27:GLU:O	3:N:28:LYS:HD2	2.13	0.48
3:N:820:GLU:HA	3:N:825:ALA:O	2.14	0.48
5:P:214:GLN:O	5:P:217:ASN:HB2	2.13	0.48
1:A:20:TYR:CD2	1:A:21:GLY:N	2.80	0.48
1:A:99:LEU:HB3	1:A:114:PHE:HD2	1.78	0.48
1:B:124:ASN:HA	9:B:9533:HOH:O	2.14	0.48
1:B:81:ASN:HD21	1:B:127:LEU:HG	1.78	0.48
2:C:108:ILE:HD12	2:C:108:ILE:N	2.28	0.48
2:C:196:LEU:HD11	2:C:303:PHE:CE1	2.49	0.48
2:C:299:LYS:HB3	9:C:9713:HOH:O	2.12	0.48
2:C:459:ALA:HB1	2:C:467:ILE:CG2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:458:TYR:HB3	2:C:470:PRO:HG3	1.95	0.48
2:C:480:THR:HG22	2:C:481:ASP:N	2.28	0.48
2:C:677:MET:HE3	3:D:943:THR:O	2.13	0.48
2:C:952:LEU:HB3	2:C:966:LEU:HD11	1.95	0.48
3:D:1232:PRO:HB3	3:D:1361:VAL:CG2	2.38	0.48
3:D:1432:LYS:HA	9:D:9581:HOH:O	2.13	0.48
3:D:10:ILE:HD13	3:D:1447:LEU:HG	1.95	0.48
3:D:183:GLU:O	3:D:186:VAL:HG12	2.14	0.48
3:D:213:VAL:HG22	3:D:214:GLU:H	1.79	0.48
2:C:1029:GLY:O	3:D:622:ARG:HD3	2.14	0.48
3:D:639:LEU:HD12	3:D:640:HIS:H	1.78	0.48
3:D:699:VAL:H	3:D:756:GLN:HE21	1.57	0.48
3:D:785:ILE:HG22	3:D:789:LEU:HD12	1.94	0.48
5:F:261:PRO:O	5:F:265:VAL:HG23	2.14	0.48
1:K:83:LYS:HE2	1:K:168:ASP:N	2.27	0.48
1:L:185:ARG:HG3	1:L:190:THR:CG2	2.39	0.48
1:L:191:ASP:O	1:L:192:LEU:HG	2.13	0.48
2:M:1043:TYR:HA	9:O:4679:HOH:O	2.13	0.48
2:M:1081:VAL:HB	2:M:1086:ARG:HE	1.78	0.48
2:M:195:LEU:HG	2:M:238:LEU:HG	1.96	0.48
2:M:431:HIS:HD2	2:M:433:THR:H	1.58	0.48
2:M:722:ILE:HG21	2:M:821:GLU:OE1	2.14	0.48
3:N:103:TRP:CH2	3:N:1447:LEU:HD23	2.48	0.48
3:N:1305:LEU:HD21	3:N:1326:THR:OG1	2.14	0.48
3:N:152:LEU:CD2	3:N:152:LEU:H	2.25	0.48
3:N:515:GLU:HB2	9:N:9820:HOH:O	2.13	0.48
3:N:629:SER:OG	3:N:726:ILE:HG13	2.14	0.48
3:N:633:VAL:HG22	3:N:635:PRO:CD	2.43	0.48
5:P:346:THR:HA	9:P:4114:HOH:O	2.12	0.48
2:C:64:LEU:HD12	2:C:100:LEU:HD13	1.95	0.48
2:C:1051:GLU:HG3	2:C:1055:LEU:HD12	1.96	0.48
2:C:1089:VAL:O	2:C:1093:GLN:HG3	2.13	0.48
2:C:42:VAL:HG12	2:C:43:GLY:N	2.26	0.48
2:C:627:ARG:HG3	2:C:628:PHE:H	1.77	0.48
2:C:931:GLY:HA3	9:C:2360:HOH:O	2.14	0.48
3:D:1223:ILE:HD12	3:D:1223:ILE:N	2.20	0.48
2:C:1115:LEU:HB3	3:D:85:VAL:CG1	2.44	0.48
4:E:54:LEU:O	4:E:54:LEU:HD23	2.14	0.48
5:F:128:ARG:HG2	9:F:9497:HOH:O	2.12	0.48
1:K:50:GLY:O	1:K:146:ARG:HA	2.13	0.48
1:L:20:TYR:HE2	1:L:198:ARG:HB3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:1040:LEU:HG	2:M:1045:ALA:HB3	1.95	0.48
2:M:54:ILE:HA	9:M:9582:HOH:O	2.13	0.48
2:M:666:LEU:HD12	2:M:667:ALA:N	2.29	0.48
2:M:873:PRO:O	2:M:876:VAL:HG23	2.13	0.48
3:N:1087:ARG:HA	3:N:1090:ASP:HB2	1.95	0.48
3:N:1353:GLN:HE21	3:N:1357:ARG:HE	1.61	0.48
3:N:186:VAL:HG13	3:N:187:LYS:N	2.29	0.48
3:N:462:GLN:HB2	3:N:513:ILE:HG21	1.95	0.48
3:N:694:VAL:HG13	9:N:2371:HOH:O	2.13	0.48
3:N:796:ARG:HA	9:N:9559:HOH:O	2.14	0.48
3:N:897:TRP:CZ2	3:N:902:LEU:HD21	2.48	0.48
3:N:967:ALA:O	3:N:995:LEU:HD21	2.13	0.48
5:P:287:THR:C	5:P:289:GLU:H	2.16	0.48
2:M:1021:LEU:HD22	5:P:331:ASP:O	2.14	0.48
9:M:9830:HOH:O	5:P:351:SER:HA	2.14	0.48
1:A:14:ARG:HH12	1:A:24:VAL:HG23	1.79	0.48
2:C:1067:TYR:CE1	3:D:655:PRO:HG3	2.49	0.48
2:C:649:VAL:HG23	9:C:9833:HOH:O	2.13	0.48
2:C:769:PRO:HB3	9:F:9559:HOH:O	2.12	0.48
2:C:444:PRO:HB3	7:C:8001:RPT:C30	2.44	0.48
3:D:792:ILE:O	3:D:878:GLY:HA3	2.13	0.48
5:F:131:VAL:HG22	5:F:178:ARG:HD3	1.95	0.48
2:M:1015:LEU:HB3	2:M:1016:ILE:HD13	1.95	0.48
2:M:1033:GLY:O	2:M:1037:VAL:HG23	2.14	0.48
2:M:278:GLU:HB3	9:M:2020:HOH:O	2.14	0.48
2:M:455:LEU:HD13	2:M:459:ALA:HB3	1.94	0.48
2:M:54:ILE:HB	9:M:2245:HOH:O	2.14	0.48
2:M:614:ARG:HG3	2:M:620:LEU:HD12	1.96	0.48
2:M:726:ILE:HG22	2:M:726:ILE:O	2.12	0.48
2:M:564:MET:HG2	2:M:840:ALA:HB3	1.94	0.48
3:N:1023:MET:O	3:N:1028:ALA:HB3	2.14	0.48
3:N:1036:ARG:NH2	9:N:9654:HOH:O	2.47	0.48
3:N:525:ARG:HD2	3:N:541:ASN:OD1	2.14	0.48
3:N:557:LEU:HD11	5:P:214:GLN:NE2	2.28	0.48
3:N:674:ARG:HG2	3:N:674:ARG:NH1	2.29	0.48
3:N:989:TYR:CZ	3:N:993:LEU:HD11	2.49	0.48
5:P:93:LEU:HG	5:P:190:ALA:HB1	1.95	0.48
1:A:184:THR:HG23	1:A:192:LEU:HD12	1.96	0.48
1:A:86:VAL:CG1	1:A:124:ASN:HB2	2.43	0.48
1:A:36:LEU:HD11	1:B:221:HIS:HB3	1.95	0.48
2:C:144:PRO:HG2	2:C:265:ARG:NH1	2.25	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:184:MET:HB2	2:C:193:LEU:CD1	2.44	0.48
2:C:260:LEU:HA	2:C:291:ALA:HB2	1.95	0.48
2:C:380:ALA:O	2:C:384:GLU:HB2	2.13	0.48
2:C:445:GLU:HB2	2:C:559:LEU:HD21	1.95	0.48
2:C:630:ARG:HA	2:C:705:ILE:CD1	2.44	0.48
2:C:91:GLN:OE1	2:C:117:HIS:HB3	2.13	0.48
3:D:1169:ASP:HB3	9:D:2071:HOH:O	2.13	0.48
3:D:1258:ARG:NH2	3:D:1262:LEU:HD11	2.28	0.48
3:D:1280:VAL:HG12	3:D:1281:VAL:N	2.29	0.48
3:D:1404:ASN:HB2	9:D:9939:HOH:O	2.14	0.48
3:D:1418:LYS:HG3	9:D:9914:HOH:O	2.13	0.48
3:D:1379:VAL:HA	3:D:1420:LEU:HB3	1.95	0.48
3:D:27:GLU:HG3	3:D:28:LYS:HD2	1.96	0.48
3:D:42:ASP:O	3:D:46:ASP:HB2	2.13	0.48
2:C:1036:GLU:HA	3:D:707:THR:HG21	1.96	0.48
5:F:277:GLN:O	5:F:280:GLN:HB3	2.14	0.48
5:F:388:ALA:HB1	9:F:9483:HOH:O	2.12	0.48
1:K:48:ILE:HD13	1:K:210:ALA:HB1	1.95	0.48
1:K:41:ARG:HH11	1:K:41:ARG:HG3	1.79	0.48
1:L:132:LEU:HD21	1:L:136:GLY:O	2.14	0.48
1:L:73:GLU:HB3	1:L:77:GLU:CG	2.43	0.48
2:M:1043:TYR:OH	3:N:711:LEU:HD23	2.13	0.48
2:M:189:ARG:HH22	2:M:243:ARG:HG2	1.78	0.48
2:M:432:ARG:NE	2:M:519:GLY:HA3	2.29	0.48
2:M:863:ASP:O	2:M:865:THR:N	2.47	0.48
2:M:953:VAL:HA	2:M:965:GLU:OE1	2.13	0.48
3:N:1003:VAL:O	3:N:1006:ALA:HB3	2.13	0.48
3:N:1096:ARG:NH1	3:N:1096:ARG:HG2	2.29	0.48
3:N:1102:THR:HG22	3:N:1222:GLY:CA	2.44	0.48
3:N:1263:PHE:CE2	3:N:1371:VAL:HG11	2.49	0.48
3:N:493:ARG:NH2	3:N:1388:ARG:HB3	2.28	0.48
3:N:1104:GLU:HA	3:N:1461:GLY:HA2	1.94	0.48
3:N:794:GLN:NE2	3:N:795:VAL:O	2.47	0.48
3:N:970:LYS:HB2	3:N:970:LYS:NZ	2.29	0.48
5:P:350:LEU:HD23	5:P:351:SER:N	2.29	0.48
1:A:143:ARG:HD2	1:A:145:ASP:OD1	2.14	0.47
1:A:63:HIS:HB3	2:C:746:GLY:CA	2.34	0.47
1:A:72:LYS:HB3	1:A:73:GLU:OE2	2.13	0.47
1:B:86:VAL:HG22	9:B:9508:HOH:O	2.14	0.47
2:C:182:VAL:HG11	9:C:9507:HOH:O	2.13	0.47
2:C:189:ARG:HH22	2:C:243:ARG:NH2	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:290:LEU:HB3	2:C:302:VAL:CG1	2.44	0.47
9:C:9669:HOH:O	3:D:1075:HIS:HE1	1.96	0.47
3:D:1259:VAL:O	3:D:1263:PHE:HD1	1.97	0.47
3:D:421:LEU:HD11	3:D:437:VAL:HG22	1.95	0.47
3:D:523:ASP:O	3:D:526:PRO:HG3	2.14	0.47
3:D:957:PRO:CD	3:D:1007:VAL:HG12	2.44	0.47
5:F:299:TRP:CE3	5:F:303:ARG:HD3	2.49	0.47
1:L:19:GLU:HG3	1:L:201:THR:O	2.14	0.47
2:M:1067:TYR:CE2	5:P:342:VAL:HA	2.49	0.47
2:M:1082:PRO:HG3	9:M:9510:HOH:O	2.13	0.47
2:M:345:ARG:HA	2:M:348:LEU:HB2	1.94	0.47
2:M:607:ASP:HB3	2:M:609:ASN:H	1.78	0.47
2:M:781:LYS:HG3	9:M:2053:HOH:O	2.14	0.47
3:N:1209:LEU:HD22	3:N:1211:MET:HB3	1.96	0.47
3:N:122:GLU:O	3:N:126:VAL:HG23	2.13	0.47
3:N:1238:MET:HE1	3:N:1257:PRO:HG3	1.96	0.47
3:N:1290:LEU:CD2	3:N:1291:SER:H	2.23	0.47
3:N:1292:VAL:O	3:N:1303:TYR:HB2	2.14	0.47
3:N:1493:LYS:HB2	9:N:9693:HOH:O	2.13	0.47
2:M:1118:LYS:HB3	3:N:23:TYR:CE1	2.49	0.47
3:N:633:VAL:C	3:N:635:PRO:HD3	2.34	0.47
3:N:730:PRO:HA	3:N:733:CYS:SG	2.54	0.47
3:N:80:VAL:HG12	3:N:81:THR:H	1.77	0.47
3:N:965:GLU:HA	3:N:968:ASP:HB2	1.96	0.47
5:P:234:LYS:CD	5:P:236:SER:H	2.27	0.47
5:P:417:LYS:HD2	9:P:4364:HOH:O	2.13	0.47
1:A:117:VAL:HB	1:A:120:VAL:CG1	2.41	0.47
1:B:133:GLU:HG3	9:B:9692:HOH:O	2.13	0.47
1:B:151:VAL:HA	1:B:155:LYS:HZ3	1.79	0.47
2:C:1030:GLN:NE2	2:C:1030:GLN:HA	2.29	0.47
2:C:1086:ARG:HD3	2:C:1112:PHE:HD2	1.80	0.47
2:C:244:PRO:HG2	2:C:246:ASP:CG	2.33	0.47
2:C:876:VAL:O	2:C:879:ARG:O	2.32	0.47
3:D:1020:LEU:HA	3:D:1023:MET:HE3	1.96	0.47
3:D:1044:LEU:HD21	3:D:1056:PRO:HG3	1.95	0.47
3:D:1087:ARG:HB2	3:D:1087:ARG:CZ	2.44	0.47
3:D:110:SER:HB2	9:D:9697:HOH:O	2.13	0.47
3:D:1173:LEU:HD23	3:D:1174:LEU:HD23	1.97	0.47
3:D:1240:THR:O	3:D:1257:PRO:HB3	2.13	0.47
3:D:1402:ALA:HB2	3:D:1415:VAL:CG2	2.44	0.47
3:D:1491:THR:HG22	9:E:9496:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:39:PRO:HB2	9:D:9934:HOH:O	2.14	0.47
3:D:445:ARG:HB3	9:D:9781:HOH:O	2.13	0.47
3:D:671:LYS:O	3:D:671:LYS:HD3	2.14	0.47
3:D:756:GLN:HG2	9:E:9480:HOH:O	2.13	0.47
4:E:49:GLN:HA	4:E:51:LEU:O	2.14	0.47
5:F:352:GLU:HG2	9:F:9594:HOH:O	2.13	0.47
1:K:23:PHE:O	1:K:196:THR:HA	2.14	0.47
2:M:208:ALA:HA	2:M:218:VAL:HG22	1.96	0.47
2:M:381:ALA:HA	9:M:9949:HOH:O	2.13	0.47
2:M:139:GLN:HE22	2:M:418:LEU:HD13	1.79	0.47
2:M:331:ARG:NH1	2:M:427:VAL:HG13	2.29	0.47
2:M:474:VAL:HG23	2:M:478:VAL:O	2.14	0.47
2:M:66:LEU:HD13	2:M:100:LEU:HB2	1.95	0.47
2:M:678:PRO:HA	2:M:683:ASN:HD21	1.79	0.47
2:M:881:ASN:N	2:M:881:ASN:ND2	2.61	0.47
3:N:1111:ASP:HA	9:N:9807:HOH:O	2.13	0.47
3:N:572:ARG:NH1	5:P:80:PRO:HD3	2.29	0.47
3:N:591:VAL:HG12	3:N:592:THR:O	2.14	0.47
3:N:668:PRO:HA	9:N:9706:HOH:O	2.14	0.47
4:O:48:MET:CB	4:O:54:LEU:HB2	2.44	0.47
4:O:70:THR:CG2	4:O:72:ARG:HH21	2.27	0.47
5:P:193:ARG:HD2	9:P:3462:HOH:O	2.14	0.47
1:A:133:GLU:HA	9:A:9594:HOH:O	2.13	0.47
1:B:151:VAL:HB	1:B:169:ALA:HB3	1.96	0.47
2:C:1090:LYS:HG2	2:C:1112:PHE:HZ	1.78	0.47
2:C:197:LEU:HA	9:C:9888:HOH:O	2.14	0.47
2:C:285:LEU:HD23	2:C:285:LEU:O	2.14	0.47
2:C:367:LEU:HD22	9:C:2175:HOH:O	2.14	0.47
2:C:52:PHE:HA	9:C:9979:HOH:O	2.13	0.47
2:C:892:LEU:HD21	2:C:967:PHE:CE1	2.49	0.47
3:D:1243:THR:HG22	3:D:1244:GLY:H	1.79	0.47
3:D:1394:VAL:HG21	3:D:1397:LYS:NZ	2.28	0.47
3:D:477:LEU:HD22	3:D:492:ALA:CB	2.42	0.47
3:D:473:LEU:HD11	3:D:495:ARG:NH1	2.29	0.47
3:D:843:PHE:CZ	3:D:864:VAL:HG11	2.49	0.47
9:D:2394:HOH:O	4:E:54:LEU:HD11	2.14	0.47
4:E:59:ASN:HB3	4:E:62:THR:OG1	2.13	0.47
2:M:551:GLU:OE1	2:M:906:PHE:HA	2.14	0.47
2:M:643:VAL:HG13	2:M:647:GLN:CD	2.35	0.47
3:N:474:GLU:O	3:N:478:LEU:HG	2.15	0.47
3:N:491:LYS:HG3	9:N:9963:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:664:LYS:HA	9:N:2138:HOH:O	2.14	0.47
3:N:776:GLU:OE1	3:N:912:LYS:HD3	2.14	0.47
4:O:54:LEU:HG	4:O:58:PRO:HD2	1.94	0.47
1:A:30:ARG:HH22	1:A:191:ASP:HB2	1.79	0.47
1:B:173:PRO:HB2	1:B:205:VAL:HG22	1.96	0.47
2:C:110:GLU:H	2:C:368:THR:HG21	1.79	0.47
2:C:134:ARG:HH21	2:C:394:PHE:N	2.12	0.47
3:D:1310:ARG:HG3	3:D:1327:ARG:CB	2.44	0.47
3:D:114:THR:O	3:D:495:ARG:HG3	2.15	0.47
3:D:501:ALA:HA	3:D:504:ASP:HB2	1.97	0.47
3:D:658:LEU:HD11	3:D:674:ARG:NH1	2.29	0.47
3:D:836:VAL:HG12	9:D:9486:HOH:O	2.14	0.47
9:C:9961:HOH:O	5:F:350:LEU:HD21	2.14	0.47
3:D:672:ALA:HA	5:F:420:ASP:OD2	2.15	0.47
2:M:478:VAL:HG13	2:M:506:ASN:HB3	1.95	0.47
2:M:63:GLY:CA	2:M:103:LYS:HE2	2.45	0.47
2:M:841:ASN:HD22	2:M:843:HIS:H	1.60	0.47
3:N:1280:VAL:HG12	3:N:1281:VAL:N	2.29	0.47
3:N:1472:ILE:HG22	3:N:1474:ALA:H	1.78	0.47
3:N:834:THR:HB	3:N:838:ARG:HB3	1.95	0.47
2:C:16:PRO:HG2	2:C:460:ARG:HH12	1.79	0.47
2:C:19:THR:HG22	2:C:19:THR:O	2.15	0.47
2:C:256:TYR:HE1	2:C:293:PHE:HB2	1.76	0.47
2:C:352:ALA:O	2:C:355:VAL:HG12	2.15	0.47
2:C:413:LEU:H	2:C:413:LEU:CD1	2.25	0.47
2:C:420:ARG:HG2	2:C:421:GLU:H	1.79	0.47
2:C:945:ARG:HD3	2:C:949:LYS:HE3	1.96	0.47
3:D:1326:THR:HG22	3:D:1327:ARG:N	2.30	0.47
3:D:1468:LEU:CD1	3:D:1470:ARG:HD3	2.43	0.47
3:D:171:LEU:HA	3:D:390:PRO:HA	1.96	0.47
3:D:584:ASN:HA	9:D:9901:HOH:O	2.15	0.47
3:D:659:LYS:HD3	3:D:659:LYS:O	2.14	0.47
3:D:891:GLU:N	9:D:9484:HOH:O	2.47	0.47
1:K:102:LYS:HG2	9:K:3922:HOH:O	2.13	0.47
1:K:34:VAL:HG21	9:M:2370:HOH:O	2.15	0.47
1:L:84:GLU:HG3	1:L:127:LEU:CD2	2.44	0.47
2:M:1030:GLN:HB2	3:N:626:SER:HB2	1.96	0.47
2:M:393:GLN:HB3	7:M:8002:RPT:H343	1.97	0.47
2:M:602:GLU:HA	2:M:647:GLN:O	2.14	0.47
2:M:773:LEU:HD21	5:P:354:LEU:HD22	1.95	0.47
3:N:1382:THR:HG21	3:N:1418:LYS:HZ2	1.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:656:PHE:CE2	3:N:698:LYS:HE3	2.49	0.47
3:N:728:LEU:HD12	3:N:729:HIS:N	2.30	0.47
3:N:826:PRO:HD2	3:N:829:VAL:HG22	1.95	0.47
3:N:848:GLU:HB3	9:N:9763:HOH:O	2.14	0.47
3:N:996:TRP:CE3	3:N:999:THR:HG21	2.50	0.47
2:M:1102:LEU:HD11	3:N:9:ARG:HB2	1.97	0.47
5:P:236:SER:HB3	9:P:3697:HOH:O	2.14	0.47
5:P:361:LEU:HD21	5:P:404:ALA:HB1	1.95	0.47
1:A:38:ASN:HB3	1:A:39:PRO:HD3	1.95	0.47
1:A:57:TYR:CD1	1:A:161:ARG:HB3	2.50	0.47
1:B:191:ASP:O	1:B:192:LEU:HG	2.13	0.47
1:A:219:ARG:NH1	1:B:219:ARG:HG2	2.29	0.47
2:C:1047:HIS:CD2	3:D:1471:LEU:HD11	2.50	0.47
2:C:1081:VAL:CG1	2:C:1086:ARG:HE	2.27	0.47
2:C:114:PHE:HB2	9:C:9593:HOH:O	2.14	0.47
2:C:537:LYS:HD2	2:C:537:LYS:H	1.80	0.47
2:C:752:GLY:C	2:C:791:ARG:HH12	2.18	0.47
3:D:952:ASP:HA	3:D:1062:ARG:NH2	2.29	0.47
3:D:1302:GLU:OE2	3:D:1304:LYS:HG2	2.15	0.47
3:D:399:ARG:HH21	3:D:432:TYR:HE2	1.61	0.47
3:D:543:LEU:HA	3:D:546:ARG:HG3	1.96	0.47
3:D:601:ARG:CD	3:D:606:ILE:HD13	2.45	0.47
3:D:709:HIS:CD2	3:D:711:LEU:HB2	2.49	0.47
3:D:970:LYS:HD2	3:D:995:LEU:HD13	1.95	0.47
1:K:18:ARG:O	1:K:201:THR:OG1	2.32	0.47
2:M:1019:GLN:NE2	3:N:621:LYS:HA	2.28	0.47
2:M:196:LEU:O	2:M:199:VAL:HB	2.15	0.47
2:M:197:LEU:CD1	2:M:207:LEU:HD11	2.45	0.47
2:M:227:PHE:HA	2:M:230:ARG:NE	2.22	0.47
2:M:269:LEU:HD11	2:M:287:GLY:HA2	1.97	0.47
2:M:802:ARG:HH11	2:M:802:ARG:CB	2.28	0.47
3:N:1352:ILE:CG2	3:N:1368:ILE:HD13	2.45	0.47
3:N:563:PRO:O	3:N:567:ILE:HG13	2.13	0.47
3:N:719:VAL:N	9:N:9610:HOH:O	2.47	0.47
3:N:96:ALA:HB2	9:N:9830:HOH:O	2.13	0.47
5:P:142:ARG:NH1	5:P:150:THR:HG21	2.30	0.47
1:B:190:THR:HG22	9:B:9536:HOH:O	2.14	0.47
1:B:32:PHE:HA	1:B:35:THR:OG1	2.15	0.47
2:C:1006:HIS:N	2:C:1006:HIS:ND1	2.63	0.47
2:C:1016:ILE:HD12	3:D:526:PRO:HG2	1.96	0.47
2:C:200:LEU:HD13	2:C:300:ASP:OD2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:212:GLY:C	2:C:215:GLY:H	2.18	0.47
2:C:269:LEU:HD23	9:C:2225:HOH:O	2.15	0.47
2:C:285:LEU:HD12	2:C:288:ARG:O	2.14	0.47
2:C:451:LEU:H	2:C:451:LEU:HD12	1.79	0.47
2:C:48:PHE:O	2:C:52:PHE:HB2	2.15	0.47
2:C:55:GLU:HG2	9:C:2379:HOH:O	2.14	0.47
2:C:654:LEU:HD13	2:C:664:GLY:N	2.29	0.47
2:C:676:ILE:CG2	2:C:988:VAL:HG22	2.45	0.47
2:C:673:LEU:CD2	2:C:867:VAL:HG12	2.45	0.47
3:D:1151:ARG:HB2	9:D:9606:HOH:O	2.15	0.47
3:D:229:ALA:HB1	9:D:9916:HOH:O	2.14	0.47
3:D:501:ALA:HB1	3:D:1453:ALA:HA	1.97	0.47
3:D:894:LYS:HB2	9:D:9872:HOH:O	2.13	0.47
3:D:969:ARG:O	3:D:972:LEU:HB3	2.14	0.47
1:L:111:ALA:HB3	1:L:124:ASN:O	2.15	0.47
2:M:194:VAL:HG21	2:M:221:LEU:HA	1.97	0.47
2:M:279:GLU:HA	9:M:9687:HOH:O	2.13	0.47
2:M:544:THR:O	2:M:547:ILE:HG13	2.15	0.47
2:M:741:GLY:HA3	9:M:9845:HOH:O	2.13	0.47
2:M:768:THR:O	2:M:772:ARG:HB3	2.15	0.47
2:M:910:LYS:HD2	2:M:910:LYS:N	2.30	0.47
3:N:1326:THR:HG22	3:N:1327:ARG:N	2.30	0.47
3:N:440:VAL:HG12	3:N:441:ARG:N	2.30	0.47
3:N:610:LYS:HG2	3:N:611:GLN:HG2	1.96	0.47
3:N:75:ARG:NH1	3:N:75:ARG:HG3	2.27	0.47
5:P:151:LEU:HB2	5:P:155:THR:OG1	2.15	0.47
3:N:550:ARG:HH21	5:P:211:ASP:CG	2.18	0.47
5:P:412:GLU:OE1	5:P:418:LEU:HD13	2.15	0.47
1:A:127:LEU:HD12	1:A:127:LEU:C	2.34	0.47
1:A:36:LEU:O	1:A:40:LEU:HG	2.15	0.47
1:B:171:PHE:HD2	9:B:9528:HOH:O	1.96	0.47
1:B:72:LYS:HG2	9:B:9498:HOH:O	2.14	0.47
2:C:389:SER:C	2:C:391:LEU:N	2.68	0.47
2:C:328:LEU:HD11	2:C:434:HIS:HD2	1.79	0.47
2:C:612:VAL:HG22	2:C:622:GLU:HB2	1.97	0.47
2:C:816:LYS:HB3	9:C:9840:HOH:O	2.15	0.47
3:D:1220:ALA:HB1	3:D:1223:ILE:CD1	2.41	0.47
3:D:421:LEU:HD12	3:D:435:VAL:CG1	2.44	0.47
3:D:572:ARG:HH12	5:F:79:ASP:CG	2.18	0.47
3:D:601:ARG:HE	3:D:606:ILE:HA	1.78	0.47
2:C:1020:PRO:O	3:D:622:ARG:HD2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:955:VAL:HB	3:D:1011:PHE:CE1	2.43	0.47
3:D:995:LEU:HA	9:D:2036:HOH:O	2.14	0.47
9:D:2189:HOH:O	5:F:145:PRO:HB3	2.14	0.47
2:M:431:HIS:HB3	2:M:434:HIS:CD2	2.49	0.47
2:M:619:ARG:HG3	9:M:9814:HOH:O	2.15	0.47
2:M:772:ARG:CD	5:P:373:LYS:HD2	2.44	0.47
2:M:833:LEU:HB2	9:M:9662:HOH:O	2.14	0.47
2:M:897:LEU:CD1	2:M:921:ALA:HA	2.44	0.47
3:N:58:CYS:SG	3:N:59:ALA:N	2.88	0.47
3:N:684:LYS:HB3	3:N:686:GLU:HG3	1.96	0.47
3:N:704:ARG:CD	3:N:705:ALA:H	2.26	0.47
2:M:984:GLU:HG3	3:N:944:THR:O	2.15	0.47
3:N:982:PHE:HZ	9:N:2480:HOH:O	1.98	0.47
5:P:82:ARG:HG2	9:P:4186:HOH:O	2.13	0.47
1:A:33:GLY:O	1:A:195:LEU:HD22	2.14	0.47
1:A:83:LYS:HE2	1:A:167:VAL:HG12	1.97	0.47
1:A:224:TYR:HB3	1:B:9:PRO:HB2	1.97	0.47
2:C:232:GLU:O	2:C:235:LEU:HB2	2.14	0.47
2:C:129:ILE:HG12	2:C:386:PHE:HB3	1.97	0.47
2:C:137:VAL:O	2:C:391:LEU:HD11	2.15	0.47
2:C:83:CYS:CA	2:C:88:LEU:HB3	2.39	0.47
3:D:1495:ILE:N	3:D:1495:ILE:HD12	2.29	0.47
3:D:28:LYS:O	3:D:43:GLY:HA2	2.15	0.47
3:D:436:GLU:HB2	3:D:445:ARG:HB3	1.95	0.47
3:D:539:ASP:OD2	5:F:318:GLU:HB2	2.14	0.47
2:C:886:LEU:CD2	3:D:951:ILE:HG13	2.44	0.47
5:F:141:VAL:O	5:F:145:PRO:HD2	2.15	0.47
5:F:316:SER:C	5:F:318:GLU:N	2.68	0.47
5:F:358:LEU:HD13	5:F:370:LYS:HG3	1.97	0.47
5:F:367:MET:HA	5:F:370:LYS:NZ	2.30	0.47
5:F:74:LYS:HG3	9:F:9539:HOH:O	2.14	0.47
2:M:220:GLY:HA3	9:M:9540:HOH:O	2.15	0.47
2:M:277:ALA:HB1	9:M:2036:HOH:O	2.14	0.47
3:N:1223:ILE:N	3:N:1223:ILE:HD12	2.25	0.47
3:N:139:GLY:N	3:N:147:VAL:HG21	2.30	0.47
3:N:98:PRO:HG3	3:N:515:GLU:HB3	1.96	0.47
2:M:1076:VAL:HG21	3:N:752:SER:HB3	1.97	0.47
1:L:65:PHE:CD1	3:N:813:LEU:HD22	2.50	0.47
3:N:933:ALA:O	3:N:937:TYR:HD1	1.96	0.47
5:P:361:LEU:HD13	5:P:366:ALA:HB1	1.97	0.47
1:A:101:LEU:HD12	1:A:114:PHE:CD1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:MET:CE	1:B:204:SER:HA	2.45	0.47
1:B:41:ARG:HB2	1:B:177:VAL:HG21	1.95	0.47
2:C:1013:TYR:CE1	2:C:1020:PRO:HG3	2.49	0.47
2:C:1018:GLN:HG3	2:C:1060:ILE:HD13	1.97	0.47
2:C:346:VAL:HB	9:C:2037:HOH:O	2.15	0.47
2:C:52:PHE:O	2:C:54:ILE:N	2.48	0.47
2:C:776:SER:HA	2:C:780:GLU:HB3	1.97	0.47
2:C:877:PRO:HG3	3:D:1020:LEU:CD1	2.44	0.47
3:D:1425:THR:HG23	3:D:1426:LYS:N	2.30	0.47
3:D:843:PHE:CD1	3:D:849:ALA:HA	2.50	0.47
1:K:97:VAL:HG12	1:K:99:LEU:HD12	1.97	0.47
1:K:225:PHE:CE1	1:L:25:LEU:HD22	2.50	0.47
1:L:94:LEU:HD11	1:L:119:ASP:HB3	1.96	0.47
2:M:167:LYS:HD3	2:M:168:ARG:N	2.30	0.47
2:M:164:PRO:HD2	2:M:170:PRO:O	2.15	0.47
2:M:202:TYR:OH	2:M:304:LEU:HD22	2.14	0.47
2:M:371:LYS:HB2	9:M:9512:HOH:O	2.14	0.47
2:M:423:ALA:HB1	9:M:9593:HOH:O	2.15	0.47
2:M:543:ASN:ND2	2:M:562:SER:HB3	2.30	0.47
3:N:137:PRO:HD2	3:N:453:ASP:HB2	1.97	0.47
3:N:36:THR:O	3:N:38:LYS:N	2.46	0.47
5:P:184:ARG:NH2	9:P:3604:HOH:O	2.46	0.47
5:P:409:LYS:HE3	5:P:410:TYR:CD1	2.49	0.47
2:C:144:PRO:HB2	9:C:9808:HOH:O	2.15	0.47
2:C:444:PRO:HG3	2:C:452:ILE:HD12	1.96	0.47
2:C:47:ALA:HA	2:C:50:GLU:OE2	2.15	0.47
2:C:515:ALA:C	2:C:516:ARG:HG2	2.35	0.47
2:C:56:GLU:CG	2:C:64:LEU:HD23	2.45	0.47
2:C:603:VAL:H	2:C:647:GLN:H	1.63	0.47
2:C:715:THR:HG22	9:C:2002:HOH:O	2.14	0.47
2:C:71:TYR:HD1	9:C:9517:HOH:O	1.97	0.47
3:D:1026:SER:C	3:D:1028:ALA:H	2.16	0.47
3:D:584:ASN:HB3	9:D:9515:HOH:O	2.15	0.47
3:D:730:PRO:HA	3:D:733:CYS:HG	1.80	0.47
5:F:188:ILE:HA	9:F:9537:HOH:O	2.15	0.47
5:F:287:THR:HG23	5:F:289:GLU:H	1.80	0.47
5:F:340:SER:OG	5:F:342:VAL:HG23	2.15	0.47
5:F:85:LEU:HB2	9:F:9663:HOH:O	2.14	0.47
1:L:189:ARG:HG3	1:L:189:ARG:NH1	2.30	0.47
2:M:1098:ASP:HB2	3:N:21:TRP:HZ2	1.78	0.47
2:M:470:PRO:HB2	2:M:534:VAL:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:96:ALA:HB3	9:M:9996:HOH:O	2.14	0.47
3:N:1101:VAL:HG22	3:N:1428:ALA:HB2	1.97	0.47
3:N:135:LEU:CD1	3:N:147:VAL:HG23	2.42	0.47
3:N:186:VAL:HG11	3:N:213:VAL:HB	1.97	0.47
3:N:510:GLU:O	3:N:513:ILE:HD12	2.14	0.47
3:N:639:LEU:HD12	3:N:639:LEU:H	1.80	0.47
3:N:64:LYS:HE3	9:N:9919:HOH:O	2.14	0.47
3:N:703:ASN:ND2	3:N:704:ARG:H	2.13	0.47
3:N:698:LYS:HA	3:N:756:GLN:NE2	2.30	0.47
3:N:844:ALA:HB3	3:N:848:GLU:OE2	2.15	0.47
4:O:5:GLY:HA3	4:O:8:LYS:HD2	1.96	0.47
1:A:206:THR:HG22	1:A:209:GLU:H	1.80	0.46
2:C:305:PRO:HG3	2:C:308:ARG:HH22	1.80	0.46
2:C:471:TYR:CD2	2:C:533:ASP:HA	2.50	0.46
2:C:721:ARG:O	2:C:758:ARG:HA	2.14	0.46
2:C:7:GLY:HA3	2:C:907:ASP:O	2.15	0.46
3:D:104:PHE:CE2	3:D:1448:THR:HG23	2.49	0.46
3:D:1102:THR:HG22	3:D:1222:GLY:CA	2.44	0.46
3:D:210:ARG:NH1	3:D:398:ALA:HB3	2.30	0.46
3:D:650:LEU:HD22	3:D:688:TRP:CH2	2.50	0.46
3:D:95:LEU:CD2	3:D:574:LEU:HD11	2.45	0.46
4:E:12:MET:HA	4:E:12:MET:CE	2.45	0.46
4:E:70:THR:HB	9:E:9533:HOH:O	2.14	0.46
5:F:209:PHE:HE2	5:F:213:ILE:HD11	1.80	0.46
1:K:12:THR:HG23	1:K:24:VAL:HB	1.97	0.46
1:L:57:TYR:CE1	1:L:163:ASN:HB2	2.41	0.46
1:L:99:LEU:HA	9:L:4955:HOH:O	2.15	0.46
2:M:170:PRO:HA	9:M:9800:HOH:O	2.14	0.46
2:M:50:GLU:HA	2:M:266:ARG:NH1	2.31	0.46
2:M:269:LEU:HD12	2:M:288:ARG:HG3	1.97	0.46
2:M:929:ARG:HH11	2:M:929:ARG:HG3	1.80	0.46
2:M:966:LEU:HD11	2:M:986:PRO:HG2	1.96	0.46
2:M:671:ASN:ND2	2:M:993:PHE:HB2	2.30	0.46
3:N:1026:SER:C	3:N:1028:ALA:H	2.17	0.46
2:M:1097:LEU:HD11	3:N:103:TRP:CZ3	2.50	0.46
3:N:551:ASN:O	3:N:555:LYS:HG3	2.14	0.46
3:N:87:ARG:HG3	3:N:88:TYR:CD2	2.50	0.46
3:N:968:ASP:O	3:N:971:LEU:HB3	2.15	0.46
3:N:972:LEU:O	3:N:976:GLN:HG3	2.14	0.46
5:P:122:LEU:HA	9:P:4063:HOH:O	2.14	0.46
1:A:23:PHE:CD1	1:A:211:LEU:HD23	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:VAL:HG13	1:B:142:VAL:HG12	1.96	0.46
1:B:85:LEU:HD13	1:B:127:LEU:HD23	1.97	0.46
2:C:208:ALA:HB1	2:C:218:VAL:CG1	2.45	0.46
2:C:110:GLU:HB2	2:C:368:THR:CG2	2.45	0.46
2:C:49:ARG:HH11	2:C:49:ARG:CB	2.23	0.46
1:A:178:ALA:CB	2:C:864:GLY:H	2.28	0.46
2:C:8:ARG:HB2	2:C:8:ARG:HH11	1.80	0.46
2:C:911:GLU:HB3	2:C:912:PRO:HD3	1.97	0.46
2:C:993:PHE:CD1	2:C:993:PHE:C	2.88	0.46
3:D:105:VAL:HG23	9:D:9538:HOH:O	2.15	0.46
3:D:1235:GLN:C	3:D:1359:GLN:HE22	2.18	0.46
3:D:1402:ALA:HB2	3:D:1415:VAL:HG23	1.96	0.46
3:D:1437:ALA:O	3:D:1446:VAL:HG21	2.15	0.46
3:D:168:THR:HA	9:D:9616:HOH:O	2.15	0.46
3:D:442:ASN:HA	9:D:9677:HOH:O	2.14	0.46
3:D:503:LEU:HD23	3:D:508:ARG:HH12	1.80	0.46
3:D:574:LEU:O	3:D:577:ALA:HB3	2.15	0.46
3:D:720:LEU:CD1	3:D:720:LEU:H	2.23	0.46
5:F:292:ALA:HB1	5:F:299:TRP:O	2.15	0.46
5:F:321:ILE:O	5:F:327:SER:HB3	2.15	0.46
1:L:5:LYS:HZ1	1:L:5:LYS:HA	1.81	0.46
2:M:101:ILE:HG22	2:M:102:HIS:H	1.80	0.46
2:M:185:LYS:HB3	2:M:188:LYS:O	2.15	0.46
2:M:205:GLU:CD	2:M:206:THR:N	2.68	0.46
2:M:352:ALA:O	2:M:356:ARG:HG3	2.16	0.46
2:M:498:GLN:CG	2:M:516:ARG:HH21	2.27	0.46
2:M:517:ARG:HG3	2:M:522:VAL:HG21	1.96	0.46
2:M:592:LEU:HD13	9:M:2275:HOH:O	2.14	0.46
2:M:770:GLU:HG2	3:N:65:ARG:HH22	1.79	0.46
2:M:810:ASP:HA	2:M:811:PRO:HD3	1.81	0.46
2:M:820:ARG:HG2	2:M:820:ARG:NH1	2.30	0.46
2:M:897:LEU:HD11	2:M:921:ALA:HA	1.96	0.46
3:N:196:VAL:HG12	9:N:9691:HOH:O	2.14	0.46
3:N:50:PHE:HB3	3:N:522:PRO:HG2	1.97	0.46
5:P:77:THR:O	5:P:81:VAL:HG23	2.15	0.46
1:A:205:VAL:HG23	1:A:206:THR:N	2.31	0.46
1:A:91:ASN:OD1	1:A:92:PRO:HD2	2.15	0.46
2:C:16:PRO:CG	2:C:460:ARG:HH12	2.28	0.46
2:C:642:ARG:HA	9:C:9967:HOH:O	2.15	0.46
2:C:757:GLY:HA2	2:C:789:SER:HB3	1.96	0.46
2:C:911:GLU:O	2:C:915:LYS:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:104:PHE:HB2	9:D:9538:HOH:O	2.15	0.46
3:D:1264:GLU:CD	3:D:1425:THR:H	2.19	0.46
3:D:171:LEU:HD13	3:D:389:GLU:C	2.35	0.46
3:D:196:VAL:HG13	3:D:202:VAL:CG1	2.46	0.46
2:C:1109:VAL:CG2	3:D:3:LYS:HG2	2.43	0.46
3:D:654:LYS:HD3	3:D:674:ARG:HH22	1.80	0.46
9:B:9616:HOH:O	3:D:813:LEU:HD21	2.15	0.46
3:D:844:ALA:O	3:D:867:ARG:HD2	2.15	0.46
3:D:859:ASP:O	3:D:877:PRO:HG2	2.16	0.46
5:F:123:ASP:HB2	5:F:126:LEU:HD13	1.98	0.46
1:L:133:GLU:HG3	1:L:134:GLU:HG2	1.97	0.46
2:M:342:ASP:O	2:M:346:VAL:HG23	2.16	0.46
2:M:403:SER:O	2:M:407:LYS:HG3	2.15	0.46
3:N:1020:LEU:HA	3:N:1023:MET:HE2	1.97	0.46
3:N:1124:GLN:HA	3:N:1125:PRO:HD3	1.70	0.46
3:N:1366:LYS:O	3:N:1370:ILE:HG12	2.16	0.46
3:N:1403:LEU:O	3:N:1407:LEU:HB2	2.16	0.46
3:N:1382:THR:OG1	3:N:1418:LYS:HE3	2.15	0.46
3:N:1465:ASN:HA	3:N:1465:ASN:HD22	1.49	0.46
3:N:54:LYS:HG3	3:N:55:ASP:OD1	2.16	0.46
4:O:86:GLN:HB3	4:O:86:GLN:HE21	1.59	0.46
5:P:139:ALA:HA	9:P:3321:HOH:O	2.15	0.46
5:P:320:PRO:CB	5:P:324:GLU:HG2	2.45	0.46
2:M:1067:TYR:HE2	5:P:342:VAL:HA	1.81	0.46
1:A:7:LYS:HD2	9:A:9499:HOH:O	2.15	0.46
2:C:961:GLU:HA	2:C:961:GLU:OE2	2.16	0.46
3:D:422:ALA:O	3:D:427:VAL:HG21	2.16	0.46
3:D:552:ASN:HA	3:D:555:LYS:HE3	1.96	0.46
3:D:56:TYR:CE2	3:D:66:GLN:HA	2.50	0.46
3:D:68:PHE:O	3:D:71:LYS:HG2	2.15	0.46
1:B:150:TYR:HD2	3:D:857:ILE:HG13	1.77	0.46
3:D:960:LYS:HG2	3:D:964:LEU:HD12	1.98	0.46
4:E:58:PRO:HB2	9:E:9487:HOH:O	2.16	0.46
5:F:287:THR:C	5:F:289:GLU:H	2.18	0.46
9:D:9547:HOH:O	5:F:349:LEU:HD12	2.15	0.46
1:L:34:VAL:HG12	9:M:9557:HOH:O	2.15	0.46
2:M:22:GLN:HE22	2:M:336:VAL:HG21	1.79	0.46
2:M:861:LEU:HD22	2:M:863:ASP:OD1	2.16	0.46
2:M:897:LEU:HG	2:M:920:GLN:HE21	1.77	0.46
3:N:957:PRO:HG3	3:N:1007:VAL:HA	1.98	0.46
3:N:1129:THR:HG23	3:N:1130:ARG:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1256:LEU:HA	3:N:1259:VAL:HG23	1.98	0.46
3:N:1431:THR:OG1	3:N:1432:LYS:N	2.49	0.46
3:N:580:ALA:HA	3:N:584:ASN:OD1	2.15	0.46
3:N:647:ARG:CZ	9:N:2258:HOH:O	2.63	0.46
5:P:317:LEU:O	5:P:329:TYR:HB3	2.15	0.46
5:P:416:ARG:CZ	5:P:419:ARG:HB3	2.46	0.46
1:A:101:LEU:HG	1:A:114:PHE:CA	2.43	0.46
1:A:30:ARG:NH1	1:A:191:ASP:HB2	2.31	0.46
1:A:9:PRO:HB3	1:A:25:LEU:CG	2.45	0.46
1:B:111:ALA:HB3	1:B:124:ASN:O	2.15	0.46
1:B:71:VAL:HG22	1:B:132:LEU:HD12	1.97	0.46
2:C:127:PHE:O	2:C:133:ASP:HA	2.16	0.46
2:C:39:ARG:HG3	9:C:9773:HOH:O	2.15	0.46
2:C:625:LEU:HB3	2:C:639:GLN:HB2	1.97	0.46
2:C:777:ILE:HG22	2:C:778:PHE:HD1	1.81	0.46
2:C:915:LYS:O	2:C:968:LEU:HD22	2.14	0.46
2:C:676:ILE:HG21	2:C:988:VAL:HG22	1.97	0.46
3:D:1046:GLN:HB2	9:D:9695:HOH:O	2.15	0.46
3:D:1295:GLU:HG2	9:D:9793:HOH:O	2.15	0.46
3:D:1299:PHE:N	3:D:1299:PHE:CD2	2.84	0.46
3:D:1306:PRO:HG3	9:D:9577:HOH:O	2.16	0.46
3:D:1486:VAL:HG12	3:D:1487:VAL:N	2.30	0.46
3:D:667:ALA:HB2	3:D:676:MET:HE1	1.97	0.46
3:D:708:LEU:HD23	3:D:708:LEU:HA	1.73	0.46
3:D:820:GLU:HA	3:D:825:ALA:O	2.16	0.46
3:D:829:VAL:HG11	9:D:2252:HOH:O	2.15	0.46
2:M:1104:GLU:H	2:M:1104:GLU:CD	2.19	0.46
2:M:17:PRO:O	2:M:20:GLU:N	2.46	0.46
2:M:429:ASP:HB3	9:M:9514:HOH:O	2.15	0.46
2:M:437:ARG:C	2:M:438:ILE:HD12	2.35	0.46
2:M:680:ASP:HB2	2:M:682:TYR:CE2	2.50	0.46
2:M:790:LEU:C	2:M:790:LEU:HD23	2.35	0.46
2:M:565:GLN:OE1	2:M:842:ARG:HG2	2.14	0.46
2:M:861:LEU:HD23	2:M:862:PRO:N	2.31	0.46
2:M:904:PRO:HG3	9:M:9623:HOH:O	2.16	0.46
3:N:1008:PHE:HB3	3:N:1012:GLU:OE2	2.15	0.46
3:N:1342:GLU:HB3	9:N:9577:HOH:O	2.15	0.46
3:N:416:ALA:HB3	3:N:417:PRO:HD3	1.97	0.46
3:N:562:ALA:HB1	3:N:567:ILE:CD1	2.45	0.46
5:P:127:ILE:HD11	9:P:4895:HOH:O	2.16	0.46
5:P:314:PRO:HD2	9:P:4162:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:1016:ILE:HD12	5:P:317:LEU:HD21	1.97	0.46
1:A:43:ILE:HA	1:A:47:SER:OG	2.16	0.46
2:C:1013:TYR:HB2	5:F:335:ASP:OD2	2.15	0.46
2:C:1101:THR:O	2:C:1102:LEU:HD12	2.15	0.46
2:C:129:ILE:HG12	2:C:386:PHE:O	2.16	0.46
2:C:115:LEU:HD12	2:C:378:LEU:HD22	1.97	0.46
2:C:3:ILE:CD1	2:C:900:ARG:HB2	2.46	0.46
2:C:777:ILE:HG22	2:C:778:PHE:CD1	2.51	0.46
2:C:93:PRO:HB2	9:C:9537:HOH:O	2.14	0.46
3:D:1139:ASP:O	3:D:1142:ALA:HB3	2.15	0.46
3:D:1258:ARG:HG3	3:D:1262:LEU:HD13	1.96	0.46
3:D:1331:ASP:OD1	3:D:1333:HIS:HB2	2.15	0.46
3:D:1346:ARG:HB2	3:D:1346:ARG:NH1	2.30	0.46
3:D:22:SER:HB3	9:D:9666:HOH:O	2.16	0.46
3:D:208:PRO:CB	3:D:395:VAL:HG13	2.45	0.46
3:D:397:LYS:NZ	3:D:399:ARG:HH21	2.13	0.46
3:D:396:VAL:CG2	3:D:447:VAL:HB	2.42	0.46
3:D:581:LEU:HD12	3:D:603:LEU:HD12	1.96	0.46
3:D:860:LEU:O	3:D:877:PRO:HD2	2.16	0.46
3:D:93:ILE:HG12	3:D:548:ILE:HD12	1.98	0.46
3:D:983:LEU:HB2	9:D:9513:HOH:O	2.16	0.46
5:F:353:GLU:OE1	5:F:356:LYS:HD2	2.16	0.46
1:K:9:PRO:HG2	1:L:224:TYR:CD2	2.51	0.46
1:L:159:LYS:N	1:L:159:LYS:HD3	2.31	0.46
2:M:409:ARG:HG2	9:M:2089:HOH:O	2.16	0.46
2:M:4:LYS:HE3	9:M:9956:HOH:O	2.15	0.46
2:M:428:ARG:O	3:N:1078:ARG:NH1	2.49	0.46
3:N:1383:ASP:HB3	3:N:1416:ALA:H	1.81	0.46
3:N:434:ARG:HG3	9:N:9784:HOH:O	2.14	0.46
3:N:608:SER:OG	3:N:609:GLY:N	2.46	0.46
3:N:899:LEU:CD1	3:N:900:ILE:HG23	2.46	0.46
3:N:928:ALA:O	3:N:931:LEU:HB2	2.16	0.46
4:O:4:PRO:HG3	9:O:5463:HOH:O	2.15	0.46
4:O:5:GLY:O	4:O:9:LEU:HG	2.15	0.46
3:N:388:HIS:H	5:P:97:GLU:HG3	1.79	0.46
1:A:86:VAL:HG23	1:A:202:ASP:OD1	2.16	0.46
1:B:123:MET:CG	9:B:9635:HOH:O	2.64	0.46
2:C:1049:LEU:HG	2:C:1053:LEU:HD11	1.96	0.46
2:C:1092:LEU:HD22	2:C:1099:VAL:CG2	2.46	0.46
2:C:289:THR:HG22	2:C:290:LEU:H	1.80	0.46
2:C:289:THR:HG22	2:C:290:LEU:HD22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1496:GLU:HA	3:D:1499:ARG:CD	2.45	0.46
3:D:468:LEU:HB3	9:D:9997:HOH:O	2.16	0.46
3:D:847:ASP:OD1	3:D:848:GLU:N	2.49	0.46
3:D:867:ARG:CB	3:D:867:ARG:HH11	2.29	0.46
3:D:919:PHE:O	3:D:919:PHE:HD2	1.98	0.46
4:E:54:LEU:HG	4:E:58:PRO:HG2	1.97	0.46
1:L:123:MET:O	1:L:125:PRO:HD3	2.16	0.46
1:L:69:PRO:HB3	9:L:5138:HOH:O	2.16	0.46
2:M:575:GLN:HB3	2:M:670:GLN:HA	1.97	0.46
2:M:73:LEU:HB2	9:M:2197:HOH:O	2.15	0.46
2:M:952:LEU:HD22	2:M:952:LEU:N	2.29	0.46
3:N:1000:THR:HG23	3:N:1001:GLU:N	2.30	0.46
3:N:1300:SER:HB2	9:N:2406:HOH:O	2.15	0.46
3:N:1304:LYS:HB3	9:N:9487:HOH:O	2.15	0.46
3:N:42:ASP:O	3:N:46:ASP:HB2	2.16	0.46
3:N:558:LEU:HD13	5:P:145:PRO:CB	2.41	0.46
3:N:82:LYS:NZ	3:N:82:LYS:HB2	2.31	0.46
9:M:2201:HOH:O	4:O:32:ARG:HD3	2.16	0.46
4:O:61:GLU:HG3	4:O:61:GLU:H	1.49	0.46
5:P:215:GLU:O	5:P:218:GLN:HB3	2.16	0.46
5:P:343:ASP:HA	9:P:5842:HOH:O	2.15	0.46
1:B:89:PHE:CD1	1:B:120:VAL:HG22	2.50	0.46
2:C:524:VAL:HG22	9:C:2060:HOH:O	2.15	0.46
2:C:630:ARG:HE	2:C:705:ILE:CG1	2.29	0.46
2:C:705:ILE:HG22	2:C:827:VAL:O	2.16	0.46
3:D:1003:VAL:O	3:D:1007:VAL:HG13	2.16	0.46
3:D:1209:LEU:HD23	3:D:1211:MET:H	1.80	0.46
3:D:1359:GLN:HE21	3:D:1359:GLN:HB3	1.51	0.46
3:D:1101:VAL:HG12	3:D:1374:GLN:HB3	1.97	0.46
3:D:44:LEU:HB3	3:D:525:ARG:NH2	2.22	0.46
2:C:1005:MET:CB	3:D:629:SER:HB2	2.45	0.46
3:D:984:THR:HG22	3:D:987:GLU:CD	2.35	0.46
1:K:58:ILE:HD13	1:K:140:MET:HB3	1.96	0.46
1:L:23:PHE:CE1	1:L:208:LEU:HD13	2.50	0.46
2:M:1054:THR:HG21	2:M:1079:PRO:HB3	1.96	0.46
2:M:343:GLN:HB2	9:M:9681:HOH:O	2.15	0.46
2:M:137:VAL:O	2:M:391:LEU:HD21	2.15	0.46
2:M:636:ALA:HB2	2:M:703:ILE:HG22	1.97	0.46
2:M:669:GLY:O	2:M:670:GLN:HG2	2.15	0.46
2:M:841:ASN:HD22	2:M:843:HIS:N	2.14	0.46
3:N:1252:ILE:HG22	3:N:1253:THR:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:181:ASP:O	3:N:185:VAL:HG23	2.16	0.46
3:N:191:LEU:HD22	3:N:195:VAL:CG2	2.45	0.46
3:N:441:ARG:O	3:N:443:VAL:N	2.49	0.46
3:N:669:ASN:O	3:N:672:ALA:HB3	2.15	0.46
4:O:45:ARG:HB2	4:O:46:PRO:CD	2.45	0.46
5:P:226:LYS:HB2	5:P:238:TYR:OH	2.16	0.46
5:P:319:THR:HG21	9:P:5402:HOH:O	2.16	0.46
1:A:13:VAL:HG12	1:A:15:THR:HG22	1.96	0.46
2:C:252:LYS:HZ2	2:C:296:GLY:HA3	1.81	0.46
2:C:319:GLY:HA3	9:C:2214:HOH:O	2.16	0.46
2:C:595:LEU:HB2	9:C:2223:HOH:O	2.15	0.46
2:C:682:TYR:N	9:C:9490:HOH:O	2.49	0.46
2:C:72:ARG:HB3	9:C:2179:HOH:O	2.15	0.46
2:C:705:ILE:HA	2:C:827:VAL:O	2.16	0.46
3:D:1277:ILE:CD1	3:D:1301:LYS:HB2	2.44	0.46
3:D:413:ASP:OD1	3:D:421:LEU:HD22	2.15	0.46
3:D:827:ILE:O	3:D:837:GLY:HA3	2.16	0.46
5:F:289:GLU:O	5:F:293:GLU:HG3	2.16	0.46
2:M:305:PRO:CG	2:M:308:ARG:HH21	2.25	0.46
2:M:329:GLY:N	2:M:488:ALA:HB3	2.31	0.46
2:M:599:GLU:HB2	9:M:9583:HOH:O	2.15	0.46
2:M:918:LEU:HD23	2:M:968:LEU:HA	1.96	0.46
3:N:704:ARG:CZ	3:N:737:ASN:O	2.64	0.46
5:P:422:LEU:HD11	9:P:3715:HOH:O	2.16	0.46
1:A:86:VAL:HG12	1:A:124:ASN:HB2	1.98	0.46
1:A:195:LEU:CD1	1:A:197:LEU:HD22	2.40	0.46
2:C:118:ILE:HG22	2:C:382:ILE:HD13	1.98	0.46
2:C:242:LEU:HA	9:C:9503:HOH:O	2.16	0.46
2:C:136:ILE:CG2	2:C:336:VAL:HG13	2.43	0.46
2:C:761:PHE:CD1	2:C:761:PHE:N	2.84	0.46
3:D:1258:ARG:HH21	3:D:1351:GLU:HG2	1.81	0.46
3:D:591:VAL:HG12	3:D:592:THR:O	2.16	0.46
3:D:694:VAL:HG13	9:D:2053:HOH:O	2.16	0.46
3:D:68:PHE:HA	3:D:71:LYS:NZ	2.31	0.46
2:M:1090:LYS:HE2	2:M:1112:PHE:CE1	2.51	0.46
2:M:146:VAL:HG11	2:M:306:THR:HG22	1.98	0.46
2:M:205:GLU:O	2:M:209:ARG:HD2	2.15	0.46
2:M:311:PHE:HB2	9:M:2157:HOH:O	2.16	0.46
2:M:438:ILE:HG22	2:M:439:CYS:O	2.16	0.46
2:M:708:TYR:N	2:M:708:TYR:CD1	2.79	0.46
2:M:91:GLN:CD	2:M:117:HIS:HB3	2.37	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:675:ALA:CA	2:M:989:VAL:HG12	2.37	0.46
3:N:1114:THR:HA	9:N:2201:HOH:O	2.16	0.46
3:N:1481:VAL:HG13	4:O:18:ARG:NE	2.27	0.46
3:N:213:VAL:HG22	3:N:214:GLU:H	1.81	0.46
3:N:31:THR:HB	3:N:32:ILE:H	1.62	0.46
3:N:411:THR:HG22	9:N:2263:HOH:O	2.16	0.46
3:N:630:VAL:HG12	3:N:631:ILE:N	2.30	0.46
3:N:667:ALA:HB2	9:N:2385:HOH:O	2.15	0.46
5:P:102:LEU:HD22	5:P:183:ALA:O	2.15	0.46
9:M:2448:HOH:O	5:P:283:GLY:HA2	2.15	0.46
1:A:9:PRO:HB3	1:A:25:LEU:HG	1.98	0.45
1:B:89:PHE:CD1	1:B:120:VAL:HG13	2.51	0.45
2:C:207:LEU:HD22	2:C:221:LEU:CD2	2.46	0.45
2:C:354:GLY:HA2	9:C:9624:HOH:O	2.15	0.45
2:C:860:HIS:HE2	2:C:975:TYR:HB2	1.81	0.45
3:D:1043:GLY:O	3:D:1056:PRO:HB3	2.15	0.45
3:D:1106:VAL:HG21	3:D:1474:ALA:HB2	1.99	0.45
3:D:1346:ARG:HB2	3:D:1346:ARG:HH11	1.81	0.45
3:D:1403:LEU:HD12	9:D:2493:HOH:O	2.15	0.45
3:D:235:ALA:HB3	9:D:2112:HOH:O	2.16	0.45
3:D:531:ASP:HB2	9:D:2123:HOH:O	2.16	0.45
3:D:564:GLU:HB2	9:F:9561:HOH:O	2.16	0.45
5:F:226:LYS:HE3	9:F:9804:HOH:O	2.17	0.45
1:L:153:ALA:HA	1:L:156:HIS:NE2	2.30	0.45
2:M:60:GLY:HA2	9:M:9972:HOH:O	2.16	0.45
2:M:822:VAL:HG13	9:M:9775:HOH:O	2.15	0.45
3:N:1122:LEU:HD23	3:N:1178:ALA:HB2	1.98	0.45
3:N:1495:ILE:O	3:N:1498:ALA:HB3	2.16	0.45
3:N:586:ARG:HG2	9:N:2658:HOH:O	2.16	0.45
1:A:211:LEU:HD12	1:A:211:LEU:O	2.16	0.45
1:A:216:GLU:HG3	1:A:220:GLU:OE1	2.16	0.45
1:B:87:VAL:HA	9:B:9635:HOH:O	2.16	0.45
2:C:339:LEU:HB3	2:C:385:PHE:HZ	1.81	0.45
2:C:43:GLY:HA2	2:C:341:THR:OG1	2.16	0.45
2:C:471:TYR:HE1	2:C:491:GLU:OE2	1.99	0.45
2:C:578:VAL:HG21	2:C:991:GLN:O	2.16	0.45
2:C:742:VAL:HG23	9:C:2181:HOH:O	2.15	0.45
2:C:773:LEU:O	2:C:777:ILE:HG13	2.16	0.45
3:D:1007:VAL:HG23	3:D:1008:PHE:N	2.32	0.45
3:D:1290:LEU:CD2	3:D:1291:SER:H	2.28	0.45
3:D:29:PRO:HG3	3:D:549:ASN:ND2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:1051:GLU:HG2	2:M:1056:LYS:CD	2.44	0.45
2:M:1086:ARG:HH11	2:M:1112:PHE:HA	1.82	0.45
2:M:603:VAL:HG23	2:M:647:GLN:O	2.16	0.45
2:M:811:PRO:HD3	9:M:9734:HOH:O	2.16	0.45
2:M:83:CYS:CA	2:M:88:LEU:HB3	2.42	0.45
2:M:893:ALA:O	2:M:897:LEU:HD22	2.16	0.45
2:M:890:LEU:HA	2:M:914:ILE:HD13	1.96	0.45
3:N:1087:ARG:HG2	3:N:1087:ARG:HH11	1.81	0.45
3:N:1246:VAL:HG21	9:N:2444:HOH:O	2.16	0.45
3:N:1272:ALA:CA	3:N:1326:THR:HB	2.44	0.45
3:N:1365:ASP:O	3:N:1369:GLU:HG3	2.16	0.45
3:N:156:GLU:O	3:N:159:ARG:HB3	2.17	0.45
3:N:523:ASP:O	3:N:526:PRO:HG3	2.17	0.45
3:N:765:SER:O	3:N:767:HIS:N	2.49	0.45
3:N:827:ILE:O	3:N:837:GLY:HA3	2.16	0.45
4:O:61:GLU:O	4:O:65:MET:HE2	2.16	0.45
4:O:69:LEU:O	4:O:69:LEU:HD23	2.16	0.45
5:P:132:ARG:NH1	5:P:136:LEU:HD21	2.27	0.45
1:A:206:THR:CG2	1:A:209:GLU:H	2.30	0.45
1:A:9:PRO:HD2	1:B:224:TYR:CE1	2.52	0.45
2:C:1021:LEU:HG	2:C:1022:GLY:N	2.31	0.45
2:C:10:ARG:HH11	2:C:11:GLU:H	1.63	0.45
2:C:16:PRO:O	2:C:18:LEU:HD12	2.16	0.45
2:C:238:LEU:HD23	2:C:241:LEU:HB3	1.99	0.45
2:C:30:LEU:HD12	2:C:30:LEU:O	2.16	0.45
2:C:68:PHE:HZ	2:C:71:TYR:HB3	1.80	0.45
2:C:873:PRO:O	2:C:876:VAL:HG23	2.16	0.45
2:C:675:ALA:CA	2:C:989:VAL:HG12	2.40	0.45
3:D:115:LEU:HD22	3:D:502:PHE:HE1	1.80	0.45
3:D:1256:LEU:HA	3:D:1259:VAL:HG23	1.98	0.45
3:D:618:LEU:HD11	3:D:1463:LYS:HD2	1.97	0.45
3:D:411:THR:HG23	9:D:9915:HOH:O	2.16	0.45
3:D:135:LEU:HA	3:D:453:ASP:O	2.16	0.45
3:D:493:ARG:HG2	3:D:493:ARG:NH1	2.30	0.45
3:D:750:PRO:O	3:D:756:GLN:OE1	2.35	0.45
3:D:799:LYS:N	3:D:826:PRO:HG2	2.31	0.45
5:F:104:ARG:CZ	9:F:9749:HOH:O	2.64	0.45
5:F:220:LEU:O	5:F:224:VAL:HG23	2.15	0.45
1:K:184:THR:O	1:K:192:LEU:HB2	2.16	0.45
1:L:206:THR:HG23	1:L:208:LEU:N	2.31	0.45
2:M:52:PHE:O	2:M:54:ILE:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:713:ARG:NH2	2:M:819:VAL:HG22	2.32	0.45
2:M:768:THR:CG2	2:M:771:GLU:HB3	2.46	0.45
2:M:77:PRO:HD3	2:M:93:PRO:HD3	1.98	0.45
2:M:950:LEU:HB3	2:M:952:LEU:HD23	1.98	0.45
2:M:68:PHE:CE1	2:M:96:ALA:HB1	2.44	0.45
3:N:1012:GLU:HG3	3:N:1021:TYR:OH	2.15	0.45
3:N:128:TYR:HB3	3:N:129:PHE:CD1	2.51	0.45
3:N:1380:GLU:HB2	3:N:1420:LEU:HD23	1.98	0.45
3:N:1425:THR:CG2	3:N:1426:LYS:N	2.79	0.45
3:N:1500:LYS:O	3:N:1503:VAL:HG23	2.16	0.45
3:N:65:ARG:H	3:N:68:PHE:HZ	1.64	0.45
3:N:696:HIS:HB2	4:O:48:MET:CE	2.47	0.45
5:P:338:LEU:HB2	9:P:5459:HOH:O	2.16	0.45
1:A:111:ALA:HB3	1:A:124:ASN:O	2.16	0.45
1:B:189:ARG:HG3	9:B:9505:HOH:O	2.16	0.45
2:C:165:LEU:HA	2:C:166:PRO:O	2.16	0.45
2:C:261:ILE:HA	9:C:2458:HOH:O	2.17	0.45
2:C:455:LEU:O	2:C:541:SER:HB3	2.16	0.45
2:C:598:GLU:HB2	2:C:615:TYR:OH	2.17	0.45
2:C:64:LEU:HB2	2:C:359:MET:SD	2.56	0.45
2:C:80:GLN:O	2:C:83:CYS:HB2	2.17	0.45
2:C:939:ARG:HG3	9:C:9564:HOH:O	2.16	0.45
3:D:1278:ASP:HB2	3:D:1318:TYR:CE1	2.51	0.45
3:D:153:LEU:HD11	3:D:157:GLU:HB2	1.97	0.45
3:D:191:LEU:HD22	3:D:195:VAL:HG11	1.98	0.45
3:D:427:VAL:HB	3:D:435:VAL:HB	1.99	0.45
3:D:462:GLN:HB2	3:D:513:ILE:HG21	1.98	0.45
3:D:661:MET:SD	3:D:687:VAL:HG22	2.57	0.45
3:D:862:ASP:O	3:D:877:PRO:HD3	2.16	0.45
3:D:926:LYS:HE3	9:D:9911:HOH:O	2.16	0.45
3:D:957:PRO:HG3	3:D:1010:ASN:HD22	1.81	0.45
3:D:965:GLU:HB2	9:D:9490:HOH:O	2.16	0.45
4:E:37:ASN:HD22	4:E:89:MET:HE2	1.81	0.45
5:F:270:LYS:HB3	5:F:295:MET:CE	2.46	0.45
1:K:30:ARG:HG3	1:K:30:ARG:NH1	2.31	0.45
2:M:127:PHE:O	2:M:133:ASP:HA	2.16	0.45
2:M:435:TYR:C	2:M:437:ARG:H	2.18	0.45
2:M:626:ARG:HG2	9:M:2116:HOH:O	2.15	0.45
2:M:905:ILE:HG22	2:M:906:PHE:CD1	2.52	0.45
3:N:1326:THR:HG22	3:N:1327:ARG:H	1.81	0.45
3:N:171:LEU:HB2	3:N:390:PRO:CA	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:171:LEU:HA	3:N:390:PRO:HA	1.97	0.45
3:N:427:VAL:HB	3:N:435:VAL:CG2	2.47	0.45
3:N:95:LEU:HA	3:N:551:ASN:OD1	2.15	0.45
1:A:182:GLU:HB3	9:A:9489:HOH:O	2.17	0.45
1:A:59:GLU:HG3	1:A:139:ASN:CG	2.37	0.45
2:C:1039:ALA:O	2:C:1043:TYR:HD1	1.98	0.45
2:C:115:LEU:HD22	2:C:373:VAL:CG1	2.46	0.45
2:C:410:ILE:HD12	2:C:410:ILE:N	2.32	0.45
2:C:140:ILE:CD1	2:C:412:ALA:HA	2.47	0.45
2:C:716:LYS:HE3	9:C:9571:HOH:O	2.16	0.45
2:C:839:LEU:N	2:C:839:LEU:HD23	2.31	0.45
2:C:9:ILE:O	2:C:9:ILE:HG13	2.16	0.45
3:D:1341:PRO:O	3:D:1344:VAL:HG23	2.17	0.45
3:D:153:LEU:HD13	3:D:157:GLU:HB2	1.98	0.45
3:D:521:PRO:C	3:D:525:ARG:HH11	2.20	0.45
5:F:113:ILE:HG23	5:F:127:ILE:CG2	2.47	0.45
5:F:215:GLU:N	9:F:9503:HOH:O	2.48	0.45
5:F:393:THR:O	5:F:397:ILE:HG13	2.16	0.45
1:L:110:LYS:HD3	9:L:4382:HOH:O	2.16	0.45
2:M:1036:GLU:O	2:M:1039:ALA:HB3	2.16	0.45
2:M:1085:PHE:O	2:M:1089:VAL:HG23	2.17	0.45
2:M:164:PRO:HG2	9:M:9517:HOH:O	2.17	0.45
2:M:267:TYR:HB2	2:M:272:ALA:CB	2.47	0.45
2:M:64:LEU:HB2	2:M:359:MET:SD	2.56	0.45
2:M:110:GLU:CG	2:M:369:PRO:HG3	2.29	0.45
3:N:1033:GLN:HB3	9:N:9622:HOH:O	2.17	0.45
3:N:1240:THR:O	3:N:1257:PRO:HB3	2.17	0.45
3:N:28:LYS:O	3:N:43:GLY:HA2	2.16	0.45
3:N:806:PHE:CG	3:N:806:PHE:O	2.69	0.45
3:N:950:GLY:O	3:N:951:ILE:C	2.54	0.45
3:N:984:THR:HG22	3:N:987:GLU:CG	2.40	0.45
1:A:128:HIS:CE1	1:A:131:THR:HG23	2.51	0.45
1:B:86:VAL:HG13	1:B:123:MET:HB2	1.98	0.45
1:B:27:PRO:HG2	1:B:186:LEU:CD1	2.46	0.45
1:A:218:LEU:HD23	1:B:222:LEU:HD21	1.99	0.45
2:C:1101:THR:HB	3:D:5:VAL:CG1	2.46	0.45
2:C:165:LEU:HD12	2:C:166:PRO:C	2.37	0.45
2:C:286:SER:HB3	2:C:299:LYS:HE3	1.98	0.45
2:C:41:ASN:N	2:C:41:ASN:HD22	1.97	0.45
2:C:631:SER:HB3	2:C:637:LEU:HD21	1.99	0.45
2:C:863:ASP:O	2:C:865:THR:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1467:ILE:HG13	9:D:9868:HOH:O	2.16	0.45
3:D:171:LEU:HD11	3:D:388:HIS:CB	2.46	0.45
3:D:169:TYR:HA	3:D:392:SER:HA	1.99	0.45
3:D:399:ARG:HB3	3:D:402:PRO:HG3	1.98	0.45
2:C:713:ARG:NH1	3:D:532:GLY:HA2	2.31	0.45
3:D:566:ILE:CG1	5:F:192:LEU:HD11	2.46	0.45
3:D:619:LEU:HB2	9:D:9516:HOH:O	2.15	0.45
3:D:729:HIS:ND1	3:D:730:PRO:N	2.64	0.45
