



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 04:06 PM UTC

PDB ID : 2A6E / pdb_00002a6e
Title : Crystal structure of the T. Thermophilus RNA polymerase holoenzyme
Authors : Artsimovitch, I.; Vassilyeva, M.N.; Svetlov, D.; Svetlov, V.; Perederina, A.;
Igarashi, N.; Matsugaki, N.; Wakatsuki, S.; Tahirov, T.H.; Vassilyev, D.G.;
RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2005-07-02
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

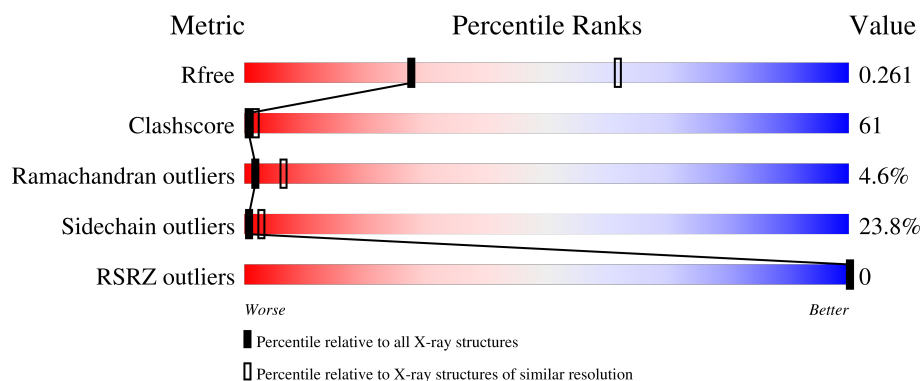
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	315	
1	B	315	
1	K	315	
1	L	315	
2	C	1119	

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Mol	Chain	Length	Quality of chain
2	M	1119	
3	D	1524	
3	N	1524	
4	E	99	
4	O	99	
5	F	423	
5	P	423	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 58679 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 8 is water.

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

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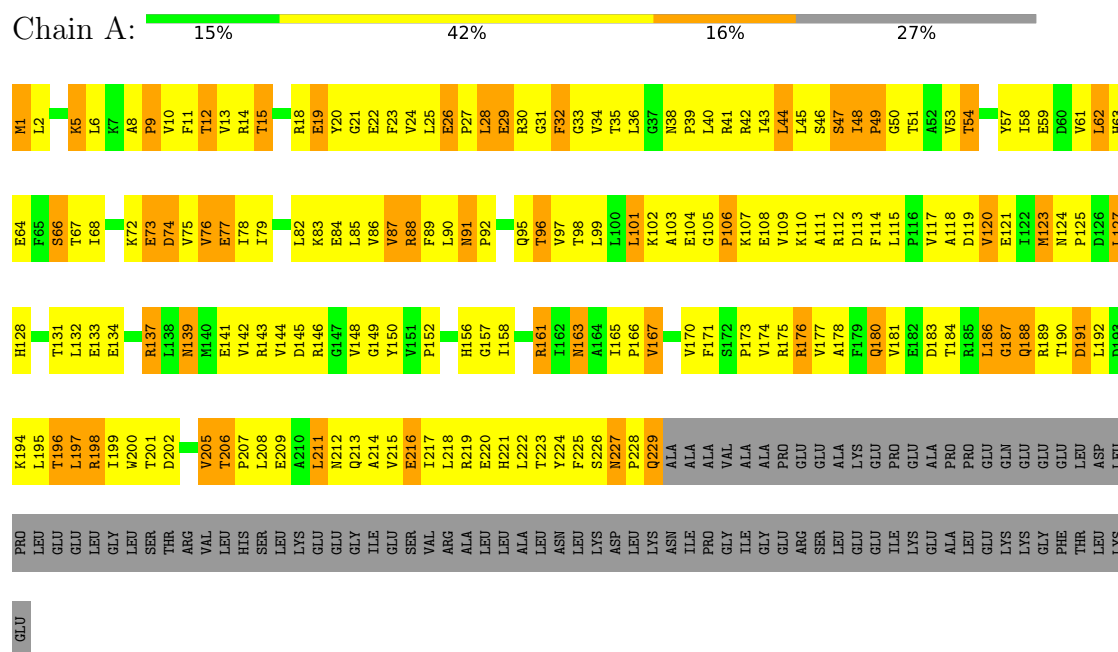
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	N	1038	Total 1038	O 1038	0	0
8	O	78	Total 78	O 78	0	0
8	P	267	Total 267	O 267	0	0

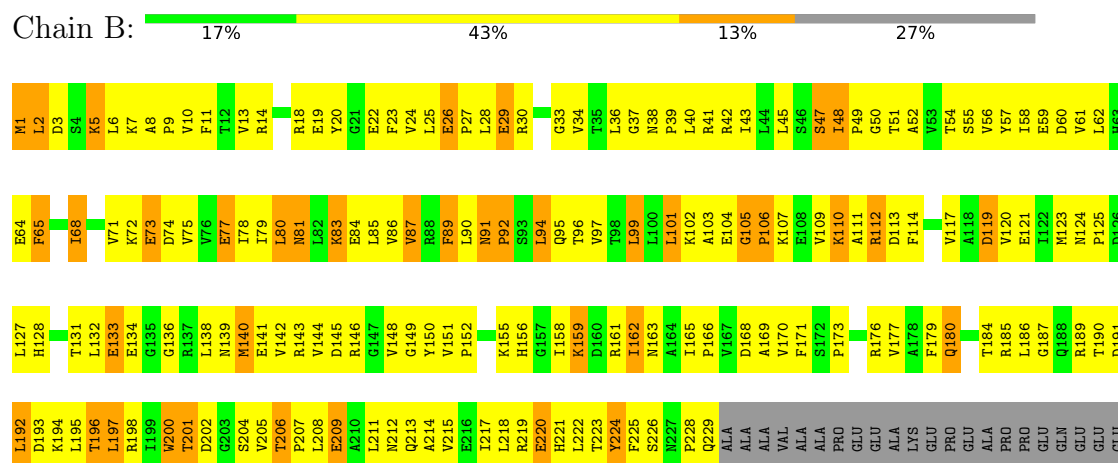
3 Residue-property plots

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

• Molecule 1: DNA-directed RNA polymerase alpha chain



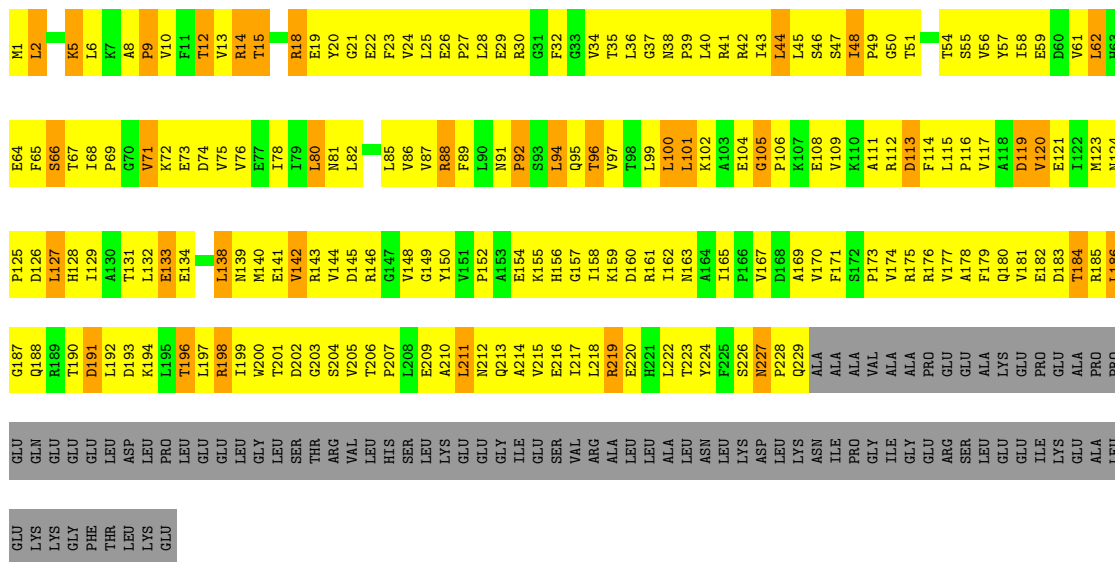
• Molecule 1: DNA-directed RNA polymerase alpha chain



THR	LEU	ASP	PRO	GLU	LEU	GLY	SER	THR	ARG	VAL	HIS	SER	LEU	LYS	GLU	GLY	ILE	GLU	SER	VAL	ARG	ALA	LEU	LEU	ALA	ASN	LEU	LYS	ASP	LEU	LYS	ASN	ILE	PRO	GLY	ILE	GLY	ARG	SER	LEU	GLU	ILE	LYS	LYS	LYS	GLY	PRO
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

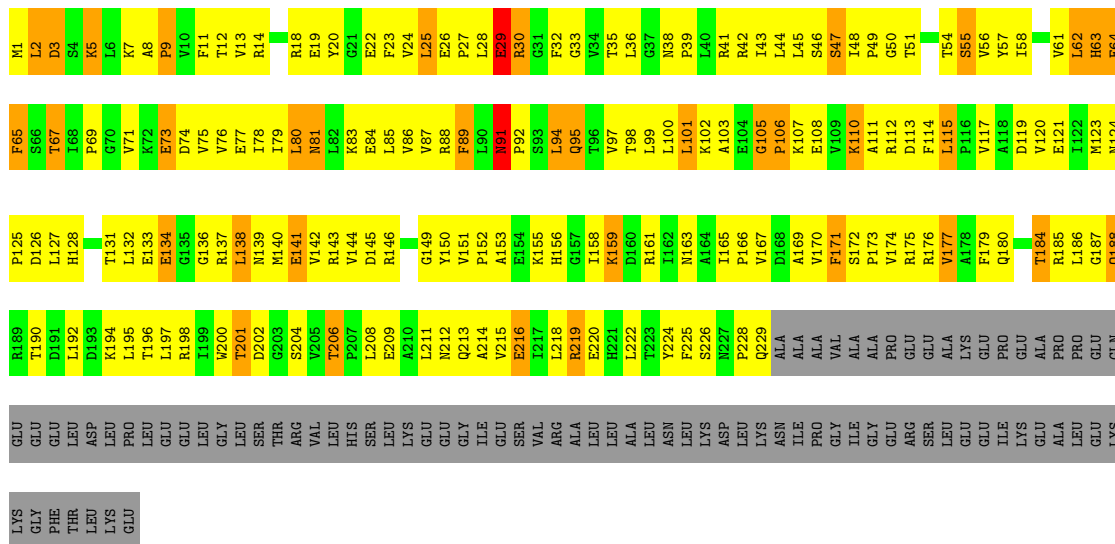
- Molecule 1: DNA-directed RNA polymerase alpha chain

Chain K:

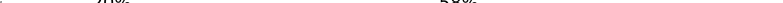


- Molecule 1: DNA-directed RNA polymerase alpha chain

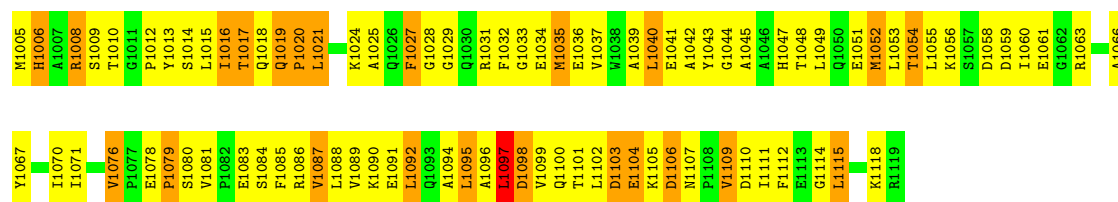
Chain L:



- Molecule 2: DNA-directed RNA polymerase beta chain

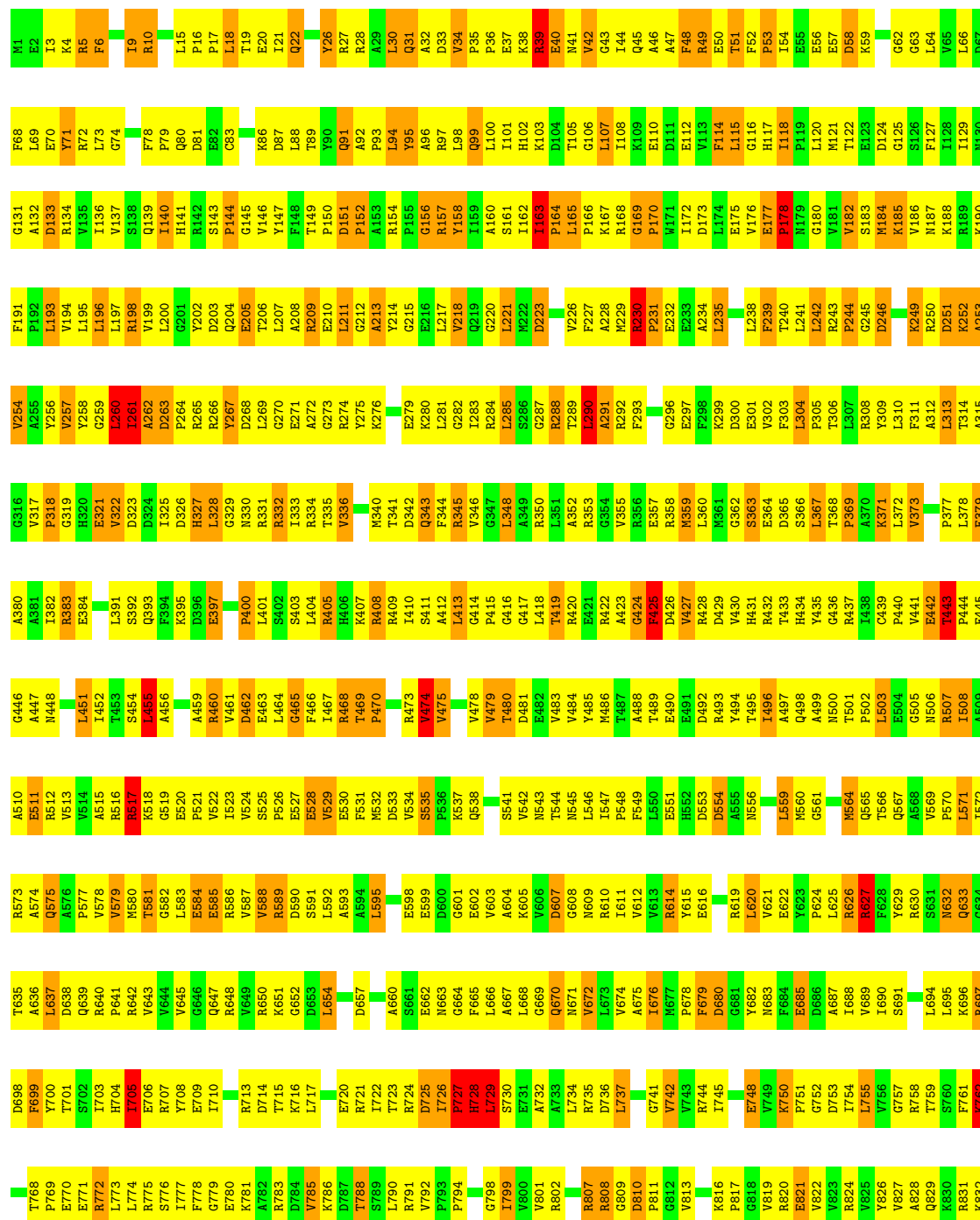
Chain C:  20% 58% 20%

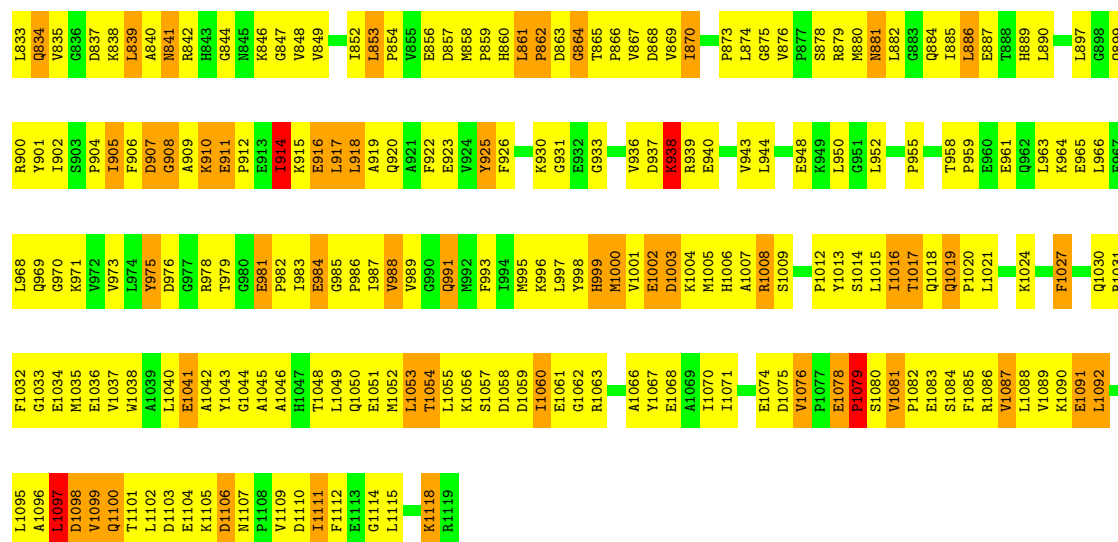
V943	R879	K816	V749	V689	Q565	P502	V441	L378	A315	D251	N187	D124	G62	W1
L944	M880	P817	K750	L690	T566	L503	E442	E379	G316	K252	K188	G125	G63	E2
R945	N881	G818	P751	S691	Q567	E504	T443	A380	P317	K252	K189	G125	L64	I3
R946	L882	V819	G752	E692	A568	G505	P444	A381	P318	K190	K190	F127	V65	K4
A947	G883	R820	D753	E693	V569	M506	E445	R383	G319	V254	F191	I128	L66	R5
E948	Q884	E821	L754	L694	P570	R507	E446	R383	H320	A255	P192	I129	D67	F6
K949	T885	V822	L755	L695	L571	L508	A447	E384	E321	Y256	L193	G7	F68	G7
L950	L886	V823		K696	L572	A509	K448	F386	T325	Y257	V194	D133	L69	R8
G951	E887	R824	R758	R697	R573	A510	L449	F386	L195	Y258	L195	E70	E70	I9
L952	L890	V825	T759	D698	A574	E511	L450	G387	D326	G259	L196	Y71	R71	E11
V953	P953	V826	S760	F699	Q575	R512	L451	R388	G327	L260	L197	Y136	R72	E11
T954	G891	V827	F761	Y700	Q576	V513	L452	L391	L328	L261	R198	V137	L73	V12
P955	L892	A828	K762	T701	P577	V514	T453	L391	G329	A262	V199	S138	G74	I13
G956			G763	S702	V578	A515	S454	S392	R330	D263	L200	Q139	E75	F14
K957	Y895	R831	E764	L703	V579	A516	L455	Q393	R331	P264	G201	I140	P76	L15
T958	F896	K832		H704	M580	R517	L456	Q393	R332	R265	Y202	H141	P77	P16
P959	L897	L833	T768	L705	T581	G518	A457	K395	L333	R266	D203	R142	F78	P17
E960	G898	Q834	P769	E706	G582	G519	Y458	D396	R334	Y267	Q204	S143	P79	L18
E961	Q899	V835	V770	R707	L583	F520	A459	E397	T335	D268	E205	P144	Q80	T19
G962	R900	G836	E771	Y708	E584	P521	R460	T398	V336	L269	T206	G145	D81	E20
L963	Y901	D837	R772	E709	E585	V522	V461	R399	G337	G270	L207	V146	E82	I21
K964	F898	K838	L773	L710	R586	T523	D462	P400	R346	E271	A208	Y147	C83	Q22
E965	S902	L839	L774	E711	V587	V524	E463	L401	L339	A272	R209	F148	R84	V23
L966	E903	R840	R775	A712	G588	S525	L464	S402	M340	G273	E210	T149		E24
F967	P904	A840	S776	R713	R589	P526	G465	S403	T341	R274	L211	P150	L88	S25
L968	L905	K841	I777	D714	D590	E527	F466	L404	D342	Y275	G212	D151	T89	Y26
Q969	D907	R842	F778	L715	S591	E528	L467	R405	Q343	K276	A213	P152	Y90	R27
G970	G908	G843	G779	K716	L592	V529	R468	H406	Y214		G215		Y90	R28
K971	A909	N845	E780	L717	D657	E530	T469	K407	G216	E279	G215	P155	A92	A29
V972	K910	K846	K781	G718	G658	F531	P470	R408	V346	K280	E216	G156	P93	L30
G973	E911	Q847	A783	P719	V659	M532	Y471	R409	G347	L281	L217	R157	L94	Q31
L974	P912	V848	R783	E720	A660	D533	R472	T410	L348	G282	V218	Y158	Y95	A32
Y975	E913	V849	R784	R721	S661	V534	R473	S411	A349	I283	Q219	I159	A96	D33
D976	L914		V785	I722	E662	P536	V474	A412	R350	R284	G220	A160	R97	V34
K977	K915	L853	G776	L723	N663	S535	V475	L413	L351	L285	L221	S161	L98	P35
R978	E916	P854	D787	R724	G664	E602	V476	G414	A352	S286	M222	I162	Q99	P36
T979	L917	V855	T788	D725	F665	V603	V478	P415		G287	D223	I163	E37	E37
G980	L918	E856	S789	L726	L666	A604	V479	G416	V355	K288	E224	P164	L101	K38
E981	A919	D857	L790	P727	A667	R605	T480	G417	R356	T289	S225	P165	H102	K39
P982	Q920	K858	R791	H728	L668	V606	D481	L418	E357	L290	V226	P166	K103	E40
L983	A921	P859	V792	L729	D607	D607	E482	T419	R358	A291	F227	K167	D104	N41
E984	F922	H860	P793	S730	G670	G608	V483	R420	M359	R292	A228	R168	T105	V42
G985	E923	L861	P794	E731	N609	R610	V484	E421	L360	M229	G169	G169	G106	V42
P986	V924	P862	G795	A732	V672	R610	Y485	R422	K361		R230	P170	L107	I44
L987	Y925	D663	E796	A733	L673	L611	M486		G362	K299	P231	W171	L108	Q45
V988	F926	G864	G797	L734	V674	V612	T487	P425	S363	D300	E232	I172	K109	A46
G990	G927	T865	G798	R735	A675	E551	A488	D426	E364	E301	E233	D173	E110	A47
K991	Q930	P866	I799	D736	L676	R614	T489	V427	D365	V302	A234	L174	D111	F48
M992	G931	V867		L737	N677	Y615	E490	R428	S366	F303	L235	E175	E112	R49
F993	E932	D868	R802	D738	P678	E616	E491	D429	L367	L304	I236	V176	V113	F50
L994	S932	V669	T803	E739	F679	A555	V492	V430	T368	P305	R237	E177	F114	T51
M995	G933	R870	V804	E740	D680	R556	R493	H431	P369	T306	L238	P178	L115	F52
K996	F934	L871	R805	G741	G681	V621	Y494	R432	A370	L307	F239	M179	G116	P53
L997	D937	N872	P873	V742	V682	E622	T433	T433	K371	R308	T240	G180	H117	I54
	Q938	P873	D810	V743	N683	V623	I496	H434	S366	F303	L241	V181	I118	E55
R999	E937	L874	P811	R744	F684	P624	A967	Y435	V373	Y309	L242	V182	P119	E56
V1001	R939	G875	G812	L745	E685	G581	Q498	G436	N374	F311	R243	S183	L120	E57
E1002	E940	V876	V813	G746	R626	S562	A499	R437	S375	A312	P244	M184	M121	D58
D1003	V941	P877	E814	A747	A687	R627	M500		R376	L313	G245	K185	T122	K59
K1004	E942	S878	L815	E748	F628	M564	T501	P440	P377	T314	D246	V186	E123	



• Molecule 2: DNA-directed RNA polymerase beta chain

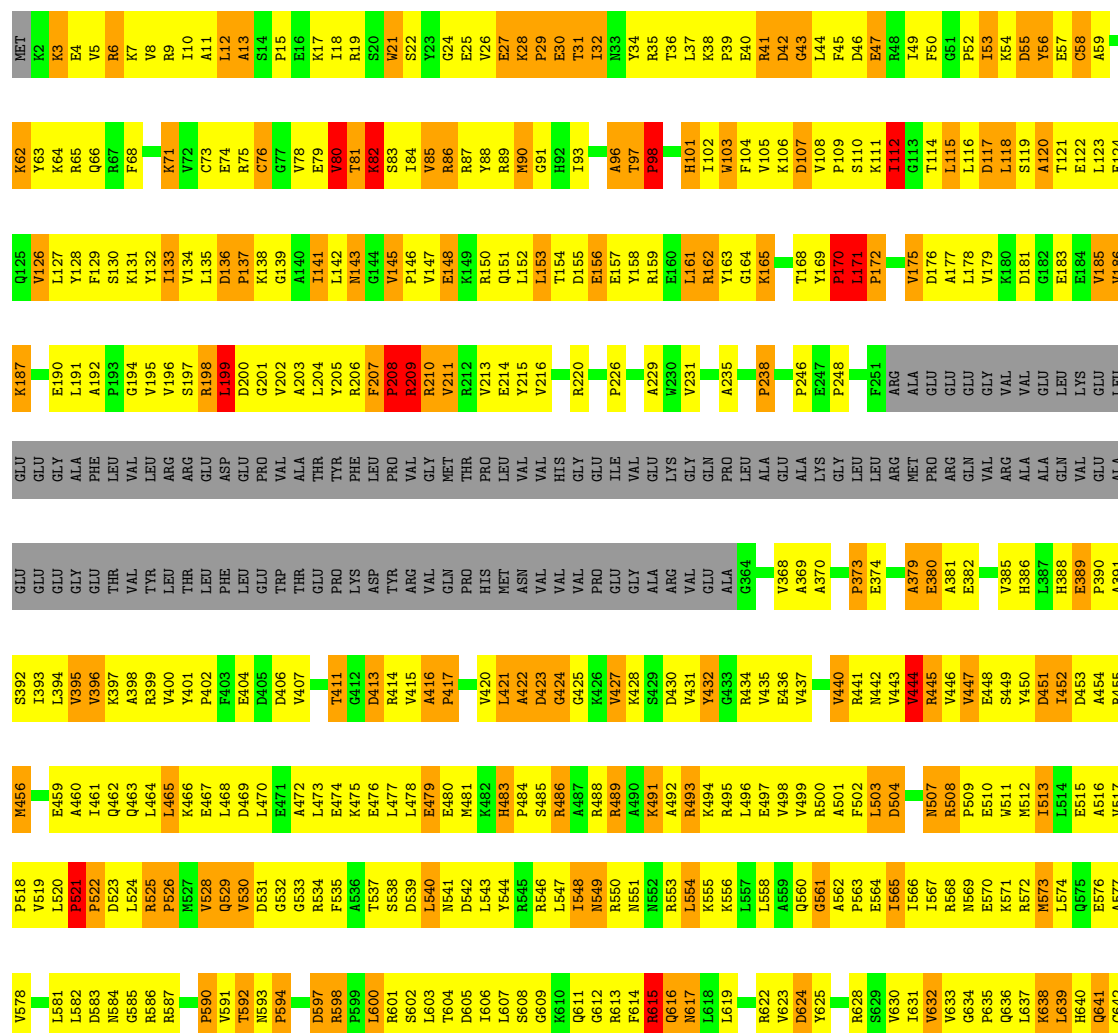
Chain M: 24% 56% 19%





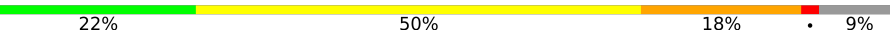
• Molecule 3: DNA-directed RNA polymerase beta' chain

Chain D: 21% 49% 19% 9%

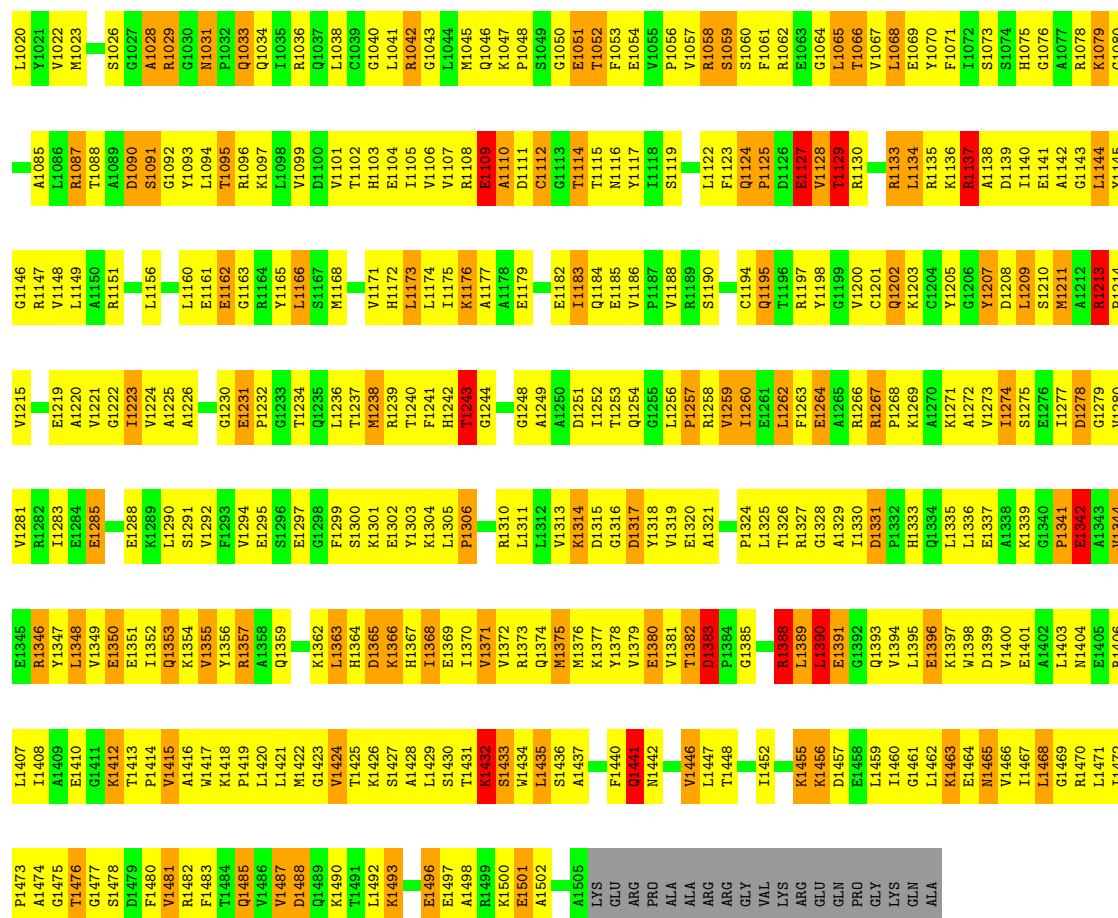


T1476	G1477	S1478	D1479	V1480	F1481	R1482	F1483	T1484	V1485	V1486	V1487	D1488	T1491	L1492	K1493	A1494	L1495	E1496	E1497	K1500	E1501	E1504	A1505	LVS	GLU	GLU	GLU	PRG	ALA	ALA	ALA	ARG	ARG	GLY	VAL	LVS	ARG	GLU	GLM	PRG	GLY	LVS	GLN	ALA																	
T1413	P1414	V1415	A1416	W1417	P1418	P1419	L1420	L1421	M1422	G1423	G1424	V1425	K1426	S1427	A1428	L1429	K1430	L1431	K1432	S1433	W1434	L1435	A1438	S1439	F1440	Q1441	L1442	T1443	A1444	H1445	V1446	L1447	T1448	L1452	A1453	G1454	K1455	K1456	D1457	E1458	L1459	T1460	G1461	L1462	K1463	E1464	N1465	V1466	I1467	L1468	G1469	R1470	L1471	T1472	P1473	A1474	G1475				
E1351	I1352	L1353	K1354	V1355	R1356	A1357	Q1358	G1359	K1360	F1361	K1362	L1363	H1364	D1365	K1366	H1367	I1368	E1369	I1370	V1371	V1372	L1373	Q1374	M1375	M1376	K1377	V1378	L1379	E1380	V1381	A1382	D1383	P1384	G1385	R1388	L1389	L1390	E1391	G1392	K1393	V1394	L1395	E1396	K1397	W1398	D1399	V1400	K1339	E1401	A1402	L1403	N1404	E1405	R1406	L1407	I1408	L1409	E1410	G1411	L1412	
E1289	L1290	Q1291	V1292	L1293	V1294	E1295	G1296	E1297	F1298	P1299	S1300	K1301	T1302	V1303	K1304	L1305	P1306	K1307	T1308	H1309	L1310	L1311	L1312	V1313	K1314	D1315	G1316	D1317	V1318	L1319	V1320	L1321	L1322	L1323	P1324	L1325	T1326	R1327	G1328	A1329	D1330	P1331	L1332	R1333	E1334	L1335	W1336	E1337	K1338	L1339	V1340	A1341	E1342	A1343	V1344	L1345	L1346	L1347	L1348	E1349	E1350
E1219	A1220	V1221	G1222	V1223	I1224	G1230	E1231	P1232	G1233	L1234	Q1235	L1236	T1237	M1238	P1239	F1240	H1241	L1242	T1243	G1244	G1248	A1249	A1250	D1251	L1252	T1253	Q1254	G1255	L1256	L1257	R1258	L1259	I1260	E1261	L1262	F1263	A1264	A1265	R1266	P1267	K1268	K1269	A1270	K1271	A1272	V1273	L1274	T1277	D1278	G1279	V1280	V1281	R1282	L1283	E1284	E1285					
V1155	L1156	K1157	V1158	L1159	L1160	E1161	G1162	L1163	R1164	V1165	L1166	M1167	D1168	D1169	L1170	V1171	L1174	L1175	K1176	A1177	A1178	E1182	L1183	Q1184	L1185	V1186	P1187	L1188	E1189	S1190	P1191	L1192	Q1195	L1196	R1197	V1198	L1199	V1200	K1201	Q1202	K1203	G1204	V1205	L1206	V1207	L1208	L1209	S1210	M1211	A1212	L1213	V1214	V1215	S1216	L1217	G1218					
L1094	T1095	R1096	K1097	L1098	V1099	D1100	V1101	T1102	H1103	E1104	L1105	V1106	V1107	R1108	E1109	L1110	D1111	G1112	G1113	T1114	N1115	Y1116	Y1117	S1118	S1119	P1120	P1121	L1122	F1123	Q1124	P1125	L1126	V1127	T1128	T1129	R1130	S1131	L1132	R1133	L1134	R1135	L1136	R1137	A1138	D1139	I1140	A1141	A1142	G1143	L1144	L1145	G1146	R1147	V1148	R1151	E1152	V1153	E1154			
Q1033	Q1034	I1035	R1036	Q1037	L1038	C1039	G1040	L1041	G1042	L1043	L1044	M1045	Q1046	P1047	E1048	S1049	G1050	E1051	L1052	F1053	E1054	P1055	V1056	L1057	R1058	S1059	W1060	T1061	R1062	E1063	L1064	L1065	T1066	V1067	L1068	E1069	V1070	F1071	L1072	S1073	S1074	H1075	G1076	A1077	K1078	L1082	D1083	T1084	L1085	L1086	R1087	T1088	A1089	D1090	S1091	G1092	Y1093				
E965	E966	A967	D968	R969	K970	L971	L972	Q973	L974	E975	Q976	A977	Y978	E979	M980	T984	D985	R986	E987	R988	I992	L993	Q994	L995	W996	T997	E998	T999	T1000	E1001	K1002	V1003	A1006	V1007	F1008	K1009	N1010	F1011	E1012	E1013	H1014	Y1015	P1019	Y1021	M1022	A1023	Q1025	E988	R989	S1026	K990	A1028	R1029	P1032							
R832	E833	T834	S835	R836	G837	R838	L839	K840	V841	R842	F843	A844	D847	E848	I849	A850	L851	A852	V853	I857	V858	E859	L860	R861	D862	F863	V864	R865	E866	R867	Y868	M869	E874	T875	S876	P877	G878	R879	I880	A883	R884	E888	A889	V890	E891	D892	E893	K894	R895	S1026	K960	K961	E898	L899	I900						
Q901	L902	D903	V904	P905	Q906	E907	K908	M909	L910	S911	K912	D913	L914	V915	M980	Q917	A918	F919	L920	R921	L922	G923	N924	E925	K926	T927	A928	R929	V863	L930	L931	Y936	Y937	G938	F939	T940	F941	S942	T943	T944	S945	G946	T947	T948	I949	D952	V955	L956	P957	E958	R959	K960	K961	Q962	L964						
L769	L770	S771	P772	A773	S774	G775	E776	F777	L778	A779	K780	R783	D784	I785	L786	L787	G788	L789	Y790	Y791	I792	T793	Q794	V795	R796	R797	E798	K799	K800	G803	L804	E805	F806	T808	P809	E810	E811	A812	L813	A814	E817	R818	G819	E820	V821	A822	L823	M824	A825	P826	M827	L828	V829	A830	G831						
R704	A705	P706	T707	L708	H709	R710	L711	G712	L713	Q714	A715	F716	Q717	V718	L719	L720	V721	E722	Q723	S725	I726	Q727	L728	H729	L730	L731	E734	A735	F736	N737	A738	D739	F740	D741	Q744	M745	V749	S752	S753	F754	A755	Q756	A757	E758	F759	A760	H696	I761	Q762	M763	L764	S765	A766	L701	L702	H767	N768				
G643	L644	P645	K646	R647	M648	A649	E650	L651	F652	L653	K654	P655	F656	L657	L658	K659	K660	E661	E662	E663	I666	A667	P668	N669	V670	K671	A672	A673	R674	R675	M676	L677	E678	R679	Q680	R681	D682	L683	D685	V687	W688	D689	A690	L691	E692	E693	V694	L695	H696	G697	K698	M699	V700	L701	L702	H767	N768				

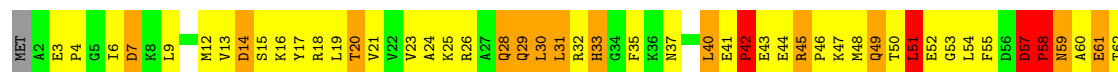
• Molecule 3: DNA-directed RNA polymerase beta' chain

Chain N:  22% 50% 18% 9%

I949	R884	E820	S763	D689	B628	I566	S505	V444	A381	ARG	GLU	G182	E122	G61	MET
G950	I885	V621	F754	A690	S629	I567	G506	R445	E382	GLN	GLU	E183	L123	K62	K2
I951	V886	A822	A755	A691	V630	R568	R507	V446	E383	VAL	GLY	E184	L124	Y63	K3
D952	A887	L823	Q756	E692	I631	N569	R508	V447	V385	ARG	VAL	V185	Q125	R64	E4
D953	E888	N824	Q757	E693	V632	E570	P509	E448		ALA	VAL	V186	V126	R65	V5
A954	A889	A825	A759	V694	V633	K571	E510	S449	H388	ALA	GLN	K187	L127	Q66	R6
V955	V980	P826	R760	I695	G634	R572	U511	V450	E389	GLN	LEU	G188	Y128	R67	K7
E991	E891	I827	I761	H696	P635	K573	K612	D451	P390	VAL	LYS		F129	P68	V8
P957	D992	K828	Q762	G697	Q636	L574	I513	I452	A391	GLU	GLU	L191	E129	E69	R9
E958	E893	V829	M763	K698	L637	K575	I514	D453	A392	ALA	LEU	A192	K131	G70	I10
E959	K894	A830	L764	V699	K638	E576	E515	A454	I393	GLU	GLU	P193	Y132	K71	A11
K960	V895	G831	S765	V700	L639	A577	A516	R455	I394	GLU	GLY	G194	I133	V72	L12
K961	A896	R832	A766	L701	H640	V578	V517	V456	L394	GLU	GLY	V195	C73	C73	A13
Q962	V897	E833	H767	L702	Q641	D579	P518		V396	GLY	ALA	V196	L135	E74	S14
V963	T634	T634	L770	N703	C642	A580	V519	E459	K397	GLU	PHE	S197	D136		P15
L964	L899	S835	L964	R704	C643	L581	L520	A460	A398	THR	LEU	R198	P137	C76	E16
E965	V836	V836	A705	A705	L644	L582	P521	I461	R399	VAL	VAL	L199	K138	G77	K17
	Q901	G837	S774	P706	P645	D583	P522	Q462	V400	TYR	LEU	D200	G139	V78	I18
D968	R838	R838	G775	L707	K646	N584	D523	Q463	Y401	LEU	ARG	G201	I140	E79	R19
R969	L839	L839	E776	L708	R647	S585	L524	L464	P402	THR	ARG	V202	I141	V80	S20
K970			P777	H709	K648	R586	R525	L465	F403	LEU	GLU	A203	L142	T81	W21
L971	E907	V842	L778	R710	A649	R587	P526	K466	E404	PHE	ASP	V211	M143	R82	Y22
L972	K908	F843	A779	L711	L650	G588	M527	E467	D405	LEU	GLU	Y205	G144	S83	Y23
Q973	N909	A844	K780	G712	E851	A589	V528	L468	D406	GLU	PRO	R206	V145	T84	G24
L974	S910	V845	P781	I713		P590	O529	D469	V407	TRP	VAL	F207	P146	V85	E25
E975	L911	P846	S782	Q714	K654	V591	V636	L470	E408	THR	ALA	P208	V147	R86	V26
Q976	E912	D847	R783	A715	P655	T592	D531	E471		GLU	THR	R209	E148	R87	E27
	D912	E848	D784	F716	F656	N593	G532	A472	T411	PRO	PRO	R210	K149	Y88	K28
E979	L914	F843	L778	Q717	L657	P594	G533	E473	G412	LYS	PHE	Y212	G150	R89	P29
M980	V915	L850	I786	P718	L658	G595	R534	L474	D413	ASP	LEU	R213	Q151	E90	E30
	Y916	L851	L787	V719	K659	S596	F535	K475	R414	TYR	PRO	V213	L152	T91	T31
Q917	Q917	A852	G788	L720	K660	D597	A536	E476	V415	ARG	VAL	E214	L153	I93	I32
A918	E918	V853	L789	V721	K661	R598	A537	L477	A416	VAL	GLY	Y215	T154	E94	N33
F919	F919		E722	E722	P599	P599	S538	E478	P417	GLN	MET	V216	D155	L95	Y34
L920	L920		T793	Q724	E663	L600	D539	E479	G418	PRO	THR	K217	E156	A96	R35
R988	R921	V858	Q794	S725	K664	R601		E480	D419	HIS	PRO		E157	T97	T36
Y989	L922	D659	V795	L726	G665	S602	D542	M481	V420	MET	LEU	R220	Y158	P98	L37
	G923	L860	R796	Q727	T666	L603	L543	K482	L421	ASN	VAL	A221	R159	A99	K38
L992	N924	Q861	R797	L728	A697	T604	V544	H483	A422	VAL	VAL	G222	E160	A100	P39
L993	E925	D862	K797	P668	P668	D605	G545	P484	D423	VAL	HIS	L223	L161	H101	E40
Q994	K926	V663	E798	H729	N669	L606	R546	R485	C424	VAL	GLY		R162	I102	R41
L995	T927	V664	K799	P730	V670	L607	L547	R486	C425	PRO	GLU	P226	Y163	W103	D42
W996	A928	T865	K800	L731	K671	S608	I548	A487	K426	GLU	ILE		G164	F104	G43
T997	R929	V666		Q732	A672	G609	N549	R488	V427	GLY	VAL	V231	K165	V105	L44
E998	L930	R667	G803	C733	A673	K610	R550	R489	K428	ALA	GLU		Q166	K106	F45
T999	L931	Y868	L804	E734	R674	Q611	N551	R490	S429	ARG	LYS	P238	E167	D107	D46
T1000	D932		E805	A735	R675	G612	N552	K491	D430	VAL	GLY	G239	T168	E108	E47
E1001	A933	K871	F806	F736	N676	R613	R553	A492	V431	GLU	GLN	E240	Y169	P109	R48
K1002	L834	R872	A807	N737	L677	F614	L554	R493	Y432	ALA	PRO		P170	S110	I49
V1003	K935	L873	T808	A738	E678	R615	K555	X494	C433		LEU	A243	L171	K111	F50
T1004	Y937	E874	P809	D739	R679	R616	K556	R495	C434	G364	ALA	E244	P172	I112	G51
Q1005	Q937	T875	E810		R679	R617	L587	L496	V436	D365	ALA	L245	P173	G113	P52
A1006	T940	S876	E811	Q744	R681	K621	A559	L497	V437	V368	ALA	L246	G174	T114	E47
V1007		P877	A812	M745	D682	R622	L558	V498	V437	A369	LYS	E247	V175	L115	S53
K1008	G878	G878	L813	M745	L683	R623	G561	Y499	D438	A370	GLY	P248	D176	L116	K54
K1009	R879	R879	A814		K684	G623	G561	R500	L439		LEU		A177	D117	D55
N1010	S945	T880	E817	V749	P685	D624	A562	A501	V440	P873	LEU	F251	L178	L118	E57
	G946	L881	E817	P750	E686	T625	P563	F502	R441		ARG	ARG	V179	L119	C88
M1018	I947	P882	R818	L751	V687	T626	E564	L503	A379	A379	ARG	ALA	K180	A120	E58
P1019	T948	A883	G819	S752	V688	G627	I565	D504	V443	E380	PRO	GLU	D181	T121	C60



Chain E: 22% 53% 17%



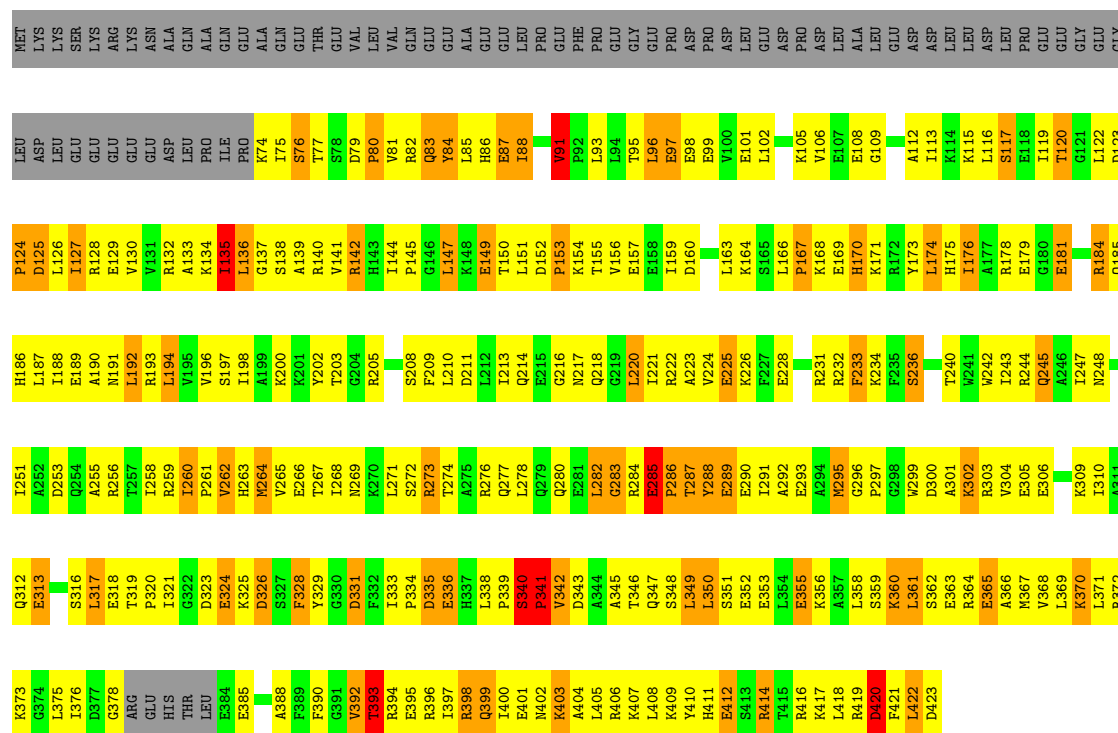
• Molecule 4: RNA polymerase omega chain

Chain O: 27% 42% 24%



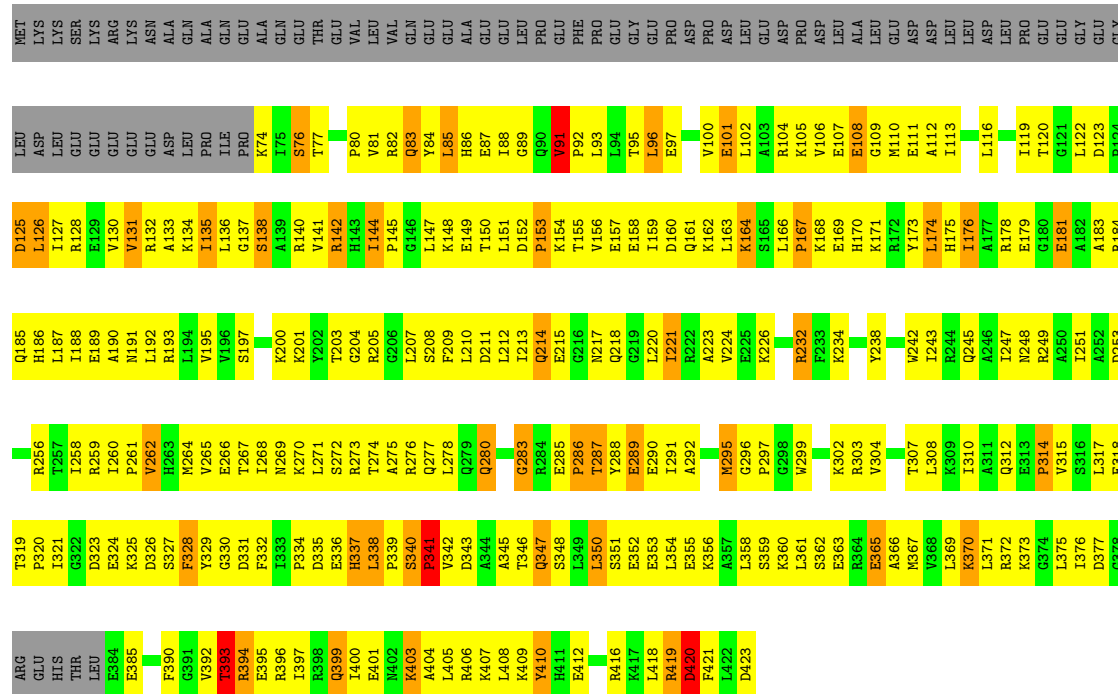
• Molecule 5: RNA polymerase sigma factor rpoD

Chain F: 18% 46% 16% 18%



• Molecule 5: RNA polymerase sigma factor rpoD

Chain P: 22% 49% 10% 18%



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	239.50Å 239.50Å 253.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.80 25.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.80) 92.0 (25.00-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.231 , 0.268 0.226 , 0.261	Depositor DCC
R_{free} test set	21166 reflections (5.78%)	wwPDB-VP
Wilson B-factor (Å ²)	58.9	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 77.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.499 for -h,-k,l 0.068 for h,-h-k,-l 0.068 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	58679	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.88	3/1838 (0.2%)	1.22	9/2498 (0.4%)
1	B	0.78	0/1838	1.09	7/2498 (0.3%)
1	K	0.79	0/1838	1.15	7/2498 (0.3%)
1	L	0.75	1/1838 (0.1%)	1.08	9/2498 (0.4%)
2	C	0.91	5/8997 (0.1%)	1.28	73/12164 (0.6%)
2	M	0.89	6/8997 (0.1%)	1.27	72/12164 (0.6%)
3	D	0.95	11/10975 (0.1%)	1.33	99/14836 (0.7%)
3	N	0.92	13/10975 (0.1%)	1.32	95/14836 (0.6%)
4	E	0.92	0/783	1.36	6/1054 (0.6%)
4	O	0.95	2/783 (0.3%)	1.39	10/1054 (0.9%)
5	F	0.81	2/2812 (0.1%)	1.19	13/3781 (0.3%)
5	P	0.80	0/2812	1.17	11/3781 (0.3%)
All	All	0.89	43/54486 (0.1%)	1.27	411/73662 (0.6%)

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

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

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	48	ILE	C-N	9.24	1.44	1.33
3	D	82	LYS	CA-C	8.55	1.64	1.52
2	C	163	ILE	CA-CB	8.41	1.62	1.53
2	M	163	ILE	CA-CB	8.23	1.62	1.53
1	A	48	ILE	CA-C	8.08	1.60	1.52
3	N	126	VAL	CA-CB	6.89	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	126	VAL	CA-CB	6.81	1.62	1.54
3	D	112	ILE	CA-CB	6.57	1.63	1.54
3	N	1091	SER	N-CA	6.44	1.54	1.46
3	D	984	THR	CA-CB	6.27	1.63	1.53
3	N	13	ALA	CA-CB	-6.15	1.45	1.53
2	C	191	PHE	C-N	6.09	1.41	1.33
2	M	914	ILE	CA-CB	6.06	1.61	1.54
3	N	1114	THR	CA-CB	6.01	1.60	1.52
3	D	13	ALA	CA-CB	-6.00	1.45	1.53
5	F	135	ILE	CA-CB	5.97	1.61	1.54
2	M	742	VAL	CA-CB	5.73	1.62	1.54
3	D	1091	SER	N-CA	-5.72	1.39	1.46
4	O	24	ALA	CA-CB	-5.72	1.44	1.53
3	N	498	VAL	CA-CB	5.64	1.60	1.54
2	C	468	ARG	CA-C	-5.64	1.45	1.52
3	N	207	PHE	CA-C	5.62	1.59	1.52
3	N	83	SER	N-CA	-5.58	1.39	1.46
1	A	49	PRO	N-CA	5.51	1.53	1.46
2	M	226	VAL	CA-CB	5.51	1.61	1.54
2	C	474	VAL	CA-CB	5.51	1.61	1.54
3	D	444	VAL	CA-CB	5.43	1.59	1.53
3	N	1375	MET	SD-CE	-5.36	1.66	1.79
3	D	207	PHE	CA-C	5.36	1.59	1.52
2	M	474	VAL	CA-CB	5.32	1.61	1.54
3	D	141	ILE	CA-CB	5.29	1.59	1.54
2	C	191	PHE	CA-C	5.23	1.59	1.52
3	N	141	ILE	CA-CB	5.19	1.59	1.54
1	L	172	SER	CA-C	-5.14	1.46	1.52
5	F	75	ILE	CA-CB	5.12	1.60	1.54
3	N	1260	ILE	CA-CB	5.10	1.61	1.54
3	N	880	ILE	CA-CB	5.10	1.60	1.54
4	O	41	GLU	CA-C	5.08	1.58	1.52
2	M	535	SER	CA-C	5.07	1.58	1.52
3	N	172	PRO	CA-C	5.07	1.56	1.52
3	D	1424	VAL	CA-CB	5.06	1.60	1.54
3	N	1177	ALA	CA-CB	-5.04	1.45	1.53
3	D	82	LYS	N-CA	5.00	1.52	1.46