3:D:553:ARG:HH22	5:F:211:ASP:CG	2.19	0.45
5:F:241:TRP:HA	5:F:244:ARG:NH1	2.31	0.45
5:F:263:HIS:HB2	9:F:9611:HOH:O	2.17	0.45
5:F:282:LEU:HB2	5:F:284:ARG:H	1.81	0.45
1:L:189:ARG:HG3	1:L:189:ARG:HH11	1.81	0.45
1:L:9:PRO:HB3	1:L:25:LEU:HG	1.98	0.45
1:L:94:LEU:HD11	9:L:4208:HOH:O	2.16	0.45
2:M:380:ALA:HA	2:M:383:ARG:HG2	1.99	0.45
2:M:516:ARG:NH2	3:N:1068:LEU:HB2	2.32	0.45
2:M:626:ARG:HB2	2:M:639:GLN:NE2	2.31	0.45
2:M:704:HIS:CG	2:M:831:ARG:HH21	2.34	0.45
2:M:68:PHE:CZ	2:M:71:TYR:HB3	2.49	0.45
2:M:897:LEU:HD22	2:M:921:ALA:HB2	1.98	0.45
3:N:1114:THR:HG23	3:N:1114:THR:O	2.16	0.45
3:N:1213:ARG:HD3	9:N:2343:HOH:O	2.15	0.45
3:N:1353:GLN:HE21	3:N:1353:GLN:HB3	1.54	0.45
3:N:1353:GLN:HE21	3:N:1357:ARG:NE	2.15	0.45
3:N:179:VAL:HG22	3:N:389:GLU:HG3	1.99	0.45
3:N:651:GLU:HA	3:N:651:GLU:OE1	2.17	0.45
2:M:1104:GLU:HA	3:N:6:ARG:HD3	1.97	0.45
3:N:729:HIS:CE1	3:N:731:LEU:HG	2.47	0.45
3:N:728:LEU:HD11	3:N:732:VAL:CG2	2.46	0.45
4:O:17:TYR:O	4:O:21:VAL:HG23	2.16	0.45
5:P:128:ARG:O	5:P:132:ARG:HG3	2.16	0.45
5:P:141:VAL:O	5:P:145:PRO:HD2	2.15	0.45
1:B:101:LEU:HB2	1:B:114:PHE:CD2	2.51	0.45
1:B:44:LEU:HD23	1:B:48:ILE:CD1	2.47	0.45
2:C:1060:ILE:HG23	2:C:1061:GLU:N	2.31	0.45
2:C:326:ASP:HB2	2:C:431:HIS:ND1	2.32	0.45
2:C:693:GLU:OE2	2:C:855:VAL:HG21	2.17	0.45
2:C:817:PRO:C	2:C:819:VAL:H	2.20	0.45
2:C:704:HIS:CG	2:C:831:ARG:HE	2.34	0.45
3:D:1084:THR:HG22	9:D:9646:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1094:LEU:HD23	9:D:9776:HOH:O	2.16	0.45
3:D:1258:ARG:NE	3:D:1262:LEU:HD11	2.32	0.45
3:D:1312:LEU:HB2	9:D:2444:HOH:O	2.16	0.45
3:D:1383:ASP:HB3	3:D:1416:ALA:H	1.82	0.45
3:D:507:ASN:HB3	9:D:9971:HOH:O	2.17	0.45
3:D:639:LEU:CD1	3:D:640:HIS:H	2.29	0.45
3:D:666:ILE:HG13	3:D:666:ILE:H	1.61	0.45
3:D:700:VAL:HB	3:D:748:HIS:O	2.17	0.45
4:E:13:VAL:HG21	4:E:19:LEU:HB2	1.98	0.45
3:D:767:HIS:CD2	4:E:6:ILE:HG12	2.52	0.45
5:F:374:GLY:N	9:F:9672:HOH:O	2.49	0.45
1:K:20:TYR:CE2	1:K:22:GLU:HG2	2.52	0.45
2:M:3:ILE:HG21	9:M:2314:HOH:O	2.16	0.45
2:M:688:ILE:N	2:M:688:ILE:HD12	2.31	0.45
2:M:861:LEU:HD21	2:M:925:TYR:CE2	2.51	0.45
3:N:1312:LEU:CB	9:N:9707:HOH:O	2.64	0.45
3:N:1432:LYS:HG3	3:N:1432:LYS:H	1.48	0.45
3:N:1435:LEU:HD23	3:N:1464:GLU:HB2	1.98	0.45
3:N:197:SER:HB2	3:N:205:TYR:OH	2.17	0.45
3:N:379:ALA:HB2	9:N:9717:HOH:O	2.15	0.45
3:N:130:SER:O	3:N:568:ARG:NH2	2.50	0.45
3:N:647:ARG:CZ	3:N:680:GLN:HE21	2.29	0.45
3:N:683:ILE:HG22	9:N:2260:HOH:O	2.16	0.45
3:N:701:LEU:H	3:N:701:LEU:HD22	1.82	0.45
3:N:989:TYR:HB2	9:N:9817:HOH:O	2.17	0.45
4:O:70:THR:CB	4:O:72:ARG:HE	2.29	0.45
4:O:75:PHE:HD1	9:O:5601:HOH:O	1.99	0.45
5:P:392:VAL:CG1	5:P:396:ARG:HG3	2.47	0.45
1:A:100:LEU:N	9:A:9585:HOH:O	2.48	0.45
1:B:102:LYS:HE2	1:B:104:GLU:OE1	2.17	0.45
2:C:114:PHE:CD1	2:C:114:PHE:N	2.84	0.45
2:C:4:LYS:HB2	9:C:9680:HOH:O	2.17	0.45
2:C:886:LEU:CG	3:D:951:ILE:HG13	2.46	0.45
3:D:1264:GLU:OE2	3:D:1264:GLU:HA	2.16	0.45
3:D:127:LEU:HD21	3:D:461:ILE:CD1	2.44	0.45
3:D:637:LEU:HD11	3:D:641:GLN:HB2	1.99	0.45
3:D:728:LEU:HD13	3:D:745:MET:CE	2.45	0.45
3:D:764:LEU:HD12	3:D:765:SER:N	2.32	0.45
4:E:25:LYS:HA	4:E:28:GLN:NE2	2.32	0.45
5:F:193:ARG:NH2	9:F:9492:HOH:O	2.50	0.45
5:F:84:TYR:CD2	5:F:192:LEU:HD13	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:1034:GLU:CA	2:M:1037:VAL:HG23	2.47	0.45
3:N:996:TRP:O	3:N:1000:THR:HG22	2.17	0.45
3:N:1348:LEU:HA	3:N:1348:LEU:HD13	1.81	0.45
3:N:963:TYR:CE2	3:N:1002:LYS:HB3	2.52	0.45
4:O:43:GLU:HG2	4:O:44:GLU:N	2.32	0.45
4:O:33:HIS:CD2	4:O:89:MET:HG2	2.52	0.45
4:O:87:LYS:HE2	4:O:91:ARG:CZ	2.47	0.45
5:P:154:LYS:HE3	5:P:158:GLU:HG2	1.98	0.45
5:P:270:LYS:HE2	9:P:5582:HOH:O	2.17	0.45
3:N:598:ARG:NH2	5:P:318:GLU:O	2.48	0.45
5:P:372:ARG:HG2	9:P:6083:HOH:O	2.17	0.45
2:C:1060:ILE:CG2	2:C:1061:GLU:N	2.80	0.45
2:C:1088:LEU:HA	2:C:1091:GLU:OE1	2.17	0.45
2:C:20:GLU:HG2	2:C:21:ILE:N	2.31	0.45
2:C:532:MET:HG3	2:C:533:ASP:N	2.32	0.45
2:C:70:GLU:HB2	2:C:97:ARG:HD2	1.98	0.45
2:C:89:THR:HG21	2:C:383:ARG:HH22	1.82	0.45
3:D:180:LYS:HG3	9:D:2419:HOH:O	2.17	0.45
3:D:127:LEU:CD1	3:D:457:GLY:H	2.30	0.45
3:D:853:VAL:HG22	3:D:858:VAL:HG23	1.99	0.45
3:D:90:MET:N	9:D:9497:HOH:O	2.50	0.45
5:F:132:ARG:HG2	5:F:181:GLU:CD	2.36	0.45
5:F:196:VAL:HG13	5:F:213:ILE:CD1	2.46	0.45
5:F:370:LYS:HZ3	5:F:371:LEU:HG	1.81	0.45
1:K:41:ARG:NH1	1:K:177:VAL:HB	2.32	0.45
1:K:91:ASN:H	1:K:94:LEU:HD12	1.82	0.45
1:K:89:PHE:CB	1:K:94:LEU:HD13	2.45	0.45
2:M:1039:ALA:O	2:M:1043:TYR:HD1	2.00	0.45
2:M:290:LEU:HB3	2:M:302:VAL:HG12	1.98	0.45
2:M:52:PHE:HB3	2:M:53:PRO:HD3	1.99	0.45
2:M:842:ARG:HB2	9:M:9551:HOH:O	2.16	0.45
2:M:987:ILE:HG12	3:N:948:THR:CG2	2.47	0.45
3:N:1038:LEU:O	3:N:1060:SER:HB2	2.17	0.45
3:N:1175:ILE:O	3:N:1179:GLU:HG3	2.16	0.45
3:N:1211:MET:HG2	3:N:1213:ARG:NE	2.32	0.45
3:N:1390:LEU:HD22	9:N:2508:HOH:O	2.16	0.45
9:M:2262:HOH:O	3:N:3:LYS:HB3	2.17	0.45
3:N:411:THR:HG21	9:N:9532:HOH:O	2.17	0.45
3:N:637:LEU:HD11	3:N:641:GLN:HB2	1.99	0.45
3:N:82:LYS:HD3	5:P:337:HIS:HB3	1.99	0.45
3:N:55:ASP:HA	3:N:82:LYS:HE3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:972:LEU:HD21	3:N:976:GLN:HE21	1.82	0.45
5:P:134:LYS:HA	9:P:4179:HOH:O	2.16	0.45
1:A:99:LEU:C	1:A:100:LEU:HD12	2.37	0.45
1:A:133:GLU:CG	1:A:134:GLU:N	2.76	0.45
1:A:197:LEU:HD23	1:A:197:LEU:H	1.82	0.45
1:B:77:GLU:HB2	3:D:872:ARG:NH2	2.30	0.45
2:C:1051:GLU:HG2	2:C:1056:LYS:HG3	1.98	0.45
2:C:196:LEU:HD21	2:C:303:PHE:CG	2.52	0.45
2:C:211:LEU:HD11	2:C:308:ARG:CB	2.37	0.45
2:C:810:ASP:HA	2:C:811:PRO:HD3	1.78	0.45
2:C:896:PHE:O	2:C:924:VAL:HG11	2.17	0.45
3:D:1115:THR:HG21	3:D:1151:ARG:NH2	2.32	0.45
3:D:1283:ILE:HB	3:D:1315:ASP:OD2	2.17	0.45
3:D:1462:LEU:N	3:D:1462:LEU:HD23	2.31	0.45
3:D:1466:VAL:CG2	3:D:1472:ILE:HD11	2.39	0.45
3:D:141:ILE:CG2	3:D:161:LEU:HD21	2.45	0.45
3:D:188:GLY:HA2	9:D:2289:HOH:O	2.17	0.45
3:D:165:LYS:CB	3:D:395:VAL:HG11	2.44	0.45
3:D:87:ARG:CB	3:D:523:ASP:HB2	2.35	0.45
3:D:645:PRO:HG3	3:D:725:SER:O	2.16	0.45
3:D:795:VAL:HG11	3:D:863:VAL:HG13	1.99	0.45
3:D:895:VAL:O	3:D:899:LEU:HG	2.17	0.45
5:F:291:ILE:CG2	5:F:304:VAL:HG21	2.46	0.45
5:F:416:ARG:NH1	9:F:9866:HOH:O	2.46	0.45
1:K:111:ALA:HB3	1:K:124:ASN:O	2.17	0.45
1:L:122:ILE:HD12	1:L:122:ILE:N	2.32	0.45
2:M:227:PHE:HB3	9:M:9899:HOH:O	2.17	0.45
2:M:283:ILE:HG23	9:M:2206:HOH:O	2.17	0.45
2:M:571:LEU:HD12	2:M:701:THR:O	2.17	0.45
2:M:770:GLU:HB2	9:N:2049:HOH:O	2.17	0.45
3:N:18:ILE:HG21	3:N:516:ALA:O	2.17	0.45
3:N:161:LEU:HD13	3:N:452:ILE:HD13	1.99	0.45
3:N:55:ASP:HB3	3:N:82:LYS:HE3	1.98	0.45
2:M:1029:GLY:HA3	3:N:623:VAL:O	2.17	0.45
3:N:52:PRO:CB	3:N:80:VAL:HG13	2.30	0.45
3:N:882:PHE:O	3:N:886:VAL:HG23	2.17	0.45
3:N:696:HIS:HB2	4:O:48:MET:HE1	1.99	0.45
2:C:186:VAL:HG23	2:C:187:ASN:N	2.25	0.44
2:C:359:MET:HA	9:C:2175:HOH:O	2.17	0.44
2:C:648:ARG:HG2	9:C:9825:HOH:O	2.17	0.44
2:C:98:LEU:N	2:C:98:LEU:HD12	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:578:VAL:HG11	2:C:991:GLN:HB3	2.00	0.44
3:D:1090:ASP:HA	3:D:1093:TYR:HB2	1.97	0.44
3:D:1392:GLY:N	9:D:9923:HOH:O	2.49	0.44
3:D:1418:LYS:HB3	9:D:9806:HOH:O	2.16	0.44
3:D:1492:LEU:HD12	3:D:1493:LYS:NZ	2.31	0.44
3:D:396:VAL:HG13	3:D:447:VAL:HA	1.98	0.44
3:D:39:PRO:HG2	3:D:47:GLU:OE2	2.17	0.44
3:D:685:ASP:HB3	9:D:9826:HOH:O	2.16	0.44
3:D:804:LEU:HD23	3:D:804:LEU:N	2.30	0.44
3:D:83:SER:O	3:D:86:ARG:HB3	2.17	0.44
1:K:199:ILE:HD12	1:K:199:ILE:N	2.32	0.44
2:M:1085:PHE:CZ	3:N:1468:LEU:HG	2.52	0.44
2:M:1088:LEU:HD23	2:M:1089:VAL:N	2.31	0.44
2:M:239:PHE:HD1	9:M:9955:HOH:O	1.99	0.44
2:M:473:ARG:HG2	2:M:473:ARG:HH11	1.81	0.44
2:M:542:VAL:HG23	9:M:9944:HOH:O	2.16	0.44
2:M:686:ASP:N	9:N:2186:HOH:O	2.49	0.44
2:M:983:ILE:CG2	2:M:987:ILE:HD11	2.45	0.44
3:N:1149:LEU:HD11	3:N:1160:LEU:HB3	1.99	0.44
3:N:1237:THR:N	9:N:2360:HOH:O	2.49	0.44
3:N:462:GLN:HB3	9:N:9521:HOH:O	2.17	0.44
3:N:601:ARG:HG2	3:N:606:ILE:CD1	2.46	0.44
3:N:6:ARG:C	3:N:7:LYS:HG3	2.38	0.44
3:N:895:VAL:HG11	3:N:922:LEU:HD21	1.99	0.44
2:M:772:ARG:HH21	5:P:378:GLY:HA2	1.81	0.44
1:B:150:TYR:HE1	1:B:168:ASP:HB3	1.82	0.44
2:C:176:VAL:HG11	9:C:9635:HOH:O	2.17	0.44
2:C:405:ARG:HB3	9:C:9528:HOH:O	2.16	0.44
3:D:1244:GLY:HA2	9:D:2331:HOH:O	2.17	0.44
3:D:1271:LYS:HB2	9:D:2687:HOH:O	2.17	0.44
3:D:1263:PHE:CZ	3:D:1352:ILE:HD13	2.52	0.44
3:D:506:GLY:HA3	3:D:1454:GLY:HA3	2.00	0.44
3:D:520:LEU:CD2	3:D:540:LEU:HD22	2.47	0.44
3:D:553:ARG:NH1	5:F:211:ASP:HA	2.32	0.44
3:D:587:ARG:HD3	9:D:9502:HOH:O	2.18	0.44
4:E:37:ASN:HD22	4:E:89:MET:CE	2.30	0.44
5:F:172:ARG:O	5:F:176:ILE:HD13	2.16	0.44
5:F:192:LEU:O	5:F:196:VAL:HG23	2.17	0.44
5:F:229:TYR:HE1	9:F:9586:HOH:O	2.00	0.44
5:F:234:LYS:HD3	5:F:236:SER:H	1.82	0.44
5:F:222:ARG:HD2	5:F:242:TRP:CE3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:303:ARG:NH2	9:F:9668:HOH:O	2.50	0.44
2:M:1008:ARG:NH2	2:M:1020:PRO:HB3	2.32	0.44
2:M:428:ARG:HD3	2:M:449:ILE:O	2.17	0.44
2:M:753:ASP:O	2:M:792:VAL:HG23	2.17	0.44
3:N:1045:MET:HG2	3:N:1073:SER:CA	2.41	0.44
3:N:22:SER:HA	3:N:90:MET:O	2.18	0.44
3:N:416:ALA:H	3:N:417:PRO:CD	2.31	0.44
3:N:111:LYS:NZ	3:N:498:VAL:HG12	2.32	0.44
3:N:610:LYS:HB3	9:N:2113:HOH:O	2.16	0.44
1:L:150:TYR:H	3:N:855:HIS:CE1	2.35	0.44
1:A:165:ILE:O	1:A:165:ILE:HD12	2.16	0.44
1:A:85:LEU:HD12	1:A:86:VAL:N	2.32	0.44
1:A:97:VAL:HG12	1:A:99:LEU:HD12	1.99	0.44
1:B:95:GLN:HG3	1:B:146:ARG:HD2	2.00	0.44
2:C:136:ILE:HG23	2:C:391:LEU:CD2	2.47	0.44
2:C:433:THR:CG2	2:C:488:ALA:HB1	2.40	0.44
2:C:543:ASN:HD21	2:C:562:SER:C	2.19	0.44
3:D:131:LYS:HE2	5:F:83:GLN:NE2	2.29	0.44
3:D:1379:VAL:CG1	3:D:1395:LEU:HD23	2.47	0.44
3:D:1472:ILE:HA	3:D:1473:PRO:HD3	1.84	0.44
3:D:1491:THR:HG22	9:E:9527:HOH:O	2.17	0.44
3:D:168:THR:OG1	3:D:393:ILE:HB	2.17	0.44
3:D:477:LEU:HD11	3:D:495:ARG:HD3	1.98	0.44
3:D:619:LEU:HD12	9:D:9516:HOH:O	2.16	0.44
3:D:619:LEU:HD23	3:D:619:LEU:O	2.18	0.44
3:D:61:GLY:HA2	3:D:64:LYS:HE3	1.98	0.44
3:D:785:ILE:HD12	3:D:785:ILE:N	2.32	0.44
5:F:307:THR:HA	5:F:310:ILE:HD11	1.98	0.44
9:C:9809:HOH:O	5:F:349:LEU:HB2	2.16	0.44
1:K:198:ARG:HG2	9:K:3473:HOH:O	2.18	0.44
1:K:63:HIS:HB3	9:K:5125:HOH:O	2.16	0.44
2:M:422:ARG:NH1	9:M:2004:HOH:O	2.51	0.44
2:M:557:ARG:NE	2:M:560:MET:SD	2.90	0.44
2:M:58:ASP:O	2:M:59:LYS:HG3	2.17	0.44
2:M:720:GLU:CD	2:M:758:ARG:HD2	2.38	0.44
2:M:794:PRO:HB2	2:M:1027:PHE:HZ	1.82	0.44
3:N:1377:LYS:HE2	9:N:9728:HOH:O	2.16	0.44
3:N:44:LEU:HB3	3:N:525:ARG:NH2	2.26	0.44
3:N:978:TYR:HD1	9:N:9888:HOH:O	2.00	0.44
4:O:33:HIS:HB2	4:O:37:ASN:ND2	2.32	0.44
5:P:376:ILE:HG22	5:P:377:ASP:OD1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:GLU:HB3	9:A:9622:HOH:O	2.15	0.44
1:A:198:ARG:HB2	1:A:200:TRP:CH2	2.52	0.44
1:A:63:HIS:HA	9:A:9482:HOH:O	2.17	0.44
2:C:140:ILE:HD11	2:C:412:ALA:HA	1.99	0.44
2:C:492:ASP:HB3	2:C:518:LYS:HD2	1.99	0.44
2:C:913:GLU:O	2:C:916:GLU:HB3	2.17	0.44
3:D:1239:ARG:HH22	3:D:1254:GLN:HB2	1.82	0.44
3:D:432:TYR:HB3	3:D:448:GLU:HA	1.99	0.44
3:D:699:VAL:CG2	3:D:760:ARG:HB3	2.47	0.44
3:D:805:GLU:HA	9:D:9963:HOH:O	2.16	0.44
3:D:838:ARG:HE	3:D:838:ARG:HB2	1.54	0.44
3:D:843:PHE:CE1	3:D:864:VAL:HG11	2.53	0.44
3:D:995:LEU:HD12	9:D:2036:HOH:O	2.16	0.44
3:D:996:TRP:HE3	3:D:999:THR:CG2	2.26	0.44
4:E:40:LEU:O	4:E:40:LEU:HD22	2.17	0.44
4:E:70:THR:HG22	4:E:71:GLY:N	2.32	0.44
1:L:73:GLU:HB3	1:L:77:GLU:HG3	1.97	0.44
2:M:1060:ILE:CG2	2:M:1061:GLU:N	2.80	0.44
2:M:212:GLY:C	2:M:215:GLY:H	2.21	0.44
2:M:208:ALA:HB1	2:M:218:VAL:CG1	2.47	0.44
2:M:611:ILE:N	2:M:611:ILE:HD12	2.32	0.44
2:M:723:THR:HG23	2:M:725:ASP:HB2	1.98	0.44
3:N:1153:VAL:HG12	3:N:1155:VAL:HG22	2.00	0.44
3:N:1173:LEU:CD2	3:N:1174:LEU:HD23	2.47	0.44
3:N:1114:THR:CG2	3:N:1195:GLN:HB3	2.48	0.44
3:N:546:ARG:CZ	3:N:550:ARG:NH2	2.81	0.44
3:N:29:PRO:HG3	3:N:549:ASN:ND2	2.33	0.44
3:N:129:PHE:C	3:N:568:ARG:HH21	2.20	0.44
3:N:800:LYS:HG2	9:N:9629:HOH:O	2.17	0.44
2:M:1115:LEU:HD21	3:N:84:ILE:HD12	2.00	0.44
3:N:864:VAL:HG12	3:N:865:THR:N	2.30	0.44
4:O:49:GLN:HA	4:O:51:LEU:O	2.18	0.44
5:P:141:VAL:HB	9:P:4054:HOH:O	2.18	0.44
5:P:173:TYR:HE2	9:P:5021:HOH:O	2.00	0.44
5:P:273:ARG:NH2	9:P:3957:HOH:O	2.50	0.44
1:A:88:ARG:HG2	1:A:88:ARG:O	2.17	0.44
2:C:309:TYR:CE2	2:C:321:GLU:HB3	2.53	0.44
1:A:72:LYS:HA	2:C:608:GLY:N	2.32	0.44
2:C:73:LEU:O	2:C:73:LEU:HD12	2.16	0.44
2:C:79:PRO:HB3	9:C:2096:HOH:O	2.16	0.44
2:C:93:PRO:HB3	9:C:9910:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1045:MET:HG2	3:D:1072:ILE:O	2.17	0.44
3:D:1209:LEU:HD22	3:D:1211:MET:SD	2.57	0.44
3:D:1288:GLU:OE1	3:D:1289:LYS:HG3	2.17	0.44
3:D:10:ILE:HD11	3:D:1434:TRP:NE1	2.33	0.44
3:D:630:VAL:O	3:D:726:ILE:HG13	2.17	0.44
3:D:630:VAL:CA	3:D:744:GLN:HG2	2.47	0.44
1:L:41:ARG:NH1	1:L:177:VAL:HG23	2.32	0.44
2:M:1086:ARG:HB3	2:M:1112:PHE:HE2	1.82	0.44
2:M:159:ILE:C	9:M:9990:HOH:O	2.55	0.44
2:M:253:ALA:O	2:M:256:TYR:HB2	2.17	0.44
2:M:769:PRO:HB2	3:N:65:ARG:CZ	2.48	0.44
3:N:396:VAL:HG13	3:N:446:VAL:O	2.18	0.44
3:N:519:VAL:N	9:N:9660:HOH:O	2.50	0.44
3:N:29:PRO:HG3	3:N:549:ASN:HD21	1.82	0.44
4:O:33:HIS:HA	9:O:5072:HOH:O	2.18	0.44
5:P:100:VAL:HG12	5:P:104:ARG:HH12	1.82	0.44
5:P:203:THR:HG22	5:P:204:GLY:N	2.32	0.44
5:P:286:PRO:HD3	9:P:4921:HOH:O	2.17	0.44
5:P:84:TYR:HD1	9:P:3565:HOH:O	2.00	0.44
1:A:191:ASP:O	1:A:191:ASP:CG	2.56	0.44
1:A:7:LYS:NZ	1:A:188:GLN:HE22	2.15	0.44
1:B:142:VAL:HG23	1:B:142:VAL:O	2.17	0.44
1:B:143:ARG:CD	1:B:158:ILE:HG21	2.48	0.44
1:B:143:ARG:HD3	1:B:158:ILE:HG21	1.98	0.44
1:B:83:LYS:HE3	1:B:167:VAL:HG12	1.99	0.44
2:C:195:LEU:HB3	9:C:9594:HOH:O	2.16	0.44
2:C:313:LEU:HD12	2:C:313:LEU:O	2.17	0.44
2:C:525:SER:OG	2:C:527:GLU:HG3	2.17	0.44
2:C:726:ILE:O	2:C:726:ILE:HG22	2.17	0.44
2:C:816:LYS:O	2:C:819:VAL:HB	2.18	0.44
3:D:1173:LEU:HD23	3:D:1174:LEU:N	2.32	0.44
3:D:156:GLU:CD	3:D:156:GLU:N	2.70	0.44
3:D:211:VAL:HG13	3:D:393:ILE:HG23	1.99	0.44
3:D:441:ARG:O	3:D:443:VAL:N	2.50	0.44
3:D:780:LYS:HE2	9:D:2356:HOH:O	2.18	0.44
3:D:917:GLN:HA	9:D:9488:HOH:O	2.16	0.44
5:F:398:ARG:HB3	9:F:9487:HOH:O	2.18	0.44
5:F:412:GLU:HG3	5:F:418:LEU:HD22	1.99	0.44
1:K:216:GLU:OE1	1:K:219:ARG:HD2	2.17	0.44
1:K:91:ASN:CG	1:K:92:PRO:HD2	2.38	0.44
2:M:189:ARG:HH22	2:M:243:ARG:CD	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:211:LEU:CD1	2:M:308:ARG:HG3	2.48	0.44
2:M:428:ARG:HH21	2:M:451:LEU:HD21	1.82	0.44
2:M:498:GLN:HB3	2:M:500:ASN:OD1	2.18	0.44
2:M:816:LYS:HB2	2:M:819:VAL:CG2	2.46	0.44
2:M:817:PRO:C	2:M:819:VAL:H	2.20	0.44
2:M:561:GLY:HA3	2:M:842:ARG:O	2.17	0.44
3:N:102:ILE:HG13	9:N:2374:HOH:O	2.15	0.44
3:N:526:PRO:HB2	5:P:317:LEU:HD11	2.00	0.44
5:P:101:GLU:O	5:P:105:LYS:HG3	2.17	0.44
1:B:1:MET:HE1	9:B:9547:HOH:O	2.16	0.44
2:C:1087:VAL:HG13	2:C:1091:GLU:OE2	2.17	0.44
2:C:41:ASN:HA	2:C:45:GLN:OE1	2.17	0.44
2:C:597:ALA:HB2	2:C:655:LEU:CD2	2.45	0.44
3:D:1155:VAL:CG1	3:D:1177:ALA:HB1	2.46	0.44
3:D:1374:GLN:HG2	9:D:9769:HOH:O	2.17	0.44
3:D:719:VAL:O	3:D:719:VAL:HG23	2.18	0.44
3:D:643:GLY:CA	3:D:727:GLN:HB2	2.46	0.44
4:E:9:LEU:HD22	4:E:19:LEU:CD1	2.47	0.44
5:F:226:LYS:HD2	5:F:242:TRP:CZ2	2.52	0.44
5:F:256:ARG:NE	5:F:260:ILE:HD12	2.33	0.44
5:F:370:LYS:HB3	5:F:370:LYS:HZ3	1.82	0.44
5:F:372:ARG:HD3	9:F:9526:HOH:O	2.17	0.44
5:F:94:LEU:HD23	5:F:95:THR:N	2.33	0.44
1:L:124:ASN:ND2	1:L:127:LEU:HD22	2.32	0.44
2:M:1013:TYR:CE1	2:M:1020:PRO:HG3	2.52	0.44
2:M:1038:TRP:HD1	2:M:1041:GLU:OE1	2.00	0.44
2:M:1083:GLU:N	9:M:9532:HOH:O	2.47	0.44
2:M:113:VAL:HG12	2:M:115:LEU:HD23	1.98	0.44
2:M:309:TYR:HA	2:M:312:ALA:HB3	1.99	0.44
2:M:438:ILE:HD11	2:M:467:ILE:HD12	1.99	0.44
2:M:964:LYS:HE2	9:M:9902:HOH:O	2.17	0.44
3:N:1063:GLU:HB3	9:N:2380:HOH:O	2.17	0.44
3:N:1156:LEU:HD13	3:N:1176:LYS:HD2	2.00	0.44
3:N:1217:ILE:H	3:N:1217:ILE:HG13	1.44	0.44
3:N:1353:GLN:HB3	3:N:1357:ARG:NE	2.32	0.44
3:N:1503:VAL:HG22	9:N:2327:HOH:O	2.18	0.44
3:N:175:VAL:HA	3:N:389:GLU:OE1	2.17	0.44
3:N:484:PRO:O	3:N:489:ARG:HD2	2.18	0.44
3:N:681:ARG:HH11	3:N:681:ARG:CB	2.30	0.44
3:N:666:ILE:HG23	3:N:686:GLU:OE2	2.17	0.44
3:N:824:ASN:HB3	9:N:9554:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:128:ARG:HB2	5:P:128:ARG:CZ	2.48	0.44
5:P:413:SER:HA	5:P:416:ARG:HD3	1.98	0.44
1:A:106:PRO:HG3	1:A:133:GLU:O	2.18	0.44
1:B:158:ILE:HA	1:B:158:ILE:HD13	1.84	0.44
2:C:1103:ASP:N	2:C:1107:ASN:O	2.51	0.44
2:C:444:PRO:HD2	2:C:452:ILE:O	2.18	0.44
2:C:493:ARG:HD2	9:C:9650:HOH:O	2.17	0.44
2:C:474:VAL:HG13	2:C:530:GLU:O	2.18	0.44
2:C:565:GLN:HA	2:C:995:MET:HE3	2.00	0.44
2:C:890:LEU:HD23	2:C:890:LEU:C	2.37	0.44
3:D:1087:ARG:HB3	3:D:1234:THR:HG23	1.99	0.44
3:D:1236:LEU:HD12	3:D:1256:LEU:CD1	2.47	0.44
3:D:1310:ARG:HG3	3:D:1327:ARG:HB3	1.99	0.44
3:D:470:LEU:HD11	3:D:509:PRO:HG3	2.00	0.44
3:D:50:PHE:HB3	3:D:522:PRO:HG2	1.99	0.44
3:D:629:SER:OG	3:D:630:VAL:N	2.50	0.44
3:D:867:ARG:HB3	3:D:867:ARG:HH11	1.83	0.44
1:K:30:ARG:HD2	9:K:4362:HOH:O	2.17	0.44
1:K:88:ARG:HB3	9:K:3485:HOH:O	2.16	0.44
2:M:1032:PHE:HA	9:M:2368:HOH:O	2.17	0.44
2:M:264:PRO:HB3	2:M:289:THR:CG2	2.46	0.44
2:M:704:HIS:O	2:M:705:ILE:HG23	2.17	0.44
2:M:925:TYR:C	2:M:925:TYR:CD1	2.91	0.44
3:N:951:ILE:HG23	3:N:1062:ARG:HH21	1.82	0.44
3:N:1209:LEU:HD21	4:O:16:LYS:NZ	2.33	0.44
3:N:126:VAL:HG12	3:N:132:TYR:HB2	1.99	0.44
3:N:29:PRO:HG3	9:N:9768:HOH:O	2.17	0.44
3:N:506:GLY:C	3:N:507:ASN:HD22	2.21	0.44
3:N:525:ARG:HB2	3:N:538:SER:OG	2.18	0.44
3:N:546:ARG:NH1	3:N:550:ARG:NH2	2.65	0.44
3:N:679:ARG:NH2	3:N:681:ARG:HD2	2.33	0.44
3:N:641:GLN:HB3	3:N:717:GLN:O	2.18	0.44
3:N:645:PRO:HB3	3:N:723:GLY:O	2.17	0.44
1:B:109:VAL:HG22	9:B:9571:HOH:O	2.17	0.44
1:B:112:ARG:CZ	1:B:112:ARG:HB3	2.47	0.44
1:B:48:ILE:HD13	1:B:210:ALA:HB1	2.00	0.44
2:C:139:GLN:HE22	2:C:415:PRO:CD	2.31	0.44
2:C:139:GLN:HE22	2:C:415:PRO:HD3	1.82	0.44
2:C:25:SER:OG	2:C:337:GLY:N	2.48	0.44
2:C:333:ILE:O	2:C:465:GLY:HA3	2.17	0.44
2:C:630:ARG:HE	2:C:705:ILE:HG13	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:816:LYS:HB2	2:C:819:VAL:CG2	2.47	0.44
3:D:1068:LEU:HD23	3:D:1068:LEU:O	2.18	0.44
3:D:1281:VAL:HG23	3:D:1317:ASP:O	2.18	0.44
3:D:1332:PRO:HB2	3:D:1421:LEU:HD22	2.00	0.44
3:D:1455:LYS:C	3:D:1455:LYS:HD3	2.37	0.44
3:D:175:VAL:HG11	3:D:218:LYS:H	1.83	0.44
3:D:396:VAL:HG13	3:D:446:VAL:O	2.18	0.44
3:D:400:VAL:HA	3:D:442:ASN:O	2.18	0.44
1:K:198:ARG:HB2	1:K:200:TRP:CH2	2.53	0.44
1:L:151:VAL:HB	1:L:169:ALA:HB3	1.99	0.44
2:M:165:LEU:HD12	2:M:165:LEU:HA	1.88	0.44
2:M:269:LEU:O	2:M:269:LEU:HD23	2.18	0.44
2:M:464:LEU:HA	2:M:464:LEU:HD12	1.80	0.44
2:M:62:GLY:O	2:M:103:LYS:HG3	2.18	0.44
2:M:704:HIS:CG	2:M:831:ARG:HE	2.36	0.44
2:M:910:LYS:HB3	2:M:912:PRO:HD2	2.00	0.44
2:M:930:LYS:HA	9:M:9525:HOH:O	2.18	0.44
2:M:979:THR:HG23	2:M:981:GLU:HB2	1.99	0.44
3:N:1109:GLU:HG2	3:N:1202:GLN:H	1.83	0.44
3:N:1192:LEU:HD22	3:N:1345:GLU:OE2	2.18	0.44
3:N:1438:ALA:N	3:N:1446:VAL:HG11	2.33	0.44
3:N:33:ASN:O	3:N:36:THR:O	2.36	0.44
3:N:456:MET:C	9:N:2390:HOH:O	2.56	0.44
3:N:661:MET:SD	3:N:673:ALA:HB1	2.57	0.44
2:M:1042:ALA:CB	3:N:710:ARG:HE	2.29	0.44
3:N:832:ARG:HG2	9:N:9674:HOH:O	2.18	0.44
4:O:61:GLU:C	4:O:65:MET:HE2	2.38	0.44
3:N:767:HIS:NE2	4:O:6:ILE:HD13	2.33	0.44
2:C:110:GLU:HB2	2:C:368:THR:HG22	1.99	0.43
2:C:195:LEU:HD12	2:C:234:ALA:HB1	1.99	0.43
2:C:235:LEU:HA	9:C:2083:HOH:O	2.18	0.43
2:C:360:LEU:HD12	9:C:9600:HOH:O	2.18	0.43
2:C:712:ALA:HB1	9:C:2168:HOH:O	2.18	0.43
2:C:71:TYR:H	2:C:71:TYR:HD2	1.65	0.43
2:C:863:ASP:OD1	2:C:865:THR:HG22	2.18	0.43
3:D:101:HIS:ND1	3:D:103:TRP:HB2	2.31	0.43
3:D:1393:GLN:HB2	3:D:1398:TRP:HZ2	1.81	0.43
3:D:1406:ARG:HD3	3:D:1406:ARG:C	2.39	0.43
3:D:1496:GLU:O	3:D:1500:LYS:HG3	2.17	0.43
3:D:16:GLU:HA	3:D:19:ARG:NH1	2.33	0.43
3:D:191:LEU:HB3	3:D:195:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:216:VAL:HG12	9:D:9947:HOH:O	2.17	0.43
3:D:525:ARG:N	3:D:526:PRO:HD3	2.33	0.43
3:D:569:ASN:HD21	5:F:210:LEU:HD22	1.82	0.43
3:D:669:ASN:HB3	9:D:9547:HOH:O	2.17	0.43
3:D:650:LEU:HD22	3:D:688:TRP:CZ3	2.53	0.43
4:E:52:GLU:HB3	4:E:55:PHE:CZ	2.53	0.43
5:F:319:THR:HB	5:F:321:ILE:HD11	1.99	0.43
2:M:1090:LYS:HD2	3:N:90:MET:SD	2.58	0.43
2:M:195:LEU:CD2	2:M:238:LEU:HG	2.48	0.43
2:M:241:LEU:HD23	9:M:9797:HOH:O	2.18	0.43
2:M:380:ALA:O	2:M:383:ARG:HG2	2.18	0.43
2:M:418:LEU:N	2:M:418:LEU:HD12	2.33	0.43
2:M:670:GLN:HG3	2:M:700:TYR:CE2	2.53	0.43
2:M:916:GLU:O	2:M:919:ALA:HB3	2.18	0.43
3:N:1047:LYS:HB3	3:N:1048:PRO:HD2	2.00	0.43
3:N:1109:GLU:CD	3:N:1202:GLN:H	2.21	0.43
3:N:1112:CYS:HB3	3:N:1201:CYS:SG	2.57	0.43
3:N:637:LEU:HD12	3:N:641:GLN:OE1	2.16	0.43
3:N:994:GLN:HA	3:N:994:GLN:HE21	1.83	0.43
5:P:134:LYS:HG3	5:P:178:ARG:NH2	2.33	0.43
5:P:223:ALA:HB2	5:P:242:TRP:HB2	1.99	0.43
5:P:358:LEU:HD11	5:P:370:LYS:NZ	2.33	0.43
1:A:2:LEU:O	1:A:6:LEU:HB3	2.18	0.43
1:A:63:HIS:HE1	9:C:2299:HOH:O	2.00	0.43
1:B:143:ARG:NH1	1:B:158:ILE:HG23	2.33	0.43
2:C:111:ASP:HB3	2:C:112:GLU:OE2	2.18	0.43
2:C:232:GLU:HG3	2:C:235:LEU:CD1	2.48	0.43
2:C:443:THR:HG23	2:C:449:ILE:HG13	1.99	0.43
2:C:460:ARG:HD2	2:C:485:TYR:CD2	2.52	0.43
2:C:535:SER:HB2	2:C:537:LYS:HD3	2.00	0.43
2:C:557:ARG:NH1	2:C:879:ARG:HG2	2.33	0.43
2:C:572:ILE:CG2	2:C:703:ILE:HD13	2.49	0.43
2:C:674:VAL:HG12	2:C:990:GLY:O	2.18	0.43
2:C:689:VAL:HB	2:C:870:ILE:CG1	2.36	0.43
2:C:68:PHE:HE1	2:C:96:ALA:HB1	1.82	0.43
2:C:838:LYS:O	2:C:838:LYS:HG3	2.18	0.43
3:D:1023:MET:O	3:D:1028:ALA:HB3	2.18	0.43
3:D:1031:ASN:O	3:D:1034:GLN:HB2	2.17	0.43
3:D:1042:ARG:O	3:D:1057:VAL:HB	2.18	0.43
3:D:1219:GLU:HG2	3:D:1220:ALA:N	2.33	0.43
3:D:1267:ARG:HH22	3:D:1333:HIS:HD2	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:513:ILE:HA	9:D:9738:HOH:O	2.18	0.43
3:D:6:ARG:HH11	3:D:6:ARG:CB	2.24	0.43
3:D:705:ALA:CB	3:D:706:PRO:HD3	2.45	0.43
4:E:54:LEU:HA	4:E:58:PRO:HG2	2.01	0.43
9:D:9603:HOH:O	5:F:337:HIS:HB3	2.18	0.43
5:F:359:SER:C	5:F:361:LEU:H	2.21	0.43
1:K:209:GLU:O	1:K:213:GLN:HG3	2.19	0.43
2:M:728:HIS:CE1	2:M:775:ARG:HH12	2.36	0.43
3:N:1096:ARG:HH11	3:N:1096:ARG:HG2	1.82	0.43
3:N:115:LEU:HD12	3:N:499:VAL:HG22	1.99	0.43
3:N:661:MET:HE2	3:N:677:LEU:HD11	1.99	0.43
3:N:661:MET:HE1	3:N:677:LEU:HD11	2.01	0.43
4:O:82:GLU:O	4:O:85:LEU:HD22	2.18	0.43
5:P:85:LEU:HD22	5:P:193:ARG:CD	2.48	0.43
1:A:18:ARG:NH2	1:A:88:ARG:NH2	2.65	0.43
1:A:66:SER:O	1:A:75:VAL:HG23	2.19	0.43
2:C:1044:GLY:HA3	4:E:17:TYR:CE1	2.53	0.43
2:C:190:LYS:HG3	9:C:9876:HOH:O	2.19	0.43
2:C:577:PRO:HG3	2:C:993:PHE:CE2	2.54	0.43
3:D:1154:GLU:HB2	9:D:9708:HOH:O	2.18	0.43
3:D:1413:THR:HG22	9:D:2035:HOH:O	2.18	0.43
3:D:553:ARG:CZ	9:F:9503:HOH:O	2.65	0.43
3:D:553:ARG:NE	9:D:9572:HOH:O	2.51	0.43
3:D:805:GLU:O	3:D:805:GLU:OE1	2.37	0.43
3:D:853:VAL:CG2	3:D:858:VAL:HG23	2.48	0.43
4:E:61:GLU:OE2	4:E:62:THR:N	2.52	0.43
5:F:115:LYS:HG3	5:F:173:TYR:HE2	1.82	0.43
5:F:230:LYS:HD3	9:F:9882:HOH:O	2.17	0.43
5:F:241:TRP:HA	5:F:244:ARG:HH12	1.83	0.43
5:F:282:LEU:CD1	5:F:286:PRO:HG3	2.49	0.43
5:F:295:MET:HB3	5:F:299:TRP:CG	2.53	0.43
5:F:305:GLU:O	5:F:309:LYS:HG3	2.18	0.43
1:L:100:LEU:HB2	1:L:115:LEU:CD2	2.44	0.43
1:K:9:PRO:HD2	1:L:224:TYR:CZ	2.53	0.43
2:M:1097:LEU:HD22	2:M:1097:LEU:H	1.83	0.43
2:M:287:GLY:O	2:M:288:ARG:C	2.56	0.43
2:M:252:LYS:HZ2	2:M:296:GLY:HA3	1.83	0.43
2:M:461:VAL:HG13	2:M:465:GLY:HA2	1.99	0.43
2:M:625:LEU:HD22	2:M:639:GLN:HB3	2.00	0.43
2:M:707:ARG:HH12	2:M:709:GLU:CB	2.21	0.43
2:M:674:VAL:O	2:M:989:VAL:HA	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:153:LEU:HD11	3:N:158:TYR:CA	2.48	0.43
3:N:852:ALA:O	3:N:857:ILE:HG12	2.18	0.43
3:N:899:LEU:HD12	3:N:900:ILE:HG23	1.99	0.43
3:N:915:VAL:HG13	3:N:931:LEU:HD21	2.00	0.43
3:N:996:TRP:HE3	3:N:999:THR:HG21	1.83	0.43
5:P:211:ASP:OD1	5:P:211:ASP:N	2.51	0.43
1:A:18:ARG:HD3	1:A:123:MET:CE	2.48	0.43
2:C:580:MET:HB2	2:C:902:ILE:HG12	1.99	0.43
2:C:607:ASP:HB3	2:C:610:ARG:H	1.84	0.43
2:C:861:LEU:HD23	2:C:862:PRO:N	2.34	0.43
2:C:938:LYS:N	9:C:9976:HOH:O	2.51	0.43
3:D:1107:VAL:O	3:D:1218:GLY:N	2.49	0.43
3:D:1495:ILE:O	3:D:1498:ALA:HB3	2.18	0.43
3:D:130:SER:O	3:D:568:ARG:NH2	2.50	0.43
3:D:703:ASN:ND2	3:D:704:ARG:N	2.66	0.43
3:D:762:GLN:HE21	4:E:20:THR:HG21	1.83	0.43
3:D:838:ARG:HD3	3:D:874:GLU:HB3	2.00	0.43
3:D:890:VAL:HG21	3:D:922:LEU:CD1	2.49	0.43
1:K:101:LEU:HG	1:K:114:PHE:CA	2.43	0.43
1:K:156:HIS:CD2	1:K:157:GLY:N	2.86	0.43
1:K:197:LEU:H	1:K:197:LEU:CD2	2.30	0.43
2:M:1005:MET:HE3	3:N:645:PRO:HB2	2.01	0.43
2:M:1100:GLN:HB2	2:M:1100:GLN:HE21	1.69	0.43
2:M:132:ALA:HB2	9:M:2414:HOH:O	2.18	0.43
2:M:175:GLU:HB3	2:M:183:SER:OG	2.18	0.43
2:M:36:PRO:HG2	2:M:70:GLU:CB	2.46	0.43
2:M:389:SER:HB2	9:M:9823:HOH:O	2.17	0.43
2:M:603:VAL:H	2:M:647:GLN:H	1.66	0.43
2:M:957:LYS:HA	9:M:2387:HOH:O	2.18	0.43
3:N:1135:ARG:HD3	3:N:1139:ASP:HB2	1.98	0.43
3:N:1403:LEU:HD23	3:N:1407:LEU:CD2	2.47	0.43
3:N:1449:GLU:HG2	9:N:9651:HOH:O	2.18	0.43
2:M:1067:TYR:CE1	3:N:655:PRO:HB3	2.54	0.43
3:N:835:SER:N	9:N:9806:HOH:O	2.52	0.43
5:P:412:GLU:HA	9:P:3726:HOH:O	2.17	0.43
1:A:109:VAL:O	1:A:129:ILE:HB	2.18	0.43
1:A:32:PHE:HD2	9:A:9505:HOH:O	2.01	0.43
1:A:42:ARG:CZ	9:A:9609:HOH:O	2.66	0.43
1:A:73:GLU:N	1:A:73:GLU:OE2	2.52	0.43
1:A:89:PHE:HB2	9:A:9536:HOH:O	2.17	0.43
1:B:27:PRO:HG2	1:B:186:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:174:LEU:CD2	2:C:184:MET:HG3	2.48	0.43
2:C:443:THR:OG1	2:C:444:PRO:HD2	2.18	0.43
2:C:598:GLU:HB2	2:C:615:TYR:CZ	2.53	0.43
2:C:752:GLY:H	2:C:792:VAL:HB	1.83	0.43
2:C:3:ILE:HA	2:C:900:ARG:O	2.19	0.43
3:D:131:LYS:HG3	3:D:568:ARG:HG2	2.00	0.43
3:D:210:ARG:HG3	3:D:398:ALA:HB3	2.00	0.43
3:D:459:GLU:O	3:D:463:GLN:HG2	2.18	0.43
3:D:520:LEU:HD12	3:D:521:PRO:CD	2.38	0.43
3:D:537:THR:HG22	9:F:9527:HOH:O	2.17	0.43
3:D:129:PHE:CD2	3:D:587:ARG:CZ	3.01	0.43
3:D:591:VAL:HG11	9:D:2452:HOH:O	2.17	0.43
3:D:615:ARG:HG3	3:D:615:ARG:HH11	1.82	0.43
3:D:625:TYR:CD1	3:D:625:TYR:N	2.86	0.43
2:C:1036:GLU:HG3	3:D:707:THR:OG1	2.18	0.43
3:D:639:LEU:HD22	3:D:766:ALA:CB	2.48	0.43
3:D:569:ASN:ND2	5:F:210:LEU:HD22	2.33	0.43
3:D:566:ILE:HG12	5:F:217:ASN:ND2	2.33	0.43
2:M:1015:LEU:HD12	5:P:335:ASP:OD1	2.19	0.43
2:M:1075:ASP:HB2	4:O:31:LEU:HD12	2.00	0.43
2:M:189:ARG:HG2	2:M:189:ARG:HH11	1.83	0.43
2:M:385:PHE:O	2:M:389:SER:HB3	2.19	0.43
2:M:610:ARG:HG3	2:M:610:ARG:HH11	1.83	0.43
2:M:625:LEU:HD22	2:M:639:GLN:CB	2.48	0.43
2:M:802:ARG:HH11	2:M:802:ARG:HB3	1.84	0.43
2:M:913:GLU:O	2:M:916:GLU:HB3	2.19	0.43
3:N:1031:ASN:O	3:N:1035:ILE:HG12	2.18	0.43
3:N:1203:LYS:HB2	9:N:9807:HOH:O	2.18	0.43
5:P:245:GLN:HA	9:P:3671:HOH:O	2.17	0.43
1:B:84:GLU:HB3	1:B:127:LEU:HD21	2.00	0.43
1:B:23:PHE:O	1:B:196:THR:HA	2.19	0.43
2:C:1036:GLU:O	2:C:1039:ALA:HB3	2.18	0.43
2:C:1115:LEU:CB	3:D:85:VAL:HG13	2.48	0.43
2:C:10:ARG:NH1	2:C:11:GLU:H	2.16	0.43
2:C:27:ARG:HD2	9:C:9549:HOH:O	2.18	0.43
2:C:44:ILE:HA	2:C:344:PHE:CE1	2.54	0.43
2:C:525:SER:OG	2:C:528:GLU:HG3	2.18	0.43
2:C:722:ILE:HD12	2:C:805:ARG:NH2	2.32	0.43
3:D:1114:THR:O	3:D:1114:THR:HG23	2.17	0.43
3:D:112:ILE:O	3:D:116:LEU:HB2	2.18	0.43
3:D:1264:GLU:HG2	3:D:1266:ARG:NH2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1364:HIS:CE1	3:D:1366:LYS:HG3	2.53	0.43
3:D:1394:VAL:HB	3:D:1397:LYS:CD	2.47	0.43
3:D:187:LYS:HG2	9:D:9853:HOH:O	2.19	0.43
3:D:178:LEU:CG	3:D:200:ASP:H	2.28	0.43
3:D:440:VAL:HG12	3:D:441:ARG:N	2.33	0.43
3:D:475:LYS:O	3:D:479:GLU:HG2	2.18	0.43
3:D:746:ALA:HB2	9:D:9498:HOH:O	2.19	0.43
3:D:908:LYS:HA	3:D:911:LEU:HD22	2.01	0.43
2:C:679:PHE:O	3:D:943:THR:HG22	2.18	0.43
4:E:26:ARG:HA	4:E:29:GLN:OE1	2.18	0.43
5:F:187:LEU:HD21	9:F:9584:HOH:O	2.17	0.43
5:F:205:ARG:HD2	5:F:251:ILE:HG21	2.01	0.43
3:D:598:ARG:NH2	5:F:318:GLU:O	2.51	0.43
1:K:32:PHE:O	1:K:36:LEU:HG	2.19	0.43
1:K:66:SER:O	1:K:75:VAL:HG23	2.18	0.43
1:L:124:ASN:HD22	1:L:127:LEU:HD22	1.83	0.43
2:M:1008:ARG:HB2	2:M:1027:PHE:HB2	2.00	0.43
2:M:1086:ARG:NH1	2:M:1112:PHE:HA	2.33	0.43
2:M:148:PHE:HB2	9:M:9837:HOH:O	2.19	0.43
2:M:150:PRO:CA	2:M:158:TYR:HB3	2.43	0.43
2:M:21:ILE:HD12	2:M:21:ILE:N	2.33	0.43
2:M:230:ARG:HB2	9:M:9523:HOH:O	2.19	0.43
2:M:243:ARG:HG2	9:M:9816:HOH:O	2.18	0.43
2:M:301:GLU:O	2:M:305:PRO:HG2	2.19	0.43
2:M:26:TYR:CD2	2:M:30:LEU:HD11	2.54	0.43
2:M:335:THR:CG2	2:M:461:VAL:HG11	2.49	0.43
2:M:433:THR:CG2	2:M:488:ALA:HB1	2.47	0.43
2:M:578:VAL:HG13	2:M:671:ASN:CG	2.39	0.43
2:M:697:ARG:HB2	9:M:9519:HOH:O	2.19	0.43
3:N:1033:GLN:NE2	3:N:1036:ARG:HH11	2.10	0.43
3:N:1123:PHE:CD1	3:N:1134:LEU:HA	2.54	0.43
3:N:1294:VAL:O	3:N:1300:SER:HA	2.19	0.43
3:N:1312:LEU:HD21	9:N:2005:HOH:O	2.18	0.43
3:N:469:ASP:OD1	3:N:471:GLU:HB2	2.19	0.43
3:N:96:ALA:CB	9:N:9830:HOH:O	2.66	0.43
3:N:992:ILE:O	3:N:995:LEU:HB3	2.19	0.43
5:P:100:VAL:HG11	9:P:6003:HOH:O	2.17	0.43
5:P:358:LEU:HD11	5:P:367:MET:SD	2.58	0.43
5:P:363:GLU:HA	5:P:367:MET:HE2	2.00	0.43
1:A:227:ASN:HD22	1:A:227:ASN:N	2.16	0.43
1:A:90:LEU:HD21	9:A:9569:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:PRO:C	1:B:28:LEU:HD23	2.39	0.43
2:C:162:ILE:HD12	2:C:172:ILE:CB	2.49	0.43
2:C:551:GLU:HG3	2:C:552:HIS:CD2	2.54	0.43
2:C:602:GLU:HA	2:C:647:GLN:O	2.19	0.43
2:C:854:PRO:C	2:C:856:GLU:N	2.71	0.43
2:C:890:LEU:HD21	2:C:901:TYR:CD1	2.53	0.43
2:C:877:PRO:HG2	3:D:1023:MET:CE	2.48	0.43
2:C:874:LEU:CD2	3:D:1023:MET:SD	3.06	0.43
3:D:1299:PHE:H	3:D:1299:PHE:HD2	1.66	0.43
3:D:130:SER:HB2	9:D:9649:HOH:O	2.18	0.43
3:D:1487:VAL:O	4:E:73:LEU:HA	2.18	0.43
3:D:570:GLU:HB2	5:F:214:GLN:NE2	2.34	0.43
3:D:965:GLU:OE1	3:D:965:GLU:HA	2.18	0.43
5:F:194:LEU:N	5:F:194:LEU:HD22	2.33	0.43
5:F:209:PHE:HD1	9:F:9815:HOH:O	2.01	0.43
5:F:214:GLN:O	5:F:217:ASN:HB2	2.19	0.43
5:F:274:THR:O	5:F:278:LEU:HG	2.18	0.43
1:L:127:LEU:HD12	1:L:128:HIS:H	1.84	0.43
1:L:132:LEU:HG	1:L:136:GLY:HA3	1.99	0.43
2:M:185:LYS:HG2	2:M:190:LYS:HG2	2.01	0.43
2:M:189:ARG:HH22	2:M:243:ARG:CG	2.32	0.43
2:M:431:HIS:HB3	2:M:434:HIS:NE2	2.34	0.43
2:M:566:THR:O	2:M:566:THR:HG22	2.19	0.43
2:M:911:GLU:OE2	3:N:1062:ARG:NE	2.51	0.43
3:N:1144:LEU:HA	3:N:1147:ARG:HG3	2.01	0.43
3:N:436:GLU:HB2	3:N:445:ARG:CB	2.48	0.43
3:N:481:MET:SD	3:N:493:ARG:HA	2.58	0.43
3:N:693:GLU:HA	4:O:48:MET:CE	2.48	0.43
3:N:643:GLY:CA	3:N:727:GLN:HB2	2.42	0.43
5:P:258:ILE:HG13	9:P:3765:HOH:O	2.18	0.43
5:P:401:GLU:O	5:P:405:LEU:HD13	2.19	0.43
1:B:88:ARG:NH1	9:B:9562:HOH:O	2.51	0.43
2:C:1005:MET:O	2:C:1005:MET:HG3	2.18	0.43
2:C:199:VAL:HG13	2:C:235:LEU:CD2	2.48	0.43
2:C:100:LEU:HD22	2:C:372:LEU:HD22	2.01	0.43
2:C:660:ALA:O	2:C:667:ALA:O	2.37	0.43
2:C:552:HIS:CD2	2:C:886:LEU:HD12	2.52	0.43
3:D:1377:LYS:HB3	3:D:1378:TYR:CE1	2.54	0.43
3:D:1472:ILE:HG22	3:D:1474:ALA:O	2.19	0.43
3:D:33:ASN:O	3:D:36:THR:O	2.36	0.43
3:D:2:LYS:HB3	3:D:3:LYS:NZ	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:55:ASP:HB3	3:D:56:TYR:H	1.57	0.43
3:D:637:LEU:HD11	3:D:642:CYS:N	2.34	0.43
3:D:781:PRO:HB3	3:D:785:ILE:CG2	2.49	0.43
3:D:884:ARG:HA	9:D:9724:HOH:O	2.18	0.43
5:F:316:SER:HB2	5:F:319:THR:OG1	2.19	0.43
1:K:203:GLY:HA2	9:K:4352:HOH:O	2.19	0.43
1:K:220:GLU:HB2	9:K:5313:HOH:O	2.18	0.43
1:L:145:ASP:O	1:L:171:PHE:HE1	2.02	0.43
1:L:84:GLU:HB2	9:N:9942:HOH:O	2.18	0.43
2:M:1018:GLN:HE21	2:M:1063:ARG:HH22	1.66	0.43
2:M:1103:ASP:N	2:M:1107:ASN:O	2.52	0.43
2:M:218:VAL:HG22	2:M:221:LEU:CD2	2.48	0.43
2:M:663:ASN:HD22	2:M:663:ASN:HA	1.65	0.43
3:N:1264:GLU:CD	3:N:1425:THR:HB	2.38	0.43
3:N:422:ALA:O	3:N:427:VAL:HG21	2.18	0.43
3:N:644:LEU:N	9:N:9610:HOH:O	2.50	0.43
3:N:834:THR:HG22	3:N:838:ARG:HD2	2.01	0.43
3:N:890:VAL:HG11	3:N:922:LEU:HD13	1.99	0.43
3:N:99:ALA:HA	3:N:575:GLN:HE22	1.83	0.43
4:O:70:THR:CG2	4:O:72:ARG:HE	2.31	0.43
5:P:169:GLU:CD	5:P:169:GLU:H	2.22	0.43
5:P:393:THR:O	5:P:397:ILE:HG13	2.18	0.43
2:C:22:GLN:O	2:C:121:MET:HE1	2.19	0.43
2:C:432:ARG:HG2	2:C:432:ARG:H	1.65	0.43
2:C:689:VAL:O	2:C:869:VAL:HG23	2.19	0.43
2:C:854:PRO:O	2:C:856:GLU:N	2.52	0.43
3:D:1047:LYS:HE3	3:D:1051:GLU:HB2	2.01	0.43
3:D:1066:THR:O	3:D:1070:TYR:HB2	2.19	0.43
3:D:1148:VAL:HG13	3:D:1163:GLY:O	2.19	0.43
3:D:1292:VAL:O	3:D:1303:TYR:HB2	2.19	0.43
3:D:1264:GLU:OE2	3:D:1424:VAL:HG12	2.19	0.43
3:D:639:LEU:N	3:D:729:HIS:CD2	2.86	0.43
3:D:641:GLN:HG2	9:D:9590:HOH:O	2.18	0.43
3:D:734:GLU:HA	9:D:9487:HOH:O	2.19	0.43
4:E:29:GLN:CB	4:E:33:HIS:NE2	2.82	0.43
5:F:313:GLU:HG2	5:F:313:GLU:H	1.47	0.43
3:D:535:PHE:O	5:F:315:VAL:HG22	2.18	0.43
1:L:58:ILE:HD13	1:L:140:MET:HB3	2.01	0.43
2:M:1115:LEU:N	2:M:1115:LEU:CD1	2.82	0.43
2:M:65:VAL:HB	2:M:101:ILE:HB	2.00	0.43
2:M:85:GLU:HA	9:M:9565:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:926:PHE:O	2:M:930:LYS:HG3	2.18	0.43
3:N:1033:GLN:NE2	3:N:1036:ARG:HD3	2.27	0.43
3:N:1125:PRO:HB2	3:N:1126:ASP:H	1.64	0.43
3:N:1334:GLN:HG3	9:N:2654:HOH:O	2.18	0.43
3:N:1264:GLU:OE2	3:N:1425:THR:HB	2.19	0.43
3:N:45:PHE:N	9:N:9567:HOH:O	2.51	0.43
3:N:693:GLU:O	4:O:48:MET:HE1	2.19	0.43
3:N:749:VAL:HA	3:N:750:PRO:HD3	1.86	0.43
5:P:143:HIS:HB2	5:P:152:ASP:OD1	2.19	0.43
5:P:197:SER:O	5:P:200:LYS:HB3	2.18	0.43
5:P:287:THR:O	5:P:289:GLU:N	2.51	0.43
1:A:176:ARG:O	1:A:200:TRP:HE3	2.02	0.43
1:A:99:LEU:HB3	1:A:114:PHE:CD2	2.54	0.43
1:B:72:LYS:HD3	9:B:9705:HOH:O	2.18	0.43
2:C:1008:ARG:NH2	2:C:1021:LEU:O	2.50	0.43
2:C:1034:GLU:CA	2:C:1037:VAL:HG23	2.48	0.43
2:C:172:ILE:N	2:C:172:ILE:HD12	2.33	0.43
2:C:289:THR:HB	9:C:9939:HOH:O	2.19	0.43
2:C:327:HIS:O	2:C:330:ASN:HB2	2.19	0.43
2:C:357:GLU:HB2	9:C:9624:HOH:O	2.19	0.43
3:D:957:PRO:HG2	3:D:1007:VAL:HG12	2.01	0.43
3:D:1106:VAL:HG12	3:D:1107:VAL:N	2.34	0.43
3:D:1239:ARG:NH2	3:D:1254:GLN:HB2	2.34	0.43
3:D:1274:ILE:H	3:D:1274:ILE:HG13	1.54	0.43
3:D:1314:LYS:HZ3	3:D:1317:ASP:H	1.67	0.43
3:D:473:LEU:HD11	3:D:495:ARG:HH12	1.82	0.43
3:D:563:PRO:HB3	9:D:9517:HOH:O	2.18	0.43
9:C:2220:HOH:O	3:D:758:GLU:HB3	2.18	0.43
3:D:806:PHE:O	3:D:806:PHE:CD1	2.72	0.43
1:L:92:PRO:HB3	9:L:5570:HOH:O	2.19	0.43
2:M:1004:LYS:O	2:M:1006:HIS:ND1	2.52	0.43
2:M:227:PHE:O	2:M:230:ARG:HD3	2.19	0.43
2:M:651:LYS:HD2	9:M:2254:HOH:O	2.19	0.43
2:M:859:PRO:O	2:M:867:VAL:HG22	2.19	0.43
2:M:1109:VAL:HG21	3:N:3:LYS:O	2.19	0.43
3:N:452:ILE:HG23	3:N:452:ILE:O	2.19	0.43
3:N:500:ARG:HG3	3:N:500:ARG:HH11	1.84	0.43
3:N:957:PRO:CG	3:N:1007:VAL:HG12	2.49	0.43
2:M:1021:LEU:CD2	5:P:332:PHE:HA	2.45	0.43
1:B:41:ARG:HG3	1:B:42:ARG:N	2.34	0.42
2:C:1049:LEU:HG	2:C:1053:LEU:CD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1067:TYR:CZ	2:C:1071:ILE:HD11	2.54	0.42
2:C:1105:LYS:O	2:C:1107:ASN:N	2.52	0.42
2:C:308:ARG:HH11	2:C:308:ARG:HG2	1.84	0.42
2:C:36:PRO:CB	2:C:70:GLU:HG2	2.48	0.42
2:C:441:VAL:O	2:C:559:LEU:HD12	2.18	0.42
2:C:674:VAL:O	2:C:989:VAL:HA	2.19	0.42
2:C:925:TYR:C	2:C:925:TYR:CD1	2.92	0.42
2:C:979:THR:HG23	2:C:981:GLU:HB2	2.00	0.42
3:D:474:GLU:CG	3:D:500:ARG:HE	2.32	0.42
9:C:9491:HOH:O	3:D:613:ARG:HG3	2.18	0.42
3:D:647:ARG:HD3	3:D:647:ARG:O	2.19	0.42
3:D:952:ASP:HA	3:D:1062:ARG:HH21	1.83	0.42
3:D:984:THR:CG2	3:D:987:GLU:H	2.31	0.42
5:F:234:LYS:HD2	5:F:236:SER:HB3	2.00	0.42
5:F:373:LYS:HG2	9:F:9532:HOH:O	2.19	0.42
5:F:392:VAL:HA	9:F:9723:HOH:O	2.18	0.42
1:L:143:ARG:NH1	1:L:158:ILE:HG23	2.33	0.42
2:M:250:ARG:HG2	9:M:2207:HOH:O	2.19	0.42
2:M:331:ARG:CZ	2:M:427:VAL:HG13	2.49	0.42
3:N:1282:ARG:NH1	9:N:2080:HOH:O	2.51	0.42
3:N:1379:VAL:HG12	3:N:1419:PRO:HA	2.01	0.42
3:N:1471:LEU:HD12	3:N:1472:ILE:N	2.31	0.42
3:N:1493:LYS:HA	3:N:1496:GLU:HG2	1.99	0.42
3:N:754:PHE:CG	4:O:24:ALA:HB1	2.54	0.42
3:N:783:ARG:HE	3:N:1029:ARG:HD3	1.84	0.42
3:N:989:TYR:HA	9:N:9914:HOH:O	2.19	0.42
5:P:102:LEU:HD23	5:P:183:ALA:HA	2.01	0.42
1:A:18:ARG:HD3	1:A:123:MET:HE3	2.00	0.42
1:A:143:ARG:HG3	1:A:144:VAL:N	2.32	0.42
1:B:36:LEU:C	1:B:39:PRO:HD2	2.37	0.42
2:C:1010:THR:HG21	5:F:341:PRO:CG	2.49	0.42
2:C:91:GLN:HG2	2:C:119:PRO:HG3	2.01	0.42
2:C:378:LEU:HD11	2:C:382:ILE:HD11	2.01	0.42
2:C:676:ILE:HG22	2:C:988:VAL:O	2.19	0.42
2:C:708:TYR:HE2	2:C:793:PRO:CD	2.30	0.42
2:C:715:THR:CG2	2:C:717:LEU:HG	2.49	0.42
2:C:69:LEU:HB2	2:C:97:ARG:HB2	2.01	0.42
3:D:1403:LEU:HD23	3:D:1407:LEU:HD22	2.00	0.42
3:D:10:ILE:CD1	3:D:1447:LEU:HG	2.49	0.42
3:D:426:LYS:HB2	9:D:2623:HOH:O	2.20	0.42
3:D:462:GLN:NE2	3:D:513:ILE:HB	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:498:VAL:HG12	9:D:9841:HOH:O	2.18	0.42
3:D:591:VAL:CG1	3:D:597:ASP:HA	2.49	0.42
3:D:996:TRP:CG	3:D:1056:PRO:HG2	2.54	0.42
5:F:340:SER:O	5:F:342:VAL:N	2.52	0.42
5:F:367:MET:HA	5:F:370:LYS:HZ2	1.83	0.42
5:F:401:GLU:O	5:F:405:LEU:HD13	2.18	0.42
1:K:58:ILE:HG21	1:K:68:ILE:CD1	2.48	0.42
1:K:11:PHE:HD2	1:L:228:PRO:HA	1.84	0.42
2:M:1043:TYR:HA	3:N:710:ARG:NH2	2.34	0.42
2:M:1090:LYS:HG2	2:M:1112:PHE:HZ	1.83	0.42
2:M:166:PRO:HB2	9:M:9802:HOH:O	2.19	0.42
2:M:380:ALA:HB2	9:M:2136:HOH:O	2.19	0.42
2:M:751:PRO:HA	2:M:792:VAL:CG1	2.49	0.42
3:N:1144:LEU:HD13	3:N:1174:LEU:HD12	2.01	0.42
3:N:1319:VAL:O	3:N:1319:VAL:HG23	2.19	0.42
3:N:1478:SER:OG	3:N:1480:PHE:HB3	2.19	0.42
3:N:42:ASP:O	3:N:49:ILE:HD12	2.18	0.42
3:N:777:PRO:HD2	3:N:912:LYS:HG2	2.01	0.42
3:N:793:THR:O	3:N:879:ARG:NH1	2.52	0.42
3:N:799:LYS:HE2	3:N:824:ASN:O	2.19	0.42
2:M:984:GLU:OE1	3:N:945:SER:HA	2.19	0.42
5:P:161:GLN:NE2	9:P:3901:HOH:O	2.52	0.42
5:P:169:GLU:HA	5:P:172:ARG:NH2	2.34	0.42
5:P:240:THR:O	5:P:244:ARG:HG3	2.20	0.42
2:M:1015:LEU:HA	5:P:335:ASP:HB2	2.01	0.42
1:B:107:LYS:HB2	9:B:9631:HOH:O	2.19	0.42
1:B:124:ASN:OD1	1:B:127:LEU:HB2	2.19	0.42
1:B:150:TYR:HD1	1:B:169:ALA:O	2.02	0.42
2:C:1090:LYS:NZ	3:D:90:MET:HG3	2.34	0.42
2:C:474:VAL:HG23	2:C:478:VAL:O	2.18	0.42
2:C:663:ASN:HA	2:C:663:ASN:HD22	1.60	0.42
2:C:697:ARG:O	2:C:699:PHE:N	2.53	0.42
2:C:72:ARG:HG3	2:C:72:ARG:NH1	2.32	0.42
3:D:955:VAL:O	3:D:1039:CYS:HB3	2.20	0.42
3:D:119:SER:HB2	3:D:123:LEU:CB	2.48	0.42
3:D:167:GLU:HB2	9:D:9804:HOH:O	2.19	0.42
3:D:513:ILE:HG13	9:D:2007:HOH:O	2.18	0.42
3:D:613:ARG:HA	3:D:613:ARG:HD2	1.90	0.42
4:E:46:PRO:CB	4:E:63:TRP:NE1	2.83	0.42
5:F:135:ILE:O	5:F:135:ILE:HD13	2.19	0.42
5:F:348:SER:OG	5:F:349:LEU:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:370:LYS:NZ	5:F:370:LYS:HB3	2.34	0.42
5:F:401:GLU:HG3	5:F:405:LEU:HD22	2.01	0.42
1:K:173:PRO:HB3	1:K:204:SER:HB3	2.01	0.42
1:L:101:LEU:HD12	1:L:114:PHE:CD1	2.55	0.42
1:L:206:THR:CG2	1:L:209:GLU:H	2.26	0.42
2:M:352:ALA:O	2:M:355:VAL:HG12	2.19	0.42
2:M:437:ARG:HG2	2:M:467:ILE:HG22	2.02	0.42
2:M:690:ILE:CG2	2:M:852:ILE:HG12	2.49	0.42
2:M:802:ARG:HB3	2:M:802:ARG:NH1	2.34	0.42
2:M:897:LEU:CD2	2:M:921:ALA:HB2	2.50	0.42
3:N:951:ILE:HG23	3:N:1062:ARG:NH2	2.35	0.42
3:N:1106:VAL:HB	3:N:1108:ARG:HH21	1.84	0.42
3:N:127:LEU:HB3	3:N:132:TYR:O	2.18	0.42
3:N:1476:THR:C	3:N:1478:SER:H	2.23	0.42
3:N:520:LEU:CD1	3:N:521:PRO:HD2	2.49	0.42
3:N:520:LEU:O	3:N:525:ARG:NH1	2.52	0.42
3:N:734:GLU:OE1	3:N:782:SER:HB2	2.18	0.42
4:O:44:GLU:HG3	9:O:5061:HOH:O	2.20	0.42
4:O:59:ASN:ND2	9:O:5180:HOH:O	2.52	0.42
4:O:79:LEU:HA	4:O:79:LEU:HD12	1.93	0.42
5:P:409:LYS:HG3	5:P:410:TYR:N	2.35	0.42
1:A:26:GLU:HG2	1:A:27:PRO:HG3	2.00	0.42
1:A:9:PRO:HB3	1:A:25:LEU:CD2	2.49	0.42
1:B:207:PRO:HB2	9:B:9532:HOH:O	2.18	0.42
1:B:213:GLN:HB2	1:B:213:GLN:HE21	1.58	0.42
1:B:86:VAL:O	1:B:86:VAL:HG13	2.17	0.42
2:C:11:GLU:HG2	2:C:537:LYS:NZ	2.34	0.42
2:C:253:ALA:O	2:C:256:TYR:HB2	2.19	0.42
2:C:270:GLY:O	2:C:271:GLU:HG2	2.18	0.42