All (411) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	207	PHE	CA-C-N	16.60	140.59	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	207	PHE	C-N-CA	16.60	140.59	119.84
3	N	207	PHE	CA-C-N	16.53	140.50	119.84
3	N	207	PHE	C-N-CA	16.53	140.50	119.84
2	C	177	GLU	CA-C-N	14.79	138.33	119.84
2	C	177	GLU	C-N-CA	14.79	138.33	119.84
3	N	508	ARG	CA-C-N	14.76	138.29	119.84
3	N	508	ARG	C-N-CA	14.76	138.29	119.84
2	M	177	GLU	CA-C-N	14.72	138.24	119.84
2	M	177	GLU	C-N-CA	14.72	138.24	119.84
3	D	508	ARG	CA-C-N	13.59	136.83	119.84
3	D	508	ARG	C-N-CA	13.59	136.83	119.84
1	A	48	ILE	CA-C-N	11.87	135.47	120.51
1	A	48	ILE	C-N-CA	11.87	135.47	120.51
3	N	705	ALA	CA-C-N	-11.09	105.98	119.84
3	N	705	ALA	C-N-CA	-11.09	105.98	119.84
3	N	423	ASP	N-CA-C	10.95	124.25	111.11
3	D	423	ASP	N-CA-C	10.92	124.55	111.33
3	D	705	ALA	CA-C-N	-10.87	106.26	119.84
3	D	705	ALA	C-N-CA	-10.87	106.26	119.84
2	C	6	PHE	N-CA-C	10.38	124.06	111.40
2	M	6	PHE	N-CA-C	10.16	123.79	111.40
1	A	105	GLY	CA-C-N	9.98	132.32	119.84
1	A	105	GLY	C-N-CA	9.98	132.32	119.84
3	N	1209	LEU	N-CA-C	-9.83	95.13	110.36
2	C	726	ILE	CA-C-N	9.65	131.90	119.84
2	C	726	ILE	C-N-CA	9.65	131.90	119.84
3	N	1124	GLN	CA-C-N	9.60	131.84	119.84
3	N	1124	GLN	C-N-CA	9.60	131.84	119.84
3	D	1209	LEU	N-CA-C	-9.54	95.06	109.86
3	N	1213	ARG	CA-C-N	-9.54	111.05	120.21
3	N	1213	ARG	C-N-CA	-9.54	111.05	120.21
2	C	230	ARG	CA-C-N	9.53	131.75	119.84
2	C	230	ARG	C-N-CA	9.53	131.75	119.84
1	A	48	ILE	N-CA-C	9.52	117.87	109.02
1	B	105	GLY	CA-C-N	9.50	131.72	119.84
1	B	105	GLY	C-N-CA	9.50	131.72	119.84
1	K	105	GLY	CA-C-N	9.48	131.69	119.84
1	K	105	GLY	C-N-CA	9.48	131.69	119.84
3	D	1383	ASP	CA-C-N	9.44	130.02	119.92
3	D	1383	ASP	C-N-CA	9.44	130.02	119.92
5	F	91	VAL	CA-C-N	-9.33	111.17	120.31
5	F	91	VAL	C-N-CA	-9.33	111.17	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	105	GLY	CA-C-N	9.29	131.46	119.84
1	L	105	GLY	C-N-CA	9.29	131.46	119.84
3	N	171	LEU	CA-C-N	9.27	129.93	120.38
3	N	171	LEU	C-N-CA	9.27	129.93	120.38
2	M	726	ILE	CA-C-N	9.27	131.42	119.84
2	M	726	ILE	C-N-CA	9.27	131.42	119.84
2	M	1078	GLU	CA-C-N	9.22	131.37	119.84
2	M	1078	GLU	C-N-CA	9.22	131.37	119.84
5	P	91	VAL	CA-C-N	-9.21	111.28	120.31
5	P	91	VAL	C-N-CA	-9.21	111.28	120.31
3	D	561	GLY	CA-C-N	-9.11	111.95	122.52
3	D	561	GLY	C-N-CA	-9.11	111.95	122.52
3	D	171	LEU	CA-C-N	9.10	129.75	120.38
3	D	171	LEU	C-N-CA	9.10	129.75	120.38
4	O	49	GLN	N-CA-C	9.08	124.22	112.41
2	M	230	ARG	CA-C-N	9.04	131.15	119.84
2	M	230	ARG	C-N-CA	9.04	131.15	119.84
3	D	517	VAL	N-CA-C	9.01	115.76	107.56
3	N	1383	ASP	CA-C-N	9.00	129.55	119.92
3	N	1383	ASP	C-N-CA	9.00	129.55	119.92
3	N	80	VAL	CA-C-N	8.93	136.82	121.64
3	N	80	VAL	C-N-CA	8.93	136.82	121.64
3	D	1213	ARG	CA-C-N	-8.89	111.67	120.21
3	D	1213	ARG	C-N-CA	-8.89	111.67	120.21
4	E	49	GLN	N-CA-C	8.78	123.82	112.41
2	C	1078	GLU	CA-C-N	8.74	130.77	119.84
2	C	1078	GLU	C-N-CA	8.74	130.77	119.84
2	M	728	HIS	N-CA-C	8.74	124.07	113.41
2	C	728	HIS	N-CA-C	8.74	124.07	113.41
2	M	762	LYS	N-CA-C	8.73	120.48	110.97
5	F	296	GLY	CA-C-N	8.63	130.62	119.84
5	F	296	GLY	C-N-CA	8.63	130.62	119.84
2	C	535	SER	N-CA-C	8.56	115.69	108.07
3	N	380	GLU	N-CA-C	-8.49	95.07	109.24
3	D	187	LYS	N-CA-C	8.48	120.21	110.97
1	K	48	ILE	CA-C-N	8.41	129.06	120.14
1	K	48	ILE	C-N-CA	8.41	129.06	120.14
3	D	186	VAL	N-CA-C	8.20	119.08	111.45
3	D	172	PRO	CA-C-N	8.18	130.06	119.84
3	D	172	PRO	C-N-CA	8.18	130.06	119.84
3	N	186	VAL	N-CA-C	8.09	118.97	111.45
3	D	634	GLY	CA-C-N	8.05	129.91	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	634	GLY	C-N-CA	8.05	129.91	119.84
3	N	172	PRO	CA-C-N	8.03	129.88	119.84
3	N	172	PRO	C-N-CA	8.03	129.88	119.84
3	D	1285	GLU	N-CA-C	8.01	123.59	112.45
3	N	805	GLU	N-CA-C	8.00	121.45	112.97
2	M	317	VAL	CA-C-N	-7.93	110.78	119.19
2	M	317	VAL	C-N-CA	-7.93	110.78	119.19
3	D	380	GLU	N-CA-C	-7.86	96.11	109.24
2	M	39	ARG	N-CA-C	7.85	119.91	111.36
2	C	169	GLY	CA-C-N	7.83	129.63	119.84
2	C	169	GLY	C-N-CA	7.83	129.63	119.84
3	N	517	VAL	N-CA-C	7.82	115.30	107.55
3	D	199	LEU	N-CA-C	7.79	122.56	112.12
3	N	187	LYS	N-CA-C	7.76	119.43	110.97
2	C	163	ILE	N-CA-C	7.75	115.22	107.55
2	M	169	GLY	CA-C-N	7.72	129.49	119.84
2	M	169	GLY	C-N-CA	7.72	129.49	119.84
2	M	260	LEU	N-CA-C	7.69	123.33	111.56
5	P	296	GLY	CA-C-N	7.69	129.45	119.84
5	P	296	GLY	C-N-CA	7.69	129.45	119.84
3	N	198	ARG	CA-C-N	-7.68	110.34	122.17
3	N	198	ARG	C-N-CA	-7.68	110.34	122.17
3	N	198	ARG	N-CA-C	7.68	122.85	113.17
2	C	260	LEU	N-CA-C	7.67	123.30	111.56
3	D	80	VAL	CA-C-N	7.66	138.36	121.81
3	D	80	VAL	C-N-CA	7.66	138.36	121.81
2	C	317	VAL	CA-C-N	-7.55	111.18	119.19
2	C	317	VAL	C-N-CA	-7.55	111.18	119.19
2	M	163	ILE	N-CA-C	7.48	114.95	107.55
5	F	76	SER	N-CA-C	7.48	120.31	111.71
2	M	1027	PHE	N-CA-C	7.47	120.31	111.71
2	C	1027	PHE	N-CA-C	7.43	120.25	111.71
3	D	198	ARG	CA-C-N	-7.42	110.75	122.17
3	D	198	ARG	C-N-CA	-7.42	110.75	122.17
2	C	39	ARG	N-CA-C	7.38	119.41	111.36
3	D	80	VAL	N-CA-C	7.36	121.12	108.90
3	D	1109	GLU	N-CA-C	7.32	117.90	108.24
1	A	47	SER	N-CA-C	7.31	119.33	111.36
2	C	443	THR	CA-C-N	7.31	127.27	120.03
2	C	443	THR	C-N-CA	7.31	127.27	120.03
3	N	80	VAL	N-CA-C	7.29	120.98	108.95
3	D	198	ARG	N-CA-C	7.28	122.35	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	634	GLY	CA-C-N	7.27	128.93	119.84
3	N	634	GLY	C-N-CA	7.27	128.93	119.84
3	N	1109	GLU	N-CA-C	7.27	117.83	108.24
5	P	76	SER	N-CA-C	7.22	120.02	111.71
3	D	1124	GLN	CA-C-N	7.18	126.81	119.19
3	D	1124	GLN	C-N-CA	7.18	126.81	119.19
3	N	199	LEU	N-CA-C	7.18	121.74	112.12
1	K	47	SER	N-CA-C	7.15	119.16	111.36
2	C	373	VAL	N-CA-C	7.13	118.15	108.17
3	D	1110	ALA	N-CA-C	-7.12	98.19	109.23
2	C	547	ILE	CA-C-N	7.09	128.71	119.84
2	C	547	ILE	C-N-CA	7.09	128.71	119.84
2	C	191	PHE	CA-C-N	7.05	127.02	119.76
2	C	191	PHE	C-N-CA	7.05	127.02	119.76
3	N	1285	GLU	N-CA-C	6.99	121.93	113.41
3	D	1125	PRO	CA-C-N	-6.95	111.98	123.04
3	D	1125	PRO	C-N-CA	-6.95	111.98	123.04
2	M	938	LYS	N-CA-C	-6.94	103.77	111.82
2	C	762	LYS	N-CA-C	6.93	119.48	111.02
3	N	951	ILE	N-CA-C	-6.93	102.72	110.62
3	N	209	ARG	N-CA-C	6.89	125.48	110.80
2	C	318	PRO	N-CA-C	-6.84	104.61	113.57
3	D	238	PRO	N-CA-CB	6.83	110.43	103.25
2	M	1019	GLN	CA-C-N	6.83	127.23	119.93
2	M	1019	GLN	C-N-CA	6.83	127.23	119.93
3	D	1109	GLU	CA-C-N	6.82	133.54	122.29
3	D	1109	GLU	C-N-CA	6.82	133.54	122.29
2	C	535	SER	CA-C-N	-6.78	112.00	119.19
2	C	535	SER	C-N-CA	-6.78	112.00	119.19
2	M	443	THR	CA-C-N	6.77	126.73	120.03
2	M	443	THR	C-N-CA	6.77	126.73	120.03
3	D	28	LYS	CA-C-N	6.76	128.29	119.84
3	D	28	LYS	C-N-CA	6.76	128.29	119.84
2	C	58	ASP	CA-C-N	6.73	134.40	121.54
2	C	58	ASP	C-N-CA	6.73	134.40	121.54
2	M	365	ASP	N-CA-C	6.73	118.70	111.36
3	D	81	THR	N-CA-C	-6.73	98.30	108.46
3	D	1344	VAL	CB-CA-C	-6.71	103.11	111.70
3	D	53	ILE	N-CA-CB	-6.71	104.54	112.39
3	D	209	ARG	N-CA-C	6.69	125.06	110.80
1	L	47	SER	N-CA-C	6.67	118.35	111.14
2	M	729	LEU	N-CA-C	6.65	124.97	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	263	ASP	CA-C-N	-6.64	113.12	119.76
2	C	263	ASP	C-N-CA	-6.64	113.12	119.76
2	M	318	PRO	N-CA-C	-6.63	104.88	113.57
2	M	373	VAL	N-CA-C	6.63	117.45	108.17
2	C	399	ASN	CA-C-N	6.61	128.11	119.84
2	C	399	ASN	C-N-CA	6.61	128.11	119.84
3	N	238	PRO	N-CA-CB	6.61	110.19	103.25
2	C	938	LYS	N-CA-C	-6.55	104.22	111.82
3	N	486	ARG	N-CA-C	6.52	119.20	111.71
2	M	243	ARG	CA-C-N	6.50	127.96	119.84
2	M	243	ARG	C-N-CA	6.50	127.96	119.84
3	D	1251	ASP	N-CA-C	6.48	119.30	111.40
2	C	729	LEU	N-CA-C	6.47	124.58	110.80
5	P	283	GLY	N-CA-C	-6.45	106.34	115.30
1	B	47	SER	N-CA-C	6.43	118.08	111.14
2	M	263	ASP	CA-C-N	-6.43	113.33	119.76
2	M	263	ASP	C-N-CA	-6.43	113.33	119.76
2	C	591	SER	N-CA-C	-6.42	102.25	110.53
2	M	591	SER	N-CA-C	-6.42	102.25	110.53
2	C	365	ASP	N-CA-C	6.41	118.27	111.28
3	N	143	ASN	N-CA-C	-6.41	105.77	113.97
3	N	1128	VAL	N-CA-C	-6.40	100.72	109.55
3	N	593	ASN	CA-C-N	6.39	127.83	119.84
3	N	593	ASN	C-N-CA	6.39	127.83	119.84
3	N	1109	GLU	CA-C-N	6.39	133.36	122.37
3	N	1109	GLU	C-N-CA	6.39	133.36	122.37
3	N	1116	ASN	N-CA-C	-6.39	97.87	108.34
5	F	283	GLY	N-CA-C	-6.38	106.43	115.30
2	M	58	ASP	CA-C-N	6.38	133.72	121.54
2	M	58	ASP	C-N-CA	6.38	133.72	121.54
3	N	1110	ALA	N-CA-C	-6.35	98.26	109.06
1	L	172	SER	CA-C-N	-6.35	113.27	119.87
1	L	172	SER	C-N-CA	-6.35	113.27	119.87
3	N	798	GLU	N-CA-C	6.34	120.66	111.02
3	N	82	LYS	CA-C-N	-6.33	109.45	121.54
3	N	82	LYS	C-N-CA	-6.33	109.45	121.54
3	D	248	PRO	N-CA-CB	6.32	109.84	102.76
1	L	171	PHE	CA-C-N	-6.27	111.18	122.28
1	L	171	PHE	C-N-CA	-6.27	111.18	122.28
2	C	1019	GLN	CA-C-N	6.27	126.64	119.93
2	C	1019	GLN	C-N-CA	6.27	126.64	119.93
2	M	442	GLU	N-CA-C	6.23	118.59	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	226	PRO	N-CA-CB	6.22	109.41	103.19
3	D	593	ASN	CA-C-N	6.22	127.61	119.84
3	D	593	ASN	C-N-CA	6.22	127.61	119.84
4	O	41	GLU	N-CA-C	6.22	120.68	112.35
3	D	208	PRO	CA-C-N	6.21	133.40	121.54
3	D	208	PRO	C-N-CA	6.21	133.40	121.54
2	M	755	LEU	N-CA-C	-6.20	105.85	113.41
3	D	798	GLU	N-CA-C	6.20	120.44	111.02
2	C	330	ASN	N-CA-C	-6.18	106.28	113.88
3	D	1128	VAL	N-CA-C	-6.18	101.03	109.55
3	N	248	PRO	N-CA-CB	6.16	109.66	102.76
3	N	81	THR	N-CA-C	-6.14	98.25	108.32
3	D	143	ASN	N-CA-C	-6.12	106.14	113.97
3	N	1251	ASP	N-CA-C	6.08	118.82	111.40
2	C	151	ASP	CA-C-N	6.08	127.44	119.84
2	C	151	ASP	C-N-CA	6.08	127.44	119.84
3	D	1116	ASN	N-CA-C	-6.05	98.42	108.34
3	N	726	ILE	CB-CA-C	-6.04	102.79	111.19
5	P	287	THR	N-CA-C	-6.04	102.56	110.53
2	C	58	ASP	N-CA-C	6.03	119.37	108.69
3	D	208	PRO	CA-N-CD	-6.01	103.59	112.00
3	D	199	LEU	CA-CB-CG	-6.00	95.30	116.30
1	K	48	ILE	N-CA-C	5.98	115.48	108.96
2	C	1118	LYS	N-CA-C	5.98	119.57	109.76
2	C	165	LEU	CA-C-N	5.96	141.31	127.00
2	C	165	LEU	C-N-CA	5.96	141.31	127.00
4	E	51	LEU	N-CA-C	-5.94	100.03	108.23
2	M	58	ASP	N-CA-C	5.93	119.19	108.69
3	D	486	ARG	N-CA-C	5.92	119.60	112.38
3	N	422	ALA	CA-C-N	5.91	128.51	120.54
3	N	422	ALA	C-N-CA	5.91	128.51	120.54
3	D	1317	ASP	CA-C-N	5.90	129.66	120.75
3	D	1317	ASP	C-N-CA	5.90	129.66	120.75
2	C	9	ILE	N-CA-C	-5.89	99.05	107.77
4	O	51	LEU	N-CA-C	-5.89	100.09	108.23
2	M	547	ILE	CA-C-N	5.84	127.14	119.84
2	M	547	ILE	C-N-CA	5.84	127.14	119.84
5	F	340	SER	CA-C-N	5.84	127.14	119.84
5	F	340	SER	C-N-CA	5.84	127.14	119.84
3	D	79	GLU	CA-C-N	-5.83	114.41	122.69
3	D	79	GLU	C-N-CA	-5.83	114.41	122.69
3	N	28	LYS	CA-C-N	5.82	127.12	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	28	LYS	C-N-CA	5.82	127.12	119.84
3	N	589	ALA	CA-C-N	5.82	125.73	119.85
3	N	589	ALA	C-N-CA	5.82	125.73	119.85
2	M	165	LEU	C-N-CD	-5.82	107.80	120.60
3	D	1472	ILE	CA-C-N	5.82	125.68	119.28
3	D	1472	ILE	C-N-CA	5.82	125.68	119.28
3	D	54	LYS	N-CA-C	5.82	118.13	108.13
2	M	165	LEU	CA-C-N	5.80	140.91	127.00
2	M	165	LEU	C-N-CA	5.80	140.91	127.00
3	D	1126	ASP	N-CA-C	5.78	120.50	108.53
2	C	315	ALA	N-CA-C	5.77	119.63	112.59
2	M	18	LEU	N-CA-C	5.74	118.28	111.33
4	E	57	ASP	CA-C-N	-5.74	112.67	119.84
4	E	57	ASP	C-N-CA	-5.74	112.67	119.84
2	C	728	HIS	CA-C-N	-5.73	110.59	121.54
2	C	728	HIS	C-N-CA	-5.73	110.59	121.54
2	M	213	ALA	N-CA-C	-5.73	105.11	111.36
5	F	287	THR	N-CA-C	-5.70	103.01	110.53
2	C	243	ARG	CA-C-N	5.70	126.96	119.84
2	C	243	ARG	C-N-CA	5.70	126.96	119.84
5	F	285	GLU	CA-C-N	5.69	126.95	119.84
5	F	285	GLU	C-N-CA	5.69	126.95	119.84
5	P	285	GLU	CA-C-N	5.68	126.94	119.84
5	P	285	GLU	C-N-CA	5.68	126.94	119.84
3	D	422	ALA	CA-C-N	5.66	128.14	120.38
3	D	422	ALA	C-N-CA	5.66	128.14	120.38
3	D	592	THR	N-CA-C	-5.65	103.08	110.53
1	B	47	SER	CA-C-O	-5.64	114.89	120.70
3	N	592	THR	N-CA-C	-5.64	103.09	110.53
3	D	617	ASN	N-CA-C	-5.63	106.36	113.18
2	C	213	ALA	N-CA-C	-5.63	105.14	111.28
3	N	208	PRO	CA-C-N	5.62	132.27	121.54
3	N	208	PRO	C-N-CA	5.62	132.27	121.54
2	M	508	ILE	N-CA-C	-5.61	103.87	110.21
2	C	796	GLU	N-CA-C	5.61	116.78	108.60
3	N	1476	THR	N-CA-C	-5.60	105.71	112.54
3	N	208	PRO	CA-N-CD	-5.60	104.17	112.00
2	M	728	HIS	CA-C-O	-5.59	113.09	119.41
3	D	379	ALA	N-CA-C	-5.58	104.21	111.02
3	N	226	PRO	N-CA-CB	5.58	108.77	103.19
3	D	863	VAL	CB-CA-C	-5.58	105.89	111.80
2	M	318	PRO	CA-C-N	5.56	131.47	120.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	318	PRO	C-N-CA	5.56	131.47	120.84
3	D	406	ASP	N-CA-C	5.56	119.77	113.15
1	L	2	LEU	N-CA-C	5.54	119.81	112.72
2	C	679	PHE	CA-C-O	-5.53	114.11	121.46
3	D	1476	THR	N-CA-C	-5.53	106.38	113.01
3	N	1317	ASP	CA-C-N	5.51	129.07	120.75
3	N	1317	ASP	C-N-CA	5.51	129.07	120.75
1	L	91	ASN	N-CA-C	5.50	114.64	108.25
2	C	318	PRO	CA-C-N	5.50	131.34	120.84
2	C	318	PRO	C-N-CA	5.50	131.34	120.84
2	M	727	PRO	CA-C-N	-5.49	112.26	122.09
2	M	727	PRO	C-N-CA	-5.49	112.26	122.09
2	M	608	GLY	N-CA-C	-5.47	106.26	115.62
3	N	373	PRO	N-CA-CB	5.47	109.00	103.25
5	F	88	ILE	CB-CA-C	-5.47	104.67	112.22
3	D	1469	GLY	N-CA-C	-5.46	106.67	115.08
2	C	506	ASN	N-CA-C	-5.45	106.30	113.17
3	D	915	VAL	CB-CA-C	-5.45	104.72	111.70
5	P	340	SER	CA-C-N	5.45	126.65	119.84
5	P	340	SER	C-N-CA	5.45	126.65	119.84
3	D	1109	GLU	CA-C-O	5.45	126.77	121.05
3	N	1331	ASP	CA-C-N	5.43	125.51	119.32
3	N	1331	ASP	C-N-CA	5.43	125.51	119.32
4	O	47	LYS	N-CA-C	5.42	117.33	108.55
2	M	728	HIS	CA-C-N	-5.42	111.19	121.54
2	M	728	HIS	C-N-CA	-5.42	111.19	121.54
2	M	810	ASP	CA-C-N	5.42	126.61	119.84
2	M	810	ASP	C-N-CA	5.42	126.61	119.84
1	B	2	LEU	N-CA-C	5.41	119.65	112.72
2	M	261	ILE	N-CA-C	5.40	120.57	109.34
2	M	1118	LYS	N-CA-C	5.40	118.61	109.76
2	C	684	PHE	CA-C-N	-5.38	112.48	122.60
2	C	684	PHE	C-N-CA	-5.38	112.48	122.60
2	M	253	ALA	N-CA-C	5.38	117.00	111.03
4	O	57	ASP	CA-C-N	-5.38	113.12	119.84
4	O	57	ASP	C-N-CA	-5.38	113.12	119.84
2	C	261	ILE	N-CA-C	5.37	120.51	109.34
3	D	726	ILE	CB-CA-C	-5.37	103.73	111.19
3	D	1317	ASP	N-CA-C	5.37	118.40	110.46
3	N	1371	VAL	CB-CA-C	-5.36	104.95	111.87
3	N	133	ILE	N-CA-C	5.35	116.48	109.58
3	D	373	PRO	N-CA-CB	5.34	108.86	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	79	GLU	CA-C-N	-5.34	114.24	122.68
3	N	79	GLU	C-N-CA	-5.34	114.24	122.68
3	N	1190	SER	N-CA-C	5.34	112.94	108.13
3	N	824	ASN	N-CA-C	5.34	117.91	111.40
3	D	1190	SER	CA-C-N	5.31	124.94	119.05
3	D	1190	SER	C-N-CA	5.31	124.94	119.05
2	M	18	LEU	CA-C-N	-5.30	113.45	122.56
2	M	18	LEU	C-N-CA	-5.30	113.45	122.56
2	C	291	ALA	N-CA-C	5.29	118.06	109.06
2	M	730	SER	N-CA-C	5.28	117.28	108.99
3	D	810	GLU	N-CA-C	-5.26	106.70	113.23
3	D	1043	GLY	CA-C-N	-5.26	115.35	122.77
3	D	1043	GLY	C-N-CA	-5.26	115.35	122.77
3	D	561	GLY	N-CA-C	-5.25	103.22	111.00
3	N	379	ALA	N-CA-C	-5.25	104.61	111.02
2	C	1110	ASP	N-CA-C	5.24	116.94	108.34
3	N	811	GLU	N-CA-C	-5.24	106.39	112.89
3	N	406	ASP	N-CA-C	5.24	119.39	113.15
3	N	1114	THR	CA-C-N	-5.24	115.56	122.85
3	N	1114	THR	C-N-CA	-5.24	115.56	122.85
1	B	91	ASN	CA-C-N	5.23	126.38	119.84
1	B	91	ASN	C-N-CA	5.23	126.38	119.84
5	F	333	ILE	CB-CA-C	-5.23	106.08	110.94
3	D	811	GLU	N-CA-C	-5.23	106.41	112.89
4	O	50	THR	CA-C-N	5.22	132.18	121.95
4	O	50	THR	C-N-CA	5.22	132.18	121.95
1	A	91	ASN	CA-C-N	5.22	126.36	119.84
1	A	91	ASN	C-N-CA	5.22	126.36	119.84
3	D	1460	ILE	N-CA-C	-5.21	101.47	108.35
3	D	1091	SER	N-CA-C	-5.20	105.61	111.28
2	M	291	ALA	N-CA-C	5.20	117.91	109.06
4	E	50	THR	CA-C-N	5.19	132.12	121.95
4	E	50	THR	C-N-CA	5.19	132.12	121.95
2	C	810	ASP	CA-C-N	5.19	126.32	119.84
2	C	810	ASP	C-N-CA	5.19	126.32	119.84
3	N	108	VAL	CA-C-N	-5.18	113.36	119.84
3	N	108	VAL	C-N-CA	-5.18	113.36	119.84
3	N	810	GLU	N-CA-C	-5.18	106.80	113.23
3	N	1209	LEU	CA-C-O	-5.18	115.55	121.82
3	N	201	GLY	N-CA-C	-5.18	100.77	110.77
1	A	2	LEU	N-CA-C	5.16	119.32	112.72
2	C	730	SER	N-CA-C	5.14	117.06	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	393	ILE	CB-CA-C	-5.14	105.07	111.08
2	C	685	GLU	N-CA-C	-5.13	105.85	112.68
3	D	380	GLU	CA-C-O	-5.12	114.77	120.66
3	N	246	PRO	N-CA-CB	5.12	108.62	103.25
3	N	1127	GLU	N-CA-C	-5.12	99.90	110.80
1	K	2	LEU	N-CA-C	5.11	119.26	112.72
3	D	201	GLY	N-CA-C	-5.11	101.08	113.18
3	D	21	TRP	CA-CB-CG	5.10	123.29	113.60
2	M	1110	ASP	N-CA-C	5.09	116.69	108.34
2	M	243	ARG	N-CA-C	5.09	121.06	109.81
3	N	76	CYS	CA-CB-SG	5.09	126.11	114.40
3	N	1043	GLY	CA-C-N	-5.09	115.60	122.77
3	N	1043	GLY	C-N-CA	-5.09	115.60	122.77
2	M	1057	SER	CA-C-N	-5.08	114.26	122.24
2	M	1057	SER	C-N-CA	-5.08	114.26	122.24
3	N	199	LEU	CA-C-N	-5.07	114.43	121.99
3	N	199	LEU	C-N-CA	-5.07	114.43	121.99
2	C	795	GLY	N-CA-C	-5.07	101.16	113.18
3	D	805	GLU	N-CA-C	5.06	121.58	110.80
3	D	824	ASN	N-CA-C	5.06	117.91	111.69
3	D	396	VAL	N-CA-C	5.06	116.53	109.55
2	C	737	LEU	N-CA-C	-5.05	101.36	109.39
2	M	315	ALA	N-CA-C	5.05	118.75	112.59
2	M	151	ASP	CA-C-N	5.05	126.15	119.84
2	M	151	ASP	C-N-CA	5.05	126.15	119.84
4	O	93	TYR	CA-C-N	5.04	126.15	120.66
4	O	93	TYR	C-N-CA	5.04	126.15	120.66
3	D	561	GLY	CA-C-O	-5.03	116.10	122.39
2	M	679	PHE	CA-C-O	-5.03	115.21	121.55
2	M	685	GLU	N-CA-C	-5.02	106.00	112.68
3	N	1328	GLY	N-CA-C	5.02	116.43	111.21
2	C	728	HIS	CA-C-O	-5.01	113.75	119.41

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	N	132	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1806	0	1861	219	0
1	B	1806	0	1861	208	0
1	K	1806	0	1861	212	0
1	L	1806	0	1861	208	0
2	C	8829	0	8933	1217	0
2	M	8829	0	8933	1131	0
3	D	10797	0	10873	1489	0
3	N	10797	0	10873	1385	0
4	E	769	0	775	99	0
4	O	769	0	775	113	0
5	F	2771	0	2844	345	0
5	P	2771	0	2844	346	0
6	D	2	0	0	0	0
6	N	2	0	0	0	0
7	D	1	0	0	0	0
7	N	1	0	0	0	0
8	A	191	0	0	37	0
8	B	181	0	0	35	0
8	C	767	0	0	175	0
8	D	1100	0	0	235	0
8	E	93	0	0	14	0
8	F	333	0	0	58	0
8	K	151	0	0	30	0
8	L	179	0	0	49	0
8	M	739	0	0	195	0
8	N	1038	0	0	224	0
8	O	78	0	0	24	0
8	P	267	0	0	62	0
All	All	58679	0	54294	6567	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 61.

All (6567) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:1054:THR:HG21	2:M:1079:PRO:HB3	1.28	1.11
1:A:95:GLN:HA	1:A:146:ARG:HH12	1.12	1.08
2:C:135:VAL:HG11	2:C:407:LYS:HA	1.36	1.04
1:A:42:ARG:HH12	2:C:857:ASP:HB3	1.14	1.04
3:N:1036:ARG:HH21	3:N:1042:ARG:HA	1.20	1.04
3:N:1481:VAL:HG13	4:O:18:ARG:HE	1.16	1.02
3:D:197:SER:HB3	3:D:203:ALA:HB3	1.42	1.02
3:N:197:SER:HB3	3:N:203:ALA:HB3	1.41	1.02
2:M:169:GLY:HA2	2:M:263:ASP:HB3	1.42	1.01
2:C:358:ARG:HH22	2:C:374:ASN:HB3	1.26	1.00
2:C:979:THR:HG23	2:C:981:GLU:H	1.26	1.00
2:C:328:LEU:HD13	2:C:433:THR:HB	1.41	0.99
3:N:1101:VAL:HG21	3:N:1424:VAL:HG22	1.40	0.99
3:D:1045:MET:HG2	3:D:1073:SER:HA	1.41	0.99
2:C:110:GLU:HG2	2:C:369:PRO:HB3	1.41	0.98
3:D:1376:MET:HE3	3:D:1421:LEU:HB2	1.44	0.98
2:M:409:ARG:HA	2:M:454:SER:HA	1.44	0.98
3:N:52:PRO:HB2	3:N:80:VAL:HG13	1.45	0.98
3:N:1144:LEU:HD12	3:N:1171:VAL:HG13	1.44	0.98
2:M:157:ARG:HD2	2:M:314:THR:HG22	1.46	0.98
2:C:1114:GLY:H	2:C:1115:LEU:HD12	1.27	0.97
2:C:47:ALA:HB1	2:C:345:ARG:HB3	1.47	0.97
2:C:281:LEU:HD11	2:C:306:THR:HA	1.47	0.97
3:D:141:ILE:HG12	3:D:449:SER:HA	1.46	0.97
2:C:1008:ARG:HH21	2:C:1028:GLY:HA2	1.30	0.96
2:M:129:ILE:HD13	2:M:134:ARG:HB2	1.46	0.96
5:P:347:GLN:HA	5:P:350:LEU:HD22	1.47	0.96
3:D:422:ALA:HB3	3:D:427:VAL:HG22	1.45	0.96
2:M:110:GLU:HG2	2:M:369:PRO:HG3	1.46	0.96
1:K:89:PHE:HB2	1:K:94:LEU:HD13	1.48	0.96
2:C:630:ARG:HH21	2:C:705:ILE:HG22	1.27	0.95
3:N:1432:LYS:HD2	3:N:1433:SER:H	1.29	0.95
2:M:405:ARG:HG2	2:M:409:ARG:HH21	1.29	0.95
2:C:719:PRO:HB3	2:C:820:ARG:HE	1.29	0.95
2:C:773:LEU:HB2	5:F:373:LYS:HB3	1.47	0.95
2:C:332:ARG:HH11	2:C:332:ARG:HB3	1.32	0.95
5:P:88:ILE:HD13	5:P:193:ARG:HB2	1.45	0.95
5:P:164:LYS:HA	5:P:171:LYS:HE2	1.49	0.94
2:C:1090:LYS:HZ2	3:D:90:MET:HG3	1.31	0.93
3:N:55:ASP:HA	3:N:82:LYS:HG3	1.48	0.93
2:C:150:PRO:HA	2:C:158:TYR:HB3	1.50	0.93
1:A:95:GLN:HG2	1:A:146:ARG:HH22	1.33	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:517:ARG:HH11	2:C:522:VAL:HG11	1.33	0.93
2:C:1054:THR:HG21	2:C:1079:PRO:HB3	1.46	0.93
2:M:16:PRO:HB3	2:M:460:ARG:HH22	1.33	0.93
3:N:422:ALA:HB3	3:N:427:VAL:HG22	1.50	0.93
2:M:564:MET:HG3	2:M:997:LEU:HD21	1.50	0.93
4:E:67:GLU:HB2	4:E:73:LEU:HD11	1.51	0.93
3:D:493:ARG:HH21	3:D:1388:ARG:HB3	1.30	0.93
2:C:479:VAL:HG21	2:C:503:LEU:HD11	1.51	0.92
3:D:1101:VAL:HG21	3:D:1424:VAL:HG22	1.52	0.92
3:N:500:ARG:HH12	3:N:1388:ARG:HH11	1.13	0.92
3:D:698:LYS:HA	3:D:756:GLN:HE22	1.32	0.92
3:D:18:ILE:HG23	3:D:518:PRO:HG3	1.51	0.92
1:A:14:ARG:HH21	1:A:22:GLU:HB3	1.32	0.92
3:D:654:LYS:HB3	3:D:655:PRO:HD3	1.52	0.92
1:K:19:GLU:HB3	1:K:175:ARG:HH22	1.34	0.92
2:C:1005:MET:HE1	3:D:648:MET:HB2	1.51	0.91
1:B:179:PHE:HB3	1:B:197:LEU:HD12	1.51	0.91
4:O:47:LYS:HA	8:O:4983:HOH:O	1.68	0.91
3:D:1066:THR:HG23	3:D:1069:GLU:H	1.34	0.91
3:D:630:VAL:HA	3:D:744:GLN:HG2	1.51	0.91
3:D:400:VAL:HG21	3:D:441:ARG:HH11	1.35	0.91
5:P:394:ARG:HA	5:P:397:ILE:HD12	1.51	0.91
3:D:908:LYS:HB3	3:D:1027:GLY:HA3	1.51	0.91
3:N:422:ALA:HB1	5:P:178:ARG:HH12	1.34	0.91
1:K:227:ASN:HD22	1:K:227:ASN:H	1.15	0.91
5:P:266:GLU:HA	5:P:269:ASN:HD22	1.35	0.91
1:B:152:PRO:HD2	1:B:155:LYS:HD3	1.51	0.91
2:C:282:GLY:HA2	2:C:308:ARG:HH22	1.32	0.90
3:D:143:ASN:HD21	3:D:145:VAL:HG12	1.35	0.90
2:M:92:ALA:HB2	2:M:120:LEU:HD11	1.53	0.90
2:C:724:ARG:HG3	2:C:741:GLY:H	1.36	0.90
3:D:118:LEU:HB3	3:D:123:LEU:HD22	1.54	0.90
5:F:268:ILE:HA	5:F:271:LEU:HD12	1.53	0.90
2:M:1111:ILE:HD12	2:M:1112:PHE:H	1.36	0.90
3:N:133:ILE:HG21	3:N:454:ALA:HB1	1.53	0.90
2:C:274:ARG:HD2	2:C:285:LEU:HB3	1.53	0.90
3:D:12:LEU:HD13	3:D:511:TRP:HB2	1.53	0.90
3:N:658:LEU:HA	3:N:661:MET:HE3	1.54	0.90
2:C:860:HIS:HB2	8:C:1175:HOH:O	1.72	0.89
5:F:392:VAL:HG11	5:F:396:ARG:HD2	1.55	0.89
3:N:9:ARG:HH12	3:N:506:GLY:HA2	1.37	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:131:LYS:HG3	3:N:568:ARG:HG2	1.53	0.89
3:N:928:ALA:HA	3:N:931:LEU:HD12	1.55	0.89
2:C:905:ILE:HD12	2:C:905:ILE:H	1.37	0.89
3:D:493:ARG:NH2	3:D:1388:ARG:HB3	1.87	0.89
3:N:787:LEU:HD11	3:N:947:ILE:HG12	1.53	0.89
2:M:150:PRO:HA	2:M:158:TYR:HB3	1.54	0.89
3:N:1290:LEU:HD23	3:N:1291:SER:H	1.37	0.89
3:D:119:SER:HB2	3:D:123:LEU:H	1.38	0.88
2:M:176:VAL:HG12	2:M:182:VAL:HG13	1.53	0.88
2:M:1054:THR:HG22	2:M:1059:ASP:HB2	1.55	0.88
2:M:979:THR:HG23	2:M:981:GLU:H	1.38	0.88
2:C:478:VAL:HG13	2:C:506:ASN:HB3	1.54	0.88
3:N:633:VAL:HG22	3:N:635:PRO:HD3	1.54	0.88
1:K:186:LEU:HB2	1:K:192:LEU:HD11	1.56	0.88
2:M:861:LEU:HD23	2:M:862:PRO:HD2	1.56	0.88
3:N:699:VAL:H	3:N:756:GLN:NE2	1.72	0.88
1:L:126:ASP:HA	8:L:4849:HOH:O	1.72	0.88
3:D:667:ALA:HB2	3:D:676:MET:HE2	1.56	0.88
3:N:565:ILE:H	3:N:565:ILE:HD12	1.39	0.88
3:N:141:ILE:HG12	3:N:449:SER:HA	1.54	0.88
3:D:191:LEU:HD12	3:D:211:VAL:HG21	1.54	0.87
3:N:1476:THR:HG23	4:O:21:VAL:HG22	1.56	0.87
5:F:76:SER:O	5:F:80:PRO:HD2	1.73	0.87
5:F:350:LEU:HD12	5:F:422:LEU:HD12	1.56	0.87
1:B:24:VAL:HG13	1:B:196:THR:HG22	1.55	0.87
3:D:136:ASP:HB3	3:D:137:PRO:HD3	1.57	0.87
2:C:1095:LEU:HD11	3:D:607:LEU:HD11	1.54	0.87
3:D:145:VAL:HG22	3:D:146:PRO:HD2	1.54	0.87
2:M:689:VAL:HB	2:M:870:ILE:HG13	1.56	0.87
2:M:704:HIS:HB2	2:M:831:ARG:HE	1.40	0.87
2:M:904:PRO:HD2	2:M:908:GLY:HA2	1.57	0.86
2:C:689:VAL:HB	2:C:870:ILE:HG13	1.58	0.86
3:D:1087:ARG:HG2	3:D:1234:THR:HA	1.54	0.86
3:N:536:ALA:HA	5:P:315:VAL:H	1.40	0.86
3:N:535:PHE:HB3	5:P:314:PRO:HB3	1.55	0.86
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.57	0.86
2:C:1090:LYS:HE2	2:C:1112:PHE:HE1	1.39	0.86
2:M:614:ARG:HD2	2:M:620:LEU:HD12	1.54	0.86
1:B:87:VAL:HG21	1:B:144:VAL:HG11	1.58	0.86
1:B:41:ARG:HG3	1:B:177:VAL:HG21	1.57	0.85
2:C:376:ARG:HH22	5:F:285:GLU:HB3	1.40	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:148:GLU:HB3	3:D:151:GLN:HB2	1.58	0.85
3:N:838:ARG:HA	8:N:9349:HOH:O	1.76	0.85
2:C:145:GLY:H	2:C:163:ILE:HG23	1.41	0.85
3:N:817:GLU:HG3	3:N:839:LEU:HD13	1.57	0.85
1:A:54:THR:HG23	1:A:158:ILE:HG13	1.59	0.85
3:D:1330:ILE:HA	8:D:9063:HOH:O	1.75	0.85
5:F:273:ARG:HA	5:F:276:ARG:HD2	1.59	0.85
3:D:1096:ARG:HH11	3:D:1096:ARG:HB2	1.39	0.85
2:M:772:ARG:HD2	5:P:373:LYS:HD2	1.59	0.85
2:C:701:THR:HG23	2:C:832:LYS:HG3	1.59	0.85
2:M:139:GLN:HE21	2:M:334:ARG:HH11	1.22	0.85
2:C:597:ALA:HB2	2:C:655:LEU:HD21	1.55	0.85
8:C:1350:HOH:O	3:D:532:GLY:HA2	1.76	0.85
3:D:800:LYS:HE3	3:D:830:ALA:HB3	1.58	0.85
1:L:87:VAL:HG21	1:L:144:VAL:HG11	1.60	0.84
1:L:57:TYR:HB3	1:L:141:GLU:HG3	1.57	0.84
1:A:145:ASP:HB3	8:A:330:HOH:O	1.76	0.84
3:D:615:ARG:HH21	3:D:619:LEU:HD12	1.40	0.84
3:N:971:LEU:HA	3:N:974:ILE:HD12	1.59	0.84
3:N:1481:VAL:HG11	4:O:18:ARG:HA	1.58	0.84
1:B:103:ALA:HB1	1:B:107:LYS:HE3	1.57	0.84
2:M:512:ARG:HB3	2:M:523:ILE:HD11	1.59	0.84
2:C:768:THR:HB	2:C:771:GLU:HB3	1.60	0.84
2:M:274:ARG:HD2	2:M:285:LEU:HD22	1.58	0.84
3:N:661:MET:HE1	3:N:677:LEU:HD11	1.59	0.84
3:N:1422:MET:HE2	3:N:1427:SER:HA	1.60	0.84
1:A:206:THR:HG22	1:A:209:GLU:H	1.43	0.84
2:M:115:LEU:HD22	2:M:373:VAL:HG11	1.57	0.84
5:P:132:ARG:HH21	5:P:184:ARG:HH12	1.25	0.84
1:A:95:GLN:HA	1:A:146:ARG:NH1	1.92	0.84
3:D:1438:ALA:O	3:D:1443:THR:HG22	1.77	0.84
1:L:180:GLN:HB2	1:L:198:ARG:HH22	1.43	0.84
3:N:186:VAL:HG21	3:N:213:VAL:HB	1.59	0.84
2:C:129:ILE:HD13	2:C:134:ARG:HB2	1.60	0.83
2:C:579:VAL:HB	2:C:890:LEU:HD22	1.61	0.83
2:C:724:ARG:HH12	2:C:734:LEU:HD23	1.42	0.83
3:D:397:LYS:HE2	3:D:399:ARG:HE	1.44	0.83
5:F:363:GLU:HA	5:F:367:MET:HE3	1.60	0.83
5:P:358:LEU:HD13	5:P:370:LYS:HG3	1.59	0.83
2:C:126:SER:HB3	2:C:407:LYS:HE3	1.60	0.83
1:K:24:VAL:HG22	1:K:196:THR:HB	1.58	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:260:LEU:HG	2:M:261:ILE:HG13	1.60	0.83
2:M:710:ILE:HB	2:M:790:LEU:HD12	1.58	0.83
1:B:86:VAL:HG12	1:B:124:ASN:HD22	1.44	0.83
2:C:500:ASN:HD21	3:D:1067:VAL:HG23	1.42	0.83
3:D:520:LEU:HD12	3:D:521:PRO:HD2	1.60	0.83
3:D:1057:VAL:HG13	3:D:1069:GLU:HB3	1.60	0.83
1:K:78:ILE:HA	1:K:81:ASN:ND2	1.93	0.83
3:D:928:ALA:HA	3:D:931:LEU:HD12	1.59	0.83
1:A:87:VAL:HG21	1:A:144:VAL:HG11	1.61	0.83
1:K:89:PHE:HZ	1:K:146:ARG:HB2	1.43	0.83
3:N:212:ARG:HD3	3:N:445:ARG:HH12	1.43	0.83
3:D:1481:VAL:HG11	4:E:18:ARG:HA	1.61	0.83
5:F:394:ARG:HA	5:F:397:ILE:HD12	1.59	0.83
2:M:380:ALA:HA	2:M:383:ARG:HD2	1.61	0.83
3:N:704:ARG:HD2	3:N:705:ALA:H	1.43	0.83
2:C:578:VAL:HG11	2:C:991:GLN:HB3	1.60	0.82
1:K:87:VAL:HG21	1:K:144:VAL:HG11	1.61	0.82
2:C:1097:LEU:HD22	2:C:1097:LEU:H	1.44	0.82
3:D:1095:THR:O	3:D:1099:VAL:HG23	1.78	0.82
3:N:139:GLY:HA3	3:N:452:ILE:HD12	1.62	0.82
3:D:573:MET:HE3	5:F:210:LEU:HB3	1.59	0.82
3:D:1141:GLU:HG2	3:D:1168:MET:HE2	1.60	0.82
5:F:85:LEU:HA	5:F:88:ILE:HD12	1.59	0.82
1:L:56:VAL:HG13	1:L:142:VAL:HG12	1.62	0.82
2:M:534:VAL:H	2:M:538:GLN:HE22	1.27	0.82
3:N:422:ALA:H	3:N:427:VAL:HG11	1.44	0.82
5:P:166:LEU:HB3	5:P:170:HIS:HB2	1.61	0.82
2:C:232:GLU:HA	2:C:235:LEU:HD12	1.58	0.82
2:M:1009:SER:HB2	3:N:651:GLU:O	1.80	0.82
3:N:907:GLU:HA	8:N:9094:HOH:O	1.78	0.82
1:A:186:LEU:HB2	1:A:192:LEU:HD11	1.60	0.82
2:C:25:SER:HB2	2:C:335:THR:HB	1.62	0.82
3:D:187:LYS:HE2	3:D:213:VAL:HG12	1.62	0.82
2:M:1051:GLU:HG2	2:M:1056:LYS:HE3	1.61	0.82
5:F:125:ASP:HA	5:F:128:ARG:NH1	1.95	0.82
5:P:406:ARG:HA	5:P:409:LYS:HG2	1.60	0.82
2:C:176:VAL:HG12	2:C:182:VAL:HG13	1.62	0.81
1:L:65:PHE:HD1	3:N:813:LEU:HD22	1.45	0.81
2:M:905:ILE:H	2:M:905:ILE:HD12	1.43	0.81
1:A:8:ALA:HB1	1:B:224:TYR:HE1	1.44	0.81
2:C:802:ARG:HG2	2:C:826:TYR:HB2	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:785:ILE:H	3:D:785:ILE:HD12	1.44	0.81
3:N:628:ARG:HD3	3:N:744:GLN:HE22	1.45	0.81
2:C:675:ALA:HB2	2:C:867:VAL:HG11	1.61	0.81
3:N:420:VAL:HA	5:P:164:LYS:HD3	1.61	0.81
3:N:187:LYS:HE2	3:N:213:VAL:HG12	1.62	0.81
2:C:710:ILE:HB	2:C:790:LEU:HD13	1.61	0.81
3:D:1310:ARG:H	3:D:1310:ARG:HD3	1.46	0.81
1:A:42:ARG:NH1	2:C:857:ASP:HB3	1.94	0.81
2:C:313:LEU:HA	2:C:321:GLU:HG3	1.63	0.81
3:D:179:VAL:HG13	3:D:389:GLU:HG3	1.62	0.81
3:D:1262:LEU:HD23	3:D:1352:ILE:HG13	1.61	0.81
2:M:1096:ALA:O	3:N:13:ALA:HB2	1.80	0.81
2:C:873:PRO:HG2	3:D:947:ILE:HD12	1.62	0.81
2:M:328:LEU:HD22	2:M:433:THR:HG22	1.63	0.81
3:N:1045:MET:HG2	3:N:1073:SER:HA	1.62	0.81
3:N:906:GLN:HB3	3:N:911:LEU:HD11	1.61	0.81
4:O:12:MET:HB3	8:O:3864:HOH:O	1.81	0.80
2:C:367:LEU:HD22	2:C:371:LYS:HG2	1.63	0.80
3:D:611:GLN:HA	3:D:615:ARG:HD2	1.62	0.80
3:N:475:LYS:HA	3:N:478:LEU:HD12	1.64	0.80
3:N:865:THR:HG23	3:N:874:GLU:HG3	1.63	0.80
3:D:87:ARG:HA	8:D:9040:HOH:O	1.81	0.80
1:L:32:PHE:HB2	8:L:4886:HOH:O	1.81	0.80
5:P:120:THR:HG22	5:P:122:LEU:HD13	1.63	0.80
3:N:500:ARG:NH1	3:N:1388:ARG:HH11	1.79	0.80
2:C:281:LEU:HD12	2:C:309:TYR:HB2	1.63	0.80
3:N:850:LEU:H	3:N:850:LEU:HD12	1.46	0.80
2:M:537:LYS:HA	2:M:545:ASN:HD21	1.46	0.80
1:A:102:LYS:HG3	1:A:139:ASN:HB2	1.61	0.80
2:C:461:VAL:HG13	2:C:465:GLY:HA2	1.62	0.80
2:M:578:VAL:HG23	2:M:579:VAL:HG12	1.63	0.80
2:M:857:ASP:HB2	2:M:978:ARG:HG2	1.64	0.80
2:M:983:ILE:HG21	2:M:987:ILE:HD11	1.61	0.80
5:P:163:LEU:HD13	5:P:174:LEU:HD21	1.63	0.80
2:C:611:ILE:HD11	2:C:625:LEU:HD11	1.62	0.80
3:N:1352:ILE:O	3:N:1355:VAL:HG23	1.81	0.80
3:N:1393:GLN:HB2	3:N:1398:TRP:HE1	1.46	0.80
2:M:507:ARG:HB2	2:M:507:ARG:HH11	1.45	0.79
3:N:152:LEU:HD23	3:N:152:LEU:H	1.44	0.79
3:D:1422:MET:HE2	3:D:1427:SER:HA	1.63	0.79
3:D:656:PHE:HB3	3:D:694:VAL:HG11	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1350:GLU:HG3	3:D:1354:LYS:HE3	1.65	0.79
2:C:347:GLY:HA2	2:C:350:ARG:HD2	1.64	0.79
2:C:719:PRO:HB3	2:C:820:ARG:NE	1.96	0.79
3:D:1277:ILE:HD12	3:D:1301:LYS:HB2	1.65	0.79
2:M:146:VAL:HG22	2:M:162:ILE:HA	1.65	0.79
3:D:546:ARG:O	3:D:550:ARG:HG2	1.81	0.79
2:C:772:ARG:HG2	5:F:378:GLY:HA2	1.64	0.79
3:D:562:ALA:HB1	3:D:567:ILE:HD11	1.65	0.79
2:M:36:PRO:HG2	2:M:70:GLU:HB3	1.64	0.79
3:N:18:ILE:HG23	3:N:518:PRO:HG3	1.62	0.79
5:F:156:VAL:HA	5:F:159:ILE:HD12	1.63	0.79
2:M:182:VAL:HG12	2:M:193:LEU:HD13	1.65	0.79
2:M:244:PRO:HD2	2:M:245:GLY:H	1.48	0.79
3:N:53:ILE:HG23	3:N:54:LYS:H	1.48	0.79
3:N:470:LEU:HD23	3:N:470:LEU:H	1.46	0.79
3:N:1057:VAL:HG13	3:N:1069:GLU:HB3	1.64	0.79
1:L:219:ARG:HB3	1:L:219:ARG:HH11	1.48	0.79
1:A:24:VAL:HG13	1:A:196:THR:HG22	1.64	0.78
2:M:68:PHE:HE1	2:M:96:ALA:HB1	1.48	0.78
3:N:615:ARG:HH11	3:N:615:ARG:HB2	1.46	0.78
2:C:1090:LYS:NZ	3:D:90:MET:HG3	1.97	0.78
3:D:1383:ASP:HB2	3:D:1416:ALA:HB3	1.64	0.78
2:M:242:LEU:HB3	8:M:1549:HOH:O	1.83	0.78
3:N:806:PHE:CE1	3:N:813:LEU:HB3	2.18	0.78
1:B:13:VAL:HG23	8:B:493:HOH:O	1.82	0.78
3:D:1087:ARG:HA	3:D:1090:ASP:HB2	1.63	0.78
2:M:670:GLN:O	2:M:672:VAL:HG12	1.83	0.78
2:M:752:GLY:H	2:M:792:VAL:HB	1.45	0.78
2:C:1009:SER:HA	8:D:9195:HOH:O	1.82	0.78
2:M:397:GLU:H	2:M:633:GLN:NE2	1.81	0.78
2:C:71:TYR:HB2	8:C:1125:HOH:O	1.82	0.78
3:D:806:PHE:CE1	3:D:813:LEU:HB3	2.18	0.78
2:M:413:LEU:H	2:M:413:LEU:HD12	1.48	0.78
1:A:83:LYS:HE2	1:A:167:VAL:HG12	1.64	0.78
2:C:413:LEU:H	2:C:413:LEU:HD12	1.46	0.78
2:C:1111:ILE:HG13	2:C:1112:PHE:H	1.49	0.78
3:N:119:SER:HB2	3:N:123:LEU:HB2	1.66	0.78
1:B:184:THR:HB	1:B:194:LYS:HZ3	1.49	0.78
3:D:86:ARG:O	3:D:522:PRO:HD2	1.83	0.78
3:D:152:LEU:HD23	3:D:152:LEU:H	1.48	0.78
3:D:422:ALA:H	3:D:427:VAL:HG11	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:130:VAL:HG21	5:F:159:ILE:HG21	1.64	0.78
2:M:710:ILE:HD12	2:M:790:LEU:HB2	1.64	0.78
2:M:966:LEU:HD11	2:M:986:PRO:HG2	1.66	0.78
1:A:63:HIS:HB3	2:C:746:GLY:HA2	1.66	0.78
2:C:876:VAL:HA	8:C:1494:HOH:O	1.84	0.78
3:N:1095:THR:O	3:N:1099:VAL:HG23	1.83	0.78
3:N:1112:CYS:HB2	3:N:1195:GLN:OE1	1.84	0.78
5:P:291:ILE:HG21	5:P:304:VAL:HG11	1.65	0.78
3:D:127:LEU:HD11	3:D:461:ILE:HD11	1.65	0.78
4:O:51:LEU:HG	4:O:53:GLY:H	1.49	0.78
1:A:175:ARG:HH11	1:A:202:ASP:HA	1.49	0.77
1:K:25:LEU:HD23	1:K:28:LEU:HD11	1.64	0.77
5:P:358:LEU:HD11	5:P:370:LYS:HZ2	1.49	0.77
3:D:1272:ALA:HA	3:D:1326:THR:HB	1.66	0.77
3:N:631:ILE:HG21	3:N:745:MET:HG3	1.66	0.77
2:C:773:LEU:HB2	5:F:373:LYS:CB	2.15	0.77
2:C:871:LEU:HD12	2:C:992:MET:HE1	1.65	0.77
3:D:1238:MET:HE2	3:D:1257:PRO:HG3	1.66	0.77
5:F:205:ARG:HD2	5:F:251:ILE:HD13	1.66	0.77
2:M:1021:LEU:HD21	5:P:332:PHE:HA	1.66	0.77
2:C:137:VAL:HG23	2:C:391:LEU:HG	1.66	0.77
2:C:468:ARG:HG2	8:C:1431:HOH:O	1.82	0.77
5:P:260:ILE:HG23	5:P:264:MET:HB2	1.65	0.77
2:C:30:LEU:HB3	2:C:44:ILE:HD12	1.67	0.77
2:C:678:PRO:O	3:D:943:THR:HA	1.84	0.77
3:D:1166:LEU:HD12	3:D:1171:VAL:HG22	1.67	0.77
2:M:250:ARG:HG2	2:M:253:ALA:HB3	1.67	0.77
5:P:321:ILE:HD11	5:P:329:TYR:HB2	1.66	0.77
1:A:150:TYR:HE2	1:A:152:PRO:HG3	1.49	0.77
3:D:877:PRO:HA	8:D:9153:HOH:O	1.84	0.77
3:D:901:GLN:HB2	8:D:9514:HOH:O	1.84	0.77
3:N:119:SER:H	3:N:123:LEU:HD22	1.50	0.77
2:C:462:ASP:HB3	2:C:468:ARG:HD2	1.66	0.77
3:D:131:LYS:HB3	3:D:456:MET:HE3	1.67	0.77
3:D:1312:LEU:HB2	8:D:9354:HOH:O	1.84	0.77
3:D:1468:LEU:HD13	3:D:1470:ARG:HD3	1.67	0.77
5:F:117:SER:HA	8:F:433:HOH:O	1.84	0.77
3:N:569:ASN:HD22	3:N:573:MET:HE1	1.47	0.77
2:C:312:ALA:HB1	2:C:318:PRO:HG2	1.65	0.77
2:C:693:GLU:HA	2:C:696:LYS:HG3	1.65	0.77
2:C:846:LYS:HD3	3:D:741:ASP:HB2	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:412:GLU:HG3	5:F:418:LEU:HD22	1.67	0.77
3:D:131:LYS:HG2	3:D:568:ARG:HG2	1.66	0.76
3:D:1381:VAL:HB	3:D:1389:LEU:O	1.84	0.76
3:D:41:ARG:HD3	3:D:42:ASP:H	1.47	0.76
3:D:876:SER:HA	8:D:9288:HOH:O	1.86	0.76
5:F:163:LEU:HB3	5:F:174:LEU:HG	1.67	0.76
2:M:263:ASP:HB2	2:M:264:PRO:HD3	1.67	0.76
2:M:1054:THR:HG21	2:M:1079:PRO:CB	2.11	0.76
3:N:107:ASP:HB2	8:N:9202:HOH:O	1.85	0.76
3:N:699:VAL:H	3:N:756:GLN:HE22	1.33	0.76
2:C:609:ASN:ND2	2:C:627:ARG:HH21	1.82	0.76
3:D:1209:LEU:HD21	4:E:16:LYS:NZ	1.99	0.76
3:D:1223:ILE:H	3:D:1223:ILE:HD12	1.49	0.76
2:M:816:LYS:HE2	2:M:819:VAL:HG21	1.66	0.76
3:N:1381:VAL:HB	3:N:1389:LEU:O	1.84	0.76
3:N:610:LYS:HG2	3:N:611:GLN:HE21	1.50	0.76
2:C:108:ILE:HB	2:C:368:THR:OG1	1.84	0.76
3:D:9:ARG:HE	3:D:11:ALA:HB2	1.51	0.76
2:M:709:GLU:HG3	2:M:824:ARG:HG3	1.67	0.76
3:N:890:VAL:HG11	3:N:922:LEU:HD13	1.65	0.76
1:A:109:VAL:HG23	8:A:356:HOH:O	1.85	0.76
2:C:1067:TYR:HA	2:C:1070:ILE:HD12	1.67	0.76
3:D:633:VAL:HG22	3:D:635:PRO:HD3	1.67	0.76
3:N:12:LEU:HD23	3:N:13:ALA:H	1.50	0.76
2:C:630:ARG:NH2	2:C:705:ILE:HG22	2.01	0.76
3:D:698:LYS:HA	3:D:756:GLN:NE2	2.01	0.76
2:M:943:VAL:HG23	2:M:985:GLY:H	1.51	0.76
3:N:639:LEU:H	3:N:639:LEU:HD12	1.51	0.76
2:C:62:GLY:HA2	2:C:359:MET:HE1	1.68	0.76
2:C:41:ASN:HD22	2:C:41:ASN:H	1.30	0.76
2:C:944:LEU:HD21	2:C:963:LEU:HD22	1.67	0.76
3:D:1236:LEU:HD12	3:D:1256:LEU:HD12	1.67	0.76
2:M:199:VAL:HG13	2:M:235:LEU:HG	1.66	0.76
2:M:736:ASP:O	2:M:744:ARG:HG2	1.86	0.75
3:N:1040:GLY:O	3:N:1060:SER:HB3	1.86	0.75
3:N:1111:ASP:HB2	3:N:1203:LYS:HG3	1.67	0.75
2:C:534:VAL:H	2:C:538:GLN:HE22	1.34	0.75
2:M:154:ARG:HH21	2:M:156:GLY:HA3	1.50	0.75
2:M:186:VAL:HG23	2:M:187:ASN:H	1.51	0.75
3:N:145:VAL:HG22	3:N:146:PRO:HD2	1.69	0.75
3:N:1066:THR:HG23	3:N:1068:LEU:H	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:457:ALA:HB3	2:C:538:GLN:HA	1.67	0.75
3:D:658:LEU:HA	3:D:661:MET:HE3	1.68	0.75
3:D:842:VAL:HG23	8:D:9407:HOH:O	1.86	0.75
3:D:73:CYS:HB3	3:D:76:CYS:O	1.85	0.75
5:F:125:ASP:HA	5:F:128:ARG:HH12	1.51	0.75
2:M:22:GLN:NE2	2:M:336:VAL:HG21	2.01	0.75
2:M:490:GLU:HB3	8:M:1436:HOH:O	1.86	0.75
2:M:683:ASN:HA	2:M:687:ALA:HB3	1.68	0.75
1:A:28:LEU:HD13	1:A:32:PHE:HB3	1.69	0.75
2:C:987:ILE:HG23	3:D:948:THR:HG21	1.69	0.75
3:D:55:ASP:HA	3:D:82:LYS:HG3	1.69	0.75
3:D:1412:LYS:O	3:D:1414:PRO:HD3	1.86	0.75
2:M:626:ARG:NH1	2:M:637:LEU:HD12	2.01	0.75
1:K:54:THR:HG22	1:K:158:ILE:HG13	1.68	0.75
1:L:206:THR:HG22	1:L:209:GLU:H	1.52	0.75
3:N:44:LEU:HB3	3:N:525:ARG:HH21	1.50	0.75
3:N:1223:ILE:H	3:N:1223:ILE:HD12	1.51	0.75
1:A:191:ASP:HB3	8:A:483:HOH:O	1.86	0.75
2:M:378:LEU:HG	2:M:382:ILE:HD11	1.69	0.75
2:M:447:ALA:HA	3:N:1085:ALA:HB1	1.67	0.75
3:N:58:CYS:HA	3:N:78:VAL:HG11	1.68	0.75
3:N:558:LEU:HD13	5:P:145:PRO:HB3	1.67	0.75
3:N:948:THR:HG22	3:N:949:ILE:H	1.51	0.75
5:P:76:SER:O	5:P:80:PRO:HD2	1.87	0.75
3:D:1109:GLU:HG2	3:D:1201:CYS:HA	1.67	0.75
3:N:1066:THR:HG22	3:N:1069:GLU:HG3	1.69	0.75
2:C:36:PRO:HG2	2:C:70:GLU:HB3	1.69	0.75
2:C:557:ARG:NH2	2:C:879:ARG:HD3	2.00	0.75
3:D:65:ARG:HG3	3:D:66:GLN:H	1.52	0.75
3:D:971:LEU:HA	3:D:974:ILE:HD12	1.69	0.75
1:A:8:ALA:HB1	1:B:224:TYR:CE1	2.22	0.74
3:D:493:ARG:NH1	3:D:1390:LEU:HB2	2.03	0.74
2:M:479:VAL:HG21	2:M:503:LEU:HD11	1.69	0.74
3:N:1393:GLN:HB2	3:N:1398:TRP:NE1	2.01	0.74
5:F:123:ASP:HB2	5:F:126:LEU:HD13	1.67	0.74
1:L:45:LEU:HD21	1:L:177:VAL:HG22	1.66	0.74
5:P:404:ALA:HB3	8:P:4587:HOH:O	1.87	0.74
1:A:189:ARG:HB3	8:A:366:HOH:O	1.86	0.74
1:B:85:LEU:HD12	1:B:124:ASN:HB3	1.68	0.74
3:D:194:GLY:H	3:D:206:ARG:HA	1.51	0.74
2:M:864:GLY:HA2	8:M:1164:HOH:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:470:LEU:HD12	3:N:503:LEU:HG	1.68	0.74
2:M:598:GLU:O	2:M:651:LYS:HG3	1.87	0.74
3:N:875:THR:HG21	3:N:902:LEU:HD13	1.67	0.74
3:N:1271:LYS:HG2	3:N:1272:ALA:H	1.51	0.74
3:D:1147:ARG:HB2	3:D:1166:LEU:HD21	1.69	0.74
3:D:1291:SER:HB2	3:D:1293:PHE:HE1	1.52	0.74
3:N:171:LEU:HB2	3:N:390:PRO:HA	1.68	0.74
3:D:1046:GLN:HG2	3:D:1052:THR:HG22	1.68	0.74
1:L:27:PRO:HB3	1:L:192:LEU:HD22	1.68	0.74
2:M:282:GLY:HA2	2:M:308:ARG:HH21	1.51	0.74
2:M:675:ALA:HA	2:M:989:VAL:HG12	1.70	0.74
3:N:135:LEU:HD13	3:N:147:VAL:HG23	1.68	0.74
2:C:603:VAL:HG21	2:C:643:VAL:HG11	1.67	0.74
2:M:197:LEU:HA	2:M:200:LEU:HD12	1.68	0.74
2:M:313:LEU:HD23	2:M:314:THR:HG23	1.68	0.74
2:C:115:LEU:HD13	2:C:351:LEU:HD21	1.70	0.74
3:D:1109:GLU:OE1	3:D:1201:CYS:HB2	1.88	0.74
5:F:88:ILE:HD13	5:F:193:ARG:HB2	1.67	0.74
5:F:247:ILE:HG22	5:F:251:ILE:HD11	1.69	0.74
2:M:282:GLY:HA2	2:M:308:ARG:NH2	2.01	0.74
2:M:605:LYS:HD3	2:M:610:ARG:CZ	2.18	0.74
2:M:671:ASN:HD21	2:M:993:PHE:HD2	1.32	0.74
3:N:486:ARG:HE	3:N:489:ARG:HD3	1.50	0.74
2:C:521:PRO:HB2	3:D:1055:VAL:HB	1.68	0.74
2:M:312:ALA:HB1	2:M:318:PRO:HG2	1.68	0.74
2:M:486:MET:HB3	8:M:1436:HOH:O	1.88	0.74
3:N:1259:VAL:HG22	3:N:1355:VAL:HG21	1.68	0.74
2:C:83:CYS:HA	2:C:88:LEU:HB3	1.70	0.74
3:D:715:ALA:HB3	3:D:764:LEU:HA	1.70	0.74
2:C:683:ASN:HA	2:C:687:ALA:HB3	1.69	0.73
2:C:124:ASP:HB3	2:C:592:LEU:HD12	1.69	0.73
3:D:1112:CYS:HB2	3:D:1195:GLN:OE1	1.88	0.73
1:L:133:GLU:HG3	1:L:134:GLU:HG2	1.70	0.73
2:M:436:GLY:HA2	2:M:538:GLN:O	1.88	0.73
2:C:269:LEU:HD23	2:C:285:LEU:HD21	1.69	0.73
3:D:795:VAL:HG11	3:D:863:VAL:HG13	1.70	0.73
2:M:89:THR:O	2:M:91:GLN:HG3	1.88	0.73
2:C:676:ILE:HG23	3:D:948:THR:HB	1.68	0.73
3:D:537:THR:C	5:F:317:LEU:HB2	2.12	0.73
3:D:1289:LYS:HE3	3:D:1307:LYS:HE2	1.69	0.73
5:F:411:HIS:HA	5:F:414:ARG:HG3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:362:GLY:HA3	2:M:367:LEU:HD23	1.68	0.73
3:N:661:MET:HG2	3:N:666:ILE:HD12	1.71	0.73
1:B:45:LEU:HA	8:B:343:HOH:O	1.88	0.73
1:B:58:ILE:HD13	1:B:140:MET:HB3	1.70	0.73
2:C:818:GLY:HA3	8:C:1350:HOH:O	1.88	0.73
3:D:459:GLU:HB3	8:D:9187:HOH:O	1.89	0.73
3:D:530:VAL:HB	3:D:534:ARG:HB2	1.70	0.73
1:L:63:HIS:HB2	8:L:3671:HOH:O	1.88	0.73
2:M:18:LEU:HD23	2:M:404:LEU:HD21	1.70	0.73
2:M:92:ALA:HB1	8:M:1276:HOH:O	1.89	0.73
2:M:1085:PHE:CD2	3:N:1468:LEU:HA	2.23	0.73
8:M:1349:HOH:O	3:N:651:GLU:HG3	1.88	0.73
3:N:644:LEU:HD12	3:N:645:PRO:HD2	1.68	0.73
5:P:358:LEU:HD21	5:P:370:LYS:HE3	1.70	0.73
1:B:56:VAL:HG13	1:B:142:VAL:HG12	1.71	0.73
1:B:206:THR:HG22	1:B:209:GLU:HB2	1.68	0.73
2:C:182:VAL:HG21	8:C:1366:HOH:O	1.89	0.73
5:P:247:ILE:HG22	5:P:251:ILE:HD11	1.70	0.73
1:B:131:THR:HG22	8:B:423:HOH:O	1.89	0.73
2:C:943:VAL:HG23	2:C:985:GLY:H	1.53	0.73
3:D:637:LEU:HD21	3:D:642:CYS:HA	1.70	0.73
3:D:1045:MET:CG	3:D:1073:SER:HA	2.17	0.73
2:M:589:ARG:HH11	2:M:589:ARG:HB2	1.51	0.73
3:N:214:GLU:HB2	3:N:390:PRO:HD2	1.71	0.73
5:P:403:LYS:HA	5:P:403:LYS:NZ	2.03	0.73
1:A:98:THR:HG21	8:A:348:HOH:O	1.89	0.73
3:D:101:HIS:HD1	3:D:103:TRP:HB2	1.53	0.73
3:D:186:VAL:HG21	3:D:213:VAL:HB	1.71	0.73
3:D:478:LEU:HD22	3:D:1388:ARG:CZ	2.18	0.73
3:D:572:ARG:HH12	5:F:79:ASP:CG	1.97	0.73
3:N:643:GLY:HA3	3:N:727:GLN:HB2	1.69	0.73
3:N:760:ARG:HH21	4:O:3:GLU:CD	1.97	0.73
2:M:292:ARG:HB2	2:M:299:LYS:HE2	1.70	0.73
2:M:371:LYS:HA	8:M:1338:HOH:O	1.87	0.73
3:N:194:GLY:H	3:N:206:ARG:HA	1.53	0.73
3:N:1194:CYS:HB3	3:N:1373:ARG:NH2	2.03	0.73
2:C:366:SER:HA	8:C:1205:HOH:O	1.87	0.73
2:C:433:THR:HG21	2:C:488:ALA:HB1	1.70	0.73
2:C:874:LEU:HD21	3:D:787:LEU:HD22	1.71	0.73
2:M:1080:SER:HB2	8:M:1849:HOH:O	1.87	0.73
3:N:1481:VAL:HG13	4:O:18:ARG:NE	2.00	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:328:LEU:HD23	2:M:437:ARG:HD3	1.71	0.72
3:D:462:GLN:HA	3:D:513:ILE:HD13	1.71	0.72
1:K:150:TYR:HE2	1:K:152:PRO:HG3	1.51	0.72
3:N:1264:GLU:OE2	3:N:1424:VAL:HG12	1.88	0.72
1:A:14:ARG:NH2	1:A:22:GLU:HB3	2.03	0.72
2:C:704:HIS:HB2	2:C:831:ARG:HE	1.53	0.72
2:C:1091:GLU:OE1	3:D:613:ARG:HG2	1.88	0.72
3:D:628:ARG:HD3	3:D:744:GLN:NE2	2.04	0.72
3:D:1209:LEU:HD22	3:D:1211:MET:HB3	1.71	0.72
2:C:166:PRO:HA	8:C:1305:HOH:O	1.88	0.72
3:D:171:LEU:HB2	3:D:390:PRO:HA	1.70	0.72
2:M:54:ILE:HG21	8:M:1182:HOH:O	1.89	0.72
2:M:565:GLN:HA	2:M:995:MET:HE1	1.72	0.72
3:N:1210:SER:HA	8:N:9113:HOH:O	1.87	0.72
3:N:1429:LEU:HG	3:N:1441:GLN:HG3	1.70	0.72
2:C:54:ILE:HA	8:C:1491:HOH:O	1.89	0.72
3:N:669:ASN:HB3	8:N:9139:HOH:O	1.89	0.72
8:N:9109:HOH:O	5:P:319:THR:HA	1.88	0.72
3:D:1235:GLN:C	3:D:1359:GLN:HE22	1.98	0.72
2:M:573:ARG:HG3	2:M:698:ASP:O	1.90	0.72
3:N:656:PHE:CE2	3:N:698:LYS:HE3	2.23	0.72
3:N:715:ALA:HB3	3:N:764:LEU:HA	1.71	0.72
1:B:36:LEU:O	1:B:39:PRO:HD2	1.89	0.72
3:D:1267:ARG:HH22	3:D:1333:HIS:HD2	1.38	0.72
3:D:1462:LEU:HD22	3:D:1472:ILE:HG23	1.70	0.72
1:K:133:GLU:HG2	1:K:134:GLU:N	2.05	0.72
3:N:1209:LEU:HD23	3:N:1210:SER:H	1.54	0.72
5:P:151:LEU:HB3	8:P:3247:HOH:O	1.89	0.72
5:F:93:LEU:HD22	5:F:98:GLU:HB3	1.69	0.72
1:K:89:PHE:CZ	1:K:146:ARG:HB2	2.25	0.72
3:N:207:PHE:HB3	3:N:208:PRO:HD2	1.70	0.72
2:C:473:ARG:HE	2:C:531:PHE:HE1	1.35	0.72
3:D:153:LEU:HD12	3:D:154:THR:N	2.05	0.72
3:D:699:VAL:HG21	3:D:760:ARG:HB3	1.72	0.72
1:L:23:PHE:HA	8:L:3037:HOH:O	1.90	0.72
2:M:1092:LEU:HD13	2:M:1099:VAL:HG21	1.72	0.72
3:N:1160:LEU:HD11	3:N:1174:LEU:HD21	1.70	0.72
2:C:64:LEU:HB2	2:C:359:MET:SD	2.30	0.72
2:C:244:PRO:HD2	2:C:245:GLY:H	1.53	0.72
3:D:671:LYS:HG3	5:F:422:LEU:HA	1.72	0.72
5:F:93:LEU:HG	5:F:190:ALA:CB	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:55:SER:OG	1:K:158:ILE:HB	1.90	0.72
4:O:51:LEU:HD12	4:O:52:GLU:H	1.55	0.72
5:P:132:ARG:NH2	5:P:184:ARG:HH12	1.86	0.72
2:C:29:ALA:HB2	2:C:337:GLY:CA	2.20	0.71
2:C:897:LEU:HB3	2:C:899:GLN:HE21	1.55	0.71
3:D:907:GLU:O	3:D:911:LEU:HD22	1.89	0.71
2:C:833:LEU:HD11	2:C:849:VAL:HG21	1.71	0.71
3:D:520:LEU:HD23	3:D:540:LEU:HD22	1.71	0.71
3:D:996:TRP:HA	3:D:999:THR:HG22	1.72	0.71
5:F:128:ARG:HG2	8:F:754:HOH:O	1.88	0.71
1:K:88:ARG:HD2	1:K:123:MET:HE2	1.70	0.71
2:M:83:CYS:HA	2:M:88:LEU:HB3	1.73	0.71
3:N:1412:LYS:O	3:N:1414:PRO:HD3	1.89	0.71
5:P:404:ALA:HA	8:P:4644:HOH:O	1.90	0.71
1:A:14:ARG:NH2	1:A:24:VAL:HG23	2.05	0.71
2:C:157:ARG:HD2	2:C:314:THR:HG22	1.73	0.71
3:D:796:ARG:NH1	3:D:861:GLN:HB2	2.06	0.71
4:E:45:ARG:HA	8:E:180:HOH:O	1.88	0.71
3:N:171:LEU:HD22	3:N:390:PRO:HG3	1.72	0.71
3:D:153:LEU:CD1	3:D:157:GLU:HB2	2.20	0.71
3:D:374:GLU:HA	8:D:9065:HOH:O	1.90	0.71
3:D:737:ASN:HA	8:D:9006:HOH:O	1.89	0.71
2:M:31:GLN:HB3	2:M:71:TYR:OH	1.91	0.71
3:N:117:ASP:HB2	3:N:495:ARG:NH2	2.05	0.71
3:N:192:ALA:O	3:N:195:VAL:HG23	1.90	0.71
3:N:637:LEU:HD21	3:N:642:CYS:HA	1.71	0.71
3:N:808:THR:HB	3:N:809:PRO:HD3	1.72	0.71
3:N:1415:VAL:HG23	8:N:9265:HOH:O	1.89	0.71
1:A:175:ARG:NH1	1:A:202:ASP:HA	2.06	0.71
2:C:52:PHE:HA	8:C:1788:HOH:O	1.91	0.71
3:D:513:ILE:HA	8:D:9491:HOH:O	1.91	0.71
3:D:1087:ARG:CG	3:D:1234:THR:HA	2.21	0.71
2:M:1115:LEU:HD23	3:N:85:VAL:HG13	1.73	0.71
3:N:215:TYR:O	3:N:389:GLU:HB3	1.89	0.71
3:N:1342:GLU:H	3:N:1342:GLU:CD	1.99	0.71
3:D:1046:GLN:HA	3:D:1052:THR:HA	1.72	0.71
3:D:1273:VAL:HG22	3:D:1326:THR:OG1	1.90	0.71
2:M:786:LYS:HA	8:M:1174:HOH:O	1.88	0.71
3:N:984:THR:HG22	3:N:987:GLU:HG3	1.72	0.71
5:P:361:LEU:HG	5:P:408:LEU:HD21	1.71	0.71
3:D:1251:ASP:O	3:D:1270:ALA:HB3	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:139:GLY:O	3:N:147:VAL:HB	1.91	0.71
3:N:1109:GLU:HG2	3:N:1201:CYS:HA	1.73	0.71
1:A:222:LEU:HD12	1:B:215:VAL:HB	1.71	0.71
2:C:113:VAL:HG13	8:C:1336:HOH:O	1.91	0.71
2:C:672:VAL:HG23	2:C:868:ASP:HB2	1.71	0.71
3:D:172:PRO:HD2	3:D:389:GLU:O	1.91	0.71
3:D:661:MET:HA	3:D:666:ILE:HD12	1.72	0.71
4:O:54:LEU:HG	4:O:58:PRO:HG2	1.73	0.71
5:P:160:ASP:HA	5:P:163:LEU:HD12	1.73	0.71
1:A:18:ARG:HH12	1:A:88:ARG:HH21	1.37	0.71
2:C:343:GLN:HG2	2:C:385:PHE:HB2	1.72	0.71
1:K:224:TYR:HB3	1:L:9:PRO:HB2	1.72	0.71
2:M:1051:GLU:HG3	2:M:1055:LEU:HD12	1.71	0.71
3:N:1173:LEU:HD23	3:N:1174:LEU:HD23	1.72	0.71
2:C:460:ARG:HB3	2:C:460:ARG:HH11	1.55	0.70
3:D:601:ARG:HD2	5:F:328:PHE:HE1	1.54	0.70
2:M:603:VAL:HG21	2:M:643:VAL:HG11	1.73	0.70
3:N:26:VAL:HG11	3:N:44:LEU:HD23	1.73	0.70
3:N:1488:ASP:HA	8:O:4394:HOH:O	1.91	0.70
2:C:264:PRO:HB3	2:C:289:THR:HG21	1.71	0.70
2:M:139:GLN:HG3	2:M:140:ILE:H	1.56	0.70
2:M:157:ARG:HE	2:M:158:TYR:H	1.36	0.70
2:M:535:SER:O	2:M:538:GLN:HG2	1.91	0.70
3:N:483:HIS:HB2	3:N:484:PRO:HD3	1.73	0.70
5:P:366:ALA:HB3	5:P:367:MET:HE2	1.73	0.70
5:F:291:ILE:HG21	5:F:304:VAL:HG11	1.73	0.70
2:M:755:LEU:HB2	2:M:790:LEU:HD22	1.73	0.70
2:C:710:ILE:HD11	2:C:758:ARG:HH21	1.56	0.70
2:C:1067:TYR:O	2:C:1071:ILE:HG12	1.92	0.70
3:D:131:LYS:HD2	5:F:83:GLN:NE2	2.06	0.70
3:D:929:ARG:HB2	8:D:9499:HOH:O	1.90	0.70
3:D:1077:ALA:HB2	8:D:2073:HOH:O	1.91	0.70
5:F:260:ILE:HG23	5:F:264:MET:HB2	1.74	0.70
2:C:511:GLU:O	2:C:526:PRO:HD3	1.91	0.70
3:D:1209:LEU:HD21	4:E:16:LYS:HZ3	1.54	0.70
5:F:77:THR:O	5:F:81:VAL:HG23	1.91	0.70
2:M:884:GLN:HG3	2:M:885:ILE:HD13	1.72	0.70
2:C:108:ILE:HG21	8:C:1205:HOH:O	1.92	0.70
2:C:127:PHE:HA	8:C:1442:HOH:O	1.90	0.70
2:C:284:ARG:HG2	2:C:285:LEU:H	1.57	0.70
3:D:570:GLU:HB2	5:F:214:GLN:NE2	2.07	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:41:GLU:O	4:O:45:ARG:HG2	1.91	0.70
1:A:141:GLU:HG3	8:A:346:HOH:O	1.92	0.70
1:L:143:ARG:NH1	1:L:158:ILE:HD12	2.07	0.70
3:N:52:PRO:HG3	3:N:78:VAL:HG22	1.72	0.70
3:N:1220:ALA:HB1	3:N:1223:ILE:HD13	1.73	0.70
2:C:101:ILE:HG23	2:C:107:LEU:HD22	1.73	0.70
2:C:256:TYR:CE1	2:C:293:PHE:HB2	2.26	0.70
2:C:512:ARG:HB3	2:C:523:ILE:HD11	1.73	0.70
5:F:396:ARG:HG2	8:F:468:HOH:O	1.92	0.70
2:C:299:LYS:HB2	8:C:1374:HOH:O	1.90	0.70
3:D:1166:LEU:HD23	3:D:1166:LEU:H	1.56	0.70
3:D:1395:LEU:HB3	8:D:9369:HOH:O	1.91	0.70
1:L:58:ILE:HB	1:L:61:VAL:HB	1.73	0.70
1:L:97:VAL:HG11	1:L:120:VAL:HG21	1.74	0.70
2:M:218:VAL:HA	2:M:221:LEU:HD23	1.74	0.70
2:M:1115:LEU:HD11	8:M:1678:HOH:O	1.90	0.70
3:N:796:ARG:HD3	3:N:861:GLN:HB2	1.73	0.70
3:N:965:GLU:HG3	3:N:969:ARG:HH21	1.56	0.70
1:B:97:VAL:HG11	1:B:120:VAL:HG21	1.74	0.70
5:F:372:ARG:HB2	8:F:635:HOH:O	1.91	0.70
2:M:1098:ASP:HB2	3:N:21:TRP:HZ2	1.57	0.70
1:B:156:HIS:ND1	1:B:158:ILE:HG12	2.06	0.69
2:C:49:ARG:HH11	2:C:49:ARG:HB2	1.57	0.69
2:C:318:PRO:HB3	8:C:1564:HOH:O	1.90	0.69
2:C:455:LEU:HD12	2:C:459:ALA:HB3	1.72	0.69
2:C:517:ARG:NH1	2:C:522:VAL:HG11	2.05	0.69
2:C:958:THR:HG23	2:C:961:GLU:H	1.56	0.69
3:D:132:TYR:HA	8:D:9333:HOH:O	1.91	0.69
1:L:209:GLU:HB3	8:L:4878:HOH:O	1.92	0.69
2:M:343:GLN:HG3	8:M:1267:HOH:O	1.92	0.69
2:C:358:ARG:NH2	2:C:374:ASN:HB3	2.06	0.69
3:D:1352:ILE:HG21	3:D:1368:ILE:HG21	1.74	0.69
5:F:234:LYS:HD3	5:F:236:SER:HB3	1.72	0.69
2:C:580:MET:HB3	2:C:584:GLU:CD	2.16	0.69
2:C:1044:GLY:HA3	4:E:17:TYR:HE1	1.57	0.69
3:D:210:ARG:HB3	3:D:210:ARG:HH11	1.57	0.69
3:D:704:ARG:HD3	3:D:738:ALA:HB2	1.73	0.69
4:E:51:LEU:HD12	4:E:52:GLU:H	1.57	0.69
2:C:92:ALA:HB1	8:C:1294:HOH:O	1.92	0.69
3:D:793:THR:HB	3:D:879:ARG:HD3	1.74	0.69
1:L:161:ARG:HA	8:L:3450:HOH:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:511:GLU:O	2:M:526:PRO:HD3	1.92	0.69
3:N:15:PRO:HA	3:N:18:ILE:HG12	1.74	0.69
3:N:834:THR:HB	3:N:838:ARG:HB3	1.74	0.69
1:B:94:LEU:HD21	1:B:119:ASP:HB2	1.75	0.69
2:C:405:ARG:NH2	2:C:566:THR:HG21	2.08	0.69
2:C:1056:LYS:HD3	3:D:623:VAL:HG13	1.73	0.69
3:D:611:GLN:HG3	5:F:326:ASP:HB2	1.75	0.69
1:K:9:PRO:HB2	1:L:224:TYR:HB3	1.73	0.69
2:M:478:VAL:HA	2:M:506:ASN:O	1.92	0.69
3:N:468:LEU:HB3	8:N:9407:HOH:O	1.92	0.69
3:D:215:TYR:O	3:D:389:GLU:HB2	1.93	0.69
3:D:1462:LEU:HB3	3:D:1472:ILE:HD12	1.75	0.69
4:E:48:MET:HB2	4:E:54:LEU:HD12	1.73	0.69
5:F:120:THR:HB	8:F:433:HOH:O	1.91	0.69
5:F:335:ASP:OD2	5:F:338:LEU:HB2	1.92	0.69
3:N:119:SER:HB2	3:N:123:LEU:H	1.57	0.69
3:N:1389:LEU:HD12	3:N:1390:LEU:H	1.57	0.69
2:C:197:LEU:HA	2:C:200:LEU:HD12	1.75	0.69
2:C:670:GLN:O	2:C:672:VAL:HG12	1.93	0.69
3:D:811:GLU:HA	8:D:9196:HOH:O	1.93	0.69
3:D:929:ARG:HD3	8:D:9607:HOH:O	1.93	0.69
1:K:62:LEU:HD12	8:K:3844:HOH:O	1.91	0.69
2:M:516:ARG:HD2	2:M:521:PRO:HA	1.73	0.69
3:N:1033:GLN:HE21	3:N:1036:ARG:HD3	1.58	0.69
3:N:1314:LYS:HZ3	3:N:1317:ASP:H	1.38	0.69
1:A:177:VAL:O	2:C:864:GLY:HA3	1.92	0.69
2:C:193:LEU:HD21	8:C:1760:HOH:O	1.93	0.69
2:C:971:LYS:HA	2:C:988:VAL:HA	1.74	0.69
3:D:663:GLU:HA	8:D:9541:HOH:O	1.93	0.69
3:D:756:GLN:O	3:D:760:ARG:HG2	1.91	0.69
3:D:996:TRP:CD2	3:D:1056:PRO:HG2	2.28	0.69
2:M:172:ILE:HG23	2:M:184:MET:HE3	1.73	0.69
3:N:211:VAL:HG22	3:N:393:ILE:HG23	1.75	0.69
2:C:720:GLU:HG2	2:C:760:SER:HB3	1.75	0.69
2:C:958:THR:HG22	8:C:1364:HOH:O	1.92	0.69
2:C:1067:TYR:CG	5:F:341:PRO:HB3	2.28	0.69
3:D:178:LEU:HG	3:D:200:ASP:H	1.58	0.69
3:D:964:LEU:HD13	3:D:1058:ARG:NH1	2.08	0.69
2:M:136:ILE:HG21	2:M:336:VAL:HG13	1.75	0.69
2:M:1000:MET:SD	2:M:1001:VAL:HG22	2.32	0.69
1:B:57:TYR:HB3	1:B:141:GLU:CG	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:62:LYS:HE2	3:D:75:ARG:HH12	1.58	0.69
3:D:393:ILE:H	3:D:393:ILE:HD12	1.58	0.69
3:N:761:ILE:HG21	8:O:3197:HOH:O	1.93	0.69
3:N:906:GLN:HB3	3:N:911:LEU:CD1	2.22	0.69
3:N:1372:VAL:HA	3:N:1375:MET:HE3	1.75	0.69
5:P:100:VAL:CG1	5:P:104:ARG:HH21	2.06	0.69
1:A:218:LEU:HD23	1:B:222:LEU:HD21	1.74	0.68
1:A:226:SER:O	1:A:228:PRO:HD3	1.93	0.68
1:K:100:LEU:HB2	1:K:115:LEU:HD11	1.75	0.68
2:M:526:PRO:HG2	8:M:1259:HOH:O	1.92	0.68
3:N:430:ASP:HB3	8:N:9241:HOH:O	1.93	0.68
3:N:542:ASP:O	3:N:546:ARG:HG2	1.94	0.68
3:N:1031:ASN:HB3	3:N:1034:GLN:CD	2.19	0.68
3:N:1205:TYR:CD2	3:N:1215:VAL:HG21	2.28	0.68
2:C:282:GLY:HA2	2:C:308:ARG:NH2	2.07	0.68
2:C:437:ARG:HA	2:C:467:ILE:HG21	1.73	0.68
2:C:567:GLN:HA	8:C:1666:HOH:O	1.93	0.68
2:C:609:ASN:HD21	2:C:627:ARG:HH21	1.40	0.68
2:C:1060:ILE:HD12	2:C:1063:ARG:NH1	2.08	0.68
5:F:108:GLU:HG3	5:F:176:ILE:HG21	1.74	0.68
2:M:311:PHE:HB3	8:M:1560:HOH:O	1.93	0.68
2:M:672:VAL:HG23	2:M:868:ASP:HB2	1.74	0.68
2:M:704:HIS:CB	2:M:831:ARG:HE	2.05	0.68
2:C:479:VAL:CG2	2:C:503:LEU:HD11	2.21	0.68
2:C:777:ILE:HG23	5:F:405:LEU:HD11	1.74	0.68
2:C:1066:ALA:O	2:C:1070:ILE:HG13	1.93	0.68
3:D:808:THR:HB	3:D:809:PRO:HD3	1.73	0.68
3:D:1495:ILE:HG12	4:E:80:VAL:HG11	1.76	0.68
1:L:85:LEU:HD12	1:L:124:ASN:HB3	1.75	0.68
3:N:1205:TYR:HD2	3:N:1215:VAL:HG21	1.59	0.68
5:P:376:ILE:HG23	8:P:3758:HOH:O	1.93	0.68
1:B:123:MET:C	1:B:125:PRO:HD3	2.19	0.68
2:C:244:PRO:HG2	2:C:246:ASP:OD2	1.93	0.68
3:D:87:ARG:HB3	3:D:523:ASP:HB2	1.76	0.68
3:D:478:LEU:HD21	3:D:500:ARG:NH2	2.08	0.68
1:K:92:PRO:HD3	8:K:3642:HOH:O	1.92	0.68
1:L:58:ILE:HG23	8:L:4138:HOH:O	1.93	0.68
1:L:156:HIS:ND1	1:L:158:ILE:HG12	2.08	0.68
2:M:726:ILE:HG22	8:M:1255:HOH:O	1.92	0.68
5:P:100:VAL:HG12	5:P:104:ARG:HH21	1.58	0.68
5:P:248:ASN:HA	5:P:251:ILE:HD12	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:LEU:HG	1:B:136:GLY:HA3	1.75	0.68
2:C:151:ASP:HB2	2:C:157:ARG:O	1.94	0.68
3:D:161:LEU:HD13	3:D:452:ILE:HD12	1.75	0.68
5:F:144:ILE:HB	5:F:145:PRO:HD3	1.76	0.68
2:M:368:THR:HB	2:M:369:PRO:HD3	1.74	0.68
2:M:675:ALA:HB2	2:M:867:VAL:HG11	1.75	0.68
2:M:983:ILE:HA	8:M:1335:HOH:O	1.92	0.68
5:P:403:LYS:NZ	5:P:406:ARG:HD2	2.08	0.68
1:A:206:THR:HG22	1:A:209:GLU:HG3	1.76	0.68
1:B:151:VAL:HG13	1:B:155:LYS:HE2	1.76	0.68
2:C:610:ARG:HB2	8:C:1501:HOH:O	1.93	0.68
2:C:1096:ALA:O	3:D:13:ALA:HB2	1.93	0.68
3:D:477:LEU:HD22	3:D:492:ALA:HB1	1.76	0.68
4:E:30:LEU:O	4:E:35:PHE:HA	1.94	0.68
1:A:9:PRO:HD2	1:B:224:TYR:CZ	2.28	0.68
1:A:198:ARG:HB2	1:A:200:TRP:CH2	2.29	0.68
2:C:428:ARG:HG2	2:C:449:ILE:O	1.94	0.68
2:C:1060:ILE:HD12	2:C:1063:ARG:HH12	1.58	0.68
3:D:1406:ARG:NH2	3:D:1407:LEU:HG	2.09	0.68
1:L:208:LEU:HD23	8:L:3127:HOH:O	1.94	0.68
2:M:300:ASP:HB2	8:M:1252:HOH:O	1.93	0.68
3:N:108:VAL:HG23	3:N:109:PRO:HD3	1.76	0.68
1:A:74:ASP:OD1	1:A:77:GLU:HB2	1.93	0.68
3:D:539:ASP:OD2	5:F:318:GLU:HB2	1.93	0.68
3:N:1273:VAL:HG22	3:N:1326:THR:OG1	1.93	0.68
2:C:64:LEU:HD13	2:C:359:MET:HG3	1.74	0.68
2:C:1109:VAL:HG23	3:D:3:LYS:HG2	1.75	0.68
5:F:119:ILE:HD13	5:F:170:HIS:ND1	2.09	0.68
1:K:18:ARG:NH1	1:K:123:MET:HE1	2.09	0.68
2:M:841:ASN:C	2:M:841:ASN:HD22	2.02	0.68
2:C:516:ARG:HD3	2:C:521:PRO:HA	1.75	0.68
3:D:46:ASP:HB3	3:D:49:ILE:HG13	1.75	0.68
3:D:133:ILE:HG21	3:D:454:ALA:HB1	1.75	0.68
1:L:184:THR:HG23	1:L:192:LEU:HB3	1.76	0.68
3:N:535:PHE:O	5:P:315:VAL:N	2.26	0.68
3:N:1058:ARG:HG3	3:N:1058:ARG:HH11	1.59	0.68
2:C:605:LYS:HD3	2:C:610:ARG:NH1	2.09	0.67
3:D:401:TYR:HB2	8:D:9802:HOH:O	1.93	0.67
3:D:422:ALA:HB3	3:D:427:VAL:CG2	2.21	0.67
3:D:1459:LEU:HD22	3:D:1465:ASN:ND2	2.09	0.67
1:L:100:LEU:HB2	1:L:115:LEU:HD21	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:112:ARG:HD2	8:L:4849:HOH:O	1.93	0.67
3:N:86:ARG:O	3:N:522:PRO:HD2	1.93	0.67
3:N:543:LEU:HD22	3:N:580:ALA:HB1	1.74	0.67
3:N:961:LYS:HG2	8:N:9231:HOH:O	1.93	0.67
2:C:36:PRO:HB3	8:C:1554:HOH:O	1.94	0.67
2:C:186:VAL:HG23	2:C:187:ASN:H	1.58	0.67
2:C:478:VAL:HA	2:C:506:ASN:O	1.94	0.67
3:D:156:GLU:H	3:D:156:GLU:CD	2.00	0.67
3:D:1082:ALA:O	3:D:1086:LEU:HD13	1.94	0.67
3:D:1318:TYR:HB3	8:D:9569:HOH:O	1.94	0.67
2:M:144:PRO:HA	2:M:163:ILE:HG12	1.76	0.67
2:M:952:LEU:HD12	2:M:969:GLN:NE2	2.09	0.67
3:N:1046:GLN:HA	3:N:1052:THR:HA	1.76	0.67
5:P:87:GLU:O	5:P:91:VAL:HG23	1.94	0.67
2:C:227:PHE:HD2	2:C:230:ARG:HH21	1.42	0.67
2:C:598:GLU:O	2:C:651:LYS:HG3	1.94	0.67
3:D:547:LEU:HD11	3:D:578:VAL:HG22	1.74	0.67
4:E:60:ALA:O	4:E:63:TRP:HB2	1.94	0.67
4:E:86:GLN:HB2	8:E:158:HOH:O	1.94	0.67
1:K:43:ILE:HD11	1:L:35:THR:HG21	1.76	0.67
2:M:165:LEU:O	2:M:265:ARG:HB2	1.93	0.67
3:N:75:ARG:HB3	8:N:9208:HOH:O	1.94	0.67
5:P:234:LYS:HG3	8:P:4168:HOH:O	1.94	0.67
1:A:24:VAL:HG22	1:A:196:THR:HB	1.75	0.67
3:D:175:VAL:HG12	3:D:176:ASP:OD1	1.94	0.67
3:D:707:THR:HA	8:D:9216:HOH:O	1.93	0.67
3:D:1336:LEU:HA	3:D:1344:VAL:HG22	1.75	0.67
5:F:351:SER:O	5:F:355:GLU:HB2	1.93	0.67
2:M:260:LEU:HB2	2:M:291:ALA:HB1	1.77	0.67
3:N:400:VAL:HG12	3:N:401:TYR:HD1	1.59	0.67
1:B:38:ASN:OD1	2:C:979:THR:HA	1.95	0.67
3:D:93:ILE:HD11	3:D:548:ILE:HD13	1.76	0.67
3:D:523:ASP:N	8:D:9040:HOH:O	2.27	0.67
3:D:834:THR:HG22	3:D:838:ARG:HD2	1.76	0.67
3:D:1095:THR:HG23	3:D:1230:GLY:HA3	1.75	0.67
2:M:205:GLU:O	2:M:209:ARG:HD2	1.94	0.67
2:M:546:LEU:HA	2:M:581:THR:HG21	1.76	0.67
2:M:736:ASP:HA	2:M:744:ARG:HD3	1.75	0.67
3:N:153:LEU:HD11	3:N:158:TYR:N	2.08	0.67
3:N:1420:LEU:HD12	3:N:1421:LEU:N	2.09	0.67
2:C:100:LEU:HB2	8:C:1196:HOH:O	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:1040:LEU:HG	2:M:1045:ALA:HB3	1.77	0.67
3:N:105:VAL:HG21	3:N:128:TYR:HE2	1.60	0.67
3:N:730:PRO:HA	3:N:733:CYS:SG	2.35	0.67
3:N:1127:GLU:HG3	3:N:1133:ARG:HH12	1.60	0.67
3:N:1383:ASP:HB2	3:N:1416:ALA:HB3	1.77	0.67
3:D:1087:ARG:HB3	3:D:1234:THR:HG23	1.75	0.67
3:D:1389:LEU:HD13	8:D:9579:HOH:O	1.94	0.67
1:L:65:PHE:HB2	8:L:3211:HOH:O	1.94	0.67
2:M:630:ARG:HH21	2:M:707:ARG:N	1.93	0.67
3:N:1397:LYS:HG2	8:N:9561:HOH:O	1.93	0.67
3:N:1485:GLN:HE21	4:O:80:VAL:H	1.43	0.67
1:A:20:TYR:HD2	1:A:21:GLY:N	1.93	0.67
2:C:777:ILE:HG22	2:C:778:PHE:HD1	1.59	0.67
3:D:793:THR:HG22	3:D:879:ARG:HA	1.77	0.67
1:K:99:LEU:HB3	1:K:114:PHE:HD2	1.57	0.67
3:N:654:LYS:HD3	3:N:674:ARG:HH22	1.59	0.67
5:F:112:ALA:HA	5:F:173:TYR:HD2	1.59	0.67
1:K:99:LEU:HB3	1:K:114:PHE:CD2	2.30	0.67
1:L:62:LEU:HD13	1:L:63:HIS:ND1	2.10	0.67
3:N:124:GLU:HB2	8:N:9808:HOH:O	1.94	0.67
3:N:1314:LYS:H	3:N:1314:LYS:HD3	1.60	0.67
4:O:60:ALA:O	4:O:63:TRP:HB2	1.95	0.67
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.76	0.66
3:D:156:GLU:HB3	8:D:9191:HOH:O	1.95	0.66
3:D:210:ARG:CZ	3:D:398:ALA:HB3	2.25	0.66
3:D:821:VAL:HG21	8:D:9498:HOH:O	1.96	0.66
3:D:1144:LEU:HB3	3:D:1166:LEU:HD11	1.77	0.66
3:D:1271:LYS:HG2	3:D:1272:ALA:H	1.60	0.66
5:F:282:LEU:HD11	5:F:286:PRO:HG3	1.76	0.66
2:M:140:ILE:HA	2:M:332:ARG:O	1.94	0.66
2:M:911:GLU:O	2:M:915:LYS:HG2	1.94	0.66
2:C:328:LEU:HB2	2:C:433:THR:HG21	1.77	0.66
2:C:498:GLN:NE2	3:D:1068:LEU:HD12	2.10	0.66
1:K:227:ASN:HD22	1:K:227:ASN:N	1.91	0.66
2:M:367:LEU:HB3	2:M:371:LYS:HG2	1.78	0.66
2:M:1085:PHE:O	2:M:1089:VAL:HG23	1.95	0.66
3:N:120:ALA:HB1	8:N:9749:HOH:O	1.94	0.66
3:N:423:ASP:OD1	5:P:174:LEU:HD13	1.95	0.66
3:N:807:ALA:HB2	3:N:833:GLU:OE1	1.94	0.66
5:P:148:LYS:HG2	8:P:3932:HOH:O	1.95	0.66
5:P:208:SER:HB3	8:P:3885:HOH:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ARG:NH1	1:A:161:ARG:HB2	2.10	0.66
1:B:52:ALA:HB1	8:B:430:HOH:O	1.94	0.66
2:C:290:LEU:HA	8:C:1381:HOH:O	1.96	0.66
2:M:52:PHE:CE1	2:M:66:LEU:HG	2.31	0.66
2:M:660:ALA:HB1	2:M:667:ALA:O	1.96	0.66
3:N:1376:MET:SD	3:N:1421:LEU:HD12	2.36	0.66
2:C:750:LYS:HB3	8:C:1606:HOH:O	1.93	0.66
2:C:930:LYS:HA	8:C:1252:HOH:O	1.96	0.66
3:D:1169:ASP:HB3	8:D:9030:HOH:O	1.95	0.66
1:L:131:THR:HA	8:L:2956:HOH:O	1.95	0.66
3:N:209:ARG:NH2	3:N:397:LYS:HG3	2.11	0.66
3:N:863:VAL:HG23	8:N:9129:HOH:O	1.94	0.66