2:C:352:ALA:C	2:C:355:VAL:HG12	2.39	0.42
2:C:578:VAL:HG13	2:C:671:ASN:OD1	2.19	0.42
2:C:31:GLN:HB3	2:C:71:TYR:OH	2.19	0.42
2:C:852:ILE:N	2:C:852:ILE:HD12	2.34	0.42
2:C:69:LEU:HD12	2:C:97:ARG:HB2	2.01	0.42
3:D:1205:TYR:HE1	3:D:1221:VAL:HG13	1.84	0.42
3:D:1467:ILE:HG22	9:D:9522:HOH:O	2.19	0.42
3:D:581:LEU:CD1	3:D:603:LEU:HD12	2.50	0.42
3:D:704:ARG:CD	3:D:705:ALA:H	2.32	0.42
3:D:765:SER:OG	3:D:766:ALA:N	2.52	0.42
3:D:844:ALA:HB3	3:D:848:GLU:OE2	2.18	0.42
3:D:914:LEU:HD22	3:D:930:LEU:HD21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:14:ASP:HB2	9:E:9493:HOH:O	2.18	0.42
3:D:757:ALA:CB	4:E:24:ALA:HB2	2.50	0.42
5:F:87:GLU:HB3	9:F:9506:HOH:O	2.20	0.42
2:M:1115:LEU:CD1	2:M:1115:LEU:H	2.31	0.42
2:M:246:ASP:HB2	9:M:9955:HOH:O	2.19	0.42
2:M:352:ALA:HA	2:M:355:VAL:CG1	2.49	0.42
2:M:35:PRO:HD2	2:M:38:LYS:CG	2.49	0.42
2:M:361:MET:HG2	9:M:2349:HOH:O	2.18	0.42
2:M:706:GLU:HB3	2:M:708:TYR:CE1	2.54	0.42
2:M:1000:MET:HG3	7:M:8002:RPT:H472	2.00	0.42
2:M:808:ARG:HA	9:M:9526:HOH:O	2.19	0.42
2:M:80:GLN:O	2:M:83:CYS:HB2	2.19	0.42
3:N:1111:ASP:HB2	3:N:1203:LYS:HG3	2.02	0.42
3:N:1133:ARG:HB2	9:N:9762:HOH:O	2.18	0.42
3:N:1402:ALA:HB1	9:N:2424:HOH:O	2.18	0.42
3:N:9:ARG:HG3	3:N:1456:LYS:HG2	2.01	0.42
3:N:95:LEU:HD11	3:N:517:VAL:CG2	2.50	0.42
3:N:93:ILE:HD13	3:N:548:ILE:HD11	2.01	0.42
3:N:563:PRO:HG2	3:N:566:ILE:HB	2.01	0.42
3:N:765:SER:C	3:N:767:HIS:H	2.22	0.42
3:N:82:LYS:C	3:N:83:SER:HG	2.22	0.42
3:N:892:ASP:HB3	3:N:895:VAL:CG2	2.49	0.42
5:P:122:LEU:HD12	9:P:4063:HOH:O	2.18	0.42
9:N:9815:HOH:O	5:P:140:ARG:HB2	2.19	0.42
5:P:361:LEU:HD23	5:P:362:SER:N	2.35	0.42
1:B:103:ALA:HB1	1:B:107:LYS:CE	2.49	0.42
1:B:49:PRO:HB3	1:B:148:VAL:HG13	2.01	0.42
2:C:1008:ARG:NH2	2:C:1021:LEU:C	2.73	0.42
2:C:1067:TYR:CE1	2:C:1071:ILE:HD11	2.55	0.42
2:C:1090:LYS:HZ1	3:D:90:MET:HG3	1.85	0.42
2:C:276:LYS:HG2	9:C:2408:HOH:O	2.19	0.42
2:C:431:HIS:CD2	2:C:433:THR:HG1	2.38	0.42
2:C:577:PRO:HB2	2:C:580:MET:HG3	2.01	0.42
2:C:636:ALA:C	2:C:637:LEU:HD23	2.40	0.42
2:C:710:ILE:HD12	2:C:790:LEU:HB2	2.01	0.42
2:C:744:ARG:HA	9:C:9908:HOH:O	2.19	0.42
2:C:774:LEU:HD21	9:C:9684:HOH:O	2.18	0.42
2:C:77:PRO:HD2	2:C:91:GLN:O	2.20	0.42
2:C:876:VAL:HG11	2:C:885:ILE:HD11	2.02	0.42
2:C:956:GLY:HA2	9:C:9712:HOH:O	2.19	0.42
3:D:102:ILE:HG13	9:D:9521:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1041:LEU:HD12	3:D:1058:ARG:C	2.40	0.42
3:D:1183:ILE:O	3:D:1183:ILE:HD12	2.20	0.42
3:D:1087:ARG:CG	3:D:1234:THR:HA	2.19	0.42
3:D:1274:ILE:HA	9:D:9544:HOH:O	2.17	0.42
3:D:1412:LYS:HG3	9:D:9570:HOH:O	2.18	0.42
3:D:1434:TRP:CZ3	3:D:1455:LYS:HB3	2.54	0.42
3:D:500:ARG:HG3	9:D:9797:HOH:O	2.20	0.42
3:D:704:ARG:NH1	3:D:737:ASN:O	2.53	0.42
1:K:229:GLN:HB2	1:K:229:GLN:HE21	1.68	0.42
1:L:119:ASP:HB3	9:L:4208:HOH:O	2.17	0.42
1:L:142:VAL:HG23	1:L:142:VAL:O	2.20	0.42
1:L:68:ILE:HG23	9:L:6170:HOH:O	2.18	0.42
2:M:50:GLU:HA	2:M:266:ARG:CZ	2.50	0.42
2:M:444:PRO:HB3	7:M:8002:RPT:H302	2.01	0.42
2:M:798:GLY:HA2	9:M:2295:HOH:O	2.18	0.42
3:N:1047:LYS:HG2	3:N:1053:PHE:CE1	2.55	0.42
3:N:106:LYS:HB3	3:N:586:ARG:NH1	2.34	0.42
3:N:1122:LEU:O	3:N:1135:ARG:N	2.45	0.42
3:N:1231:GLU:HB3	3:N:1232:PRO:HD3	2.00	0.42
3:N:209:ARG:NH2	3:N:397:LYS:HG3	2.34	0.42
3:N:508:ARG:HG3	9:N:2034:HOH:O	2.18	0.42
3:N:679:ARG:HB3	9:N:9725:HOH:O	2.19	0.42
3:N:838:ARG:HD3	3:N:874:GLU:HB3	2.00	0.42
4:O:31:LEU:HD23	4:O:35:PHE:CD1	2.54	0.42
5:P:131:VAL:HG13	5:P:178:ARG:HG2	2.02	0.42
5:P:88:ILE:HG21	5:P:193:ARG:CZ	2.50	0.42
5:P:411:HIS:HA	5:P:414:ARG:HG3	2.01	0.42
1:A:32:PHE:HB2	9:A:9526:HOH:O	2.19	0.42
1:A:9:PRO:HG2	1:B:224:TYR:CD2	2.55	0.42
1:B:123:MET:HG2	9:B:9635:HOH:O	2.20	0.42
1:B:140:MET:HG3	9:B:9666:HOH:O	2.19	0.42
2:C:172:ILE:HA	2:C:185:LYS:O	2.18	0.42
2:C:254:VAL:HG13	2:C:258:TYR:HE1	1.84	0.42
2:C:614:ARG:HG3	2:C:620:LEU:HB3	2.02	0.42
2:C:658:GLY:N	2:C:661:SER:OG	2.52	0.42
2:C:964:LYS:HB2	9:C:2350:HOH:O	2.19	0.42
3:D:1040:GLY:O	3:D:1060:SER:HB3	2.20	0.42
3:D:1074:SER:O	3:D:1077:ALA:HB3	2.20	0.42
3:D:1109:GLU:HG2	3:D:1202:GLN:H	1.85	0.42
3:D:1344:VAL:HG11	3:D:1421:LEU:HD13	2.01	0.42
3:D:501:ALA:HB1	3:D:1453:ALA:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:715:ALA:HB3	3:D:764:LEU:CA	2.47	0.42
1:K:18:ARG:HG2	9:K:4001:HOH:O	2.19	0.42
2:M:1078:GLU:HA	2:M:1079:PRO:HD3	1.93	0.42
2:M:90:TYR:CE2	2:M:120:LEU:HB2	2.55	0.42
2:M:393:GLN:HB2	7:M:8002:RPT:O9	2.20	0.42
2:M:405:ARG:HD2	2:M:442:GLU:OE1	2.19	0.42
2:M:729:LEU:HB3	9:M:2237:HOH:O	2.20	0.42
2:M:86:LYS:CE	2:M:813:VAL:HG12	2.49	0.42
2:M:546:LEU:HD23	2:M:842:ARG:HH11	1.85	0.42
2:M:689:VAL:O	2:M:869:VAL:HG23	2.20	0.42
2:M:928:LYS:HD2	9:M:2219:HOH:O	2.18	0.42
3:N:964:LEU:HD22	3:N:1058:ARG:HH12	1.81	0.42
3:N:1283:ILE:N	3:N:1315:ASP:OD1	2.52	0.42
3:N:1341:PRO:HA	3:N:1344:VAL:HG23	2.01	0.42
3:N:1394:VAL:HG21	3:N:1397:LYS:HE3	2.02	0.42
3:N:645:PRO:HA	3:N:721:VAL:O	2.19	0.42
3:N:739:ASP:O	3:N:743:ASP:OD2	2.37	0.42
5:P:136:LEU:HD12	5:P:137:GLY:N	2.35	0.42
5:P:352:GLU:O	5:P:356:LYS:HG3	2.19	0.42
2:C:137:VAL:O	2:C:391:LEU:HD21	2.20	0.42
2:C:559:LEU:HD23	2:C:560:MET:N	2.35	0.42
2:C:798:GLY:HA3	2:C:828:ALA:O	2.20	0.42
2:C:841:ASN:C	2:C:841:ASN:HD22	2.23	0.42
2:C:833:LEU:HD11	2:C:849:VAL:HG21	2.02	0.42
2:C:886:LEU:HD23	2:C:886:LEU:HA	1.92	0.42
2:C:94:LEU:HD21	9:C:9517:HOH:O	2.19	0.42
3:D:1034:GLN:O	3:D:1037:GLN:HG3	2.19	0.42
3:D:1041:LEU:HD23	3:D:1041:LEU:O	2.19	0.42
3:D:1065:LEU:HD12	3:D:1066:THR:N	2.34	0.42
3:D:1129:THR:C	3:D:1130:ARG:HD2	2.40	0.42
3:D:1109:GLU:CG	3:D:1202:GLN:H	2.33	0.42
3:D:1463:LYS:HA	3:D:1463:LYS:HD3	1.85	0.42
3:D:169:TYR:N	3:D:170:PRO:HD2	2.35	0.42
3:D:584:ASN:HD21	3:D:589:ALA:CA	2.30	0.42
3:D:93:ILE:HD12	3:D:519:VAL:HG22	2.02	0.42
1:L:116:PRO:HD3	9:L:6307:HOH:O	2.19	0.42
1:L:95:GLN:H	1:L:95:GLN:NE2	2.18	0.42
2:M:141:HIS:HB2	9:M:9692:HOH:O	2.19	0.42
2:M:391:LEU:HD23	2:M:391:LEU:C	2.40	0.42
2:M:455:LEU:HD12	2:M:459:ALA:HB3	2.00	0.42
2:M:654:LEU:HD11	2:M:657:ASP:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:815:LEU:HD21	2:M:820:ARG:O	2.19	0.42
2:M:838:LYS:CD	2:M:846:LYS:HZ3	2.33	0.42
2:M:93:PRO:HG3	2:M:117:HIS:HE1	1.83	0.42
3:N:1037:GLN:OE1	3:N:1042:ARG:HB3	2.20	0.42
3:N:1148:VAL:HG21	3:N:1203:LYS:HA	2.02	0.42
3:N:1283:ILE:HG23	3:N:1290:LEU:HD21	2.00	0.42
3:N:1315:ASP:HB2	9:N:9493:HOH:O	2.20	0.42
3:N:135:LEU:HD11	3:N:139:GLY:HA3	2.02	0.42
3:N:154:THR:HG23	3:N:157:GLU:H	1.83	0.42
3:N:187:LYS:HA	3:N:187:LYS:HD3	1.87	0.42
3:N:411:THR:HG23	3:N:429:SER:CB	2.49	0.42
3:N:957:PRO:CD	3:N:1007:VAL:HG12	2.49	0.42
4:O:43:GLU:H	4:O:43:GLU:CD	2.23	0.42
1:A:7:LYS:HB2	9:A:9499:HOH:O	2.18	0.42
1:B:84:GLU:HG2	1:B:127:LEU:CD1	2.49	0.42
2:C:101:ILE:HG22	2:C:102:HIS:H	1.85	0.42
2:C:1102:LEU:HD23	2:C:1106:ASP:CA	2.50	0.42
2:C:343:GLN:HA	9:C:2037:HOH:O	2.19	0.42
2:C:135:VAL:O	2:C:392:SER:HA	2.19	0.42
2:C:420:ARG:HG2	2:C:421:GLU:N	2.34	0.42
2:C:755:LEU:CD2	2:C:825:VAL:HG11	2.47	0.42
2:C:881:ASN:H	2:C:881:ASN:ND2	2.15	0.42
3:D:1047:LYS:HA	3:D:1053:PHE:CZ	2.55	0.42
3:D:1292:VAL:N	3:D:1305:LEU:HD21	2.35	0.42
3:D:209:ARG:CZ	3:D:397:LYS:HG3	2.49	0.42
3:D:23:TYR:OH	3:D:89:ARG:NE	2.53	0.42
3:D:415:VAL:N	9:D:2009:HOH:O	2.51	0.42
3:D:491:LYS:HB2	9:D:9973:HOH:O	2.19	0.42
4:E:87:LYS:HD2	9:E:9516:HOH:O	2.20	0.42
5:F:131:VAL:CG1	5:F:181:GLU:HG3	2.48	0.42
1:L:103:ALA:O	1:L:138:LEU:HD23	2.19	0.42
1:L:18:ARG:O	1:L:207:PRO:HD3	2.19	0.42
1:L:85:LEU:HD12	1:L:86:VAL:N	2.35	0.42
2:M:1008:ARG:NH1	2:M:1011:GLY:CA	2.82	0.42
2:M:1032:PHE:HD1	9:M:2368:HOH:O	2.03	0.42
2:M:290:LEU:HD22	2:M:302:VAL:HG11	2.00	0.42
2:M:316:GLY:O	2:M:318:PRO:HD3	2.19	0.42
2:M:380:ALA:HA	2:M:383:ARG:CD	2.50	0.42
2:M:405:ARG:HH21	2:M:409:ARG:NH2	2.18	0.42
2:M:443:THR:HG23	2:M:449:ILE:HG13	2.02	0.42
2:M:496:ILE:HD12	2:M:496:ILE:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:537:LYS:HE3	2:M:905:ILE:HD11	2.02	0.42
2:M:660:ALA:O	2:M:667:ALA:O	2.38	0.42
2:M:721:ARG:HG3	2:M:721:ARG:HH11	1.85	0.42
2:M:727:PRO:HB3	9:M:2452:HOH:O	2.19	0.42
2:M:815:LEU:HD11	2:M:819:VAL:HG12	2.02	0.42
3:N:115:LEU:CD1	3:N:498:VAL:HG23	2.50	0.42
3:N:1459:LEU:HD22	3:N:1465:ASN:HA	2.01	0.42
3:N:799:LYS:N	3:N:826:PRO:HG2	2.34	0.42
5:P:276:ARG:HB2	9:P:4488:HOH:O	2.19	0.42
5:P:356:LYS:HZ1	5:P:417:LYS:HE2	1.85	0.42
1:B:28:LEU:HB2	1:B:193:ASP:HB2	2.01	0.42
2:C:14:PRO:HA	9:C:2347:HOH:O	2.20	0.42
2:C:150:PRO:CA	2:C:158:TYR:HB3	2.34	0.42
2:C:287:GLY:O	2:C:288:ARG:C	2.58	0.42
2:C:384:GLU:HA	2:C:388:ARG:HH21	1.85	0.42
2:C:406:HIS:ND1	2:C:406:HIS:O	2.52	0.42
2:C:599:GLU:HG2	2:C:600:ASP:H	1.84	0.42
2:C:75:GLU:O	2:C:93:PRO:HG2	2.19	0.42
3:D:1011:PHE:HZ	3:D:1039:CYS:SG	2.42	0.42
3:D:1031:ASN:OD1	3:D:1033:GLN:N	2.53	0.42
3:D:203:ALA:HB2	9:D:9843:HOH:O	2.20	0.42
3:D:491:LYS:HG3	9:D:9655:HOH:O	2.19	0.42
5:F:220:LEU:HB2	5:F:243:ILE:HD11	2.01	0.42
5:F:326:ASP:HB2	9:F:9660:HOH:O	2.20	0.42
1:K:44:LEU:CD2	1:K:199:ILE:HG12	2.49	0.42
1:K:32:PHE:HB2	9:K:4346:HOH:O	2.20	0.42
1:K:53:VAL:HG21	1:K:82:LEU:HB3	2.01	0.42
2:M:103:LYS:HG2	9:M:9553:HOH:O	2.19	0.42
2:M:1059:ASP:OD2	2:M:1079:PRO:HA	2.20	0.42
2:M:199:VAL:HG13	2:M:235:LEU:CG	2.44	0.42
2:M:305:PRO:HA	2:M:308:ARG:HB2	2.01	0.42
2:M:495:THR:HG21	2:M:524:VAL:HG21	2.01	0.42
2:M:571:LEU:HD12	2:M:701:THR:N	2.34	0.42
3:N:1074:SER:O	3:N:1077:ALA:HB3	2.19	0.42
3:N:120:ALA:HB1	9:N:2018:HOH:O	2.20	0.42
3:N:1317:ASP:OD2	3:N:1317:ASP:N	2.49	0.42
3:N:477:LEU:HD21	3:N:495:ARG:HD3	2.00	0.42
3:N:546:ARG:NH2	3:N:550:ARG:HH22	2.17	0.42
3:N:654:LYS:CB	3:N:655:PRO:HD3	2.48	0.42
3:N:6:ARG:HG2	9:N:9676:HOH:O	2.19	0.42
3:N:782:SER:N	3:N:785:ILE:HD13	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:828:LYS:HD3	3:N:828:LYS:N	2.34	0.42
5:P:113:ILE:HG23	5:P:127:ILE:HG22	2.01	0.42
5:P:175:HIS:O	5:P:179:GLU:HG2	2.20	0.42
1:A:110:LYS:HB2	9:A:9528:HOH:O	2.19	0.42
1:A:199:ILE:N	9:A:9498:HOH:O	2.52	0.42
1:B:132:LEU:CD1	1:B:138:LEU:HD22	2.48	0.42
1:B:217:ILE:O	1:B:221:HIS:ND1	2.53	0.42
2:C:137:VAL:HG22	2:C:391:LEU:O	2.20	0.42
2:C:218:VAL:HG22	2:C:221:LEU:HD23	2.00	0.42
2:C:207:LEU:HD13	2:C:221:LEU:HD13	2.02	0.42
2:C:258:TYR:O	2:C:290:LEU:HG	2.20	0.42
2:C:289:THR:O	2:C:291:ALA:N	2.53	0.42
2:C:466:PHE:HD2	9:C:9744:HOH:O	2.03	0.42
2:C:64:LEU:HD13	2:C:359:MET:CG	2.50	0.42
2:C:742:VAL:HG12	2:C:743:VAL:H	1.84	0.42
2:C:498:GLN:CD	3:D:1068:LEU:HD12	2.41	0.42
3:D:1118:ILE:HG21	3:D:1346:ARG:CZ	2.50	0.42
3:D:1128:VAL:O	3:D:1129:THR:C	2.58	0.42
3:D:1176:LYS:HA	3:D:1179:GLU:OE1	2.19	0.42
3:D:142:LEU:HD12	3:D:142:LEU:O	2.20	0.42
3:D:159:ARG:HB2	3:D:159:ARG:NH1	2.34	0.42
3:D:15:PRO:HG3	9:D:9862:HOH:O	2.20	0.42
3:D:434:ARG:HB2	3:D:447:VAL:CG2	2.50	0.42
2:C:1056:LYS:CD	3:D:623:VAL:HG13	2.45	0.42
3:D:634:GLY:O	3:D:637:LEU:HB3	2.19	0.42
3:D:681:ARG:NH1	9:D:2081:HOH:O	2.53	0.42
3:D:992:ILE:O	3:D:995:LEU:HB3	2.20	0.42
5:F:138:SER:HB2	5:F:140:ARG:HG2	2.02	0.42
3:D:675:ARG:HH22	5:F:420:ASP:HA	1.84	0.42
1:L:165:ILE:HA	1:L:166:PRO:HD3	1.94	0.42
1:L:195:LEU:HD12	1:L:196:THR:N	2.34	0.42
2:M:1050:GLN:HA	2:M:1053:LEU:HD12	2.02	0.42
2:M:172:ILE:HD12	2:M:172:ILE:N	2.35	0.42
2:M:276:LYS:HE3	9:M:9970:HOH:O	2.20	0.42
2:M:405:ARG:HH21	2:M:409:ARG:HH21	1.68	0.42
2:M:430:VAL:HG13	3:N:1075:HIS:ND1	2.35	0.42
2:M:47:ALA:O	2:M:50:GLU:HB3	2.20	0.42
2:M:591:SER:HB2	9:M:2161:HOH:O	2.18	0.42
2:M:790:LEU:HD23	2:M:791:ARG:N	2.34	0.42
2:M:841:ASN:ND2	2:M:841:ASN:C	2.73	0.42
3:N:1007:VAL:CG2	3:N:1008:PHE:N	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1423:GLY:O	3:N:1426:LYS:N	2.53	0.42
3:N:1441:GLN:NE2	3:N:1442:ASN:HB2	2.35	0.42
3:N:28:LYS:HD3	3:N:41:ARG:NH1	2.34	0.42
3:N:450:TYR:HA	9:N:9669:HOH:O	2.18	0.42
5:P:340:SER:O	5:P:342:VAL:N	2.52	0.42
1:A:64:GLU:O	1:A:64:GLU:HG2	2.20	0.41
1:B:19:GLU:O	1:B:200:TRP:HA	2.20	0.41
2:C:244:PRO:CD	2:C:245:GLY:N	2.82	0.41
2:C:555:ALA:HB2	3:D:1070:TYR:CE2	2.55	0.41
2:C:666:LEU:HG	2:C:668:LEU:HD11	2.02	0.41
2:C:713:ARG:HH12	3:D:532:GLY:HA2	1.85	0.41
3:D:1238:MET:HE1	3:D:1257:PRO:HG3	2.02	0.41
3:D:123:LEU:HD12	9:D:9569:HOH:O	2.19	0.41
3:D:1351:GLU:HA	3:D:1354:LYS:HG2	2.01	0.41
3:D:672:ALA:HB2	9:F:9494:HOH:O	2.18	0.41
3:D:683:ILE:HA	9:D:9956:HOH:O	2.19	0.41
3:D:765:SER:C	3:D:767:HIS:H	2.24	0.41
4:E:84:ARG:NH1	4:E:84:ARG:HB2	2.35	0.41
5:F:281:GLU:HB3	9:F:9529:HOH:O	2.20	0.41
5:F:350:LEU:O	5:F:354:LEU:HB2	2.20	0.41
5:F:370:LYS:NZ	5:F:371:LEU:HG	2.35	0.41
1:K:156:HIS:HD2	1:K:157:GLY:N	2.18	0.41
1:L:156:HIS:HE1	1:L:166:PRO:HB3	1.84	0.41
1:L:188:GLN:N	9:L:5782:HOH:O	2.53	0.41
2:M:203:ASP:OD1	2:M:205:GLU:HG3	2.19	0.41
2:M:460:ARG:HD2	2:M:485:TYR:CD2	2.55	0.41
2:M:525:SER:HA	9:M:2109:HOH:O	2.20	0.41
2:M:744:ARG:HE	2:M:747:ALA:HB2	1.86	0.41
2:M:877:PRO:HG3	3:N:1023:MET:CE	2.49	0.41
3:N:105:VAL:HG12	3:N:106:LYS:HZ1	1.85	0.41
3:N:1066:THR:HG22	3:N:1069:GLU:OE1	2.20	0.41
3:N:1259:VAL:HG22	3:N:1355:VAL:HG21	2.02	0.41
3:N:153:LEU:HD12	3:N:154:THR:N	2.35	0.41
3:N:605:ASP:HB3	9:N:9598:HOH:O	2.19	0.41
3:N:653:PHE:CE2	3:N:695:ILE:HG13	2.53	0.41
3:N:734:GLU:HB2	9:N:9534:HOH:O	2.19	0.41
3:N:63:TYR:HE1	3:N:74:GLU:OE1	2.03	0.41
2:M:1044:GLY:HA3	4:O:17:TYR:CD1	2.55	0.41
4:O:54:LEU:HA	4:O:58:PRO:HG2	2.00	0.41
9:M:9879:HOH:O	5:P:334:PRO:HG2	2.18	0.41
5:P:392:VAL:HG12	5:P:396:ARG:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:PHE:HZ	1:A:146:ARG:HB2	1.83	0.41
1:A:23:PHE:O	1:A:196:THR:HA	2.19	0.41
1:A:30:ARG:NH1	2:C:938:LYS:HE2	2.35	0.41
1:A:79:ILE:O	1:A:83:LYS:HG3	2.20	0.41
1:B:34:VAL:HA	9:B:9725:HOH:O	2.19	0.41
2:C:124:ASP:OD1	2:C:125:GLY:N	2.53	0.41
2:C:578:VAL:N	2:C:671:ASN:OD1	2.53	0.41
3:D:106:LYS:HD3	3:D:106:LYS:HA	1.81	0.41
3:D:1090:ASP:HA	3:D:1093:TYR:CB	2.49	0.41
3:D:1129:THR:O	3:D:1130:ARG:HD2	2.20	0.41
3:D:1294:VAL:O	3:D:1300:SER:HA	2.19	0.41
3:D:1465:ASN:ND2	3:D:1470:ARG:NH1	2.66	0.41
3:D:196:VAL:HG13	3:D:202:VAL:HG13	2.01	0.41
3:D:953:ASP:N	3:D:953:ASP:OD2	2.54	0.41
3:D:983:LEU:CB	9:D:9513:HOH:O	2.68	0.41
5:F:149:GLU:HA	5:F:149:GLU:OE1	2.19	0.41
5:F:82:ARG:HD3	9:F:9734:HOH:O	2.20	0.41
1:K:156:HIS:CD2	1:K:157:GLY:H	2.33	0.41
1:K:57:TYR:CZ	1:K:161:ARG:HD2	2.55	0.41
1:K:36:LEU:HB2	1:K:195:LEU:CD2	2.50	0.41
1:K:197:LEU:N	1:K:197:LEU:HD23	2.33	0.41
1:K:25:LEU:C	1:K:25:LEU:HD23	2.40	0.41
1:L:44:LEU:O	1:L:174:VAL:HG21	2.18	0.41
1:L:177:VAL:HB	9:L:4703:HOH:O	2.20	0.41
2:M:167:LYS:HE3	2:M:168:ARG:NH2	2.35	0.41
2:M:162:ILE:HG21	2:M:172:ILE:HD13	2.02	0.41
2:M:260:LEU:HG	2:M:261:ILE:CG1	2.49	0.41
2:M:398:THR:O	2:M:399:ASN:HB3	2.20	0.41
2:M:459:ALA:HB1	2:M:467:ILE:CG2	2.50	0.41
2:M:474:VAL:HG13	2:M:530:GLU:C	2.40	0.41
2:M:54:ILE:HG12	2:M:56:GLU:HG2	2.02	0.41
2:M:654:LEU:HD11	2:M:657:ASP:CG	2.40	0.41
2:M:933:GLY:HA2	9:M:9889:HOH:O	2.19	0.41
3:N:1084:THR:HG23	9:N:9666:HOH:O	2.20	0.41
3:N:1495:ILE:HG12	4:O:80:VAL:HG11	2.00	0.41
3:N:235:ALA:HB1	9:N:9519:HOH:O	2.20	0.41
3:N:481:MET:HB2	3:N:1388:ARG:HH21	1.84	0.41
2:M:1007:ALA:HB2	3:N:648:MET:CG	2.50	0.41
9:M:9622:HOH:O	3:N:791:TYR:HE2	2.03	0.41
3:N:871:LYS:HB3	3:N:873:LEU:HD11	2.02	0.41
5:P:321:ILE:HG13	5:P:332:PHE:HE1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:PRO:HA	1:B:146:ARG:CZ	2.50	0.41
1:B:26:GLU:HG3	1:B:194:LYS:HZ2	1.85	0.41
2:C:145:GLY:O	2:C:163:ILE:HG23	2.20	0.41
2:C:185:LYS:HG2	2:C:190:LYS:HG2	2.03	0.41
2:C:193:LEU:HB2	9:C:9507:HOH:O	2.21	0.41
2:C:194:VAL:HG21	2:C:221:LEU:HA	2.01	0.41
2:C:461:VAL:N	9:C:9546:HOH:O	2.53	0.41
2:C:734:LEU:HA	2:C:737:LEU:HD12	2.02	0.41
2:C:768:THR:HG23	9:C:9533:HOH:O	2.20	0.41
2:C:769:PRO:O	2:C:772:ARG:HB3	2.20	0.41
2:C:943:VAL:HG11	2:C:973:VAL:HG22	2.03	0.41
3:D:1378:TYR:CD1	3:D:1378:TYR:N	2.87	0.41
3:D:1429:LEU:HG	3:D:1441:GLN:OE1	2.19	0.41
3:D:146:PRO:HA	9:D:9718:HOH:O	2.20	0.41
3:D:389:GLU:HG2	3:D:389:GLU:O	2.20	0.41
3:D:396:VAL:HG23	9:D:9579:HOH:O	2.20	0.41
3:D:49:ILE:HB	3:D:50:PHE:CE1	2.55	0.41
3:D:521:PRO:HA	3:D:522:PRO:HD3	1.84	0.41
3:D:940:THR:O	3:D:943:THR:HG23	2.20	0.41
2:M:1008:ARG:HH21	2:M:1029:GLY:H	1.68	0.41
2:M:208:ALA:HA	2:M:221:LEU:HD21	2.01	0.41
2:M:211:LEU:HD13	2:M:308:ARG:HG3	2.02	0.41
2:M:339:LEU:HD22	2:M:391:LEU:HD13	2.02	0.41
2:M:403:SER:OG	2:M:404:LEU:N	2.54	0.41
2:M:498:GLN:O	2:M:532:MET:SD	2.79	0.41
3:N:1061:PHE:HE1	3:N:1065:LEU:HD23	1.85	0.41
3:N:1472:ILE:HA	3:N:1473:PRO:HD3	1.87	0.41
3:N:2:LYS:HB3	3:N:3:LYS:CE	2.50	0.41
3:N:56:TYR:HB3	9:N:2129:HOH:O	2.20	0.41
3:N:678:GLU:HG3	3:N:679:ARG:HG3	2.03	0.41
3:N:681:ARG:NH1	3:N:681:ARG:HB3	2.36	0.41
3:N:684:LYS:HG2	9:N:2365:HOH:O	2.20	0.41
3:N:639:LEU:N	3:N:729:HIS:CD2	2.88	0.41
3:N:813:LEU:HD12	3:N:814:ALA:N	2.35	0.41
5:P:303:ARG:HG2	9:P:3308:HOH:O	2.20	0.41
5:P:364:ARG:NH1	5:P:392:VAL:HG21	2.35	0.41
1:A:128:HIS:NE2	1:A:131:THR:HG23	2.34	0.41
2:C:1019:GLN:HG2	2:C:1019:GLN:H	1.65	0.41
2:C:1020:PRO:HD2	2:C:1057:SER:OG	2.21	0.41
2:C:145:GLY:C	2:C:163:ILE:HG23	2.40	0.41
2:C:239:PHE:CE1	2:C:250:ARG:HB3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:308:ARG:HG3	9:C:9545:HOH:O	2.20	0.41
2:C:332:ARG:CZ	2:C:464:LEU:HD11	2.50	0.41
2:C:63:GLY:HA3	2:C:103:LYS:CG	2.50	0.41
2:C:717:LEU:HD11	9:C:2279:HOH:O	2.20	0.41
2:C:843:HIS:CD2	2:C:884:GLN:HA	2.55	0.41
2:C:3:ILE:HD13	2:C:900:ARG:HB2	2.02	0.41
3:D:1031:ASN:O	3:D:1035:ILE:HG12	2.20	0.41
3:D:493:ARG:HE	3:D:1388:ARG:HB3	1.80	0.41
3:D:145:VAL:CG2	3:D:146:PRO:HD2	2.37	0.41
3:D:441:ARG:HG2	3:D:442:ASN:N	2.35	0.41
3:D:468:LEU:HD22	9:D:2533:HOH:O	2.20	0.41
3:D:683:ILE:N	3:D:683:ILE:HD12	2.35	0.41
3:D:786:ILE:HD13	3:D:908:LYS:HB3	2.02	0.41
3:D:984:THR:HG22	3:D:987:GLU:H	1.84	0.41
5:F:115:LYS:HG2	9:F:9676:HOH:O	2.20	0.41
1:K:184:THR:HG23	1:K:192:LEU:CB	2.50	0.41
1:L:7:LYS:HA	9:L:5355:HOH:O	2.20	0.41
2:M:207:LEU:HD22	2:M:221:LEU:HD13	2.02	0.41
2:M:367:LEU:HD23	2:M:371:LYS:NZ	2.31	0.41
2:M:865:THR:HA	2:M:866:PRO:HD3	1.90	0.41
3:N:107:ASP:O	3:N:108:VAL:C	2.59	0.41
3:N:1275:SER:HB3	3:N:1325:LEU:HD11	2.01	0.41
3:N:1352:ILE:HG22	3:N:1368:ILE:HD13	2.03	0.41
3:N:1396:GLU:O	3:N:1400:VAL:HG23	2.20	0.41
3:N:196:VAL:HG13	3:N:202:VAL:HG11	2.02	0.41
3:N:30:GLU:HB3	3:N:40:GLU:CB	2.50	0.41
3:N:501:ALA:HA	3:N:504:ASP:HB2	2.02	0.41
5:P:163:LEU:HB3	5:P:174:LEU:HD11	2.01	0.41
2:C:1115:LEU:CD1	2:C:1115:LEU:H	2.31	0.41
2:C:208:ALA:HA	2:C:221:LEU:HD21	2.02	0.41
2:C:413:LEU:CD2	2:C:448:ASN:HD21	2.17	0.41
2:C:462:ASP:CG	2:C:463:GLU:H	2.24	0.41
2:C:634:GLY:HA3	9:C:2295:HOH:O	2.20	0.41
2:C:668:LEU:O	2:C:993:PHE:CZ	2.73	0.41
3:D:1098:LEU:N	3:D:1098:LEU:HD12	2.35	0.41
3:D:1314:LYS:NZ	3:D:1317:ASP:HB2	2.35	0.41
3:D:1319:VAL:HG11	3:D:1325:LEU:HD11	2.02	0.41
3:D:1369:GLU:HA	3:D:1372:VAL:HG12	2.02	0.41
3:D:1379:VAL:HA	3:D:1420:LEU:CB	2.50	0.41
3:D:1481:VAL:HB	9:E:9482:HOH:O	2.20	0.41
3:D:459:GLU:HA	9:D:9482:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:525:ARG:HA	3:D:538:SER:CB	2.51	0.41
3:D:591:VAL:HG22	9:D:9851:HOH:O	2.18	0.41
3:D:89:ARG:HB3	9:D:9497:HOH:O	2.20	0.41
5:F:119:ILE:HG12	9:F:9493:HOH:O	2.20	0.41
5:F:226:LYS:HB2	5:F:238:TYR:OH	2.20	0.41
5:F:256:ARG:HD3	5:F:260:ILE:HB	2.02	0.41
1:K:212:ASN:O	1:K:215:VAL:HG22	2.21	0.41
1:K:211:LEU:O	1:K:214:ALA:HB3	2.20	0.41
1:K:44:LEU:HD21	1:K:199:ILE:HG12	2.03	0.41
1:K:59:GLU:HG3	1:K:139:ASN:HB3	2.03	0.41
1:L:100:LEU:HD12	1:L:115:LEU:HD21	2.02	0.41
1:L:208:LEU:H	1:L:208:LEU:CD2	2.33	0.41
2:M:444:PRO:HD2	2:M:452:ILE:O	2.20	0.41
2:M:462:ASP:N	9:M:2120:HOH:O	2.54	0.41
2:M:545:ASN:HB3	2:M:583:LEU:HD13	2.02	0.41
2:M:742:VAL:HG12	2:M:743:VAL:H	1.85	0.41
2:M:899:GLN:HG3	2:M:901:TYR:OH	2.20	0.41
3:N:105:VAL:HG12	3:N:106:LYS:HZ2	1.86	0.41
3:N:1263:PHE:HA	3:N:1375:MET:HE1	2.02	0.41
3:N:1310:ARG:HB3	9:N:9491:HOH:O	2.20	0.41
3:N:177:ALA:HB1	3:N:199:LEU:HB3	2.03	0.41
3:N:444:VAL:O	3:N:446:VAL:HG23	2.20	0.41
3:N:50:PHE:CB	3:N:522:PRO:HG2	2.51	0.41
5:P:290:GLU:CD	5:P:290:GLU:H	2.23	0.41
1:A:121:GLU:HB3	9:A:9529:HOH:O	2.20	0.41
1:B:123:MET:HE3	1:B:204:SER:HA	2.02	0.41
2:C:1044:GLY:HA3	4:E:17:TYR:HE1	1.85	0.41
2:C:107:LEU:HB3	9:C:2236:HOH:O	2.19	0.41
2:C:1105:LYS:HD2	2:C:1107:ASN:HD21	1.86	0.41
2:C:1111:ILE:HG13	2:C:1112:PHE:N	2.29	0.41
2:C:279:GLU:HG3	2:C:280:LYS:N	2.34	0.41
2:C:435:TYR:C	2:C:437:ARG:H	2.24	0.41
2:C:684:PHE:HA	3:D:784:ASP:OD1	2.21	0.41
2:C:630:ARG:NH2	2:C:707:ARG:HB2	2.36	0.41
2:C:813:VAL:HG12	9:C:9512:HOH:O	2.21	0.41
2:C:92:ALA:HB2	9:C:2288:HOH:O	2.21	0.41
2:C:937:ASP:HB2	2:C:940:GLU:H	1.86	0.41
3:D:1303:TYR:CD1	3:D:1325:LEU:HD23	2.56	0.41
3:D:168:THR:O	3:D:393:ILE:N	2.52	0.41
3:D:400:VAL:HG21	3:D:441:ARG:NH1	2.28	0.41
3:D:578:VAL:O	3:D:582:LEU:HD12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:614:PHE:HB3	9:D:9835:HOH:O	2.20	0.41
5:F:108:GLU:HA	5:F:108:GLU:OE1	2.20	0.41
1:K:208:LEU:O	1:K:211:LEU:HB3	2.21	0.41
1:K:28:LEU:HD11	1:K:36:LEU:HD12	2.02	0.41
1:L:23:PHE:HZ	1:L:207:PRO:HB2	1.86	0.41
2:M:1032:PHE:CD2	2:M:1052:MET:HG2	2.56	0.41
2:M:172:ILE:HD12	2:M:172:ILE:H	1.84	0.41
2:M:367:LEU:HA	2:M:371:LYS:HB2	2.03	0.41
2:M:374:ASN:ND2	2:M:377:PRO:HD3	2.36	0.41
2:M:512:ARG:HA	9:M:2109:HOH:O	2.20	0.41
2:M:872:ASN:OD1	2:M:873:PRO:HD2	2.20	0.41
3:N:176:ASP:HB2	9:N:2270:HOH:O	2.19	0.41
3:N:603:LEU:O	3:N:607:LEU:HD12	2.20	0.41
3:N:637:LEU:CD1	3:N:641:GLN:HB2	2.50	0.41
3:N:943:THR:HA	9:N:9516:HOH:O	2.20	0.41
4:O:72:ARG:N	9:O:3347:HOH:O	2.53	0.41
5:P:151:LEU:HB2	5:P:155:THR:H	1.86	0.41
1:A:30:ARG:CZ	1:A:191:ASP:HB2	2.50	0.41
1:B:156:HIS:CE1	1:B:158:ILE:H	2.39	0.41
1:B:81:ASN:ND2	1:B:128:HIS:O	2.54	0.41
2:C:66:LEU:HD13	2:C:100:LEU:HB2	2.03	0.41
2:C:1083:GLU:O	2:C:1087:VAL:HB	2.21	0.41
2:C:399:ASN:ND2	2:C:399:ASN:N	2.66	0.41
2:C:48:PHE:HE2	9:C:9738:HOH:O	2.03	0.41
2:C:504:GLU:HB2	2:C:507:ARG:HB2	2.01	0.41
2:C:509:ALA:HB1	9:C:9815:HOH:O	2.21	0.41
1:A:72:LYS:HA	2:C:608:GLY:CA	2.50	0.41
2:C:710:ILE:HD11	2:C:758:ARG:HH21	1.84	0.41
2:C:945:ARG:O	2:C:948:GLU:HG3	2.20	0.41
3:D:1348:LEU:O	3:D:1349:VAL:C	2.58	0.41
3:D:1362:LYS:HA	3:D:1362:LYS:HD3	1.93	0.41
3:D:95:LEU:CD1	3:D:517:VAL:HG23	2.51	0.41
3:D:826:PRO:HB3	3:D:828:LYS:HZ3	1.85	0.41
4:E:93:TYR:HA	4:E:94:PRO:HD3	1.80	0.41
5:F:273:ARG:HG2	5:F:276:ARG:NH1	2.35	0.41
5:F:278:LEU:HB3	5:F:286:PRO:HG2	2.03	0.41
5:F:409:LYS:HG3	5:F:410:TYR:N	2.35	0.41
1:K:127:LEU:HD12	1:K:128:HIS:N	2.35	0.41
1:K:185:ARG:HD3	9:K:4032:HOH:O	2.21	0.41
1:L:176:ARG:NH2	3:N:884:ARG:NE	2.69	0.41
1:L:29:GLU:OE2	1:L:189:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:1025:ALA:HA	9:M:9518:HOH:O	2.20	0.41
2:M:22:GLN:O	2:M:121:MET:HE1	2.21	0.41
2:M:290:LEU:H	2:M:290:LEU:HD23	1.86	0.41
2:M:31:GLN:O	2:M:34:VAL:HG23	2.21	0.41
2:M:627:ARG:HA	9:M:9521:HOH:O	2.19	0.41
2:M:707:ARG:HH11	2:M:824:ARG:CG	2.33	0.41
3:N:1243:THR:HG1	3:N:1253:THR:HB	1.85	0.41
3:N:462:GLN:HE21	3:N:513:ILE:CD1	2.34	0.41
3:N:668:PRO:HD2	3:N:672:ALA:CB	2.50	0.41
3:N:639:LEU:HD12	3:N:729:HIS:NE2	2.35	0.41
3:N:838:ARG:HH11	3:N:874:GLU:HB3	1.84	0.41
3:N:92:HIS:HA	3:N:519:VAL:HG23	2.02	0.41
3:N:956:ILE:HD13	3:N:960:LYS:NZ	2.36	0.41
5:P:370:LYS:NZ	5:P:370:LYS:HB3	2.36	0.41
2:M:775:ARG:NH1	5:P:423:ASP:O	2.54	0.41
1:A:150:TYR:CD1	2:C:696:LYS:HG2	2.55	0.41
1:B:106:PRO:HG3	1:B:134:GLU:CD	2.40	0.41
1:B:165:ILE:HG12	9:B:9537:HOH:O	2.20	0.41
1:B:22:GLU:HG2	1:B:198:ARG:CG	2.51	0.41
1:B:45:LEU:HD21	1:B:177:VAL:HG13	2.02	0.41
1:B:44:LEU:HD23	1:B:48:ILE:HD12	2.03	0.41
2:C:1008:ARG:HH21	2:C:1028:GLY:CA	2.32	0.41
2:C:22:GLN:NE2	2:C:336:VAL:HG21	2.36	0.41
2:C:347:GLY:HA2	9:C:9903:HOH:O	2.19	0.41
2:C:352:ALA:HA	2:C:355:VAL:CG1	2.50	0.41
2:C:355:VAL:HB	9:C:9756:HOH:O	2.20	0.41
2:C:376:ARG:HH22	5:F:285:GLU:CB	2.33	0.41
2:C:438:ILE:HG22	2:C:439:CYS:O	2.21	0.41
2:C:472:ARG:HD2	2:C:480:THR:O	2.21	0.41
2:C:759:THR:HA	9:C:9930:HOH:O	2.21	0.41
2:C:881:ASN:N	2:C:881:ASN:HD22	2.07	0.41
2:C:889:HIS:CD2	2:C:970:GLY:HA3	2.56	0.41
3:D:101:HIS:CE1	3:D:582:LEU:HD13	2.56	0.41
3:D:1046:GLN:HG2	3:D:1052:THR:HG22	2.03	0.41
3:D:107:ASP:O	3:D:108:VAL:C	2.59	0.41
3:D:482:LYS:HB3	3:D:483:HIS:ND1	2.36	0.41
3:D:553:ARG:HD3	9:F:9503:HOH:O	2.20	0.41
3:D:800:LYS:HG2	9:D:2552:HOH:O	2.20	0.41
3:D:847:ASP:HA	3:D:850:LEU:HD13	2.03	0.41
3:D:760:ARG:NH1	4:E:59:ASN:OD1	2.53	0.41
5:F:215:GLU:HG3	5:F:250:ALA:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:324:GLU:HA	9:F:9742:HOH:O	2.21	0.41
1:K:227:ASN:ND2	1:K:227:ASN:H	2.07	0.41
1:K:86:VAL:HG12	1:K:124:ASN:HB2	2.02	0.41
2:M:195:LEU:O	2:M:199:VAL:HG23	2.20	0.41
2:M:374:ASN:HD21	2:M:377:PRO:HD3	1.85	0.41
2:M:443:THR:OG1	2:M:444:PRO:HD2	2.19	0.41
2:M:18:LEU:HD22	2:M:590:ASP:HB2	2.02	0.41
3:N:1053:PHE:HD2	9:N:9968:HOH:O	2.02	0.41
3:N:400:VAL:HA	3:N:442:ASN:O	2.20	0.41
3:N:534:ARG:HD2	5:P:315:VAL:CG2	2.51	0.41
3:N:694:VAL:HG22	9:N:2371:HOH:O	2.20	0.41
5:P:309:LYS:HA	5:P:312:GLN:NE2	2.35	0.41
5:P:328:PHE:HA	5:P:328:PHE:HD2	1.77	0.41
2:M:1064:ASN:ND2	5:P:344:ALA:HB2	2.36	0.41
5:P:370:LYS:HZ2	5:P:370:LYS:HB3	1.85	0.41
1:A:184:THR:HG23	1:A:192:LEU:CB	2.49	0.41
1:B:219:ARG:HD3	9:B:9524:HOH:O	2.20	0.41
2:C:127:PHE:HE1	2:C:386:PHE:HE2	1.68	0.41
2:C:129:ILE:HB	2:C:134:ARG:HG3	2.01	0.41
2:C:242:LEU:HD23	2:C:242:LEU:HA	1.92	0.41
2:C:29:ALA:HB2	2:C:337:GLY:HA2	2.01	0.41
2:C:378:LEU:O	2:C:382:ILE:HG13	2.21	0.41
2:C:471:TYR:HD2	2:C:533:ASP:HA	1.85	0.41
2:C:597:ALA:O	2:C:652:GLY:N	2.54	0.41
2:C:745:ILE:HD12	9:C:2126:HOH:O	2.21	0.41
3:D:1060:SER:O	3:D:1063:GLU:O	2.39	0.41
3:D:1143:GLY:HA2	9:D:9689:HOH:O	2.20	0.41
3:D:1156:LEU:HD21	3:D:1177:ALA:HA	2.02	0.41
3:D:1171:VAL:HG12	3:D:1171:VAL:O	2.21	0.41
3:D:1221:VAL:O	3:D:1222:GLY:C	2.58	0.41
3:D:1376:MET:HE3	3:D:1421:LEU:HA	2.02	0.41
3:D:1438:ALA:N	3:D:1446:VAL:HG11	2.35	0.41
3:D:1480:PHE:HE2	9:E:9493:HOH:O	2.04	0.41
3:D:156:GLU:O	3:D:159:ARG:HB3	2.21	0.41
3:D:399:ARG:HG3	9:D:9991:HOH:O	2.21	0.41
3:D:53:ILE:O	3:D:53:ILE:HG12	2.20	0.41
3:D:653:PHE:CD1	3:D:653:PHE:N	2.86	0.41
3:D:704:ARG:CB	3:D:736:PHE:HB3	2.51	0.41
3:D:806:PHE:O	3:D:807:ALA:C	2.59	0.41
3:D:818:ARG:HD2	9:D:9809:HOH:O	2.20	0.41
4:E:26:ARG:NH1	4:E:29:GLN:NE2	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:227:PHE:CZ	5:F:229:TYR:HA	2.56	0.41
5:F:74:LYS:HD3	5:F:74:LYS:HA	1.95	0.41
5:F:79:ASP:HB3	5:F:80:PRO:HD2	2.02	0.41
1:K:102:LYS:HD2	9:K:3447:HOH:O	2.19	0.41
1:K:133:GLU:OE2	2:M:605:LYS:HB3	2.21	0.41
2:M:132:ALA:HA	9:M:2436:HOH:O	2.20	0.41
2:M:172:ILE:HA	2:M:185:LYS:O	2.20	0.41
2:M:352:ALA:C	2:M:355:VAL:HG12	2.41	0.41
2:M:492:ASP:HB3	2:M:518:LYS:HG2	2.02	0.41
2:M:64:LEU:HD22	2:M:359:MET:SD	2.61	0.41
2:M:669:GLY:C	2:M:670:GLN:HG2	2.41	0.41
2:M:911:GLU:O	2:M:914:ILE:HG22	2.21	0.41
2:M:917:LEU:HD12	9:M:2374:HOH:O	2.19	0.41
3:N:1106:VAL:HA	9:N:9633:HOH:O	2.21	0.41
3:N:1154:GLU:HG3	3:N:1159:ARG:HG2	2.02	0.41
3:N:1282:ARG:HA	3:N:1315:ASP:OD1	2.21	0.41
3:N:1462:LEU:CD2	3:N:1473:PRO:HD2	2.51	0.41
3:N:179:VAL:HG23	9:N:9797:HOH:O	2.21	0.41
3:N:223:LEU:N	3:N:365:ASP:O	2.50	0.41
3:N:413:ASP:OD1	3:N:419:ASP:HA	2.21	0.41
3:N:827:ILE:HB	3:N:828:LYS:HD3	2.02	0.41
9:N:2443:HOH:O	5:P:337:HIS:HA	2.20	0.41
5:P:337:HIS:H	5:P:337:HIS:HD2	1.68	0.41
1:A:135:GLY:HA2	9:A:9515:HOH:O	2.20	0.41
1:A:156:HIS:HE1	1:A:167:VAL:O	2.03	0.41
1:B:103:ALA:HB1	1:B:107:LYS:CD	2.51	0.41
1:B:12:THR:OG1	1:B:24:VAL:HB	2.21	0.41
2:C:176:VAL:O	2:C:178:PRO:HD3	2.20	0.41
2:C:170:PRO:HG2	2:C:258:TYR:CD2	2.56	0.41
2:C:267:TYR:HB2	2:C:272:ALA:CB	2.51	0.41
2:C:593:ALA:HB1	2:C:658:GLY:HA3	2.02	0.41
2:C:881:ASN:N	2:C:881:ASN:ND2	2.69	0.41
2:C:862:PRO:CG	2:C:975:TYR:HE1	2.34	0.41
3:D:1047:LYS:HD2	3:D:1051:GLU:OE1	2.21	0.41
3:D:1299:PHE:N	3:D:1299:PHE:HD2	2.19	0.41
3:D:1325:LEU:C	9:D:2444:HOH:O	2.58	0.41
3:D:1383:ASP:HB2	3:D:1416:ALA:HB3	2.02	0.41
3:D:185:VAL:CG1	3:D:191:LEU:HD21	2.51	0.41
3:D:441:ARG:O	3:D:443:VAL:HG23	2.21	0.41
3:D:60:CYS:HA	9:D:2600:HOH:O	2.20	0.41
3:D:783:ARG:NE	3:D:1029:ARG:CZ	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:890:VAL:HG13	3:D:926:LYS:HD3	2.03	0.41
3:D:967:ALA:HB2	9:D:2079:HOH:O	2.21	0.41
4:E:90:GLU:HB3	9:E:9562:HOH:O	2.20	0.41
5:F:362:SER:C	5:F:364:ARG:H	2.23	0.41
1:K:30:ARG:HG2	9:K:4745:HOH:O	2.21	0.41
2:M:798:GLY:HA3	2:M:828:ALA:O	2.20	0.41
2:M:808:ARG:NH1	2:M:808:ARG:HG2	2.35	0.41
2:M:854:PRO:O	2:M:856:GLU:N	2.54	0.41
3:N:178:LEU:HD11	9:N:9572:HOH:O	2.21	0.41
3:N:400:VAL:C	3:N:402:PRO:HD3	2.42	0.41
3:N:44:LEU:HG	9:N:9808:HOH:O	2.19	0.41
3:N:115:LEU:CD1	3:N:499:VAL:HG22	2.51	0.41
3:N:31:THR:HG21	3:N:527:MET:CE	2.51	0.41
5:P:119:ILE:HD13	5:P:170:HIS:CG	2.56	0.41
5:P:409:LYS:HE3	5:P:410:TYR:HD1	1.85	0.41
2:C:1067:TYR:CB	5:F:341:PRO:HB3	2.50	0.41
2:C:264:PRO:HB3	2:C:289:THR:CG2	2.48	0.41
2:C:51:THR:O	2:C:51:THR:HG22	2.21	0.41
2:C:585:GLU:HB2	9:C:2332:HOH:O	2.21	0.41
2:C:605:LYS:HG2	2:C:612:VAL:HB	2.03	0.41
2:C:601:GLY:HA3	2:C:615:TYR:HA	2.03	0.41
2:C:660:ALA:O	2:C:667:ALA:HB3	2.21	0.41
2:C:722:ILE:HG23	2:C:805:ARG:NH2	2.36	0.41
2:C:878:SER:HB3	3:D:1029:ARG:NH1	2.35	0.41
2:C:91:GLN:HA	2:C:119:PRO:HA	2.03	0.41
2:C:958:THR:CG2	2:C:961:GLU:HG2	2.50	0.41
3:D:27:GLU:O	3:D:27:GLU:HG3	2.20	0.41
3:D:393:ILE:HD12	3:D:393:ILE:N	2.31	0.41
3:D:29:PRO:HG3	3:D:549:ASN:HD21	1.86	0.41
3:D:606:ILE:O	3:D:613:ARG:HB2	2.21	0.41
3:D:683:ILE:H	3:D:683:ILE:HD12	1.86	0.41
2:C:1039:ALA:HB2	3:D:707:THR:HG21	2.02	0.41
3:D:645:PRO:HB3	3:D:723:GLY:O	2.21	0.41
3:D:629:SER:HB3	3:D:726:ILE:HD11	2.03	0.41
5:F:115:LYS:HD3	5:F:118:GLU:OE2	2.21	0.41
5:F:244:ARG:HB2	5:F:244:ARG:HH11	1.86	0.41
5:F:317:LEU:HD23	5:F:317:LEU:O	2.21	0.41
5:F:399:GLN:HB3	9:F:9591:HOH:O	2.19	0.41
5:F:408:LEU:HA	5:F:411:HIS:ND1	2.36	0.41
1:K:185:ARG:O	1:K:185:ARG:HD2	2.21	0.41
1:K:19:GLU:O	1:K:200:TRP:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:136:ILE:CG2	2:M:336:VAL:HG13	2.46	0.41
2:M:512:ARG:HD3	2:M:523:ILE:HD11	2.01	0.41
2:M:739:GLU:HG3	9:M:9499:HOH:O	2.21	0.41
2:M:78:PHE:CB	2:M:88:LEU:HD21	2.49	0.41
3:N:1335:LEU:HD21	3:N:1343:ALA:CB	2.51	0.41
3:N:1425:THR:CG2	3:N:1426:LYS:H	2.33	0.41
3:N:1503:VAL:HG13	9:N:2327:HOH:O	2.20	0.41
3:N:125:GLN:NE2	3:N:587:ARG:HH21	2.16	0.41
3:N:965:GLU:HB2	9:N:2437:HOH:O	2.19	0.41
4:O:42:PRO:HD3	9:O:4549:HOH:O	2.19	0.41
4:O:73:LEU:N	9:O:3347:HOH:O	2.54	0.41
5:P:151:LEU:O	5:P:155:THR:HB	2.21	0.41
5:P:218:GLN:HA	5:P:221:ILE:CD1	2.52	0.41
9:M:9830:HOH:O	5:P:354:LEU:HD12	2.21	0.41
1:A:150:TYR:CE2	1:A:152:PRO:HG3	2.55	0.40
1:B:191:ASP:OD1	1:B:191:ASP:N	2.55	0.40
1:B:89:PHE:HD1	1:B:120:VAL:HG13	1.85	0.40
2:C:1002:GLU:HA	2:C:1006:HIS:CE1	2.56	0.40
2:C:1033:GLY:O	2:C:1037:VAL:HG23	2.21	0.40
2:C:1102:LEU:HD23	2:C:1106:ASP:C	2.42	0.40
2:C:252:LYS:HZ3	2:C:296:GLY:HA3	1.85	0.40
2:C:307:LEU:HG	2:C:311:PHE:CE2	2.56	0.40
2:C:396:ASP:O	2:C:403:SER:N	2.54	0.40
2:C:333:ILE:HD11	2:C:467:ILE:HG13	2.02	0.40
2:C:479:VAL:HG23	2:C:506:ASN:CA	2.51	0.40
3:D:1120:VAL:HA	3:D:1121:PRO:HD3	1.84	0.40
3:D:1339:LYS:HB3	3:D:1343:ALA:CB	2.51	0.40
3:D:1393:GLN:CB	3:D:1398:TRP:HE1	2.33	0.40
3:D:34:TYR:O	3:D:37:LEU:HD23	2.21	0.40
3:D:769:LEU:N	3:D:769:LEU:HD12	2.36	0.40
3:D:836:VAL:HA	3:D:839:LEU:HB2	2.04	0.40
3:D:912:LYS:HE3	9:D:2356:HOH:O	2.21	0.40
4:E:36:LYS:HD3	4:E:36:LYS:HA	1.82	0.40
5:F:105:LYS:HE2	5:F:179:GLU:O	2.21	0.40
5:F:336:GLU:HB2	9:F:9817:HOH:O	2.21	0.40
1:K:46:SER:HA	9:K:5849:HOH:O	2.21	0.40
1:L:110:LYS:NZ	1:L:110:LYS:HB2	2.36	0.40
1:L:86:VAL:O	1:L:86:VAL:HG13	2.20	0.40
2:M:1049:LEU:O	2:M:1053:LEU:HG	2.21	0.40
2:M:1105:LYS:O	2:M:1107:ASN:N	2.54	0.40
2:M:276:LYS:H	2:M:276:LYS:CD	2.32	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:418:LEU:H	2:M:418:LEU:HD12	1.86	0.40
2:M:5:ARG:H	2:M:5:ARG:HG3	1.77	0.40
2:M:601:GLY:HA3	2:M:615:TYR:HA	2.02	0.40
2:M:63:GLY:HA3	2:M:103:LYS:CG	2.51	0.40
2:M:654:LEU:HD21	2:M:657:ASP:OD2	2.20	0.40
2:M:900:ARG:NE	9:M:2073:HOH:O	2.54	0.40
2:M:922:PHE:CD2	2:M:964:LYS:HD3	2.57	0.40
3:N:1065:LEU:HD12	3:N:1066:THR:N	2.37	0.40
3:N:1128:VAL:O	3:N:1129:THR:C	2.58	0.40
3:N:1171:VAL:HG12	3:N:1171:VAL:O	2.21	0.40
3:N:1346:ARG:HG2	9:N:9698:HOH:O	2.21	0.40
3:N:1362:LYS:HB3	9:N:9810:HOH:O	2.21	0.40
3:N:134:VAL:HG12	3:N:152:LEU:HB3	2.03	0.40
3:N:40:GLU:HA	3:N:40:GLU:OE1	2.21	0.40
3:N:550:ARG:NE	9:N:9529:HOH:O	2.54	0.40
3:N:702:LEU:HD23	3:N:716:PHE:CD1	2.55	0.40
3:N:706:PRO:HA	9:N:9787:HOH:O	2.21	0.40
3:N:838:ARG:HG2	3:N:865:THR:OG1	2.22	0.40
3:N:53:ILE:HB	3:N:86:ARG:HD3	2.02	0.40
3:N:881:LEU:HD12	9:N:9868:HOH:O	2.20	0.40
3:N:731:LEU:CD1	3:N:931:LEU:HB3	2.51	0.40
3:N:980:MET:HB3	3:N:982:PHE:CE1	2.56	0.40
5:P:147:LEU:HG	9:P:3632:HOH:O	2.20	0.40
1:A:179:PHE:HD2	9:A:9593:HOH:O	2.03	0.40
1:B:101:LEU:HB2	1:B:114:PHE:CE2	2.56	0.40
2:C:1045:ALA:HB1	2:C:1048:THR:HB	2.03	0.40
2:C:1068:GLU:HG2	9:C:2111:HOH:O	2.21	0.40
2:C:267:TYR:CD2	2:C:267:TYR:N	2.89	0.40
2:C:265:ARG:HD3	2:C:267:TYR:HB3	2.04	0.40
2:C:2:GLU:HG2	9:C:9602:HOH:O	2.21	0.40
2:C:379:GLU:HG3	9:C:2275:HOH:O	2.20	0.40
2:C:605:LYS:CG	2:C:612:VAL:HB	2.52	0.40
1:A:150:TYR:HD1	2:C:696:LYS:HG2	1.87	0.40
2:C:70:GLU:N	9:C:9625:HOH:O	2.53	0.40
2:C:1096:ALA:HB2	3:D:101:HIS:CD2	2.56	0.40
3:D:1047:LYS:HD2	3:D:1051:GLU:CD	2.42	0.40
3:D:1087:ARG:NH1	3:D:1234:THR:O	2.54	0.40
3:D:1254:GLN:OE1	3:D:1254:GLN:HA	2.21	0.40
3:D:1432:LYS:HZ3	3:D:1460:ILE:HG13	1.83	0.40
3:D:31:THR:HB	3:D:32:ILE:H	1.63	0.40
3:D:603:LEU:HA	3:D:606:ILE:HG13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:421:PHE:C	5:F:423:ASP:N	2.73	0.40
1:K:34:VAL:HG23	9:K:3503:HOH:O	2.20	0.40
1:L:105:GLY:O	1:L:132:LEU:HB3	2.21	0.40
2:M:129:ILE:HD12	2:M:129:ILE:N	2.36	0.40
2:M:408:ARG:O	2:M:454:SER:HB2	2.21	0.40
2:M:547:ILE:HA	2:M:548:PRO:HD3	1.90	0.40
2:M:771:GLU:HB2	9:P:5420:HOH:O	2.21	0.40
2:M:942:GLU:O	2:M:945:ARG:HB3	2.21	0.40
3:N:1295:GLU:HB2	3:N:1300:SER:OG	2.22	0.40
3:N:1379:VAL:HA	3:N:1420:LEU:CB	2.50	0.40
3:N:463:GLN:HE21	3:N:463:GLN:HA	1.86	0.40
3:N:471:GLU:HG2	9:N:2578:HOH:O	2.21	0.40
3:N:502:PHE:CD1	3:N:509:PRO:HB3	2.56	0.40
3:N:809:PRO:O	3:N:812:ALA:HB3	2.21	0.40
3:N:849:ALA:O	3:N:853:VAL:HG23	2.21	0.40
3:N:927:THR:O	3:N:931:LEU:HG	2.21	0.40
2:C:1039:ALA:HB2	3:D:707:THR:CG2	2.51	0.40
2:C:1037:VAL:HG13	2:C:1049:LEU:HD11	2.02	0.40
2:C:1055:LEU:CD2	2:C:1079:PRO:HG3	2.51	0.40
2:C:1115:LEU:HD23	3:D:85:VAL:HG13	2.03	0.40
2:C:140:ILE:HD12	2:C:140:ILE:H	1.86	0.40
2:C:258:TYR:HD2	9:C:2316:HOH:O	2.04	0.40
2:C:732:ALA:HB2	9:C:9752:HOH:O	2.21	0.40
2:C:677:MET:CE	2:C:983:ILE:HD13	2.51	0.40
3:D:1026:SER:C	3:D:1028:ALA:N	2.75	0.40
3:D:1097:LYS:NZ	9:D:9536:HOH:O	2.53	0.40
3:D:1148:VAL:HG21	3:D:1203:LYS:HA	2.03	0.40
3:D:770:LEU:HB2	3:D:1210:SER:O	2.21	0.40
3:D:1264:GLU:HG2	3:D:1266:ARG:HH21	1.86	0.40
3:D:1432:LYS:CG	3:D:1433:SER:N	2.83	0.40
3:D:671:LYS:N	9:D:9547:HOH:O	2.46	0.40
3:D:929:ARG:HB3	9:D:2176:HOH:O	2.21	0.40
1:K:106:PRO:HB3	9:K:3754:HOH:O	2.20	0.40
1:K:152:PRO:HB3	2:M:832:LYS:NZ	2.36	0.40
1:L:30:ARG:HG2	1:L:30:ARG:HH11	1.86	0.40
2:M:1002:GLU:HG3	2:M:1002:GLU:H	1.57	0.40
2:M:109:LYS:HE2	9:M:2096:HOH:O	2.21	0.40
2:M:163:ILE:HB	2:M:171:TRP:CZ2	2.56	0.40
2:M:212:GLY:HA3	2:M:218:VAL:CG2	2.49	0.40
2:M:200:LEU:HD22	2:M:300:ASP:OD1	2.21	0.40
2:M:642:ARG:HG2	2:M:642:ARG:HH11	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:693:GLU:HA	2:M:693:GLU:OE1	2.21	0.40
3:N:1043:GLY:N	9:N:9654:HOH:O	2.53	0.40
3:N:1264:GLU:HG2	3:N:1266:ARG:CZ	2.51	0.40
3:N:1192:LEU:HD13	3:N:1345:GLU:HB3	2.03	0.40
3:N:823:LEU:N	3:N:823:LEU:HD23	2.36	0.40
3:N:866:VAL:HG12	3:N:867:ARG:N	2.37	0.40
3:N:87:ARG:HD2	3:N:88:TYR:HE2	1.86	0.40
3:N:8:VAL:HG12	3:N:9:ARG:N	2.37	0.40
5:P:155:THR:HG22	5:P:156:VAL:N	2.35	0.40
1:A:19:GLU:O	1:A:200:TRP:HA	2.21	0.40
1:B:62:LEU:HG	1:B:163:ASN:CG	2.41	0.40
2:C:1051:GLU:HG2	2:C:1056:LYS:HD2	2.03	0.40
2:C:1069:ALA:HA	9:C:2111:HOH:O	2.21	0.40
2:C:34:VAL:HB	2:C:38:LYS:HG3	2.02	0.40
2:C:54:ILE:HG12	2:C:56:GLU:HG2	2.03	0.40
2:C:916:GLU:O	2:C:919:ALA:HB3	2.22	0.40
3:D:1000:THR:CG2	3:D:1001:GLU:N	2.84	0.40
3:D:1037:GLN:OE1	3:D:1042:ARG:NE	2.53	0.40
3:D:1066:THR:HG22	3:D:1069:GLU:H	1.86	0.40
3:D:1238:MET:CE	3:D:1257:PRO:HG3	2.50	0.40
3:D:1258:ARG:HE	3:D:1351:GLU:HG3	1.86	0.40
3:D:598:ARG:HD3	5:F:320:PRO:HD3	2.03	0.40
3:D:659:LYS:HD3	3:D:659:LYS:C	2.41	0.40
3:D:742:GLY:HA3	9:D:9931:HOH:O	2.22	0.40
5:F:163:LEU:HB3	5:F:174:LEU:CG	2.50	0.40
5:F:343:ASP:O	5:F:346:THR:HB	2.21	0.40
5:F:85:LEU:HA	9:F:9492:HOH:O	2.21	0.40
1:K:23:PHE:HB2	1:K:197:LEU:HD23	2.03	0.40
2:M:1030:GLN:CB	3:N:626:SER:HB2	2.52	0.40
2:M:1046:ALA:HB3	3:N:1476:THR:HG22	2.02	0.40
2:M:126:SER:HB3	2:M:395:LYS:NZ	2.37	0.40
2:M:230:ARG:HA	2:M:231:PRO:HD3	1.80	0.40
2:M:323:ASP:HA	9:M:9868:HOH:O	2.21	0.40
2:M:410:ILE:N	2:M:410:ILE:HD12	2.37	0.40
2:M:520:GLU:HA	2:M:521:PRO:HD3	1.80	0.40
2:M:602:GLU:HB3	9:M:9999:HOH:O	2.21	0.40
3:N:1133:ARG:HG2	3:N:1134:LEU:N	2.36	0.40
3:N:1161:GLU:HG2	3:N:1164:ARG:HB2	2.02	0.40
3:N:1166:LEU:HD12	3:N:1171:VAL:CG2	2.50	0.40
3:N:210:ARG:O	3:N:394:LEU:O	2.40	0.40
3:N:562:ALA:HB1	3:N:567:ILE:HD11	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:867:ARG:NH1	9:N:9942:HOH:O	2.54	0.40
5:P:210:LEU:HA	5:P:213:ILE:HD12	2.03	0.40
5:P:215:GLU:OE2	5:P:254:GLN:NE2	2.53	0.40
5:P:408:LEU:HA	5:P:411:HIS:CE1	2.55	0.40
2:C:1008:ARG:HH22	2:C:1021:LEU:C	2.25	0.40
2:C:1013:TYR:CZ	2:C:1063:ARG:NE	2.89	0.40
2:C:527:GLU:HB3	9:C:9801:HOH:O	2.21	0.40
3:D:1362:LYS:HB3	9:D:9652:HOH:O	2.22	0.40
3:D:1423:GLY:O	3:D:1426:LYS:N	2.54	0.40
3:D:1497:GLU:OE1	3:D:1500:LYS:HD2	2.22	0.40
3:D:169:TYR:HA	3:D:392:SER:CB	2.52	0.40
3:D:396:VAL:HG22	9:D:9613:HOH:O	2.20	0.40
3:D:3:LYS:CD	3:D:3:LYS:H	2.34	0.40
2:C:1016:ILE:CD1	3:D:526:PRO:HG2	2.52	0.40
3:D:704:ARG:HB2	3:D:736:PHE:HB3	2.02	0.40
3:D:773:ALA:HB2	3:D:1228:SER:HB3	2.04	0.40
3:D:52:PRO:HG3	3:D:78:VAL:HG13	2.03	0.40
4:E:17:TYR:N	4:E:17:TYR:HD2	2.17	0.40
3:D:566:ILE:HG13	5:F:192:LEU:HD11	2.04	0.40
5:F:194:LEU:H	5:F:194:LEU:CD2	2.34	0.40
1:K:217:ILE:HG13	1:K:217:ILE:H	1.70	0.40
1:L:152:PRO:HG2	3:N:857:ILE:HD12	2.03	0.40
2:M:285:LEU:HG	2:M:287:GLY:O	2.21	0.40
2:M:44:ILE:HA	9:M:2405:HOH:O	2.22	0.40
2:M:728:HIS:HE1	2:M:775:ARG:HH12	1.68	0.40
2:M:979:THR:HG23	2:M:981:GLU:N	2.19	0.40
3:N:1280:VAL:HG12	3:N:1281:VAL:H	1.86	0.40
3:N:1320:GLU:HG2	3:N:1339:LYS:NZ	2.36	0.40
3:N:1422:MET:CE	3:N:1427:SER:HA	2.52	0.40
3:N:172:PRO:HA	3:N:173:PRO:HD3	1.66	0.40
5:P:179:GLU:HG3	9:P:5874:HOH:O	2.21	0.40
5:P:361:LEU:HD12	5:P:408:LEU:HG	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	227/315 (72%)	201 (88%)	21 (9%)	5 (2%)	6	10
1	B	227/315 (72%)	198 (87%)	23 (10%)	6 (3%)	5	8
1	K	227/315 (72%)	200 (88%)	23 (10%)	4 (2%)	8	14
1	L	227/315 (72%)	203 (89%)	20 (9%)	4 (2%)	8	14
2	C	1117/1119 (100%)	907 (81%)	157 (14%)	53 (5%)	2	2
2	M	1117/1119 (100%)	906 (81%)	158 (14%)	53 (5%)	2	2
3	D	1388/1524 (91%)	1108 (80%)	207 (15%)	73 (5%)	2	2
3	N	1388/1524 (91%)	1105 (80%)	208 (15%)	75 (5%)	2	2
4	E	93/99 (94%)	75 (81%)	15 (16%)	3 (3%)	4	5
4	O	93/99 (94%)	75 (81%)	15 (16%)	3 (3%)	4	5
5	F	341/423 (81%)	285 (84%)	38 (11%)	18 (5%)	2	2
5	P	341/423 (81%)	287 (84%)	38 (11%)	16 (5%)	2	2
All	All	6786/7590 (89%)	5550 (82%)	923 (14%)	313 (5%)	2	2