3:N:1080:GLY:HA3	8:N:9701:HOH:O	1.95	0.66
3:N:1434:TRP:CZ3	3:N:1457:ASP:HB2	2.29	0.66
2:C:480:THR:HG22	2:C:482:GLU:H	1.61	0.66
3:D:528:VAL:O	3:D:535:PHE:HA	1.95	0.66
3:D:1349:VAL:HG11	8:D:9752:HOH:O	1.94	0.66
3:D:1468:LEU:HD22	3:D:1470:ARG:HB2	1.77	0.66
4:E:26:ARG:O	4:E:29:GLN:HG3	1.95	0.66
1:L:95:GLN:HE21	1:L:95:GLN:H	1.43	0.66
3:N:191:LEU:HD12	3:N:211:VAL:HG21	1.77	0.66
3:N:209:ARG:HH22	3:N:397:LYS:HG3	1.60	0.66
1:A:198:ARG:NH2	2:C:932:GLU:HG2	2.11	0.66
2:C:155:PRO:HB2	8:C:1225:HOH:O	1.95	0.66
3:D:89:ARG:O	3:D:521:PRO:HG3	1.96	0.66
3:D:783:ARG:HE	3:D:1029:ARG:NE	1.91	0.66
3:D:1413:THR:HG21	8:D:9279:HOH:O	1.94	0.66
1:L:74:ASP:HA	8:L:3261:HOH:O	1.94	0.66
2:M:513:VAL:HB	8:M:1319:HOH:O	1.95	0.66
3:N:1004:THR:HG21	8:N:9281:HOH:O	1.93	0.66
3:N:1459:LEU:HA	3:N:1464:GLU:OE1	1.95	0.66
5:P:325:LYS:HE2	8:P:2932:HOH:O	1.94	0.66
5:P:371:LEU:HD22	5:P:375:LEU:HD22	1.77	0.66
2:C:41:ASN:H	2:C:41:ASN:ND2	1.92	0.66
2:C:95:TYR:CD2	2:C:114:PHE:HB3	2.30	0.66
2:C:455:LEU:HD23	2:C:455:LEU:H	1.60	0.66
2:C:504:GLU:OE2	2:C:509:ALA:HB2	1.94	0.66
2:M:516:ARG:HE	3:N:1068:LEU:HD13	1.61	0.66
1:A:20:TYR:HD2	1:A:21:GLY:H	1.44	0.66
1:A:161:ARG:HB2	1:A:161:ARG:HH11	1.59	0.66
1:A:219:ARG:CZ	1:B:219:ARG:HG2	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:722:ILE:HG23	2:C:805:ARG:HH21	1.60	0.66
3:D:652:LEU:HA	8:D:9195:HOH:O	1.95	0.66
3:N:570:GLU:HA	3:N:573:MET:HE2	1.77	0.66
3:N:1105:ILE:HD11	3:N:1374:GLN:NE2	2.10	0.66
3:D:148:GLU:HG2	3:D:151:GLN:NE2	2.11	0.66
3:D:964:LEU:HD13	3:D:1058:ARG:HH11	1.61	0.66
5:F:171:LYS:HE3	5:F:175:HIS:NE2	2.11	0.66
1:K:86:VAL:HG23	8:K:3038:HOH:O	1.95	0.66
2:M:197:LEU:HD13	2:M:207:LEU:HD11	1.78	0.66
2:C:42:VAL:HG12	2:C:43:GLY:H	1.61	0.66
2:C:325:ILE:HG22	8:C:1411:HOH:O	1.96	0.66
2:C:328:LEU:HD22	2:C:433:THR:HG22	1.77	0.66
2:C:710:ILE:HD11	2:C:758:ARG:NH2	2.11	0.66
3:D:424:GLY:HA2	3:D:436:GLU:HA	1.78	0.66
3:D:562:ALA:HB1	3:D:567:ILE:CD1	2.25	0.66
3:D:598:ARG:HH22	5:F:318:GLU:C	2.04	0.66
5:F:160:ASP:HA	5:F:163:LEU:HD12	1.78	0.66
1:L:19:GLU:HG3	1:L:201:THR:O	1.96	0.66
2:M:151:ASP:HB2	2:M:157:ARG:O	1.96	0.66
2:M:584:GLU:CD	2:M:584:GLU:H	2.02	0.66
3:N:642:CYS:SG	3:N:716:PHE:HB2	2.36	0.66
3:N:1094:LEU:HD23	3:N:1230:GLY:HA2	1.78	0.66
3:N:1281:VAL:HG21	3:N:1313:VAL:HG21	1.77	0.66
1:B:99:LEU:HD12	1:B:114:PHE:HB3	1.77	0.65
3:D:1087:ARG:HD2	3:D:1256:LEU:HD22	1.78	0.65
1:L:152:PRO:HD2	1:L:155:LYS:HD2	1.76	0.65
2:M:137:VAL:HG23	2:M:391:LEU:HG	1.78	0.65
2:M:1040:LEU:HD21	2:M:1048:THR:HG22	1.78	0.65
3:N:656:PHE:HE2	3:N:698:LYS:HE3	1.59	0.65
3:N:877:PRO:O	3:N:880:ILE:HG22	1.95	0.65
5:P:323:ASP:HB3	8:P:3957:HOH:O	1.94	0.65
2:C:197:LEU:HD12	2:C:207:LEU:HD11	1.78	0.65
3:D:850:LEU:HD12	3:D:850:LEU:H	1.60	0.65
3:D:908:LYS:CB	3:D:1027:GLY:HA3	2.24	0.65
3:D:955:VAL:HB	3:D:1011:PHE:HE1	1.61	0.65
5:F:248:ASN:HA	5:F:251:ILE:HD12	1.78	0.65
2:M:211:LEU:HD12	2:M:308:ARG:HG3	1.76	0.65
3:N:35:ARG:HG3	3:N:36:THR:N	2.10	0.65
3:N:141:ILE:HD11	8:N:9550:HOH:O	1.95	0.65
3:N:656:PHE:HB3	3:N:694:VAL:HG11	1.77	0.65
3:N:844:ALA:O	3:N:867:ARG:HB3	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1272:ALA:HA	3:N:1326:THR:HB	1.76	0.65
1:B:38:ASN:HB3	1:B:39:PRO:HD3	1.78	0.65
3:D:396:VAL:HA	8:D:9468:HOH:O	1.96	0.65
5:F:113:ILE:HA	5:F:116:LEU:HD12	1.78	0.65
1:L:106:PRO:HD3	8:L:3583:HOH:O	1.97	0.65
2:M:3:ILE:HG23	8:M:1340:HOH:O	1.94	0.65
2:M:73:LEU:HB3	2:M:94:LEU:HB2	1.79	0.65
2:M:773:LEU:O	2:M:777:ILE:HG13	1.95	0.65
2:M:859:PRO:O	2:M:867:VAL:HG22	1.96	0.65
3:N:161:LEU:HD22	3:N:452:ILE:HG21	1.78	0.65
2:C:265:ARG:HG2	2:C:267:TYR:H	1.61	0.65
3:D:1455:LYS:HD3	3:D:1456:LYS:N	2.11	0.65
3:D:1492:LEU:HA	8:D:2041:HOH:O	1.96	0.65
3:N:576:GLU:HB2	8:N:9391:HOH:O	1.95	0.65
3:N:1087:ARG:HA	3:N:1090:ASP:HB2	1.79	0.65
3:N:1294:VAL:HB	8:N:9539:HOH:O	1.95	0.65
5:P:85:LEU:HA	5:P:88:ILE:HD12	1.79	0.65
5:P:104:ARG:HB3	8:P:3870:HOH:O	1.97	0.65
5:P:175:HIS:O	5:P:179:GLU:HG3	1.97	0.65
5:P:352:GLU:O	5:P:356:LYS:HG3	1.96	0.65
2:C:185:LYS:HG2	2:C:190:LYS:HG2	1.79	0.65
2:C:838:LYS:HG3	2:C:997:LEU:HB2	1.78	0.65
3:D:434:ARG:HB2	3:D:447:VAL:HG13	1.77	0.65
3:D:704:ARG:NE	3:D:705:ALA:H	1.94	0.65
3:D:1120:VAL:HB	3:D:1144:LEU:HD21	1.77	0.65
1:K:54:THR:HG21	8:K:3561:HOH:O	1.96	0.65
2:M:274:ARG:HB2	2:M:285:LEU:HD13	1.77	0.65
3:N:520:LEU:HD12	3:N:521:PRO:HD2	1.78	0.65
3:N:655:PRO:HA	3:N:658:LEU:HD12	1.78	0.65
1:B:90:LEU:HD23	8:B:356:HOH:O	1.97	0.65
1:B:110:LYS:HZ3	1:B:112:ARG:HD2	1.61	0.65
2:C:186:VAL:HG23	8:C:1357:HOH:O	1.95	0.65
2:C:926:PHE:O	2:C:930:LYS:HG3	1.96	0.65
3:D:111:LYS:HE2	3:D:1452:ILE:HG12	1.78	0.65
3:D:1160:LEU:HD11	3:D:1174:LEU:HD21	1.78	0.65
5:F:166:LEU:O	5:F:171:LYS:HB2	1.96	0.65
2:M:45:GLN:HA	8:M:1223:HOH:O	1.95	0.65
8:N:9970:HOH:O	5:P:135:ILE:HD11	1.97	0.65
5:P:163:LEU:HB3	5:P:174:LEU:HG	1.78	0.65
2:C:678:PRO:HB2	3:D:942:SER:OG	1.97	0.65
2:C:798:GLY:H	2:C:827:VAL:CG1	2.09	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:427:VAL:CG2	3:D:435:VAL:HB	2.26	0.65
3:D:1154:GLU:HG3	3:D:1159:ARG:HG3	1.78	0.65
1:K:117:VAL:HB	1:K:120:VAL:HG12	1.78	0.65
2:M:816:LYS:HB2	2:M:819:VAL:HG21	1.79	0.65
3:N:14:SER:H	3:N:17:LYS:NZ	1.94	0.65
3:N:119:SER:H	3:N:123:LEU:HB2	1.61	0.65
1:A:27:PRO:HD2	8:A:350:HOH:O	1.97	0.65
3:D:537:THR:HA	5:F:317:LEU:HD12	1.77	0.65
3:D:570:GLU:HB2	5:F:214:GLN:HE21	1.62	0.65
3:N:187:LYS:HA	8:N:9174:HOH:O	1.97	0.65
3:N:434:ARG:HB2	3:N:447:VAL:HG22	1.78	0.65
5:P:154:LYS:O	5:P:158:GLU:HG3	1.97	0.65
1:B:47:SER:O	1:B:49:PRO:N	2.29	0.65
2:C:29:ALA:HB2	2:C:337:GLY:HA3	1.78	0.65
2:C:405:ARG:HH12	2:C:563:ASN:ND2	1.94	0.65
3:D:398:ALA:HB2	3:D:445:ARG:HE	1.61	0.65
3:D:817:GLU:HG3	3:D:840:LYS:NZ	2.12	0.65
3:D:1036:ARG:HH21	3:D:1042:ARG:HA	1.61	0.65
3:D:1264:GLU:OE1	3:D:1424:VAL:HG12	1.97	0.65
4:E:59:ASN:HB3	4:E:62:THR:OG1	1.97	0.65
2:M:416:GLY:HA3	8:M:1698:HOH:O	1.96	0.65
2:M:690:ILE:HG23	2:M:852:ILE:HA	1.78	0.65
3:N:654:LYS:HB3	3:N:655:PRO:HD3	1.79	0.65
3:N:783:ARG:HH21	3:N:1029:ARG:CG	2.09	0.65
2:M:918:LEU:HD23	2:M:968:LEU:HA	1.78	0.65
5:P:260:ILE:HD11	5:P:310:ILE:HG22	1.79	0.65
5:P:275:ALA:HA	5:P:278:LEU:HD12	1.79	0.65
3:D:26:VAL:HG11	3:D:44:LEU:HD23	1.79	0.64
3:D:90:MET:HE3	3:D:519:VAL:O	1.96	0.64
3:D:116:LEU:HB3	3:D:118:LEU:HD21	1.79	0.64
3:D:483:HIS:HB2	3:D:484:PRO:HD3	1.79	0.64
2:M:157:ARG:HD2	2:M:314:THR:CG2	2.23	0.64
2:M:304:LEU:HD21	8:M:1371:HOH:O	1.96	0.64
3:N:147:VAL:HG21	8:N:9806:HOH:O	1.96	0.64
3:N:708:LEU:HA	8:N:9285:HOH:O	1.96	0.64
1:B:73:GLU:HB3	1:B:77:GLU:CG	2.27	0.64
2:C:771:GLU:O	2:C:775:ARG:HG2	1.98	0.64
2:C:1090:LYS:HE2	2:C:1112:PHE:CE1	2.27	0.64
3:D:550:ARG:NH1	3:D:573:MET:HB3	2.11	0.64
3:D:701:LEU:HD21	3:D:763:MET:HE3	1.78	0.64
1:L:123:MET:C	1:L:125:PRO:HD3	2.22	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:1018:GLN:HG3	2:M:1060:ILE:HD11	1.79	0.64
3:N:487:ALA:HB3	8:N:9323:HOH:O	1.97	0.64
3:N:890:VAL:HG13	3:N:926:LYS:HD3	1.79	0.64
1:B:58:ILE:HB	1:B:61:VAL:HB	1.77	0.64
1:B:184:THR:HB	1:B:194:LYS:NZ	2.12	0.64
2:C:12:VAL:HG13	2:C:13:ILE:HG23	1.78	0.64
3:D:699:VAL:HG12	3:D:717:GLN:HA	1.79	0.64
3:D:1243:THR:HB	3:D:1253:THR:HG22	1.78	0.64
3:D:1274:ILE:HD11	3:D:1334:GLN:HB3	1.79	0.64
4:E:33:HIS:CD2	4:E:89:MET:HG2	2.33	0.64
2:M:35:PRO:HD2	2:M:38:LYS:HG2	1.77	0.64
2:M:498:GLN:O	2:M:501:THR:HG23	1.97	0.64
2:M:669:GLY:O	2:M:670:GLN:HG3	1.97	0.64
2:M:1037:VAL:HG13	2:M:1049:LEU:HD11	1.79	0.64
3:N:911:LEU:O	3:N:915:VAL:HG23	1.98	0.64
3:N:1310:ARG:O	3:N:1327:ARG:HG3	1.97	0.64
4:O:25:LYS:HA	4:O:28:GLN:NE2	2.12	0.64
2:C:342:ASP:O	2:C:346:VAL:HG23	1.96	0.64
2:C:660:ALA:HB1	2:C:667:ALA:O	1.98	0.64
2:C:685:GLU:HG3	3:D:783:ARG:HD2	1.78	0.64
3:D:85:VAL:HG21	8:D:9019:HOH:O	1.96	0.64
3:D:1075:HIS:HB3	8:D:9589:HOH:O	1.98	0.64
2:M:1082:PRO:HG2	3:N:1469:GLY:HA3	1.78	0.64
2:M:1084:SER:O	2:M:1087:VAL:HG12	1.97	0.64
1:A:101:LEU:HG	1:A:114:PHE:HA	1.79	0.64
2:C:881:ASN:H	2:C:881:ASN:HD22	1.42	0.64
3:D:135:LEU:HD13	3:D:147:VAL:HG23	1.77	0.64
3:D:810:GLU:O	3:D:813:LEU:HG	1.98	0.64
2:M:565:GLN:OE1	2:M:842:ARG:HG2	1.98	0.64
2:M:678:PRO:HD2	8:N:9142:HOH:O	1.96	0.64
3:D:448:GLU:HG3	8:D:9492:HOH:O	1.98	0.64
3:D:1306:PRO:HB3	3:D:1307:LYS:HE3	1.79	0.64
2:M:627:ARG:HA	8:M:1225:HOH:O	1.96	0.64
2:M:636:ALA:HB2	2:M:703:ILE:HG22	1.80	0.64
3:N:448:GLU:HG2	8:N:9338:HOH:O	1.98	0.64
3:N:560:GLN:NE2	5:P:221:ILE:HB	2.13	0.64
1:A:18:ARG:HH12	1:A:88:ARG:NH2	1.96	0.64
1:A:30:ARG:NH1	1:A:191:ASP:HB2	2.13	0.64
1:B:37:GLY:HA2	1:B:40:LEU:HD12	1.79	0.64
1:B:156:HIS:CE1	1:B:166:PRO:HB3	2.33	0.64
3:D:544:TYR:O	3:D:548:ILE:HG12	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:996:TRP:CE3	3:D:999:THR:HG21	2.32	0.64
3:D:1129:THR:O	3:D:1130:ARG:HD2	1.98	0.64
3:D:1501:GLU:HA	8:D:9088:HOH:O	1.95	0.64
1:K:35:THR:HG21	1:L:43:ILE:HD11	1.79	0.64
3:N:400:VAL:HG21	3:N:441:ARG:HH11	1.61	0.64
3:N:443:VAL:HG11	3:N:445:ARG:HE	1.63	0.64
3:N:615:ARG:HB2	3:N:615:ARG:NH1	2.13	0.64
3:N:698:LYS:HA	8:N:9643:HOH:O	1.98	0.64
3:N:1137:ARG:HA	3:N:1140:ILE:HD12	1.79	0.64
1:A:30:ARG:HH11	1:A:191:ASP:HB2	1.62	0.64
2:C:56:GLU:HG3	2:C:64:LEU:HD23	1.80	0.64
2:C:172:ILE:H	2:C:172:ILE:HD12	1.62	0.64
2:C:675:ALA:HA	2:C:989:VAL:HG12	1.80	0.64
3:D:139:GLY:H	3:D:147:VAL:HG21	1.62	0.64
3:D:208:PRO:HB2	3:D:395:VAL:HG22	1.80	0.64
3:D:836:VAL:HG12	8:D:9602:HOH:O	1.96	0.64
3:D:1261:GLU:OE1	3:D:1268:PRO:HA	1.97	0.64
3:D:1384:PRO:HD3	8:D:9043:HOH:O	1.98	0.64
3:D:1466:VAL:HG23	3:D:1472:ILE:HD11	1.79	0.64
5:F:273:ARG:HB3	8:F:555:HOH:O	1.97	0.64
2:M:16:PRO:HG2	2:M:460:ARG:HH12	1.61	0.64
2:M:93:PRO:HA	8:M:1237:HOH:O	1.97	0.64
2:M:95:TYR:CD2	2:M:114:PHE:HB3	2.32	0.64
2:M:612:VAL:HG22	2:M:622:GLU:HA	1.80	0.64
3:N:907:GLU:O	3:N:911:LEU:HD13	1.98	0.64
1:B:103:ALA:O	1:B:138:LEU:HD23	1.98	0.64
2:C:709:GLU:CD	2:C:824:ARG:HH12	2.05	0.64
2:C:838:LYS:HD2	2:C:846:LYS:NZ	2.13	0.64
3:D:804:LEU:HB2	3:D:830:ALA:O	1.98	0.64
1:K:36:LEU:O	1:K:39:PRO:HD2	1.98	0.64
1:K:100:LEU:HG	8:K:3093:HOH:O	1.97	0.64
2:M:367:LEU:O	2:M:372:LEU:HD13	1.97	0.64
2:M:1114:GLY:H	2:M:1115:LEU:HD12	1.62	0.64
3:N:396:VAL:HG21	3:N:447:VAL:HB	1.80	0.64
3:N:422:ALA:HB3	3:N:427:VAL:CG2	2.26	0.64
3:N:899:LEU:HD12	3:N:900:ILE:HG23	1.79	0.64
3:N:917:GLN:HA	8:N:9246:HOH:O	1.98	0.64
5:P:317:LEU:HD23	5:P:330:GLY:HA3	1.79	0.64
5:P:403:LYS:HZ1	5:P:406:ARG:HD2	1.61	0.64
1:B:59:GLU:HG2	1:B:139:ASN:O	1.98	0.64
2:C:886:LEU:HD23	3:D:951:ILE:HG13	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:904:PRO:HD2	2:C:908:GLY:HA2	1.80	0.64
3:D:136:ASP:CB	3:D:137:PRO:HD3	2.27	0.64
3:D:501:ALA:HB1	3:D:1453:ALA:HA	1.80	0.64
3:D:590:PRO:HA	8:D:2066:HOH:O	1.98	0.64
3:D:1215:VAL:HG23	8:D:9465:HOH:O	1.97	0.64
3:D:1459:LEU:HB2	3:D:1470:ARG:HH12	1.63	0.64
5:F:225:GLU:HB3	8:F:496:HOH:O	1.96	0.64
2:M:188:LYS:HD3	8:M:1768:HOH:O	1.96	0.64
2:M:860:HIS:CE1	2:M:975:TYR:HB2	2.33	0.64
2:M:1000:MET:O	2:M:1003:ASP:HB3	1.97	0.64
3:N:6:ARG:NH1	3:N:6:ARG:HB3	2.13	0.64
3:N:87:ARG:CB	3:N:523:ASP:HB2	2.27	0.64
3:N:188:GLY:HA3	8:N:9237:HOH:O	1.97	0.64
3:N:422:ALA:H	3:N:427:VAL:CG1	2.11	0.64
3:N:693:GLU:HG3	4:O:48:MET:SD	2.38	0.64
3:N:1018:ASN:O	3:N:1022:VAL:HG23	1.98	0.64
3:N:1243:THR:OG1	3:N:1253:THR:HB	1.98	0.64
3:N:1279:GLY:O	3:N:1318:TYR:HA	1.98	0.64
5:P:95:THR:HB	5:P:96:LEU:HD23	1.78	0.64
1:A:27:PRO:HG2	1:A:186:LEU:HD22	1.80	0.63
2:M:1013:TYR:HE1	2:M:1020:PRO:HG3	1.62	0.63
4:O:30:LEU:O	4:O:35:PHE:HA	1.97	0.63
5:P:416:ARG:NH1	5:P:419:ARG:HB2	2.13	0.63
1:A:58:ILE:HG21	1:A:68:ILE:HD11	1.79	0.63
2:C:704:HIS:CB	2:C:831:ARG:HE	2.10	0.63
2:C:716:LYS:HE2	8:F:558:HOH:O	1.98	0.63
3:D:97:THR:HG21	3:D:571:LYS:HD3	1.80	0.63
3:D:804:LEU:HD23	3:D:804:LEU:H	1.63	0.63
2:M:34:VAL:HB	2:M:38:LYS:HG3	1.80	0.63
2:M:290:LEU:HB3	2:M:302:VAL:CG1	2.28	0.63
2:M:1115:LEU:HD12	2:M:1115:LEU:N	2.14	0.63
3:N:65:ARG:HG3	3:N:66:GLN:H	1.61	0.63
3:N:1147:ARG:HB3	3:N:1188:VAL:HG21	1.79	0.63
5:P:351:SER:O	5:P:355:GLU:HB2	1.97	0.63
1:B:27:PRO:O	1:B:28:LEU:HD23	1.99	0.63
1:B:206:THR:HG22	1:B:209:GLU:H	1.63	0.63
2:C:470:PRO:HB3	2:C:485:TYR:CZ	2.33	0.63
2:C:663:ASN:HB2	8:C:1359:HOH:O	1.97	0.63
2:C:859:PRO:O	2:C:867:VAL:HG22	1.97	0.63
3:D:510:GLU:O	3:D:513:ILE:HD12	1.99	0.63
3:D:1481:VAL:HG13	4:E:18:ARG:HE	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:108:GLU:HG2	8:L:2956:HOH:O	1.98	0.63
2:M:431:HIS:CD2	2:M:433:THR:H	2.16	0.63
2:M:461:VAL:HG13	2:M:465:GLY:HA2	1.81	0.63
3:N:424:GLY:HA2	3:N:436:GLU:HA	1.80	0.63
3:N:984:THR:H	3:N:987:GLU:CD	2.07	0.63
4:O:16:LYS:HD3	4:O:17:TYR:HE2	1.62	0.63
1:A:97:VAL:HG23	8:A:316:HOH:O	1.99	0.63
1:A:128:HIS:HB2	8:A:408:HOH:O	1.96	0.63
3:D:64:LYS:HD3	5:F:376:ILE:O	1.99	0.63
3:D:178:LEU:HD21	8:D:9071:HOH:O	1.97	0.63
3:D:1399:ASP:O	3:D:1403:LEU:HB2	1.99	0.63
5:F:321:ILE:HD11	5:F:329:TYR:HB2	1.78	0.63
1:L:89:PHE:HB2	1:L:94:LEU:HD13	1.79	0.63
2:M:571:LEU:HD21	2:M:700:TYR:HD2	1.62	0.63
2:M:1050:GLN:HG2	2:M:1079:PRO:HG2	1.80	0.63
3:N:11:ALA:HB1	3:N:507:ASN:OD1	1.98	0.63
3:N:496:LEU:HD23	3:N:1388:ARG:HG2	1.80	0.63
3:D:177:ALA:HB1	3:D:199:LEU:HD22	1.79	0.63
3:D:1311:LEU:HA	8:D:9045:HOH:O	1.99	0.63
3:D:1350:GLU:O	3:D:1354:LYS:HG2	1.98	0.63
1:K:157:GLY:HA3	8:K:5051:HOH:O	1.99	0.63
1:K:197:LEU:HD23	1:K:197:LEU:H	1.62	0.63
2:M:432:ARG:HD2	2:M:519:GLY:HA3	1.80	0.63
2:M:833:LEU:HD11	2:M:849:VAL:HG21	1.79	0.63
2:M:1101:THR:HB	3:N:5:VAL:CG1	2.29	0.63
3:N:25:GLU:HB2	8:N:9156:HOH:O	1.98	0.63
3:N:178:LEU:HD21	8:N:9082:HOH:O	1.97	0.63
3:N:240:GLU:HA	8:N:9487:HOH:O	1.97	0.63
3:N:1123:PHE:HE2	3:N:1184:GLN:HA	1.62	0.63
1:A:36:LEU:O	1:A:39:PRO:HD2	1.98	0.63
1:B:80:LEU:HD21	8:D:9557:HOH:O	1.99	0.63
2:C:579:VAL:HB	2:C:890:LEU:CD2	2.28	0.63
3:D:9:ARG:HA	3:D:1434:TRP:HH2	1.63	0.63
3:D:1047:LYS:HD2	3:D:1051:GLU:OE1	1.99	0.63
2:M:157:ARG:NE	2:M:158:TYR:H	1.95	0.63
2:M:899:GLN:HA	8:M:1664:HOH:O	1.97	0.63
3:N:116:LEU:O	3:N:118:LEU:HG	1.98	0.63
3:N:417:PRO:HA	5:P:168:LYS:NZ	2.13	0.63
3:N:699:VAL:HG12	3:N:717:GLN:HG3	1.80	0.63
2:C:220:GLY:HA3	8:C:1329:HOH:O	1.98	0.63
2:C:777:ILE:HG22	2:C:778:PHE:CD1	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:13:VAL:HA	8:L:3037:HOH:O	1.98	0.63
2:M:958:THR:OG1	2:M:961:GLU:HG2	1.98	0.63
2:M:983:ILE:CG2	2:M:987:ILE:HD11	2.29	0.63
1:A:35:THR:HG21	1:B:43:ILE:HD11	1.81	0.63
3:D:139:GLY:O	3:D:147:VAL:HB	1.99	0.63
3:D:208:PRO:HB2	3:D:395:VAL:HG13	1.79	0.63
3:D:616:GLN:OE1	3:D:619:LEU:HB3	1.98	0.63
3:D:1096:ARG:HH11	3:D:1096:ARG:CB	2.11	0.63
5:F:317:LEU:O	5:F:329:TYR:HB3	1.99	0.63
2:M:397:GLU:H	2:M:633:GLN:HE22	1.47	0.63
2:M:1081:VAL:HG11	2:M:1111:ILE:HG22	1.81	0.63
3:N:1310:ARG:HD2	3:N:1327:ARG:NH2	2.12	0.63
4:O:93:TYR:HB2	8:O:3948:HOH:O	1.99	0.63
1:B:170:VAL:HG22	8:B:430:HOH:O	1.97	0.63
2:C:113:VAL:HG22	8:C:1632:HOH:O	1.97	0.63
2:C:462:ASP:HA	8:C:1164:HOH:O	1.97	0.63
2:C:1004:LYS:HE3	2:C:1027:PHE:HE1	1.62	0.63
3:D:165:LYS:HB3	3:D:395:VAL:HG11	1.81	0.63
2:M:329:GLY:HA3	2:M:489:THR:HG23	1.81	0.63
2:M:601:GLY:HA2	2:M:616:GLU:HG2	1.79	0.63
3:N:197:SER:HB2	3:N:205:TYR:CZ	2.34	0.63
4:O:5:GLY:O	4:O:9:LEU:HG	1.99	0.63
5:P:278:LEU:HD22	5:P:290:GLU:HB3	1.79	0.63
1:A:184:THR:HG23	1:A:192:LEU:HD12	1.79	0.62
5:F:283:GLY:HA3	8:F:696:HOH:O	1.98	0.62
2:M:31:GLN:HA	8:M:1127:HOH:O	1.98	0.62
2:M:71:TYR:H	2:M:71:TYR:HD2	1.47	0.62
3:N:536:ALA:HA	5:P:315:VAL:O	1.99	0.62
3:N:728:LEU:HD22	3:N:745:MET:HE2	1.80	0.62
3:N:810:GLU:O	3:N:813:LEU:HG	1.98	0.62
3:N:975:GLU:O	3:N:979:GLU:HG3	1.99	0.62
5:P:112:ALA:HA	5:P:173:TYR:HD2	1.64	0.62
1:A:14:ARG:HH22	1:A:24:VAL:HG23	1.63	0.62
1:A:91:ASN:HB2	8:A:426:HOH:O	1.98	0.62
2:C:162:ILE:O	2:C:164:PRO:HD3	1.99	0.62
2:C:910:LYS:HB2	2:C:913:GLU:OE1	1.99	0.62
3:D:90:MET:HE1	3:D:518:PRO:HB3	1.81	0.62
3:D:817:GLU:O	3:D:821:VAL:HG23	1.99	0.62
3:D:1406:ARG:HA	8:D:2023:HOH:O	1.98	0.62
2:M:379:GLU:O	2:M:383:ARG:HB3	1.99	0.62
3:N:610:LYS:HG2	3:N:611:GLN:NE2	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:928:ALA:CA	3:N:931:LEU:HD12	2.29	0.62
3:N:1026:SER:HA	8:N:9094:HOH:O	1.99	0.62
3:D:1209:LEU:HD23	3:D:1210:SER:N	2.13	0.62
1:K:42:ARG:HH12	2:M:857:ASP:HB3	1.65	0.62
1:L:78:ILE:HA	8:L:2800:HOH:O	1.99	0.62
2:M:846:LYS:HE3	8:M:1413:HOH:O	1.99	0.62
2:M:890:LEU:HA	2:M:914:ILE:HD13	1.81	0.62
3:N:102:ILE:HD11	8:N:9432:HOH:O	1.99	0.62
3:N:423:ASP:HB2	5:P:178:ARG:HD2	1.80	0.62
1:B:212:ASN:O	1:B:215:VAL:HG22	2.00	0.62
2:C:150:PRO:CA	2:C:158:TYR:HB3	2.28	0.62
2:C:650:ARG:HG3	2:C:653:ASP:HB2	1.80	0.62
2:C:937:ASP:HB2	2:C:940:GLU:HG3	1.80	0.62
3:D:142:LEU:HA	8:D:9173:HOH:O	1.97	0.62
5:F:196:VAL:HG22	5:F:213:ILE:HD13	1.81	0.62
1:L:30:ARG:HH11	1:L:30:ARG:HB2	1.64	0.62
2:M:809:GLY:HA2	8:M:1515:HOH:O	1.98	0.62
3:N:1123:PHE:CE2	3:N:1184:GLN:HA	2.34	0.62
3:N:1277:ILE:HD12	3:N:1301:LYS:HB2	1.81	0.62
1:A:41:ARG:O	1:A:45:LEU:HD12	1.98	0.62
3:D:119:SER:HB2	3:D:123:LEU:N	2.11	0.62
3:D:1337:GLU:HA	8:D:2052:HOH:O	1.98	0.62
3:D:1372:VAL:HA	3:D:1375:MET:SD	2.39	0.62
5:F:196:VAL:HG13	5:F:213:ILE:HD11	1.81	0.62
2:M:971:LYS:HA	2:M:988:VAL:HA	1.80	0.62
3:N:728:LEU:HA	8:N:9469:HOH:O	1.99	0.62
3:N:1166:LEU:H	3:N:1166:LEU:HD23	1.63	0.62
3:N:1435:LEU:HD23	3:N:1464:GLU:HB2	1.80	0.62
2:C:254:VAL:HG13	2:C:258:TYR:HE1	1.64	0.62
2:C:328:LEU:HD11	2:C:434:HIS:HD2	1.64	0.62
2:C:338:GLU:HA	2:C:341:THR:HG22	1.81	0.62
2:C:640:ARG:NH1	2:C:642:ARG:HH22	1.96	0.62
2:C:1035:MET:HE1	8:D:9330:HOH:O	2.00	0.62
3:D:9:ARG:HA	3:D:1434:TRP:CH2	2.35	0.62
1:K:91:ASN:O	1:K:94:LEU:HD12	1.98	0.62
1:L:57:TYR:HE1	1:L:163:ASN:HB2	1.64	0.62
1:L:185:ARG:HG3	1:L:190:THR:HG22	1.80	0.62
2:M:48:PHE:HD2	8:M:1223:HOH:O	1.82	0.62
2:M:676:ILE:O	2:M:676:ILE:HG23	1.98	0.62
3:N:62:LYS:HE2	3:N:75:ARG:NH1	2.15	0.62
3:N:783:ARG:HH21	3:N:1029:ARG:HG2	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1122:LEU:HD11	3:N:1186:VAL:HG23	1.81	0.62
1:A:42:ARG:NH1	2:C:978:ARG:HA	2.14	0.62
2:C:72:ARG:NH1	2:C:72:ARG:HB2	2.15	0.62
2:C:162:ILE:HB	2:C:172:ILE:HD13	1.82	0.62
3:D:207:PHE:HB3	3:D:208:PRO:HD2	1.81	0.62
3:D:1214:PRO:HB2	8:D:2011:HOH:O	1.98	0.62
3:D:1285:GLU:CD	3:D:1285:GLU:H	2.08	0.62
2:M:580:MET:HB3	2:M:584:GLU:CD	2.23	0.62
3:N:41:ARG:HD3	3:N:42:ASP:H	1.65	0.62
3:N:478:LEU:HD21	3:N:500:ARG:HH21	1.65	0.62
3:N:488:ARG:NH1	3:N:488:ARG:HB3	2.15	0.62
5:P:396:ARG:HB2	8:P:2872:HOH:O	2.00	0.62
2:C:3:ILE:HG22	8:C:1178:HOH:O	1.99	0.62
2:C:516:ARG:CZ	3:D:1068:LEU:HD22	2.30	0.62
2:C:704:HIS:CD2	2:C:831:ARG:HH21	2.18	0.62
3:D:723:GLY:HA3	8:D:9008:HOH:O	1.99	0.62
3:D:1279:GLY:O	3:D:1318:TYR:HA	1.99	0.62
1:K:94:LEU:HD21	1:K:119:ASP:HB3	1.81	0.62
2:M:777:ILE:HG22	8:M:1241:HOH:O	2.00	0.62
3:N:95:LEU:CD2	3:N:574:LEU:HD11	2.30	0.62
3:N:421:LEU:HD12	3:N:435:VAL:HG11	1.80	0.62
3:N:704:ARG:HG3	3:N:736:PHE:HB3	1.82	0.62
2:C:706:GLU:HB3	2:C:708:TYR:CE1	2.34	0.62
3:D:28:LYS:HD3	3:D:41:ARG:CZ	2.29	0.62
3:D:537:THR:O	5:F:317:LEU:HB2	1.99	0.62
3:D:570:GLU:OE2	5:F:214:GLN:HG3	1.98	0.62
4:E:26:ARG:HA	4:E:29:GLN:OE1	2.00	0.62
1:L:212:ASN:O	1:L:215:VAL:HG22	2.00	0.62
2:M:254:VAL:HG11	8:M:1850:HOH:O	1.99	0.62
3:N:178:LEU:HB2	8:N:9874:HOH:O	1.99	0.62
3:N:441:ARG:O	3:N:443:VAL:HG23	1.99	0.62
3:N:1129:THR:HG23	3:N:1130:ARG:H	1.65	0.62
3:D:161:LEU:HD22	3:D:452:ILE:HG21	1.81	0.62
3:D:625:TYR:O	3:D:749:VAL:HG23	1.98	0.62
3:D:696:HIS:CD2	4:E:59:ASN:HB2	2.35	0.62
3:D:844:ALA:O	3:D:867:ARG:HB3	1.98	0.62
3:D:1280:VAL:HG23	3:D:1295:GLU:O	2.00	0.62
3:D:1389:LEU:HD12	3:D:1390:LEU:N	2.15	0.62
5:F:361:LEU:CD2	5:F:362:SER:H	2.13	0.62
1:K:20:TYR:HD2	1:K:21:GLY:H	1.47	0.62
2:M:232:GLU:HA	2:M:235:LEU:HD12	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:495:THR:HB	2:M:530:GLU:HG3	1.82	0.62
2:M:768:THR:HB	2:M:771:GLU:HB3	1.82	0.62
3:N:136:ASP:CB	3:N:137:PRO:HD3	2.30	0.62
3:N:705:ALA:HB3	3:N:706:PRO:HD3	1.81	0.62
5:P:277:GLN:O	5:P:280:GLN:HB3	1.99	0.62
5:P:361:LEU:HD23	5:P:362:SER:H	1.65	0.62
2:C:71:TYR:H	2:C:71:TYR:HD2	1.48	0.61
2:C:686:ASP:H	3:D:740:PHE:HD1	1.48	0.61
2:C:816:LYS:HB2	2:C:819:VAL:HG21	1.81	0.61
3:D:605:ASP:HB3	8:D:2071:HOH:O	2.00	0.61
2:M:197:LEU:HB3	2:M:202:TYR:HB2	1.82	0.61
2:M:775:ARG:HD3	8:M:1274:HOH:O	1.99	0.61
2:M:910:LYS:HB3	2:M:912:PRO:HD2	1.81	0.61
2:M:976:ASP:CB	2:M:979:THR:HG22	2.29	0.61
8:M:1274:HOH:O	5:P:421:PHE:HE2	1.83	0.61
3:N:12:LEU:HD11	3:N:512:MET:HG2	1.81	0.61
3:N:529:GLN:HG2	3:N:535:PHE:HE2	1.65	0.61
3:N:561:GLY:HA3	5:P:184:ARG:NH2	2.14	0.61
5:P:142:ARG:HD2	8:P:2896:HOH:O	1.99	0.61
5:P:347:GLN:HA	5:P:350:LEU:CD2	2.27	0.61
1:B:206:THR:CG2	1:B:209:GLU:H	2.13	0.61
2:C:89:THR:HG21	2:C:383:ARG:HH21	1.65	0.61
2:C:243:ARG:HB3	8:C:1850:HOH:O	1.99	0.61
3:D:85:VAL:O	3:D:89:ARG:HD3	1.99	0.61
3:D:117:ASP:HA	8:D:9025:HOH:O	2.00	0.61
3:D:1169:ASP:HB2	8:D:9180:HOH:O	1.99	0.61
3:D:1197:ARG:HG3	3:D:1198:TYR:H	1.64	0.61
1:K:41:ARG:HH11	1:K:177:VAL:HB	1.64	0.61
2:M:16:PRO:CG	2:M:460:ARG:HH12	2.13	0.61
2:M:101:ILE:HG23	2:M:107:LEU:HD22	1.82	0.61
2:M:261:ILE:HD13	8:M:1497:HOH:O	2.00	0.61
8:M:1241:HOH:O	5:P:409:LYS:HB2	1.99	0.61
3:D:127:LEU:HD21	3:D:461:ILE:HD11	1.82	0.61
3:D:153:LEU:HD11	3:D:158:TYR:N	2.15	0.61
3:D:661:MET:HE3	3:D:673:ALA:HB1	1.82	0.61
1:L:80:LEU:HD23	3:N:867:ARG:HH12	1.65	0.61
2:M:158:TYR:HD1	2:M:313:LEU:HD21	1.65	0.61
2:M:839:LEU:HD21	2:M:849:VAL:HG23	1.81	0.61
3:N:543:LEU:HA	3:N:546:ARG:HG3	1.82	0.61
1:B:97:VAL:HG13	8:B:346:HOH:O	2.00	0.61
2:C:49:ARG:HB2	2:C:49:ARG:NH1	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:78:PHE:HB2	2:C:88:LEU:HD21	1.81	0.61
2:C:94:LEU:HD21	8:C:1125:HOH:O	1.99	0.61
2:C:409:ARG:HA	2:C:454:SER:HA	1.80	0.61
2:C:1018:GLN:HE21	2:C:1063:ARG:HH22	1.48	0.61
3:D:15:PRO:HA	3:D:18:ILE:HG12	1.82	0.61
3:D:675:ARG:HH21	5:F:421:PHE:N	1.97	0.61
2:M:244:PRO:HB2	8:M:1637:HOH:O	2.00	0.61
2:M:492:ASP:HB3	2:M:518:LYS:HD2	1.81	0.61
2:M:545:ASN:O	2:M:581:THR:HG21	2.00	0.61
2:M:549:PHE:CD2	2:M:886:LEU:HB3	2.35	0.61
2:M:625:LEU:HB3	2:M:639:GLN:HB2	1.82	0.61
3:N:400:VAL:HG21	3:N:441:ARG:NH1	2.15	0.61
3:N:1000:THR:O	3:N:1003:VAL:HG22	2.00	0.61
5:P:262:VAL:HG12	5:P:266:GLU:OE1	2.00	0.61
1:A:123:MET:O	1:A:125:PRO:HD3	2.01	0.61
2:C:208:ALA:O	2:C:218:VAL:HG21	2.01	0.61
2:C:651:LYS:HA	8:C:1288:HOH:O	2.01	0.61
3:D:4:GLU:HA	8:D:9462:HOH:O	2.01	0.61
3:D:778:LEU:O	3:D:778:LEU:HD23	2.00	0.61
3:D:998:GLU:HA	8:D:9447:HOH:O	1.99	0.61
3:D:1021:TYR:CE1	3:D:1025:GLN:HG3	2.35	0.61
3:D:1236:LEU:HD23	3:D:1359:GLN:NE2	2.16	0.61
3:D:1302:GLU:HB3	8:D:2003:HOH:O	1.99	0.61
2:M:332:ARG:HG2	2:M:332:ARG:NH1	2.15	0.61
2:M:350:ARG:HD3	2:M:353:ARG:NH2	2.16	0.61
2:M:605:LYS:HD3	2:M:610:ARG:NH1	2.15	0.61
3:N:9:ARG:HG3	3:N:1455:LYS:O	2.01	0.61
3:N:427:VAL:CG2	3:N:435:VAL:HB	2.30	0.61
5:P:400:ILE:HA	8:P:3326:HOH:O	1.99	0.61
1:A:54:THR:CG2	1:A:158:ILE:HG13	2.30	0.61
1:A:86:VAL:HG21	1:A:202:ASP:O	2.00	0.61
2:C:532:MET:HG3	2:C:533:ASP:N	2.16	0.61
3:D:965:GLU:O	3:D:968:ASP:HB2	2.00	0.61
3:D:1147:ARG:O	3:D:1165:TYR:HA	2.01	0.61
5:F:361:LEU:HD22	5:F:362:SER:H	1.65	0.61
2:M:1007:ALA:HB2	3:N:648:MET:HG3	1.83	0.61
3:N:130:SER:HB3	3:N:132:TYR:CE1	2.35	0.61
5:P:144:ILE:HB	5:P:145:PRO:HD3	1.81	0.61
3:D:705:ALA:HB3	3:D:706:PRO:HD3	1.83	0.61
3:D:1487:VAL:HG11	3:D:1492:LEU:HD23	1.81	0.61
1:L:100:LEU:O	1:L:115:LEU:HG	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:110:GLU:CG	2:M:369:PRO:HG3	2.28	0.61
3:N:99:ALA:HA	3:N:575:GLN:HE22	1.65	0.61
3:N:100:ALA:HA	8:N:9084:HOH:O	1.99	0.61
3:N:116:LEU:HB3	3:N:118:LEU:HD21	1.82	0.61
3:N:208:PRO:HB2	3:N:395:VAL:HG13	1.82	0.61
5:P:337:HIS:CD2	5:P:337:HIS:H	2.19	0.61
2:C:140:ILE:HD11	2:C:412:ALA:HA	1.82	0.61
3:D:652:LEU:HB3	3:D:653:PHE:HD1	1.65	0.61
3:D:1033:GLN:HE22	3:D:1036:ARG:NH1	1.97	0.61
4:E:25:LYS:O	4:E:29:GLN:HG2	2.01	0.61
5:F:220:LEU:HB2	5:F:243:ILE:HD11	1.83	0.61
1:K:102:LYS:HE2	1:K:139:ASN:CG	2.26	0.61
1:L:188:GLN:HG3	8:N:9878:HOH:O	2.01	0.61
2:M:251:ASP:HB3	2:M:252:LYS:HD2	1.81	0.61
3:N:123:LEU:HD11	3:N:152:LEU:HD21	1.82	0.61
3:N:172:PRO:HD2	3:N:389:GLU:O	2.01	0.61
5:P:156:VAL:HA	5:P:159:ILE:HD12	1.81	0.61
2:C:56:GLU:CG	2:C:64:LEU:HD23	2.31	0.61
2:C:64:LEU:HD22	2:C:359:MET:HG3	1.81	0.61
2:C:431:HIS:H	2:C:434:HIS:CE1	2.18	0.61
2:C:575:GLN:N	2:C:667:ALA:HB1	2.15	0.61
2:C:976:ASP:CB	2:C:979:THR:HG22	2.31	0.61
3:D:133:ILE:HG22	3:D:455:ARG:N	2.15	0.61
3:D:1394:VAL:HB	3:D:1397:LYS:HD2	1.83	0.61
2:M:63:GLY:HA3	2:M:103:LYS:HE2	1.82	0.61
2:M:807:ARG:CZ	2:M:807:ARG:HB2	2.30	0.61
3:N:164:GLY:HA2	8:N:9338:HOH:O	2.00	0.61
3:N:817:GLU:O	3:N:821:VAL:HG23	2.00	0.61
3:N:984:THR:HG22	3:N:987:GLU:H	1.65	0.61
3:N:1147:ARG:O	3:N:1165:TYR:HA	2.00	0.61
3:N:1422:MET:HE3	3:N:1426:LYS:HG3	1.83	0.61
2:C:605:LYS:HG3	2:C:612:VAL:HB	1.81	0.61
2:C:861:LEU:HG	2:C:862:PRO:HD2	1.83	0.61
1:K:216:GLU:O	1:K:220:GLU:HG3	2.00	0.61
1:L:84:GLU:HB2	8:N:9025:HOH:O	2.01	0.61
3:N:842:VAL:HG23	8:N:9576:HOH:O	2.01	0.61
3:N:1324:PRO:HA	8:N:9087:HOH:O	2.00	0.61
1:A:150:TYR:CE1	2:C:696:LYS:HA	2.36	0.60
2:C:537:LYS:H	2:C:537:LYS:HD2	1.65	0.60
2:C:1018:GLN:HG3	2:C:1060:ILE:HD13	1.82	0.60
2:C:1044:GLY:HA3	4:E:17:TYR:CE1	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1299:PHE:HB2	8:D:9130:HOH:O	2.01	0.60
3:N:1493:LYS:HA	3:N:1493:LYS:NZ	2.16	0.60
1:A:11:PHE:CD1	1:B:225:PHE:HA	2.36	0.60
2:C:682:TYR:HE2	8:D:9907:HOH:O	1.85	0.60
2:C:724:ARG:CD	2:C:740:GLU:HA	2.31	0.60
2:C:724:ARG:HD2	2:C:740:GLU:HA	1.81	0.60
2:C:833:LEU:HD12	2:C:834:GLN:N	2.17	0.60
2:C:837:ASP:OD1	2:C:996:LYS:HE3	2.01	0.60
3:D:190:GLU:HB3	8:D:9257:HOH:O	2.01	0.60
3:D:214:GLU:CD	3:D:390:PRO:HB2	2.26	0.60
3:D:1107:VAL:HG12	3:D:1217:ILE:HA	1.82	0.60
1:K:102:LYS:HE2	1:K:139:ASN:ND2	2.15	0.60
1:L:86:VAL:HG12	1:L:124:ASN:HD22	1.66	0.60
2:M:567:GLN:HB2	2:M:997:LEU:HD23	1.83	0.60
3:N:119:SER:N	3:N:123:LEU:HB2	2.16	0.60
3:N:130:SER:O	3:N:568:ARG:NH2	2.34	0.60
3:N:1468:LEU:HD13	3:N:1470:ARG:HB2	1.83	0.60
4:O:70:THR:HG21	4:O:72:ARG:NH2	2.16	0.60
5:P:403:LYS:HA	5:P:403:LYS:HZ2	1.65	0.60
1:A:5:LYS:O	1:A:8:ALA:HB2	2.01	0.60
1:B:5:LYS:O	1:B:8:ALA:HB2	2.02	0.60
2:C:91:GLN:HG2	2:C:119:PRO:HG3	1.83	0.60
3:D:119:SER:HB2	3:D:123:LEU:HB2	1.81	0.60
3:D:658:LEU:HD11	3:D:674:ARG:NH1	2.16	0.60
3:D:966:GLU:HA	3:D:969:ARG:HD2	1.83	0.60
3:D:1320:GLU:HB2	3:D:1323:GLN:HE21	1.65	0.60
3:D:1393:GLN:HB2	3:D:1398:TRP:CZ2	2.36	0.60
4:E:48:MET:N	4:E:54:LEU:HB2	2.15	0.60
1:K:5:LYS:O	1:K:8:ALA:HB2	2.01	0.60
1:K:58:ILE:HB	1:K:61:VAL:HB	1.83	0.60
1:L:2:LEU:HD12	1:L:3:ASP:H	1.66	0.60
2:M:39:ARG:HA	2:M:39:ARG:NE	2.16	0.60
2:M:52:PHE:CD2	2:M:68:PHE:HB2	2.37	0.60
3:N:35:ARG:HG3	3:N:36:THR:H	1.66	0.60
3:N:767:HIS:CD2	4:O:6:ILE:HG12	2.35	0.60
3:N:1314:LYS:HD3	3:N:1314:LYS:N	2.17	0.60
1:B:132:LEU:HD21	1:B:136:GLY:O	2.01	0.60
1:B:158:ILE:HD13	8:B:396:HOH:O	2.01	0.60
2:C:176:VAL:C	2:C:178:PRO:HD3	2.25	0.60
2:C:327:HIS:CE1	2:C:489:THR:HA	2.35	0.60
2:C:1005:MET:HE1	3:D:648:MET:CB	2.29	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:162:ARG:CZ	3:D:162:ARG:HB2	2.31	0.60
3:D:561:GLY:HA3	5:F:184:ARG:HH12	1.65	0.60
3:D:608:SER:HB3	3:D:1443:THR:OG1	2.01	0.60
3:D:1307:LYS:H	3:D:1307:LYS:CD	2.14	0.60
5:F:112:ALA:O	5:F:116:LEU:HG	2.01	0.60
2:M:395:LYS:HE3	2:M:403:SER:OG	2.01	0.60
2:M:515:ALA:O	2:M:516:ARG:HD3	2.01	0.60
2:M:564:MET:HG2	2:M:840:ALA:HB3	1.83	0.60
3:N:9:ARG:NH1	3:N:506:GLY:HA2	2.14	0.60
3:N:566:ILE:HD11	5:P:192:LEU:HD21	1.84	0.60
3:N:658:LEU:HD11	3:N:674:ARG:NH1	2.16	0.60
3:N:831:GLY:HA3	8:N:9080:HOH:O	2.01	0.60
3:N:950:GLY:H	3:N:953:ASP:HB2	1.66	0.60
3:N:1146:GLY:HA3	3:N:1207:TYR:HB2	1.83	0.60
4:O:31:LEU:HD23	4:O:35:PHE:CE1	2.36	0.60
5:P:82:ARG:HG2	5:P:86:HIS:CD2	2.36	0.60
2:C:162:ILE:HD12	2:C:172:ILE:HB	1.83	0.60
2:C:193:LEU:HB2	8:C:1179:HOH:O	2.01	0.60
2:C:625:LEU:HD22	2:C:639:GLN:HB2	1.84	0.60
3:D:3:LYS:HE2	8:D:9538:HOH:O	2.01	0.60
3:D:1267:ARG:HH22	3:D:1333:HIS:CD2	2.17	0.60
3:D:1406:ARG:HH21	3:D:1407:LEU:HG	1.67	0.60
5:F:278:LEU:HB3	5:F:286:PRO:HG2	1.83	0.60
5:F:287:THR:HG23	5:F:289:GLU:HB2	1.83	0.60
5:F:363:GLU:HA	5:F:367:MET:CE	2.31	0.60
1:K:227:ASN:H	1:K:227:ASN:ND2	1.94	0.60
1:L:36:LEU:O	1:L:39:PRO:HD2	2.02	0.60
2:M:902:ILE:HG13	8:M:1340:HOH:O	2.00	0.60
3:N:1124:GLN:N	3:N:1133:ARG:O	2.34	0.60
1:A:43:ILE:HG13	8:A:322:HOH:O	2.01	0.60
2:C:433:THR:HG21	2:C:488:ALA:CB	2.32	0.60
3:D:58:CYS:HA	3:D:78:VAL:HG11	1.84	0.60
3:D:566:ILE:HG23	5:F:214:GLN:OE1	2.02	0.60
3:D:1109:GLU:CD	3:D:1202:GLN:H	2.09	0.60
3:D:1341:PRO:HA	3:D:1344:VAL:HG23	1.83	0.60
4:E:45:ARG:O	4:E:47:LYS:HE3	2.02	0.60
2:M:31:GLN:HB2	8:M:1418:HOH:O	2.00	0.60
2:M:154:ARG:NH2	2:M:156:GLY:HA3	2.15	0.60
2:M:775:ARG:HA	8:M:1274:HOH:O	2.01	0.60
2:M:914:ILE:HD11	2:M:918:LEU:HD13	1.84	0.60
3:N:1301:LYS:HB3	8:N:9539:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:146:VAL:HG22	2:C:162:ILE:HA	1.84	0.60
2:C:1034:GLU:HA	2:C:1037:VAL:HG23	1.84	0.60
3:D:65:ARG:HG2	8:D:9136:HOH:O	2.00	0.60
3:D:1428:ALA:O	3:D:1431:THR:HG23	2.02	0.60
8:D:2041:HOH:O	4:E:80:VAL:HG21	2.00	0.60
1:L:57:TYR:CE1	1:L:163:ASN:HB2	2.37	0.60
2:M:367:LEU:HD23	2:M:371:LYS:HZ2	1.65	0.60
3:N:659:LYS:HE3	3:N:663:GLU:CD	2.27	0.60
3:N:699:VAL:HG21	3:N:760:ARG:HB3	1.83	0.60
1:B:29:GLU:HG3	8:B:446:HOH:O	2.00	0.60
2:C:542:VAL:HG23	2:C:543:ASN:H	1.65	0.60
2:C:698:ASP:HA	8:C:1248:HOH:O	2.00	0.60
2:C:1115:LEU:HD12	2:C:1115:LEU:H	1.67	0.60
3:D:402:PRO:HG2	3:D:444:VAL:HG11	1.83	0.60
3:D:491:LYS:HD3	3:D:492:ALA:N	2.17	0.60
3:D:891:GLU:HG3	8:D:2090:HOH:O	2.01	0.60
2:M:455:LEU:HD12	2:M:456:ALA:O	2.01	0.60
3:N:584:ASN:ND2	3:N:590:PRO:HD2	2.15	0.60
3:N:865:THR:CG2	3:N:874:GLU:HG3	2.32	0.60
3:N:1271:LYS:HG2	3:N:1272:ALA:N	2.16	0.60
5:P:416:ARG:CZ	5:P:419:ARG:HB2	2.31	0.60
2:C:19:THR:O	2:C:23:VAL:HG23	2.02	0.60
2:C:241:LEU:HB2	8:C:1346:HOH:O	2.02	0.60
2:C:493:ARG:HD2	8:C:1692:HOH:O	2.02	0.60
2:C:569:VAL:HG12	2:C:996:LYS:O	2.01	0.60
2:C:583:LEU:O	2:C:587:VAL:HG23	2.02	0.60
2:C:1014:SER:OG	5:F:331:ASP:HA	2.01	0.60
3:D:660:LYS:HA	3:D:660:LYS:HE3	1.84	0.60
3:D:1144:LEU:HA	3:D:1147:ARG:HG3	1.84	0.60
3:D:1262:LEU:HD23	3:D:1352:ILE:CG1	2.32	0.60
1:L:98:THR:HB	8:L:4416:HOH:O	2.02	0.60
2:M:64:LEU:HA	8:M:1327:HOH:O	2.00	0.60
2:M:367:LEU:HD11	8:M:1686:HOH:O	2.01	0.60
2:M:774:LEU:HA	2:M:777:ILE:HD12	1.83	0.60
2:M:1080:SER:HA	8:M:1763:HOH:O	2.02	0.60
3:N:127:LEU:HD21	3:N:461:ILE:HD11	1.83	0.60
3:N:630:VAL:HA	3:N:744:GLN:HG2	1.82	0.60
3:N:1262:LEU:HD21	3:N:1351:GLU:HG3	1.83	0.60
3:N:1389:LEU:HD12	3:N:1390:LEU:N	2.16	0.60
5:P:226:LYS:HB2	5:P:238:TYR:OH	2.02	0.60
1:A:198:ARG:HH21	2:C:932:GLU:HG2	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:408:ARG:NH1	2:C:455:LEU:HG	2.17	0.60
3:D:560:GLN:HG3	5:F:221:ILE:HG21	1.81	0.60
3:D:796:ARG:HH11	3:D:861:GLN:HB2	1.67	0.60
3:D:1310:ARG:NE	3:D:1327:ARG:HB3	2.17	0.60
3:D:1459:LEU:HD13	3:D:1470:ARG:NH1	2.16	0.60
5:F:85:LEU:HD12	8:F:574:HOH:O	2.01	0.60
5:F:356:LYS:O	5:F:360:LYS:HG2	2.02	0.60
1:L:219:ARG:HB3	1:L:219:ARG:NH1	2.14	0.60
2:M:208:ALA:O	2:M:218:VAL:HG21	2.02	0.60
2:M:1048:THR:O	2:M:1052:MET:HE2	2.02	0.60
5:P:261:PRO:O	5:P:265:VAL:HG23	2.02	0.60
5:P:359:SER:HA	8:P:4306:HOH:O	2.02	0.60
2:C:68:PHE:HE1	2:C:96:ALA:HB1	1.67	0.59
2:C:211:LEU:HD11	2:C:308:ARG:HA	1.83	0.59
2:C:516:ARG:HH11	2:C:521:PRO:HB3	1.66	0.59
2:C:585:GLU:O	2:C:588:VAL:HG22	2.01	0.59
3:D:540:LEU:HA	3:D:543:LEU:HD12	1.84	0.59
3:D:584:ASN:ND2	3:D:590:PRO:HD2	2.17	0.59
3:D:820:GLU:HB2	3:D:836:VAL:HG11	1.84	0.59
3:D:1045:MET:HA	3:D:1045:MET:HE3	1.83	0.59
3:D:1243:THR:OG1	3:D:1253:THR:HB	2.02	0.59
3:D:1412:LYS:HG2	3:D:1414:PRO:HG3	1.84	0.59
3:D:1463:LYS:O	3:D:1467:ILE:HD12	2.01	0.59
5:F:126:LEU:O	5:F:130:VAL:HG23	2.02	0.59
5:F:278:LEU:CB	5:F:286:PRO:HG2	2.32	0.59
2:M:769:PRO:HB2	8:N:9172:HOH:O	2.02	0.59
2:M:1043:TYR:HE1	3:N:710:ARG:O	1.85	0.59
2:M:1054:THR:CG2	2:M:1079:PRO:HB3	2.18	0.59
2:M:1097:LEU:H	2:M:1097:LEU:HD22	1.67	0.59
4:O:43:GLU:CD	4:O:43:GLU:H	2.10	0.59
2:C:398:THR:OG1	2:C:633:GLN:HG3	2.02	0.59
3:D:601:ARG:NH2	3:D:612:GLY:HA2	2.17	0.59
3:D:734:GLU:HB3	8:D:9079:HOH:O	2.03	0.59
2:M:41:ASN:O	2:M:46:ALA:HB2	2.02	0.59
2:M:89:THR:HA	2:M:129:ILE:O	2.03	0.59
2:M:626:ARG:H	2:M:639:GLN:NE2	2.00	0.59
2:M:643:VAL:HG13	2:M:647:GLN:CD	2.27	0.59
3:N:471:GLU:O	3:N:475:LYS:HD2	2.02	0.59
3:N:1462:LEU:HD22	3:N:1472:ILE:HG23	1.84	0.59
5:P:404:ALA:O	5:P:408:LEU:HD23	2.02	0.59
2:C:116:GLY:HA3	2:C:378:LEU:HD23	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:181:VAL:HB	8:C:1316:HOH:O	2.02	0.59
2:C:317:VAL:HG12	8:C:1247:HOH:O	2.02	0.59
2:C:530:GLU:HA	8:C:1268:HOH:O	2.03	0.59
2:C:755:LEU:HD21	2:C:792:VAL:HG22	1.82	0.59
3:D:168:THR:HA	8:D:9120:HOH:O	2.02	0.59
3:D:775:GLY:HA3	3:D:1145:TYR:HE1	1.67	0.59
3:D:1213:ARG:HB2	3:D:1214:PRO:CD	2.32	0.59
1:K:156:HIS:HD2	1:K:157:GLY:H	1.49	0.59
1:L:175:ARG:O	3:N:851:LEU:HD21	2.03	0.59
2:M:455:LEU:CD1	2:M:459:ALA:HB3	2.32	0.59
2:M:1002:GLU:HG2	8:P:3095:HOH:O	2.02	0.59
3:N:397:LYS:HD3	8:N:9216:HOH:O	2.01	0.59
2:C:263:ASP:HB2	2:C:264:PRO:HD3	1.84	0.59
2:C:602:GLU:HA	2:C:647:GLN:O	2.03	0.59
2:C:1052:MET:HG3	3:D:623:VAL:CG2	2.32	0.59
3:D:1385:GLY:HA2	8:D:9279:HOH:O	2.01	0.59
1:L:180:GLN:HG2	8:N:9258:HOH:O	2.02	0.59
2:M:69:LEU:HB2	2:M:97:ARG:HB2	1.84	0.59
2:M:342:ASP:O	2:M:346:VAL:HG23	2.02	0.59
2:M:904:PRO:HA	8:M:1161:HOH:O	2.01	0.59
2:M:1095:LEU:HD23	3:N:582:LEU:HD22	1.84	0.59
3:N:572:ARG:HH22	5:P:83:GLN:HG3	1.68	0.59
3:N:847:ASP:HA	3:N:850:LEU:HD13	1.84	0.59
3:N:907:GLU:HG2	3:N:908:LYS:N	2.18	0.59
3:N:1147:ARG:HB3	3:N:1188:VAL:CG2	2.32	0.59
2:C:25:SER:CB	2:C:335:THR:HB	2.32	0.59
2:C:895:TYR:HD1	2:C:991:GLN:HE21	1.51	0.59
3:D:1061:PHE:HA	8:D:9283:HOH:O	2.01	0.59
3:D:1157:GLY:HA2	8:D:9700:HOH:O	2.02	0.59
3:D:1272:ALA:CA	3:D:1326:THR:HB	2.31	0.59
1:K:141:GLU:HA	8:K:3093:HOH:O	2.00	0.59
1:L:180:GLN:HA	8:N:9258:HOH:O	2.02	0.59
3:N:152:LEU:HD23	3:N:152:LEU:N	2.15	0.59
3:N:462:GLN:HG3	3:N:513:ILE:HD13	1.83	0.59
3:N:983:LEU:HA	3:N:987:GLU:OE2	2.02	0.59
3:N:1267:ARG:HB2	3:N:1267:ARG:HH11	1.67	0.59
2:C:720:GLU:HA	2:C:759:THR:O	2.03	0.59
2:C:983:ILE:HG23	3:D:944:THR:O	2.02	0.59
3:D:36:THR:C	3:D:38:LYS:H	2.11	0.59
3:D:491:LYS:HB2	8:D:9725:HOH:O	2.02	0.59
3:D:764:LEU:HB3	8:D:9083:HOH:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:860:LEU:HA	3:D:877:PRO:HB2	1.83	0.59
3:D:1354:LYS:HD2	8:D:9706:HOH:O	2.03	0.59
1:K:10:VAL:HG12	1:K:12:THR:HG22	1.85	0.59
1:K:14:ARG:HG3	1:K:22:GLU:HB2	1.85	0.59
1:L:5:LYS:O	1:L:8:ALA:HB2	2.02	0.59
2:M:212:GLY:HA3	2:M:218:VAL:HG23	1.83	0.59
2:M:332:ARG:HG2	2:M:332:ARG:HH11	1.67	0.59
2:M:603:VAL:HG21	2:M:643:VAL:CG1	2.33	0.59
2:M:798:GLY:H	2:M:827:VAL:CG1	2.15	0.59
2:M:1014:SER:HB3	2:M:1017:THR:O	2.02	0.59
3:N:705:ALA:HB2	8:N:9482:HOH:O	2.02	0.59
3:N:843:PHE:HE1	3:N:864:VAL:HG11	1.67	0.59
2:C:51:THR:HB	2:C:348:LEU:HD23	1.85	0.59
2:C:135:VAL:O	2:C:392:SER:HA	2.03	0.59
3:D:126:VAL:HG12	3:D:132:TYR:HB2	1.85	0.59
3:D:1304:LYS:HA	8:D:9240:HOH:O	2.02	0.59
3:D:1406:ARG:C	3:D:1406:ARG:HE	2.11	0.59
1:K:222:LEU:HD11	1:L:218:LEU:HD23	1.85	0.59
2:M:938:LYS:HB3	2:M:939:ARG:HH21	1.67	0.59
3:N:36:THR:C	3:N:38:LYS:H	2.10	0.59
3:N:149:LYS:HD3	8:N:9307:HOH:O	2.02	0.59
5:P:166:LEU:O	5:P:171:LYS:HB2	2.02	0.59
1:A:133:GLU:HG2	1:A:134:GLU:N	2.16	0.59
2:C:290:LEU:HB3	2:C:302:VAL:CG1	2.33	0.59
2:C:905:ILE:H	2:C:905:ILE:CD1	2.07	0.59
3:D:1050:GLY:HA2	8:D:9344:HOH:O	2.02	0.59
1:K:209:GLU:C	1:K:213:GLN:HE21	2.10	0.59
8:K:3080:HOH:O	1:L:36:LEU:HD12	2.02	0.59
1:L:64:GLU:HG3	8:L:3767:HOH:O	2.01	0.59
1:L:80:LEU:HD23	3:N:867:ARG:NH1	2.18	0.59
1:L:117:VAL:HG13	8:L:3779:HOH:O	2.02	0.59
2:M:173:ASP:O	2:M:184:MET:HA	2.03	0.59
2:M:274:ARG:NH2	2:M:284:ARG:HG2	2.17	0.59
2:M:685:GLU:HG2	3:N:739:ASP:HB2	1.85	0.59
2:M:1015:LEU:HB2	5:P:334:PRO:O	2.02	0.59
3:N:133:ILE:HG21	3:N:454:ALA:CB	2.31	0.59
3:N:169:TYR:H	3:N:169:TYR:HD1	1.49	0.59
3:N:588:GLY:HA2	8:N:9699:HOH:O	2.03	0.59
3:N:629:SER:C	3:N:744:GLN:HG2	2.28	0.59
3:N:679:ARG:HB2	3:N:682:ASP:OD1	2.02	0.59
3:N:920:LEU:HB2	8:N:9246:HOH:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:70:GLU:HA	8:C:1554:HOH:O	2.03	0.59
2:C:328:LEU:HB2	2:C:488:ALA:HB2	1.84	0.59
2:C:470:PRO:HB2	2:C:534:VAL:HG21	1.83	0.59
2:C:682:TYR:HB3	2:C:689:VAL:HG22	1.85	0.59
2:C:778:PHE:CZ	5:F:409:LYS:HB2	2.38	0.59
3:D:128:TYR:CE1	3:D:461:ILE:HG13	2.37	0.59
3:D:380:GLU:O	3:D:382:GLU:N	2.35	0.59
3:D:477:LEU:HD11	3:D:495:ARG:HD3	1.84	0.59
3:D:553:ARG:HH22	5:F:211:ASP:CG	2.11	0.59
3:D:817:GLU:HG3	3:D:840:LYS:HZ2	1.68	0.59
3:D:1320:GLU:H	3:D:1323:GLN:NE2	2.01	0.59
4:E:31:LEU:HD12	4:E:32:ARG:HD3	1.84	0.59
5:F:102:LEU:O	5:F:106:VAL:HG23	2.03	0.59
2:M:62:GLY:HA2	2:M:359:MET:HE1	1.84	0.59
3:N:984:THR:HB	3:N:987:GLU:OE1	2.01	0.59
3:N:1036:ARG:HH21	3:N:1042:ARG:CA	2.07	0.59
3:N:1091:SER:HA	8:N:9056:HOH:O	2.02	0.59
5:P:245:GLN:HB3	8:P:4764:HOH:O	2.02	0.59
1:B:73:GLU:HB3	1:B:77:GLU:HG3	1.85	0.59
1:B:101:LEU:HG	1:B:114:PHE:HA	1.84	0.59
2:C:313:LEU:HD13	2:C:321:GLU:O	2.02	0.59
2:C:798:GLY:HA3	2:C:828:ALA:O	2.03	0.59
2:C:1115:LEU:HD23	3:D:85:VAL:HG13	1.85	0.59
3:D:500:ARG:HG3	3:D:500:ARG:HH11	1.68	0.59
4:E:88:GLU:OE1	4:E:91:ARG:HD2	2.03	0.59
5:F:416:ARG:HB3	8:F:511:HOH:O	2.02	0.59
5:F:420:ASP:O	5:F:422:LEU:HD23	2.03	0.59
2:M:691:SER:HB2	2:M:858:MET:SD	2.42	0.59
2:M:714:ASP:HB2	8:M:1654:HOH:O	2.03	0.59
3:N:125:GLN:HE22	3:N:587:ARG:HH21	1.51	0.59
3:N:434:ARG:HB2	3:N:447:VAL:CG2	2.33	0.59
2:C:549:PHE:CE2	2:C:886:LEU:HB3	2.38	0.58
3:D:130:SER:HB3	3:D:132:TYR:CE1	2.38	0.58
3:D:424:GLY:HA2	3:D:435:VAL:O	2.02	0.58
1:L:62:LEU:HD12	1:L:62:LEU:H	1.67	0.58
2:M:1090:LYS:HE3	3:N:88:TYR:O	2.03	0.58
3:N:629:SER:O	3:N:744:GLN:HG2	2.03	0.58
5:P:85:LEU:HD22	5:P:193:ARG:HD3	1.84	0.58
1:A:216:GLU:HG2	8:A:475:HOH:O	2.02	0.58
2:C:49:ARG:HG3	2:C:266:ARG:HH22	1.68	0.58
3:D:154:THR:HG22	3:D:157:GLU:CD	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:403:LYS:HA	5:F:403:LYS:NZ	2.18	0.58
1:K:126:ASP:HB3	8:K:4974:HOH:O	2.03	0.58
2:M:604:ALA:HB3	2:M:612:VAL:O	2.03	0.58
3:N:584:ASN:CG	3:N:590:PRO:HD2	2.28	0.58
3:N:1104:GLU:O	3:N:1106:VAL:HG23	2.04	0.58
2:C:113:VAL:HG11	2:C:373:VAL:HB	1.84	0.58
2:C:578:VAL:HG13	2:C:671:ASN:HB3	1.86	0.58
3:D:150:ARG:HH11	3:D:150:ARG:HG3	1.68	0.58
3:D:420:VAL:HG23	8:D:9627:HOH:O	2.02	0.58
3:D:637:LEU:HD11	3:D:641:GLN:HB2	1.84	0.58
3:D:1412:LYS:HG3	8:D:9515:HOH:O	2.03	0.58
5:F:168:LYS:HG3	8:F:516:HOH:O	2.03	0.58
1:L:132:LEU:HG	1:L:136:GLY:HA3	1.84	0.58
2:M:54:ILE:HG22	2:M:66:LEU:HB3	1.84	0.58
2:M:203:ASP:OD1	2:M:205:GLU:HG3	2.02	0.58
3:N:1124:GLN:HG2	3:N:1133:ARG:HG2	1.85	0.58
1:B:102:LYS:HE2	1:B:104:GLU:OE1	2.02	0.58
3:D:907:GLU:HG2	3:D:1027:GLY:N	2.17	0.58
3:D:1146:GLY:HA3	3:D:1207:TYR:HB2	1.85	0.58
3:D:1209:LEU:HD23	3:D:1211:MET:H	1.68	0.58
4:E:26:ARG:HD2	4:E:29:GLN:OE1	2.02	0.58
1:K:18:ARG:HH11	1:K:123:MET:HE1	1.68	0.58
2:M:162:ILE:O	2:M:164:PRO:HD3	2.02	0.58
2:M:176:VAL:C	2:M:178:PRO:HD3	2.28	0.58
2:M:357:GLU:O	2:M:360:LEU:HG	2.04	0.58
2:M:575:GLN:H	2:M:667:ALA:HB1	1.68	0.58
2:M:579:VAL:HG11	2:M:887:GLU:HG3	1.84	0.58
2:M:722:ILE:HG13	2:M:757:GLY:O	2.02	0.58
2:M:862:PRO:HG3	2:M:975:TYR:HE1	1.67	0.58
3:N:947:ILE:O	3:N:947:ILE:HD12	2.03	0.58
3:N:1304:LYS:HA	8:N:2011:HOH:O	2.03	0.58
5:P:152:ASP:HA	8:P:2840:HOH:O	2.03	0.58
5:P:152:ASP:HB2	5:P:153:PRO:HD3	1.84	0.58
5:P:163:LEU:HB3	5:P:174:LEU:CG	2.33	0.58
5:P:393:THR:HG22	5:P:394:ARG:H	1.66	0.58
2:C:139:GLN:HE22	2:C:415:PRO:CD	2.17	0.58
2:C:139:GLN:HA	2:C:411:SER:O	2.03	0.58