All (313) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	B	29	GLU
1	B	48	ILE
2	C	152	PRO
2	C	178	PRO
2	C	231	PRO
2	C	244	PRO
2	C	262	ALA
2	C	288	ARG
2	C	290	LEU
2	C	422	ARG
2	C	462	ASP
2	C	465	GLY
2	C	548	PRO
2	C	680	ASP
2	C	864	GLY
2	C	908	GLY
2	C	1004	LYS

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Mol	Chain	Res	Type
3	D	40	GLU
3	D	43	GLY
3	D	55	ASP
3	D	82	LYS
3	D	137	PRO
3	D	208	PRO
3	D	209	ARG
3	D	238	PRO
3	D	246	PRO
3	D	370	ALA
3	D	373	PRO
3	D	381	ALA
3	D	385	VAL
3	D	440	VAL
3	D	504	ASP
3	D	705	ALA
3	D	766	ALA
3	D	832	ARG
3	D	844	ALA
3	D	1028	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	147	LEU
5	F	153	PRO
5	F	324	GLU
5	F	341	PRO
5	F	390	PHE
1	K	29	GLU
1	L	29	GLU
2	M	152	PRO
2	M	178	PRO
2	M	231	PRO
2	M	244	PRO
2	M	261	ILE
2	M	262	ALA
2	M	288	ARG
2	M	290	LEU
2	M	422	ARG