2:C:487:THR:HA	8:C:1431:HOH:O	2.02	0.58
3:D:810:GLU:HA	3:D:813:LEU:HD23	1.83	0.58
5:F:129:GLU:HB3	5:F:142:ARG:HH21	1.67	0.58
5:F:166:LEU:HB3	5:F:170:HIS:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:52:PRO:CG	3:N:78:VAL:HG13	2.32	0.58
5:P:358:LEU:HD11	5:P:370:LYS:NZ	2.19	0.58
1:B:57:TYR:HE1	1:B:163:ASN:HB2	1.68	0.58
2:C:115:LEU:HD22	2:C:373:VAL:HG11	1.86	0.58
2:C:166:PRO:HD3	2:C:265:ARG:HE	1.68	0.58
2:C:437:ARG:O	2:C:467:ILE:HD13	2.04	0.58
2:C:690:ILE:HD13	2:C:833:LEU:HD21	1.84	0.58
2:C:881:ASN:HD22	2:C:881:ASN:N	1.99	0.58
2:C:1032:PHE:CE1	2:C:1052:MET:HG2	2.37	0.58
2:C:1054:THR:HG22	2:C:1059:ASP:HB2	1.86	0.58
3:D:28:LYS:HB2	8:D:9050:HOH:O	2.03	0.58
3:D:111:LYS:HB3	3:D:512:MET:HE1	1.85	0.58
3:D:523:ASP:O	3:D:526:PRO:HG3	2.04	0.58
3:D:704:ARG:HE	3:D:705:ALA:H	1.50	0.58
3:D:877:PRO:O	3:D:880:ILE:HG22	2.03	0.58
3:D:1104:GLU:HA	3:D:1461:GLY:HA2	1.86	0.58
5:F:79:ASP:HB3	5:F:80:PRO:CD	2.33	0.58
5:F:278:LEU:O	5:F:282:LEU:HG	2.03	0.58
5:F:282:LEU:HD12	5:F:284:ARG:O	2.03	0.58
3:N:134:VAL:HG12	3:N:152:LEU:HB3	1.86	0.58
3:N:208:PRO:HB2	3:N:395:VAL:HG22	1.84	0.58
3:N:1122:LEU:O	3:N:1134:LEU:HD23	2.04	0.58
3:N:1478:SER:O	3:N:1482:ARG:HG3	2.04	0.58
4:O:47:LYS:HE2	4:O:47:LYS:N	2.19	0.58
1:B:41:ARG:HG3	1:B:177:VAL:CG2	2.33	0.58
2:C:110:GLU:HB2	2:C:368:THR:HB	1.86	0.58
3:D:41:ARG:HD2	8:D:9050:HOH:O	2.03	0.58
3:D:584:ASN:CG	3:D:590:PRO:HD2	2.28	0.58
2:M:210:GLU:HA	8:M:1749:HOH:O	2.03	0.58
3:N:756:GLN:O	3:N:760:ARG:HG2	2.04	0.58
4:O:70:THR:HG21	4:O:72:ARG:CZ	2.34	0.58
1:B:10:VAL:HA	8:B:381:HOH:O	2.02	0.58
1:B:80:LEU:HD11	8:D:9557:HOH:O	2.04	0.58
2:C:44:ILE:HB	8:C:1185:HOH:O	2.04	0.58
2:C:897:LEU:HG	2:C:920:GLN:NE2	2.19	0.58
3:D:430:ASP:CG	3:D:431:VAL:H	2.12	0.58
3:D:865:THR:HG23	3:D:874:GLU:HG2	1.84	0.58
3:D:1129:THR:HG23	3:D:1130:ARG:H	1.68	0.58
2:M:460:ARG:HD2	2:M:485:TYR:CE2	2.38	0.58
3:N:131:LYS:HA	3:N:456:MET:HG3	1.86	0.58
5:P:392:VAL:HG12	8:P:2872:HOH:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:GLU:HG3	1:A:139:ASN:CG	2.29	0.58
1:A:91:ASN:OD1	1:A:92:PRO:HD2	2.04	0.58
2:C:159:ILE:HG22	8:C:1786:HOH:O	2.03	0.58
2:C:758:ARG:HB3	2:C:788:THR:O	2.04	0.58
2:C:946:ARG:HB2	8:C:1715:HOH:O	2.03	0.58
3:D:207:PHE:CB	3:D:208:PRO:HD2	2.33	0.58
3:D:1277:ILE:CD1	3:D:1301:LYS:HB2	2.33	0.58
5:F:82:ARG:HG2	5:F:86:HIS:CD2	2.39	0.58
5:F:291:ILE:O	5:F:295:MET:HB2	2.03	0.58
1:L:23:PHE:HD1	8:L:3037:HOH:O	1.86	0.58
2:M:342:ASP:O	2:M:345:ARG:HG3	2.04	0.58
2:M:807:ARG:HB2	2:M:807:ARG:NH1	2.18	0.58
3:N:104:PHE:CD2	3:N:1448:THR:HG23	2.39	0.58
3:N:998:GLU:HG3	8:N:9582:HOH:O	2.04	0.58
5:P:93:LEU:HD12	5:P:191:ASN:HD21	1.68	0.58
5:P:232:ARG:HB3	8:P:3790:HOH:O	2.03	0.58
1:A:36:LEU:O	1:A:40:LEU:HG	2.03	0.58
1:A:57:TYR:CE2	1:A:59:GLU:HA	2.39	0.58
2:C:276:LYS:O	2:C:280:LYS:HB2	2.04	0.58
2:C:678:PRO:HG3	3:D:947:ILE:HD11	1.84	0.58
2:C:691:SER:HA	2:C:858:MET:HE3	1.86	0.58
2:C:695:LEU:HD22	2:C:832:LYS:HG2	1.86	0.58
2:C:1040:LEU:HD21	2:C:1048:THR:HG22	1.84	0.58
2:C:1085:PHE:O	2:C:1089:VAL:HG23	2.04	0.58
3:D:28:LYS:HG2	8:D:9642:HOH:O	2.04	0.58
3:D:178:LEU:HD21	3:D:199:LEU:H	1.69	0.58
3:D:470:LEU:HD11	3:D:509:PRO:HG3	1.86	0.58
3:D:619:LEU:HB2	8:D:9069:HOH:O	2.04	0.58
3:D:1341:PRO:O	3:D:1344:VAL:HG23	2.04	0.58
3:D:1491:THR:O	3:D:1495:ILE:HD13	2.04	0.58
5:F:218:GLN:HE21	5:F:221:ILE:HD12	1.67	0.58
5:F:220:LEU:O	5:F:224:VAL:HG23	2.03	0.58
1:K:39:PRO:O	1:K:43:ILE:HG12	2.04	0.58
1:K:152:PRO:HD2	1:K:155:LYS:HG3	1.85	0.58
2:M:166:PRO:HD3	2:M:265:ARG:HG3	1.85	0.58
2:M:276:LYS:O	2:M:280:LYS:HB2	2.02	0.58
2:M:1111:ILE:CD1	2:M:1112:PHE:H	2.14	0.58
3:N:184:GLU:HA	8:N:9224:HOH:O	2.04	0.58
3:N:1356:TYR:CD2	3:N:1363:LEU:HD23	2.39	0.58
5:P:154:LYS:HB3	8:P:3247:HOH:O	2.03	0.58
5:P:220:LEU:O	5:P:224:VAL:HG23	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ALA:HB2	8:A:343:HOH:O	2.03	0.57
1:A:211:LEU:O	1:A:215:VAL:HG13	2.04	0.57
2:C:29:ALA:HB2	2:C:337:GLY:HA2	1.86	0.57
2:C:66:LEU:HD22	2:C:372:LEU:HD23	1.86	0.57
2:C:433:THR:HA	8:C:1154:HOH:O	2.02	0.57
2:C:847:GLY:HA3	8:C:1126:HOH:O	2.04	0.57
3:D:675:ARG:O	3:D:678:GLU:HG2	2.04	0.57
3:D:920:LEU:HD21	8:D:9121:HOH:O	2.03	0.57
3:D:957:PRO:HB3	3:D:959:GLU:OE1	2.04	0.57
3:D:1047:LYS:HA	3:D:1053:PHE:CE1	2.38	0.57
3:D:1164:ARG:HH11	3:D:1164:ARG:HG3	1.68	0.57
3:D:1205:TYR:HE1	3:D:1221:VAL:HG13	1.67	0.57
5:F:93:LEU:HG	5:F:190:ALA:HB1	1.86	0.57
2:M:611:ILE:HD11	2:M:641:PRO:HG3	1.86	0.57
3:N:119:SER:OG	3:N:123:LEU:HD13	2.03	0.57
3:N:810:GLU:HA	3:N:813:LEU:HD23	1.84	0.57
5:P:187:LEU:HD23	5:P:191:ASN:ND2	2.18	0.57
1:A:178:ALA:CB	2:C:864:GLY:H	2.18	0.57
1:A:191:ASP:O	1:A:192:LEU:HD23	2.04	0.57
1:B:150:TYR:CD2	3:D:857:ILE:HG13	2.38	0.57
2:C:200:LEU:HB2	8:C:1211:HOH:O	2.04	0.57
2:C:383:ARG:HB2	2:C:383:ARG:NH1	2.19	0.57
2:C:752:GLY:H	2:C:792:VAL:HB	1.70	0.57
3:D:576:GLU:C	3:D:576:GLU:CD	2.72	0.57
3:D:1472:ILE:HG22	3:D:1474:ALA:H	1.68	0.57
1:L:38:ASN:HB3	1:L:39:PRO:HD3	1.86	0.57
1:L:65:PHE:CD1	3:N:813:LEU:HD22	2.33	0.57
2:M:503:LEU:HB3	8:M:1190:HOH:O	2.04	0.57
2:M:678:PRO:HG2	3:N:947:ILE:HD11	1.85	0.57
2:M:759:THR:HB	2:M:785:VAL:HG21	1.87	0.57
2:C:320:HIS:HB2	8:C:1663:HOH:O	2.04	0.57
3:D:153:LEU:HD12	3:D:154:THR:H	1.69	0.57
3:D:1232:PRO:HA	3:D:1235:GLN:OE1	2.04	0.57
5:F:113:ILE:HG23	5:F:127:ILE:CG2	2.34	0.57
5:F:152:ASP:HB2	5:F:153:PRO:HD3	1.85	0.57
2:M:328:LEU:H	2:M:433:THR:HG21	1.69	0.57
2:M:1101:THR:HB	3:N:5:VAL:HG13	1.87	0.57
3:N:661:MET:CE	3:N:677:LEU:HD11	2.31	0.57
3:N:774:SER:C	3:N:776:GLU:H	2.13	0.57
3:N:957:PRO:CG	3:N:1007:VAL:HA	2.35	0.57
5:P:81:VAL:HG12	5:P:85:LEU:HG	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:SER:HB3	2:C:856:GLU:HG3	1.86	0.57
2:C:57:GLU:OE1	2:C:63:GLY:HA2	2.05	0.57
2:C:110:GLU:HG2	2:C:369:PRO:CB	2.26	0.57
2:C:1051:GLU:HG2	2:C:1056:LYS:HD2	1.86	0.57
3:D:774:SER:C	3:D:776:GLU:H	2.12	0.57
3:D:1209:LEU:HD11	4:E:16:LYS:HD3	1.87	0.57
1:L:143:ARG:HH12	1:L:158:ILE:HD12	1.68	0.57
2:M:27:ARG:HD2	8:M:1403:HOH:O	2.04	0.57
2:M:874:LEU:CD1	3:N:783:ARG:HB2	2.35	0.57
3:N:823:LEU:HD11	8:N:9446:HOH:O	2.03	0.57
3:N:1127:GLU:HG3	3:N:1133:ARG:NH1	2.18	0.57
3:N:1379:VAL:HG11	3:N:1395:LEU:HD23	1.85	0.57
3:N:1433:SER:HB2	3:N:1457:ASP:OD1	2.04	0.57
5:P:93:LEU:HG	5:P:190:ALA:CB	2.34	0.57
1:A:123:MET:C	1:A:125:PRO:HD3	2.29	0.57
1:B:89:PHE:HB3	1:B:94:LEU:HD13	1.86	0.57
2:C:157:ARG:HA	8:C:1144:HOH:O	2.04	0.57
2:C:177:GLU:HB3	8:C:1316:HOH:O	2.02	0.57
2:C:750:LYS:HB2	3:D:681:ARG:NH2	2.19	0.57
2:C:954:THR:OG1	2:C:957:LYS:HG3	2.03	0.57
3:D:105:VAL:HG13	3:D:124:GLU:OE1	2.05	0.57
3:D:159:ARG:HB2	3:D:159:ARG:HH11	1.69	0.57
3:D:955:VAL:HG21	3:D:1015:TYR:CE2	2.39	0.57
5:F:120:THR:HA	8:F:562:HOH:O	2.04	0.57
5:F:365:GLU:CD	5:F:397:ILE:HA	2.29	0.57
1:K:162:ILE:HG13	1:K:163:ASN:OD1	2.04	0.57
2:M:318:PRO:HD3	8:M:1200:HOH:O	2.05	0.57
3:N:399:ARG:HG2	8:N:9313:HOH:O	2.04	0.57
3:N:1143:GLY:HA2	3:N:1365:ASP:OD1	2.05	0.57
2:C:157:ARG:CZ	2:C:314:THR:HA	2.34	0.57
2:C:575:GLN:H	2:C:667:ALA:HB1	1.68	0.57
2:C:626:ARG:H	2:C:639:GLN:HE21	1.51	0.57
2:C:769:PRO:O	2:C:772:ARG:HB3	2.05	0.57
2:C:885:ILE:HG23	3:D:949:ILE:O	2.05	0.57
2:C:1092:LEU:HD13	2:C:1099:VAL:HG21	1.86	0.57
3:D:42:ASP:O	3:D:46:ASP:HB2	2.04	0.57
3:D:159:ARG:HB2	3:D:159:ARG:NH1	2.20	0.57
3:D:478:LEU:HD23	3:D:496:LEU:HD21	1.86	0.57
3:D:531:ASP:C	3:D:533:GLY:H	2.11	0.57
3:D:840:LYS:HD2	8:D:9835:HOH:O	2.05	0.57
1:L:29:GLU:C	8:L:4886:HOH:O	2.46	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:473:ARG:HD2	2:M:475:VAL:HG22	1.85	0.57
2:M:534:VAL:N	2:M:538:GLN:HE22	2.01	0.57
3:N:421:LEU:HD11	3:N:437:VAL:HG22	1.86	0.57
3:N:524:LEU:HD23	8:N:9282:HOH:O	2.04	0.57
3:N:899:LEU:HB3	3:N:921:ARG:NH1	2.19	0.57
3:N:924:MET:HE1	4:O:10:PHE:CE1	2.39	0.57
4:O:54:LEU:O	4:O:54:LEU:HD23	2.04	0.57
5:P:385:GLU:O	5:P:397:ILE:HD13	2.04	0.57
1:A:127:LEU:HD12	1:A:128:HIS:N	2.18	0.57
1:B:112:ARG:HB3	1:B:112:ARG:NH1	2.20	0.57
2:C:724:ARG:NE	2:C:737:LEU:O	2.38	0.57
3:D:30:GLU:HA	8:D:9510:HOH:O	2.05	0.57
3:D:56:TYR:CE2	3:D:66:GLN:HA	2.39	0.57
3:D:601:ARG:HD2	5:F:328:PHE:CE1	2.38	0.57
3:D:1377:LYS:HE2	3:D:1394:VAL:HG22	1.87	0.57
3:D:1389:LEU:HD12	3:D:1390:LEU:H	1.68	0.57
8:D:2049:HOH:O	5:F:168:LYS:HE3	2.03	0.57
1:L:143:ARG:HH11	1:L:158:ILE:CG2	2.17	0.57
2:M:10:ARG:CZ	2:M:10:ARG:HA	2.34	0.57
2:M:78:PHE:HB2	2:M:88:LEU:HD21	1.86	0.57
2:M:139:GLN:NE2	2:M:418:LEU:HD22	2.19	0.57
2:M:182:VAL:CG1	2:M:193:LEU:HD13	2.33	0.57
2:M:516:ARG:NE	3:N:1068:LEU:HD22	2.20	0.57
3:N:477:LEU:HD21	3:N:495:ARG:HD3	1.86	0.57
3:N:843:PHE:CE1	3:N:864:VAL:HG11	2.39	0.57
3:N:1128:VAL:HB	8:N:9347:HOH:O	2.05	0.57
1:A:101:LEU:HD21	1:A:113:ASP:HB3	1.85	0.57
2:C:300:ASP:HB2	8:C:1289:HOH:O	2.04	0.57
3:D:235:ALA:HB3	8:D:2026:HOH:O	2.04	0.57
3:D:397:LYS:HG3	8:D:9912:HOH:O	2.05	0.57
3:D:637:LEU:CD1	3:D:641:GLN:HB2	2.33	0.57
3:D:1220:ALA:HB1	3:D:1223:ILE:HD13	1.87	0.57
3:D:1266:ARG:O	3:D:1268:PRO:HD3	2.04	0.57
4:E:54:LEU:HD23	4:E:54:LEU:O	2.05	0.57
5:F:385:GLU:O	5:F:397:ILE:HD13	2.05	0.57
2:M:145:GLY:O	2:M:163:ILE:HG23	2.04	0.57
2:M:150:PRO:CA	2:M:158:TYR:HB3	2.31	0.57
2:M:252:LYS:NZ	2:M:296:GLY:HA3	2.20	0.57
2:M:820:ARG:HD3	2:M:821:GLU:HB3	1.86	0.57
2:M:1106:ASP:OD1	3:N:7:LYS:HD2	2.05	0.57
3:N:380:GLU:O	3:N:382:GLU:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1231:GLU:OE1	3:N:1232:PRO:HG3	2.04	0.57
4:O:17:TYR:CD2	4:O:17:TYR:N	2.72	0.57
5:P:207:LEU:HB3	5:P:212:LEU:HG	1.87	0.57
1:A:137:ARG:HD2	1:A:137:ARG:H	1.68	0.57
1:B:196:THR:HG23	8:B:382:HOH:O	2.05	0.57
2:C:41:ASN:O	2:C:46:ALA:HB2	2.05	0.57
2:C:882:LEU:HD22	3:D:951:ILE:HD13	1.85	0.57
3:D:519:VAL:HA	3:D:544:TYR:OH	2.05	0.57
3:D:1491:THR:HG23	8:D:9315:HOH:O	2.03	0.57
5:F:260:ILE:HD11	5:F:310:ILE:HG22	1.86	0.57
1:K:68:ILE:HD13	1:K:138:LEU:HD11	1.86	0.57
1:K:198:ARG:HB2	1:K:200:TRP:CZ3	2.40	0.57
3:N:119:SER:N	3:N:123:LEU:HD22	2.18	0.57
3:N:191:LEU:HB3	3:N:195:VAL:HG21	1.86	0.57
3:N:1379:VAL:HA	3:N:1420:LEU:HB3	1.85	0.57
2:C:200:LEU:HD13	2:C:300:ASP:CG	2.30	0.57
2:C:498:GLN:OE1	3:D:1067:VAL:HB	2.05	0.57
2:C:945:ARG:NH1	2:C:945:ARG:HB3	2.20	0.57
3:D:210:ARG:HB3	3:D:210:ARG:NH1	2.20	0.57
3:D:427:VAL:HB	3:D:435:VAL:HB	1.87	0.57
3:D:659:LYS:C	3:D:659:LYS:HD3	2.29	0.57
3:D:1364:HIS:CE1	3:D:1366:LYS:HG3	2.39	0.57
4:E:43:GLU:HG2	4:E:44:GLU:H	1.69	0.57
5:F:139:ALA:HB2	8:F:644:HOH:O	2.04	0.57
1:K:198:ARG:HB2	1:K:200:TRP:CH2	2.40	0.57
1:L:27:PRO:O	1:L:28:LEU:HD23	2.03	0.57
2:M:680:ASP:HB2	2:M:682:TYR:CD2	2.40	0.57
3:N:53:ILE:HG23	3:N:54:LYS:N	2.19	0.57
3:N:171:LEU:HD13	3:N:389:GLU:C	2.30	0.57
3:N:679:ARG:HD2	8:N:9182:HOH:O	2.03	0.57
3:N:899:LEU:HB3	3:N:921:ARG:HH12	1.70	0.57
3:N:988:ARG:HD2	3:N:989:TYR:N	2.20	0.57
3:N:1406:ARG:HD2	3:N:1412:LYS:HD2	1.86	0.57
1:B:228:PRO:O	1:B:229:GLN:HG3	2.05	0.56
2:C:352:ALA:HA	2:C:355:VAL:HG12	1.87	0.56
2:C:604:ALA:HB3	2:C:612:VAL:O	2.04	0.56
2:C:674:VAL:HG23	2:C:869:VAL:O	2.05	0.56
2:C:1042:ALA:CB	3:D:710:ARG:HB3	2.35	0.56
3:D:525:ARG:HB2	3:D:541:ASN:HD21	1.69	0.56
3:D:1147:ARG:HB3	3:D:1188:VAL:CG2	2.35	0.56
2:M:26:TYR:HD2	2:M:121:MET:HB2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:206:THR:HA	8:M:1787:HOH:O	2.05	0.56
3:N:799:LYS:H	3:N:826:PRO:HG2	1.70	0.56
4:O:31:LEU:HD21	4:O:60:ALA:HB2	1.86	0.56
2:C:630:ARG:NH1	2:C:630:ARG:HG2	2.20	0.56
2:C:728:HIS:HB3	2:C:729:LEU:HD12	1.87	0.56
3:D:133:ILE:HG23	3:D:456:MET:SD	2.46	0.56
3:D:952:ASP:HA	3:D:1062:ARG:HH21	1.70	0.56
3:D:1198:TYR:OH	3:D:1432:LYS:HG2	2.05	0.56
1:L:14:ARG:HG2	8:L:3275:HOH:O	2.04	0.56
2:M:569:VAL:HG12	2:M:996:LYS:O	2.05	0.56
2:M:674:VAL:HG23	2:M:869:VAL:O	2.05	0.56
2:M:1040:LEU:HG	2:M:1045:ALA:CB	2.35	0.56
3:N:197:SER:CB	3:N:203:ALA:HB3	2.27	0.56
3:N:486:ARG:HB3	8:N:9366:HOH:O	2.05	0.56
5:P:350:LEU:HG	5:P:354:LEU:HD12	1.87	0.56
1:A:150:TYR:HE1	2:C:696:LYS:HA	1.71	0.56
1:B:57:TYR:HB3	1:B:141:GLU:HG2	1.86	0.56
2:C:97:ARG:HD2	8:C:1601:HOH:O	2.06	0.56
2:C:231:PRO:HB3	8:C:1721:HOH:O	2.04	0.56
2:C:672:VAL:CG2	2:C:868:ASP:HB2	2.34	0.56
2:C:874:LEU:HD23	3:D:1023:MET:SD	2.45	0.56
3:D:7:LYS:HD3	3:D:1456:LYS:HZ2	1.70	0.56
3:D:44:LEU:HB3	3:D:525:ARG:NH2	2.21	0.56
3:D:386:HIS:HA	8:D:9065:HOH:O	2.04	0.56
3:D:879:ARG:HH21	3:D:903:ASP:C	2.14	0.56
3:D:996:TRP:HE3	3:D:999:THR:HG21	1.68	0.56
3:D:1200:VAL:HG22	3:D:1373:ARG:NH1	2.20	0.56
3:D:1324:PRO:HG3	3:D:1330:ILE:HD11	1.86	0.56
3:D:1379:VAL:HG12	3:D:1419:PRO:HA	1.87	0.56
5:F:370:LYS:HZ3	5:F:371:LEU:HG	1.69	0.56
1:K:46:SER:HB3	2:M:856:GLU:CD	2.30	0.56
1:K:123:MET:O	1:K:125:PRO:HD3	2.05	0.56
1:K:123:MET:C	1:K:125:PRO:HD3	2.31	0.56
2:M:460:ARG:NH1	2:M:460:ARG:HB3	2.20	0.56
3:N:835:SER:HA	8:N:9080:HOH:O	2.05	0.56
3:N:860:LEU:HD22	3:N:878:GLY:HA2	1.86	0.56
4:O:48:MET:HG2	4:O:49:GLN:H	1.70	0.56
5:P:88:ILE:CD1	5:P:193:ARG:HB2	2.30	0.56
5:P:131:VAL:HG12	5:P:181:GLU:HG3	1.86	0.56
5:P:134:LYS:HG3	5:P:178:ARG:NH2	2.20	0.56
5:P:361:LEU:HD22	5:P:366:ALA:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:LEU:O	1:A:44:LEU:HD12	2.05	0.56
2:C:184:MET:HE1	2:C:196:LEU:HD13	1.87	0.56
3:D:93:ILE:CD1	3:D:548:ILE:HD13	2.36	0.56
3:D:214:GLU:HB2	3:D:390:PRO:HD2	1.88	0.56
3:D:703:ASN:ND2	3:D:704:ARG:H	2.03	0.56
4:E:54:LEU:HG	4:E:58:PRO:HG2	1.88	0.56
2:M:139:GLN:HE22	2:M:415:PRO:HG2	1.69	0.56
2:M:139:GLN:O	2:M:333:ILE:HA	2.05	0.56
2:M:200:LEU:HD13	2:M:300:ASP:CG	2.30	0.56
2:M:580:MET:SD	2:M:584:GLU:HG3	2.46	0.56
2:M:1042:ALA:HB3	3:N:710:ARG:HB3	1.87	0.56
3:N:42:ASP:O	3:N:46:ASP:HB2	2.06	0.56
3:N:633:VAL:HG22	3:N:635:PRO:CD	2.30	0.56
3:N:953:ASP:HA	8:N:9114:HOH:O	2.05	0.56
3:N:1341:PRO:O	3:N:1344:VAL:HG23	2.04	0.56
1:A:62:LEU:HD12	8:A:375:HOH:O	2.04	0.56
2:C:736:ASP:HA	2:C:744:ARG:NH1	2.21	0.56
2:C:987:ILE:HG23	3:D:948:THR:CG2	2.36	0.56
3:D:422:ALA:H	3:D:427:VAL:CG1	2.18	0.56
3:D:639:LEU:HD22	3:D:766:ALA:HA	1.87	0.56
3:D:916:TYR:HE2	3:D:920:LEU:HD13	1.69	0.56
3:D:1307:LYS:H	3:D:1307:LYS:HD3	1.71	0.56
5:F:120:THR:HG22	5:F:122:LEU:HD13	1.87	0.56
1:K:20:TYR:CD2	1:K:21:GLY:N	2.74	0.56
2:M:479:VAL:CG2	2:M:503:LEU:HD11	2.35	0.56
3:N:459:GLU:HG3	3:N:460:ALA:N	2.20	0.56
3:N:628:ARG:HD3	3:N:744:GLN:NE2	2.17	0.56
3:N:695:ILE:HG21	3:N:720:LEU:HD11	1.88	0.56
3:N:1036:ARG:NH2	3:N:1042:ARG:HA	2.05	0.56
3:N:1038:LEU:O	3:N:1060:SER:HB2	2.05	0.56
3:N:1066:THR:HG22	3:N:1069:GLU:CG	2.33	0.56
3:N:1136:LYS:O	3:N:1139:ASP:HB2	2.06	0.56
4:O:21:VAL:O	4:O:25:LYS:HG3	2.06	0.56
5:P:358:LEU:CD2	5:P:370:LYS:HE3	2.34	0.56
2:C:129:ILE:HG12	2:C:386:PHE:O	2.05	0.56
2:C:173:ASP:O	2:C:184:MET:HA	2.06	0.56
2:C:979:THR:HG23	2:C:981:GLU:N	2.09	0.56
3:D:1003:VAL:O	3:D:1006:ALA:HB3	2.06	0.56
5:F:226:LYS:HD2	5:F:242:TRP:CZ2	2.40	0.56
1:K:8:ALA:HB1	1:L:224:TYR:CE1	2.41	0.56
1:K:44:LEU:O	1:K:174:VAL:HG21	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:150:TYR:HE1	2:M:696:LYS:HA	1.70	0.56
2:M:26:TYR:O	2:M:30:LEU:HD12	2.06	0.56
2:M:208:ALA:HB1	2:M:218:VAL:HG13	1.87	0.56
2:M:577:PRO:HG3	2:M:993:PHE:CE2	2.40	0.56
2:M:630:ARG:HD3	2:M:705:ILE:HG13	1.87	0.56
2:M:798:GLY:H	2:M:827:VAL:HG11	1.70	0.56
2:M:948:GLU:HB3	8:M:1188:HOH:O	2.04	0.56
2:M:1046:ALA:HB1	3:N:1471:LEU:HD11	1.87	0.56
3:N:84:ILE:HG12	8:N:9092:HOH:O	2.06	0.56
3:N:87:ARG:HD2	3:N:88:TYR:HE2	1.71	0.56
3:N:116:LEU:HD23	3:N:468:LEU:HD11	1.87	0.56
3:N:706:PRO:HA	8:N:9170:HOH:O	2.06	0.56
3:N:953:ASP:OD1	3:N:1019:PRO:HG2	2.06	0.56
3:N:989:TYR:CZ	3:N:993:LEU:HD11	2.40	0.56
3:N:1031:ASN:HB3	3:N:1034:GLN:NE2	2.21	0.56
5:P:407:LYS:HB2	8:P:4644:HOH:O	2.05	0.56
3:D:423:ASP:HB2	5:F:178:ARG:HD2	1.87	0.56
3:D:475:LYS:HA	3:D:478:LEU:HG	1.87	0.56
3:D:829:VAL:HG21	8:D:9103:HOH:O	2.05	0.56
3:D:1087:ARG:O	3:D:1091:SER:HB2	2.06	0.56
3:D:1478:SER:O	3:D:1482:ARG:HG3	2.06	0.56
4:E:91:ARG:HB3	8:E:105:HOH:O	2.05	0.56
2:M:63:GLY:CA	2:M:103:LYS:HE2	2.36	0.56
2:M:269:LEU:HG	2:M:288:ARG:N	2.19	0.56
2:M:602:GLU:HA	2:M:647:GLN:O	2.06	0.56
3:N:423:ASP:OD2	5:P:174:LEU:HD22	2.05	0.56
3:N:434:ARG:HB2	3:N:447:VAL:HG13	1.88	0.56
3:N:1490:LYS:HB3	8:O:4026:HOH:O	2.05	0.56
2:C:189:ARG:HB3	8:C:1497:HOH:O	2.06	0.56
2:C:633:GLN:NE2	2:C:633:GLN:H	2.04	0.56
2:C:724:ARG:HG3	2:C:741:GLY:N	2.14	0.56
2:C:918:LEU:HB3	2:C:968:LEU:HD23	1.88	0.56
3:D:607:LEU:HB3	3:D:614:PHE:HE2	1.70	0.56
3:D:1217:ILE:HD13	3:D:1480:PHE:CE2	2.41	0.56
2:M:21:ILE:H	2:M:21:ILE:HD12	1.70	0.56
2:M:49:ARG:HH11	2:M:49:ARG:HB2	1.71	0.56
2:M:1015:LEU:HA	5:P:335:ASP:HB3	1.88	0.56
3:N:524:LEU:C	3:N:526:PRO:HD3	2.31	0.56
3:N:552:ASN:HA	3:N:555:LYS:HD2	1.87	0.56
3:N:928:ALA:O	3:N:931:LEU:HB2	2.06	0.56
3:N:1404:ASN:ND2	3:N:1408:ILE:HD12	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:33:HIS:HB2	4:O:37:ASN:ND2	2.20	0.56
4:O:73:LEU:HD23	8:O:4394:HOH:O	2.06	0.56
1:B:2:LEU:HD12	1:B:3:ASP:N	2.21	0.56
1:B:86:VAL:HG12	1:B:124:ASN:ND2	2.19	0.56
2:C:289:THR:HG22	2:C:290:LEU:HD22	1.86	0.56
2:C:352:ALA:O	2:C:356:ARG:HG3	2.05	0.56
2:C:987:ILE:HD11	3:D:946:GLY:HA3	1.86	0.56
2:C:1042:ALA:HB3	3:D:710:ARG:HB3	1.88	0.56
3:D:153:LEU:HD13	3:D:157:GLU:HB2	1.87	0.56
3:D:1206:GLY:HA3	3:D:1366:LYS:HZ1	1.71	0.56
5:F:166:LEU:HD13	5:F:170:HIS:HB2	1.88	0.56
1:L:41:ARG:CZ	1:L:177:VAL:HG23	2.36	0.56
3:N:493:ARG:O	3:N:497:GLU:HG3	2.06	0.56
3:N:560:GLN:HE21	5:P:218:GLN:NE2	2.04	0.56
3:N:1087:ARG:NE	3:N:1238:MET:HB2	2.21	0.56
3:N:1478:SER:OG	3:N:1480:PHE:HB3	2.05	0.56
5:P:82:ARG:HG2	5:P:86:HIS:NE2	2.21	0.56
5:P:135:ILE:O	5:P:135:ILE:HD13	2.06	0.56
5:P:144:ILE:HA	8:P:4865:HOH:O	2.05	0.56
5:P:401:GLU:O	5:P:405:LEU:HB2	2.05	0.56
2:C:39:ARG:HE	2:C:39:ARG:HA	1.71	0.56
2:C:212:GLY:HA3	2:C:218:VAL:HG23	1.88	0.56
2:C:281:LEU:CD1	2:C:306:THR:HA	2.28	0.56
2:C:445:GLU:HB2	8:C:1296:HOH:O	2.06	0.56
2:C:679:PHE:C	3:D:943:THR:HG22	2.31	0.56
2:C:724:ARG:CG	2:C:740:GLU:HA	2.36	0.56
3:D:654:LYS:HB3	3:D:655:PRO:CD	2.32	0.56
3:D:969:ARG:O	3:D:972:LEU:HB3	2.06	0.56
5:F:328:PHE:HB3	8:F:674:HOH:O	2.05	0.56
5:F:417:LYS:HG3	8:F:684:HOH:O	2.06	0.56
1:L:143:ARG:HH11	1:L:158:ILE:HG23	1.70	0.56
2:M:404:LEU:O	2:M:407:LYS:HB2	2.06	0.56
2:M:493:ARG:HD2	8:M:1824:HOH:O	2.06	0.56
2:M:1067:TYR:CE1	2:M:1071:ILE:HD11	2.40	0.56
3:N:28:LYS:HB2	3:N:41:ARG:HD2	1.87	0.56
3:N:82:LYS:HE2	8:N:9124:HOH:O	2.05	0.56
3:N:875:THR:HG23	3:N:879:ARG:HE	1.71	0.56
3:N:1176:LYS:HA	3:N:1179:GLU:CD	2.30	0.56
3:N:1310:ARG:HG3	3:N:1327:ARG:HB2	1.86	0.56
5:P:153:PRO:HG2	5:P:154:LYS:H	1.71	0.56
1:A:178:ALA:HB2	2:C:864:GLY:H	1.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:290:LEU:HB3	2:C:302:VAL:HG11	1.88	0.55
2:C:313:LEU:CA	2:C:321:GLU:HG3	2.33	0.55
3:D:116:LEU:HD23	3:D:468:LEU:HD11	1.88	0.55
3:D:434:ARG:HB2	3:D:447:VAL:CG1	2.35	0.55
3:D:728:LEU:HD22	3:D:745:MET:SD	2.46	0.55
4:E:54:LEU:HG	4:E:58:PRO:CG	2.36	0.55
1:K:101:LEU:HD21	1:K:113:ASP:HB3	1.87	0.55
1:K:224:TYR:CD2	1:L:9:PRO:HG2	2.41	0.55
2:M:5:ARG:HB3	2:M:902:ILE:HB	1.88	0.55
2:M:773:LEU:HG	2:M:777:ILE:HD11	1.88	0.55
3:N:245:LEU:HA	8:N:9639:HOH:O	2.06	0.55
3:N:530:VAL:HG23	3:N:534:ARG:O	2.06	0.55
3:N:894:LYS:HG3	8:N:9120:HOH:O	2.06	0.55
3:N:1047:LYS:HB3	3:N:1048:PRO:CD	2.36	0.55
3:N:1262:LEU:HD11	3:N:1351:GLU:HG2	1.88	0.55
5:P:201:LYS:HG2	8:P:3872:HOH:O	2.04	0.55
5:P:264:MET:O	5:P:268:ILE:HG13	2.06	0.55
1:B:150:TYR:CE2	3:D:857:ILE:HG13	2.40	0.55
2:C:902:ILE:O	2:C:904:PRO:HD3	2.06	0.55
2:C:956:GLY:HA2	8:C:1408:HOH:O	2.05	0.55
2:C:1029:GLY:O	3:D:622:ARG:HD3	2.07	0.55
3:D:29:PRO:HG3	3:D:549:ASN:HD21	1.71	0.55
3:D:524:LEU:C	3:D:526:PRO:HD3	2.31	0.55
3:D:1290:LEU:HD22	3:D:1291:SER:H	1.71	0.55
5:F:132:ARG:O	5:F:136:LEU:HG	2.06	0.55
5:F:366:ALA:HB3	5:F:367:MET:HE2	1.86	0.55
2:M:5:ARG:HG3	8:M:1295:HOH:O	2.05	0.55
2:M:410:ILE:HD11	2:M:455:LEU:HB3	1.88	0.55
2:M:571:LEU:HD12	2:M:701:THR:C	2.31	0.55
2:M:575:GLN:OE1	2:M:670:GLN:HB3	2.06	0.55
3:N:80:VAL:HG12	3:N:81:THR:N	2.21	0.55
3:N:183:GLU:HA	3:N:186:VAL:HG12	1.87	0.55
3:N:1102:THR:HG22	3:N:1222:GLY:HA2	1.87	0.55
3:D:112:ILE:HG13	3:D:124:GLU:OE2	2.06	0.55
3:D:604:THR:HA	3:D:607:LEU:HD12	1.88	0.55
3:D:890:VAL:HA	8:D:9150:HOH:O	2.06	0.55
3:D:980:MET:HG3	8:D:9110:HOH:O	2.06	0.55
1:K:37:GLY:HA3	1:K:179:PHE:CD1	2.41	0.55
1:L:18:ARG:HG3	8:L:3742:HOH:O	2.06	0.55
2:M:97:ARG:HG3	8:M:1631:HOH:O	2.06	0.55
2:M:549:PHE:CE2	2:M:886:LEU:HB3	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:488:ARG:HH22	3:N:491:LYS:NZ	2.04	0.55
3:N:834:THR:HG22	3:N:838:ARG:HD2	1.86	0.55
3:N:1042:ARG:O	3:N:1057:VAL:HB	2.05	0.55
3:N:1428:ALA:O	3:N:1431:THR:HG23	2.05	0.55
5:P:351:SER:HA	8:P:3059:HOH:O	2.06	0.55
5:P:355:GLU:HA	8:P:2808:HOH:O	2.06	0.55
1:A:222:LEU:HD12	1:B:215:VAL:CB	2.37	0.55
1:B:184:THR:O	1:B:192:LEU:HB2	2.07	0.55
2:C:197:LEU:HB3	2:C:202:TYR:HB2	1.88	0.55
2:C:802:ARG:HD2	8:C:1186:HOH:O	2.06	0.55
2:C:1033:GLY:HA3	8:C:1885:HOH:O	2.07	0.55
3:D:211:VAL:HG11	8:D:9373:HOH:O	2.06	0.55
3:D:584:ASN:OD1	3:D:590:PRO:HD2	2.06	0.55
5:F:398:ARG:HG2	5:F:402:ASN:HD22	1.72	0.55
1:K:38:ASN:HB3	1:K:39:PRO:HD3	1.87	0.55
1:K:104:GLU:HG2	1:K:105:GLY:N	2.21	0.55
1:L:206:THR:CG2	1:L:209:GLU:H	2.18	0.55
2:M:140:ILE:HD11	2:M:412:ALA:HA	1.88	0.55
2:M:583:LEU:O	2:M:587:VAL:HG23	2.06	0.55
2:M:979:THR:HG23	2:M:981:GLU:HB2	1.88	0.55
3:N:414:ARG:HG2	8:N:9890:HOH:O	2.06	0.55
3:N:1109:GLU:OE1	3:N:1201:CYS:HB2	2.06	0.55
3:N:1462:LEU:HD22	3:N:1472:ILE:CG2	2.36	0.55
5:P:218:GLN:NE2	5:P:221:ILE:HD12	2.21	0.55
5:P:264:MET:O	5:P:267:THR:HB	2.07	0.55
5:P:403:LYS:HD3	8:P:4835:HOH:O	2.07	0.55
1:A:219:ARG:NH2	1:B:223:THR:HG23	2.22	0.55
1:B:27:PRO:HD2	8:B:363:HOH:O	2.06	0.55
1:B:148:VAL:HA	8:B:322:HOH:O	2.05	0.55
2:C:113:VAL:HG21	2:C:373:VAL:HG21	1.89	0.55
2:C:666:LEU:CD2	2:C:668:LEU:HD11	2.36	0.55
3:D:29:PRO:HG3	3:D:549:ASN:ND2	2.21	0.55
3:D:183:GLU:HA	3:D:186:VAL:HG12	1.88	0.55
3:D:210:ARG:HG3	3:D:398:ALA:H	1.72	0.55
3:D:592:THR:N	3:D:600:LEU:HD21	2.22	0.55
3:D:1152:GLU:CD	3:D:1159:ARG:HH12	2.15	0.55
4:E:4:PRO:HB3	8:E:138:HOH:O	2.07	0.55
1:K:150:TYR:CE2	1:K:152:PRO:HG3	2.38	0.55
2:M:114:PHE:HD1	2:M:114:PHE:H	1.52	0.55
2:M:140:ILE:CG2	2:M:333:ILE:HG13	2.35	0.55
2:M:207:LEU:HD22	2:M:221:LEU:HD13	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:585:GLU:HG2	2:M:665:PHE:HD2	1.70	0.55
2:M:697:ARG:HG3	2:M:699:PHE:CD1	2.41	0.55
3:N:1200:VAL:HG22	3:N:1373:ARG:NH1	2.22	0.55
1:A:180:GLN:HB3	8:A:328:HOH:O	2.06	0.55
2:C:51:THR:HG22	8:C:1597:HOH:O	2.06	0.55
2:C:64:LEU:HD11	8:C:1196:HOH:O	2.05	0.55
2:C:203:ASP:HB3	8:C:1639:HOH:O	2.05	0.55
2:C:478:VAL:HG11	8:C:1719:HOH:O	2.06	0.55
2:C:534:VAL:H	2:C:538:GLN:NE2	2.02	0.55
2:C:595:LEU:O	2:C:655:LEU:HG	2.07	0.55
2:C:716:LYS:HG2	8:C:1417:HOH:O	2.06	0.55
2:C:918:LEU:HD23	2:C:967:PHE:O	2.07	0.55
2:C:976:ASP:HB2	2:C:979:THR:HG22	1.89	0.55
3:D:108:VAL:HB	3:D:109:PRO:HD3	1.88	0.55
3:D:1278:ASP:HA	3:D:1319:VAL:O	2.05	0.55
1:K:9:PRO:HD2	1:L:224:TYR:CE1	2.41	0.55
2:M:397:GLU:HG3	2:M:633:GLN:NE2	2.22	0.55
2:M:517:ARG:HB2	8:M:1758:HOH:O	2.07	0.55
2:M:601:GLY:O	2:M:648:ARG:HA	2.06	0.55
2:M:770:GLU:HA	8:M:1825:HOH:O	2.06	0.55
3:N:1047:LYS:HE2	8:N:9823:HOH:O	2.06	0.55
3:N:1278:ASP:HB2	3:N:1318:TYR:OH	2.07	0.55
3:N:1290:LEU:HD11	3:N:1311:LEU:HD22	1.89	0.55
3:N:1357:ARG:HD3	8:N:9210:HOH:O	2.06	0.55
5:P:208:SER:HB2	5:P:211:ASP:CG	2.31	0.55
5:P:287:THR:C	5:P:289:GLU:H	2.15	0.55
1:A:219:ARG:NH1	1:B:223:THR:HG23	2.22	0.55
2:C:732:ALA:HB2	8:C:1371:HOH:O	2.07	0.55
3:D:134:VAL:HG12	3:D:152:LEU:HB3	1.89	0.55
3:D:551:ASN:O	3:D:555:LYS:HG3	2.06	0.55
3:D:695:ILE:HG21	3:D:720:LEU:HD11	1.88	0.55
3:D:704:ARG:HG2	3:D:736:PHE:HB3	1.89	0.55
3:D:842:VAL:HG12	8:D:9557:HOH:O	2.07	0.55
3:D:899:LEU:HD12	3:D:900:ILE:HG23	1.89	0.55
3:D:1397:LYS:O	3:D:1400:VAL:HB	2.07	0.55
2:M:196:LEU:HB2	8:M:1510:HOH:O	2.05	0.55
2:M:520:GLU:HB2	8:M:1758:HOH:O	2.07	0.55
2:M:585:GLU:HG2	2:M:665:PHE:CD2	2.42	0.55
2:M:878:SER:HB3	3:N:1029:ARG:HD3	1.89	0.55
3:N:402:PRO:HG2	3:N:444:VAL:HG11	1.87	0.55
3:N:1097:LYS:HA	8:N:9081:HOH:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:33:HIS:HB3	8:O:3948:HOH:O	2.06	0.55
5:P:218:GLN:HA	5:P:221:ILE:CD1	2.37	0.55
2:C:160:ALA:O	2:C:173:ASP:HA	2.07	0.55
2:C:195:LEU:HD23	2:C:238:LEU:HG	1.89	0.55
2:C:251:ASP:HB3	2:C:252:LYS:HD2	1.89	0.55
3:D:809:PRO:HB2	3:D:812:ALA:HB2	1.88	0.55
5:F:82:ARG:HA	8:F:574:HOH:O	2.06	0.55
5:F:222:ARG:HA	8:F:496:HOH:O	2.07	0.55
2:M:722:ILE:HG21	2:M:821:GLU:OE2	2.07	0.55
3:N:131:LYS:CG	3:N:568:ARG:HG2	2.31	0.55
3:N:178:LEU:HG	3:N:200:ASP:H	1.71	0.55
3:N:838:ARG:HH11	3:N:874:GLU:HG2	1.71	0.55
3:N:1220:ALA:O	3:N:1224:VAL:HG23	2.07	0.55
4:O:69:LEU:HB3	8:O:3383:HOH:O	2.05	0.55
1:A:218:LEU:O	1:A:222:LEU:HD23	2.06	0.55
2:C:436:GLY:HA3	2:C:469:THR:OG1	2.06	0.55
3:D:10:ILE:HG13	3:D:1434:TRP:CZ2	2.42	0.55
3:D:631:ILE:HG21	3:D:745:MET:HG3	1.89	0.55
3:D:722:GLU:HB3	8:D:9352:HOH:O	2.07	0.55
3:D:764:LEU:HD12	3:D:765:SER:N	2.22	0.55
4:E:47:LYS:HA	4:E:54:LEU:HB3	1.88	0.55
2:M:51:THR:OG1	2:M:348:LEU:HD23	2.07	0.55
2:M:132:ALA:HB1	2:M:632:ASN:HD21	1.71	0.55
2:M:209:ARG:O	2:M:213:ALA:HB2	2.07	0.55
2:M:244:PRO:HD3	8:M:1549:HOH:O	2.06	0.55
2:M:902:ILE:O	2:M:904:PRO:HD3	2.07	0.55
3:N:154:THR:HA	8:N:9161:HOH:O	2.07	0.55
3:N:181:ASP:OD2	3:N:199:LEU:HB2	2.07	0.55
3:N:795:VAL:HG11	3:N:863:VAL:HG13	1.88	0.55
1:B:60:ASP:HB2	8:B:383:HOH:O	2.07	0.55
2:C:52:PHE:O	2:C:54:ILE:HG13	2.05	0.55
2:C:139:GLN:HB3	2:C:334:ARG:HD2	1.89	0.55
2:C:290:LEU:HD12	8:C:1289:HOH:O	2.06	0.55
2:C:355:VAL:CG2	2:C:372:LEU:HG	2.37	0.55
3:D:460:ALA:O	3:D:464:LEU:HG	2.07	0.55
3:D:644:LEU:HD12	3:D:645:PRO:HD2	1.89	0.55
5:F:369:LEU:HD11	5:F:401:GLU:HB2	1.88	0.55
1:L:180:GLN:CB	1:L:198:ARG:HH22	2.16	0.55
2:M:49:ARG:HB3	2:M:266:ARG:HH12	1.71	0.55
2:M:1115:LEU:HB3	3:N:85:VAL:HG13	1.88	0.55
3:N:421:LEU:HD12	3:N:435:VAL:CG1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:573:MET:SD	5:P:210:LEU:HD13	2.47	0.55
3:N:676:MET:HE2	3:N:684:LYS:HD2	1.89	0.55
3:N:933:ALA:O	3:N:937:TYR:HD1	1.90	0.55
3:N:1278:ASP:HA	3:N:1319:VAL:O	2.07	0.55
3:N:1346:ARG:CZ	3:N:1346:ARG:HA	2.37	0.55
5:P:268:ILE:HA	5:P:271:LEU:HD12	1.89	0.55
1:A:176:ARG:O	1:A:200:TRP:HE3	1.90	0.54
2:C:1115:LEU:HD12	2:C:1115:LEU:N	2.22	0.54
8:C:1147:HOH:O	3:D:943:THR:HG21	2.07	0.54
3:D:49:ILE:HB	3:D:50:PHE:CD1	2.41	0.54
3:D:192:ALA:O	3:D:195:VAL:HG23	2.07	0.54
3:D:553:ARG:HD3	5:F:214:GLN:HB3	1.89	0.54
3:D:565:ILE:HD11	5:F:189:GLU:OE1	2.07	0.54
3:D:790:TYR:CD2	3:D:1026:SER:HB3	2.42	0.54
3:D:1066:THR:HG22	3:D:1069:GLU:HB2	1.88	0.54
4:E:33:HIS:HB2	4:E:37:ASN:ND2	2.22	0.54
1:L:102:LYS:HG3	1:L:139:ASN:HB2	1.89	0.54
2:M:496:ILE:H	2:M:496:ILE:HD12	1.72	0.54
3:N:1369:GLU:O	3:N:1372:VAL:HG12	2.07	0.54
5:P:323:ASP:HB2	8:P:2932:HOH:O	2.07	0.54
2:C:1014:SER:HB3	2:C:1017:THR:O	2.07	0.54
3:D:126:VAL:O	3:D:132:TYR:HD1	1.91	0.54
3:D:213:VAL:HG22	3:D:214:GLU:H	1.71	0.54
3:D:842:VAL:HG12	8:D:9009:HOH:O	2.07	0.54
4:E:40:LEU:HD22	8:E:184:HOH:O	2.05	0.54
5:F:218:GLN:NE2	5:F:221:ILE:HD12	2.22	0.54
1:K:58:ILE:HG21	1:K:68:ILE:HD11	1.87	0.54
1:K:91:ASN:H	1:K:94:LEU:HD12	1.73	0.54
1:K:101:LEU:HG	1:K:114:PHE:HA	1.88	0.54
2:M:54:ILE:O	2:M:54:ILE:HG23	2.07	0.54
2:M:160:ALA:O	2:M:173:ASP:HA	2.08	0.54
2:M:254:VAL:O	2:M:257:VAL:HG23	2.08	0.54
2:M:431:HIS:H	2:M:434:HIS:CE1	2.25	0.54
2:M:1015:LEU:HB3	2:M:1016:ILE:HD13	1.90	0.54
2:M:1049:LEU:HG	2:M:1053:LEU:HD12	1.88	0.54
3:N:73:CYS:HB3	3:N:76:CYS:O	2.07	0.54
3:N:419:ASP:OD2	5:P:171:LYS:HE3	2.08	0.54
3:N:637:LEU:HD11	3:N:642:CYS:N	2.22	0.54
3:N:863:VAL:HG21	8:N:9257:HOH:O	2.06	0.54
3:N:970:LYS:NZ	3:N:970:LYS:HB2	2.22	0.54
5:P:162:LYS:HA	8:P:1319:HOH:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:VAL:HG21	1:A:82:LEU:HD22	1.88	0.54
1:B:78:ILE:HA	8:B:366:HOH:O	2.05	0.54
1:B:159:LYS:HD3	1:B:159:LYS:N	2.23	0.54
2:C:196:LEU:HD11	2:C:303:PHE:CE1	2.43	0.54
2:C:486:MET:SD	2:C:491:GLU:HA	2.48	0.54
3:D:462:GLN:HG2	8:D:9662:HOH:O	2.07	0.54
3:D:787:LEU:HD21	3:D:947:ILE:HD13	1.88	0.54
3:D:794:GLN:HG2	3:D:905:PRO:HB3	1.90	0.54
3:D:974:ILE:HG22	8:D:9303:HOH:O	2.06	0.54
3:D:1404:ASN:ND2	3:D:1408:ILE:HD12	2.22	0.54
1:L:108:GLU:HB3	8:L:3562:HOH:O	2.07	0.54
2:M:9:ILE:HG12	2:M:907:ASP:OD2	2.07	0.54
2:M:688:ILE:HD11	2:M:847:GLY:HA3	1.89	0.54
2:M:1082:PRO:HA	8:M:1607:HOH:O	2.06	0.54
3:N:28:LYS:HG3	3:N:29:PRO:HD2	1.90	0.54
3:N:56:TYR:HE2	3:N:69:GLU:HB3	1.72	0.54
3:N:68:PHE:O	3:N:71:LYS:HG2	2.08	0.54
3:N:614:PHE:O	3:N:617:ASN:HB2	2.07	0.54
3:N:809:PRO:HB2	3:N:812:ALA:HB2	1.89	0.54
3:N:838:ARG:NH1	3:N:874:GLU:HG2	2.22	0.54
5:P:161:GLN:HA	5:P:164:LYS:NZ	2.22	0.54
2:C:196:LEU:HD21	2:C:303:PHE:CD1	2.41	0.54
2:C:724:ARG:HB2	2:C:740:GLU:HG3	1.89	0.54
3:D:529:GLN:OE1	3:D:533:GLY:HA2	2.08	0.54
3:D:584:ASN:HB2	3:D:602:SER:HB3	1.90	0.54
3:D:615:ARG:HD3	3:D:616:GLN:N	2.22	0.54
3:D:957:PRO:HG2	3:D:1007:VAL:HG12	1.90	0.54
3:D:1068:LEU:HD23	3:D:1072:ILE:HG12	1.89	0.54
5:F:108:GLU:HG3	5:F:176:ILE:CG2	2.38	0.54
5:F:369:LEU:HD23	8:F:443:HOH:O	2.07	0.54
1:K:133:GLU:HG2	1:K:134:GLU:H	1.71	0.54
2:M:710:ILE:CD1	2:M:790:LEU:HB2	2.37	0.54
2:M:838:LYS:HB3	2:M:848:VAL:HG22	1.88	0.54
2:M:1034:GLU:HA	2:M:1037:VAL:HG23	1.89	0.54
3:N:804:LEU:HB2	3:N:830:ALA:O	2.06	0.54
3:N:1110:ALA:HB2	8:N:9805:HOH:O	2.07	0.54
3:N:1380:GLU:HG3	3:N:1381:VAL:N	2.23	0.54
2:C:89:THR:HA	2:C:129:ILE:O	2.08	0.54
2:C:146:VAL:HG22	2:C:162:ILE:HG23	1.90	0.54
2:C:732:ALA:HA	2:C:735:ARG:CZ	2.37	0.54
2:C:945:ARG:HD3	2:C:949:LYS:NZ	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1012:PRO:HD2	2:C:1021:LEU:O	2.07	0.54
3:D:116:LEU:CD2	3:D:468:LEU:HD11	2.38	0.54
3:D:628:ARG:HD3	3:D:744:GLN:HE21	1.71	0.54
3:D:754:PHE:HZ	4:E:21:VAL:HG13	1.72	0.54
3:D:795:VAL:HG23	3:D:879:ARG:HH12	1.73	0.54
3:D:1333:HIS:CE1	3:D:1421:LEU:HD23	2.43	0.54
3:D:1367:HIS:O	3:D:1371:VAL:HG23	2.07	0.54
1:L:81:ASN:O	1:L:84:GLU:HB3	2.07	0.54
1:L:186:LEU:O	1:L:186:LEU:HD23	2.07	0.54
2:M:227:PHE:HA	2:M:230:ARG:HE	1.71	0.54
3:N:9:ARG:HG3	3:N:1455:LYS:C	2.33	0.54
3:N:167:GLU:HG3	8:N:9466:HOH:O	2.06	0.54
3:N:601:ARG:NH2	3:N:606:ILE:HA	2.23	0.54
3:N:1290:LEU:HD23	3:N:1291:SER:N	2.17	0.54
2:C:749:VAL:HG11	2:C:755:LEU:HD23	1.88	0.54
2:C:820:ARG:HG2	8:C:1605:HOH:O	2.08	0.54
3:D:1232:PRO:HB3	3:D:1361:VAL:HG21	1.90	0.54
3:D:1468:LEU:HD22	3:D:1470:ARG:CB	2.38	0.54
5:F:245:GLN:HA	8:F:572:HOH:O	2.06	0.54
1:K:20:TYR:HD2	1:K:21:GLY:N	2.05	0.54
2:M:185:LYS:HB3	2:M:188:LYS:O	2.07	0.54
2:M:358:ARG:HB3	2:M:371:LYS:O	2.08	0.54
2:M:408:ARG:NH1	2:M:542:VAL:HG23	2.23	0.54
2:M:424:GLY:O	2:M:427:VAL:HG23	2.08	0.54
2:M:455:LEU:HD12	2:M:459:ALA:HB3	1.89	0.54
2:M:607:ASP:HB3	2:M:609:ASN:H	1.72	0.54
3:N:702:LEU:HD13	3:N:716:PHE:CD1	2.43	0.54
3:N:1104:GLU:HA	3:N:1461:GLY:HA2	1.89	0.54
5:P:167:PRO:HB2	5:P:169:GLU:OE2	2.08	0.54
1:A:90:LEU:HD12	1:A:119:ASP:O	2.07	0.54
2:C:194:VAL:HG23	8:C:1179:HOH:O	2.06	0.54
2:C:242:LEU:HD23	8:C:1853:HOH:O	2.08	0.54
2:C:333:ILE:CD1	2:C:467:ILE:HG13	2.37	0.54
2:C:341:THR:CG2	2:C:345:ARG:HH21	2.20	0.54
2:C:555:ALA:HA	3:D:1070:TYR:OH	2.06	0.54
2:C:631:SER:HB3	2:C:637:LEU:HD21	1.89	0.54
2:C:886:LEU:CD2	3:D:951:ILE:HG13	2.38	0.54
3:D:948:THR:O	3:D:949:ILE:HD13	2.08	0.54
3:D:1047:LYS:HG2	3:D:1053:PHE:CE2	2.42	0.54
3:D:1314:LYS:HB2	8:D:9676:HOH:O	2.06	0.54
3:D:1465:ASN:HD21	3:D:1470:ARG:HD3	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:287:THR:C	5:F:289:GLU:H	2.15	0.54
1:K:30:ARG:HD3	8:K:3174:HOH:O	2.07	0.54
1:K:43:ILE:HD12	1:L:32:PHE:CZ	2.43	0.54
2:M:202:TYR:HA	8:M:1314:HOH:O	2.07	0.54
2:M:204:GLN:HG3	8:M:1527:HOH:O	2.08	0.54
2:M:210:GLU:HB3	8:M:1386:HOH:O	2.07	0.54
2:M:672:VAL:CG2	2:M:868:ASP:HB2	2.37	0.54
3:N:211:VAL:HG13	3:N:393:ILE:HA	1.90	0.54
3:N:523:ASP:O	3:N:526:PRO:HG3	2.08	0.54
3:N:828:LYS:HB3	8:N:9129:HOH:O	2.08	0.54
3:N:860:LEU:HA	3:N:877:PRO:HB2	1.89	0.54
3:N:1277:ILE:HA	8:N:9618:HOH:O	2.07	0.54
5:P:323:ASP:C	5:P:325:LYS:H	2.15	0.54
1:A:212:ASN:O	1:A:215:VAL:HG22	2.07	0.54
2:C:73:LEU:HB3	2:C:94:LEU:HB2	1.90	0.54
2:C:83:CYS:HA	2:C:88:LEU:HD23	1.90	0.54
2:C:535:SER:H	2:C:538:GLN:NE2	2.06	0.54
2:C:580:MET:HB3	2:C:584:GLU:OE2	2.08	0.54
8:C:1147:HOH:O	3:D:940:THR:HA	2.07	0.54
3:D:135:LEU:CD1	3:D:147:VAL:HG23	2.38	0.54
3:D:530:VAL:HG12	3:D:531:ASP:H	1.72	0.54
3:D:929:ARG:HH11	3:D:929:ARG:HG3	1.73	0.54
3:D:1205:TYR:CD2	3:D:1215:VAL:HG21	2.42	0.54
4:E:9:LEU:HD22	4:E:19:LEU:HD11	1.90	0.54
1:K:218:LEU:O	1:K:222:LEU:HD23	2.07	0.54
1:L:67:THR:HA	8:L:3261:HOH:O	2.07	0.54
2:M:42:VAL:HG12	2:M:43:GLY:H	1.72	0.54
2:M:103:LYS:HD2	8:M:1331:HOH:O	2.06	0.54
2:M:328:LEU:CD2	2:M:437:ARG:HD3	2.37	0.54
2:M:397:GLU:OE2	2:M:632:ASN:HB2	2.08	0.54
2:M:630:ARG:HH21	2:M:707:ARG:H	1.54	0.54
2:M:1013:TYR:HD1	2:M:1020:PRO:HA	1.73	0.54
2:M:1090:LYS:HE2	2:M:1112:PHE:CE1	2.43	0.54
2:M:1109:VAL:HG11	3:N:5:VAL:HG22	1.90	0.54
3:N:478:LEU:HD21	3:N:500:ARG:NH2	2.22	0.54
3:N:567:ILE:C	3:N:571:LYS:HZ2	2.16	0.54
3:N:834:THR:CG2	3:N:838:ARG:HD2	2.38	0.54
3:N:1280:VAL:O	3:N:1294:VAL:HA	2.08	0.54
2:C:3:ILE:HD13	2:C:900:ARG:O	2.07	0.54
2:C:214:TYR:HB3	8:C:1697:HOH:O	2.08	0.54
2:C:691:SER:HB3	2:C:868:ASP:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:715:THR:HG22	2:C:717:LEU:HG	1.89	0.54
2:C:722:ILE:HG22	8:C:1846:HOH:O	2.06	0.54
3:D:379:ALA:HB3	8:D:9652:HOH:O	2.08	0.54
3:D:503:LEU:HA	3:D:508:ARG:HH22	1.73	0.54
3:D:1102:THR:HG22	3:D:1222:GLY:HA2	1.90	0.54
3:D:1114:THR:HG23	3:D:1114:THR:O	2.08	0.54
3:D:1382:THR:HG21	3:D:1418:LYS:NZ	2.23	0.54
5:F:99:GLU:HB2	8:F:540:HOH:O	2.08	0.54
2:M:37:GLU:HG2	8:M:1585:HOH:O	2.08	0.54
3:N:121:THR:C	8:N:9808:HOH:O	2.51	0.54
3:N:217:LYS:HA	8:N:9812:HOH:O	2.08	0.54
3:N:852:ALA:O	3:N:857:ILE:HG12	2.08	0.54
3:N:864:VAL:HA	8:N:9349:HOH:O	2.07	0.54
3:N:892:ASP:HB3	3:N:895:VAL:CG2	2.38	0.54
3:N:1156:LEU:CD1	3:N:1176:LYS:HD2	2.38	0.54
3:N:1382:THR:HG22	8:N:9076:HOH:O	2.08	0.54
3:N:1425:THR:HG23	3:N:1426:LYS:N	2.23	0.54
1:A:128:HIS:CE1	1:A:131:THR:HG23	2.43	0.54
1:B:65:PHE:CD1	3:D:813:LEU:HD22	2.43	0.54
2:C:1090:LYS:HE3	3:D:88:TYR:O	2.08	0.54
3:D:28:LYS:HB2	3:D:41:ARG:HD2	1.89	0.54
3:D:391:ALA:HB3	8:D:9451:HOH:O	2.08	0.54
3:D:767:HIS:CD2	4:E:6:ILE:HG12	2.43	0.54
3:D:860:LEU:HD23	3:D:877:PRO:HB2	1.91	0.54
3:D:992:ILE:O	3:D:995:LEU:HB3	2.08	0.54
3:D:1271:LYS:HG2	8:D:9063:HOH:O	2.07	0.54
4:E:63:TRP:O	4:E:67:GLU:HG3	2.08	0.54
1:K:19:GLU:HB3	1:K:175:ARG:NH2	2.15	0.54
1:K:159:LYS:HE2	8:K:3739:HOH:O	2.07	0.54
2:M:158:TYR:CD1	2:M:313:LEU:HD21	2.42	0.54
2:M:165:LEU:HD12	2:M:166:PRO:C	2.32	0.54
2:M:290:LEU:HB3	2:M:302:VAL:HG11	1.89	0.54
2:M:578:VAL:HG13	2:M:671:ASN:OD1	2.08	0.54
2:M:1012:PRO:HD2	2:M:1021:LEU:O	2.08	0.54
2:M:1015:LEU:HD13	5:P:335:ASP:HA	1.89	0.54
2:M:1067:TYR:O	2:M:1071:ILE:HG12	2.08	0.54
3:N:424:GLY:HA2	3:N:435:VAL:O	2.08	0.54
3:N:1066:THR:CG2	3:N:1069:GLU:HG3	2.36	0.54
3:N:1220:ALA:HB1	3:N:1223:ILE:CD1	2.37	0.54
3:N:1321:ALA:HB3	3:N:1339:LYS:HE2	1.90	0.54
3:N:1472:ILE:HG22	3:N:1474:ALA:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:48:MET:HB2	4:O:54:LEU:HB2	1.90	0.54
5:P:74:LYS:HE3	8:P:2868:HOH:O	2.07	0.54
5:P:376:ILE:HG22	5:P:377:ASP:OD1	2.08	0.54
1:A:18:ARG:O	1:A:207:PRO:HD3	2.08	0.53
1:B:214:ALA:HA	1:B:217:ILE:HD12	1.89	0.53
2:C:405:ARG:HD3	2:C:543:ASN:OD1	2.08	0.53
2:C:487:THR:HG23	8:C:1431:HOH:O	2.08	0.53
2:C:798:GLY:H	2:C:827:VAL:HG11	1.70	0.53
2:C:848:VAL:HG23	3:D:740:PHE:O	2.08	0.53
3:D:154:THR:CG2	3:D:156:GLU:HG2	2.37	0.53
3:D:156:GLU:CD	3:D:156:GLU:N	2.66	0.53
3:D:1236:LEU:HA	3:D:1359:GLN:OE1	2.08	0.53
3:D:1463:LYS:HG2	8:D:9761:HOH:O	2.08	0.53
1:L:24:VAL:HG12	1:L:26:GLU:OE2	2.08	0.53
1:L:86:VAL:HG12	1:L:124:ASN:ND2	2.22	0.53
2:M:431:HIS:HD2	2:M:433:THR:H	1.56	0.53
2:M:473:ARG:HA	2:M:531:PHE:HD1	1.73	0.53
2:M:499:ALA:HA	8:M:1410:HOH:O	2.08	0.53
2:M:549:PHE:CZ	2:M:886:LEU:HD12	2.43	0.53
2:M:697:ARG:HB2	8:M:1159:HOH:O	2.07	0.53
2:M:876:VAL:O	2:M:879:ARG:O	2.26	0.53
3:N:165:LYS:HE2	3:N:165:LYS:HA	1.89	0.53
3:N:396:VAL:HG13	3:N:447:VAL:HA	1.90	0.53
3:N:1420:LEU:HD12	3:N:1421:LEU:H	1.70	0.53
1:A:108:GLU:HB3	8:A:384:HOH:O	2.07	0.53
2:C:138:SER:HB2	2:C:410:ILE:HG13	1.90	0.53
2:C:184:MET:HE2	2:C:191:PHE:CE2	2.43	0.53
2:C:193:LEU:HD11	8:C:1760:HOH:O	2.08	0.53
2:C:216:GLU:HA	8:C:1237:HOH:O	2.07	0.53
2:C:554:ASP:HB2	2:C:880:MET:HB2	1.89	0.53
2:C:586:ARG:HG2	8:C:1243:HOH:O	2.08	0.53
2:C:812:GLY:HA3	8:C:1432:HOH:O	2.07	0.53
2:C:1060:ILE:CG2	2:C:1061:GLU:N	2.71	0.53
2:C:1100:GLN:HG3	2:C:1101:THR:O	2.08	0.53
3:D:400:VAL:HG21	3:D:441:ARG:NH1	2.14	0.53
3:D:650:LEU:HD22	3:D:688:TRP:CZ3	2.43	0.53
3:D:674:ARG:HD2	8:F:469:HOH:O	2.09	0.53
3:D:704:ARG:HH11	3:D:738:ALA:HB2	1.73	0.53
3:D:903:ASP:HB2	8:D:9514:HOH:O	2.07	0.53
3:D:1095:THR:N	8:D:9051:HOH:O	2.41	0.53
3:D:1264:GLU:OE2	3:D:1425:THR:HG22	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:28:GLN:O	4:E:31:LEU:HG	2.07	0.53
1:K:2:LEU:HB2	8:K:5032:HOH:O	2.08	0.53
1:L:153:ALA:HA	1:L:156:HIS:NE2	2.23	0.53
1:L:185:ARG:HA	8:L:4811:HOH:O	2.08	0.53
2:M:572:ILE:O	2:M:573:ARG:HG2	2.08	0.53
3:N:127:LEU:HD12	3:N:128:TYR:N	2.23	0.53
3:N:690:ALA:O	3:N:694:VAL:HG23	2.08	0.53
3:N:1273:VAL:O	3:N:1325:LEU:HB2	2.08	0.53
5:P:201:LYS:HD2	8:P:3919:HOH:O	2.08	0.53
1:B:109:VAL:HG21	1:B:138:LEU:HD21	1.89	0.53
2:C:69:LEU:HB2	2:C:97:ARG:HB2	1.91	0.53
2:C:145:GLY:N	2:C:163:ILE:HG23	2.18	0.53
2:C:195:LEU:HD12	2:C:234:ALA:HB1	1.89	0.53
2:C:332:ARG:HD3	2:C:465:GLY:HA3	1.91	0.53
2:C:839:LEU:HD21	2:C:849:VAL:HG22	1.89	0.53
3:D:847:ASP:O	3:D:851:LEU:HG	2.09	0.53
3:D:959:GLU:H	3:D:959:GLU:CD	2.16	0.53
5:F:362:SER:C	5:F:364:ARG:H	2.15	0.53
2:M:571:LEU:HG	2:M:700:TYR:HA	1.91	0.53
2:M:1013:TYR:CE1	2:M:1020:PRO:HG3	2.43	0.53
3:N:18:ILE:HG23	3:N:518:PRO:CG	2.37	0.53
3:N:105:VAL:HG21	3:N:128:TYR:CE2	2.43	0.53
3:N:514:LEU:HD23	8:N:9079:HOH:O	2.08	0.53
3:N:534:ARG:HH11	3:N:534:ARG:HG3	1.74	0.53
3:N:656:PHE:HB3	3:N:694:VAL:CG1	2.38	0.53
3:N:1108:ARG:HH21	3:N:1198:TYR:C	2.16	0.53
3:N:1502:ALA:HA	8:N:9322:HOH:O	2.09	0.53
4:O:66:LYS:HE3	8:O:3745:HOH:O	2.08	0.53
5:P:138:SER:O	5:P:141:VAL:HG12	2.08	0.53
1:A:198:ARG:C	1:A:199:ILE:HD12	2.34	0.53
2:C:52:PHE:CG	2:C:68:PHE:HB2	2.44	0.53
2:C:102:HIS:HB2	2:C:106:GLY:O	2.09	0.53
2:C:944:LEU:HD21	2:C:963:LEU:CD2	2.37	0.53
3:D:1041:LEU:HD12	3:D:1058:ARG:HA	1.90	0.53
5:F:79:ASP:HB3	5:F:80:PRO:HD3	1.90	0.53
5:F:306:GLU:O	5:F:310:ILE:HG13	2.08	0.53
1:K:222:LEU:HD12	1:L:215:VAL:HB	1.91	0.53
2:M:198:ARG:HB3	8:M:1370:HOH:O	2.09	0.53
2:M:380:ALA:HA	2:M:383:ARG:CD	2.35	0.53
2:M:1054:THR:HG22	2:M:1059:ASP:CB	2.34	0.53
3:N:165:LYS:HB3	3:N:395:VAL:HG11	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:951:ILE:HG23	3:N:1062:ARG:HE	1.74	0.53
3:N:1498:ALA:HB3	8:N:9099:HOH:O	2.09	0.53
4:O:86:GLN:O	4:O:90:GLU:HG3	2.07	0.53
1:B:226:SER:O	1:B:228:PRO:HD3	2.07	0.53
2:C:601:GLY:O	2:C:648:ARG:HA	2.09	0.53
2:C:1009:SER:HB2	3:D:651:GLU:OE1	2.08	0.53
2:C:1063:ARG:O	2:C:1066:ALA:HB3	2.09	0.53
3:D:652:LEU:HB3	3:D:653:PHE:CD1	2.44	0.53
3:D:786:ILE:HD13	3:D:908:LYS:HB3	1.89	0.53
3:D:1000:THR:O	3:D:1003:VAL:HG22	2.07	0.53
3:D:1295:GLU:HB3	3:D:1300:SER:OG	2.09	0.53
4:E:61:GLU:O	4:E:65:MET:HG3	2.08	0.53
5:F:305:GLU:O	5:F:309:LYS:HG3	2.08	0.53
5:F:402:ASN:O	5:F:406:ARG:HG3	2.08	0.53
1:L:42:ARG:HB3	8:L:3652:HOH:O	2.08	0.53
1:L:115:LEU:HD12	1:L:115:LEU:O	2.08	0.53
2:M:790:LEU:C	2:M:790:LEU:HD23	2.34	0.53
8:M:1680:HOH:O	3:N:1088:THR:HG21	2.09	0.53
3:N:196:VAL:HG13	3:N:202:VAL:CG1	2.38	0.53
3:N:1423:GLY:HA3	8:N:9011:HOH:O	2.08	0.53
5:P:393:THR:O	5:P:397:ILE:HG13	2.09	0.53
1:A:66:SER:O	1:A:75:VAL:HG23	2.08	0.53
1:B:146:ARG:HG3	1:B:146:ARG:O	2.08	0.53
2:C:384:GLU:HG3	2:C:388:ARG:HE	1.74	0.53
3:D:63:TYR:HB3	3:D:68:PHE:CE1	2.44	0.53
3:D:168:THR:OG1	3:D:393:ILE:HB	2.09	0.53
3:D:1192:LEU:HD22	3:D:1345:GLU:OE2	2.08	0.53
3:D:1351:GLU:OE1	3:D:1354:LYS:HG3	2.07	0.53
2:M:139:GLN:HE22	2:M:415:PRO:CG	2.21	0.53
2:M:411:SER:HA	2:M:452:ILE:HA	1.90	0.53
3:N:554:LEU:HD12	3:N:558:LEU:HD11	1.89	0.53
3:N:738:ALA:HB3	8:N:9159:HOH:O	2.08	0.53
3:N:1197:ARG:HG3	3:N:1198:TYR:H	1.73	0.53
4:O:51:LEU:HD12	4:O:52:GLU:N	2.24	0.53
5:P:270:LYS:HA	5:P:273:ARG:HD2	1.89	0.53
1:A:31:GLY:HA2	2:C:939:ARG:HH22	1.73	0.53
1:A:117:VAL:HG12	8:A:360:HOH:O	2.07	0.53
1:A:150:TYR:CE2	1:A:152:PRO:HG3	2.37	0.53
2:C:141:HIS:HB3	2:C:418:LEU:HB3	1.90	0.53
2:C:577:PRO:HB2	2:C:580:MET:HG3	1.91	0.53
2:C:673:LEU:CD2	2:C:867:VAL:HA	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:945:ARG:HB3	2:C:945:ARG:HH11	1.74	0.53
2:C:1003:ASP:O	2:C:1005:MET:N	2.41	0.53
2:C:1025:ALA:HA	8:C:1228:HOH:O	2.07	0.53
3:D:420:VAL:HA	5:F:164:LYS:HE3	1.91	0.53
3:D:714:GLN:OE1	3:D:765:SER:HB2	2.08	0.53
3:D:1209:LEU:HD13	3:D:1211:MET:HE2	1.91	0.53
3:D:1242:HIS:CE1	3:D:1266:ARG:HD3	2.43	0.53
3:D:1349:VAL:HG21	8:D:9752:HOH:O	2.07	0.53
2:M:139:GLN:HG2	2:M:418:LEU:HD22	1.90	0.53
2:M:271:GLU:OE1	2:M:275:TYR:HB2	2.09	0.53
2:M:630:ARG:HA	2:M:705:ILE:HD11	1.89	0.53
2:M:752:GLY:N	2:M:792:VAL:HB	2.21	0.53
3:N:104:PHE:CE2	3:N:1448:THR:HG23	2.44	0.53
3:N:137:PRO:HD2	3:N:453:ASP:CB	2.39	0.53
3:N:197:SER:HA	8:N:9553:HOH:O	2.09	0.53
3:N:1253:THR:OG1	3:N:1258:ARG:HD3	2.07	0.53
3:N:1314:LYS:HZ1	3:N:1317:ASP:HB2	1.74	0.53
5:P:155:THR:HA	5:P:158:GLU:OE2	2.09	0.53
5:P:163:LEU:HB3	5:P:174:LEU:CD1	2.39	0.53
5:P:209:PHE:O	5:P:213:ILE:HG13	2.08	0.53
1:B:27:PRO:HG2	1:B:186:LEU:HD12	1.90	0.53
2:C:274:ARG:HG2	8:C:1235:HOH:O	2.08	0.53
2:C:444:PRO:HD2	2:C:452:ILE:HG13	1.91	0.53
2:C:496:ILE:H	2:C:496:ILE:HD12	1.74	0.53
2:C:874:LEU:HD13	3:D:783:ARG:HB2	1.90	0.53
2:C:964:LYS:HD2	8:C:1456:HOH:O	2.09	0.53
2:C:1058:ASP:OD2	2:C:1083:GLU:HB2	2.09	0.53
3:D:191:LEU:HB3	3:D:195:VAL:HG21	1.91	0.53
3:D:477:LEU:HD13	3:D:492:ALA:O	2.08	0.53
3:D:1009:LYS:HA	3:D:1012:GLU:CD	2.34	0.53
3:D:1097:LYS:O	3:D:1101:VAL:HG23	2.09	0.53
4:E:64:ALA:HA	4:E:67:GLU:CD	2.34	0.53
1:K:182:GLU:O	1:K:194:LYS:HB3	2.09	0.53
2:M:129:ILE:HD13	2:M:134:ARG:CB	2.29	0.53
2:M:489:THR:HG21	8:M:1667:HOH:O	2.07	0.53
2:M:500:ASN:HD21	3:N:1067:VAL:CG2	2.22	0.53
2:M:571:LEU:HD12	2:M:701:THR:O	2.08	0.53
2:M:758:ARG:NH1	2:M:788:THR:HB	2.24	0.53
2:M:905:ILE:HG22	2:M:906:PHE:CD1	2.44	0.53
3:N:480:GLU:O	3:N:484:PRO:HD2	2.09	0.53
3:N:1101:VAL:HG22	3:N:1428:ALA:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1459:LEU:HD13	3:N:1465:ASN:ND2	2.24	0.53
5:P:205:ARG:HH11	5:P:251:ILE:HG21	1.74	0.53
5:P:253:ASP:HA	5:P:259:ARG:NH1	2.24	0.53
5:P:269:ASN:O	5:P:273:ARG:HG3	2.09	0.53
1:B:143:ARG:HD2	1:B:158:ILE:HG21	1.91	0.53
2:C:115:LEU:HA	2:C:375:SER:HB3	1.90	0.53
2:C:329:GLY:HA3	2:C:489:THR:HG23	1.91	0.53
2:C:358:ARG:HB3	2:C:371:LYS:O	2.09	0.53
2:C:380:ALA:O	2:C:384:GLU:HB2	2.09	0.53
2:C:479:VAL:HG11	2:C:532:MET:HE2	1.91	0.53
2:C:578:VAL:HG11	2:C:991:GLN:CB	2.35	0.53
2:C:669:GLY:C	2:C:670:GLN:HG3	2.33	0.53
2:C:1043:TYR:HE1	3:D:710:ARG:O	1.91	0.53
3:D:86:ARG:HH11	3:D:86:ARG:HG2	1.72	0.53
3:D:119:SER:CB	3:D:123:LEU:HB2	2.39	0.53
3:D:880:ILE:O	3:D:883:ALA:HB3	2.09	0.53
3:D:957:PRO:CG	3:D:1007:VAL:HA	2.39	0.53
3:D:1281:VAL:HG23	3:D:1317:ASP:O	2.09	0.53
3:D:1381:VAL:HG23	3:D:1391:GLU:O	2.09	0.53
5:F:203:THR:HG22	8:F:514:HOH:O	2.07	0.53
5:F:398:ARG:HG2	5:F:402:ASN:ND2	2.24	0.53
1:L:94:LEU:HD11	1:L:119:ASP:HB3	1.89	0.53
1:L:101:LEU:HG	1:L:114:PHE:HA	1.90	0.53
2:M:167:LYS:HD3	2:M:168:ARG:HD2	1.90	0.53
2:M:217:LEU:HD12	2:M:311:PHE:CD2	2.44	0.53
2:M:326:ASP:HB2	2:M:431:HIS:ND1	2.24	0.53
2:M:639:GLN:HG3	8:M:1290:HOH:O	2.09	0.53
2:M:1005:MET:HE1	3:N:648:MET:HB2	1.91	0.53
3:N:907:GLU:CD	3:N:909:ASN:HD22	2.17	0.53
3:N:1087:ARG:HG2	3:N:1087:ARG:HH11	1.73	0.53
3:N:1432:LYS:HD2	3:N:1433:SER:N	2.12	0.53
4:O:8:LYS:HG3	8:O:3467:HOH:O	2.09	0.53
5:P:337:HIS:H	5:P:337:HIS:HD2	1.56	0.53
5:P:420:ASP:HB2	8:P:2629:HOH:O	2.08	0.53
1:A:176:ARG:HG3	1:A:200:TRP:HB2	1.91	0.53
1:A:221:HIS:HA	1:A:224:TYR:CD2	2.44	0.53
2:C:302:VAL:C	2:C:305:PRO:HD2	2.34	0.53
2:C:431:HIS:CD2	2:C:433:THR:H	2.27	0.53
2:C:525:SER:OG	2:C:528:GLU:HG3	2.08	0.53
2:C:690:ILE:HD12	2:C:849:VAL:HG13	1.91	0.53
2:C:1054:THR:HG22	2:C:1059:ASP:OD2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:90:MET:HE1	3:D:518:PRO:CB	2.39	0.53
3:D:122:GLU:O	3:D:126:VAL:HG23	2.09	0.53
3:D:478:LEU:HD22	3:D:1388:ARG:NH1	2.23	0.53
3:D:890:VAL:HG13	3:D:926:LYS:HE2	1.91	0.53
3:D:1164:ARG:HH21	3:D:1170:ASP:CG	2.16	0.53
4:E:26:ARG:HE	4:E:30:LEU:HD13	1.73	0.53
4:E:33:HIS:HB2	4:E:37:ASN:HD21	1.73	0.53
2:M:16:PRO:HA	8:M:1782:HOH:O	2.08	0.53
2:M:296:GLY:HA2	8:M:1743:HOH:O	2.09	0.53
2:M:520:GLU:O	2:M:522:VAL:HG23	2.08	0.53
2:M:925:TYR:CD1	2:M:925:TYR:C	2.87	0.53
3:N:462:GLN:CG	3:N:513:ILE:HD13	2.38	0.53
3:N:699:VAL:CG1	3:N:717:GLN:HE21	2.20	0.53
3:N:1278:ASP:OD1	3:N:1321:ALA:HB2	2.08	0.53
5:P:191:ASN:HA	8:P:2854:HOH:O	2.09	0.53
1:A:197:LEU:N	1:A:197:LEU:HD23	2.25	0.52
2:C:140:ILE:CD1	2:C:412:ALA:HA	2.38	0.52
2:C:985:GLY:O	2:C:987:ILE:HD12	2.09	0.52
2:C:1054:THR:CG2	2:C:1079:PRO:HB3	2.30	0.52
3:D:52:PRO:HG3	3:D:78:VAL:HG13	1.91	0.52
3:D:669:ASN:HD21	5:F:417:LYS:HA	1.74	0.52
3:D:684:LYS:HD3	3:D:686:GLU:OE1	2.09	0.52
3:D:720:LEU:H	3:D:720:LEU:HD12	1.75	0.52
3:D:1230:GLY:CA	8:D:9051:HOH:O	2.57	0.52
4:E:95:GLY:HA3	8:E:104:HOH:O	2.08	0.52
5:F:388:ALA:HB1	8:F:443:HOH:O	2.08	0.52
1:L:9:PRO:HB3	1:L:25:LEU:HG	1.91	0.52
1:L:74:ASP:O	1:L:78:ILE:HG13	2.09	0.52
2:M:172:ILE:H	2:M:172:ILE:HD12	1.74	0.52
2:M:380:ALA:O	2:M:384:GLU:HB2	2.09	0.52
2:M:510:ALA:HB1	8:M:1203:HOH:O	2.09	0.52
2:M:627:ARG:O	2:M:638:ASP:HB3	2.09	0.52
2:M:710:ILE:HD11	2:M:758:ARG:HH21	1.73	0.52
2:M:720:GLU:HA	2:M:759:THR:O	2.08	0.52
8:M:1245:HOH:O	3:N:603:LEU:HD11	2.09	0.52
3:N:799:LYS:O	3:N:799:LYS:HD3	2.09	0.52
3:N:950:GLY:O	3:N:953:ASP:N	2.38	0.52
3:N:1106:VAL:HG22	8:N:9413:HOH:O	2.10	0.52
4:O:45:ARG:HB2	4:O:46:PRO:CD	2.39	0.52
1:A:53:VAL:HG12	1:A:167:VAL:HG21	1.91	0.52
2:C:19:THR:HG21	2:C:124:ASP:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:260:LEU:HB2	2:C:291:ALA:HB1	1.90	0.52
2:C:292:ARG:HD2	2:C:299:LYS:HE2	1.91	0.52
2:C:685:GLU:H	3:D:740:PHE:HE1	1.57	0.52
2:C:1039:ALA:O	2:C:1043:TYR:HD1	1.92	0.52
2:C:1049:LEU:O	2:C:1053:LEU:HG	2.08	0.52
2:C:1056:LYS:HB3	3:D:624:ASP:H	1.74	0.52
3:D:911:LEU:O	3:D:915:VAL:HG23	2.09	0.52
3:D:955:VAL:HG21	3:D:1015:TYR:HE2	1.74	0.52
5:F:323:ASP:C	5:F:325:LYS:H	2.17	0.52
1:L:184:THR:O	1:L:192:LEU:HB2	2.08	0.52
2:M:102:HIS:HB2	2:M:106:GLY:O	2.09	0.52
2:M:170:PRO:HG2	2:M:258:TYR:CD2	2.44	0.52
3:N:507:ASN:HA	8:N:9017:HOH:O	2.08	0.52
3:N:702:LEU:HD13	3:N:716:PHE:HD1	1.74	0.52
3:N:1087:ARG:HE	3:N:1238:MET:HB2	1.74	0.52
1:A:10:VAL:HG12	1:A:12:THR:HG22	1.91	0.52
1:A:20:TYR:CD2	1:A:21:GLY:N	2.76	0.52
1:A:58:ILE:HB	1:A:61:VAL:HB	1.91	0.52
1:B:22:GLU:HG2	1:B:198:ARG:HG2	1.91	0.52
2:C:559:LEU:HD23	2:C:560:MET:HG3	1.90	0.52
2:C:671:ASN:ND2	2:C:671:ASN:H	2.06	0.52
2:C:732:ALA:O	2:C:735:ARG:HG3	2.10	0.52
2:C:861:LEU:HD23	2:C:862:PRO:N	2.24	0.52
2:C:1111:ILE:HG13	2:C:1112:PHE:N	2.19	0.52
3:D:98:PRO:HG3	3:D:515:GLU:HB3	1.90	0.52
3:D:131:LYS:CG	3:D:568:ARG:HG2	2.36	0.52
3:D:564:GLU:HA	3:D:567:ILE:HD12	1.91	0.52
3:D:607:LEU:HB3	3:D:614:PHE:CE2	2.44	0.52
3:D:895:VAL:O	3:D:899:LEU:HG	2.10	0.52
3:D:956:ILE:HG12	3:D:1039:CYS:O	2.08	0.52
3:D:1128:VAL:O	3:D:1129:THR:C	2.52	0.52
5:F:191:ASN:HB3	5:F:220:LEU:HD11	1.91	0.52
5:F:263:HIS:HB2	8:F:604:HOH:O	2.08	0.52
5:F:340:SER:OG	5:F:342:VAL:HG23	2.09	0.52
2:M:19:THR:HG21	2:M:125:GLY:HA3	1.92	0.52
2:M:352:ALA:HA	2:M:355:VAL:HG12	1.90	0.52
2:M:411:SER:HB2	2:M:452:ILE:HG23	1.91	0.52
2:M:629:TYR:HB2	2:M:637:LEU:HG	1.92	0.52
2:M:798:GLY:HA3	2:M:828:ALA:O	2.09	0.52
3:N:697:GLY:HA3	8:O:2665:HOH:O	2.08	0.52
3:N:1033:GLN:HB3	8:N:9763:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1103:HIS:CD2	3:N:1463:LYS:H	2.28	0.52
3:N:1366:LYS:O	3:N:1370:ILE:HG12	2.10	0.52
5:P:278:LEU:CB	5:P:286:PRO:HG2	2.39	0.52
1:A:23:PHE:HE1	1:A:208:LEU:HD13	1.73	0.52
2:C:468:ARG:HD3	2:C:485:TYR:HB3	1.90	0.52
2:C:625:LEU:HD13	2:C:639:GLN:O	2.10	0.52
2:C:687:ALA:C	2:C:688:ILE:HD12	2.35	0.52
2:C:777:ILE:HG23	5:F:405:LEU:CD1	2.39	0.52
2:C:1092:LEU:HA	2:C:1095:LEU:HD12	1.90	0.52
2:C:1095:LEU:CD1	3:D:607:LEU:HD11	2.32	0.52
3:D:116:LEU:O	3:D:118:LEU:HG	2.08	0.52
3:D:537:THR:CA	5:F:317:LEU:HD12	2.39	0.52
3:D:799:LYS:H	3:D:826:PRO:HG2	1.74	0.52
3:D:858:VAL:HG11	3:D:864:VAL:HG21	1.92	0.52
3:D:884:ARG:HG2	8:D:9790:HOH:O	2.10	0.52
3:D:996:TRP:O	3:D:999:THR:HG22	2.08	0.52
3:D:1448:THR:O	3:D:1452:ILE:HD13	2.09	0.52
8:D:9510:HOH:O	5:F:259:ARG:HB2	2.07	0.52
5:F:401:GLU:O	5:F:405:LEU:HB2	2.10	0.52
1:K:91:ASN:HA	8:K:3642:HOH:O	2.09	0.52
1:K:219:ARG:HG3	1:K:219:ARG:HH11	1.74	0.52
1:L:123:MET:O	1:L:125:PRO:HD3	2.10	0.52
1:L:156:HIS:CE1	1:L:166:PRO:HB3	2.44	0.52
2:M:15:LEU:HD11	2:M:583:LEU:HD11	1.90	0.52
2:M:56:GLU:CG	2:M:64:LEU:HD23	2.39	0.52
2:M:165:LEU:HB2	8:M:1197:HOH:O	2.09	0.52
2:M:378:LEU:HG	2:M:382:ILE:CD1	2.40	0.52
2:M:694:LEU:HD11	2:M:868:ASP:HB3	1.91	0.52
2:M:772:ARG:CD	5:P:373:LYS:HD2	2.37	0.52
2:M:842:ARG:HB2	8:M:1165:HOH:O	2.07	0.52
3:N:420:VAL:HG23	8:N:9890:HOH:O	2.07	0.52
3:N:631:ILE:HD13	3:N:745:MET:HG3	1.91	0.52
3:N:1168:MET:HE2	3:N:1172:HIS:CE1	2.43	0.52
5:P:169:GLU:H	5:P:169:GLU:CD	2.17	0.52
5:P:185:GLN:O	5:P:189:GLU:HG3	2.09	0.52
1:B:5:LYS:HA	1:B:5:LYS:HE3	1.90	0.52
2:C:630:ARG:HH22	2:C:707:ARG:HB2	1.73	0.52
2:C:673:LEU:HD22	2:C:867:VAL:HA	1.90	0.52
2:C:778:PHE:HB2	8:C:1741:HOH:O	2.09	0.52
2:C:1104:GLU:HA	3:D:6:ARG:HH12	1.75	0.52
3:D:399:ARG:HB2	3:D:444:VAL:HG13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:584:ASN:HB3	8:D:9062:HOH:O	2.08	0.52
3:D:643:GLY:CA	3:D:727:GLN:HB2	2.35	0.52
5:F:234:LYS:CD	5:F:236:SER:HB3	2.37	0.52
1:K:94:LEU:HD11	1:K:119:ASP:OD1	2.09	0.52
1:K:97:VAL:HG23	8:K:3015:HOH:O	2.07	0.52
2:M:162:ILE:HB	2:M:172:ILE:HB	1.90	0.52
2:M:428:ARG:HE	2:M:451:LEU:HD21	1.75	0.52
2:M:687:ALA:C	2:M:688:ILE:HD12	2.35	0.52
3:N:712:GLY:HA2	8:N:9111:HOH:O	2.09	0.52
3:N:853:VAL:HG13	3:N:858:VAL:O	2.10	0.52
3:N:1381:VAL:HG23	3:N:1391:GLU:O	2.10	0.52
5:P:93:LEU:HG	5:P:190:ALA:HB1	1.90	0.52
2:C:332:ARG:HA	2:C:465:GLY:O	2.10	0.52
2:C:567:GLN:HB2	2:C:997:LEU:HD22	1.91	0.52
2:C:627:ARG:HG3	2:C:628:PHE:H	1.75	0.52
2:C:777:ILE:HG12	5:F:405:LEU:HD11	1.91	0.52
2:C:899:GLN:HG3	2:C:901:TYR:CZ	2.45	0.52
2:C:1024:LYS:HB2	8:C:1173:HOH:O	2.08	0.52
2:C:1047:HIS:CD2	3:D:1471:LEU:HD11	2.45	0.52
2:C:1109:VAL:HG22	8:D:9538:HOH:O	2.10	0.52
3:D:996:TRP:HB2	3:D:1044:LEU:HD11	1.92	0.52
3:D:1147:ARG:HB3	3:D:1188:VAL:HG21	1.90	0.52
2:M:52:PHE:CG	2:M:68:PHE:HB2	2.45	0.52
2:M:139:GLN:HE22	2:M:415:PRO:HD2	1.73	0.52
2:M:269:LEU:HD23	2:M:285:LEU:HD21	1.90	0.52
3:N:87:ARG:HG3	3:N:88:TYR:CD2	2.44	0.52
3:N:1047:LYS:HG2	3:N:1053:PHE:CE1	2.45	0.52
1:A:205:VAL:HG23	1:A:206:THR:N	2.23	0.52
1:B:138:LEU:HB2	1:B:140:MET:HE1	1.92	0.52
2:C:118:ILE:HG22	2:C:382:ILE:HD13	1.92	0.52
2:C:384:GLU:CD	2:C:388:ARG:HH21	2.18	0.52
2:C:480:THR:HG22	2:C:481:ASP:N	2.24	0.52
2:C:510:ALA:HB3	2:C:513:VAL:HG23	1.91	0.52
2:C:730:SER:O	2:C:734:LEU:HD13	2.10	0.52
2:C:862:PRO:HG3	2:C:975:TYR:HE1	1.73	0.52
3:D:38:LYS:HD3	8:D:9533:HOH:O	2.09	0.52
3:D:679:ARG:HD3	3:D:682:ASP:OD2	2.10	0.52
3:D:1033:GLN:HA	3:D:1033:GLN:HE21	1.74	0.52
1:K:18:ARG:O	1:K:207:PRO:HD3	2.08	0.52
1:K:68:ILE:HA	8:K:4050:HOH:O	2.09	0.52
2:M:645:VAL:HG22	8:M:1487:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:180:LYS:O	3:N:184:GLU:HG3	2.09	0.52
3:N:490:ALA:HB2	8:N:9895:HOH:O	2.10	0.52
3:N:1330:ILE:HD12	3:N:1330:ILE:N	2.25	0.52
4:O:74:VAL:HG12	4:O:79:LEU:HD21	1.90	0.52
5:P:102:LEU:HD22	5:P:183:ALA:O	2.09	0.52
5:P:365:GLU:OE1	5:P:400:ILE:HD12	2.09	0.52
5:P:367:MET:HA	5:P:370:LYS:NZ	2.24	0.52
2:C:22:GLN:NE2	2:C:336:VAL:HG21	2.24	0.52
2:C:32:ALA:HB2	2:C:73:LEU:HD21	1.91	0.52
2:C:208:ALA:HA	2:C:218:VAL:HG22	1.92	0.52
2:C:402:SER:OG	2:C:566:THR:HG22	2.10	0.52
2:C:551:GLU:OE1	2:C:906:PHE:HA	2.09	0.52
2:C:884:GLN:HG3	2:C:885:ILE:N	2.22	0.52
2:C:897:LEU:HG	2:C:920:GLN:HE21	1.75	0.52
3:D:148:GLU:CB	3:D:151:GLN:HB2	2.34	0.52
3:D:819:GLY:HA3	8:D:9099:HOH:O	2.08	0.52
5:F:247:ILE:O	5:F:251:ILE:HG13	2.10	0.52
1:K:80:LEU:HB3	8:K:3096:HOH:O	2.10	0.52
1:L:226:SER:O	1:L:228:PRO:HD3	2.09	0.52
2:M:97:ARG:HD2	8:M:1366:HOH:O	2.10	0.52
2:M:412:ALA:CB	2:M:451:LEU:HB3	2.40	0.52
2:M:473:ARG:HA	2:M:531:PHE:CD1	2.45	0.52
2:M:1101:THR:O	2:M:1102:LEU:HD23	2.10	0.52
3:N:434:ARG:HB2	3:N:447:VAL:CG1	2.40	0.52
3:N:500:ARG:HH12	3:N:1388:ARG:HD2	1.75	0.52
3:N:951:ILE:HG23	3:N:1062:ARG:HH21	1.75	0.52
3:N:1041:LEU:HD12	3:N:1057:VAL:O	2.08	0.52
3:N:1047:LYS:HA	3:N:1053:PHE:CE1	2.44	0.52
3:N:1102:THR:HG22	3:N:1222:GLY:CA	2.40	0.52
3:N:1109:GLU:HG2	3:N:1202:GLN:H	1.75	0.52
3:N:1240:THR:O	3:N:1257:PRO:HB3	2.10	0.52
3:N:1344:VAL:HG12	3:N:1348:LEU:CD2	2.40	0.52
5:P:167:PRO:HG2	8:P:3728:HOH:O	2.10	0.52
1:B:204:SER:HB2	8:B:371:HOH:O	2.09	0.52
2:C:114:PHE:HB2	8:C:1287:HOH:O	2.10	0.52
2:C:139:GLN:OE1	2:C:415:PRO:HD2	2.09	0.52
2:C:232:GLU:O	2:C:235:LEU:HB2	2.09	0.52
2:C:305:PRO:HG3	2:C:308:ARG:HH21	1.75	0.52
2:C:333:ILE:N	2:C:333:ILE:HD12	2.25	0.52
2:C:612:VAL:HG22	2:C:622:GLU:HA	1.91	0.52
2:C:722:ILE:HD12	2:C:805:ARG:HH21	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:724:ARG:HG3	2:C:740:GLU:HA	1.91	0.52
2:C:841:ASN:HD21	2:C:845:ASN:H	1.58	0.52
2:C:1060:ILE:HG23	2:C:1061:GLU:N	2.24	0.52
3:D:136:ASP:HB3	3:D:137:PRO:CD	2.35	0.52
3:D:191:LEU:HD13	3:D:195:VAL:HG11	1.91	0.52
3:D:211:VAL:HG13	3:D:393:ILE:HA	1.91	0.52
3:D:918:ALA:O	3:D:922:LEU:HG	2.10	0.52
3:D:972:LEU:HD23	3:D:973:GLN:N	2.24	0.52
3:D:1318:TYR:HD1	3:D:1319:VAL:H	1.56	0.52
5:F:274:THR:O	5:F:278:LEU:HG	2.10	0.52
1:K:123:MET:HE3	1:K:203:GLY:O	2.10	0.52
1:K:219:ARG:HG3	1:K:219:ARG:NH1	2.25	0.52
1:K:226:SER:O	1:K:228:PRO:HD3	2.10	0.52
2:M:244:PRO:CD	2:M:245:GLY:H	2.17	0.52
2:M:322:VAL:HA	8:M:1189:HOH:O	2.09	0.52
2:M:442:GLU:HG2	2:M:454:SER:OG	2.10	0.52
2:M:571:LEU:HD23	2:M:670:GLN:NE2	2.25	0.52
2:M:1034:GLU:HB2	8:M:1373:HOH:O	2.09	0.52
3:N:963:TYR:CD2	3:N:1002:LYS:HB3	2.45	0.52
3:N:1068:LEU:C	3:N:1070:TYR:N	2.67	0.52
3:N:1112:CYS:HA	3:N:1195:GLN:HE22	1.74	0.52
5:P:363:GLU:HA	5:P:367:MET:HG2	1.92	0.52
1:B:151:VAL:HB	1:B:169:ALA:HB3	1.92	0.52
2:C:41:ASN:HD22	2:C:41:ASN:N	1.97	0.52
2:C:399:ASN:HD22	2:C:399:ASN:N	2.08	0.52
2:C:470:PRO:HD3	2:C:485:TYR:CE2	2.45	0.52
2:C:584:GLU:CD	2:C:584:GLU:H	2.16	0.52
2:C:597:ALA:CB	2:C:655:LEU:HD21	2.35	0.52
2:C:625:LEU:CD1	2:C:641:PRO:HG3	2.40	0.52
2:C:724:ARG:HB3	2:C:724:ARG:HH11	1.73	0.52
2:C:1084:SER:O	2:C:1087:VAL:HG12	2.10	0.52
3:D:58:CYS:SG	3:D:59:ALA:N	2.83	0.52
3:D:445:ARG:HG2	3:D:445:ARG:HH11	1.75	0.52
3:D:573:MET:HE1	5:F:214:GLN:CG	2.40	0.52
4:E:19:LEU:O	4:E:23:VAL:HG23	2.10	0.52
5:F:408:LEU:HA	5:F:411:HIS:CE1	2.44	0.52
1:K:143:ARG:HG3	1:K:144:VAL:N	2.25	0.52
1:L:46:SER:HB2	8:L:3700:HOH:O	2.09	0.52
1:L:85:LEU:HD13	1:L:127:LEU:HD23	1.92	0.52
2:M:451:LEU:HD12	2:M:451:LEU:H	1.75	0.52
2:M:564:MET:HE1	8:M:1413:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:15:PRO:HG3	8:N:9079:HOH:O	2.10	0.52
3:N:81:THR:HG22	8:N:9092:HOH:O	2.10	0.52
3:N:97:THR:HG21	3:N:571:LYS:HD3	1.92	0.52
3:N:126:VAL:O	3:N:132:TYR:HD1	1.92	0.52
3:N:411:THR:HB	8:N:9297:HOH:O	2.10	0.52
3:N:750:PRO:HB2	3:N:756:GLN:OE1	2.09	0.52
3:N:1194:CYS:HB3	3:N:1373:ARG:CZ	2.40	0.52
3:N:1194:CYS:HB3	3:N:1373:ARG:HH22	1.74	0.52
5:P:253:ASP:HA	5:P:259:ARG:HH12	1.75	0.52
5:P:321:ILE:HB	5:P:327:SER:OG	2.10	0.52
5:P:323:ASP:O	5:P:325:LYS:N	2.43	0.52
2:C:554:ASP:HA	3:D:1061:PHE:CZ	2.45	0.51
3:D:213:VAL:HG21	8:D:9600:HOH:O	2.09	0.51
3:D:529:GLN:HG2	3:D:535:PHE:CE1	2.45	0.51
3:D:542:ASP:O	3:D:546:ARG:HG2	2.10	0.51
3:D:543:LEU:HD21	3:D:600:LEU:HD12	1.92	0.51
3:D:777:PRO:HG2	3:D:915:VAL:HB	1.92	0.51
3:D:819:GLY:O	3:D:822:ALA:HB3	2.10	0.51
3:D:1076:GLY:O	3:D:1079:LYS:HG2	2.10	0.51
3:D:1277:ILE:HG21	8:D:9249:HOH:O	2.10	0.51
3:D:1333:HIS:ND1	3:D:1421:LEU:HD23	2.26	0.51
3:D:1403:LEU:HG	8:D:9163:HOH:O	2.10	0.51
5:F:87:GLU:O	5:F:91:VAL:HG23	2.10	0.51
1:K:62:LEU:HD12	1:K:62:LEU:H	1.75	0.51
2:M:52:PHE:HB3	2:M:53:PRO:HD3	1.92	0.51
2:M:290:LEU:HD13	8:M:1252:HOH:O	2.10	0.51
2:M:626:ARG:HB2	8:M:1290:HOH:O	2.11	0.51
2:M:817:PRO:C	2:M:819:VAL:H	2.18	0.51
3:N:30:GLU:HG3	3:N:41:ARG:HG2	1.91	0.51
3:N:119:SER:HB2	3:N:123:LEU:N	2.24	0.51
3:N:1210:SER:HB2	8:O:3546:HOH:O	2.10	0.51
1:A:117:VAL:HB	1:A:120:VAL:HG12	1.91	0.51
1:B:83:LYS:HE2	1:B:168:ASP:HB2	1.91	0.51
2:C:269:LEU:HG	2:C:288:ARG:N	2.24	0.51
2:C:911:GLU:HG2	2:C:915:LYS:HZ2	1.75	0.51
2:C:1097:LEU:HD21	3:D:103:TRP:CZ3	2.45	0.51
3:D:1045:MET:HG2	3:D:1073:SER:CA	2.27	0.51
3:D:1242:HIS:HE1	3:D:1266:ARG:HB3	1.75	0.51
1:K:58:ILE:HG21	1:K:68:ILE:CD1	2.40	0.51
1:L:170:VAL:HG23	8:L:3287:HOH:O	2.10	0.51
2:M:103:LYS:HB2	8:M:1613:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:309:TYR:HA	2:M:312:ALA:HB3	1.92	0.51
2:M:405:ARG:HE	2:M:543:ASN:ND2	2.08	0.51
2:M:958:THR:HA	8:M:1596:HOH:O	2.09	0.51
2:M:1071:ILE:O	3:N:659:LYS:HB2	2.10	0.51
3:N:87:ARG:HB3	3:N:523:ASP:HB2	1.91	0.51
3:N:610:LYS:HG2	3:N:611:GLN:HG2	1.92	0.51
3:N:637:LEU:HD21	8:N:9469:HOH:O	2.10	0.51
3:N:963:TYR:CE2	3:N:1002:LYS:HB3	2.45	0.51
3:N:1033:GLN:HE21	3:N:1036:ARG:HH11	1.57	0.51
3:N:1133:ARG:HB2	8:N:9380:HOH:O	2.09	0.51
5:P:303:ARG:O	5:P:307:THR:HG23	2.10	0.51
5:P:335:ASP:CG	5:P:338:LEU:HD12	2.35	0.51
1:A:106:PRO:HG3	1:A:133:GLU:O	2.11	0.51
2:C:198:ARG:HD2	8:C:1571:HOH:O	2.09	0.51
2:C:208:ALA:HB1	2:C:218:VAL:HG13	1.92	0.51
2:C:264:PRO:HB2	8:C:1418:HOH:O	2.10	0.51
2:C:265:ARG:HG2	2:C:267:TYR:CG	2.45	0.51
2:C:329:GLY:N	2:C:488:ALA:HB3	2.24	0.51
2:C:920:GLN:HG3	8:C:1216:HOH:O	2.11	0.51
2:C:1015:LEU:HA	8:C:1202:HOH:O	2.09	0.51
2:C:1098:ASP:HB2	3:D:21:TRP:HZ2	1.75	0.51
3:D:1008:PHE:HZ	3:D:1032:PRO:HA	1.73	0.51
5:F:153:PRO:HG2	5:F:154:LYS:H	1.75	0.51
2:M:137:VAL:O	2:M:391:LEU:HD21	2.10	0.51
2:M:244:PRO:HG2	2:M:246:ASP:OD2	2.09	0.51
3:N:168:THR:HG21	8:N:9101:HOH:O	2.10	0.51
3:N:213:VAL:HG22	3:N:214:GLU:H	1.75	0.51
3:N:996:TRP:CE2	3:N:1056:PRO:HG3	2.45	0.51
3:N:1123:PHE:HA	3:N:1135:ARG:H	1.75	0.51
3:N:1310:ARG:HB2	3:N:1327:ARG:HE	1.75	0.51
3:N:1396:GLU:O	3:N:1400:VAL:HG23	2.10	0.51
4:O:88:GLU:HA	4:O:91:ARG:HD2	1.93	0.51
5:P:119:ILE:HD13	5:P:170:HIS:CG	2.44	0.51
5:P:299:TRP:CZ3	5:P:303:ARG:HG2	2.45	0.51
5:P:421:PHE:C	5:P:423:ASP:H	2.17	0.51
1:B:42:ARG:HG2	1:B:42:ARG:HH11	1.75	0.51
1:B:124:ASN:OD1	1:B:127:LEU:HB2	2.11	0.51
2:C:72:ARG:HB2	2:C:72:ARG:HH11	1.75	0.51
2:C:199:VAL:HG13	2:C:235:LEU:HG	1.92	0.51
2:C:574:ALA:HB1	2:C:667:ALA:HB3	1.92	0.51
2:C:701:THR:CG2	2:C:832:LYS:HG3	2.37	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:876:VAL:HB	2:C:877:PRO:HD3	1.92	0.51
2:C:1004:LYS:O	2:C:1006:HIS:ND1	2.42	0.51
3:D:181:ASP:O	3:D:185:VAL:HG23	2.11	0.51
3:D:507:ASN:HA	8:D:9186:HOH:O	2.11	0.51
3:D:889:ALA:O	3:D:929:ARG:HD2	2.11	0.51
3:D:1135:ARG:HB2	3:D:1140:ILE:HD11	1.92	0.51
3:D:1138:ALA:O	3:D:1141:GLU:HB2	2.10	0.51
3:D:1254:GLN:HA	3:D:1254:GLN:OE1	2.09	0.51
3:D:1382:THR:HG22	8:D:9873:HOH:O	2.09	0.51
4:E:81:PRO:HG3	8:E:183:HOH:O	2.09	0.51
1:K:72:LYS:HD2	1:K:73:GLU:OE2	2.09	0.51
1:K:115:LEU:HD13	8:K:3936:HOH:O	2.09	0.51
1:K:127:LEU:HD12	1:K:128:HIS:N	2.23	0.51
1:K:181:VAL:O	2:M:938:LYS:HD3	2.10	0.51
1:K:184:THR:O	1:K:192:LEU:HD12	2.10	0.51
2:M:4:LYS:HD3	8:M:1624:HOH:O	2.10	0.51
2:M:22:GLN:HE22	2:M:336:VAL:HG21	1.74	0.51
2:M:191:PHE:CE2	2:M:195:LEU:HB3	2.46	0.51
2:M:254:VAL:HG13	2:M:258:TYR:HE1	1.76	0.51
2:M:274:ARG:HD2	2:M:285:LEU:HB3	1.91	0.51
2:M:546:LEU:CA	2:M:581:THR:HG21	2.41	0.51
2:M:741:GLY:HA3	8:M:1430:HOH:O	2.09	0.51
2:M:1076:VAL:CG2	3:N:752:SER:HB3	2.40	0.51
3:N:127:LEU:HD11	3:N:461:ILE:HD11	1.92	0.51
3:N:491:LYS:HD3	3:N:492:ALA:N	2.25	0.51
3:N:550:ARG:HH12	3:N:577:ALA:HB2	1.76	0.51
3:N:1311:LEU:HD23	3:N:1311:LEU:H	1.74	0.51
1:A:132:LEU:HD13	8:A:356:HOH:O	2.09	0.51
2:C:183:SER:HB2	2:C:190:LYS:HD3	1.91	0.51
2:C:410:ILE:N	2:C:410:ILE:HD12	2.26	0.51
2:C:1104:GLU:HA	3:D:6:ARG:NH1	2.26	0.51
3:D:178:LEU:HD12	3:D:200:ASP:HB2	1.93	0.51
3:D:483:HIS:ND1	3:D:483:HIS:N	2.58	0.51
3:D:764:LEU:HD12	3:D:765:SER:H	1.75	0.51
3:D:1088:THR:HA	8:D:9405:HOH:O	2.10	0.51
3:D:1393:GLN:HB2	3:D:1398:TRP:HZ2	1.75	0.51
3:D:1478:SER:OG	3:D:1481:VAL:HG23	2.11	0.51
1:L:57:TYR:CE1	1:L:161:ARG:HB3	2.46	0.51
2:M:37:GLU:HA	8:M:1458:HOH:O	2.11	0.51
2:M:420:ARG:HG2	2:M:422:ARG:HG2	1.91	0.51
3:N:498:VAL:HG12	8:N:9641:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:729:HIS:HE1	3:N:731:LEU:HG	1.75	0.51
3:N:957:PRO:HG2	3:N:1007:VAL:HA	1.92	0.51
3:N:1390:LEU:HD13	8:N:9614:HOH:O	2.11	0.51
4:O:24:ALA:O	4:O:28:GLN:HG3	2.10	0.51
4:O:47:LYS:HA	4:O:54:LEU:HB3	1.93	0.51
5:P:113:ILE:O	5:P:116:LEU:HB2	2.11	0.51
5:P:214:GLN:OE1	5:P:214:GLN:HA	2.10	0.51
5:P:365:GLU:CD	5:P:397:ILE:HA	2.35	0.51
5:P:412:GLU:OE1	5:P:418:LEU:HD13	2.10	0.51
1:B:91:ASN:O	1:B:94:LEU:HD12	2.11	0.51
1:B:105:GLY:O	1:B:132:LEU:HD23	2.09	0.51
1:B:217:ILE:O	1:B:221:HIS:ND1	2.44	0.51
2:C:209:ARG:O	2:C:213:ALA:HB2	2.11	0.51
2:C:958:THR:CG2	2:C:961:GLU:HB2	2.40	0.51
2:C:1071:ILE:HD13	3:D:655:PRO:HB3	1.92	0.51
3:D:486:ARG:HA	3:D:489:ARG:HG2	1.91	0.51
3:D:543:LEU:O	3:D:546:ARG:HB2	2.11	0.51
3:D:669:ASN:HB3	5:F:349:LEU:HD11	1.92	0.51
3:D:1320:GLU:HB2	3:D:1323:GLN:NE2	2.25	0.51
4:E:48:MET:CB	4:E:54:LEU:HB2	2.41	0.51
5:F:213:ILE:HG22	5:F:217:ASN:ND2	2.26	0.51
5:F:371:LEU:HD22	5:F:375:LEU:HD22	1.91	0.51
5:F:393:THR:HG22	5:F:394:ARG:H	1.76	0.51
1:L:173:PRO:HA	1:L:202:ASP:OD2	2.10	0.51
1:L:216:GLU:HG3	1:L:219:ARG:HH12	1.76	0.51
2:M:36:PRO:HD3	8:M:1244:HOH:O	2.09	0.51
2:M:154:ARG:HH21	2:M:157:ARG:H	1.58	0.51
2:M:319:GLY:HA2	8:M:1247:HOH:O	2.11	0.51
3:N:513:ILE:HA	8:N:9084:HOH:O	2.10	0.51
3:N:720:LEU:H	3:N:720:LEU:HD12	1.75	0.51
3:N:1065:LEU:CD1	3:N:1069:GLU:HB2	2.41	0.51
4:O:48:MET:HG2	4:O:49:GLN:N	2.24	0.51
4:O:86:GLN:HG2	8:O:2986:HOH:O	2.09	0.51
5:P:153:PRO:HG3	8:P:3659:HOH:O	2.10	0.51
2:C:6:PHE:CE2	2:C:913:GLU:HB3	2.46	0.51
2:C:15:LEU:HD12	2:C:15:LEU:H	1.76	0.51
2:C:218:VAL:HA	2:C:221:LEU:HD23	1.93	0.51
2:C:693:GLU:HG3	8:C:1199:HOH:O	2.11	0.51
2:C:701:THR:HG23	2:C:832:LYS:HA	1.92	0.51
2:C:1018:GLN:NE2	2:C:1063:ARG:HH22	2.08	0.51
3:D:550:ARG:HH11	3:D:573:MET:HB3	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:671:LYS:O	3:D:671:LYS:HD3	2.11	0.51
3:D:1231:GLU:HB3	3:D:1232:PRO:HD3	1.93	0.51
3:D:1342:GLU:CD	3:D:1342:GLU:H	2.18	0.51
3:D:1420:LEU:HD12	3:D:1421:LEU:N	2.26	0.51
1:K:13:VAL:HG12	1:K:15:THR:HG22	1.93	0.51
1:L:101:LEU:HB2	1:L:114:PHE:CD2	2.46	0.51
2:M:147:TYR:HB3	2:M:323:ASP:OD2	2.11	0.51
2:M:252:LYS:HZ2	2:M:296:GLY:HA3	1.74	0.51
2:M:584:GLU:O	2:M:588:VAL:HG13	2.11	0.51
2:M:944:LEU:O	2:M:948:GLU:HG2	2.10	0.51
3:N:6:ARG:HB3	3:N:6:ARG:CZ	2.41	0.51
3:N:550:ARG:HG3	3:N:550:ARG:NH1	2.26	0.51
3:N:1109:GLU:CD	3:N:1202:GLN:H	2.18	0.51
3:N:1183:ILE:HG22	8:N:2022:HOH:O	2.10	0.51
3:N:1363:LEU:HD12	3:N:1364:HIS:O	2.11	0.51
4:O:17:TYR:N	4:O:17:TYR:HD2	2.08	0.51
5:P:291:ILE:HG23	5:P:304:VAL:HG21	1.91	0.51
1:B:101:LEU:HB2	1:B:114:PHE:CD2	2.45	0.51
2:C:42:VAL:HG12	2:C:43:GLY:N	2.26	0.51
2:C:157:ARG:NH2	2:C:314:THR:HA	2.24	0.51
3:D:81:THR:O	3:D:82:LYS:O	2.28	0.51
3:D:84:ILE:O	3:D:87:ARG:HG3	2.11	0.51
3:D:561:GLY:HA3	5:F:184:ARG:HH22	1.76	0.51
3:D:563:PRO:HG3	5:F:188:ILE:HG21	1.93	0.51
3:D:775:GLY:HA3	3:D:1145:TYR:CE1	2.46	0.51
3:D:1139:ASP:O	3:D:1142:ALA:HB3	2.11	0.51
3:D:1223:ILE:HD12	3:D:1223:ILE:N	2.23	0.51
3:D:1389:LEU:HD12	3:D:1390:LEU:HG	1.93	0.51
5:F:264:MET:O	5:F:267:THR:HB	2.10	0.51
5:F:316:SER:HB2	5:F:319:THR:OG1	2.11	0.51
3:N:191:LEU:HD22	3:N:195:VAL:HG21	1.92	0.51
3:N:550:ARG:NH1	3:N:577:ALA:HB2	2.26	0.51
3:N:554:LEU:O	3:N:558:LEU:HG	2.11	0.51
3:N:1156:LEU:HD11	3:N:1176:LYS:HD2	1.92	0.51
3:N:1372:VAL:O	3:N:1375:MET:HB2	2.10	0.51
4:O:54:LEU:HG	4:O:58:PRO:CG	2.40	0.51
5:P:203:THR:HG22	5:P:204:GLY:N	2.26	0.51
1:B:220:GLU:HG2	8:B:449:HOH:O	2.10	0.51
2:C:22:GLN:O	2:C:121:MET:HE1	2.10	0.51
2:C:34:VAL:CG1	2:C:38:LYS:HG3	2.41	0.51
2:C:64:LEU:HD22	2:C:359:MET:CG	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:113:VAL:N	8:C:1822:HOH:O	2.41	0.51
2:C:897:LEU:HD23	2:C:899:GLN:NE2	2.26	0.51
3:D:705:ALA:CB	3:D:706:PRO:HD3	2.41	0.51
3:D:790:TYR:CD1	3:D:1022:VAL:HG13	2.46	0.51
5:F:170:HIS:H	5:F:170:HIS:CD2	2.28	0.51
5:F:259:ARG:N	8:F:509:HOH:O	2.43	0.51
1:K:149:GLY:O	1:K:171:PHE:HB2	2.11	0.51
2:M:256:TYR:CE1	2:M:293:PHE:HB2	2.46	0.51
2:M:321:GLU:HG2	8:M:1221:HOH:O	2.10	0.51
2:M:885:ILE:HD12	8:N:9188:HOH:O	2.11	0.51
3:N:1059:SER:HA	8:N:9131:HOH:O	2.11	0.51
3:N:1314:LYS:NZ	3:N:1317:ASP:H	2.09	0.51
3:N:1487:VAL:HG11	3:N:1492:LEU:HD23	1.92	0.51
3:N:1500:LYS:HD3	8:N:9564:HOH:O	2.11	0.51
5:P:256:ARG:NH2	5:P:258:ILE:HB	2.26	0.51
1:A:14:ARG:CZ	1:A:24:VAL:HG23	2.41	0.51
1:A:83:LYS:HE2	1:A:167:VAL:CG1	2.40	0.51
1:B:19:GLU:HG3	1:B:201:THR:O	2.10	0.51
2:C:21:ILE:H	2:C:21:ILE:HD12	1.74	0.51
2:C:362:GLY:HA3	2:C:367:LEU:HD22	1.92	0.51
2:C:394:PHE:H	2:C:394:PHE:HD2	1.59	0.51
2:C:577:PRO:HG3	2:C:993:PHE:CE2	2.46	0.51
2:C:1054:THR:HG22	2:C:1059:ASP:CG	2.36	0.51
3:D:7:LYS:HD3	3:D:1456:LYS:NZ	2.26	0.51
3:D:152:LEU:HD23	3:D:152:LEU:N	2.23	0.51
3:D:1209:LEU:HD13	3:D:1211:MET:CE	2.41	0.51
3:D:1295:GLU:HB3	3:D:1300:SER:CB	2.41	0.51
5:F:268:ILE:HG22	8:F:510:HOH:O	2.11	0.51
5:F:336:GLU:HG2	8:F:426:HOH:O	2.11	0.51
2:M:303:PHE:HD1	8:M:1252:HOH:O	1.93	0.51
2:M:626:ARG:HB2	2:M:639:GLN:HE21	1.74	0.51
2:M:704:HIS:O	2:M:705:ILE:HG23	2.11	0.51
2:M:1006:HIS:O	3:N:648:MET:HE2	2.11	0.51
3:N:58:CYS:SG	3:N:59:ALA:N	2.84	0.51
3:N:81:THR:O	3:N:82:LYS:C	2.54	0.51
3:N:170:PRO:HA	8:N:9445:HOH:O	2.11	0.51
3:N:178:LEU:HA	3:N:181:ASP:OD2	2.11	0.51
3:N:195:VAL:HG22	8:N:9187:HOH:O	2.11	0.51
3:N:527:MET:HE1	3:N:537:THR:HB	1.93	0.51
3:N:1144:LEU:HA	3:N:1147:ARG:HG3	1.91	0.51
3:N:1288:GLU:HA	8:N:9629:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:47:LYS:N	4:O:54:LEU:HD13	2.26	0.51
4:O:83:ASP:O	4:O:86:GLN:HG3	2.11	0.51
2:C:358:ARG:HH22	2:C:374:ASN:CB	2.11	0.50
2:C:549:PHE:CD2	2:C:886:LEU:HB3	2.47	0.50
2:C:724:ARG:NH1	2:C:734:LEU:HD23	2.20	0.50
2:C:798:GLY:C	2:C:799:ILE:HD13	2.36	0.50
3:D:684:LYS:HD3	3:D:686:GLU:CD	2.35	0.50
3:D:805:GLU:OE1	3:D:809:PRO:HD2	2.11	0.50
3:D:1271:LYS:HG2	3:D:1272:ALA:N	2.25	0.50
5:F:407:LYS:HD3	8:F:437:HOH:O	2.10	0.50
1:K:9:PRO:HD2	1:L:224:TYR:CZ	2.46	0.50
1:K:32:PHE:HB2	8:K:3631:HOH:O	2.11	0.50
1:K:91:ASN:H	1:K:94:LEU:CD1	2.24	0.50
1:K:227:ASN:ND2	8:K:3074:HOH:O	2.43	0.50
1:L:23:PHE:O	1:L:196:THR:HA	2.12	0.50
1:L:176:ARG:HB2	8:N:9402:HOH:O	2.12	0.50
2:M:72:ARG:HH21	2:M:112:GLU:HG3	1.76	0.50
2:M:145:GLY:C	2:M:163:ILE:HG23	2.36	0.50
2:M:1107:ASN:HA	8:M:1421:HOH:O	2.11	0.50
3:N:564:GLU:HA	3:N:567:ILE:HD12	1.93	0.50
3:N:576:GLU:HA	3:N:579:ASP:OD2	2.11	0.50
3:N:647:ARG:HG2	8:N:9316:HOH:O	2.11	0.50
3:N:1003:VAL:O	3:N:1006:ALA:HB3	2.10	0.50
3:N:1436:SER:HB3	8:N:9153:HOH:O	2.11	0.50
1:A:96:THR:HB	8:A:441:HOH:O	2.09	0.50
2:C:128:ILE:HG22	8:C:1224:HOH:O	2.10	0.50
2:C:175:GLU:HB3	2:C:183:SER:OG	2.11	0.50
2:C:643:VAL:HG13	2:C:647:GLN:CD	2.36	0.50
2:C:838:LYS:HD2	2:C:846:LYS:HZ1	1.76	0.50
3:D:420:VAL:HA	5:F:164:LYS:CE	2.41	0.50
3:D:642:CYS:SG	3:D:716:PHE:HB2	2.51	0.50
3:D:653:PHE:CD1	3:D:653:PHE:N	2.80	0.50
3:D:1164:ARG:HG3	3:D:1164:ARG:NH1	2.25	0.50
3:D:1314:LYS:HB3	8:D:9482:HOH:O	2.10	0.50
3:D:1493:LYS:O	3:D:1497:GLU:HG2	2.10	0.50
1:K:46:SER:HB3	2:M:856:GLU:HG2	1.93	0.50
2:M:208:ALA:HA	2:M:218:VAL:HG22	1.92	0.50
2:M:208:ALA:HA	2:M:221:LEU:HD21	1.93	0.50
2:M:290:LEU:HD22	2:M:302:VAL:HG11	1.92	0.50
2:M:575:GLN:HA	2:M:662:GLU:OE2	2.11	0.50
3:N:27:GLU:N	8:N:9386:HOH:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:399:ARG:HH21	3:N:432:TYR:HE2	1.59	0.50
3:N:422:ALA:O	3:N:427:VAL:HG21	2.11	0.50
3:N:999:THR:O	3:N:1002:LYS:HB2	2.11	0.50
3:N:1119:SER:HA	3:N:1186:VAL:O	2.10	0.50
5:P:278:LEU:HB3	5:P:286:PRO:HG2	1.94	0.50
1:A:115:LEU:HD12	1:A:115:LEU:O	2.12	0.50
1:B:173:PRO:HB2	1:B:205:VAL:HG22	1.92	0.50
2:C:157:ARG:HD3	2:C:158:TYR:H	1.76	0.50
2:C:256:TYR:HE1	2:C:293:PHE:HB2	1.73	0.50
2:C:288:ARG:HB2	2:C:288:ARG:HH11	1.76	0.50
2:C:405:ARG:HH12	2:C:563:ASN:HD21	1.57	0.50
2:C:497:ALA:HA	2:C:515:ALA:HA	1.93	0.50
2:C:625:LEU:HB3	2:C:639:GLN:HG3	1.93	0.50
2:C:712:ALA:HB1	2:C:820:ARG:HH11	1.76	0.50
2:C:969:GLN:HA	8:D:9594:HOH:O	2.11	0.50
2:C:1097:LEU:H	2:C:1097:LEU:CD2	2.19	0.50
3:D:195:VAL:HG13	8:D:9005:HOH:O	2.11	0.50
3:D:428:LYS:HB3	3:D:450:TYR:CE1	2.46	0.50
3:D:480:GLU:O	3:D:484:PRO:HD2	2.11	0.50
3:D:633:VAL:HG22	3:D:635:PRO:CD	2.40	0.50
3:D:1271:LYS:HE3	3:D:1334:GLN:HE22	1.75	0.50
1:K:54:THR:HG23	1:K:156:HIS:CE1	2.46	0.50
2:M:350:ARG:HD3	2:M:353:ARG:HH22	1.76	0.50
3:N:183:GLU:HA	3:N:186:VAL:CG1	2.42	0.50
3:N:1433:SER:HB2	3:N:1457:ASP:CG	2.37	0.50
4:O:84:ARG:HB2	4:O:84:ARG:CZ	2.42	0.50
1:A:97:VAL:HG12	1:A:99:LEU:HD12	1.93	0.50
1:B:84:GLU:HB3	1:B:127:LEU:HD21	1.92	0.50
2:C:66:LEU:HB2	8:C:1196:HOH:O	2.11	0.50
2:C:175:GLU:HA	8:C:1786:HOH:O	2.11	0.50
2:C:404:LEU:O	2:C:407:LYS:HB2	2.11	0.50
2:C:670:GLN:HE22	2:C:699:PHE:C	2.20	0.50
2:C:1088:LEU:HB2	8:D:9002:HOH:O	2.10	0.50
3:D:111:LYS:CE	3:D:1452:ILE:HG12	2.40	0.50
3:D:1047:LYS:HB2	3:D:1051:GLU:OE2	2.10	0.50
3:D:1117:TYR:HE2	3:D:1151:ARG:HH21	1.59	0.50
3:D:1200:VAL:HG22	3:D:1373:ARG:HH12	1.76	0.50
4:E:17:TYR:O	4:E:21:VAL:HG23	2.11	0.50
5:F:142:ARG:HB3	5:F:142:ARG:HH11	1.77	0.50
1:K:86:VAL:HG12	1:K:124:ASN:HD22	1.76	0.50
1:L:33:GLY:O	1:L:195:LEU:HD22	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:333:ILE:O	2:M:465:GLY:HA3	2.11	0.50
2:M:706:GLU:HB3	2:M:708:TYR:CE1	2.47	0.50
2:M:1067:TYR:HA	2:M:1070:ILE:HD12	1.93	0.50
3:N:130:SER:C	3:N:568:ARG:HH21	2.20	0.50
3:N:554:LEU:HD21	3:N:571:LYS:HG3	1.93	0.50
3:N:639:LEU:HD12	3:N:639:LEU:N	2.25	0.50
3:N:1097:LYS:HD2	8:N:9081:HOH:O	2.10	0.50
3:N:1258:ARG:HG3	3:N:1262:LEU:HD22	1.92	0.50
3:N:1342:GLU:CD	3:N:1342:GLU:N	2.67	0.50
5:P:132:ARG:HE	5:P:184:ARG:NH1	2.07	0.50
5:P:164:LYS:HD2	8:P:4625:HOH:O	2.10	0.50
1:A:44:LEU:O	1:A:174:VAL:HG21	2.12	0.50
2:C:254:VAL:HG13	2:C:258:TYR:CE1	2.44	0.50
2:C:432:ARG:HD3	3:D:1048:PRO:HG2	1.92	0.50
2:C:572:ILE:CG2	2:C:703:ILE:HD13	2.41	0.50
2:C:722:ILE:O	2:C:722:ILE:HD13	2.12	0.50
2:C:876:VAL:O	2:C:879:ARG:O	2.29	0.50
3:D:526:PRO:O	3:D:537:THR:HA	2.12	0.50
3:D:762:GLN:NE2	4:E:20:THR:HG21	2.27	0.50
3:D:904:VAL:HG22	8:D:9514:HOH:O	2.09	0.50
3:D:1119:SER:HA	3:D:1186:VAL:O	2.11	0.50
3:D:1429:LEU:HG	3:D:1441:GLN:OE1	2.11	0.50
5:F:149:GLU:OE1	5:F:149:GLU:HA	2.11	0.50
5:F:373:LYS:HD3	5:F:378:GLY:C	2.36	0.50
1:K:173:PRO:HB3	1:K:204:SER:HB3	1.93	0.50
1:L:132:LEU:HD21	1:L:136:GLY:O	2.12	0.50
2:M:199:VAL:HG13	2:M:235:LEU:CG	2.39	0.50
2:M:680:ASP:HB2	2:M:682:TYR:CE2	2.46	0.50
2:M:707:ARG:HG3	2:M:826:TYR:CE2	2.46	0.50
2:M:755:LEU:HB2	2:M:790:LEU:CD2	2.40	0.50
2:M:1016:ILE:HD13	2:M:1016:ILE:N	2.27	0.50
3:N:175:VAL:HG11	8:N:9190:HOH:O	2.11	0.50
3:N:699:VAL:N	3:N:756:GLN:NE2	2.53	0.50
3:N:1090:ASP:O	3:N:1093:TYR:HB3	2.12	0.50
3:N:1263:PHE:CD2	3:N:1371:VAL:HG11	2.47	0.50
8:N:9535:HOH:O	5:P:140:ARG:HB2	2.10	0.50
5:P:102:LEU:O	5:P:106:VAL:HG23	2.12	0.50
5:P:113:ILE:HG23	5:P:127:ILE:CG2	2.41	0.50
1:A:213:GLN:O	1:A:217:ILE:HG13	2.11	0.50
1:B:11:PHE:CD1	1:B:25:LEU:HD13	2.47	0.50
1:B:158:ILE:HA	8:B:396:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:72:ARG:HD3	8:C:1601:HOH:O	2.12	0.50
2:C:479:VAL:HG23	2:C:506:ASN:C	2.37	0.50
3:D:178:LEU:CD2	3:D:199:LEU:H	2.24	0.50
3:D:470:LEU:HD12	3:D:508:ARG:HH21	1.77	0.50
3:D:902:LEU:H	3:D:902:LEU:HD12	1.76	0.50
3:D:1105:ILE:HD11	3:D:1374:GLN:NE2	2.26	0.50
3:D:1205:TYR:HE1	3:D:1221:VAL:CG1	2.23	0.50
3:D:1396:GLU:O	3:D:1400:VAL:HG23	2.12	0.50
1:K:56:VAL:HG21	1:K:82:LEU:HD12	1.93	0.50
1:K:173:PRO:HB2	1:K:205:VAL:HG22	1.93	0.50
1:L:81:ASN:HB2	8:L:2800:HOH:O	2.12	0.50
2:M:139:GLN:O	2:M:334:ARG:N	2.43	0.50
2:M:191:PHE:CD2	2:M:238:LEU:HD21	2.47	0.50
2:M:377:PRO:HA	8:M:1544:HOH:O	2.11	0.50
2:M:589:ARG:HD2	8:M:1552:HOH:O	2.12	0.50
2:M:852:ILE:N	2:M:852:ILE:HD12	2.27	0.50
2:M:853:LEU:HD23	2:M:858:MET:HB3	1.94	0.50
2:M:1005:MET:HE1	3:N:648:MET:CB	2.42	0.50
3:N:21:TRP:HZ3	3:N:518:PRO:HG2	1.77	0.50
3:N:950:GLY:O	3:N:951:ILE:C	2.54	0.50
3:N:951:ILE:CG2	3:N:1062:ARG:HH21	2.24	0.50
3:N:1335:LEU:HD23	3:N:1344:VAL:HG22	1.94	0.50
5:P:287:THR:N	5:P:290:GLU:OE1	2.44	0.50
5:P:412:GLU:HG3	5:P:418:LEU:HD22	1.92	0.50
1:A:13:VAL:HG12	1:A:15:THR:HG22	1.94	0.50
1:A:26:GLU:HG2	1:A:27:PRO:HA	1.94	0.50
1:A:156:HIS:CD2	1:A:157:GLY:H	2.29	0.50
1:A:206:THR:CG2	1:A:209:GLU:HG3	2.39	0.50
2:C:18:LEU:HB2	2:C:590:ASP:HB3	1.93	0.50
2:C:103:LYS:HG3	8:C:1421:HOH:O	2.12	0.50
2:C:136:ILE:HG21	2:C:336:VAL:HG13	1.93	0.50
2:C:195:LEU:CD2	2:C:238:LEU:HG	2.42	0.50
2:C:437:ARG:HA	2:C:467:ILE:CG2	2.40	0.50
2:C:534:VAL:HB	2:C:538:GLN:NE2	2.27	0.50
2:C:572:ILE:HG21	2:C:703:ILE:HD13	1.92	0.50
2:C:780:GLU:CD	2:C:781:LYS:H	2.18	0.50
2:C:1101:THR:HB	3:D:5:VAL:HG13	1.92	0.50
8:C:1739:HOH:O	5:F:370:LYS:HG2	2.12	0.50
3:D:396:VAL:HG13	3:D:446:VAL:O	2.12	0.50
3:D:399:ARG:NH2	3:D:432:TYR:HE2	2.09	0.50
3:D:661:MET:CE	3:D:673:ALA:HB1	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1009:LYS:O	3:D:1012:GLU:HG2	2.11	0.50
3:D:1147:ARG:O	3:D:1166:LEU:HD23	2.11	0.50
3:D:1264:GLU:CD	3:D:1425:THR:H	2.20	0.50
5:F:289:GLU:O	5:F:293:GLU:HG3	2.11	0.50
1:K:42:ARG:HG2	1:K:42:ARG:HH11	1.76	0.50
2:M:214:TYR:HB2	8:M:1457:HOH:O	2.12	0.50
2:M:428:ARG:HG2	2:M:451:LEU:HG	1.93	0.50
2:M:704:HIS:CG	2:M:831:ARG:HH21	2.30	0.50
2:M:837:ASP:O	2:M:848:VAL:HG13	2.12	0.50
2:M:889:HIS:CD2	2:M:970:GLY:HA3	2.46	0.50
2:M:1027:PHE:HA	8:M:1757:HOH:O	2.11	0.50
3:N:30:GLU:HB3	3:N:40:GLU:HB3	1.93	0.50
3:N:186:VAL:HG13	3:N:187:LYS:N	2.27	0.50
3:N:207:PHE:CB	3:N:208:PRO:HD2	2.35	0.50
3:N:502:PHE:HZ	3:N:512:MET:HE2	1.76	0.50
3:N:574:LEU:O	3:N:578:VAL:HG23	2.11	0.50
3:N:950:GLY:C	3:N:953:ASP:H	2.20	0.50
5:P:108:GLU:OE1	5:P:108:GLU:HA	2.12	0.50
2:C:197:LEU:HD22	2:C:202:TYR:HD2	1.76	0.50
2:C:404:LEU:HD22	2:C:591:SER:HB3	1.93	0.50
2:C:627:ARG:O	2:C:638:ASP:HB3	2.12	0.50
3:D:404:GLU:HB3	3:D:414:ARG:HD3	1.94	0.50
3:D:690:ALA:O	3:D:694:VAL:HG23	2.12	0.50
3:D:834:THR:HB	3:D:838:ARG:HB3	1.92	0.50
3:D:916:TYR:CE2	3:D:920:LEU:HD13	2.46	0.50
3:D:1192:LEU:HG	3:D:1369:GLU:HG2	1.92	0.50
3:D:1455:LYS:HD3	3:D:1455:LYS:C	2.36	0.50
8:D:9410:HOH:O	5:F:147:LEU:HD11	2.11	0.50
5:F:404:ALA:O	5:F:408:LEU:HD23	2.12	0.50
2:M:228:ALA:HB2	8:M:1214:HOH:O	2.11	0.50
2:M:955:PRO:HA	8:M:1188:HOH:O	2.11	0.50
3:N:148:GLU:HB3	3:N:151:GLN:HB3	1.93	0.50
3:N:421:LEU:HD11	3:N:437:VAL:CG2	2.42	0.50
3:N:462:GLN:HA	3:N:513:ILE:HD13	1.94	0.50
3:N:898:GLU:HB3	3:N:921:ARG:HH22	1.76	0.50
3:N:1114:THR:CG2	3:N:1195:GLN:HB3	2.41	0.50
3:N:1128:VAL:O	3:N:1129:THR:C	2.55	0.50
1:A:42:ARG:NH2	1:B:34:VAL:HB	2.27	0.50
2:C:157:ARG:CD	2:C:314:THR:HG22	2.40	0.50
2:C:352:ALA:C	2:C:355:VAL:HG12	2.37	0.50
2:C:437:ARG:CZ	2:C:469:THR:HG22	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:464:LEU:O	2:C:466:PHE:N	2.45	0.50
2:C:1045:ALA:HB1	2:C:1048:THR:HB	1.94	0.50
3:D:15:PRO:HA	3:D:18:ILE:CG1	2.41	0.50
3:D:42:ASP:O	3:D:43:GLY:O	2.29	0.50
3:D:462:GLN:HA	3:D:513:ILE:CD1	2.41	0.50
3:D:658:LEU:HD11	3:D:674:ARG:HH11	1.77	0.50
3:D:864:VAL:HG12	3:D:865:THR:H	1.77	0.50
3:D:965:GLU:HA	3:D:968:ASP:HB2	1.94	0.50
3:D:1230:GLY:HA3	8:D:9051:HOH:O	2.11	0.50
5:F:255:ALA:HB3	8:F:561:HOH:O	2.11	0.50
2:M:136:ILE:CG2	2:M:336:VAL:HG13	2.42	0.50
2:M:751:PRO:HA	2:M:792:VAL:CG1	2.42	0.50
2:M:1059:ASP:CG	2:M:1062:GLY:HA3	2.37	0.50
3:N:9:ARG:HH22	3:N:507:ASN:HD21	1.60	0.50
3:N:16:GLU:HB2	8:N:9939:HOH:O	2.11	0.50
3:N:428:LYS:HB3	3:N:450:TYR:CE1	2.46	0.50
3:N:813:LEU:HD12	3:N:817:GLU:OE1	2.12	0.50
3:N:846:PRO:HD3	8:N:9226:HOH:O	2.10	0.50
5:P:363:GLU:HA	5:P:367:MET:HE3	1.93	0.50
5:P:419:ARG:HG3	5:P:420:ASP:N	2.26	0.50
1:B:145:ASP:O	1:B:171:PHE:HE1	1.94	0.49
2:C:137:VAL:HG22	2:C:391:LEU:O	2.12	0.49
2:C:218:VAL:HG22	2:C:221:LEU:HD23	1.93	0.49
2:C:437:ARG:HB3	2:C:467:ILE:HB	1.93	0.49
2:C:630:ARG:HG2	2:C:630:ARG:HH11	1.76	0.49
2:C:674:VAL:HG11	2:C:992:MET:HE3	1.93	0.49
2:C:1044:GLY:CA	4:E:17:TYR:HE1	2.25	0.49
3:D:400:VAL:HG12	3:D:401:TYR:HD1	1.75	0.49
3:D:1003:VAL:O	3:D:1007:VAL:HG13	2.12	0.49
3:D:1102:THR:HG22	3:D:1222:GLY:CA	2.41	0.49
4:E:66:LYS:HB2	4:E:66:LYS:NZ	2.26	0.49
1:K:49:PRO:HB3	1:K:148:VAL:HG22	1.94	0.49
1:K:64:GLU:HB2	8:K:3487:HOH:O	2.10	0.49
2:M:86:LYS:CG	2:M:813:VAL:HG12	2.41	0.49
2:M:723:THR:HG21	2:M:783:ARG:HH22	1.77	0.49
3:N:183:GLU:O	3:N:186:VAL:HG12	2.12	0.49
3:N:427:VAL:HG21	3:N:435:VAL:HB	1.93	0.49
3:N:543:LEU:O	3:N:546:ARG:HB2	2.11	0.49
3:N:733:CYS:HA	8:N:9159:HOH:O	2.12	0.49
3:N:836:VAL:HA	3:N:839:LEU:HB2	1.94	0.49
3:N:1397:LYS:O	3:N:1400:VAL:HB	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1481:VAL:HA	4:O:18:ARG:HH21	1.77	0.49
1:A:219:ARG:CZ	1:B:223:THR:HG23	2.42	0.49
2:C:217:LEU:HA	8:C:1241:HOH:O	2.10	0.49
2:C:551:GLU:HB3	2:C:906:PHE:HD2	1.77	0.49
2:C:761:PHE:N	2:C:761:PHE:CD1	2.80	0.49
2:C:1004:LYS:HE3	2:C:1027:PHE:CE1	2.45	0.49
3:D:191:LEU:HD22	3:D:195:VAL:HG21	1.94	0.49
3:D:549:ASN:HB3	8:F:611:HOH:O	2.12	0.49
3:D:630:VAL:HG23	3:D:744:GLN:OE1	2.12	0.49
3:D:1197:ARG:HG3	8:D:9036:HOH:O	2.10	0.49
3:D:1310:ARG:HG2	3:D:1327:ARG:HB3	1.94	0.49
3:D:1363:LEU:HD12	3:D:1364:HIS:O	2.12	0.49
4:E:86:GLN:O	4:E:90:GLU:HG3	2.12	0.49
5:F:167:PRO:HD2	5:F:170:HIS:CD2	2.47	0.49
1:K:66:SER:O	1:K:75:VAL:HG23	2.12	0.49
1:K:211:LEU:O	1:K:215:VAL:HG22	2.12	0.49
2:M:49:ARG:HB2	2:M:49:ARG:NH1	2.27	0.49
2:M:157:ARG:NE	2:M:157:ARG:HA	2.27	0.49
2:M:259:GLY:HA3	8:M:1296:HOH:O	2.11	0.49
2:M:508:ILE:HG21	8:M:1319:HOH:O	2.12	0.49
2:M:745:ILE:HD11	8:M:1269:HOH:O	2.11	0.49
2:M:826:TYR:N	2:M:826:TYR:CD1	2.80	0.49
3:N:60:CYS:SG	3:N:62:LYS:HG2	2.52	0.49
3:N:583:ASP:HA	3:N:602:SER:HB2	1.93	0.49
3:N:1496:GLU:O	3:N:1500:LYS:HG3	2.12	0.49
4:O:39:VAL:HB	4:O:72:ARG:HD2	1.94	0.49
5:P:142:ARG:HB3	5:P:142:ARG:HH11	1.76	0.49
1:A:61:VAL:HG12	8:A:482:HOH:O	2.12	0.49
1:A:102:LYS:HE2	1:A:139:ASN:CG	2.37	0.49
2:C:141:HIS:ND1	2:C:418:LEU:HG	2.27	0.49
2:C:710:ILE:CB	2:C:790:LEU:HD13	2.39	0.49
3:D:197:SER:CB	3:D:203:ALA:HB3	2.28	0.49
3:D:525:ARG:HB2	3:D:541:ASN:ND2	2.26	0.49
3:D:850:LEU:O	3:D:853:VAL:HB	2.12	0.49
3:D:1205:TYR:HD2	8:D:9465:HOH:O	1.95	0.49
3:D:1209:LEU:HD21	4:E:16:LYS:HZ2	1.75	0.49
3:D:1213:ARG:HB2	3:D:1214:PRO:HD3	1.92	0.49
1:L:62:LEU:HD12	8:L:2996:HOH:O	2.12	0.49
2:M:170:PRO:HG2	2:M:258:TYR:HD2	1.76	0.49
2:M:708:TYR:CD1	2:M:708:TYR:N	2.79	0.49
3:N:379:ALA:HB2	8:N:9176:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:462:GLN:HB3	8:N:9127:HOH:O	2.12	0.49
3:N:474:GLU:O	3:N:478:LEU:HG	2.12	0.49
3:N:645:PRO:HG3	3:N:725:SER:O	2.13	0.49
3:N:844:ALA:HA	3:N:867:ARG:NH1	2.27	0.49
3:N:1225:ALA:HA	3:N:1367:HIS:ND1	2.27	0.49
3:N:1263:PHE:CE2	3:N:1371:VAL:HG11	2.48	0.49