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Mol	Chain	Res	Type
2	M	462	ASP
2	M	465	GLY
2	M	680	ASP
2	M	864	GLY
2	M	908	GLY
3	N	40	GLU
3	N	43	GLY
3	N	55	ASP
3	N	82	LYS
3	N	137	PRO
3	N	208	PRO
3	N	209	ARG
3	N	217	LYS
3	N	238	PRO
3	N	246	PRO
3	N	370	ALA
3	N	373	PRO
3	N	381	ALA
3	N	385	VAL
3	N	440	VAL
3	N	504	ASP
3	N	705	ALA
3	N	766	ALA
3	N	832	ARG
3	N	844	ALA
3	N	1028	ALA
3	N	1125	PRO
3	N	1129	THR
3	N	1208	ASP
3	N	1243	THR
3	N	1441	GLN
4	O	42	PRO
4	O	58	PRO
5	P	147	LEU
5	P	153	PRO
5	P	324	GLU
5	P	390	PHE
1	A	187	GLY
1	B	187	GLY
2	C	18	LEU
2	C	59	LYS
2	C	156	GLY

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Mol	Chain	Res	Type
2	C	170	PRO
2	C	261	ILE
2	C	363	SER
2	C	369	PRO
2	C	626	ARG
2	C	627	ARG
2	C	1106	ASP
3	D	96	ALA
3	D	98	PRO
3	D	165	LYS
3	D	220	ARG
3	D	231	VAL
3	D	417	PRO
3	D	594	PRO
3	D	609	GLY
3	D	783	ARG
3	D	803	GLY
3	D	822	ALA
3	D	1020	LEU
4	E	53	GLY
5	F	326	ASP
1	K	187	GLY
1	L	187	GLY
2	M	59	LYS
2	M	156	GLY
2	M	363	SER
2	M	369	PRO
2	M	413	LEU
2	M	447	ALA
2	M	548	PRO
2	M	626	ARG
2	M	1106	ASP
3	N	31	THR
3	N	37	LEU
3	N	98	PRO
3	N	165	LYS
3	N	220	ARG
3	N	417	PRO
3	N	594	PRO
3	N	609	GLY
3	N	783	ARG
3	N	803	GLY

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Mol	Chain	Res	Type
3	N	822	ALA
4	O	53	GLY
5	P	326	ASP
5	P	341	PRO
1	A	106	PRO
1	A	188	GLN
1	B	106	PRO
2	C	74	GLY
2	C	164	PRO
2	C	251	ASP
2	C	273	GLY
2	C	447	ALA
2	C	517	ARG
2	C	727	PRO
2	C	783	ARG
2	C	1007	ALA
3	D	31	THR
3	D	37	LEU
3	D	120	ALA
3	D	170	PRO
3	D	424	GLY
3	D	451	ASP
3	D	1248	GLY
3	D	1286	THR
3	D	1349	VAL
5	F	288	TYR
5	F	420	ASP
1	L	106	PRO
2	M	74	GLY
2	M	164	PRO
2	M	170	PRO
2	M	251	ASP
2	M	423	ALA
2	M	517	ARG
2	M	529	VAL
2	M	627	ARG
2	M	727	PRO
3	N	96	ALA
3	N	120	ALA
3	N	170	PRO
3	N	231	VAL
3	N	424	GLY

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Mol	Chain	Res	Type
3	N	530	VAL
3	N	1338	ALA
3	N	1349	VAL
3	N	1389	LEU
5	P	232	ARG
5	P	288	TYR
5	P	420	ASP
2	C	180	GLY
2	C	400	PRO
2	C	413	LEU
2	C	781	LYS
2	C	1097	LEU
3	D	46	ASP
3	D	415	VAL
3	D	416	ALA
3	D	509	PRO
3	D	522	PRO
3	D	530	VAL
3	D	1338	ALA
3	D	1385	GLY
3	D	1389	LEU
5	F	232	ARG
5	F	286	PRO
5	F	297	PRO
5	F	329	TYR
5	F	393	THR
1	K	106	PRO
2	M	180	GLY
2	M	223	ASP
2	M	273	GLY
2	M	455	LEU
2	M	781	LYS
2	M	1007	ALA
2	M	1097	LEU
3	N	24	GLY
3	N	415	VAL
3	N	416	ALA
3	N	451	ASP
3	N	509	PRO
3	N	522	PRO
3	N	782	SER
3	N	1019	PRO

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Mol	Chain	Res	Type
3	N	1064	GLY
3	N	1248	GLY
3	N	1385	GLY
5	P	286	PRO
5	P	297	PRO
1	B	188	GLN
2	C	399	ASN
2	C	529	VAL
2	C	905	ILE
3	D	24	GLY
3	D	161	LEU
3	D	808	THR
3	D	1019	PRO
3	D	1064	GLY
3	D	1213	ARG
3	D	1241	PHE
3	D	1315	ASP
3	D	1379	VAL
5	F	97	GLU
5	F	416	ARG
2	M	18	LEU
3	N	161	LEU
3	N	533	GLY
3	N	808	THR
3	N	1241	PHE
3	N	1286	THR
3	N	1315	ASP
3	N	1341	PRO
5	P	184	ARG
5	P	393	THR
1	B	9	PRO
2	C	79	PRO
2	C	779	GLY
3	D	425	GLY
3	D	782	SER
3	D	1288	GLU
5	F	167	PRO
5	F	293	GLU
2	M	79	PRO
2	M	705	ILE
2	M	779	GLY
2	M	1059	ASP

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Mol	Chain	Res	Type
3	N	1213	ARG
3	N	1390	LEU
5	P	416	ARG
2	C	424	GLY
3	D	368	VAL
3	D	1306	PRO
1	K	9	PRO
2	M	399	ASN
3	N	368	VAL
3	N	425	GLY
5	P	167	PRO
1	A	9	PRO
2	C	1076	VAL
3	D	1446	VAL
1	L	9	PRO
2	M	646	GLY
3	N	173	PRO
3	N	1306	PRO
3	N	1379	VAL
3	N	1446	VAL
5	P	314	PRO
3	D	136	ASP
2	M	767	PRO
2	M	905	ILE
2	M	1076	VAL
2	C	53	PRO
2	C	835	VAL
3	D	173	PRO
3	D	781	PRO
2	M	17	PRO
2	M	415	PRO
3	N	136	ASP
3	N	169	TYR
3	N	1268	PRO
2	C	17	PRO
2	C	377	PRO
2	C	646	GLY
2	C	767	PRO
3	D	526	PRO
5	F	314	PRO
2	M	377	PRO
2	C	166	PRO

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Mol	Chain	Res	Type
2	M	166	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	202/273 (74%)	159 (79%)	43 (21%)	1	2
1	B	202/273 (74%)	161 (80%)	41 (20%)	1	2
1	K	202/273 (74%)	158 (78%)	44 (22%)	1	1
1	L	202/273 (74%)	160 (79%)	42 (21%)	1	2
2	C	941/941 (100%)	714 (76%)	227 (24%)	0	1
2	M	941/941 (100%)	738 (78%)	203 (22%)	1	1
3	D	1123/1279 (88%)	868 (77%)	255 (23%)	1	1
3	N	1123/1279 (88%)	871 (78%)	252 (22%)	1	1
4	E	83/87 (95%)	62 (75%)	21 (25%)	0	1
4	O	83/87 (95%)	65 (78%)	18 (22%)	1	1
5	F	295/370 (80%)	233 (79%)	62 (21%)	1	2
5	P	295/370 (80%)	246 (83%)	49 (17%)	2	4
All	All	5692/6446 (88%)	4435 (78%)	1257 (22%)	1	1

All (1257) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	5	LYS
1	A	9	PRO
1	A	12	THR
1	A	15	THR
1	A	16	GLN
1	A	20	TYR
1	A	26	GLU
1	A	44	LEU

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Mol	Chain	Res	Type
1	A	45	LEU
1	A	47	SER
1	A	66	SER
1	A	73	GLU
1	A	74	ASP
1	A	89	PHE
1	A	96	THR
1	A	101	LEU
1	A	104	GLU
1	A	112	ARG
1	A	115	LEU
1	A	121	GLU
1	A	127	LEU
1	A	133	GLU
1	A	137	ARG
1	A	161	ARG
1	A	163	ASN
1	A	167	VAL
1	A	170	VAL
1	A	184	THR
1	A	186	LEU
1	A	188	GLN
1	A	190	THR
1	A	191	ASP
1	A	196	THR
1	A	197	LEU
1	A	198	ARG
1	A	205	VAL
1	A	206	THR
1	A	208	LEU
1	A	211	LEU
1	A	223	THR
1	A	227	ASN
1	A	229	GLN
1	B	1	MET
1	B	5	LYS
1	B	7	LYS
1	B	9	PRO
1	B	26	GLU
1	B	30	ARG
1	B	41	ARG
1	B	60	ASP

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Mol	Chain	Res	Type
1	B	65	PHE
1	B	68	ILE
1	B	73	GLU
1	B	77	GLU
1	B	80	LEU
1	B	88	ARG
1	B	89	PHE
1	B	92	PRO
1	B	94	LEU
1	B	95	GLN
1	B	96	THR
1	B	101	LEU
1	B	112	ARG
1	B	121	GLU
1	B	124	ASN
1	B	128	HIS
1	B	133	GLU
1	B	140	MET
1	B	141	GLU
1	B	146	ARG
1	B	159	LYS
1	B	162	ILE
1	B	189	ARG
1	B	190	THR
1	B	193	ASP
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	224	TYR
2	C	1	MET
2	C	5	ARG
2	C	8	ARG
2	C	10	ARG
2	C	20	GLU
2	C	22	GLN
2	C	26	TYR
2	C	30	LEU
2	C	31	GLN

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Mol	Chain	Res	Type
2	C	34	VAL
2	C	37	GLU
2	C	41	ASN
2	C	48	PHE
2	C	49	ARG
2	C	81	ASP
2	C	82	GLU
2	C	87	ASP
2	C	95	TYR
2	C	98	LEU
2	C	99	GLN
2	C	100	LEU
2	C	104	ASP
2	C	110	GLU
2	C	114	PHE
2	C	115	LEU
2	C	133	ASP
2	C	135	VAL
2	C	137	VAL
2	C	139	GLN
2	C	140	ILE
2	C	141	HIS
2	C	144	PRO
2	C	149	THR
2	C	150	PRO
2	C	152	PRO
2	C	157	ARG
2	C	158	TYR
2	C	161	SER
2	C	163	ILE
2	C	168	ARG
2	C	170	PRO
2	C	178	PRO
2	C	194	VAL
2	C	196	LEU
2	C	198	ARG
2	C	205	GLU
2	C	221	LEU
2	C	222	MET
2	C	223	ASP
2	C	229	MET
2	C	237	ARG

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Mol	Chain	Res	Type
2	C	238	LEU
2	C	252	LYS
2	C	254	VAL
2	C	257	VAL
2	C	267	TYR
2	C	268	ASP
2	C	275	TYR
2	C	279	GLU
2	C	285	LEU
2	C	286	SER
2	C	290	LEU
2	C	292	ARG
2	C	297	GLU
2	C	303	PHE
2	C	304	LEU
2	C	308	ARG
2	C	309	TYR
2	C	321	GLU
2	C	323	ASP
2	C	332	ARG
2	C	340	MET
2	C	342	ASP
2	C	343	GLN
2	C	350	ARG
2	C	357	GLU
2	C	359	MET
2	C	360	LEU
2	C	364	GLU
2	C	365	ASP
2	C	367	LEU
2	C	376	ARG
2	C	379	GLU
2	C	383	ARG
2	C	384	GLU
2	C	388	ARG
2	C	392	SER
2	C	393	GLN
2	C	394	PHE
2	C	399	ASN
2	C	400	PRO
2	C	408	ARG
2	C	413	LEU

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Mol	Chain	Res	Type
2	C	419	THR
2	C	420	ARG
2	C	421	GLU
2	C	422	ARG
2	C	425	PHE
2	C	426	ASP
2	C	432	ARG
2	C	443	THR
2	C	451	LEU
2	C	452	ILE
2	C	453	THR
2	C	460	ARG
2	C	474	VAL
2	C	479	VAL
2	C	482	GLU
2	C	486	MET
2	C	492	ASP
2	C	496	ILE
2	C	502	PRO
2	C	503	LEU
2	C	508	ILE
2	C	517	ARG
2	C	527	GLU
2	C	533	ASP
2	C	537	LYS
2	C	542	VAL
2	C	548	PRO
2	C	554	ASP
2	C	559	LEU
2	C	564	MET
2	C	565	GLN
2	C	584	GLU
2	C	589	ARG
2	C	620	LEU
2	C	621	VAL
2	C	622	GLU
2	C	633	GLN
2	C	640	ARG
2	C	650	ARG
2	C	654	LEU
2	C	655	LEU
2	C	657	ASP

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Mol	Chain	Res	Type
2	C	663	ASN
2	C	668	LEU
2	C	671	ASN
2	C	672	VAL
2	C	679	PHE
2	C	684	PHE
2	C	686	ASP
2	C	691	SER
2	C	693	GLU
2	C	699	PHE
2	C	714	ASP
2	C	722	ILE
2	C	724	ARG
2	C	725	ASP
2	C	727	PRO
2	C	730	SER
2	C	740	GLU
2	C	744	ARG
2	C	749	VAL
2	C	759	THR
2	C	768	THR
2	C	771	GLU
2	C	773	LEU
2	C	780	GLU
2	C	785	VAL
2	C	791	ARG
2	C	794	PRO
2	C	796	GLU
2	C	799	ILE
2	C	804	VAL
2	C	808	ARG
2	C	820	ARG
2	C	821	GLU
2	C	829	GLN
2	C	834	GLN
2	C	835	VAL
2	C	839	LEU
2	C	841	ASN
2	C	858	MET
2	C	860	HIS
2	C	862	PRO
2	C	863	ASP

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Mol	Chain	Res	Type
2	C	868	ASP
2	C	870	ILE
2	C	877	PRO
2	C	881	ASN
2	C	882	LEU
2	C	886	LEU
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	934	PHE
2	C	939	ARG
2	C	945	ARG
2	C	948	GLU
2	C	950	LEU
2	C	953	VAL
2	C	966	LEU
2	C	976	ASP
2	C	978	ARG
2	C	981	GLU
2	C	984	GLU
2	C	988	VAL
2	C	993	PHE
2	C	995	MET
2	C	1000	MET
2	C	1002	GLU
2	C	1006	HIS
2	C	1008	ARG
2	C	1016	ILE
2	C	1019	GLN
2	C	1021	LEU
2	C	1024	LYS
2	C	1026	GLN
2	C	1052	MET
2	C	1054	THR
2	C	1074	GLU
2	C	1076	VAL
2	C	1082	PRO
2	C	1083	GLU
2	C	1085	PHE

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Mol	Chain	Res	Type
2	C	1087	VAL
2	C	1092	LEU
2	C	1095	LEU
2	C	1098	ASP
2	C	1103	ASP
2	C	1104	GLU
2	C	1106	ASP
2	C	1109	VAL
3	D	3	LYS
3	D	5	VAL
3	D	6	ARG
3	D	9	ARG
3	D	12	LEU
3	D	14	SER
3	D	16	GLU
3	D	25	GLU
3	D	27	GLU
3	D	29	PRO
3	D	31	THR
3	D	41	ARG
3	D	42	ASP
3	D	47	GLU
3	D	48	ARG
3	D	53	ILE
3	D	55	ASP
3	D	56	TYR
3	D	58	CYS
3	D	62	LYS
3	D	68	PHE
3	D	71	LYS
3	D	76	CYS
3	D	80	VAL
3	D	82	LYS
3	D	85	VAL
3	D	86	ARG
3	D	87	ARG
3	D	95	LEU
3	D	101	HIS
3	D	102	ILE
3	D	112	ILE
3	D	115	LEU
3	D	117	ASP

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Mol	Chain	Res	Type
3	D	118	LEU
3	D	122	GLU
3	D	127	LEU
3	D	133	ILE
3	D	143	ASN
3	D	145	VAL
3	D	150	ARG
3	D	153	LEU
3	D	155	ASP
3	D	156	GLU
3	D	162	ARG
3	D	166	GLN
3	D	170	PRO
3	D	171	LEU
3	D	185	VAL
3	D	199	LEU
3	D	205	TYR
3	D	206	ARG
3	D	208	PRO
3	D	209	ARG
3	D	389	GLU
3	D	394	LEU
3	D	405	ASP
3	D	411	THR
3	D	413	ASP
3	D	421	LEU
3	D	432	TYR
3	D	444	VAL
3	D	445	ARG
3	D	452	ILE
3	D	455	ARG
3	D	456	MET
3	D	459	GLU
3	D	475	LYS
3	D	481	MET
3	D	483	HIS
3	D	486	ARG
3	D	488	ARG
3	D	502	PHE
3	D	504	ASP
3	D	521	PRO
3	D	528	VAL

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Mol	Chain	Res	Type
3	D	529	GLN
3	D	535	PHE
3	D	537	THR
3	D	540	LEU
3	D	542	ASP
3	D	554	LEU
3	D	565	ILE
3	D	568	ARG
3	D	569	ASN
3	D	571	LYS
3	D	576	GLU
3	D	584	ASN
3	D	590	PRO
3	D	594	PRO
3	D	613	ARG
3	D	618	LEU
3	D	624	ASP
3	D	629	SER
3	D	636	GLN
3	D	639	LEU
3	D	641	GLN
3	D	651	GLU
3	D	656	PHE
3	D	661	MET
3	D	675	ARG
3	D	676	MET
3	D	682	ASP
3	D	688	TRP
3	D	695	ILE
3	D	702	LEU
3	D	704	ARG
3	D	713	ILE
3	D	716	PHE
3	D	719	VAL
3	D	724	GLN
3	D	734	GLU
3	D	739	ASP
3	D	749	VAL
3	D	754	PHE
3	D	781	PRO
3	D	792	ILE
3	D	793	THR

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Mol	Chain	Res	Type
3	D	794	GLN
3	D	796	ARG
3	D	797	LYS
3	D	800	LYS
3	D	805	GLU
3	D	810	GLU
3	D	813	LEU
3	D	824	ASN
3	D	828	LYS
3	D	829	VAL
3	D	832	ARG
3	D	839	LEU
3	D	847	ASP
3	D	850	LEU
3	D	851	LEU
3	D	859	ASP
3	D	862	ASP
3	D	863	VAL
3	D	864	VAL
3	D	865	THR
3	D	867	ARG
3	D	879	ARG
3	D	880	ILE
3	D	888	GLU
3	D	891	GLU
3	D	902	LEU
3	D	910	SER
3	D	914	LEU
3	D	916	TYR
3	D	917	GLN
3	D	919	PHE
3	D	922	LEU
3	D	927	THR
3	D	944	THR
3	D	951	ILE
3	D	952	ASP
3	D	957	PRO
3	D	959	GLU
3	D	968	ASP
3	D	972	LEU
3	D	985	ASP
3	D	987	GLU

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Mol	Chain	Res	Type
3	D	999	THR
3	D	1001	GLU
3	D	1026	SER
3	D	1029	ARG
3	D	1032	PRO
3	D	1041	LEU
3	D	1042	ARG
3	D	1051	GLU
3	D	1058	ARG
3	D	1060	SER
3	D	1062	ARG
3	D	1065	LEU
3	D	1068	LEU
3	D	1087	ARG
3	D	1095	THR
3	D	1096	ARG
3	D	1109	GLU
3	D	1112	CYS
3	D	1116	ASN
3	D	1127	GLU
3	D	1135	ARG
3	D	1139	ASP
3	D	1144	LEU
3	D	1151	ARG
3	D	1160	LEU
3	D	1161	GLU
3	D	1164	ARG
3	D	1166	LEU
3	D	1167	SER
3	D	1173	LEU
3	D	1176	LYS
3	D	1195	GLN
3	D	1207	TYR
3	D	1209	LEU
3	D	1211	MET
3	D	1215	VAL
3	D	1223	ILE
3	D	1227	GLN
3	D	1231	GLU
3	D	1238	MET
3	D	1242	HIS
3	D	1243	THR

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Mol	Chain	Res	Type
3	D	1251	ASP
3	D	1258	ARG
3	D	1260	ILE
3	D	1264	GLU
3	D	1267	ARG
3	D	1269	LYS
3	D	1274	ILE
3	D	1276	GLU
3	D	1285	GLU
3	D	1288	GLU
3	D	1290	LEU
3	D	1299	PHE
3	D	1305	LEU
3	D	1307	LYS
3	D	1314	LYS
3	D	1317	ASP
3	D	1318	TYR
3	D	1331	ASP
3	D	1337	GLU
3	D	1344	VAL
3	D	1345	GLU
3	D	1346	ARG
3	D	1348	LEU
3	D	1353	GLN
3	D	1359	GLN
3	D	1363	LEU
3	D	1365	ASP
3	D	1368	ILE
3	D	1376	MET
3	D	1378	TYR
3	D	1382	THR
3	D	1387	SER
3	D	1388	ARG
3	D	1389	LEU
3	D	1401	GLU
3	D	1403	LEU
3	D	1406	ARG
3	D	1415	VAL
3	D	1420	LEU
3	D	1421	LEU
3	D	1424	VAL
3	D	1432	LYS

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Mol	Chain	Res	Type
3	D	1435	LEU
3	D	1440	PHE
3	D	1447	LEU
3	D	1460	ILE
3	D	1463	LYS
3	D	1465	ASN
3	D	1479	ASP
3	D	1485	GLN
3	D	1488	ASP
3	D	1496	GLU
3	D	1501	GLU
4	E	14	ASP
4	E	20	THR
4	E	28	GLN
4	E	29	GLN
4	E	30	LEU
4	E	31	LEU
4	E	32	ARG
4	E	33	HIS
4	E	40	LEU
4	E	42	PRO
4	E	43	GLU
4	E	45	ARG
4	E	56	ASP
4	E	57	ASP
4	E	59	ASN
4	E	61	GLU
4	E	66	LYS
4	E	67	GLU
4	E	81	PRO
4	E	84	ARG
4	E	87	LYS
5	F	80	PRO
5	F	83	GLN
5	F	84	TYR
5	F	86	HIS
5	F	90	GLN
5	F	91	VAL
5	F	101	GLU
5	F	111	GLU
5	F	125	ASP
5	F	126	LEU