3:N:1281:VAL:HG21	3:N:1313:VAL:CG2	2.43	0.49
1:B:27:PRO:HB3	1:B:192:LEU:HD22	1.93	0.49
2:C:15:LEU:HD13	2:C:586:ARG:HG3	1.94	0.49
2:C:146:VAL:HG13	2:C:161:SER:O	2.12	0.49
2:C:443:THR:HG23	2:C:449:ILE:HD12	1.92	0.49
2:C:503:LEU:HD13	2:C:507:ARG:O	2.12	0.49
2:C:777:ILE:HA	5:F:405:LEU:HD21	1.93	0.49
3:D:85:VAL:HG12	3:D:89:ARG:NE	2.28	0.49
3:D:87:ARG:CB	3:D:523:ASP:HB2	2.41	0.49
3:D:111:LYS:HE2	3:D:1452:ILE:HG21	1.95	0.49
3:D:395:VAL:HG12	8:D:2022:HOH:O	2.11	0.49
3:D:809:PRO:O	3:D:812:ALA:HB3	2.12	0.49
3:D:1105:ILE:HA	8:D:9253:HOH:O	2.12	0.49
3:D:1283:ILE:N	3:D:1315:ASP:OD1	2.45	0.49
4:E:55:PHE:HB3	8:E:116:HOH:O	2.12	0.49
1:K:57:TYR:CE2	1:K:161:ARG:HD2	2.47	0.49
1:K:68:ILE:HG21	1:K:138:LEU:CD1	2.42	0.49
1:L:57:TYR:CE2	1:L:161:ARG:HG2	2.47	0.49
1:L:101:LEU:HD11	1:L:113:ASP:HB2	1.95	0.49
2:M:92:ALA:HB2	2:M:120:LEU:CD1	2.34	0.49
2:M:490:GLU:HG2	2:M:494:TYR:CE1	2.47	0.49
2:M:1118:LYS:HG2	3:N:23:TYR:HE1	1.78	0.49
3:N:7:LYS:HD3	3:N:1456:LYS:NZ	2.28	0.49
3:N:203:ALA:HA	8:N:9962:HOH:O	2.13	0.49
3:N:781:PRO:HB3	3:N:785:ILE:CG2	2.42	0.49
3:N:868:TYR:HE2	3:N:880:ILE:HD11	1.78	0.49
5:P:107:GLU:HG3	8:P:4460:HOH:O	2.11	0.49
5:P:218:GLN:HE21	5:P:221:ILE:HD12	1.78	0.49
5:P:247:ILE:O	5:P:251:ILE:HG13	2.13	0.49
5:P:358:LEU:CD1	5:P:370:LYS:HG3	2.38	0.49
5:P:362:SER:O	5:P:367:MET:HE2	2.11	0.49
5:P:363:GLU:HA	5:P:367:MET:CE	2.42	0.49
1:B:101:LEU:HD12	1:B:114:PHE:CE1	2.47	0.49
2:C:327:HIS:HD2	2:C:433:THR:OG1	1.96	0.49
2:C:461:VAL:HG22	8:C:1321:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:551:GLU:HG3	2:C:552:HIS:CD2	2.48	0.49
2:C:577:PRO:HA	2:C:671:ASN:OD1	2.13	0.49
2:C:710:ILE:HB	2:C:790:LEU:HD22	1.94	0.49
3:D:44:LEU:HB3	3:D:525:ARG:HH21	1.77	0.49
3:D:473:LEU:HD21	3:D:495:ARG:CZ	2.42	0.49
3:D:543:LEU:HA	3:D:546:ARG:HG3	1.93	0.49
3:D:1107:VAL:CG1	3:D:1217:ILE:HA	2.43	0.49
3:D:1240:THR:O	3:D:1257:PRO:HB3	2.11	0.49
4:E:26:ARG:HE	4:E:30:LEU:CD1	2.25	0.49
5:F:203:THR:HB	8:F:436:HOH:O	2.11	0.49
5:F:299:TRP:CE3	5:F:303:ARG:HD3	2.47	0.49
1:K:65:PHE:CE1	2:M:799:ILE:HD11	2.46	0.49
2:M:937:ASP:HB2	2:M:940:GLU:H	1.77	0.49
3:N:119:SER:HB2	3:N:123:LEU:CB	2.38	0.49
3:N:570:GLU:OE2	5:P:214:GLN:HG3	2.12	0.49
3:N:720:LEU:HD12	8:N:9443:HOH:O	2.12	0.49
3:N:970:LYS:HE3	8:N:9931:HOH:O	2.13	0.49
3:N:1197:ARG:HD2	3:N:1198:TYR:CE1	2.48	0.49
5:P:260:ILE:CG2	5:P:264:MET:HB2	2.41	0.49
5:P:291:ILE:HB	8:P:4032:HOH:O	2.13	0.49
1:A:187:GLY:HA3	8:A:335:HOH:O	2.11	0.49
8:A:501:HOH:O	2:C:644:VAL:HG13	2.13	0.49
2:C:328:LEU:HB2	2:C:433:THR:CG2	2.42	0.49
2:C:332:ARG:NE	2:C:464:LEU:HD11	2.28	0.49
2:C:422:ARG:HG2	8:C:1141:HOH:O	2.12	0.49
2:C:479:VAL:HG22	2:C:508:ILE:HD13	1.95	0.49
2:C:515:ALA:C	2:C:516:ARG:HG2	2.38	0.49
2:C:609:ASN:ND2	2:C:627:ARG:NH2	2.58	0.49
2:C:726:ILE:O	2:C:726:ILE:HG22	2.11	0.49
2:C:896:PHE:O	2:C:924:VAL:HG11	2.12	0.49
3:D:96:ALA:CB	3:D:554:LEU:HD12	2.42	0.49
3:D:785:ILE:HG22	3:D:789:LEU:HD12	1.94	0.49
3:D:806:PHE:O	3:D:807:ALA:C	2.55	0.49
3:D:862:ASP:O	3:D:877:PRO:HD3	2.12	0.49
3:D:1289:LYS:HE3	3:D:1307:LYS:CE	2.41	0.49
5:F:277:GLN:O	5:F:280:GLN:HB3	2.12	0.49
5:F:419:ARG:O	5:F:421:PHE:N	2.46	0.49
1:L:84:GLU:HG3	1:L:127:LEU:HD22	1.94	0.49
1:L:102:LYS:HG3	1:L:139:ASN:CB	2.42	0.49
1:L:196:THR:HB	8:L:4937:HOH:O	2.11	0.49
2:M:139:GLN:HE22	2:M:415:PRO:CD	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:420:ARG:HD2	2:M:420:ARG:H	1.76	0.49
2:M:802:ARG:HD2	8:M:1213:HOH:O	2.12	0.49
2:M:861:LEU:HD21	2:M:925:TYR:CE2	2.48	0.49
2:M:882:LEU:HD12	3:N:1061:PHE:HB3	1.95	0.49
2:M:965:GLU:HA	2:M:968:LEU:HD12	1.94	0.49
2:M:1060:ILE:HG22	2:M:1061:GLU:N	2.28	0.49
3:N:28:LYS:CB	3:N:41:ARG:HD2	2.43	0.49
3:N:133:ILE:HG23	3:N:455:ARG:N	2.28	0.49
3:N:135:LEU:CD1	3:N:147:VAL:HG23	2.41	0.49
3:N:169:TYR:N	3:N:170:PRO:CD	2.76	0.49
3:N:728:LEU:HD12	8:N:9339:HOH:O	2.12	0.49
3:N:890:VAL:CG1	3:N:926:LYS:HD3	2.42	0.49
3:N:906:GLN:HA	3:N:906:GLN:OE1	2.11	0.49
3:N:1139:ASP:O	3:N:1142:ALA:HB3	2.13	0.49
1:A:72:LYS:HB3	1:A:73:GLU:OE2	2.13	0.49
2:C:274:ARG:HG3	2:C:274:ARG:O	2.13	0.49
2:C:366:SER:O	2:C:367:LEU:HD23	2.12	0.49
2:C:433:THR:HG22	2:C:433:THR:O	2.13	0.49
2:C:589:ARG:HG2	8:C:1213:HOH:O	2.12	0.49
2:C:630:ARG:NH2	2:C:706:GLU:C	2.71	0.49
3:D:124:GLU:HG2	3:D:128:TYR:CZ	2.47	0.49
3:D:1403:LEU:O	3:D:1407:LEU:HB2	2.11	0.49
4:E:51:LEU:CD1	4:E:52:GLU:H	2.26	0.49
5:F:335:ASP:CG	5:F:338:LEU:HB2	2.37	0.49
1:L:20:TYR:HE2	1:L:198:ARG:HB3	1.78	0.49
2:M:332:ARG:NE	2:M:464:LEU:HG	2.28	0.49
2:M:333:ILE:HD13	2:M:467:ILE:HG13	1.93	0.49
2:M:580:MET:HB3	2:M:584:GLU:OE2	2.13	0.49
2:M:768:THR:O	2:M:772:ARG:HB3	2.12	0.49
3:N:27:GLU:O	3:N:28:LYS:HD2	2.13	0.49
3:N:574:LEU:O	3:N:577:ALA:HB3	2.11	0.49
3:N:602:SER:O	3:N:606:ILE:HG12	2.13	0.49
3:N:957:PRO:HG2	3:N:1007:VAL:HG12	1.94	0.49
3:N:1476:THR:CG2	4:O:21:VAL:HG22	2.36	0.49
4:O:54:LEU:HB3	8:O:4983:HOH:O	2.12	0.49
5:P:142:ARG:HB3	5:P:142:ARG:NH1	2.26	0.49
5:P:184:ARG:O	5:P:188:ILE:HG13	2.12	0.49
1:B:65:PHE:HD1	3:D:813:LEU:HD22	1.76	0.49
2:C:84:ARG:HH21	2:C:128:ILE:HD11	1.78	0.49
2:C:172:ILE:HD12	2:C:172:ILE:N	2.27	0.49
2:C:412:ALA:CB	2:C:451:LEU:HB3	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:717:LEU:HB3	8:C:1140:HOH:O	2.13	0.49
2:C:751:PRO:HA	2:C:792:VAL:CG1	2.42	0.49
2:C:817:PRO:C	2:C:819:VAL:H	2.20	0.49
3:D:229:ALA:HA	8:D:2026:HOH:O	2.12	0.49
3:D:436:GLU:HB2	3:D:445:ARG:HB3	1.93	0.49
3:D:493:ARG:HD2	8:D:9698:HOH:O	2.13	0.49
3:D:696:HIS:HD2	4:E:59:ASN:HB2	1.74	0.49
3:D:790:TYR:CG	3:D:1026:SER:HB3	2.48	0.49
3:D:939:PHE:O	3:D:943:THR:HG23	2.13	0.49
3:D:1157:GLY:HA3	8:D:9057:HOH:O	2.11	0.49
3:D:1206:GLY:HA3	3:D:1366:LYS:NZ	2.27	0.49
5:F:404:ALA:HA	8:F:429:HOH:O	2.12	0.49
2:M:62:GLY:O	2:M:103:LYS:HG3	2.13	0.49
2:M:345:ARG:HB3	2:M:345:ARG:HH11	1.77	0.49
2:M:492:ASP:HB3	2:M:518:LYS:CD	2.42	0.49
2:M:571:LEU:HD23	2:M:670:GLN:HE21	1.77	0.49
2:M:770:GLU:HB2	8:N:9595:HOH:O	2.12	0.49
2:M:832:LYS:O	2:M:833:LEU:C	2.55	0.49
3:N:400:VAL:C	3:N:402:PRO:HD3	2.38	0.49
3:N:687:VAL:O	3:N:690:ALA:HB3	2.12	0.49
3:N:1007:VAL:HG23	3:N:1008:PHE:N	2.28	0.49
3:N:1314:LYS:HE2	3:N:1317:ASP:OD2	2.12	0.49
3:N:1442:ASN:HA	8:N:9244:HOH:O	2.11	0.49
5:P:128:ARG:O	5:P:132:ARG:HG2	2.13	0.49
5:P:181:GLU:O	5:P:184:ARG:HB3	2.13	0.49
1:A:95:GLN:HG2	1:A:146:ARG:NH2	2.14	0.49
1:B:57:TYR:CE1	1:B:163:ASN:HB2	2.46	0.49
2:C:100:LEU:HD12	2:C:101:ILE:O	2.12	0.49
2:C:212:GLY:C	2:C:215:GLY:H	2.21	0.49
2:C:397:GLU:HA	2:C:403:SER:HB3	1.94	0.49
2:C:536:PRO:HB3	2:C:906:PHE:HD1	1.77	0.49
2:C:637:LEU:HD13	8:C:1532:HOH:O	2.12	0.49
2:C:842:ARG:HH21	2:C:887:GLU:CD	2.21	0.49
3:D:440:VAL:HG22	8:D:9349:HOH:O	2.13	0.49
3:D:1148:VAL:HG11	3:D:1203:LYS:HD2	1.95	0.49
3:D:1290:LEU:CD2	3:D:1291:SER:H	2.25	0.49
3:D:1431:THR:HB	8:D:9481:HOH:O	2.13	0.49
3:D:1447:LEU:O	3:D:1448:THR:C	2.56	0.49
5:F:395:GLU:O	5:F:399:GLN:HB2	2.13	0.49
2:M:139:GLN:HG3	2:M:140:ILE:N	2.26	0.49
2:M:326:ASP:HB2	2:M:431:HIS:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:525:SER:H	2:M:528:GLU:HG3	1.77	0.49
2:M:565:GLN:CA	2:M:995:MET:HE1	2.42	0.49
2:M:758:ARG:HB3	2:M:788:THR:O	2.13	0.49
2:M:841:ASN:ND2	2:M:844:GLY:H	2.11	0.49
3:N:674:ARG:HG2	3:N:674:ARG:HH11	1.76	0.49
3:N:704:ARG:HG3	3:N:736:PHE:CB	2.43	0.49
3:N:1147:ARG:O	3:N:1166:LEU:HD23	2.13	0.49
1:A:62:LEU:HB3	1:A:163:ASN:HD21	1.78	0.49
2:C:207:LEU:HD22	2:C:221:LEU:HD22	1.95	0.49
2:C:603:VAL:HG12	8:C:1221:HOH:O	2.13	0.49
3:D:1101:VAL:HG22	3:D:1428:ALA:HB2	1.95	0.49
4:E:84:ARG:NH1	4:E:84:ARG:HB2	2.26	0.49
5:F:142:ARG:HG3	8:F:482:HOH:O	2.12	0.49
1:K:96:THR:HG21	8:K:3321:HOH:O	2.12	0.49
2:M:285:LEU:HD23	2:M:285:LEU:O	2.13	0.49
2:M:497:ALA:HA	2:M:515:ALA:HA	1.94	0.49
2:M:614:ARG:CD	2:M:620:LEU:HD12	2.36	0.49
2:M:722:ILE:HG23	2:M:722:ILE:O	2.13	0.49
3:N:99:ALA:HA	3:N:575:GLN:NE2	2.28	0.49
3:N:466:LYS:HB2	8:N:9423:HOH:O	2.12	0.49
3:N:558:LEU:HD13	5:P:145:PRO:CB	2.40	0.49
3:N:948:THR:O	3:N:949:ILE:HD13	2.13	0.49
4:O:48:MET:N	4:O:54:LEU:HB2	2.28	0.49
4:O:54:LEU:HD23	4:O:58:PRO:HD2	1.94	0.49
5:P:176:ILE:HD12	8:P:3516:HOH:O	2.13	0.49
1:A:191:ASP:O	1:A:191:ASP:CG	2.55	0.48
1:B:89:PHE:CD1	1:B:120:VAL:HG13	2.48	0.48
2:C:137:VAL:O	2:C:391:LEU:HD21	2.13	0.48
2:C:166:PRO:HD2	8:C:1392:HOH:O	2.13	0.48
2:C:286:SER:HB3	8:C:1755:HOH:O	2.12	0.48
2:C:292:ARG:HB2	2:C:299:LYS:HE2	1.95	0.48
2:C:352:ALA:HA	2:C:355:VAL:CG1	2.42	0.48
3:D:32:ILE:HG12	3:D:38:LYS:O	2.13	0.48
3:D:1109:GLU:HG2	3:D:1201:CYS:CA	2.39	0.48
3:D:1236:LEU:HA	3:D:1359:GLN:CD	2.38	0.48
1:K:100:LEU:HD11	8:K:4816:HOH:O	2.13	0.48
1:L:32:PHE:O	1:L:36:LEU:HD23	2.12	0.48
2:M:200:LEU:HD13	2:M:300:ASP:OD2	2.13	0.48
2:M:510:ALA:HA	8:M:1122:HOH:O	2.13	0.48
2:M:537:LYS:CA	2:M:545:ASN:HD21	2.22	0.48
2:M:589:ARG:HH11	2:M:589:ARG:CB	2.23	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:721:ARG:O	2:M:758:ARG:HA	2.13	0.48
2:M:778:PHE:HD2	8:M:1700:HOH:O	1.95	0.48
2:M:810:ASP:HB3	2:M:813:VAL:HG22	1.95	0.48
2:M:998:TYR:CZ	2:M:1000:MET:HA	2.48	0.48
3:N:433:GLY:HA3	3:N:450:TYR:HD1	1.78	0.48
3:N:550:ARG:CZ	3:N:573:MET:HB3	2.43	0.48
3:N:890:VAL:HG12	8:N:9462:HOH:O	2.12	0.48
5:P:290:GLU:H	5:P:290:GLU:CD	2.20	0.48
1:B:18:ARG:O	1:B:207:PRO:HD3	2.13	0.48
2:C:470:PRO:HB3	2:C:485:TYR:CE1	2.48	0.48
2:C:498:GLN:O	2:C:501:THR:HG23	2.12	0.48
2:C:583:LEU:O	2:C:583:LEU:HG	2.13	0.48
2:C:1013:TYR:CE1	2:C:1020:PRO:HG3	2.48	0.48
3:D:679:ARG:HB2	3:D:682:ASP:OD2	2.13	0.48
3:D:843:PHE:CD1	3:D:849:ALA:HA	2.48	0.48
3:D:971:LEU:O	3:D:975:GLU:HG3	2.12	0.48
3:D:1310:ARG:NH1	3:D:1327:ARG:HD3	2.28	0.48
3:D:1330:ILE:HB	3:D:1347:TYR:CZ	2.48	0.48
2:M:283:ILE:HG23	8:M:1216:HOH:O	2.13	0.48
2:M:397:GLU:N	2:M:633:GLN:CD	2.71	0.48
2:M:516:ARG:CZ	3:N:1068:LEU:HD22	2.43	0.48
2:M:605:LYS:HB3	8:M:1452:HOH:O	2.11	0.48
2:M:637:LEU:N	2:M:637:LEU:HD23	2.28	0.48
3:N:12:LEU:HD22	3:N:511:TRP:CB	2.44	0.48
3:N:119:SER:H	3:N:123:LEU:CD2	2.23	0.48
3:N:785:ILE:HG12	3:N:935:LYS:HA	1.96	0.48
3:N:1046:GLN:OE1	3:N:1046:GLN:N	2.46	0.48
4:O:48:MET:CB	4:O:54:LEU:HB2	2.43	0.48
5:P:193:ARG:HG2	8:P:3920:HOH:O	2.13	0.48
5:P:208:SER:HB2	5:P:211:ASP:OD1	2.13	0.48
1:B:103:ALA:HB1	1:B:107:LYS:CE	2.37	0.48
2:C:367:LEU:CD2	2:C:371:LYS:HG2	2.41	0.48
2:C:552:HIS:CD2	2:C:886:LEU:HD12	2.47	0.48
2:C:742:VAL:HG12	2:C:743:VAL:N	2.28	0.48
2:C:759:THR:HB	2:C:785:VAL:HG21	1.95	0.48
2:C:802:ARG:HB3	8:C:1186:HOH:O	2.11	0.48
2:C:971:LYS:HB3	2:C:987:ILE:C	2.38	0.48
2:C:1008:ARG:NH2	2:C:1028:GLY:HA2	2.13	0.48
2:C:1034:GLU:HA	2:C:1037:VAL:CG2	2.42	0.48
3:D:63:TYR:HE2	8:D:9643:HOH:O	1.96	0.48
3:D:104:PHE:CD2	3:D:1448:THR:HG23	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:768:ASN:N	3:D:768:ASN:ND2	2.61	0.48
3:D:829:VAL:HA	8:D:2081:HOH:O	2.13	0.48
4:E:85:LEU:HD23	4:E:86:GLN:N	2.28	0.48
5:F:142:ARG:HA	8:F:755:HOH:O	2.13	0.48
5:F:231:ARG:HB3	5:F:233:PHE:CZ	2.49	0.48
1:K:109:VAL:HG23	1:K:132:LEU:HD13	1.95	0.48
1:K:140:MET:HG3	1:K:142:VAL:HG12	1.94	0.48
1:L:143:ARG:NH1	1:L:158:ILE:HG23	2.28	0.48
2:M:407:LYS:HD2	8:M:1363:HOH:O	2.12	0.48
2:M:619:ARG:C	2:M:620:LEU:HD13	2.37	0.48
2:M:707:ARG:HD2	2:M:824:ARG:HG2	1.93	0.48
2:M:882:LEU:HD11	3:N:1038:LEU:HD23	1.94	0.48
2:M:1063:ARG:O	2:M:1066:ALA:HB3	2.12	0.48
3:N:15:PRO:HA	3:N:18:ILE:CG1	2.42	0.48
3:N:126:VAL:HG12	3:N:132:TYR:HB2	1.95	0.48
3:N:179:VAL:HG23	8:N:9425:HOH:O	2.13	0.48
3:N:668:PRO:HD2	3:N:672:ALA:CB	2.43	0.48
3:N:756:GLN:HG2	8:N:9643:HOH:O	2.12	0.48
3:N:844:ALA:HB1	8:N:9025:HOH:O	2.11	0.48
3:N:860:LEU:HB2	3:N:861:GLN:NE2	2.28	0.48
3:N:1243:THR:HG1	3:N:1253:THR:HB	1.78	0.48
3:N:1493:LYS:O	3:N:1497:GLU:HG2	2.13	0.48
1:A:118:ALA:HB3	8:A:444:HOH:O	2.14	0.48
2:C:379:GLU:O	2:C:383:ARG:HB3	2.12	0.48
2:C:435:TYR:C	2:C:437:ARG:H	2.21	0.48
2:C:500:ASN:ND2	3:D:1067:VAL:HG23	2.20	0.48
2:C:839:LEU:HD12	2:C:994:ILE:HG21	1.95	0.48
2:C:872:ASN:HB3	8:C:1870:HOH:O	2.13	0.48
3:D:139:GLY:N	3:D:147:VAL:HG21	2.27	0.48
3:D:396:VAL:HG21	3:D:447:VAL:HB	1.96	0.48
3:D:586:ARG:NH1	3:D:1444:THR:HG21	2.28	0.48
3:D:608:SER:O	3:D:612:GLY:HA3	2.14	0.48
3:D:1291:SER:HB2	3:D:1293:PHE:CE1	2.42	0.48
5:F:132:ARG:HD3	5:F:181:GLU:CD	2.39	0.48
5:F:134:LYS:HB3	5:F:178:ARG:NH1	2.28	0.48
5:F:226:LYS:HE3	8:F:741:HOH:O	2.12	0.48
5:F:310:ILE:HB	8:F:438:HOH:O	2.12	0.48
1:L:2:LEU:HD12	1:L:3:ASP:N	2.27	0.48
1:L:13:VAL:HG22	8:L:3037:HOH:O	2.13	0.48
2:M:91:GLN:CD	2:M:117:HIS:HB3	2.37	0.48
2:M:141:HIS:HB3	2:M:418:LEU:HD23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:195:LEU:CD2	2:M:238:LEU:HG	2.43	0.48
2:M:281:LEU:CD1	2:M:306:THR:HA	2.44	0.48
2:M:748:GLU:HA	2:M:799:ILE:HG22	1.95	0.48
2:M:939:ARG:HD3	2:M:982:PRO:HD3	1.95	0.48
2:M:1060:ILE:HG12	2:M:1063:ARG:HH21	1.78	0.48
3:N:566:ILE:HB	8:N:9165:HOH:O	2.13	0.48
3:N:1004:THR:O	3:N:1007:VAL:HG22	2.13	0.48
3:N:1045:MET:HG2	3:N:1073:SER:CA	2.39	0.48
3:N:1176:LYS:HA	3:N:1179:GLU:OE2	2.14	0.48
4:O:35:PHE:HB3	8:O:3746:HOH:O	2.14	0.48
5:P:132:ARG:HD3	5:P:181:GLU:CD	2.37	0.48
2:C:892:LEU:HD21	2:C:967:PHE:CE1	2.49	0.48
3:D:65:ARG:HG3	3:D:66:GLN:N	2.25	0.48
3:D:768:ASN:HD22	3:D:768:ASN:H	1.61	0.48
8:D:9332:HOH:O	5:F:80:PRO:HA	2.13	0.48
5:F:138:SER:HB2	5:F:140:ARG:HG2	1.96	0.48
5:F:194:LEU:HB2	8:F:523:HOH:O	2.12	0.48
5:F:278:LEU:HB3	5:F:286:PRO:CG	2.43	0.48
1:L:103:ALA:HB1	1:L:107:LYS:CE	2.43	0.48
1:L:173:PRO:HB3	1:L:204:SER:HB3	1.94	0.48
2:M:264:PRO:HB2	2:M:289:THR:OG1	2.13	0.48
2:M:462:ASP:CG	2:M:463:GLU:H	2.21	0.48
2:M:474:VAL:HG23	2:M:478:VAL:O	2.13	0.48
2:M:607:ASP:HB2	2:M:610:ARG:HG3	1.95	0.48
3:N:565:ILE:H	3:N:565:ILE:CD1	2.10	0.48
5:P:110:MET:HE1	8:P:4110:HOH:O	2.14	0.48
5:P:223:ALA:HB2	5:P:242:TRP:HB2	1.95	0.48
5:P:320:PRO:C	5:P:321:ILE:HD13	2.38	0.48
1:B:162:ILE:HG22	8:B:463:HOH:O	2.12	0.48
2:C:41:ASN:HB3	8:C:1231:HOH:O	2.13	0.48
2:C:115:LEU:HD22	2:C:373:VAL:CG1	2.43	0.48
2:C:127:PHE:O	2:C:133:ASP:HA	2.13	0.48
2:C:630:ARG:HH22	2:C:707:ARG:N	2.11	0.48
2:C:708:TYR:N	2:C:708:TYR:CD1	2.81	0.48
2:C:746:GLY:C	2:C:799:ILE:HG22	2.38	0.48
3:D:101:HIS:ND1	3:D:103:TRP:HB2	2.26	0.48
3:D:179:VAL:HG22	3:D:389:GLU:CD	2.38	0.48
3:D:827:ILE:O	3:D:837:GLY:HA3	2.14	0.48
3:D:1264:GLU:HB3	3:D:1266:ARG:NE	2.29	0.48
4:E:87:LYS:O	4:E:91:ARG:HG3	2.14	0.48
1:K:215:VAL:HG11	1:L:225:PHE:CD1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:19:THR:HG21	2:M:124:ASP:O	2.14	0.48
2:M:239:PHE:HE2	8:M:1222:HOH:O	1.97	0.48
2:M:301:GLU:O	2:M:305:PRO:HG2	2.13	0.48
2:M:435:TYR:C	2:M:437:ARG:H	2.20	0.48
2:M:688:ILE:HD12	2:M:688:ILE:N	2.29	0.48
2:M:759:THR:HB	2:M:785:VAL:CG2	2.43	0.48
2:M:833:LEU:HD12	2:M:834:GLN:N	2.29	0.48
2:M:879:ARG:NH1	3:N:1029:ARG:NH2	2.62	0.48
3:N:42:ASP:O	3:N:43:GLY:O	2.31	0.48
3:N:950:GLY:C	3:N:952:ASP:N	2.64	0.48
3:N:973:GLN:HG2	8:N:9252:HOH:O	2.13	0.48
4:O:45:ARG:O	4:O:47:LYS:HD3	2.13	0.48
5:P:350:LEU:HG	5:P:354:LEU:CD1	2.43	0.48
1:A:58:ILE:HG21	1:A:68:ILE:CD1	2.43	0.48
2:C:44:ILE:HG23	2:C:344:PHE:CE1	2.48	0.48
2:C:91:GLN:HE22	2:C:383:ARG:NH2	2.11	0.48
2:C:471:TYR:HA	2:C:534:VAL:HG23	1.96	0.48
2:C:603:VAL:H	2:C:647:GLN:H	1.61	0.48
2:C:810:ASP:HA	2:C:811:PRO:HD3	1.76	0.48
3:D:389:GLU:O	3:D:389:GLU:HG2	2.13	0.48
3:D:428:LYS:HB3	3:D:450:TYR:HE1	1.77	0.48
3:D:666:ILE:H	3:D:666:ILE:HG13	1.33	0.48
3:D:704:ARG:NH1	3:D:738:ALA:HA	2.28	0.48
3:D:813:LEU:O	3:D:839:LEU:HD11	2.13	0.48
3:D:860:LEU:O	3:D:877:PRO:HD2	2.13	0.48
3:D:899:LEU:HD21	3:D:922:LEU:HD21	1.96	0.48
3:D:1129:THR:HA	8:D:9218:HOH:O	2.14	0.48
3:D:1130:ARG:HG3	8:D:2021:HOH:O	2.13	0.48
4:E:17:TYR:N	4:E:17:TYR:CD2	2.82	0.48
4:E:43:GLU:HG2	4:E:44:GLU:N	2.28	0.48
5:F:320:PRO:C	5:F:321:ILE:HD13	2.38	0.48
1:K:178:ALA:HB3	1:K:198:ARG:HD3	1.94	0.48
1:K:209:GLU:O	1:K:213:GLN:HG3	2.13	0.48
2:M:57:GLU:HG3	2:M:58:ASP:OD2	2.13	0.48
2:M:80:GLN:O	2:M:83:CYS:HB2	2.13	0.48
2:M:599:GLU:OE1	2:M:651:LYS:HD2	2.14	0.48
2:M:1045:ALA:HB1	2:M:1048:THR:HB	1.96	0.48
3:N:568:ARG:O	3:N:569:ASN:C	2.57	0.48
3:N:880:ILE:O	3:N:883:ALA:HB3	2.14	0.48
3:N:1243:THR:HB	3:N:1253:THR:HG22	1.95	0.48
3:N:1441:GLN:CD	3:N:1442:ASN:HB2	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:PRO:HD2	1:B:224:TYR:CE1	2.49	0.48
1:A:85:LEU:HD12	1:A:86:VAL:N	2.29	0.48
1:A:86:VAL:HG12	1:A:124:ASN:HB2	1.96	0.48
1:A:110:LYS:HB2	8:A:442:HOH:O	2.14	0.48
1:A:161:ARG:NH2	8:A:348:HOH:O	2.46	0.48
2:C:289:THR:HB	8:C:1418:HOH:O	2.12	0.48
2:C:309:TYR:HA	2:C:312:ALA:HB3	1.95	0.48
2:C:417:GLY:C	2:C:418:LEU:HD12	2.39	0.48
2:C:773:LEU:HG	2:C:777:ILE:HD11	1.96	0.48
2:C:937:ASP:HB3	2:C:939:ARG:HG2	1.96	0.48
3:D:18:ILE:HG23	3:D:518:PRO:CG	2.33	0.48
3:D:32:ILE:O	5:F:258:ILE:HG23	2.14	0.48
3:D:494:LYS:HD3	8:D:9340:HOH:O	2.14	0.48
3:D:550:ARG:HA	8:D:9108:HOH:O	2.14	0.48
3:D:598:ARG:CZ	5:F:320:PRO:HD3	2.44	0.48
3:D:633:VAL:HB	3:D:740:PHE:CZ	2.48	0.48
3:D:1114:THR:CG2	3:D:1195:GLN:HB3	2.43	0.48
4:E:6:ILE:HA	4:E:9:LEU:HD12	1.95	0.48
4:E:54:LEU:HA	4:E:58:PRO:HG2	1.96	0.48
5:F:171:LYS:HG3	5:F:175:HIS:CD2	2.49	0.48
2:M:852:ILE:HD12	2:M:852:ILE:H	1.79	0.48
2:M:863:ASP:O	2:M:865:THR:N	2.46	0.48
2:M:975:TYR:HA	2:M:982:PRO:HA	1.95	0.48
3:N:93:ILE:HD13	3:N:548:ILE:HD11	1.95	0.48
3:N:208:PRO:CB	3:N:395:VAL:HG13	2.44	0.48
3:N:470:LEU:HD21	3:N:508:ARG:HH21	1.77	0.48
3:N:631:ILE:O	3:N:632:VAL:HG23	2.13	0.48
3:N:799:LYS:HE2	3:N:824:ASN:O	2.13	0.48
3:N:1117:TYR:N	3:N:1117:TYR:CD2	2.82	0.48
3:N:1173:LEU:CD2	3:N:1174:LEU:HD23	2.43	0.48
3:N:1264:GLU:CD	3:N:1425:THR:HB	2.39	0.48
3:N:1310:ARG:HD2	3:N:1327:ARG:HH21	1.76	0.48
5:P:125:ASP:OD2	5:P:126:LEU:HD13	2.14	0.48
1:A:137:ARG:HD2	1:A:137:ARG:N	2.29	0.48
1:B:26:GLU:HG3	1:B:194:LYS:HZ2	1.78	0.48
2:C:536:PRO:HG2	8:C:1330:HOH:O	2.14	0.48
2:C:669:GLY:HA3	2:C:995:MET:HA	1.96	0.48
2:C:694:LEU:HD11	2:C:868:ASP:HB3	1.96	0.48
2:C:715:THR:CG2	2:C:717:LEU:HG	2.44	0.48
2:C:721:ARG:O	2:C:758:ARG:HA	2.14	0.48
3:D:161:LEU:CD1	3:D:452:ILE:HD12	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:183:GLU:O	3:D:186:VAL:HG12	2.14	0.48
3:D:645:PRO:HG3	3:D:725:SER:O	2.12	0.48
3:D:1137:ARG:O	3:D:1141:GLU:HG3	2.13	0.48
3:D:1339:LYS:HB3	3:D:1343:ALA:CB	2.44	0.48
5:F:323:ASP:O	5:F:325:LYS:N	2.46	0.48
1:K:50:GLY:HA3	1:K:173:PRO:HG3	1.95	0.48
1:L:218:LEU:O	1:L:222:LEU:HG	2.14	0.48
2:M:31:GLN:HG2	2:M:34:VAL:HG23	1.96	0.48
2:M:114:PHE:CZ	5:P:283:GLY:HA3	2.49	0.48
2:M:208:ALA:HB1	2:M:218:VAL:CG1	2.43	0.48
2:M:305:PRO:HA	2:M:308:ARG:HB2	1.96	0.48
2:M:310:LEU:O	2:M:314:THR:HG23	2.14	0.48
2:M:571:LEU:C	2:M:573:ARG:H	2.21	0.48
2:M:586:ARG:HD2	2:M:590:ASP:OD2	2.14	0.48
2:M:952:LEU:HB3	2:M:969:GLN:HE22	1.78	0.48
2:M:1104:GLU:HG2	8:M:1597:HOH:O	2.13	0.48
3:N:393:ILE:HD12	3:N:393:ILE:H	1.79	0.48
3:N:661:MET:CE	3:N:673:ALA:HB1	2.43	0.48
3:N:754:PHE:CG	4:O:24:ALA:HB1	2.49	0.48
3:N:788:GLY:O	3:N:792:ILE:HG22	2.13	0.48
3:N:804:LEU:HB3	8:N:9574:HOH:O	2.13	0.48
3:N:879:ARG:NE	3:N:902:LEU:O	2.47	0.48
3:N:1020:LEU:HA	3:N:1023:MET:CE	2.44	0.48
3:N:1149:LEU:HD12	3:N:1161:GLU:O	2.13	0.48
3:N:1272:ALA:CA	3:N:1326:THR:HB	2.41	0.48
8:N:9310:HOH:O	4:O:89:MET:HA	2.14	0.48
4:O:47:LYS:HE2	4:O:47:LYS:H	1.78	0.48
5:P:267:THR:HG21	8:P:3894:HOH:O	2.14	0.48
5:P:291:ILE:O	5:P:295:MET:HB2	2.13	0.48
2:C:378:LEU:HG	2:C:382:ILE:CD1	2.44	0.48
2:C:395:LYS:HE2	2:C:403:SER:HB2	1.94	0.48
2:C:704:HIS:O	2:C:705:ILE:HG13	2.14	0.48
3:D:137:PRO:HD2	3:D:453:ASP:CB	2.44	0.48
3:D:516:ALA:O	3:D:518:PRO:HD3	2.14	0.48
3:D:1107:VAL:HG21	3:D:1215:VAL:HG11	1.94	0.48
3:D:1250:ALA:O	3:D:1269:LYS:HE2	2.14	0.48
3:D:1262:LEU:HD21	3:D:1351:GLU:HG3	1.96	0.48
3:D:1280:VAL:O	3:D:1294:VAL:HA	2.14	0.48
4:E:13:VAL:HG12	4:E:75:PHE:CE1	2.49	0.48
2:M:207:LEU:O	2:M:211:LEU:HB3	2.13	0.48
2:M:415:PRO:HB2	2:M:418:LEU:HD13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:835:VAL:HG13	3:N:725:SER:OG	2.14	0.48
3:N:684:LYS:HD3	3:N:686:GLU:CD	2.39	0.48
3:N:761:ILE:HD13	8:O:3197:HOH:O	2.13	0.48
3:N:787:LEU:HD12	3:N:787:LEU:O	2.14	0.48
3:N:1003:VAL:O	3:N:1007:VAL:HG13	2.14	0.48
3:N:1242:HIS:NE2	3:N:1266:ARG:HD3	2.29	0.48
3:N:1333:HIS:O	3:N:1336:LEU:HB3	2.14	0.48
3:N:1475:GLY:O	3:N:1478:SER:HB3	2.14	0.48
5:P:396:ARG:NH1	5:P:399:GLN:HE21	2.12	0.48
5:P:396:ARG:HH11	5:P:399:GLN:HE21	1.62	0.48
1:A:9:PRO:HB3	1:A:25:LEU:CG	2.44	0.47
1:A:184:THR:HG23	1:A:192:LEU:CD1	2.44	0.47
1:B:102:LYS:HG3	1:B:139:ASN:HB2	1.96	0.47
2:C:335:THR:CG2	2:C:461:VAL:HG11	2.44	0.47
2:C:694:LEU:O	2:C:699:PHE:HB2	2.14	0.47
2:C:776:SER:HA	2:C:780:GLU:HB3	1.96	0.47
2:C:926:PHE:CD2	2:C:930:LYS:HE2	2.49	0.47
2:C:958:THR:HG23	2:C:961:GLU:HB2	1.96	0.47
2:C:1090:LYS:HG2	2:C:1112:PHE:CZ	2.48	0.47
3:D:209:ARG:NH2	3:D:397:LYS:HG3	2.29	0.47
3:D:924:MET:O	3:D:927:THR:HB	2.14	0.47
5:F:115:LYS:HE2	5:F:115:LYS:HA	1.96	0.47
5:F:200:LYS:HE2	8:F:705:HOH:O	2.14	0.47
5:F:295:MET:HB3	5:F:299:TRP:CD1	2.48	0.47
1:L:143:ARG:HG3	8:L:3482:HOH:O	2.13	0.47
1:L:190:THR:HA	8:L:4811:HOH:O	2.14	0.47
2:M:178:PRO:HA	8:M:1432:HOH:O	2.11	0.47
2:M:367:LEU:HD23	2:M:371:LYS:NZ	2.29	0.47
2:M:575:GLN:N	2:M:667:ALA:HB1	2.29	0.47
2:M:611:ILE:HD12	2:M:611:ILE:N	2.29	0.47
2:M:728:HIS:HB3	2:M:729:LEU:HD12	1.96	0.47
2:M:735:ARG:HG2	2:M:735:ARG:HH11	1.79	0.47
2:M:808:ARG:HH21	2:M:820:ARG:HG2	1.78	0.47
2:M:810:ASP:HB3	8:M:1642:HOH:O	2.13	0.47
2:M:857:ASP:HB2	2:M:978:ARG:CG	2.42	0.47
3:N:443:VAL:CG1	3:N:445:ARG:HE	2.26	0.47
3:N:658:LEU:O	3:N:661:MET:HB2	2.14	0.47
3:N:806:PHE:O	3:N:807:ALA:C	2.56	0.47
3:N:1197:ARG:HB3	3:N:1396:GLU:OE1	2.13	0.47
5:P:80:PRO:HA	5:P:83:GLN:HB2	1.96	0.47
5:P:370:LYS:NZ	5:P:370:LYS:HB3	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:THR:HG22	1:A:143:ARG:HG2	1.95	0.47
1:B:11:PHE:HD1	1:B:25:LEU:HD13	1.79	0.47
1:B:159:LYS:HE2	8:B:396:HOH:O	2.12	0.47
2:C:103:LYS:HB2	8:C:1576:HOH:O	2.13	0.47
2:C:260:LEU:HA	2:C:291:ALA:CB	2.43	0.47
2:C:625:LEU:HD11	2:C:641:PRO:HG3	1.96	0.47
3:D:42:ASP:HA	3:D:46:ASP:OD1	2.14	0.47
3:D:43:GLY:N	8:D:9050:HOH:O	2.47	0.47
3:D:585:GLY:N	8:D:9822:HOH:O	2.47	0.47
3:D:699:VAL:HG12	3:D:717:GLN:CA	2.43	0.47
3:D:787:LEU:HD21	3:D:947:ILE:CD1	2.44	0.47
3:D:829:VAL:HG11	8:D:9103:HOH:O	2.12	0.47
3:D:1432:LYS:CG	3:D:1433:SER:H	2.27	0.47
5:F:306:GLU:HG2	8:F:517:HOH:O	2.14	0.47
2:M:19:THR:HG22	2:M:22:GLN:HB2	1.94	0.47
2:M:495:THR:H	2:M:530:GLU:CD	2.22	0.47
2:M:776:SER:HB3	8:M:1776:HOH:O	2.12	0.47
2:M:916:GLU:HG3	2:M:917:LEU:N	2.29	0.47
2:M:984:GLU:HG3	3:N:944:THR:O	2.14	0.47
3:N:169:TYR:HA	3:N:392:SER:HA	1.96	0.47
3:N:185:VAL:CG1	3:N:191:LEU:HD21	2.43	0.47
3:N:427:VAL:HB	3:N:435:VAL:CG2	2.45	0.47
3:N:471:GLU:OE2	3:N:503:LEU:HD21	2.13	0.47
3:N:583:ASP:OD2	3:N:586:ARG:HD2	2.14	0.47
3:N:761:ILE:HG23	4:O:6:ILE:HD11	1.95	0.47
3:N:792:ILE:O	3:N:878:GLY:HA3	2.14	0.47
1:A:59:GLU:HG3	1:A:139:ASN:ND2	2.30	0.47
2:C:80:GLN:O	2:C:83:CYS:HB2	2.14	0.47
2:C:553:ASP:HA	2:C:881:ASN:HA	1.97	0.47
2:C:959:PRO:O	2:C:963:LEU:HD23	2.14	0.47
3:D:169:TYR:N	3:D:170:PRO:CD	2.77	0.47
3:D:477:LEU:HD22	3:D:492:ALA:CB	2.43	0.47
3:D:633:VAL:C	3:D:635:PRO:HD3	2.39	0.47
3:D:1155:VAL:HG11	3:D:1183:ILE:HD11	1.95	0.47
3:D:1318:TYR:HD1	3:D:1319:VAL:N	2.12	0.47
3:D:1366:LYS:O	3:D:1369:GLU:HB2	2.14	0.47
4:E:37:ASN:HD22	4:E:89:MET:CE	2.27	0.47
5:F:80:PRO:HA	5:F:83:GLN:HB2	1.96	0.47
5:F:138:SER:O	5:F:141:VAL:HG12	2.14	0.47
5:F:198:ILE:HA	8:F:618:HOH:O	2.14	0.47
5:F:216:GLY:O	5:F:243:ILE:HG12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:13:VAL:HG11	1:L:208:LEU:HD11	1.96	0.47
1:L:32:PHE:N	8:L:4886:HOH:O	2.47	0.47
2:M:415:PRO:C	2:M:417:GLY:H	2.23	0.47
2:M:534:VAL:H	2:M:538:GLN:NE2	2.03	0.47
2:M:603:VAL:H	2:M:647:GLN:H	1.63	0.47
3:N:957:PRO:CD	3:N:1007:VAL:HG12	2.44	0.47
1:A:157:GLY:HA3	8:A:320:HOH:O	2.14	0.47
1:B:211:LEU:O	1:B:215:VAL:HG13	2.14	0.47
2:C:157:ARG:HD3	2:C:158:TYR:N	2.29	0.47
2:C:557:ARG:CZ	2:C:879:ARG:HD3	2.44	0.47
3:D:119:SER:H	3:D:123:LEU:HD13	1.79	0.47
3:D:214:GLU:OE2	3:D:390:PRO:HB2	2.15	0.47
3:D:568:ARG:O	3:D:569:ASN:C	2.57	0.47
3:D:638:LYS:C	3:D:729:HIS:HD2	2.23	0.47
3:D:639:LEU:HD12	3:D:640:HIS:H	1.80	0.47
3:D:711:LEU:CD1	3:D:778:LEU:HD13	2.44	0.47
3:D:1207:TYR:C	8:D:9465:HOH:O	2.56	0.47
3:D:1207:TYR:N	8:D:9465:HOH:O	2.46	0.47
3:D:1250:ALA:HB3	8:D:9181:HOH:O	2.14	0.47
3:D:1317:ASP:N	8:D:9664:HOH:O	2.47	0.47
5:F:223:ALA:HB2	5:F:242:TRP:HB2	1.96	0.47
5:F:267:THR:O	5:F:271:LEU:HG	2.14	0.47
5:F:282:LEU:HB2	5:F:284:ARG:H	1.79	0.47
5:F:303:ARG:HG3	8:F:507:HOH:O	2.14	0.47
5:F:368:VAL:HG12	8:F:443:HOH:O	2.14	0.47
1:K:95:GLN:HG3	8:K:3203:HOH:O	2.14	0.47
1:K:150:TYR:CE1	2:M:696:LYS:HA	2.48	0.47
2:M:172:ILE:HD12	2:M:172:ILE:N	2.30	0.47
2:M:198:ARG:NH1	2:M:231:PRO:HG3	2.30	0.47
2:M:302:VAL:C	2:M:305:PRO:HD2	2.39	0.47
2:M:405:ARG:HG2	2:M:409:ARG:NH2	2.11	0.47
2:M:460:ARG:HD2	2:M:485:TYR:CD2	2.49	0.47
2:M:716:LYS:HB2	8:M:1298:HOH:O	2.13	0.47
3:N:147:VAL:HG11	8:N:9806:HOH:O	2.13	0.47
3:N:827:ILE:HG23	3:N:837:GLY:CA	2.45	0.47
3:N:1475:GLY:HA2	4:O:17:TYR:CD1	2.49	0.47
3:N:1485:GLN:HE21	4:O:80:VAL:N	2.09	0.47
4:O:54:LEU:HA	4:O:58:PRO:HG2	1.95	0.47
5:P:128:ARG:NH1	5:P:128:ARG:HB2	2.30	0.47
5:P:336:GLU:HG2	5:P:337:HIS:HD2	1.80	0.47
2:C:232:GLU:HG3	2:C:235:LEU:CD1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:398:THR:HG22	2:C:568:ALA:O	2.13	0.47
2:C:473:ARG:HD2	2:C:475:VAL:HG23	1.95	0.47
2:C:510:ALA:HB2	8:C:1220:HOH:O	2.14	0.47
2:C:524:VAL:HG22	2:C:528:GLU:CD	2.39	0.47
2:C:526:PRO:HB2	8:C:1311:HOH:O	2.13	0.47
2:C:567:GLN:CB	2:C:997:LEU:HD22	2.45	0.47
2:C:773:LEU:O	2:C:777:ILE:HG13	2.14	0.47
2:C:1055:LEU:HG	2:C:1079:PRO:HG3	1.97	0.47
3:D:104:PHE:CE2	3:D:1448:THR:HG23	2.50	0.47
3:D:186:VAL:HG13	3:D:187:LYS:N	2.28	0.47
3:D:420:VAL:HA	5:F:164:LYS:NZ	2.29	0.47
3:D:432:TYR:HB3	3:D:448:GLU:HA	1.96	0.47
3:D:465:LEU:CD1	3:D:513:ILE:HD11	2.44	0.47
3:D:912:LYS:O	3:D:915:VAL:HG23	2.15	0.47
3:D:1153:VAL:O	3:D:1160:LEU:HG	2.14	0.47
3:D:1250:ALA:HB2	8:D:9571:HOH:O	2.13	0.47
5:F:209:PHE:CE2	5:F:213:ILE:HD11	2.49	0.47
5:F:358:LEU:O	5:F:367:MET:HE1	2.14	0.47
5:F:411:HIS:HB2	8:F:598:HOH:O	2.13	0.47
2:M:197:LEU:CD1	2:M:207:LEU:HD11	2.44	0.47
2:M:260:LEU:HA	2:M:291:ALA:CB	2.45	0.47
2:M:625:LEU:O	2:M:627:ARG:N	2.47	0.47
2:M:645:VAL:HG13	8:M:1487:HOH:O	2.14	0.47
2:M:862:PRO:HA	2:M:975:TYR:CE1	2.49	0.47
2:M:1059:ASP:O	2:M:1063:ARG:HG2	2.13	0.47
2:M:1090:LYS:HG2	2:M:1112:PHE:CZ	2.49	0.47
3:N:132:TYR:HA	8:N:9161:HOH:O	2.14	0.47
3:N:417:PRO:HA	5:P:168:LYS:HZ2	1.77	0.47
3:N:459:GLU:HG2	8:N:9337:HOH:O	2.14	0.47
3:N:493:ARG:NH1	3:N:1390:LEU:H	2.12	0.47
3:N:561:GLY:HA2	8:N:9133:HOH:O	2.14	0.47
3:N:568:ARG:HA	3:N:571:LYS:NZ	2.29	0.47
3:N:864:VAL:HG12	3:N:865:THR:H	1.79	0.47
3:N:871:LYS:HB3	3:N:873:LEU:HD11	1.97	0.47
3:N:886:VAL:HG13	3:N:930:LEU:HD11	1.96	0.47
3:N:1138:ALA:HA	3:N:1141:GLU:HG3	1.96	0.47
3:N:1310:ARG:HB2	8:N:9400:HOH:O	2.14	0.47
4:O:84:ARG:HG3	4:O:84:ARG:O	2.15	0.47
5:P:112:ALA:HA	5:P:173:TYR:CD2	2.48	0.47
5:P:302:LYS:HA	8:P:3021:HOH:O	2.14	0.47
5:P:392:VAL:HG21	8:P:3999:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:GLY:O	1:A:171:PHE:HB2	2.14	0.47
1:B:68:ILE:HD12	1:B:71:VAL:HG21	1.95	0.47
2:C:139:GLN:HG2	2:C:140:ILE:H	1.79	0.47
2:C:498:GLN:CD	3:D:1068:LEU:HB2	2.39	0.47
3:D:416:ALA:H	3:D:417:PRO:CD	2.26	0.47
3:D:640:HIS:HE1	4:E:3:GLU:HG2	1.79	0.47
3:D:675:ARG:HH21	5:F:421:PHE:H	1.61	0.47
3:D:852:ALA:O	3:D:857:ILE:HG12	2.14	0.47
3:D:1071:PHE:HB3	8:D:9526:HOH:O	2.14	0.47
5:F:117:SER:OG	5:F:124:PRO:HG3	2.15	0.47
5:F:371:LEU:O	5:F:375:LEU:HB3	2.15	0.47
1:K:69:PRO:O	1:K:71:VAL:HG23	2.13	0.47
1:K:228:PRO:HG3	8:K:4456:HOH:O	2.13	0.47
2:M:31:GLN:HB3	2:M:71:TYR:HH	1.80	0.47
2:M:32:ALA:HA	8:M:1342:HOH:O	2.15	0.47
2:M:820:ARG:HB2	8:M:1654:HOH:O	2.14	0.47
2:M:839:LEU:HD21	2:M:849:VAL:CG2	2.44	0.47
2:M:916:GLU:O	2:M:919:ALA:HB3	2.15	0.47
2:M:987:ILE:HG23	3:N:948:THR:HG21	1.96	0.47
2:M:1030:GLN:HB3	3:N:626:SER:HB2	1.97	0.47
3:N:80:VAL:HG12	3:N:81:THR:H	1.79	0.47
3:N:396:VAL:CG2	3:N:447:VAL:HB	2.45	0.47
3:N:572:ARG:NH1	5:P:80:PRO:HD3	2.29	0.47
3:N:607:LEU:HA	3:N:613:ARG:HB3	1.96	0.47
3:N:829:VAL:HA	8:N:9426:HOH:O	2.15	0.47
3:N:902:LEU:O	3:N:902:LEU:HD12	2.15	0.47
3:N:1054:GLU:HB2	8:N:9488:HOH:O	2.15	0.47
3:N:1123:PHE:CE2	3:N:1184:GLN:HG3	2.50	0.47
3:N:1184:GLN:HG2	8:N:9892:HOH:O	2.15	0.47
3:N:1320:GLU:HG2	3:N:1339:LYS:HE3	1.96	0.47
3:N:1447:LEU:O	3:N:1448:THR:C	2.57	0.47
3:N:1485:GLN:NE2	4:O:80:VAL:H	2.12	0.47
5:P:396:ARG:HA	5:P:399:GLN:HB2	1.95	0.47
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.97	0.47
2:C:52:PHE:O	2:C:54:ILE:N	2.47	0.47
2:C:193:LEU:HD23	2:C:307:LEU:CD1	2.45	0.47
2:C:301:GLU:O	2:C:305:PRO:HG2	2.15	0.47
2:C:372:LEU:HD21	8:C:1196:HOH:O	2.14	0.47
2:C:403:SER:O	2:C:407:LYS:HD2	2.14	0.47
2:C:739:GLU:HB2	8:C:1284:HOH:O	2.14	0.47
2:C:798:GLY:HA2	8:C:1158:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:878:SER:HB2	8:C:1420:HOH:O	2.14	0.47
2:C:1067:TYR:CE2	5:F:345:ALA:HB2	2.50	0.47
3:D:83:SER:O	3:D:86:ARG:HB3	2.14	0.47
3:D:96:ALA:HB1	3:D:554:LEU:HD12	1.97	0.47
3:D:131:LYS:HB3	3:D:456:MET:CE	2.43	0.47
3:D:488:ARG:HB3	3:D:488:ARG:NH1	2.29	0.47
3:D:502:PHE:CE2	3:D:1452:ILE:HG23	2.50	0.47
3:D:519:VAL:HG13	3:D:544:TYR:CZ	2.50	0.47
3:D:543:LEU:CD2	3:D:600:LEU:HD12	2.45	0.47
3:D:601:ARG:CD	3:D:606:ILE:HD13	2.44	0.47
3:D:647:ARG:HG2	8:D:9811:HOH:O	2.14	0.47
3:D:729:HIS:HE1	3:D:731:LEU:HG	1.79	0.47
3:D:780:LYS:HE2	8:D:9604:HOH:O	2.13	0.47
3:D:848:GLU:HB2	8:D:9179:HOH:O	2.13	0.47
3:D:890:VAL:HG11	3:D:922:LEU:HD13	1.96	0.47
3:D:1009:LYS:HE2	3:D:1013:GLU:OE1	2.14	0.47
3:D:1047:LYS:HB3	3:D:1048:PRO:CD	2.45	0.47
3:D:1393:GLN:CB	3:D:1398:TRP:HE1	2.28	0.47
4:E:69:LEU:HD11	8:E:181:HOH:O	2.15	0.47
5:F:273:ARG:HG2	8:F:571:HOH:O	2.15	0.47
1:K:9:PRO:HB3	1:K:25:LEU:HG	1.96	0.47
2:M:52:PHE:O	2:M:54:ILE:N	2.48	0.47
2:M:112:GLU:HB2	8:M:1448:HOH:O	2.15	0.47
2:M:207:LEU:HD22	2:M:221:LEU:HD22	1.97	0.47
2:M:470:PRO:HB2	2:M:534:VAL:HG21	1.96	0.47
2:M:470:PRO:HB2	2:M:483:VAL:HG11	1.97	0.47
2:M:578:VAL:HG11	2:M:991:GLN:HB3	1.96	0.47
2:M:724:ARG:HE	2:M:734:LEU:HG	1.78	0.47
2:M:762:LYS:HB2	2:M:762:LYS:NZ	2.30	0.47
2:M:770:GLU:HG2	8:N:9172:HOH:O	2.15	0.47
2:M:824:ARG:HB3	2:M:826:TYR:CE1	2.50	0.47
2:M:1038:TRP:HA	2:M:1041:GLU:HB2	1.96	0.47
2:M:1076:VAL:HG22	3:N:752:SER:HB3	1.96	0.47
2:M:1115:LEU:CD2	3:N:85:VAL:HG13	2.43	0.47
3:N:47:GLU:OE1	3:N:52:PRO:HA	2.15	0.47
3:N:89:ARG:O	3:N:521:PRO:HG3	2.14	0.47
3:N:153:LEU:CD1	3:N:157:GLU:HB2	2.45	0.47
3:N:442:ASN:HB3	8:N:9376:HOH:O	2.14	0.47
3:N:470:LEU:HD21	3:N:508:ARG:NH2	2.30	0.47
3:N:598:ARG:NE	8:N:9109:HOH:O	2.47	0.47
3:N:666:ILE:HG23	3:N:686:GLU:OE2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:770:LEU:HD13	3:N:776:GLU:C	2.40	0.47
3:N:950:GLY:H	3:N:953:ASP:CG	2.22	0.47
3:N:960:LYS:HB3	8:N:9231:HOH:O	2.13	0.47
3:N:1166:LEU:HD23	3:N:1166:LEU:N	2.29	0.47
3:N:1281:VAL:HG23	3:N:1317:ASP:O	2.15	0.47
3:N:1379:VAL:CG1	3:N:1395:LEU:HD23	2.45	0.47
3:N:1462:LEU:HD22	3:N:1473:PRO:HD2	1.95	0.47
5:P:155:THR:O	5:P:159:ILE:HG13	2.14	0.47
5:P:159:ILE:O	5:P:163:LEU:HG	2.14	0.47
1:B:57:TYR:HB3	1:B:141:GLU:HG3	1.95	0.47
2:C:285:LEU:HD12	2:C:288:ARG:O	2.15	0.47
2:C:946:ARG:NH2	3:D:859:ASP:HA	2.30	0.47
2:C:1054:THR:HG22	2:C:1059:ASP:CB	2.45	0.47
3:D:115:LEU:HD23	3:D:116:LEU:N	2.30	0.47
3:D:414:ARG:HG2	8:D:9627:HOH:O	2.13	0.47
3:D:421:LEU:HD11	3:D:437:VAL:HG22	1.95	0.47
3:D:528:VAL:HG12	8:D:9096:HOH:O	2.15	0.47
3:D:591:VAL:HG12	3:D:592:THR:O	2.15	0.47
3:D:645:PRO:HB3	3:D:723:GLY:O	2.14	0.47
3:D:996:TRP:HA	3:D:999:THR:CG2	2.43	0.47
3:D:1033:GLN:HE22	3:D:1036:ARG:HH11	1.63	0.47
3:D:1066:THR:HG23	3:D:1069:GLU:N	2.16	0.47
3:D:1312:LEU:N	8:D:9045:HOH:O	2.42	0.47
3:D:1354:LYS:HD3	8:D:9078:HOH:O	2.15	0.47
5:F:316:SER:HB3	5:F:318:GLU:O	2.15	0.47
1:L:50:GLY:O	1:L:146:ARG:HA	2.15	0.47
1:L:61:VAL:HA	8:L:2996:HOH:O	2.15	0.47
1:L:149:GLY:O	1:L:171:PHE:HB2	2.14	0.47
1:L:212:ASN:HD22	1:L:212:ASN:N	2.11	0.47
2:M:53:PRO:HD3	8:M:1173:HOH:O	2.14	0.47
2:M:206:THR:HG21	8:M:1314:HOH:O	2.15	0.47
2:M:290:LEU:HB3	2:M:302:VAL:HG12	1.97	0.47
2:M:332:ARG:HB2	2:M:466:PHE:HE1	1.78	0.47
2:M:409:ARG:HA	2:M:454:SER:CA	2.32	0.47
2:M:572:ILE:CG2	2:M:703:ILE:HD13	2.45	0.47
2:M:624:PRO:O	2:M:625:LEU:HD23	2.15	0.47
2:M:723:THR:HG23	2:M:725:ASP:HB2	1.97	0.47
3:N:486:ARG:HH21	3:N:489:ARG:CD	2.28	0.47
3:N:536:ALA:HA	5:P:315:VAL:N	2.19	0.47
3:N:587:ARG:HD3	8:N:9432:HOH:O	2.14	0.47
3:N:1110:ALA:O	3:N:1111:ASP:C	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1123:PHE:HB3	3:N:1133:ARG:O	2.15	0.47
3:N:1465:ASN:ND2	3:N:1470:ARG:HD3	2.30	0.47
4:O:10:PHE:HE2	4:O:16:LYS:HG3	1.80	0.47
5:P:110:MET:HA	5:P:113:ILE:HD12	1.97	0.47
5:P:195:VAL:HG11	5:P:217:ASN:OD1	2.15	0.47
2:C:207:LEU:HD22	2:C:221:LEU:CD2	2.45	0.47
2:C:244:PRO:CD	2:C:245:GLY:H	2.20	0.47
3:D:129:PHE:CE2	3:D:587:ARG:HD3	2.50	0.47
3:D:169:TYR:HA	3:D:392:SER:HA	1.97	0.47
3:D:171:LEU:HD22	3:D:390:PRO:HG3	1.97	0.47
3:D:434:ARG:HB2	3:D:447:VAL:HG22	1.97	0.47
3:D:476:GLU:HG2	8:D:9254:HOH:O	2.14	0.47
3:D:645:PRO:HA	3:D:721:VAL:O	2.14	0.47
3:D:843:PHE:HA	3:D:848:GLU:OE1	2.14	0.47
3:D:1148:VAL:HG13	3:D:1163:GLY:O	2.15	0.47
3:D:1152:GLU:CD	3:D:1159:ARG:NH1	2.73	0.47
3:D:1341:PRO:HD2	3:D:1342:GLU:OE2	2.14	0.47
3:D:1382:THR:HG21	3:D:1418:LYS:HE3	1.95	0.47
4:E:13:VAL:HG21	4:E:19:LEU:HB2	1.96	0.47
1:K:86:VAL:HG12	1:K:124:ASN:ND2	2.29	0.47
2:M:183:SER:C	2:M:193:LEU:HD11	2.39	0.47
2:M:515:ALA:C	2:M:516:ARG:HD3	2.40	0.47
2:M:551:GLU:HA	2:M:906:PHE:CE2	2.49	0.47
2:M:671:ASN:ND2	2:M:993:PHE:CD2	2.81	0.47
2:M:841:ASN:C	2:M:841:ASN:ND2	2.70	0.47
2:M:1105:LYS:HB2	2:M:1107:ASN:HD22	1.80	0.47
8:M:1335:HOH:O	3:N:944:THR:HA	2.14	0.47
3:N:181:ASP:O	3:N:185:VAL:HG23	2.14	0.47
3:N:188:GLY:HA2	3:N:210:ARG:NH1	2.30	0.47
3:N:204:LEU:HG	8:N:9317:HOH:O	2.14	0.47
3:N:209:ARG:HB2	3:N:395:VAL:O	2.15	0.47
3:N:463:GLN:O	3:N:467:GLU:HG3	2.15	0.47
3:N:882:PHE:CE1	3:N:906:GLN:HG3	2.49	0.47
3:N:950:GLY:H	3:N:953:ASP:CB	2.27	0.47
3:N:1267:ARG:HH11	3:N:1267:ARG:CB	2.27	0.47
4:O:54:LEU:CD2	4:O:63:TRP:HE1	2.27	0.47
5:P:109:GLY:O	5:P:113:ILE:HG13	2.14	0.47
1:B:20:TYR:OH	1:B:198:ARG:HD3	2.14	0.47
1:B:180:GLN:HB3	8:D:9039:HOH:O	2.15	0.47
2:C:269:LEU:HD22	8:C:1709:HOH:O	2.14	0.47
2:C:302:VAL:O	2:C:306:THR:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:625:LEU:O	2:C:627:ARG:N	2.48	0.47
2:C:645:VAL:HA	8:C:1221:HOH:O	2.15	0.47
2:C:690:ILE:CD1	2:C:833:LEU:HD21	2.45	0.47
2:C:722:ILE:CG2	2:C:805:ARG:HH21	2.27	0.47
3:D:80:VAL:HG12	8:D:9019:HOH:O	2.14	0.47
3:D:422:ALA:O	3:D:427:VAL:HG21	2.15	0.47
3:D:474:GLU:O	3:D:478:LEU:HG	2.15	0.47
3:D:928:ALA:O	3:D:931:LEU:HB2	2.14	0.47
3:D:1183:ILE:N	3:D:1183:ILE:HD12	2.29	0.47
3:D:1336:LEU:HA	3:D:1344:VAL:CG2	2.45	0.47
5:F:261:PRO:O	5:F:265:VAL:HG23	2.15	0.47
5:F:388:ALA:HA	8:F:635:HOH:O	2.15	0.47
1:L:54:THR:HG22	1:L:158:ILE:HG13	1.97	0.47
2:M:44:ILE:HD13	2:M:344:PHE:CE1	2.50	0.47
2:M:212:GLY:C	2:M:215:GLY:H	2.23	0.47
2:M:215:GLY:HA3	8:M:1560:HOH:O	2.15	0.47
2:M:405:ARG:HD3	2:M:543:ASN:HB2	1.97	0.47
2:M:412:ALA:HB3	2:M:451:LEU:HB3	1.97	0.47
2:M:462:ASP:HB3	2:M:468:ARG:HD2	1.97	0.47
2:M:605:LYS:HA	8:M:1487:HOH:O	2.15	0.47
2:M:926:PHE:O	2:M:930:LYS:HG3	2.15	0.47
3:N:90:MET:SD	3:N:521:PRO:HD3	2.54	0.47
3:N:397:LYS:HE2	3:N:399:ARG:HE	1.80	0.47
3:N:566:ILE:HG12	5:P:217:ASN:HD22	1.80	0.47
3:N:678:GLU:HG3	3:N:679:ARG:HG3	1.97	0.47
3:N:916:TYR:O	3:N:919:PHE:HB3	2.15	0.47
3:N:1023:MET:O	3:N:1028:ALA:HB3	2.15	0.47
3:N:1462:LEU:CD2	3:N:1473:PRO:HD2	2.45	0.47
4:O:74:VAL:CG1	4:O:79:LEU:HD21	2.45	0.47
2:C:195:LEU:CD1	2:C:234:ALA:HB1	2.46	0.46
2:C:281:LEU:HB2	2:C:309:TYR:CG	2.50	0.46
2:C:285:LEU:HD23	2:C:285:LEU:O	2.15	0.46
2:C:805:ARG:HG3	2:C:823:VAL:HG22	1.97	0.46
2:C:941:VAL:O	2:C:944:LEU:HB2	2.14	0.46
2:C:1100:GLN:O	2:C:1102:LEU:HD12	2.15	0.46
3:D:797:LYS:N	3:D:797:LYS:HD2	2.30	0.46
3:D:1124:GLN:HA	3:D:1125:PRO:HD3	1.76	0.46
3:D:1459:LEU:HD22	3:D:1465:ASN:HD22	1.79	0.46
5:F:282:LEU:N	5:F:282:LEU:HD23	2.30	0.46
5:F:363:GLU:HA	5:F:367:MET:SD	2.55	0.46
5:F:412:GLU:CD	5:F:418:LEU:HD13	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:68:ILE:CD1	1:K:138:LEU:HD11	2.45	0.46
1:K:115:LEU:HB3	8:K:4097:HOH:O	2.14	0.46
1:K:198:ARG:C	1:K:199:ILE:HD12	2.41	0.46
2:M:345:ARG:HH11	2:M:345:ARG:CB	2.27	0.46
2:M:422:ARG:HG3	8:M:1745:HOH:O	2.13	0.46
2:M:464:LEU:O	2:M:466:PHE:N	2.48	0.46
2:M:918:LEU:HD23	2:M:968:LEU:CA	2.43	0.46
3:N:44:LEU:HG	8:N:9867:HOH:O	2.16	0.46
3:N:196:VAL:HG13	3:N:202:VAL:HG11	1.97	0.46
3:N:645:PRO:HA	3:N:721:VAL:O	2.15	0.46
3:N:827:ILE:O	3:N:837:GLY:HA3	2.15	0.46
3:N:1275:SER:HB3	3:N:1325:LEU:CD1	2.45	0.46
1:A:50:GLY:O	1:A:146:ARG:HA	2.15	0.46
1:A:67:THR:HG21	2:C:609:ASN:HD21	1.80	0.46
1:A:101:LEU:HG	1:A:113:ASP:O	2.15	0.46
2:C:9:ILE:HD12	2:C:9:ILE:O	2.15	0.46
2:C:521:PRO:HB2	3:D:1055:VAL:CB	2.43	0.46
2:C:534:VAL:N	2:C:538:GLN:NE2	2.63	0.46
2:C:1054:THR:C	2:C:1059:ASP:HB2	2.40	0.46
3:D:495:ARG:O	3:D:495:ARG:HG2	2.16	0.46
3:D:962:GLN:OE1	3:D:962:GLN:N	2.47	0.46
5:F:282:LEU:HD23	5:F:282:LEU:H	1.79	0.46
5:F:370:LYS:HD2	5:F:370:LYS:C	2.39	0.46
5:F:416:ARG:NH1	5:F:419:ARG:HB2	2.30	0.46
1:K:78:ILE:O	1:K:82:LEU:HG	2.15	0.46
1:K:117:VAL:HB	1:K:120:VAL:CG1	2.42	0.46
2:M:44:ILE:HG22	8:M:1223:HOH:O	2.14	0.46
2:M:195:LEU:HD12	2:M:234:ALA:HB1	1.97	0.46
2:M:325:ILE:HG23	8:M:1502:HOH:O	2.16	0.46
2:M:397:GLU:H	2:M:633:GLN:CD	2.23	0.46
2:M:621:VAL:HG22	8:M:1199:HOH:O	2.16	0.46
2:M:1101:THR:HB	3:N:5:VAL:HG11	1.98	0.46
2:M:1118:LYS:HD3	3:N:20:SER:O	2.14	0.46
3:N:400:VAL:HA	3:N:442:ASN:O	2.15	0.46
3:N:484:PRO:O	3:N:489:ARG:HD2	2.14	0.46
3:N:551:ASN:O	3:N:555:LYS:HG3	2.15	0.46
3:N:759:ALA:HA	3:N:763:MET:HB3	1.96	0.46
3:N:1056:PRO:HD2	8:N:9483:HOH:O	2.14	0.46
3:N:1168:MET:HE3	3:N:1171:VAL:HB	1.97	0.46
3:N:1243:THR:HG22	3:N:1244:GLY:H	1.79	0.46
4:O:40:LEU:CD2	4:O:67:GLU:HA	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:GLU:O	1:A:200:TRP:HA	2.16	0.46
1:B:26:GLU:HG2	1:B:27:PRO:HA	1.97	0.46
2:C:208:ALA:HB1	2:C:218:VAL:CG1	2.45	0.46
2:C:863:ASP:O	2:C:865:THR:N	2.48	0.46
2:C:987:ILE:HG22	2:C:988:VAL:O	2.15	0.46
3:D:783:ARG:HH21	3:D:1029:ARG:CZ	2.28	0.46
3:D:907:GLU:OE1	3:D:908:LYS:HG2	2.14	0.46
3:D:1085:ALA:HA	8:D:9707:HOH:O	2.14	0.46
5:F:141:VAL:O	5:F:145:PRO:HD2	2.16	0.46
5:F:218:GLN:HA	5:F:221:ILE:HD12	1.96	0.46
1:K:115:LEU:HD12	1:K:115:LEU:O	2.15	0.46
2:M:93:PRO:HG3	2:M:117:HIS:HE1	1.80	0.46
2:M:428:ARG:HE	2:M:451:LEU:HD11	1.80	0.46
2:M:1050:GLN:CG	2:M:1079:PRO:HG2	2.44	0.46
2:M:1056:LYS:NZ	3:N:749:VAL:O	2.47	0.46
2:M:1111:ILE:HD11	8:M:1318:HOH:O	2.14	0.46
3:N:93:ILE:CD1	3:N:548:ILE:HD11	2.46	0.46
3:N:633:VAL:C	3:N:635:PRO:HD3	2.40	0.46
3:N:828:LYS:HD2	8:N:9129:HOH:O	2.15	0.46
4:O:59:ASN:HD22	4:O:59:ASN:HA	1.59	0.46
1:A:218:LEU:HB2	8:A:322:HOH:O	2.14	0.46
1:B:19:GLU:O	1:B:200:TRP:HA	2.15	0.46
1:B:73:GLU:HB2	1:B:78:ILE:HD11	1.96	0.46
1:B:86:VAL:HG22	8:B:371:HOH:O	2.15	0.46
1:B:92:PRO:HA	1:B:146:ARG:NH2	2.31	0.46
2:C:265:ARG:HG2	2:C:267:TYR:N	2.30	0.46
2:C:441:VAL:HG12	2:C:559:LEU:HA	1.96	0.46
2:C:442:GLU:HG2	2:C:454:SER:HB2	1.98	0.46
2:C:835:VAL:HG11	8:D:9008:HOH:O	2.16	0.46
3:D:68:PHE:O	3:D:71:LYS:HG2	2.15	0.46
3:D:110:SER:HB3	8:D:9091:HOH:O	2.15	0.46
3:D:396:VAL:HG13	3:D:447:VAL:HA	1.98	0.46
3:D:573:MET:HE1	5:F:214:GLN:HG2	1.96	0.46
3:D:574:LEU:O	3:D:578:VAL:HG23	2.16	0.46
3:D:704:ARG:HA	3:D:704:ARG:HD2	1.76	0.46
3:D:1093:TYR:HA	8:D:9017:HOH:O	2.16	0.46
3:D:1380:GLU:HB3	3:D:1418:LYS:HB2	1.98	0.46