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Mol	Chain	Res	Type
5	F	127	ILE
5	F	135	ILE
5	F	136	LEU
5	F	142	ARG
5	F	145	PRO
5	F	149	GLU
5	F	154	LYS
5	F	164	LYS
5	F	170	HIS
5	F	174	LEU
5	F	184	ARG
5	F	187	LEU
5	F	207	LEU
5	F	208	SER
5	F	209	PHE
5	F	218	GLN
5	F	233	PHE
5	F	234	LYS
5	F	240	THR
5	F	244	ARG
5	F	245	GLN
5	F	256	ARG
5	F	261	PRO
5	F	264	MET
5	F	280	GLN
5	F	282	LEU
5	F	290	GLU
5	F	295	MET
5	F	297	PRO
5	F	302	LYS
5	F	310	ILE
5	F	313	GLU
5	F	328	PHE
5	F	329	TYR
5	F	331	ASP
5	F	340	SER
5	F	341	PRO
5	F	347	GLN
5	F	349	LEU
5	F	355	GLU
5	F	363	GLU
5	F	365	GLU

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Mol	Chain	Res	Type
5	F	370	LYS
5	F	393	THR
5	F	396	ARG
5	F	399	GLN
5	F	403	LYS
5	F	406	ARG
5	F	408	LEU
5	F	410	TYR
5	F	414	ARG
5	F	420	ASP
1	K	5	LYS
1	K	9	PRO
1	K	12	THR
1	K	18	ARG
1	K	26	GLU
1	K	29	GLU
1	K	44	LEU
1	K	60	ASP
1	K	62	LEU
1	K	67	THR
1	K	73	GLU
1	K	84	GLU
1	K	88	ARG
1	K	89	PHE
1	K	90	LEU
1	K	92	PRO
1	K	94	LEU
1	K	101	LEU
1	K	112	ARG
1	K	115	LEU
1	K	121	GLU
1	K	127	LEU
1	K	134	GLU
1	K	142	VAL
1	K	145	ASP
1	K	146	ARG
1	K	156	HIS
1	K	165	ILE
1	K	167	VAL
1	K	176	ARG
1	K	179	PHE
1	K	180	GLN

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Mol	Chain	Res	Type
1	K	183	ASP
1	K	184	THR
1	K	186	LEU
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	219	ARG
1	K	223	THR
1	K	227	ASN
1	L	1	MET
1	L	2	LEU
1	L	4	SER
1	L	5	LYS
1	L	7	LYS
1	L	26	GLU
1	L	29	GLU
1	L	38	ASN
1	L	41	ARG
1	L	47	SER
1	L	55	SER
1	L	62	LEU
1	L	73	GLU
1	L	77	GLU
1	L	80	LEU
1	L	88	ARG
1	L	89	PHE
1	L	94	LEU
1	L	95	GLN
1	L	101	LEU
1	L	108	GLU
1	L	112	ARG
1	L	113	ASP
1	L	121	GLU
1	L	123	MET
1	L	126	ASP
1	L	138	LEU
1	L	141	GLU
1	L	159	LYS
1	L	160	ASP

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Mol	Chain	Res	Type
1	L	167	VAL
1	L	177	VAL
1	L	182	GLU
1	L	190	THR
1	L	191	ASP
1	L	201	THR
1	L	204	SER
1	L	206	THR
1	L	208	LEU
1	L	213	GLN
1	L	220	GLU
1	L	221	HIS
2	M	5	ARG
2	M	10	ARG
2	M	22	GLN
2	M	26	TYR
2	M	30	LEU
2	M	31	GLN
2	M	33	ASP
2	M	34	VAL
2	M	48	PHE
2	M	49	ARG
2	M	51	THR
2	M	71	TYR
2	M	79	PRO
2	M	86	LYS
2	M	91	GLN
2	M	95	TYR
2	M	98	LEU
2	M	99	GLN
2	M	100	LEU
2	M	102	HIS
2	M	104	ASP
2	M	105	THR
2	M	107	LEU
2	M	108	ILE
2	M	110	GLU
2	M	114	PHE
2	M	115	LEU
2	M	133	ASP
2	M	134	ARG
2	M	141	HIS

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Mol	Chain	Res	Type
2	M	143	SER
2	M	149	THR
2	M	152	PRO
2	M	157	ARG
2	M	158	TYR
2	M	163	ILE
2	M	167	LYS
2	M	168	ARG
2	M	178	PRO
2	M	182	VAL
2	M	184	MET
2	M	187	ASN
2	M	189	ARG
2	M	198	ARG
2	M	209	ARG
2	M	216	GLU
2	M	218	VAL
2	M	221	LEU
2	M	222	MET
2	M	229	MET
2	M	230	ARG
2	M	237	ARG
2	M	239	PHE
2	M	243	ARG
2	M	252	LYS
2	M	254	VAL
2	M	260	LEU
2	M	267	TYR
2	M	276	LYS
2	M	279	GLU
2	M	285	LEU
2	M	290	LEU
2	M	293	PHE
2	M	295	ASP
2	M	297	GLU
2	M	303	PHE
2	M	304	LEU
2	M	309	TYR
2	M	321	GLU
2	M	322	VAL
2	M	328	LEU
2	M	345	ARG

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Mol	Chain	Res	Type
2	M	348	LEU
2	M	359	MET
2	M	360	LEU
2	M	365	ASP
2	M	367	LEU
2	M	371	LYS
2	M	374	ASN
2	M	384	GLU
2	M	393	GLN
2	M	397	GLU
2	M	413	LEU
2	M	415	PRO
2	M	420	ARG
2	M	421	GLU
2	M	422	ARG
2	M	425	PHE
2	M	426	ASP
2	M	435	TYR
2	M	443	THR
2	M	451	LEU
2	M	455	LEU
2	M	460	ARG
2	M	468	ARG
2	M	469	THR
2	M	474	VAL
2	M	479	VAL
2	M	482	GLU
2	M	496	ILE
2	M	500	ASN
2	M	503	LEU
2	M	507	ARG
2	M	524	VAL
2	M	538	GLN
2	M	540	PHE
2	M	542	VAL
2	M	545	ASN
2	M	563	ASN
2	M	564	MET
2	M	571	LEU
2	M	583	LEU
2	M	584	GLU
2	M	586	ARG

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Mol	Chain	Res	Type
2	M	589	ARG
2	M	590	ASP
2	M	591	SER
2	M	599	GLU
2	M	605	LYS
2	M	607	ASP
2	M	620	LEU
2	M	626	ARG
2	M	627	ARG
2	M	630	ARG
2	M	633	GLN
2	M	635	THR
2	M	637	LEU
2	M	645	VAL
2	M	653	ASP
2	M	654	LEU
2	M	657	ASP
2	M	663	ASN
2	M	668	LEU
2	M	672	VAL
2	M	679	PHE
2	M	684	PHE
2	M	689	VAL
2	M	697	ARG
2	M	699	PHE
2	M	713	ARG
2	M	717	LEU
2	M	727	PRO
2	M	729	LEU
2	M	730	SER
2	M	735	ARG
2	M	737	LEU
2	M	739	GLU
2	M	749	VAL
2	M	750	LYS
2	M	755	LEU
2	M	762	LYS
2	M	772	ARG
2	M	775	ARG
2	M	780	GLU
2	M	785	VAL
2	M	799	ILE

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Mol	Chain	Res	Type
2	M	802	ARG
2	M	807	ARG
2	M	808	ARG
2	M	821	GLU
2	M	825	VAL
2	M	834	GLN
2	M	835	VAL
2	M	839	LEU
2	M	841	ASN
2	M	853	LEU
2	M	862	PRO
2	M	863	ASP
2	M	881	ASN
2	M	886	LEU
2	M	897	LEU
2	M	910	LYS
2	M	911	GLU
2	M	925	TYR
2	M	937	ASP
2	M	950	LEU
2	M	958	THR
2	M	966	LEU
2	M	981	GLU
2	M	984	GLU
2	M	988	VAL
2	M	999	HIS
2	M	1000	MET
2	M	1002	GLU
2	M	1003	ASP
2	M	1008	ARG
2	M	1009	SER
2	M	1016	ILE
2	M	1035	MET
2	M	1058	ASP
2	M	1060	ILE
2	M	1074	GLU
2	M	1076	VAL
2	M	1079	PRO
2	M	1087	VAL
2	M	1092	LEU
2	M	1095	LEU
2	M	1097	LEU

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Mol	Chain	Res	Type
2	M	1098	ASP
2	M	1100	GLN
2	M	1103	ASP
2	M	1117	SER
2	M	1118	LYS
3	N	3	LYS
3	N	6	ARG
3	N	12	LEU
3	N	15	PRO
3	N	20	SER
3	N	27	GLU
3	N	32	ILE
3	N	34	TYR
3	N	35	ARG
3	N	41	ARG
3	N	52	PRO
3	N	53	ILE
3	N	55	ASP
3	N	56	TYR
3	N	65	ARG
3	N	66	GLN
3	N	71	LYS
3	N	76	CYS
3	N	80	VAL
3	N	82	LYS
3	N	85	VAL
3	N	87	ARG
3	N	102	ILE
3	N	103	TRP
3	N	106	LYS
3	N	108	VAL
3	N	112	ILE
3	N	117	ASP
3	N	123	LEU
3	N	128	TYR
3	N	130	SER
3	N	133	ILE
3	N	142	LEU
3	N	145	VAL
3	N	153	LEU
3	N	155	ASP
3	N	160	GLU

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Mol	Chain	Res	Type
3	N	161	LEU
3	N	162	ARG
3	N	166	GLN
3	N	169	TYR
3	N	170	PRO
3	N	171	LEU
3	N	185	VAL
3	N	190	GLU
3	N	199	LEU
3	N	205	TYR
3	N	206	ARG
3	N	208	PRO
3	N	210	ARG
3	N	389	GLU
3	N	395	VAL
3	N	413	ASP
3	N	414	ARG
3	N	419	ASP
3	N	421	LEU
3	N	430	ASP
3	N	432	TYR
3	N	442	ASN
3	N	445	ARG
3	N	450	TYR
3	N	455	ARG
3	N	456	MET
3	N	459	GLU
3	N	463	GLN
3	N	465	LEU
3	N	475	LYS
3	N	481	MET
3	N	483	HIS
3	N	486	ARG
3	N	488	ARG
3	N	493	ARG
3	N	502	PHE
3	N	503	LEU
3	N	505	SER
3	N	509	PRO
3	N	511	TRP
3	N	521	PRO
3	N	530	VAL

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Mol	Chain	Res	Type
3	N	554	LEU
3	N	576	GLU
3	N	581	LEU
3	N	584	ASN
3	N	592	THR
3	N	594	PRO
3	N	601	ARG
3	N	602	SER
3	N	616	GLN
3	N	617	ASN
3	N	629	SER
3	N	641	GLN
3	N	651	GLU
3	N	652	LEU
3	N	666	ILE
3	N	674	ARG
3	N	676	MET
3	N	677	LEU
3	N	681	ARG
3	N	688	TRP
3	N	692	GLU
3	N	695	ILE
3	N	701	LEU
3	N	704	ARG
3	N	709	HIS
3	N	710	ARG
3	N	716	PHE
3	N	721	VAL
3	N	736	PHE
3	N	739	ASP
3	N	754	PHE
3	N	758	GLU
3	N	768	ASN
3	N	770	LEU
3	N	778	LEU
3	N	783	ARG
3	N	786	ILE
3	N	792	ILE
3	N	794	GLN
3	N	796	ARG
3	N	797	LYS
3	N	799	LYS

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Mol	Chain	Res	Type
3	N	800	LYS
3	N	805	GLU
3	N	823	LEU
3	N	828	LYS
3	N	836	VAL
3	N	847	ASP
3	N	863	VAL
3	N	865	THR
3	N	868	TYR
3	N	869	MET
3	N	876	SER
3	N	879	ARG
3	N	880	ILE
3	N	888	GLU
3	N	890	VAL
3	N	891	GLU
3	N	892	ASP
3	N	897	TRP
3	N	899	LEU
3	N	907	GLU
3	N	914	LEU
3	N	942	SER
3	N	951	ILE
3	N	959	GLU
3	N	971	LEU
3	N	972	LEU
3	N	984	THR
3	N	990	ASP
3	N	991	GLN
3	N	994	GLN
3	N	999	THR
3	N	1020	LEU
3	N	1033	GLN
3	N	1034	GLN
3	N	1035	ILE
3	N	1039	CYS
3	N	1045	MET
3	N	1051	GLU
3	N	1052	THR
3	N	1058	ARG
3	N	1060	SER
3	N	1062	ARG

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Mol	Chain	Res	Type
3	N	1063	GLU
3	N	1065	LEU
3	N	1068	LEU
3	N	1083	ASP
3	N	1084	THR
3	N	1087	ARG
3	N	1090	ASP
3	N	1095	THR
3	N	1096	ARG
3	N	1101	VAL
3	N	1109	GLU
3	N	1111	ASP
3	N	1112	CYS
3	N	1115	THR
3	N	1127	GLU
3	N	1129	THR
3	N	1130	ARG
3	N	1136	LYS
3	N	1141	GLU
3	N	1144	LEU
3	N	1151	ARG
3	N	1164	ARG
3	N	1166	LEU
3	N	1183	ILE
3	N	1195	GLN
3	N	1207	TYR
3	N	1208	ASP
3	N	1213	ARG
3	N	1216	SER
3	N	1217	ILE
3	N	1231	GLU
3	N	1238	MET
3	N	1243	THR
3	N	1252	ILE
3	N	1259	VAL
3	N	1262	LEU
3	N	1264	GLU
3	N	1267	ARG
3	N	1269	LYS
3	N	1285	GLU
3	N	1286	THR
3	N	1295	GLU

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Mol	Chain	Res	Type
3	N	1297	GLU
3	N	1299	PHE
3	N	1301	LYS
3	N	1306	PRO
3	N	1307	LYS
3	N	1308	GLU
3	N	1311	LEU
3	N	1312	LEU
3	N	1314	LYS
3	N	1317	ASP
3	N	1318	TYR
3	N	1331	ASP
3	N	1332	PRO
3	N	1337	GLU
3	N	1344	VAL
3	N	1346	ARG
3	N	1353	GLN
3	N	1355	VAL
3	N	1363	LEU
3	N	1372	VAL
3	N	1382	THR
3	N	1387	SER
3	N	1389	LEU
3	N	1391	GLU
3	N	1395	LEU
3	N	1399	ASP
3	N	1401	GLU
3	N	1403	LEU
3	N	1418	LYS
3	N	1419	PRO
3	N	1420	LEU
3	N	1424	VAL
3	N	1431	THR
3	N	1432	LYS
3	N	1433	SER
3	N	1435	LEU
3	N	1439	SER
3	N	1440	PHE
3	N	1441	GLN
3	N	1447	LEU
3	N	1465	ASN
3	N	1466	VAL

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Mol	Chain	Res	Type
3	N	1476	THR
3	N	1478	SER
3	N	1483	PHE
3	N	1485	GLN
3	N	1488	ASP
4	O	12	MET
4	O	14	ASP
4	O	15	SER
4	O	32	ARG
4	O	41	GLU
4	O	42	PRO
4	O	45	ARG
4	O	51	LEU
4	O	54	LEU
4	O	57	ASP
4	O	59	ASN
4	O	61	GLU
4	O	66	LYS
4	O	70	THR
4	O	72	ARG
4	O	84	ARG
4	O	85	LEU
4	O	86	GLN
5	P	83	GLN
5	P	84	TYR
5	P	86	HIS
5	P	87	GLU
5	P	91	VAL
5	P	96	LEU
5	P	101	GLU
5	P	108	GLU
5	P	125	ASP
5	P	132	ARG
5	P	135	ILE
5	P	136	LEU
5	P	142	ARG
5	P	150	THR
5	P	164	LYS
5	P	174	LEU
5	P	186	HIS
5	P	187	LEU
5	P	209	PHE

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Mol	Chain	Res	Type
5	P	211	ASP
5	P	212	LEU
5	P	214	GLN
5	P	220	LEU
5	P	225	GLU
5	P	231	ARG
5	P	234	LYS
5	P	240	THR
5	P	277	GLN
5	P	285	GLU
5	P	289	GLU
5	P	295	MET
5	P	302	LYS
5	P	319	THR
5	P	327	SER
5	P	328	PHE
5	P	337	HIS
5	P	341	PRO
5	P	347	GLN
5	P	350	LEU
5	P	353	GLU
5	P	363	GLU
5	P	365	GLU
5	P	370	LYS
5	P	393	THR
5	P	399	GLN
5	P	403	LYS
5	P	410	TYR
5	P	419	ARG
5	P	420	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (169) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	156	HIS
1	A	163	ASN
1	A	180	GLN
1	A	188	GLN
1	A	227	ASN
1	A	229	GLN
1	B	16	GLN

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Mol	Chain	Res	Type
1	B	38	ASN
1	B	81	ASN
1	B	95	GLN
1	B	124	ASN
1	B	163	ASN
1	B	212	ASN
1	B	213	GLN
1	B	227	ASN
2	C	22	GLN
2	C	31	GLN
2	C	41	ASN
2	C	117	HIS
2	C	320	HIS
2	C	399	ASN
2	C	448	ASN
2	C	498	GLN
2	C	543	ASN
2	C	552	HIS
2	C	563	ASN
2	C	565	GLN
2	C	632	ASN
2	C	663	ASN
2	C	670	GLN
2	C	834	GLN
2	C	841	ASN
2	C	845	ASN
2	C	881	ASN
2	C	884	GLN
2	C	889	HIS
2	C	899	GLN
2	C	969	GLN
2	C	999	HIS
2	C	1019	GLN
2	C	1047	HIS
2	C	1107	ASN
3	D	143	ASN
3	D	151	GLN
3	D	463	GLN
3	D	549	ASN
3	D	560	GLN
3	D	584	ASN
3	D	703	ASN

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Mol	Chain	Res	Type
3	D	724	GLN
3	D	756	GLN
3	D	768	ASN
3	D	824	ASN
3	D	917	GLN
3	D	976	GLN
3	D	994	GLN
3	D	1025	GLN
3	D	1033	GLN
3	D	1075	HIS
3	D	1103	HIS
3	D	1116	ASN
3	D	1124	GLN
3	D	1184	GLN
3	D	1202	GLN
3	D	1323	GLN
3	D	1333	HIS
3	D	1353	GLN
3	D	1359	GLN
3	D	1374	GLN
3	D	1465	ASN
4	E	37	ASN
4	E	86	GLN
5	F	83	GLN
5	F	90	GLN
5	F	185	GLN
5	F	218	GLN
5	F	312	GLN
5	F	337	HIS
5	F	402	ASN
1	K	38	ASN
1	K	156	HIS
1	K	180	GLN
1	K	213	GLN
1	K	227	ASN
1	K	229	GLN
1	L	38	ASN
1	L	95	GLN
1	L	128	HIS
1	L	212	ASN
1	L	229	GLN
2	M	22	GLN

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Mol	Chain	Res	Type
2	M	31	GLN
2	M	99	GLN
2	M	117	HIS
2	M	139	GLN
2	M	343	GLN
2	M	374	ASN
2	M	390	GLN
2	M	431	HIS
2	M	434	HIS
2	M	448	ASN
2	M	506	ASN
2	M	563	ASN
2	M	575	GLN
2	M	609	ASN
2	M	632	ASN
2	M	639	GLN
2	M	663	ASN
2	M	671	ASN
2	M	834	GLN
2	M	841	ASN
2	M	881	ASN
2	M	889	HIS
2	M	899	GLN
2	M	920	GLN
2	M	969	GLN
2	M	1018	GLN
2	M	1019	GLN
3	N	101	HIS
3	N	462	GLN
3	N	463	GLN
3	N	507	ASN
3	N	549	ASN
3	N	552	ASN
3	N	569	ASN
3	N	703	ASN
3	N	717	GLN
3	N	727	GLN
3	N	737	ASN
3	N	748	HIS
3	N	756	GLN
3	N	768	ASN
3	N	794	GLN

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Mol	Chain	Res	Type
3	N	855	HIS
3	N	906	GLN
3	N	917	GLN
3	N	976	GLN
3	N	994	GLN
3	N	1033	GLN
3	N	1103	HIS
3	N	1116	ASN
3	N	1202	GLN
3	N	1242	HIS
3	N	1323	GLN
3	N	1334	GLN
3	N	1353	GLN
3	N	1359	GLN
3	N	1393	GLN
3	N	1404	ASN
3	N	1441	GLN
3	N	1465	ASN
3	N	1485	GLN
4	O	28	GLN
4	O	29	GLN
4	O	59	ASN
4	O	86	GLN
5	P	83	GLN
5	P	90	GLN
5	P	161	GLN
5	P	185	GLN
5	P	191	ASN
5	P	245	GLN
5	P	269	ASN
5	P	279	GLN
5	P	312	GLN
5	P	337	HIS
5	P	399	GLN
5	P	402	ASN

### 5.3.3 RNA ⓘ

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 493 ligands modelled in this entry, 491 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	RPT	M	8002	-	68,68,68	2.52	22 (32%)	101,101,101	1.22	9 (8%)
7	RPT	C	8001	-	68,68,68	2.45	22 (32%)	101,101,101	1.23	11 (10%)

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	RPT	M	8002	-	-	20/64/96/96	0/6/6/6
7	RPT	C	8001	-	-	12/64/96/96	0/6/6/6

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	8002	RPT	C39-N4	6.55	1.59	1.47
7	M	8002	RPT	C42-N4	6.42	1.59	1.47
7	C	8001	RPT	O6-C27	6.22	1.58	1.43
7	C	8001	RPT	O5-C29	6.12	1.55	1.39
7	M	8002	RPT	O5-C29	5.98	1.54	1.39
7	M	8002	RPT	C2-C1	5.49	1.52	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	8001	RPT	C42-N4	5.20	1.57	1.47
7	C	8001	RPT	C39-N4	5.07	1.57	1.47
7	M	8002	RPT	O6-C27	4.95	1.55	1.43
7	M	8002	RPT	C8-C9	4.80	1.58	1.43
7	M	8002	RPT	C5-C10	4.79	1.53	1.43
7	C	8001	RPT	C10-C9	4.77	1.54	1.42
7	C	8001	RPT	C8-C9	4.76	1.57	1.43
7	C	8001	RPT	C2-C1	4.75	1.50	1.38
7	C	8001	RPT	C5-C10	4.72	1.53	1.43
7	M	8002	RPT	C10-C9	4.47	1.54	1.42
7	C	8001	RPT	C3-C4	4.44	1.48	1.40
7	M	8002	RPT	C38-N4	4.26	1.60	1.48
7	M	8002	RPT	C40-N3	3.79	1.54	1.46
7	M	8002	RPT	C3-C2	3.64	1.48	1.41
7	C	8001	RPT	O4-C11	3.55	1.27	1.21
7	M	8002	RPT	O5-C12	3.54	1.58	1.42
7	C	8001	RPT	C24-C25	3.52	1.63	1.54
7	M	8002	RPT	C3-C4	3.51	1.46	1.40
7	C	8001	RPT	O5-C12	3.39	1.57	1.42
7	M	8002	RPT	C24-C25	3.38	1.62	1.54
7	C	8001	RPT	C40-N3	3.21	1.52	1.46
7	M	8002	RPT	C8-C7	3.04	1.53	1.39
7	M	8002	RPT	O4-C11	2.97	1.26	1.21
7	C	8001	RPT	C8-C7	2.94	1.52	1.39
7	M	8002	RPT	C1-C9	2.78	1.51	1.43
7	C	8001	RPT	C3-C2	2.75	1.46	1.41
7	C	8001	RPT	C1-C9	2.71	1.51	1.43
7	M	8002	RPT	C27-C28	2.66	1.59	1.50
7	C	8001	RPT	O7-C25	2.60	1.48	1.44
7	C	8001	RPT	C3-C43	2.58	1.51	1.46
7	C	8001	RPT	C27-C28	2.57	1.59	1.50
7	C	8001	RPT	C38-N4	2.53	1.55	1.48
7	C	8001	RPT	C41-N3	2.45	1.51	1.46
7	M	8002	RPT	C3-C43	2.45	1.51	1.46
7	M	8002	RPT	C41-N3	2.42	1.51	1.46
7	C	8001	RPT	C45-C38	2.39	1.59	1.53
7	M	8002	RPT	O2-C8	-2.25	1.28	1.35
7	M	8002	RPT	C32-C22	2.23	1.58	1.53

All (20) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	8002	RPT	C24-C23-C22	3.73	121.68	115.43
7	C	8001	RPT	C24-C23-C22	3.28	120.92	115.43
7	M	8002	RPT	C20-C21-C22	3.25	121.58	114.96
7	C	8001	RPT	C25-O7-C35	3.23	122.72	117.72
7	C	8001	RPT	C2-N1-C15	3.10	134.26	124.11
7	C	8001	RPT	C20-C21-C22	3.04	121.16	114.96
7	M	8002	RPT	C34-C26-C25	-3.03	105.97	111.40
7	M	8002	RPT	C31-C20-C19	-2.88	103.02	109.99
7	M	8002	RPT	C2-N1-C15	2.73	133.05	124.11
7	C	8001	RPT	C31-C20-C19	-2.71	103.44	109.99
7	C	8001	RPT	C3-C2-N1	-2.65	114.84	119.25
7	M	8002	RPT	C25-O7-C35	2.64	121.81	117.72
7	C	8001	RPT	C26-C27-C28	2.48	117.54	112.13
7	C	8001	RPT	C34-C26-C25	-2.35	107.18	111.40
7	M	8002	RPT	C32-C22-C23	-2.18	106.97	111.39
7	C	8001	RPT	C12-O5-C29	2.18	123.22	117.84
7	M	8002	RPT	C31-C20-C21	2.17	115.85	111.31
7	C	8001	RPT	C31-C20-C21	2.04	115.59	111.31
7	M	8002	RPT	C3-C2-N1	-2.03	115.88	119.25
7	C	8001	RPT	C3-C43-N2	2.01	124.47	121.54

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	M	8002	RPT	C28-C27-O6-C37
7	M	8002	RPT	C44-C38-N4-C39
7	M	8002	RPT	C45-C38-N4-C39
7	M	8002	RPT	C45-C38-N4-C42
7	C	8001	RPT	C26-C27-C28-C29
7	C	8001	RPT	C26-C27-O6-C37
7	C	8001	RPT	C28-C27-O6-C37
7	M	8002	RPT	C3-C2-N1-C15
7	M	8002	RPT	C16-C17-C18-C19
7	C	8001	RPT	C3-C2-N1-C15
7	C	8001	RPT	C16-C17-C18-C19
7	C	8001	RPT	C18-C19-C20-C31
7	M	8002	RPT	C19-C20-C21-C22
7	M	8002	RPT	C31-C20-C21-C22
7	C	8001	RPT	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
7	M	8002	RPT	C43-N2-N3-C40
7	M	8002	RPT	C43-N2-N3-C41
7	C	8001	RPT	C43-N2-N3-C40
7	C	8001	RPT	C43-N2-N3-C41
7	C	8001	RPT	O6-C27-C28-C29
7	M	8002	RPT	C33-C24-C25-C26
7	M	8002	RPT	C18-C19-C20-C21
7	M	8002	RPT	C23-C24-C25-C26
7	M	8002	RPT	C26-C27-C28-C29
7	M	8002	RPT	O6-C27-C28-C29
7	M	8002	RPT	C18-C19-C20-C31
7	M	8002	RPT	C31-C20-C21-O10
7	M	8002	RPT	C44-C38-N4-C42
7	C	8001	RPT	C23-C24-C25-C26
7	M	8002	RPT	C28-C29-O5-C12
7	C	8001	RPT	C28-C29-O5-C12
7	M	8002	RPT	C33-C24-C25-O7

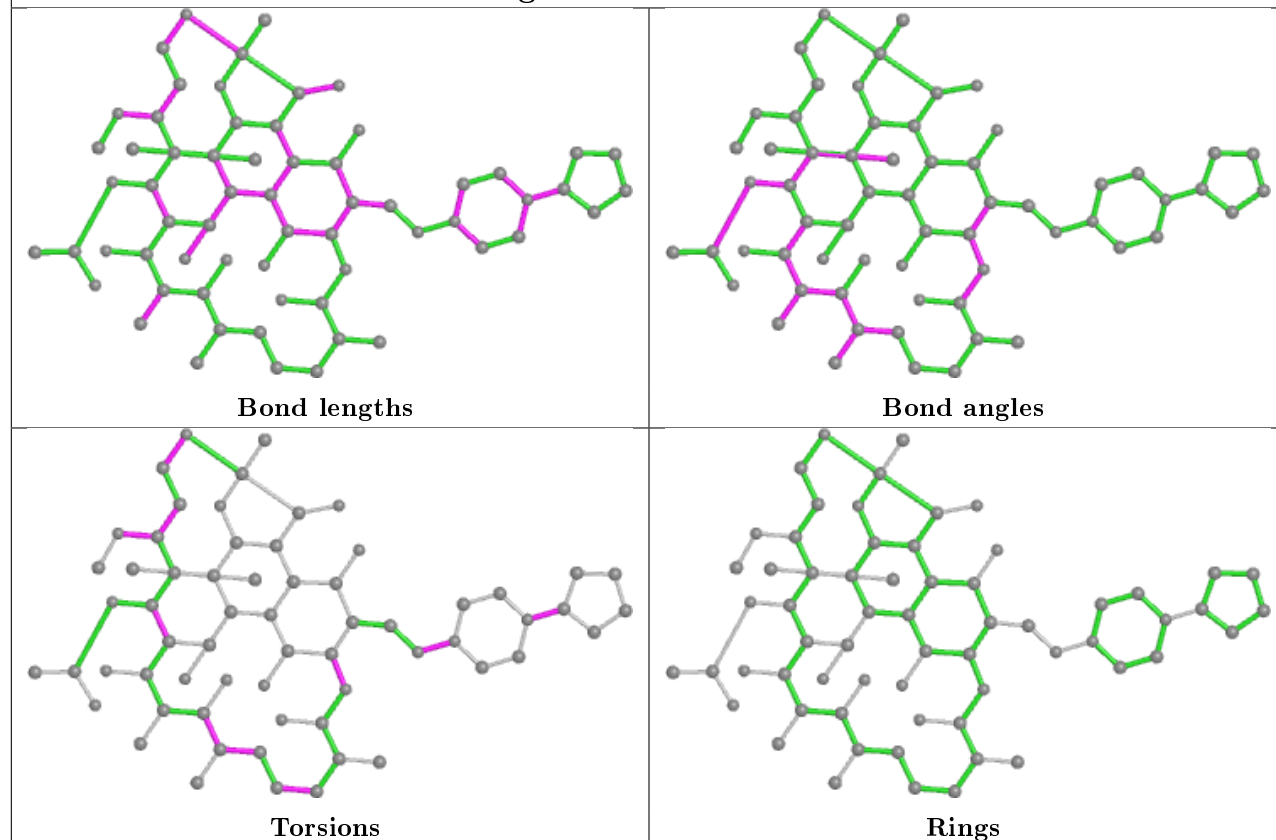
There are no ring outliers.

2 monomers are involved in 13 short contacts:

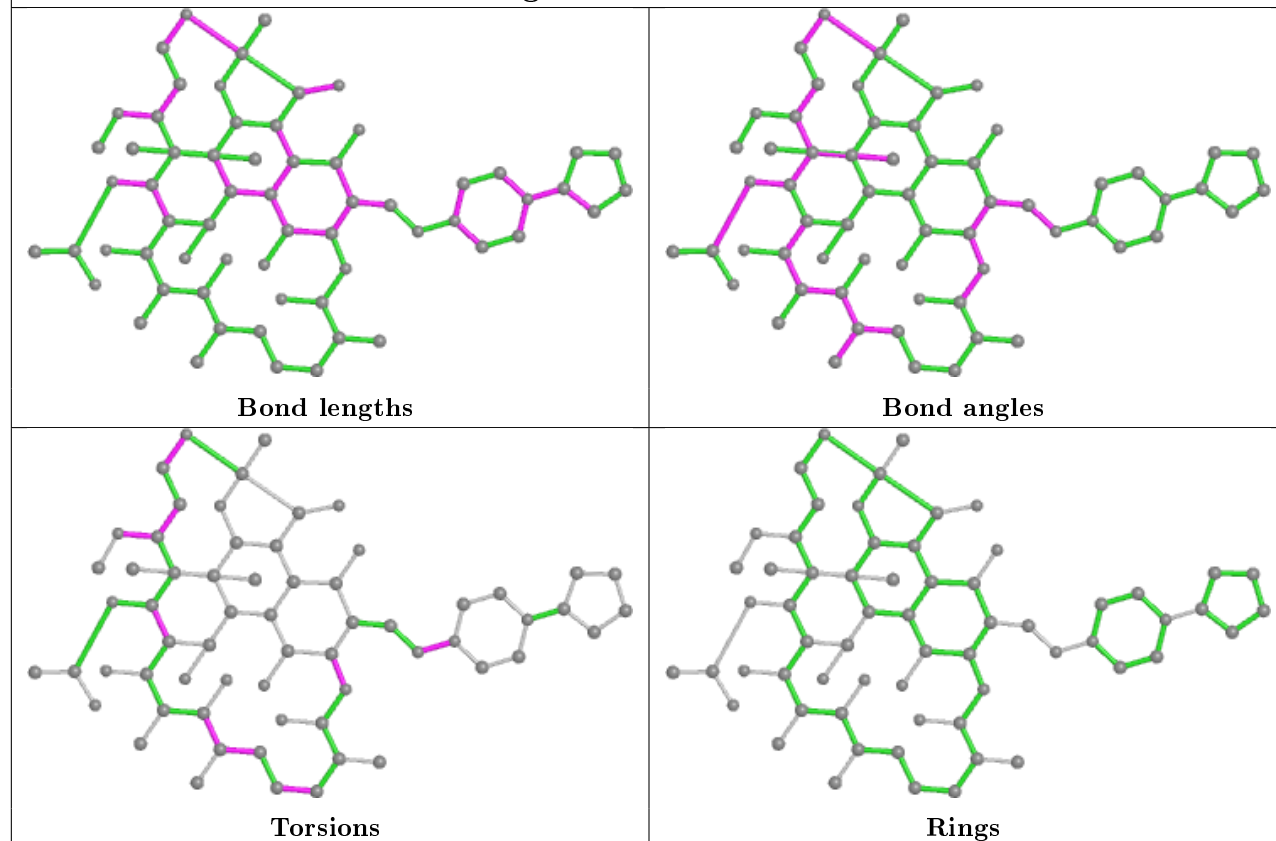
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	M	8002	RPT	7	0
7	C	8001	RPT	6	0

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.

## Ligand RPT M 8002



## Ligand RPT C 8001



## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	229/315 (72%)	-0.31	1 (0%) 92 93	27, 63, 91, 115	0
1	B	229/315 (72%)	-0.11	12 (5%) 27 29	48, 93, 115, 119	0
1	K	229/315 (72%)	-0.30	2 (0%) 84 86	34, 65, 94, 134	0
1	L	229/315 (72%)	-0.21	6 (2%) 56 59	52, 92, 110, 131	0
2	C	1119/1119 (100%)	-0.34	14 (1%) 77 79	21, 75, 106, 118	0
2	M	1119/1119 (100%)	-0.31	15 (1%) 77 79	25, 79, 109, 122	0
3	D	1392/1524 (91%)	-0.27	24 (1%) 70 72	24, 65, 112, 132	0
3	N	1392/1524 (91%)	-0.25	31 (2%) 62 65	25, 69, 117, 138	0
4	E	95/99 (95%)	-0.27	5 (5%) 26 28	42, 83, 108, 126	0
4	O	95/99 (95%)	-0.39	1 (1%) 80 82	46, 80, 107, 114	0
5	F	345/423 (81%)	-0.36	6 (1%) 70 72	49, 84, 110, 127	0
5	P	345/423 (81%)	-0.28	6 (1%) 70 72	63, 89, 114, 124	0
All	All	6818/7590 (89%)	-0.29	123 (1%) 68 71	21, 75, 112, 138	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	N	802	ALA	7.6
3	D	1240	THR	5.8
3	N	1249	ALA	5.5
2	C	180	GLY	5.3
3	D	1245	GLY	5.3
3	N	1243	THR	5.2
3	D	439	LEU	5.0
1	L	6	LEU	4.9
1	K	1	MET	4.8
1	L	1	MET	4.8
3	D	1247	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
4	E	85	LEU	4.4
5	F	145	PRO	4.4
3	N	1248	GLY	4.3
2	C	311	PHE	4.2
2	C	813	VAL	4.2
3	N	1246	VAL	4.1
3	D	1242	HIS	4.0
3	N	1242	HIS	4.0
1	K	2	LEU	4.0
1	B	129	ILE	3.9
3	D	444	VAL	3.9
3	D	247	GLU	3.9
3	D	177	ALA	3.8
1	B	58	ILE	3.8
5	P	145	PRO	3.8
2	M	98	LEU	3.7
3	D	228	ALA	3.7
5	F	291	ILE	3.7
3	N	230	TRP	3.6
3	N	177	ALA	3.6
1	B	130	ALA	3.6
3	D	388	HIS	3.6
2	C	153	ALA	3.5
1	B	82	LEU	3.5
3	N	371	ILE	3.4
3	N	1398	TRP	3.4
3	N	1408	ILE	3.3
2	C	307	LEU	3.3
2	M	211	LEU	3.2
3	D	1251	ASP	3.2
3	D	1243	THR	3.2
3	N	179	VAL	3.2
3	N	836	VAL	3.1
2	M	186	VAL	3.1
3	N	202	VAL	3.1
3	D	407	VAL	3.1
2	C	154	ARG	3.0
2	M	281	LEU	3.0
1	A	1	MET	3.0
2	M	100	LEU	2.9
4	E	93	TYR	2.9
5	P	365	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
3	N	403	PHE	2.9
3	N	1407	LEU	2.9
2	C	152	PRO	2.8
5	P	163	LEU	2.8
3	D	802	ALA	2.8
3	N	407	VAL	2.8
1	B	92	PRO	2.8
1	L	135	GLY	2.7
4	E	79	LEU	2.7
1	B	6	LEU	2.7
1	L	68	ILE	2.7
3	N	381	ALA	2.6
2	M	372	LEU	2.6
2	C	362	GLY	2.6
1	L	130	ALA	2.6
3	N	401	TYR	2.6
3	D	1241	PHE	2.5
3	N	1240	THR	2.5
3	N	1325	LEU	2.5
3	N	251	PHE	2.5
5	P	357	ALA	2.5
3	D	384	VAL	2.5
3	D	1408	ILE	2.5
1	B	62	LEU	2.5
2	C	776	SER	2.5
2	M	105	THR	2.5
1	B	120	VAL	2.5
2	M	644	VAL	2.5
5	P	144	ILE	2.5
2	M	246	ASP	2.5
3	D	803	GLY	2.5
5	F	147	LEU	2.4
3	D	77	GLY	2.4
4	E	95	GLY	2.4
3	D	128	TYR	2.4
2	C	281	LEU	2.4
3	D	202	VAL	2.3
4	E	80	VAL	2.3
2	M	245	GLY	2.3
3	N	137	PRO	2.3
3	N	1247	ALA	2.3
5	P	90	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
5	F	311	ALA	2.3
3	N	394	LEU	2.3
1	B	109	VAL	2.3
2	C	819	VAL	2.3
2	C	372	LEU	2.3
2	M	255	ALA	2.2
3	N	248	PRO	2.2
2	C	765	SER	2.2
2	M	196	LEU	2.2
3	D	204	LEU	2.2
5	F	371	LEU	2.2
2	M	180	GLY	2.2
5	F	144	ILE	2.2
3	N	803	GLY	2.2
3	D	242	LEU	2.1
1	L	2	LEU	2.1
3	N	205	TYR	2.1
3	N	801	GLY	2.1
4	O	39	VAL	2.1
3	D	251	PHE	2.1
3	N	184	GLU	2.1
1	B	71	VAL	2.0
2	M	483	VAL	2.0
2	M	101	ILE	2.0
1	B	61	VAL	2.0
2	C	293	PHE	2.0
1	B	70	GLY	2.0
3	N	418	GLY	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	ZN	D	7058	1/1	0.87	0.07	106,106,106,106	0
6	MG	M	9256	1/1	0.89	0.17	56,56,56,56	0
6	MG	C	9362	1/1	0.90	0.15	55,55,55,55	0
6	MG	N	9192	1/1	0.91	0.12	62,62,62,62	0
6	MG	D	9161	1/1	0.91	0.09	57,57,57,57	0
6	MG	C	9168	1/1	0.91	0.10	45,45,45,45	0
6	MG	K	9470	1/1	0.91	0.13	55,55,55,55	0
6	MG	N	9221	1/1	0.92	0.13	44,44,44,44	0
6	MG	D	9330	1/1	0.92	0.14	39,39,39,39	0
6	MG	F	9390	1/1	0.93	0.07	46,46,46,46	0
6	MG	C	9350	1/1	0.93	0.07	60,60,60,60	0
6	MG	P	9226	1/1	0.93	0.08	43,43,43,43	0
6	MG	A	9078	1/1	0.93	0.13	66,66,66,66	0
6	MG	D	9001	1/1	0.93	0.10	36,36,36,36	0
6	MG	F	9109	1/1	0.94	0.11	60,60,60,60	0
6	MG	N	9449	1/1	0.94	0.09	51,51,51,51	0
6	MG	M	9263	1/1	0.94	0.10	56,56,56,56	0
6	MG	A	9357	1/1	0.94	0.11	54,54,54,54	0
6	MG	L	9414	1/1	0.94	0.13	51,51,51,51	0
6	MG	C	9067	1/1	0.94	0.17	57,57,57,57	0
6	MG	O	9420	1/1	0.94	0.10	51,51,51,51	0
6	MG	C	9149	1/1	0.94	0.16	48,48,48,48	0
6	MG	P	9202	1/1	0.94	0.10	49,49,49,49	0
6	MG	D	9102	1/1	0.94	0.13	44,44,44,44	0
6	MG	C	9049	1/1	0.94	0.10	46,46,46,46	0
6	MG	M	9411	1/1	0.94	0.09	47,47,47,47	0
6	MG	L	9182	1/1	0.94	0.05	47,47,47,47	0
6	MG	N	9427	1/1	0.94	0.14	58,58,58,58	0
6	MG	N	9313	1/1	0.94	0.10	43,43,43,43	0
6	MG	M	9447	1/1	0.94	0.07	64,64,64,64	0
6	MG	N	9194	1/1	0.94	0.12	51,51,51,51	0
6	MG	M	9324	1/1	0.95	0.08	41,41,41,41	0
6	MG	N	9217	1/1	0.95	0.15	48,48,48,48	0
6	MG	N	9200	1/1	0.95	0.10	38,38,38,38	0
6	MG	M	9471	1/1	0.95	0.08	47,47,47,47	0
6	MG	D	9036	1/1	0.95	0.09	44,44,44,44	0
6	MG	N	9233	1/1	0.95	0.14	62,62,62,62	0
6	MG	N	9327	1/1	0.95	0.07	40,40,40,40	0
6	MG	F	9148	1/1	0.95	0.08	54,54,54,54	0
6	MG	N	9291	1/1	0.95	0.12	64,64,64,64	0
6	MG	C	9162	1/1	0.95	0.12	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	D	9082	1/1	0.95	0.14	60,60,60,60	0
6	MG	P	9297	1/1	0.95	0.09	45,45,45,45	0
6	MG	D	9014	1/1	0.95	0.10	41,41,41,41	0
6	MG	M	9294	1/1	0.96	0.09	52,52,52,52	0
6	MG	M	9210	1/1	0.96	0.13	41,41,41,41	0
6	MG	M	9406	1/1	0.96	0.15	67,67,67,67	0
6	MG	M	9261	1/1	0.96	0.11	47,47,47,47	0
6	MG	C	9175	1/1	0.96	0.14	68,68,68,68	0
6	MG	N	9292	1/1	0.96	0.12	56,56,56,56	0
6	MG	N	9326	1/1	0.96	0.14	62,62,62,62	0
6	MG	D	9453	1/1	0.96	0.11	38,38,38,38	0
6	MG	B	9359	1/1	0.96	0.10	52,52,52,52	0
6	MG	M	9234	1/1	0.96	0.12	53,53,53,53	0
6	MG	C	9372	1/1	0.96	0.09	61,61,61,61	0
6	MG	D	9365	1/1	0.96	0.06	41,41,41,41	0
7	RPT	M	8002	63/63	0.96	0.22	33,45,55,57	0
6	MG	L	9278	1/1	0.96	0.11	44,44,44,44	0
6	MG	F	9370	1/1	0.96	0.09	46,46,46,46	0
6	MG	M	9225	1/1	0.96	0.14	56,56,56,56	0
6	MG	D	9062	1/1	0.96	0.08	47,47,47,47	0
6	MG	C	9047	1/1	0.96	0.12	53,53,53,53	0
6	MG	D	9054	1/1	0.96	0.08	44,44,44,44	0
6	MG	C	9355	1/1	0.96	0.12	58,58,58,58	0
6	MG	A	9081	1/1	0.96	0.08	40,40,40,40	0
7	RPT	C	8001	63/63	0.96	0.23	26,40,66,82	0
6	MG	L	9218	1/1	0.96	0.09	33,33,33,33	0
6	MG	O	9198	1/1	0.96	0.12	36,36,36,36	0
6	MG	A	9013	1/1	0.96	0.12	44,44,44,44	0
6	MG	E	9074	1/1	0.96	0.09	59,59,59,59	0
6	MG	N	9426	1/1	0.96	0.09	41,41,41,41	0
6	MG	D	9096	1/1	0.96	0.15	60,60,60,60	0
6	MG	C	9381	1/1	0.96	0.08	53,53,53,53	0
6	MG	C	9391	1/1	0.96	0.06	60,60,60,60	0
6	MG	P	9209	1/1	0.96	0.15	46,46,46,46	0
6	MG	C	9019	1/1	0.96	0.13	57,57,57,57	0
6	MG	D	9009	1/1	0.96	0.09	43,43,43,43	0
6	MG	F	9172	1/1	0.96	0.11	51,51,51,51	0
6	MG	B	9059	1/1	0.96	0.07	48,48,48,48	0
6	MG	D	9373	1/1	0.97	0.12	51,51,51,51	0
6	MG	L	9289	1/1	0.97	0.14	62,62,62,62	0
6	MG	D	9073	1/1	0.97	0.12	34,34,34,34	0
6	MG	A	9352	1/1	0.97	0.10	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	D	9166	1/1	0.97	0.09	40,40,40,40	0
6	MG	C	9107	1/1	0.97	0.09	42,42,42,42	0
6	MG	C	9122	1/1	0.97	0.10	56,56,56,56	0
6	MG	D	9348	1/1	0.97	0.14	57,57,57,57	0
6	MG	M	9412	1/1	0.97	0.14	43,43,43,43	0
6	MG	D	9006	1/1	0.97	0.12	40,40,40,40	0
6	MG	M	9201	1/1	0.97	0.10	45,45,45,45	0
6	MG	N	9232	1/1	0.97	0.08	47,47,47,47	0
6	MG	F	9376	1/1	0.97	0.19	62,62,62,62	0
6	MG	D	9158	1/1	0.97	0.12	60,60,60,60	0
6	MG	P	9216	1/1	0.97	0.13	48,48,48,48	0
6	MG	M	9475	1/1	0.97	0.05	62,62,62,62	0
6	MG	B	9458	1/1	0.97	0.08	44,44,44,44	0
6	MG	C	9022	1/1	0.97	0.12	37,37,37,37	0
6	MG	C	9360	1/1	0.97	0.13	53,53,53,53	0
6	MG	C	9178	1/1	0.97	0.09	39,39,39,39	0
6	MG	C	9119	1/1	0.97	0.07	43,43,43,43	0
6	MG	D	9174	1/1	0.97	0.12	47,47,47,47	0
6	MG	A	9156	1/1	0.97	0.08	43,43,43,43	0
6	MG	M	9275	1/1	0.97	0.12	55,55,55,55	0
6	MG	N	9276	1/1	0.97	0.08	61,61,61,61	0
6	MG	P	9189	1/1	0.97	0.11	49,49,49,49	0
6	MG	D	9041	1/1	0.97	0.13	47,47,47,47	0
6	MG	D	9030	1/1	0.97	0.09	48,48,48,48	0
6	MG	M	9237	1/1	0.97	0.15	52,52,52,52	0
6	MG	C	9160	1/1	0.97	0.09	44,44,44,44	0
6	MG	K	9188	1/1	0.97	0.12	40,40,40,40	0
6	MG	D	9167	1/1	0.97	0.12	49,49,49,49	0
6	MG	B	9104	1/1	0.97	0.10	45,45,45,45	0
6	MG	L	9245	1/1	0.97	0.09	62,62,62,62	0
6	MG	D	9177	1/1	0.97	0.13	64,64,64,64	0
6	MG	F	9123	1/1	0.97	0.09	37,37,37,37	0
6	MG	K	9257	1/1	0.97	0.10	58,58,58,58	0
6	MG	A	9171	1/1	0.97	0.11	58,58,58,58	0
6	MG	D	9087	1/1	0.97	0.07	43,43,43,43	0
6	MG	L	9252	1/1	0.97	0.09	45,45,45,45	0
6	MG	K	9433	1/1	0.97	0.07	50,50,50,50	0
6	MG	D	9346	1/1	0.97	0.07	47,47,47,47	0
6	MG	K	9410	1/1	0.97	0.15	36,36,36,36	0
6	MG	N	9211	1/1	0.97	0.10	44,44,44,44	0
6	MG	F	9389	1/1	0.97	0.11	53,53,53,53	0
6	MG	M	9196	1/1	0.97	0.09	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	M	9273	1/1	0.97	0.12	44,44,44,44	0
6	MG	D	9388	1/1	0.97	0.09	37,37,37,37	0
6	MG	N	9473	1/1	0.97	0.12	51,51,51,51	0
6	MG	A	9153	1/1	0.97	0.15	66,66,66,66	0
6	MG	B	9103	1/1	0.97	0.12	43,43,43,43	0
6	MG	F	9060	1/1	0.97	0.10	41,41,41,41	0
6	MG	P	9325	1/1	0.97	0.12	49,49,49,49	0
6	MG	D	9095	1/1	0.97	0.15	30,30,30,30	0
6	MG	D	9165	1/1	0.97	0.07	32,32,32,32	0
6	MG	A	9125	1/1	0.97	0.12	36,36,36,36	0
6	MG	D	9367	1/1	0.97	0.06	31,31,31,31	0
6	MG	F	9099	1/1	0.97	0.13	56,56,56,56	0
6	MG	K	9251	1/1	0.97	0.11	43,43,43,43	0
6	MG	N	9422	1/1	0.97	0.14	56,56,56,56	0
6	MG	D	9017	1/1	0.97	0.10	42,42,42,42	0
6	MG	N	9450	1/1	0.97	0.10	48,48,48,48	0
6	MG	N	9425	1/1	0.97	0.12	46,46,46,46	0
6	MG	M	9219	1/1	0.97	0.09	47,47,47,47	0
6	MG	A	9066	1/1	0.97	0.14	47,47,47,47	0
6	MG	D	9127	1/1	0.97	0.14	48,48,48,48	0
6	MG	N	9465	1/1	0.98	0.08	49,49,49,49	0
6	MG	O	9296	1/1	0.98	0.11	42,42,42,42	0
6	MG	M	9424	1/1	0.98	0.13	34,34,34,34	0
6	MG	P	9280	1/1	0.98	0.10	51,51,51,51	0
6	MG	F	9356	1/1	0.98	0.14	37,37,37,37	0
6	MG	M	9310	1/1	0.98	0.07	46,46,46,46	0
6	MG	D	9121	1/1	0.98	0.09	35,35,35,35	0
6	MG	C	9138	1/1	0.98	0.08	43,43,43,43	0
6	MG	D	9108	1/1	0.98	0.15	51,51,51,51	0
6	MG	L	9246	1/1	0.98	0.12	52,52,52,52	0
6	MG	C	9128	1/1	0.98	0.12	52,52,52,52	0
6	MG	A	9460	1/1	0.98	0.07	55,55,55,55	0
6	MG	K	9405	1/1	0.98	0.11	56,56,56,56	0
6	MG	N	9184	1/1	0.98	0.10	29,29,29,29	0
6	MG	C	9340	1/1	0.98	0.09	60,60,60,60	0
6	MG	C	9004	1/1	0.98	0.10	39,39,39,39	0
6	MG	E	9045	1/1	0.98	0.12	61,61,61,61	0
6	MG	D	9374	1/1	0.98	0.10	41,41,41,41	0
6	MG	C	9461	1/1	0.98	0.07	50,50,50,50	0
6	MG	N	9428	1/1	0.98	0.10	42,42,42,42	0
6	MG	N	9265	1/1	0.98	0.14	61,61,61,61	0
6	MG	C	9015	1/1	0.98	0.09	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	M	9434	1/1	0.98	0.11	34,34,34,34	0
6	MG	N	9445	1/1	0.98	0.10	51,51,51,51	0
6	MG	O	9439	1/1	0.98	0.16	56,56,56,56	0
6	MG	D	9118	1/1	0.98	0.11	44,44,44,44	0
6	MG	M	9441	1/1	0.98	0.07	45,45,45,45	0
6	MG	A	9016	1/1	0.98	0.14	36,36,36,36	0
6	MG	D	9397	1/1	0.98	0.12	51,51,51,51	0
6	MG	M	9452	1/1	0.98	0.13	42,42,42,42	0
6	MG	D	9163	1/1	0.98	0.14	52,52,52,52	0
6	MG	D	9379	1/1	0.98	0.11	47,47,47,47	0
6	MG	L	9309	1/1	0.98	0.13	49,49,49,49	0
6	MG	A	9111	1/1	0.98	0.09	35,35,35,35	0
6	MG	N	9214	1/1	0.98	0.10	33,33,33,33	0
6	MG	M	9407	1/1	0.98	0.14	35,35,35,35	0
6	MG	N	9215	1/1	0.98	0.12	32,32,32,32	0
6	MG	N	9415	1/1	0.98	0.07	42,42,42,42	0
6	MG	D	9344	1/1	0.98	0.11	55,55,55,55	0
6	MG	D	9152	1/1	0.98	0.12	67,67,67,67	0
6	MG	N	9419	1/1	0.98	0.11	51,51,51,51	0
6	MG	P	9228	1/1	0.98	0.09	43,43,43,43	0
6	MG	P	9235	1/1	0.98	0.16	40,40,40,40	0
6	MG	D	9137	1/1	0.98	0.08	47,47,47,47	0
6	MG	D	9349	1/1	0.98	0.13	33,33,33,33	0
6	MG	M	9284	1/1	0.98	0.14	54,54,54,54	0
6	MG	D	9338	1/1	0.98	0.10	42,42,42,42	0
6	MG	N	9253	1/1	0.98	0.12	42,42,42,42	0
6	MG	A	9010	1/1	0.98	0.12	30,30,30,30	0
6	MG	C	9154	1/1	0.98	0.07	43,43,43,43	0
6	MG	D	9052	1/1	0.98	0.07	65,65,65,65	0
6	MG	N	9231	1/1	0.98	0.11	52,52,52,52	0
6	MG	D	9069	1/1	0.98	0.12	48,48,48,48	0
6	MG	C	9464	1/1	0.98	0.06	48,48,48,48	0
6	MG	D	9173	1/1	0.98	0.07	48,48,48,48	0
6	MG	C	9021	1/1	0.98	0.09	37,37,37,37	0
6	MG	A	9027	1/1	0.98	0.08	37,37,37,37	0
6	MG	F	9387	1/1	0.98	0.10	53,53,53,53	0
6	MG	K	9438	1/1	0.98	0.10	52,52,52,52	0
6	MG	C	9142	1/1	0.98	0.15	48,48,48,48	0
6	MG	D	9113	1/1	0.98	0.11	34,34,34,34	0
6	MG	M	9305	1/1	0.98	0.09	46,46,46,46	0
6	MG	N	9204	1/1	0.98	0.19	44,44,44,44	0
6	MG	M	9212	1/1	0.98	0.08	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	N	9243	1/1	0.98	0.09	35,35,35,35	0
6	MG	N	9185	1/1	0.98	0.14	56,56,56,56	0
6	MG	L	9314	1/1	0.98	0.07	56,56,56,56	0
6	MG	N	9435	1/1	0.98	0.23	53,53,53,53	0
6	MG	B	9080	1/1	0.98	0.10	56,56,56,56	0
6	MG	C	9112	1/1	0.98	0.11	39,39,39,39	0
6	MG	C	9090	1/1	0.98	0.10	47,47,47,47	0
6	MG	N	9404	1/1	0.98	0.12	55,55,55,55	0
6	MG	K	9301	1/1	0.98	0.12	43,43,43,43	0
6	MG	A	9012	1/1	0.98	0.10	47,47,47,47	0
6	MG	F	9383	1/1	0.98	0.11	48,48,48,48	0
6	MG	C	9394	1/1	0.98	0.09	33,33,33,33	0
6	MG	F	9159	1/1	0.98	0.15	57,57,57,57	0
6	MG	N	9270	1/1	0.98	0.05	39,39,39,39	0
6	MG	N	9181	1/1	0.98	0.16	47,47,47,47	0
6	MG	L	9283	1/1	0.98	0.12	59,59,59,59	0
6	MG	M	9241	1/1	0.98	0.11	36,36,36,36	0
6	MG	C	9065	1/1	0.98	0.10	37,37,37,37	0
6	MG	N	9287	1/1	0.98	0.09	53,53,53,53	0
6	MG	L	9421	1/1	0.98	0.12	53,53,53,53	0
6	MG	P	9285	1/1	0.98	0.09	56,56,56,56	0
6	MG	K	9290	1/1	0.98	0.12	51,51,51,51	0
6	MG	M	9205	1/1	0.98	0.11	38,38,38,38	0
6	MG	F	9105	1/1	0.98	0.14	36,36,36,36	0
6	MG	B	9478	1/1	0.98	0.12	61,61,61,61	0
6	MG	D	9459	1/1	0.98	0.05	54,54,54,54	0
6	MG	C	9037	1/1	0.98	0.16	51,51,51,51	0
6	MG	B	9056	1/1	0.98	0.13	43,43,43,43	0
6	MG	F	9098	1/1	0.98	0.11	54,54,54,54	0
6	MG	A	9477	1/1	0.98	0.18	52,52,52,52	0
6	MG	K	9264	1/1	0.98	0.08	42,42,42,42	0
6	MG	C	9025	1/1	0.98	0.14	39,39,39,39	0
6	MG	F	9008	1/1	0.98	0.09	40,40,40,40	0
6	MG	N	9267	1/1	0.98	0.12	42,42,42,42	0
6	MG	M	9440	1/1	0.98	0.10	50,50,50,50	0
6	MG	D	9064	1/1	0.98	0.14	44,44,44,44	0
6	MG	D	9369	1/1	0.98	0.10	49,49,49,49	0
6	MG	K	9191	1/1	0.98	0.15	32,32,32,32	0
6	MG	F	9375	1/1	0.98	0.13	36,36,36,36	0
6	MG	D	9018	1/1	0.98	0.11	39,39,39,39	0
6	MG	D	9063	1/1	0.98	0.08	33,33,33,33	0
6	MG	O	9197	1/1	0.98	0.04	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	N	9423	1/1	0.98	0.17	58,58,58,58	0
6	MG	M	9247	1/1	0.98	0.07	51,51,51,51	0
6	MG	N	9293	1/1	0.98	0.15	42,42,42,42	0
6	MG	D	9392	1/1	0.98	0.12	52,52,52,52	0
6	MG	N	9298	1/1	0.98	0.05	55,55,55,55	0
6	MG	N	9259	1/1	0.98	0.15	34,34,34,34	0
6	MG	A	9068	1/1	0.98	0.12	39,39,39,39	0
6	MG	F	9363	1/1	0.98	0.12	53,53,53,53	0
6	MG	M	9250	1/1	0.98	0.07	38,38,38,38	0
6	MG	D	9028	1/1	0.98	0.13	34,34,34,34	0
6	MG	N	9286	1/1	0.98	0.14	31,31,31,31	0
6	MG	N	9322	1/1	0.98	0.10	54,54,54,54	0
6	MG	A	9384	1/1	0.98	0.14	39,39,39,39	0
6	MG	M	9239	1/1	0.98	0.07	34,34,34,34	0
6	MG	C	9092	1/1	0.98	0.06	44,44,44,44	0
6	MG	D	9024	1/1	0.98	0.14	36,36,36,36	0
6	MG	N	9236	1/1	0.98	0.10	39,39,39,39	0
6	MG	D	9135	1/1	0.98	0.14	50,50,50,50	0
6	MG	D	9132	1/1	0.98	0.10	43,43,43,43	0
6	MG	E	9479	1/1	0.98	0.10	62,62,62,62	0
6	MG	K	9213	1/1	0.98	0.11	43,43,43,43	0
6	MG	E	9007	1/1	0.98	0.11	40,40,40,40	0
6	MG	N	9429	1/1	0.98	0.10	45,45,45,45	0
6	MG	P	9282	1/1	0.98	0.09	56,56,56,56	0
6	MG	B	9093	1/1	0.98	0.15	40,40,40,40	0
6	MG	B	9457	1/1	0.98	0.07	43,43,43,43	0
6	MG	N	9431	1/1	0.99	0.12	39,39,39,39	0
6	MG	N	9472	1/1	0.99	0.15	56,56,56,56	0
6	MG	C	9020	1/1	0.99	0.10	34,34,34,34	0
6	MG	D	9343	1/1	0.99	0.10	59,59,59,59	0
6	MG	M	9442	1/1	0.99	0.07	59,59,59,59	0
6	MG	K	9413	1/1	0.99	0.10	54,54,54,54	0
6	MG	D	9329	1/1	0.99	0.12	33,33,33,33	0
6	MG	D	9038	1/1	0.99	0.14	39,39,39,39	0
6	MG	D	9337	1/1	0.99	0.15	53,53,53,53	0
6	MG	D	9336	1/1	0.99	0.10	53,53,53,53	0
6	MG	A	9097	1/1	0.99	0.16	34,34,34,34	0
6	MG	D	9386	1/1	0.99	0.11	40,40,40,40	0
6	MG	M	9203	1/1	0.99	0.11	32,32,32,32	0
6	MG	C	9371	1/1	0.99	0.15	54,54,54,54	0
6	MG	N	9402	1/1	0.99	0.07	45,45,45,45	0
6	MG	A	9043	1/1	0.99	0.17	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	M	9195	1/1	0.99	0.08	34,34,34,34	0
6	MG	B	9094	1/1	0.99	0.15	38,38,38,38	0
6	MG	P	9399	1/1	0.99	0.11	34,34,34,34	0
6	MG	C	9042	1/1	0.99	0.07	47,47,47,47	0
6	MG	C	9176	1/1	0.99	0.09	28,28,28,28	0
6	MG	N	9199	1/1	0.99	0.11	35,35,35,35	0
6	MG	A	9332	1/1	0.99	0.06	35,35,35,35	0
6	MG	A	9395	1/1	0.99	0.14	50,50,50,50	0
6	MG	N	9207	1/1	0.99	0.13	41,41,41,41	0
6	MG	D	9130	1/1	0.99	0.09	51,51,51,51	0
6	MG	D	9011	1/1	0.99	0.12	33,33,33,33	0
6	MG	N	9318	1/1	0.99	0.11	34,34,34,34	0
6	MG	N	9443	1/1	0.99	0.13	54,54,54,54	0
6	MG	F	9382	1/1	0.99	0.09	40,40,40,40	0
6	MG	N	9308	1/1	0.99	0.15	55,55,55,55	0
6	MG	N	9179	1/1	0.99	0.12	33,33,33,33	0
6	MG	M	9272	1/1	0.99	0.17	45,45,45,45	0
6	MG	C	9126	1/1	0.99	0.10	46,46,46,46	0
6	MG	C	9366	1/1	0.99	0.14	41,41,41,41	0
6	MG	N	9304	1/1	0.99	0.11	47,47,47,47	0
6	MG	N	9262	1/1	0.99	0.09	51,51,51,51	0
6	MG	L	9437	1/1	0.99	0.06	40,40,40,40	0
6	MG	F	9139	1/1	0.99	0.10	38,38,38,38	0
6	MG	F	9481	1/1	0.99	0.08	57,57,57,57	0
6	MG	D	9146	1/1	0.99	0.10	31,31,31,31	0
6	MG	D	9335	1/1	0.99	0.06	52,52,52,52	0
6	MG	D	9144	1/1	0.99	0.12	39,39,39,39	0
6	MG	M	9242	1/1	0.99	0.11	35,35,35,35	0
6	MG	C	9353	1/1	0.99	0.10	48,48,48,48	0
6	MG	D	9089	1/1	0.99	0.09	36,36,36,36	0
6	MG	F	9048	1/1	0.99	0.10	41,41,41,41	0
6	MG	D	9100	1/1	0.99	0.08	43,43,43,43	0
6	MG	B	9378	1/1	0.99	0.13	47,47,47,47	0
6	MG	B	9083	1/1	0.99	0.13	40,40,40,40	0
6	MG	D	9133	1/1	0.99	0.13	42,42,42,42	0
6	MG	N	9417	1/1	0.99	0.09	39,39,39,39	0
6	MG	N	9186	1/1	0.99	0.12	49,49,49,49	0
6	MG	D	9029	1/1	0.99	0.12	33,33,33,33	0
6	MG	P	9315	1/1	0.99	0.08	35,35,35,35	0
6	MG	A	9088	1/1	0.99	0.07	36,36,36,36	0
6	MG	P	9436	1/1	0.99	0.11	49,49,49,49	0
6	MG	B	9033	1/1	0.99	0.14	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	C	9145	1/1	0.99	0.13	66,66,66,66	0
6	MG	A	9002	1/1	0.99	0.17	31,31,31,31	0
6	MG	L	9306	1/1	0.99	0.11	57,57,57,57	0
6	MG	M	9190	1/1	0.99	0.16	29,29,29,29	0
6	MG	C	9115	1/1	0.99	0.11	36,36,36,36	0
6	MG	N	9288	1/1	0.99	0.09	49,49,49,49	0
6	MG	D	9334	1/1	0.99	0.10	54,54,54,54	0
6	MG	P	9277	1/1	0.99	0.09	41,41,41,41	0
6	MG	D	9140	1/1	0.99	0.13	40,40,40,40	0
6	MG	D	9480	1/1	0.99	0.10	55,55,55,55	0
6	MG	A	9106	1/1	0.99	0.12	38,38,38,38	0
6	MG	N	9468	1/1	0.99	0.10	55,55,55,55	0
6	MG	A	9345	1/1	0.99	0.12	41,41,41,41	0
6	MG	C	9026	1/1	0.99	0.13	42,42,42,42	0
6	MG	D	9456	1/1	0.99	0.10	55,55,55,55	0
6	MG	N	9274	1/1	0.99	0.18	40,40,40,40	0
6	MG	D	9339	1/1	0.99	0.14	37,37,37,37	0
6	MG	D	9134	1/1	0.99	0.13	47,47,47,47	0
6	MG	C	9462	1/1	0.99	0.08	43,43,43,43	0
6	MG	D	9396	1/1	0.99	0.10	62,62,62,62	0
6	MG	D	9328	1/1	0.99	0.12	30,30,30,30	0
6	MG	N	9316	1/1	0.99	0.08	37,37,37,37	0
6	MG	N	9430	1/1	0.99	0.08	57,57,57,57	0
6	MG	A	9368	1/1	0.99	0.13	43,43,43,43	0
6	MG	B	9136	1/1	0.99	0.10	47,47,47,47	0
8	ZN	N	7113	1/1	0.99	0.13	84,84,84,84	0
6	MG	P	9255	1/1	0.99	0.12	34,34,34,34	0
6	MG	N	9302	1/1	0.99	0.10	31,31,31,31	0
6	MG	C	9071	1/1	0.99	0.11	42,42,42,42	0
6	MG	B	9116	1/1	0.99	0.09	38,38,38,38	0
6	MG	B	9110	1/1	0.99	0.12	49,49,49,49	0
6	MG	M	9486	1/1	0.99	0.07	48,48,48,48	0
6	MG	O	9254	1/1	0.99	0.08	39,39,39,39	0
6	MG	N	9323	1/1	0.99	0.09	38,38,38,38	0
6	MG	K	9223	1/1	0.99	0.09	32,32,32,32	0
6	MG	D	9072	1/1	0.99	0.14	32,32,32,32	0
6	MG	M	9222	1/1	0.99	0.10	35,35,35,35	0
6	MG	N	9229	1/1	0.99	0.07	41,41,41,41	0
6	MG	A	9124	1/1	0.99	0.12	39,39,39,39	0
6	MG	A	9380	1/1	0.99	0.11	44,44,44,44	0
6	MG	M	9416	1/1	0.99	0.11	45,45,45,45	0
6	MG	F	9157	1/1	0.99	0.11	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	B	9032	1/1	0.99	0.06	34,34,34,34	0
6	MG	L	9466	1/1	0.99	0.10	49,49,49,49	0
6	MG	D	9333	1/1	0.99	0.07	33,33,33,33	0
6	MG	D	9385	1/1	0.99	0.13	35,35,35,35	0
6	MG	D	9364	1/1	0.99	0.12	47,47,47,47	0
6	MG	N	9418	1/1	0.99	0.10	49,49,49,49	0
6	MG	A	9354	1/1	0.99	0.09	37,37,37,37	0
6	MG	D	9005	1/1	0.99	0.11	40,40,40,40	0
6	MG	N	9187	1/1	0.99	0.18	33,33,33,33	0
6	MG	C	9377	1/1	0.99	0.09	44,44,44,44	0
6	MG	D	9085	1/1	0.99	0.18	49,49,49,49	0
6	MG	C	9053	1/1	0.99	0.12	30,30,30,30	0
6	MG	O	9483	1/1	0.99	0.09	63,63,63,63	0
6	MG	N	9467	1/1	0.99	0.12	35,35,35,35	0
6	MG	L	9307	1/1	0.99	0.10	35,35,35,35	0
6	MG	D	9129	1/1	0.99	0.14	42,42,42,42	0
6	MG	D	9347	1/1	0.99	0.09	49,49,49,49	0
6	MG	D	9023	1/1	0.99	0.14	34,34,34,34	0
6	MG	M	9295	1/1	0.99	0.08	42,42,42,42	0
6	MG	N	9444	1/1	0.99	0.15	49,49,49,49	0
6	MG	A	9342	1/1	0.99	0.12	39,39,39,39	0
6	MG	N	9484	1/1	0.99	0.07	37,37,37,37	0
6	MG	C	9044	1/1	0.99	0.14	34,34,34,34	0
6	MG	N	9317	1/1	0.99	0.09	43,43,43,43	0
6	MG	D	9151	1/1	0.99	0.15	57,57,57,57	0
6	MG	N	9206	1/1	0.99	0.16	31,31,31,31	0
6	MG	M	9227	1/1	0.99	0.12	35,35,35,35	0
6	MG	E	9155	1/1	0.99	0.14	44,44,44,44	0
6	MG	N	9451	1/1	0.99	0.06	41,41,41,41	0
6	MG	D	9077	1/1	0.99	0.11	35,35,35,35	0
6	MG	N	9398	1/1	0.99	0.15	48,48,48,48	0
6	MG	M	9260	1/1	0.99	0.12	36,36,36,36	0
6	MG	D	9070	1/1	0.99	0.07	33,33,33,33	0
6	MG	C	9046	1/1	0.99	0.11	38,38,38,38	0
6	MG	K	9432	1/1	0.99	0.13	49,49,49,49	0
6	MG	N	9238	1/1	0.99	0.11	43,43,43,43	0
6	MG	C	9463	1/1	0.99	0.09	55,55,55,55	0
6	MG	C	9114	1/1	0.99	0.09	30,30,30,30	0
6	MG	F	9035	1/1	0.99	0.10	40,40,40,40	0
6	MG	D	9039	1/1	0.99	0.12	44,44,44,44	0
8	ZN	N	7059	1/1	0.99	0.12	93,93,93,93	0
6	MG	C	9051	1/1	0.99	0.12	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	C	9143	1/1	0.99	0.10	35,35,35,35	0
6	MG	M	9220	1/1	0.99	0.11	51,51,51,51	0
6	MG	N	9240	1/1	0.99	0.14	46,46,46,46	0
6	MG	M	9299	1/1	0.99	0.09	43,43,43,43	0
6	MG	N	9476	1/1	0.99	0.09	54,54,54,54	0
6	MG	B	9131	1/1	0.99	0.08	33,33,33,33	0
6	MG	C	9055	1/1	0.99	0.11	38,38,38,38	0
6	MG	D	9150	1/1	0.99	0.14	31,31,31,31	0
6	MG	C	9086	1/1	0.99	0.14	39,39,39,39	0
6	MG	M	9224	1/1	0.99	0.13	40,40,40,40	0
6	MG	D	9120	1/1	0.99	0.08	31,31,31,31	0
6	MG	D	9331	1/1	0.99	0.18	43,43,43,43	0
6	MG	M	9400	1/1	0.99	0.12	40,40,40,40	0
6	MG	M	9268	1/1	0.99	0.09	32,32,32,32	0
8	ZN	D	7112	1/1	0.99	0.10	80,80,80,80	0
6	MG	M	9208	1/1	0.99	0.10	39,39,39,39	0
6	MG	M	9300	1/1	0.99	0.09	39,39,39,39	0
6	MG	C	9003	1/1	0.99	0.13	38,38,38,38	0
6	MG	N	9303	1/1	0.99	0.08	54,54,54,54	0
6	MG	N	9279	1/1	0.99	0.11	54,54,54,54	0
6	MG	M	9312	1/1	0.99	0.12	37,37,37,37	0
6	MG	C	9454	1/1	0.99	0.09	55,55,55,55	0
6	MG	D	9147	1/1	0.99	0.10	41,41,41,41	0
6	MG	M	9474	1/1	0.99	0.14	49,49,49,49	0
6	MG	C	9455	1/1	0.99	0.11	40,40,40,40	0
6	MG	C	9061	1/1	0.99	0.07	34,34,34,34	0
6	MG	D	9141	1/1	0.99	0.06	50,50,50,50	0
6	MG	C	9169	1/1	0.99	0.13	42,42,42,42	0
6	MG	D	9351	1/1	0.99	0.06	43,43,43,43	0
6	MG	L	9183	1/1	0.99	0.13	37,37,37,37	0
6	MG	D	9034	1/1	0.99	0.08	41,41,41,41	0
6	MG	N	9448	1/1	0.99	0.09	51,51,51,51	0
6	MG	F	9393	1/1	0.99	0.12	38,38,38,38	0
6	MG	K	9469	1/1	0.99	0.12	50,50,50,50	0
6	MG	C	9170	1/1	0.99	0.06	41,41,41,41	0
6	MG	P	9446	1/1	0.99	0.13	34,34,34,34	0
6	MG	D	9058	1/1	0.99	0.08	38,38,38,38	0
6	MG	C	9079	1/1	0.99	0.11	38,38,38,38	0
6	MG	B	9358	1/1	0.99	0.07	39,39,39,39	0
6	MG	D	9084	1/1	0.99	0.11	37,37,37,37	0
6	MG	D	9341	1/1	0.99	0.10	41,41,41,41	0
6	MG	N	9403	1/1	0.99	0.12	34,34,34,34	0

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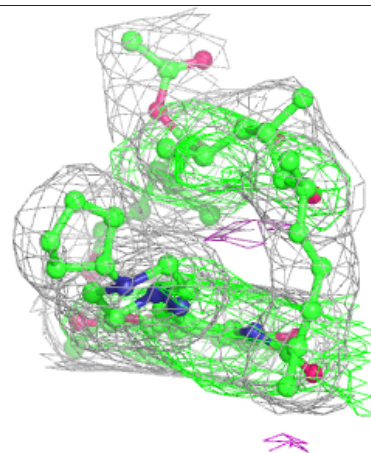
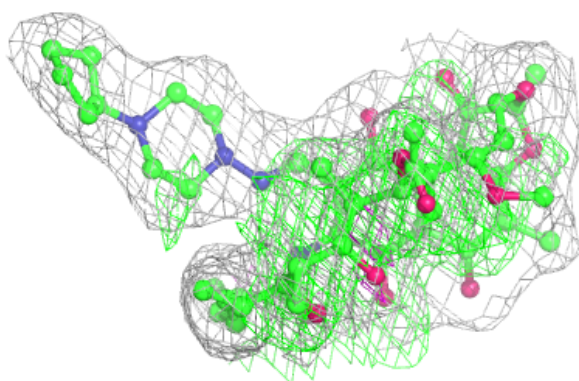
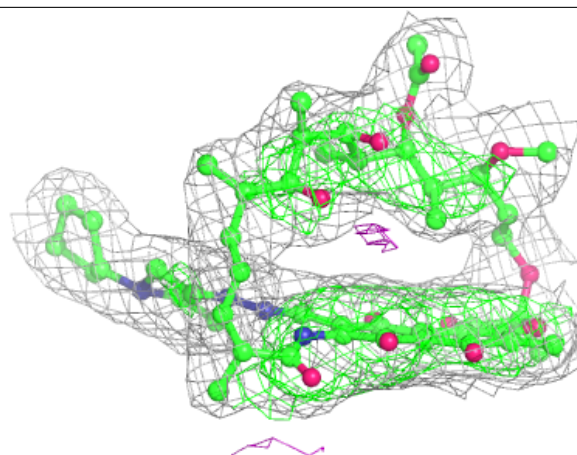
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	C	9031	1/1	0.99	0.10	40,40,40,40	0
6	MG	K	9244	1/1	0.99	0.07	44,44,44,44	0
6	MG	C	9164	1/1	0.99	0.10	49,49,49,49	0
6	MG	B	9040	1/1	0.99	0.16	36,36,36,36	0
6	MG	N	9269	1/1	0.99	0.07	42,42,42,42	0
6	MG	C	9050	1/1	0.99	0.15	37,37,37,37	0
6	MG	M	9409	1/1	0.99	0.10	36,36,36,36	0
6	MG	A	9075	1/1	0.99	0.10	36,36,36,36	0
6	MG	M	9281	1/1	0.99	0.11	49,49,49,49	0
6	MG	K	9180	1/1	1.00	0.11	42,42,42,42	0
6	MG	M	9485	1/1	1.00	0.07	54,54,54,54	0
6	MG	N	9408	1/1	1.00	0.14	45,45,45,45	0
6	MG	F	9101	1/1	1.00	0.12	44,44,44,44	0
6	MG	D	9117	1/1	1.00	0.13	48,48,48,48	0
6	MG	C	9361	1/1	1.00	0.10	41,41,41,41	0
6	MG	O	9266	1/1	1.00	0.08	47,47,47,47	0
6	MG	M	9321	1/1	1.00	0.12	41,41,41,41	0
6	MG	N	9193	1/1	1.00	0.15	34,34,34,34	0
6	MG	M	9320	1/1	1.00	0.11	34,34,34,34	0
6	MG	D	9091	1/1	1.00	0.13	27,27,27,27	0
6	MG	P	9258	1/1	1.00	0.14	51,51,51,51	0
6	MG	F	9057	1/1	1.00	0.09	30,30,30,30	0
6	MG	M	9230	1/1	1.00	0.11	50,50,50,50	0
6	MG	N	9249	1/1	1.00	0.10	45,45,45,45	0
6	MG	N	9311	1/1	1.00	0.10	39,39,39,39	0
6	MG	C	9487	1/1	1.00	0.11	32,32,32,32	0
6	MG	N	9271	1/1	1.00	0.07	43,43,43,43	0
6	MG	C	9076	1/1	1.00	0.12	33,33,33,33	0
6	MG	M	9319	1/1	1.00	0.12	41,41,41,41	0
6	MG	P	9482	1/1	1.00	0.11	48,48,48,48	0
6	MG	M	9401	1/1	1.00	0.10	37,37,37,37	0
6	MG	M	9248	1/1	1.00	0.08	48,48,48,48	0

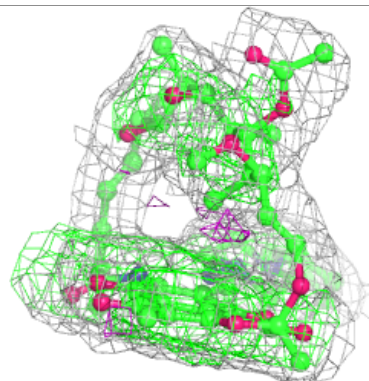
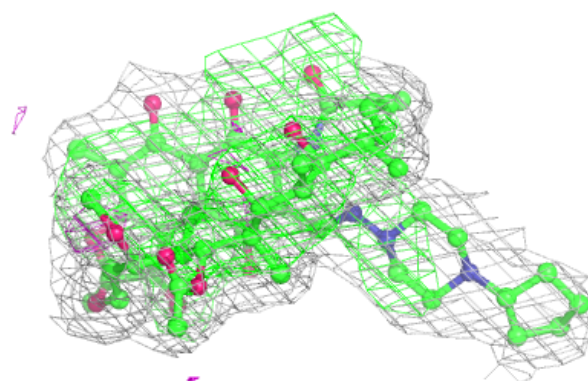
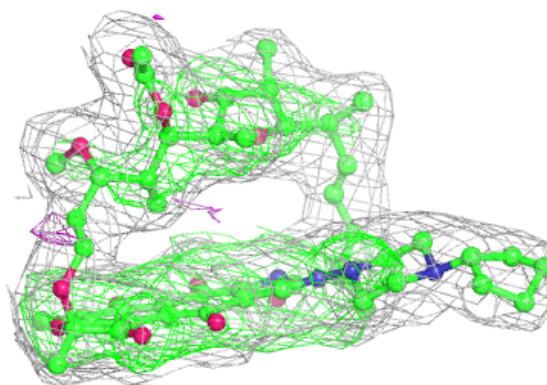
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around RPT M 8002:**

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

**Electron density around RPT C 8001:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.