4:E:41:GLU:O	4:E:45:ARG:HG2	2.15	0.46
5:F:256:ARG:NH2	5:F:310:ILE:O	2.48	0.46
5:F:276:ARG:HA	8:F:735:HOH:O	2.14	0.46
1:K:210:ALA:HA	1:K:213:GLN:NE2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:101:ILE:HG22	2:M:102:HIS:N	2.30	0.46
2:M:191:PHE:CE2	2:M:238:LEU:HD21	2.51	0.46
2:M:710:ILE:HB	2:M:790:LEU:CD1	2.38	0.46
2:M:801:VAL:HG23	8:M:1213:HOH:O	2.15	0.46
3:N:416:ALA:H	3:N:417:PRO:CD	2.28	0.46
3:N:957:PRO:HA	3:N:1010:ASN:ND2	2.30	0.46
3:N:1114:THR:HG23	3:N:1114:THR:O	2.15	0.46
3:N:1156:LEU:HD12	8:N:9485:HOH:O	2.16	0.46
5:P:370:LYS:HD2	5:P:370:LYS:C	2.40	0.46
2:C:218:VAL:HG22	2:C:221:LEU:CD2	2.46	0.46
2:C:310:LEU:O	2:C:314:THR:HG23	2.15	0.46
2:C:490:GLU:HG2	2:C:494:TYR:OH	2.15	0.46
2:C:647:GLN:HA	8:C:1176:HOH:O	2.16	0.46
2:C:979:THR:CG2	2:C:981:GLU:HB2	2.45	0.46
3:D:84:ILE:HA	3:D:87:ARG:HG2	1.97	0.46
3:D:190:GLU:HG3	3:D:210:ARG:CD	2.46	0.46
3:D:208:PRO:CB	3:D:395:VAL:HG13	2.43	0.46
3:D:501:ALA:HA	3:D:504:ASP:HB2	1.97	0.46
3:D:521:PRO:C	3:D:525:ARG:HH11	2.24	0.46
3:D:952:ASP:HA	3:D:1062:ARG:NH2	2.30	0.46
4:E:18:ARG:HD3	8:E:126:HOH:O	2.15	0.46
5:F:336:GLU:HB2	8:F:726:HOH:O	2.15	0.46
1:L:69:PRO:O	1:L:71:VAL:HG23	2.16	0.46
2:M:52:PHE:HE1	2:M:66:LEU:HG	1.75	0.46
2:M:143:SER:HB3	2:M:332:ARG:HB2	1.97	0.46
2:M:810:ASP:HA	2:M:811:PRO:HD3	1.79	0.46
2:M:842:ARG:HD3	8:M:1636:HOH:O	2.16	0.46
2:M:875:GLY:O	2:M:879:ARG:HD3	2.15	0.46
2:M:976:ASP:HB3	2:M:979:THR:HG22	1.96	0.46
3:N:28:LYS:HD3	3:N:41:ARG:NH1	2.30	0.46
3:N:404:GLU:OE1	3:N:414:ARG:HD3	2.16	0.46
3:N:560:GLN:HE21	5:P:218:GLN:HE22	1.63	0.46
3:N:891:GLU:HG2	8:N:9646:HOH:O	2.15	0.46
3:N:926:LYS:HE2	8:N:9736:HOH:O	2.16	0.46
3:N:1434:TRP:HZ3	3:N:1457:ASP:H	1.62	0.46
4:O:29:GLN:HB2	4:O:33:HIS:CD2	2.51	0.46
5:P:104:ARG:HG2	8:P:3629:HOH:O	2.15	0.46
5:P:215:GLU:OE1	5:P:215:GLU:HA	2.15	0.46
2:C:73:LEU:HD22	2:C:94:LEU:HD22	1.97	0.46
2:C:113:VAL:HG11	2:C:373:VAL:CB	2.46	0.46
3:D:1114:THR:HG22	3:D:1195:GLN:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1272:ALA:HB2	8:D:9364:HOH:O	2.16	0.46
3:D:1382:THR:HG22	8:D:9579:HOH:O	2.16	0.46
3:D:1476:THR:CG2	4:E:21:VAL:HG22	2.46	0.46
1:K:23:PHE:O	1:K:196:THR:HA	2.15	0.46
2:M:478:VAL:HG13	2:M:506:ASN:HB3	1.97	0.46
2:M:688:ILE:CD1	2:M:847:GLY:HA3	2.45	0.46
2:M:1091:GLU:OE2	3:N:613:ARG:HD2	2.15	0.46
3:N:508:ARG:HB3	3:N:510:GLU:OE2	2.16	0.46
3:N:516:ALA:O	3:N:518:PRO:HD3	2.16	0.46
3:N:550:ARG:HG3	3:N:550:ARG:HH11	1.79	0.46
3:N:608:SER:O	3:N:612:GLY:HA3	2.16	0.46
3:N:646:LYS:HA	3:N:720:LEU:HD23	1.97	0.46
3:N:809:PRO:O	3:N:812:ALA:HB3	2.16	0.46
3:N:820:GLU:HA	3:N:825:ALA:O	2.16	0.46
3:N:1342:GLU:HG2	8:N:9105:HOH:O	2.15	0.46
3:N:1353:GLN:HG2	3:N:1368:ILE:HD12	1.98	0.46
2:C:144:PRO:HA	2:C:163:ILE:HG12	1.98	0.46
2:C:328:LEU:CD2	2:C:437:ARG:HD3	2.46	0.46
2:C:376:ARG:NH2	5:F:285:GLU:HB3	2.21	0.46
2:C:925:TYR:CD1	2:C:925:TYR:C	2.94	0.46
2:C:1004:LYS:O	2:C:1005:MET:C	2.59	0.46
3:D:829:VAL:H	3:D:835:SER:HB2	1.81	0.46
3:D:1042:ARG:O	3:D:1057:VAL:HB	2.15	0.46
3:D:1274:ILE:HB	3:D:1322:GLY:HA2	1.98	0.46
4:E:69:LEU:HD21	8:E:181:HOH:O	2.15	0.46
5:F:375:LEU:HG	5:F:376:ILE:HG13	1.97	0.46
1:K:27:PRO:HG2	1:K:186:LEU:HD22	1.98	0.46
1:K:175:ARG:HH21	1:K:201:THR:H	1.62	0.46
1:L:26:GLU:HB2	1:L:27:PRO:HA	1.98	0.46
1:L:138:LEU:O	1:L:138:LEU:HD23	2.16	0.46
2:M:127:PHE:O	2:M:133:ASP:HA	2.16	0.46
2:M:218:VAL:HG22	2:M:221:LEU:CD2	2.45	0.46
2:M:253:ALA:HB3	8:M:1251:HOH:O	2.15	0.46
2:M:1033:GLY:O	2:M:1036:GLU:HB2	2.15	0.46
2:M:1040:LEU:HD23	2:M:1049:LEU:HA	1.98	0.46
3:N:136:ASP:HB3	3:N:137:PRO:HD3	1.98	0.46
3:N:470:LEU:HD12	3:N:503:LEU:CG	2.43	0.46
3:N:530:VAL:HB	3:N:531:ASP:H	1.56	0.46
3:N:586:ARG:HA	8:N:2001:HOH:O	2.15	0.46
3:N:671:LYS:N	8:N:9139:HOH:O	2.48	0.46
3:N:819:GLY:O	3:N:822:ALA:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1378:TYR:N	3:N:1378:TYR:CD1	2.84	0.46
5:P:292:ALA:HB1	5:P:299:TRP:O	2.16	0.46
5:P:319:THR:HB	5:P:321:ILE:HD11	1.96	0.46
1:A:181:VAL:O	2:C:937:ASP:HA	2.16	0.46
1:B:81:ASN:HB2	8:B:366:HOH:O	2.16	0.46
2:C:129:ILE:CG1	2:C:386:PHE:HB3	2.46	0.46
2:C:175:GLU:HB3	2:C:183:SER:HG	1.81	0.46
2:C:194:VAL:HG21	2:C:221:LEU:HA	1.98	0.46
2:C:571:LEU:C	2:C:573:ARG:H	2.22	0.46
2:C:744:ARG:HG3	2:C:747:ALA:HB2	1.97	0.46
2:C:1039:ALA:HB2	3:D:707:THR:HG21	1.98	0.46
3:D:116:LEU:HB3	3:D:118:LEU:CD2	2.46	0.46
3:D:126:VAL:O	3:D:132:TYR:CD1	2.68	0.46
3:D:842:VAL:C	8:D:9557:HOH:O	2.59	0.46
3:D:1293:PHE:CE2	3:D:1302:GLU:HB2	2.51	0.46
3:D:1432:LYS:HD2	3:D:1433:SER:N	2.29	0.46
5:F:273:ARG:O	5:F:276:ARG:HB2	2.16	0.46
2:M:146:VAL:HG13	2:M:161:SER:O	2.16	0.46
2:M:157:ARG:HG2	2:M:157:ARG:HH11	1.80	0.46
3:N:159:ARG:CZ	3:N:159:ARG:HB2	2.46	0.46
3:N:521:PRO:O	3:N:525:ARG:HG2	2.14	0.46
3:N:805:GLU:HB2	8:N:9612:HOH:O	2.16	0.46
3:N:813:LEU:HA	3:N:839:LEU:HD11	1.97	0.46
3:N:850:LEU:O	3:N:853:VAL:HB	2.15	0.46
3:N:957:PRO:HG3	3:N:1007:VAL:HA	1.97	0.46
3:N:1115:THR:HB	8:N:9719:HOH:O	2.15	0.46
3:N:1137:ARG:O	3:N:1140:ILE:N	2.49	0.46
3:N:1209:LEU:HD22	3:N:1211:MET:SD	2.55	0.46
3:N:1269:LYS:HE3	8:N:9213:HOH:O	2.16	0.46
3:N:1441:GLN:NE2	3:N:1442:ASN:H	2.14	0.46
4:O:11:GLY:HA3	8:O:3878:HOH:O	2.15	0.46
5:P:274:THR:O	5:P:278:LEU:HG	2.15	0.46
2:C:47:ALA:CB	2:C:345:ARG:HB3	2.33	0.46
2:C:495:THR:HG21	2:C:524:VAL:HG21	1.97	0.46
2:C:702:SER:OG	2:C:996:LYS:NZ	2.49	0.46
2:C:873:PRO:O	2:C:876:VAL:HG23	2.16	0.46
2:C:975:TYR:HA	2:C:982:PRO:HA	1.98	0.46
2:C:1076:VAL:HG23	3:D:752:SER:HA	1.98	0.46
2:C:1109:VAL:HG11	3:D:5:VAL:HG13	1.98	0.46
3:D:97:THR:CG2	3:D:571:LYS:HD3	2.46	0.46
3:D:569:ASN:HD21	5:F:210:LEU:HD22	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:592:THR:HA	8:D:9540:HOH:O	2.16	0.46
3:D:863:VAL:HA	8:D:2082:HOH:O	2.16	0.46
3:D:1337:GLU:HB3	8:D:9228:HOH:O	2.16	0.46
2:M:408:ARG:CZ	2:M:542:VAL:HG23	2.46	0.46
2:M:423:ALA:HB1	8:M:1764:HOH:O	2.16	0.46
2:M:473:ARG:HG2	2:M:473:ARG:HH11	1.80	0.46
2:M:602:GLU:HG2	2:M:603:VAL:N	2.31	0.46
2:M:685:GLU:CG	3:N:739:ASP:HB2	2.46	0.46
2:M:861:LEU:HD23	2:M:862:PRO:CD	2.37	0.46
2:M:983:ILE:O	2:M:984:GLU:C	2.59	0.46
3:N:600:LEU:HD12	3:N:600:LEU:H	1.81	0.46
3:N:860:LEU:HD22	3:N:878:GLY:CA	2.46	0.46
3:N:1109:GLU:HG2	3:N:1201:CYS:CA	2.43	0.46
3:N:1114:THR:HA	8:N:9054:HOH:O	2.14	0.46
5:P:163:LEU:HB3	5:P:174:LEU:HD11	1.96	0.46
5:P:302:LYS:HG3	5:P:303:ARG:N	2.31	0.46
1:A:219:ARG:HH12	1:B:223:THR:HG23	1.81	0.46
1:A:219:ARG:HH22	1:B:223:THR:HG23	1.80	0.46
1:B:74:ASP:O	1:B:78:ILE:HG13	2.16	0.46
1:B:85:LEU:CD1	1:B:124:ASN:HB3	2.42	0.46
2:C:216:GLU:OE1	2:C:217:LEU:HG	2.15	0.46
2:C:352:ALA:O	2:C:355:VAL:HG12	2.16	0.46
2:C:473:ARG:NE	2:C:531:PHE:HE1	2.09	0.46
2:C:546:LEU:HD21	2:C:587:VAL:HG21	1.97	0.46
2:C:751:PRO:HB2	3:D:680:GLN:HG3	1.98	0.46
2:C:904:PRO:HB2	2:C:907:ASP:OD2	2.16	0.46
2:C:1103:ASP:N	2:C:1107:ASN:O	2.49	0.46
3:D:186:VAL:HG11	3:D:213:VAL:HB	1.98	0.46
3:D:210:ARG:NE	3:D:398:ALA:HB3	2.31	0.46
3:D:400:VAL:HG23	8:D:9178:HOH:O	2.15	0.46
3:D:421:LEU:HD23	3:D:421:LEU:O	2.15	0.46
3:D:543:LEU:HD21	3:D:600:LEU:HB2	1.97	0.46
3:D:1122:LEU:HD23	3:D:1178:ALA:HB2	1.97	0.46
3:D:1135:ARG:NH2	8:D:9592:HOH:O	2.49	0.46
3:D:1164:ARG:HA	8:D:9221:HOH:O	2.15	0.46
3:D:1327:ARG:HG2	8:D:9891:HOH:O	2.16	0.46
3:D:1481:VAL:HG11	4:E:18:ARG:CA	2.40	0.46
5:F:421:PHE:C	5:F:423:ASP:N	2.72	0.46
1:K:18:ARG:HD3	1:K:123:MET:HE1	1.97	0.46
1:L:43:ILE:HD13	8:L:3139:HOH:O	2.16	0.46
2:M:260:LEU:HA	2:M:291:ALA:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:420:ARG:H	2:M:420:ARG:CD	2.29	0.46
2:M:455:LEU:HD13	2:M:459:ALA:HB3	1.97	0.46
2:M:575:GLN:HA	2:M:662:GLU:CD	2.41	0.46
2:M:1100:GLN:HG3	2:M:1101:THR:O	2.16	0.46
3:N:52:PRO:CB	3:N:80:VAL:HG13	2.31	0.46
3:N:500:ARG:HD2	8:N:9705:HOH:O	2.15	0.46
3:N:529:GLN:HG2	3:N:535:PHE:CE2	2.48	0.46
3:N:844:ALA:HB3	3:N:848:GLU:OE2	2.16	0.46
3:N:976:GLN:HA	3:N:979:GLU:OE1	2.15	0.46
3:N:1341:PRO:O	3:N:1344:VAL:N	2.48	0.46
5:P:342:VAL:HG23	5:P:343:ASP:OD1	2.15	0.46
5:P:361:LEU:HD21	5:P:404:ALA:HB1	1.98	0.46
1:B:149:GLY:O	1:B:171:PHE:HB2	2.16	0.45
2:C:101:ILE:HG22	2:C:102:HIS:N	2.31	0.45
2:C:338:GLU:O	2:C:341:THR:HG22	2.16	0.45
2:C:694:LEU:HD21	2:C:868:ASP:HB3	1.98	0.45
2:C:979:THR:HG23	2:C:981:GLU:HB2	1.98	0.45
3:D:183:GLU:HA	3:D:186:VAL:CG1	2.46	0.45
3:D:441:ARG:O	3:D:443:VAL:N	2.49	0.45
3:D:585:GLY:HA3	8:D:9104:HOH:O	2.16	0.45
3:D:838:ARG:HD3	3:D:874:GLU:HB3	1.97	0.45
3:D:875:THR:HG22	3:D:879:ARG:HB2	1.98	0.45
3:D:1104:GLU:O	3:D:1106:VAL:HG23	2.16	0.45
3:D:1110:ALA:O	3:D:1111:ASP:C	2.60	0.45
3:D:1397:LYS:HB3	8:D:9838:HOH:O	2.15	0.45
5:F:117:SER:N	5:F:127:ILE:HD12	2.31	0.45
5:F:202:TYR:OH	5:F:244:ARG:HD2	2.16	0.45
5:F:340:SER:O	5:F:342:VAL:N	2.49	0.45
1:K:224:TYR:HB3	1:L:9:PRO:CB	2.42	0.45
2:M:114:PHE:HE1	8:P:4072:HOH:O	1.99	0.45
2:M:157:ARG:HG2	2:M:157:ARG:NH1	2.32	0.45
2:M:169:GLY:HA2	2:M:263:ASP:CB	2.30	0.45
2:M:194:VAL:HA	2:M:197:LEU:HD12	1.97	0.45
2:M:232:GLU:O	2:M:235:LEU:HB2	2.16	0.45
2:M:446:GLY:O	2:M:447:ALA:C	2.58	0.45
2:M:473:ARG:HG2	2:M:473:ARG:NH1	2.32	0.45
2:M:704:HIS:CD2	2:M:705:ILE:H	2.33	0.45
2:M:770:GLU:OE1	5:P:354:LEU:HD13	2.17	0.45
2:M:1050:GLN:NE2	8:M:1526:HOH:O	2.48	0.45
3:N:411:THR:HG23	3:N:429:SER:OG	2.16	0.45
3:N:527:MET:CE	3:N:537:THR:HB	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:567:ILE:H	3:N:567:ILE:HG13	1.51	0.45
3:N:729:HIS:HB3	3:N:732:VAL:HG22	1.98	0.45
4:O:5:GLY:HA3	4:O:8:LYS:HD2	1.98	0.45
5:P:89:GLY:HA2	8:P:4492:HOH:O	2.15	0.45
1:A:9:PRO:HB3	1:A:25:LEU:HG	1.98	0.45
2:C:142:ARG:NH1	2:C:325:ILE:HG12	2.30	0.45
2:C:203:ASP:OD1	2:C:206:THR:HG22	2.16	0.45
2:C:502:PRO:HB2	2:C:509:ALA:HB3	1.98	0.45
2:C:598:GLU:HG3	8:C:1515:HOH:O	2.15	0.45
2:C:794:PRO:HD3	8:C:1635:HOH:O	2.15	0.45
2:C:1016:ILE:CD1	3:D:526:PRO:HG2	2.46	0.45
3:D:455:ARG:HG2	3:D:455:ARG:HH11	1.81	0.45
3:D:806:PHE:CZ	3:D:813:LEU:HB3	2.51	0.45
3:D:890:VAL:HG13	3:D:926:LYS:HD3	1.98	0.45
3:D:1211:MET:SD	3:D:1213:ARG:HD2	2.57	0.45
3:D:1377:LYS:O	3:D:1395:LEU:N	2.47	0.45
3:D:1494:ALA:HB3	8:D:9315:HOH:O	2.16	0.45
5:F:196:VAL:HG13	5:F:213:ILE:CD1	2.45	0.45
5:F:302:LYS:HG3	5:F:303:ARG:N	2.31	0.45
1:K:101:LEU:HG	1:K:113:ASP:C	2.40	0.45
1:L:188:GLN:HA	8:N:9218:HOH:O	2.17	0.45
2:M:56:GLU:HG2	2:M:64:LEU:HD23	1.97	0.45
2:M:134:ARG:HE	2:M:393:GLN:C	2.23	0.45
2:M:435:TYR:HA	3:N:1071:PHE:HE2	1.81	0.45
2:M:778:PHE:HA	8:M:1278:HOH:O	2.16	0.45
2:M:998:TYR:OH	2:M:1000:MET:HA	2.16	0.45
2:M:1078:GLU:HA	2:M:1078:GLU:OE1	2.17	0.45
3:N:701:LEU:C	3:N:702:LEU:HD12	2.41	0.45
3:N:814:ALA:HA	8:N:9843:HOH:O	2.15	0.45
3:N:1068:LEU:O	3:N:1069:GLU:C	2.59	0.45
3:N:1151:ARG:HA	3:N:1162:GLU:HG3	1.99	0.45
3:N:1223:ILE:O	3:N:1224:VAL:C	2.60	0.45
5:P:409:LYS:HG3	5:P:410:TYR:N	2.29	0.45
1:A:20:TYR:HB3	8:A:358:HOH:O	2.16	0.45
1:A:26:GLU:HG2	1:A:27:PRO:CA	2.46	0.45
1:B:36:LEU:C	1:B:39:PRO:HD2	2.41	0.45
1:B:50:GLY:O	1:B:146:ARG:HA	2.16	0.45
2:C:144:PRO:O	2:C:276:LYS:HD3	2.16	0.45
2:C:148:PHE:HD2	2:C:160:ALA:HA	1.80	0.45
2:C:207:LEU:O	2:C:211:LEU:HB3	2.16	0.45
2:C:218:VAL:HB	8:C:1237:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:254:VAL:HA	2:C:257:VAL:HG23	1.96	0.45
2:C:289:THR:HG22	2:C:290:LEU:H	1.81	0.45
2:C:456:ALA:HB1	2:C:538:GLN:O	2.16	0.45
2:C:471:TYR:CE2	2:C:496:ILE:HG21	2.51	0.45
2:C:643:VAL:HG13	2:C:647:GLN:OE1	2.17	0.45
2:C:683:ASN:OD1	2:C:683:ASN:N	2.49	0.45
2:C:837:ASP:O	2:C:849:VAL:HG23	2.16	0.45
2:C:881:ASN:N	2:C:881:ASN:ND2	2.64	0.45
2:C:897:LEU:CD1	2:C:921:ALA:HA	2.46	0.45
2:C:1015:LEU:HD12	8:C:1202:HOH:O	2.17	0.45
2:C:1105:LYS:O	2:C:1107:ASN:N	2.49	0.45
3:D:170:PRO:HG3	8:D:9430:HOH:O	2.16	0.45
3:D:400:VAL:HA	3:D:442:ASN:O	2.17	0.45
3:D:757:ALA:CB	4:E:24:ALA:HB2	2.46	0.45
3:D:770:LEU:HB2	3:D:1210:SER:O	2.17	0.45
3:D:1331:ASP:OD1	3:D:1334:GLN:HG3	2.16	0.45
3:D:1333:HIS:O	3:D:1336:LEU:HB3	2.15	0.45
5:F:253:ASP:O	5:F:259:ARG:HD2	2.17	0.45
1:K:2:LEU:O	1:K:6:LEU:HB3	2.16	0.45
1:L:62:LEU:HD22	1:L:63:HIS:CE1	2.52	0.45
2:M:17:PRO:O	2:M:20:GLU:HB3	2.16	0.45
2:M:69:LEU:HD21	2:M:99:GLN:NE2	2.31	0.45
2:M:254:VAL:HA	2:M:257:VAL:HG23	1.98	0.45
2:M:737:LEU:HD21	2:M:741:GLY:O	2.16	0.45
2:M:838:LYS:HG2	8:M:1507:HOH:O	2.16	0.45
2:M:1009:SER:OG	3:N:655:PRO:HD3	2.15	0.45
3:N:177:ALA:HB1	3:N:199:LEU:HD22	1.97	0.45
3:N:396:VAL:HG13	3:N:446:VAL:O	2.16	0.45
3:N:416:ALA:HB3	3:N:417:PRO:HD3	1.98	0.45
3:N:480:GLU:OE2	3:N:484:PRO:HG2	2.17	0.45
3:N:486:ARG:HA	3:N:489:ARG:HD3	1.96	0.45
3:N:820:GLU:HG2	3:N:825:ALA:O	2.17	0.45
3:N:875:THR:HG23	3:N:879:ARG:NE	2.32	0.45
3:N:1112:CYS:HB3	3:N:1201:CYS:SG	2.56	0.45
3:N:1290:LEU:CD2	3:N:1291:SER:H	2.20	0.45
5:P:148:LYS:HB2	8:P:4930:HOH:O	2.16	0.45
5:P:308:LEU:O	5:P:312:GLN:HG3	2.15	0.45
5:P:336:GLU:HA	8:P:2842:HOH:O	2.16	0.45
1:A:26:GLU:HG3	1:A:184:THR:HG21	1.99	0.45
1:A:33:GLY:HA2	1:A:195:LEU:HD22	1.98	0.45
1:B:14:ARG:HA	8:B:324:HOH:O	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:GLU:HG3	1:B:79:ILE:HD13	1.97	0.45
1:B:143:ARG:HB2	8:B:337:HOH:O	2.16	0.45
2:C:16:PRO:O	2:C:18:LEU:HD12	2.16	0.45
2:C:19:THR:O	2:C:19:THR:HG22	2.16	0.45
2:C:399:ASN:ND2	2:C:402:SER:HB2	2.31	0.45
2:C:535:SER:H	2:C:538:GLN:HE21	1.64	0.45
2:C:603:VAL:HG22	2:C:613:VAL:HG12	1.99	0.45
2:C:668:LEU:HD12	2:C:668:LEU:N	2.32	0.45
2:C:826:TYR:HB3	8:C:1718:HOH:O	2.15	0.45
2:C:854:PRO:C	2:C:856:GLU:N	2.74	0.45
2:C:911:GLU:O	2:C:915:LYS:HG2	2.17	0.45
2:C:1096:ALA:HB2	3:D:101:HIS:CD2	2.51	0.45
3:D:473:LEU:HD21	3:D:495:ARG:NE	2.30	0.45
3:D:581:LEU:CD1	3:D:603:LEU:HD12	2.46	0.45
3:D:704:ARG:NH1	3:D:737:ASN:O	2.50	0.45
3:D:792:ILE:O	3:D:878:GLY:HA3	2.16	0.45
3:D:827:ILE:HG23	3:D:837:GLY:HA2	1.99	0.45
3:D:868:TYR:CG	3:D:869:MET:N	2.75	0.45
3:D:900:ILE:CD1	3:D:902:LEU:HG	2.47	0.45
3:D:1094:LEU:O	3:D:1098:LEU:HD13	2.17	0.45
3:D:1192:LEU:HD21	3:D:1372:VAL:CG1	2.46	0.45
3:D:1339:LYS:HE3	8:D:2030:HOH:O	2.14	0.45
3:D:1440:PHE:HD1	3:D:1441:GLN:H	1.64	0.45
4:E:61:GLU:OE2	4:E:62:THR:N	2.50	0.45
1:K:54:THR:CG2	1:K:158:ILE:HG13	2.40	0.45
1:L:110:LYS:HE3	8:L:3562:HOH:O	2.15	0.45
2:M:217:LEU:HD12	2:M:311:PHE:HD2	1.81	0.45
2:M:437:ARG:CZ	2:M:488:ALA:HA	2.47	0.45
2:M:874:LEU:HD12	3:N:783:ARG:HB2	1.97	0.45
3:N:119:SER:CB	3:N:123:LEU:HB2	2.39	0.45
3:N:992:ILE:O	3:N:995:LEU:HB3	2.15	0.45
3:N:1075:HIS:HB3	8:N:9012:HOH:O	2.16	0.45
3:N:1171:VAL:O	3:N:1171:VAL:HG12	2.17	0.45
4:O:78:ASN:HB2	8:O:4376:HOH:O	2.16	0.45
5:P:403:LYS:HA	5:P:403:LYS:HZ3	1.81	0.45
1:A:18:ARG:NH1	1:A:88:ARG:HE	2.14	0.45
2:C:94:LEU:HD12	2:C:95:TYR:N	2.32	0.45
2:C:460:ARG:HG2	8:C:1486:HOH:O	2.16	0.45
2:C:657:ASP:HB3	8:C:1152:HOH:O	2.17	0.45
2:C:957:LYS:HE2	2:C:965:GLU:OE2	2.16	0.45
3:D:6:ARG:CB	3:D:6:ARG:HH11	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:41:ARG:CD	3:D:42:ASP:H	2.23	0.45
3:D:145:VAL:HG21	8:D:9724:HOH:O	2.16	0.45
3:D:178:LEU:CG	3:D:200:ASP:H	2.26	0.45
3:D:502:PHE:CE2	3:D:1452:ILE:HG13	2.52	0.45
3:D:583:ASP:HA	3:D:602:SER:OG	2.16	0.45
3:D:584:ASN:HD21	3:D:590:PRO:HD2	1.80	0.45
3:D:717:GLN:HE21	3:D:717:GLN:HB2	1.51	0.45
3:D:850:LEU:HB2	8:D:9338:HOH:O	2.16	0.45
3:D:890:VAL:HG21	3:D:922:LEU:CD1	2.47	0.45
3:D:972:LEU:O	3:D:976:GLN:HG3	2.17	0.45
3:D:1035:ILE:HA	3:D:1038:LEU:HD12	1.97	0.45
3:D:1281:VAL:HG21	3:D:1313:VAL:HG21	1.99	0.45
3:D:1337:GLU:HG3	8:D:2052:HOH:O	2.16	0.45
5:F:105:LYS:NZ	5:F:179:GLU:HB3	2.31	0.45
5:F:197:SER:HA	8:F:484:HOH:O	2.14	0.45
1:L:101:LEU:HD12	1:L:114:PHE:CD1	2.52	0.45
1:L:123:MET:HG2	8:L:3100:HOH:O	2.15	0.45
1:L:206:THR:HG22	1:L:209:GLU:HG3	1.99	0.45
2:M:157:ARG:CD	2:M:158:TYR:H	2.28	0.45
2:M:244:PRO:HD2	2:M:245:GLY:N	2.25	0.45
2:M:669:GLY:HA3	2:M:995:MET:HA	1.98	0.45
2:M:987:ILE:HG23	3:N:948:THR:CG2	2.47	0.45
3:N:123:LEU:HA	8:N:9192:HOH:O	2.16	0.45
3:N:569:ASN:HA	3:N:572:ARG:HD2	1.98	0.45
3:N:696:HIS:HB2	4:O:48:MET:HE2	1.97	0.45
3:N:800:LYS:HD3	3:N:804:LEU:HD22	1.98	0.45
3:N:1465:ASN:HD22	3:N:1465:ASN:HA	1.53	0.45
8:A:413:HOH:O	2:C:642:ARG:HA	2.17	0.45
1:B:156:HIS:CE1	1:B:158:ILE:H	2.35	0.45
2:C:521:PRO:CB	3:D:1055:VAL:HB	2.42	0.45
2:C:549:PHE:HE2	2:C:887:GLU:N	2.15	0.45
2:C:622:GLU:OE1	2:C:624:PRO:HG3	2.17	0.45
2:C:941:VAL:HA	2:C:944:LEU:HD12	1.98	0.45
2:C:948:GLU:HG3	2:C:949:LYS:N	2.31	0.45
3:D:36:THR:O	3:D:38:LYS:N	2.50	0.45
3:D:86:ARG:HG2	3:D:86:ARG:NH1	2.31	0.45
3:D:87:ARG:HB3	3:D:523:ASP:CB	2.45	0.45
3:D:396:VAL:CG2	3:D:447:VAL:HB	2.46	0.45
3:D:859:ASP:OD2	3:D:859:ASP:N	2.48	0.45
3:D:1233:GLY:O	3:D:1256:LEU:HD13	2.16	0.45
3:D:1291:SER:HB3	8:D:9240:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:57:TYR:CZ	1:K:161:ARG:HD2	2.52	0.45
1:K:127:LEU:HD12	1:K:127:LEU:C	2.42	0.45
1:K:176:ARG:HG3	1:K:200:TRP:CE3	2.52	0.45
1:K:183:ASP:HB2	8:K:4658:HOH:O	2.16	0.45
1:L:81:ASN:ND2	1:L:127:LEU:HD11	2.30	0.45
2:M:207:LEU:HD22	2:M:221:LEU:CD1	2.46	0.45
2:M:571:LEU:HD12	2:M:701:THR:N	2.32	0.45
2:M:863:ASP:OD1	2:M:865:THR:HG22	2.16	0.45
3:N:115:LEU:CD1	3:N:499:VAL:HG22	2.47	0.45
3:N:861:GLN:CD	3:N:861:GLN:H	2.25	0.45
3:N:1213:ARG:HB2	3:N:1214:PRO:CD	2.46	0.45
5:P:102:LEU:HD13	5:P:187:LEU:HG	1.97	0.45
5:P:272:SER:O	5:P:276:ARG:HG2	2.16	0.45
5:P:421:PHE:C	5:P:423:ASP:N	2.73	0.45
1:A:103:ALA:HB1	1:A:107:LYS:NZ	2.32	0.45
1:B:24:VAL:HG13	1:B:196:THR:CG2	2.37	0.45
2:C:124:ASP:CG	2:C:407:LYS:HZ1	2.25	0.45
2:C:251:ASP:C	2:C:252:LYS:HD2	2.42	0.45
2:C:794:PRO:HD2	8:C:1228:HOH:O	2.16	0.45
3:D:27:GLU:HG3	3:D:28:LYS:HD2	1.98	0.45
3:D:396:VAL:HG22	8:D:9882:HOH:O	2.17	0.45
3:D:503:LEU:HG	3:D:508:ARG:NH2	2.32	0.45
3:D:957:PRO:HG2	3:D:1007:VAL:HA	1.98	0.45
3:D:1155:VAL:CG1	3:D:1183:ILE:HD11	2.47	0.45
3:D:1504:GLU:HB3	8:D:9773:HOH:O	2.15	0.45
4:E:41:GLU:HG3	8:E:170:HOH:O	2.15	0.45
5:F:217:ASN:O	5:F:221:ILE:HG13	2.17	0.45
5:F:359:SER:C	5:F:361:LEU:H	2.23	0.45
2:M:73:LEU:HD12	2:M:73:LEU:O	2.17	0.45
2:M:86:LYS:HG2	2:M:813:VAL:HG12	1.99	0.45
2:M:144:PRO:HB3	8:M:1235:HOH:O	2.16	0.45
2:M:290:LEU:HD12	8:M:1503:HOH:O	2.17	0.45
2:M:943:VAL:HG11	2:M:973:VAL:HG22	1.99	0.45
3:N:13:ALA:HA	3:N:17:LYS:NZ	2.32	0.45
3:N:99:ALA:HB1	3:N:575:GLN:CD	2.42	0.45
3:N:399:ARG:HB3	3:N:402:PRO:HG3	1.98	0.45
3:N:491:LYS:HG3	8:N:9735:HOH:O	2.17	0.45
3:N:774:SER:C	3:N:776:GLU:N	2.75	0.45
3:N:866:VAL:HG12	3:N:867:ARG:N	2.32	0.45
3:N:892:ASP:HB3	3:N:895:VAL:HG23	1.99	0.45
3:N:1112:CYS:HB2	3:N:1195:GLN:CD	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1127:GLU:HB2	8:N:9303:HOH:O	2.17	0.45
3:N:1129:THR:O	3:N:1130:ARG:HD2	2.17	0.45
3:N:1175:ILE:HG22	3:N:1179:GLU:OE1	2.16	0.45
3:N:1262:LEU:HD11	3:N:1351:GLU:CG	2.46	0.45
5:P:153:PRO:O	5:P:157:GLU:HG2	2.16	0.45
1:A:20:TYR:CE2	1:A:22:GLU:HG3	2.51	0.45
1:A:184:THR:HB	1:A:194:LYS:HD2	1.98	0.45
1:A:227:ASN:ND2	1:A:227:ASN:H	2.14	0.45
1:B:20:TYR:HB3	8:B:319:HOH:O	2.15	0.45
2:C:39:ARG:HA	2:C:39:ARG:NE	2.30	0.45
2:C:265:ARG:HD2	8:C:1452:HOH:O	2.17	0.45
2:C:304:LEU:HG	2:C:305:PRO:N	2.31	0.45
2:C:874:LEU:HB3	3:D:1029:ARG:HD2	1.98	0.45
2:C:1043:TYR:CE1	3:D:710:ARG:O	2.70	0.45
2:C:1056:LYS:HE2	3:D:625:TYR:HB2	1.98	0.45
3:D:164:GLY:HA2	8:D:9127:HOH:O	2.16	0.45
3:D:168:THR:HG1	3:D:393:ILE:HB	1.82	0.45
3:D:462:GLN:NE2	3:D:513:ILE:HB	2.32	0.45
3:D:957:PRO:HG3	3:D:1007:VAL:HA	1.99	0.45
3:D:985:ASP:O	3:D:988:ARG:HD2	2.16	0.45
3:D:1314:LYS:NZ	3:D:1317:ASP:HB2	2.31	0.45
3:D:1342:GLU:O	3:D:1346:ARG:HB2	2.17	0.45
5:F:421:PHE:C	5:F:423:ASP:H	2.25	0.45
1:K:40:LEU:O	1:K:44:LEU:HD12	2.17	0.45
1:K:74:ASP:O	1:K:78:ILE:HG13	2.17	0.45
1:L:128:HIS:CE1	1:L:131:THR:HG23	2.52	0.45
1:L:194:LYS:HG2	8:L:4937:HOH:O	2.17	0.45
2:M:503:LEU:HD12	2:M:505:GLY:O	2.17	0.45
2:M:762:LYS:HD3	2:M:771:GLU:OE2	2.16	0.45
2:M:922:PHE:HD2	2:M:964:LYS:HD3	1.82	0.45
3:N:119:SER:CB	3:N:123:LEU:HD13	2.46	0.45
3:N:141:ILE:HD13	3:N:450:TYR:HB2	1.98	0.45
3:N:703:ASN:ND2	3:N:704:ARG:H	2.15	0.45
3:N:1136:LYS:HE3	3:N:1139:ASP:OD2	2.16	0.45
3:N:1200:VAL:HG22	3:N:1373:ARG:HH12	1.81	0.45
3:N:1238:MET:HG2	3:N:1256:LEU:HD23	1.98	0.45
4:O:9:LEU:CD2	4:O:69:LEU:HG	2.47	0.45
1:A:48:ILE:HG22	1:A:173:PRO:CD	2.47	0.45
1:B:28:LEU:HB2	1:B:193:ASP:HB2	1.99	0.45
2:C:5:ARG:HG2	2:C:5:ARG:HH11	1.82	0.45
2:C:98:LEU:HD11	8:C:1822:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:112:GLU:HA	8:C:1822:HOH:O	2.17	0.45
2:C:203:ASP:OD1	2:C:205:GLU:HG3	2.16	0.45
2:C:217:LEU:HD23	8:C:1241:HOH:O	2.17	0.45
2:C:333:ILE:O	2:C:465:GLY:HA3	2.17	0.45
2:C:405:ARG:CZ	2:C:566:THR:HG21	2.47	0.45
2:C:433:THR:CG2	2:C:488:ALA:HB1	2.42	0.45
2:C:1006:HIS:N	2:C:1006:HIS:HD1	2.14	0.45
2:C:1033:GLY:O	2:C:1037:VAL:HG23	2.17	0.45
3:D:22:SER:OG	3:D:91:GLY:HA2	2.17	0.45
3:D:198:ARG:HG3	8:D:9736:HOH:O	2.16	0.45
3:D:639:LEU:N	3:D:729:HIS:CD2	2.84	0.45
3:D:704:ARG:HB2	3:D:736:PHE:CD2	2.52	0.45
3:D:848:GLU:HA	3:D:851:LEU:CD1	2.46	0.45
3:D:1086:LEU:HD22	8:D:9242:HOH:O	2.16	0.45
3:D:1223:ILE:O	3:D:1224:VAL:C	2.59	0.45
5:F:362:SER:O	5:F:367:MET:HE3	2.17	0.45
5:F:364:ARG:O	5:F:368:VAL:HG23	2.17	0.45
1:K:161:ARG:NH1	1:K:161:ARG:HB2	2.32	0.45
2:M:164:PRO:HA	8:M:1235:HOH:O	2.17	0.45
2:M:210:GLU:HG3	8:M:1787:HOH:O	2.17	0.45
2:M:620:LEU:HD13	2:M:620:LEU:N	2.32	0.45
3:N:9:ARG:HA	3:N:1455:LYS:O	2.16	0.45
3:N:52:PRO:HD2	3:N:79:GLU:O	2.16	0.45
3:N:399:ARG:HB2	3:N:444:VAL:HG13	1.99	0.45
3:N:456:MET:HG2	3:N:456:MET:O	2.16	0.45
3:N:640:HIS:NE2	3:N:717:GLN:OE1	2.48	0.45
3:N:645:PRO:HB3	3:N:723:GLY:O	2.17	0.45
3:N:704:ARG:CZ	3:N:737:ASN:O	2.65	0.45
3:N:872:ARG:NH2	8:N:9086:HOH:O	2.50	0.45
3:N:1209:LEU:C	3:N:1211:MET:N	2.75	0.45
3:N:1320:GLU:HG3	8:N:9381:HOH:O	2.16	0.45
3:N:1459:LEU:HD13	3:N:1465:ASN:HD21	1.81	0.45
1:B:23:PHE:O	1:B:196:THR:HA	2.17	0.45
1:B:123:MET:HE2	1:B:204:SER:HA	1.97	0.45
2:C:115:LEU:HD12	2:C:378:LEU:HD22	1.99	0.45
2:C:374:ASN:ND2	2:C:377:PRO:HD3	2.32	0.45
2:C:535:SER:O	2:C:538:GLN:HG2	2.16	0.45
2:C:579:VAL:HG11	2:C:887:GLU:HG3	1.99	0.45
2:C:718:GLY:HA3	2:C:761:PHE:CZ	2.52	0.45
2:C:729:LEU:HD21	5:F:421:PHE:HD1	1.82	0.45
2:C:774:LEU:HA	2:C:777:ILE:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:911:GLU:HB3	2:C:912:PRO:HD3	1.99	0.45
2:C:952:LEU:HB3	2:C:966:LEU:CD1	2.47	0.45
2:C:1083:GLU:OE1	2:C:1083:GLU:HA	2.17	0.45
3:D:495:ARG:O	3:D:499:VAL:HG23	2.17	0.45
3:D:768:ASN:N	3:D:768:ASN:HD22	2.13	0.45
3:D:1495:ILE:HG12	4:E:80:VAL:CG1	2.46	0.45
8:D:9004:HOH:O	5:F:132:ARG:NH1	2.49	0.45
5:F:209:PHE:HE2	5:F:213:ILE:HD11	1.81	0.45
1:L:22:GLU:OE2	1:L:198:ARG:HG2	2.17	0.45
2:M:15:LEU:CD2	2:M:583:LEU:HD21	2.47	0.45
2:M:72:ARG:HH21	2:M:112:GLU:CD	2.25	0.45
2:M:139:GLN:NE2	2:M:418:LEU:HD13	2.32	0.45
2:M:366:SER:HB2	8:M:1234:HOH:O	2.17	0.45
2:M:437:ARG:HG2	2:M:467:ILE:HG22	1.98	0.45
2:M:498:GLN:O	2:M:532:MET:SD	2.75	0.45
2:M:679:PHE:HD2	2:M:682:TYR:HD2	1.65	0.45
2:M:1095:LEU:O	2:M:1096:ALA:C	2.60	0.45
3:N:130:SER:HB3	3:N:132:TYR:HE1	1.80	0.45
3:N:402:PRO:HG2	3:N:444:VAL:CG1	2.47	0.45
3:N:634:GLY:O	3:N:637:LEU:HB3	2.17	0.45
3:N:778:LEU:HD12	3:N:778:LEU:HA	1.78	0.45
3:N:806:PHE:O	3:N:806:PHE:CG	2.70	0.45
3:N:1087:ARG:NH1	3:N:1234:THR:O	2.50	0.45
3:N:1455:LYS:HE3	8:N:9604:HOH:O	2.17	0.45
4:O:7:ASP:HB2	8:O:3467:HOH:O	2.16	0.45
4:O:85:LEU:HD23	4:O:86:GLN:N	2.32	0.45
5:P:131:VAL:HG13	5:P:178:ARG:HG2	1.98	0.45
1:B:106:PRO:HB2	8:B:403:HOH:O	2.17	0.44
2:C:260:LEU:HA	2:C:291:ALA:HB2	1.98	0.44
2:C:405:ARG:HD2	2:C:442:GLU:OE1	2.17	0.44
2:C:499:ALA:HB1	8:C:1368:HOH:O	2.18	0.44
2:C:603:VAL:HG21	2:C:643:VAL:CG1	2.41	0.44
2:C:693:GLU:OE2	2:C:855:VAL:HG21	2.16	0.44
2:C:737:LEU:HD12	2:C:754:ILE:HB	1.98	0.44
2:C:884:GLN:HG3	2:C:885:ILE:HD13	1.98	0.44
2:C:1005:MET:HE3	2:C:1005:MET:HB2	1.84	0.44
3:D:10:ILE:HD13	3:D:1447:LEU:HG	1.99	0.44
3:D:630:VAL:O	3:D:726:ILE:HG13	2.16	0.44
3:D:756:GLN:NE2	3:D:760:ARG:HD2	2.32	0.44
3:D:795:VAL:CG1	3:D:863:VAL:HG13	2.44	0.44
3:D:1026:SER:C	3:D:1028:ALA:H	2.24	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1192:LEU:HD21	3:D:1372:VAL:HG13	1.99	0.44
3:D:1258:ARG:HH21	3:D:1351:GLU:HG2	1.82	0.44
3:D:1320:GLU:CB	3:D:1323:GLN:HE21	2.30	0.44
1:K:19:GLU:O	1:K:200:TRP:HA	2.16	0.44
1:L:76:VAL:HA	1:L:79:ILE:HG12	1.98	0.44
2:M:34:VAL:CB	2:M:38:LYS:HG3	2.47	0.44
2:M:134:ARG:HD3	2:M:393:GLN:O	2.17	0.44
2:M:139:GLN:HB3	2:M:334:ARG:HD3	1.99	0.44
2:M:332:ARG:HG3	2:M:333:ILE:N	2.33	0.44
2:M:333:ILE:N	2:M:333:ILE:HD12	2.32	0.44
2:M:429:ASP:HB3	8:M:1324:HOH:O	2.17	0.44
2:M:559:LEU:HD23	2:M:560:MET:N	2.33	0.44
2:M:1013:TYR:CD1	2:M:1020:PRO:HA	2.52	0.44
2:M:1037:VAL:HG12	2:M:1041:GLU:OE1	2.17	0.44
2:M:1040:LEU:HD23	2:M:1049:LEU:CA	2.47	0.44
2:M:1043:TYR:CE1	3:N:710:ARG:HB2	2.52	0.44
2:M:1066:ALA:O	2:M:1070:ILE:HG13	2.16	0.44
3:N:34:TYR:O	3:N:35:ARG:C	2.60	0.44
3:N:799:LYS:N	3:N:826:PRO:HG2	2.31	0.44
3:N:1197:ARG:HD2	3:N:1198:TYR:CD1	2.52	0.44
3:N:1249:ALA:HB2	8:N:9831:HOH:O	2.16	0.44
3:N:1280:VAL:HG12	3:N:1281:VAL:N	2.32	0.44
3:N:1403:LEU:O	3:N:1407:LEU:HB2	2.16	0.44
5:P:141:VAL:O	5:P:145:PRO:HD2	2.15	0.44
5:P:144:ILE:HG23	8:P:4865:HOH:O	2.17	0.44
5:P:217:ASN:O	5:P:221:ILE:HG13	2.18	0.44
1:B:173:PRO:HA	1:B:202:ASP:OD2	2.17	0.44
2:C:71:TYR:HD2	8:C:1554:HOH:O	1.99	0.44
2:C:162:ILE:HB	2:C:172:ILE:CD1	2.47	0.44
2:C:304:LEU:HD23	2:C:305:PRO:HD3	1.99	0.44
3:D:112:ILE:O	3:D:112:ILE:HD12	2.18	0.44
3:D:574:LEU:O	3:D:577:ALA:HB3	2.16	0.44
3:D:637:LEU:HD12	3:D:641:GLN:OE1	2.18	0.44
3:D:765:SER:C	3:D:767:HIS:H	2.26	0.44
3:D:1155:VAL:CG1	3:D:1177:ALA:HB1	2.47	0.44
3:D:1211:MET:CG	3:D:1213:ARG:HG2	2.47	0.44
3:D:1211:MET:HG2	3:D:1213:ARG:HG2	1.99	0.44
5:F:302:LYS:O	5:F:306:GLU:HB2	2.17	0.44
2:M:139:GLN:CG	2:M:140:ILE:N	2.80	0.44
2:M:329:GLY:N	2:M:488:ALA:HB3	2.33	0.44
2:M:873:PRO:HB3	3:N:949:ILE:HG12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:63:TYR:HB3	3:N:68:PHE:CE1	2.53	0.44
3:N:423:ASP:HB3	5:P:175:HIS:HA	1.99	0.44
3:N:500:ARG:HH12	3:N:1388:ARG:NH1	1.95	0.44
3:N:891:GLU:OE1	3:N:891:GLU:HA	2.17	0.44
3:N:951:ILE:HG23	3:N:1062:ARG:NH2	2.32	0.44
3:N:1000:THR:HG23	3:N:1001:GLU:N	2.32	0.44
3:N:1065:LEU:C	3:N:1065:LEU:HD12	2.41	0.44
5:P:367:MET:HA	5:P:370:LYS:HZ3	1.83	0.44
5:P:369:LEU:O	5:P:373:LYS:HB2	2.17	0.44
2:C:79:PRO:HG2	2:C:82:GLU:HB2	2.00	0.44
2:C:305:PRO:HG2	8:C:1135:HOH:O	2.16	0.44
2:C:338:GLU:CA	2:C:341:THR:HG22	2.46	0.44
2:C:436:GLY:O	2:C:459:ALA:HB2	2.18	0.44
2:C:601:GLY:HA2	2:C:616:GLU:CD	2.42	0.44
2:C:841:ASN:C	2:C:841:ASN:HD22	2.25	0.44
2:C:841:ASN:ND2	2:C:844:GLY:H	2.15	0.44
2:C:1067:TYR:HE2	5:F:345:ALA:HB2	1.82	0.44
3:D:62:LYS:HB2	3:D:73:CYS:SG	2.57	0.44
3:D:135:LEU:HD21	3:D:138:LYS:C	2.42	0.44
3:D:209:ARG:HB2	3:D:395:VAL:O	2.17	0.44
3:D:658:LEU:O	3:D:661:MET:HB2	2.17	0.44
3:D:978:TYR:HE1	3:D:985:ASP:HA	1.82	0.44
3:D:1328:GLY:HA2	8:D:9891:HOH:O	2.16	0.44
3:D:1369:GLU:O	3:D:1372:VAL:HG12	2.17	0.44
5:F:93:LEU:HD11	5:F:187:LEU:HG	2.00	0.44
1:L:55:SER:OG	1:L:158:ILE:HB	2.18	0.44
2:M:469:THR:HG23	2:M:470:PRO:HD2	1.99	0.44
2:M:561:GLY:HA3	2:M:842:ARG:O	2.18	0.44
2:M:713:ARG:HH11	2:M:713:ARG:HG3	1.82	0.44
3:N:436:GLU:HB2	3:N:445:ARG:HB2	1.98	0.44
3:N:465:LEU:HD22	3:N:509:PRO:O	2.17	0.44
3:N:893:GLU:O	3:N:896:ALA:HB3	2.17	0.44
3:N:899:LEU:CD1	3:N:900:ILE:HG23	2.45	0.44
3:N:1031:ASN:OD1	3:N:1033:GLN:N	2.50	0.44
3:N:1329:ALA:C	3:N:1330:ILE:HD12	2.42	0.44
3:N:1393:GLN:CB	3:N:1398:TRP:HE1	2.25	0.44
3:N:1498:ALA:HA	3:N:1501:GLU:OE2	2.18	0.44
4:O:16:LYS:HD3	4:O:17:TYR:CE2	2.46	0.44
5:P:256:ARG:HD2	8:P:3047:HOH:O	2.17	0.44
5:P:317:LEU:O	5:P:329:TYR:HB3	2.16	0.44
1:A:112:ARG:HD3	8:A:442:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:LEU:HD11	1:A:197:LEU:HD22	1.98	0.44
2:C:884:GLN:CG	2:C:885:ILE:N	2.80	0.44
2:C:1002:GLU:HB2	3:D:628:ARG:HH12	1.82	0.44
2:C:1060:ILE:CG2	2:C:1061:GLU:H	2.29	0.44
3:D:477:LEU:HD23	8:D:9254:HOH:O	2.16	0.44
3:D:581:LEU:HD12	3:D:603:LEU:HD12	2.00	0.44
3:D:970:LYS:HD2	3:D:995:LEU:HD13	1.99	0.44
3:D:1109:GLU:HG2	3:D:1202:GLN:H	1.83	0.44
3:D:1350:GLU:HG3	3:D:1354:LYS:CE	2.43	0.44
2:M:534:VAL:N	2:M:538:GLN:NE2	2.63	0.44
2:M:674:VAL:O	2:M:989:VAL:HA	2.17	0.44
2:M:816:LYS:HB2	2:M:819:VAL:CG2	2.47	0.44
2:M:975:TYR:HE2	8:M:1126:HOH:O	2.01	0.44
2:M:1114:GLY:N	2:M:1115:LEU:HD12	2.31	0.44
3:N:472:ALA:HB3	8:N:9566:HOH:O	2.17	0.44
3:N:486:ARG:CZ	8:N:9895:HOH:O	2.65	0.44
3:N:584:ASN:H	3:N:602:SER:CB	2.30	0.44
3:N:650:LEU:HD12	3:N:691:LEU:HD22	2.00	0.44
3:N:699:VAL:HG12	3:N:717:GLN:HA	1.98	0.44
5:P:123:ASP:HB2	5:P:126:LEU:HD22	1.98	0.44
5:P:276:ARG:HB2	8:P:3917:HOH:O	2.16	0.44
1:A:184:THR:O	1:A:192:LEU:HD12	2.17	0.44
1:B:14:ARG:HH21	1:B:24:VAL:HG21	1.82	0.44
1:B:71:VAL:HG22	1:B:132:LEU:HD12	1.99	0.44
2:C:129:ILE:HG13	2:C:386:PHE:HB3	1.99	0.44
2:C:447:ALA:O	2:C:449:ILE:HG22	2.18	0.44
2:C:474:VAL:HG13	2:C:530:GLU:C	2.42	0.44
2:C:917:LEU:HA	2:C:917:LEU:HD23	1.89	0.44
2:C:1033:GLY:O	2:C:1036:GLU:HB2	2.18	0.44
2:C:1035:MET:HG2	3:D:707:THR:O	2.17	0.44
3:D:548:ILE:HG12	3:D:548:ILE:H	1.47	0.44
3:D:554:LEU:O	3:D:558:LEU:HG	2.16	0.44
3:D:583:ASP:OD2	3:D:586:ARG:HD2	2.18	0.44
3:D:879:ARG:HG3	3:D:879:ARG:NH1	2.33	0.44
3:D:925:GLU:HG2	4:E:7:ASP:OD1	2.18	0.44
3:D:1092:GLY:O	3:D:1093:TYR:C	2.60	0.44
3:D:1278:ASP:HB2	3:D:1318:TYR:HE1	1.82	0.44
3:D:1394:VAL:HG21	3:D:1397:LYS:NZ	2.32	0.44
3:D:1462:LEU:N	3:D:1462:LEU:HD23	2.32	0.44
4:E:40:LEU:HD13	8:E:180:HOH:O	2.18	0.44
1:K:64:GLU:OE2	1:K:76:VAL:HG13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:156:HIS:HD2	1:K:157:GLY:N	2.15	0.44
2:M:239:PHE:HD1	8:M:1629:HOH:O	2.00	0.44
2:M:578:VAL:HG13	2:M:671:ASN:CG	2.42	0.44
2:M:854:PRO:C	2:M:856:GLU:N	2.75	0.44
2:M:908:GLY:C	2:M:910:LYS:HZ3	2.25	0.44
2:M:979:THR:CG2	2:M:981:GLU:HB2	2.46	0.44
2:M:1068:GLU:OE1	5:P:345:ALA:HA	2.17	0.44
3:N:128:TYR:HB3	3:N:129:PHE:CD1	2.53	0.44
3:N:206:ARG:HG2	3:N:206:ARG:HH11	1.82	0.44
3:N:591:VAL:CG1	3:N:597:ASP:HA	2.48	0.44
3:N:1399:ASP:O	3:N:1403:LEU:HD12	2.18	0.44
5:P:128:ARG:HB2	5:P:128:ARG:CZ	2.48	0.44
5:P:287:THR:O	5:P:289:GLU:N	2.50	0.44
5:P:395:GLU:O	5:P:399:GLN:HB2	2.18	0.44
5:P:416:ARG:HD2	5:P:419:ARG:HB3	1.99	0.44
1:A:27:PRO:HG3	1:A:186:LEU:HD13	2.00	0.44
1:A:107:LYS:HG3	8:A:494:HOH:O	2.17	0.44
1:B:54:THR:HG22	1:B:158:ILE:HG13	1.99	0.44
1:B:73:GLU:HB2	1:B:78:ILE:CG1	2.48	0.44
2:C:78:PHE:CB	2:C:88:LEU:HD21	2.48	0.44
2:C:383:ARG:HB2	2:C:383:ARG:CZ	2.46	0.44
2:C:470:PRO:HB2	2:C:483:VAL:HG11	1.99	0.44
2:C:666:LEU:HD21	2:C:668:LEU:HD11	1.99	0.44
2:C:690:ILE:HD12	2:C:849:VAL:CG1	2.47	0.44
2:C:789:SER:O	2:C:791:ARG:HG2	2.17	0.44
4:E:49:GLN:HA	4:E:51:LEU:O	2.18	0.44
5:F:81:VAL:O	5:F:85:LEU:HG	2.17	0.44
5:F:136:LEU:HD12	5:F:137:GLY:N	2.32	0.44
1:K:58:ILE:HD13	1:K:140:MET:CB	2.47	0.44
1:L:107:LYS:HB2	8:L:4739:HOH:O	2.16	0.44
2:M:428:ARG:O	3:N:1078:ARG:NH1	2.50	0.44
2:M:1061:GLU:HB3	8:M:1529:HOH:O	2.17	0.44
3:N:36:THR:C	3:N:38:LYS:N	2.76	0.44
3:N:631:ILE:HG12	3:N:743:ASP:O	2.18	0.44
3:N:759:ALA:O	3:N:763:MET:HB3	2.17	0.44
3:N:955:VAL:HA	8:N:9249:HOH:O	2.17	0.44
3:N:968:ASP:O	3:N:971:LEU:HB3	2.17	0.44
3:N:1416:ALA:HA	8:N:9145:HOH:O	2.16	0.44
1:A:49:PRO:O	1:A:173:PRO:HG3	2.18	0.44
1:A:156:HIS:CD2	1:A:157:GLY:N	2.86	0.44
2:C:41:ASN:HB2	8:C:1831:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:141:HIS:NE2	2:C:332:ARG:NH1	2.65	0.44
2:C:281:LEU:HD11	2:C:306:THR:CA	2.34	0.44
2:C:446:GLY:O	2:C:447:ALA:C	2.60	0.44
2:C:546:LEU:C	2:C:581:THR:HG21	2.43	0.44
2:C:953:VAL:HG22	2:C:966:LEU:HD13	2.00	0.44
3:D:9:ARG:HH21	3:D:11:ALA:CB	2.31	0.44
3:D:57:GLU:HG2	3:D:58:CYS:N	2.33	0.44
3:D:90:MET:CE	3:D:518:PRO:HB3	2.47	0.44
3:D:369:ALA:HB3	8:D:9717:HOH:O	2.16	0.44
3:D:400:VAL:CG1	3:D:441:ARG:HD3	2.48	0.44
3:D:999:THR:O	3:D:1002:LYS:HB2	2.17	0.44
1:L:13:VAL:HG13	1:L:23:PHE:CD1	2.53	0.44
2:M:95:TYR:N	2:M:95:TYR:CD1	2.86	0.44
2:M:129:ILE:N	2:M:129:ILE:HD12	2.31	0.44
2:M:164:PRO:HD2	2:M:170:PRO:O	2.18	0.44
2:M:211:LEU:CD1	2:M:308:ARG:HG3	2.44	0.44
2:M:391:LEU:HD23	2:M:391:LEU:C	2.43	0.44
2:M:445:GLU:HA	2:M:445:GLU:OE2	2.17	0.44
3:N:18:ILE:HG21	3:N:516:ALA:HB1	1.99	0.44
3:N:82:LYS:HE3	3:N:82:LYS:HB2	1.85	0.44
3:N:464:LEU:HD11	8:N:9491:HOH:O	2.18	0.44
3:N:563:PRO:HA	5:P:185:GLN:OE1	2.18	0.44
3:N:566:ILE:HG23	5:P:214:GLN:HE22	1.82	0.44
3:N:884:ARG:NH1	8:N:9403:HOH:O	2.49	0.44
3:N:1470:ARG:HG2	3:N:1471:LEU:N	2.32	0.44
4:O:45:ARG:HB2	4:O:46:PRO:HD2	1.99	0.44
1:A:73:GLU:OE2	1:A:73:GLU:N	2.51	0.44
1:B:1:MET:O	1:B:6:LEU:HD13	2.18	0.44
2:C:27:ARG:HG2	2:C:27:ARG:HH11	1.82	0.44
2:C:51:THR:CB	2:C:348:LEU:HD23	2.48	0.44
2:C:93:PRO:HG3	2:C:117:HIS:HE1	1.82	0.44
2:C:176:VAL:HG13	8:C:1607:HOH:O	2.17	0.44
2:C:185:LYS:HB3	2:C:188:LYS:O	2.17	0.44
2:C:244:PRO:HG2	2:C:246:ASP:CG	2.42	0.44
2:C:415:PRO:C	2:C:417:GLY:H	2.24	0.44
2:C:470:PRO:HG2	2:C:538:GLN:OE1	2.18	0.44
2:C:597:ALA:HB2	2:C:655:LEU:CD2	2.37	0.44
2:C:636:ALA:C	2:C:637:LEU:HD23	2.43	0.44
2:C:820:ARG:HB3	8:C:1508:HOH:O	2.18	0.44
2:C:1086:ARG:HG2	2:C:1112:PHE:CE2	2.52	0.44
2:C:1101:THR:HB	3:D:5:VAL:CG1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:6:ARG:HH11	3:D:6:ARG:HB3	1.83	0.44
3:D:168:THR:O	3:D:393:ILE:N	2.49	0.44
3:D:196:VAL:HG13	3:D:202:VAL:CG1	2.48	0.44
3:D:472:ALA:HB3	8:D:9440:HOH:O	2.17	0.44
3:D:600:LEU:O	3:D:601:ARG:C	2.61	0.44
3:D:653:PHE:HD1	3:D:653:PHE:N	2.16	0.44
3:D:774:SER:C	3:D:776:GLU:N	2.76	0.44
3:D:1106:VAL:O	3:D:1108:ARG:HG2	2.18	0.44
3:D:1369:GLU:HA	3:D:1372:VAL:HG12	1.99	0.44
3:D:1472:ILE:HA	3:D:1473:PRO:HD3	1.86	0.44
1:K:50:GLY:O	1:K:146:ARG:HA	2.18	0.44
1:K:175:ARG:HH21	1:K:201:THR:N	2.16	0.44
1:K:217:ILE:HA	1:K:220:GLU:CD	2.43	0.44
2:M:80:GLN:HE22	2:M:122:THR:HG23	1.83	0.44
2:M:146:VAL:HG11	2:M:306:THR:HG22	2.00	0.44
2:M:218:VAL:O	2:M:221:LEU:HG	2.18	0.44
2:M:250:ARG:HG2	8:M:1251:HOH:O	2.18	0.44
2:M:364:GLU:HG2	8:M:1471:HOH:O	2.17	0.44
2:M:625:LEU:HD13	2:M:639:GLN:O	2.18	0.44
2:M:695:LEU:HD22	2:M:832:LYS:HB3	2.00	0.44
2:M:752:GLY:O	3:N:679:ARG:HG2	2.18	0.44
2:M:1032:PHE:CE2	2:M:1052:MET:HG2	2.52	0.44
3:N:12:LEU:HD23	3:N:13:ALA:N	2.26	0.44
3:N:14:SER:H	3:N:17:LYS:HZ2	1.62	0.44
3:N:85:VAL:HG12	3:N:89:ARG:NE	2.33	0.44
3:N:119:SER:CB	3:N:123:LEU:H	2.27	0.44
3:N:459:GLU:HA	8:N:9127:HOH:O	2.17	0.44
3:N:702:LEU:HD23	3:N:745:MET:HE1	1.99	0.44
3:N:907:GLU:HG2	3:N:908:LYS:H	1.81	0.44
3:N:1123:PHE:HA	3:N:1135:ARG:N	2.32	0.44
3:N:1493:LYS:HA	3:N:1493:LYS:HZ2	1.82	0.44
4:O:10:PHE:CE2	4:O:16:LYS:HG3	2.53	0.44
4:O:33:HIS:HB2	4:O:37:ASN:HD21	1.80	0.44
5:P:133:ALA:HB2	5:P:142:ARG:CZ	2.48	0.44
1:A:107:LYS:HB3	8:A:463:HOH:O	2.18	0.44
1:B:57:TYR:CE1	1:B:161:ARG:HB3	2.53	0.44
1:B:170:VAL:O	1:B:170:VAL:HG23	2.17	0.44
2:C:31:GLN:HB3	2:C:71:TYR:OH	2.16	0.44
2:C:108:ILE:HG12	8:C:1205:HOH:O	2.18	0.44
2:C:208:ALA:HA	2:C:221:LEU:HD21	1.99	0.44
2:C:577:PRO:HG3	2:C:993:PHE:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:601:GLY:HA3	2:C:615:TYR:HA	1.99	0.44
2:C:722:ILE:HG23	2:C:805:ARG:NH2	2.30	0.44
2:C:778:PHE:HB3	8:C:1664:HOH:O	2.18	0.44
2:C:902:ILE:HD13	8:C:1742:HOH:O	2.18	0.44
2:C:916:GLU:O	2:C:919:ALA:HB3	2.18	0.44
2:C:1049:LEU:HG	2:C:1053:LEU:HD11	1.99	0.44
3:D:135:LEU:HA	3:D:453:ASP:O	2.18	0.44
3:D:611:GLN:CG	5:F:326:ASP:HB2	2.46	0.44
3:D:780:LYS:NZ	8:D:9079:HOH:O	2.48	0.44
3:D:783:ARG:NH2	3:D:1029:ARG:CZ	2.81	0.44
3:D:799:LYS:N	3:D:826:PRO:HG2	2.32	0.44
3:D:910:SER:O	3:D:913:ASP:HB2	2.18	0.44
3:D:955:VAL:HB	3:D:1011:PHE:CE1	2.46	0.44
3:D:1122:LEU:HD11	3:D:1186:VAL:HG23	1.99	0.44
3:D:1379:VAL:HA	3:D:1420:LEU:HB3	1.99	0.44
4:E:37:ASN:HD22	4:E:89:MET:HE2	1.83	0.44
5:F:287:THR:O	5:F:289:GLU:N	2.51	0.44
5:F:295:MET:HB3	5:F:299:TRP:CG	2.52	0.44
5:F:361:LEU:HD13	5:F:366:ALA:HB2	1.99	0.44
1:K:69:PRO:HA	2:M:607:ASP:OD2	2.17	0.44
2:M:474:VAL:HG13	2:M:530:GLU:C	2.43	0.44
2:M:577:PRO:HD3	8:M:1226:HOH:O	2.17	0.44
2:M:783:ARG:C	2:M:785:VAL:H	2.25	0.44
2:M:943:VAL:HG11	2:M:973:VAL:CG2	2.48	0.44
2:M:1042:ALA:HB1	3:N:710:ARG:CD	2.48	0.44
2:M:1049:LEU:O	2:M:1053:LEU:HD12	2.17	0.44
2:M:1105:LYS:O	2:M:1107:ASN:N	2.50	0.44
3:N:119:SER:H	3:N:123:LEU:CB	2.28	0.44
3:N:448:GLU:CD	3:N:448:GLU:H	2.25	0.44
3:N:664:LYS:HE3	3:N:693:GLU:OE1	2.18	0.44
3:N:1020:LEU:HA	3:N:1023:MET:HE3	2.00	0.44
3:N:1109:GLU:CG	3:N:1202:GLN:H	2.31	0.44
3:N:1231:GLU:HB3	3:N:1232:PRO:HD3	2.00	0.44
3:N:1302:GLU:OE2	3:N:1304:LYS:HG3	2.17	0.44
4:O:50:THR:HB	8:O:4472:HOH:O	2.18	0.44
5:P:376:ILE:HB	8:P:4564:HOH:O	2.18	0.44
1:A:150:TYR:HD1	2:C:696:LYS:HD3	1.83	0.43
1:A:218:LEU:HD23	1:B:222:LEU:CD2	2.44	0.43
1:B:27:PRO:C	1:B:28:LEU:HD23	2.42	0.43
2:C:162:ILE:HD12	2:C:172:ILE:CB	2.46	0.43
2:C:305:PRO:HB3	2:C:308:ARG:NH2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:786:LYS:HA	8:C:1481:HOH:O	2.17	0.43
2:C:861:LEU:HD23	2:C:863:ASP:H	1.83	0.43
2:C:873:PRO:HG2	3:D:947:ILE:CD1	2.43	0.43
2:C:927:GLY:HA2	2:C:930:LYS:HE3	1.99	0.43
2:C:961:GLU:HG3	8:C:1364:HOH:O	2.18	0.43
3:D:34:TYR:OH	5:F:261:PRO:HD2	2.18	0.43
3:D:573:MET:CE	5:F:210:LEU:HB3	2.39	0.43
3:D:639:LEU:HD22	3:D:766:ALA:CB	2.48	0.43
3:D:1098:LEU:HD12	3:D:1098:LEU:N	2.33	0.43
3:D:1135:ARG:NH1	3:D:1357:ARG:HH12	2.16	0.43
3:D:1223:ILE:H	3:D:1223:ILE:CD1	2.25	0.43
4:E:14:ASP:OD1	4:E:14:ASP:N	2.46	0.43
1:K:42:ARG:NH1	2:M:857:ASP:HB3	2.30	0.43
1:K:58:ILE:HD13	1:K:140:MET:HB2	2.00	0.43
1:L:75:VAL:O	1:L:79:ILE:HG23	2.17	0.43
1:L:176:ARG:HG3	1:L:200:TRP:CE3	2.52	0.43
2:M:47:ALA:HB3	2:M:344:PHE:CE1	2.53	0.43
2:M:176:VAL:O	2:M:178:PRO:HD3	2.17	0.43
2:M:566:THR:HG22	2:M:566:THR:O	2.18	0.43
2:M:761:PHE:HB3	8:M:1358:HOH:O	2.17	0.43
2:M:1087:VAL:HG23	3:N:524:LEU:CD2	2.48	0.43
3:N:136:ASP:HB2	3:N:137:PRO:HD3	1.98	0.43
3:N:177:ALA:HB1	3:N:199:LEU:HB3	2.00	0.43
3:N:637:LEU:HD12	3:N:641:GLN:OE1	2.18	0.43
3:N:783:ARG:HE	3:N:1029:ARG:HG3	1.83	0.43
3:N:1026:SER:C	3:N:1028:ALA:H	2.24	0.43
3:N:1350:GLU:O	3:N:1354:LYS:HG2	2.18	0.43
5:P:101:GLU:O	5:P:105:LYS:HG3	2.18	0.43
5:P:133:ALA:O	5:P:137:GLY:O	2.36	0.43
1:A:51:THR:HA	1:A:145:ASP:O	2.18	0.43
1:A:99:LEU:HB3	1:A:114:PHE:CD2	2.53	0.43
1:A:219:ARG:NE	1:B:219:ARG:HG2	2.33	0.43
2:C:65:VAL:HB	2:C:101:ILE:HB	2.00	0.43
2:C:338:GLU:HA	2:C:341:THR:CG2	2.46	0.43
2:C:754:ILE:HD13	2:C:791:ARG:CD	2.48	0.43
3:D:131:LYS:HA	3:D:456:MET:HG3	2.00	0.43
3:D:178:LEU:CD1	3:D:200:ASP:H	2.32	0.43
3:D:530:VAL:HG12	3:D:531:ASP:N	2.32	0.43
3:D:631:ILE:O	3:D:632:VAL:HG23	2.18	0.43
3:D:814:ALA:HB3	8:D:9196:HOH:O	2.17	0.43
3:D:817:GLU:O	3:D:840:LYS:NZ	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:890:VAL:HG13	3:D:926:LYS:CE	2.48	0.43
3:D:1198:TYR:HE1	8:D:9137:HOH:O	2.00	0.43
5:F:155:THR:O	5:F:159:ILE:HG13	2.17	0.43
5:F:416:ARG:HD2	5:F:419:ARG:HB3	1.98	0.43
1:K:169:ALA:HB1	1:K:171:PHE:CE1	2.53	0.43
1:L:94:LEU:HD21	1:L:119:ASP:HB2	2.01	0.43
2:M:50:GLU:OE2	2:M:345:ARG:NH1	2.52	0.43
2:M:357:GLU:HB2	8:M:1297:HOH:O	2.17	0.43
2:M:484:VAL:HG21	8:M:1124:HOH:O	2.18	0.43
2:M:603:VAL:HG23	2:M:647:GLN:O	2.17	0.43
2:M:916:GLU:HA	8:M:1178:HOH:O	2.16	0.43
3:N:163:TYR:O	3:N:447:VAL:HG21	2.18	0.43
3:N:530:VAL:HA	8:N:9503:HOH:O	2.17	0.43
3:N:560:GLN:NE2	5:P:218:GLN:NE2	2.65	0.43
3:N:644:LEU:HD12	3:N:645:PRO:CD	2.42	0.43
3:N:754:PHE:HZ	4:O:21:VAL:HG13	1.83	0.43
3:N:996:TRP:HA	3:N:996:TRP:CE3	2.53	0.43
3:N:1004:THR:OG1	3:N:1036:ARG:HG3	2.18	0.43
3:N:1353:GLN:O	3:N:1357:ARG:HD2	2.18	0.43
8:N:9109:HOH:O	5:P:319:THR:HG23	2.17	0.43
4:O:46:PRO:CB	4:O:54:LEU:HD22	2.48	0.43
5:P:130:VAL:HG21	5:P:159:ILE:HG21	2.01	0.43
1:A:107:LYS:CG	8:A:494:HOH:O	2.66	0.43
1:B:189:ARG:H	1:B:189:ARG:HG2	1.61	0.43
2:C:54:ILE:HG12	8:C:1597:HOH:O	2.19	0.43
2:C:108:ILE:H	2:C:108:ILE:HG13	1.55	0.43
2:C:688:ILE:HD12	2:C:688:ILE:N	2.33	0.43
2:C:876:VAL:HG21	3:D:949:ILE:HG13	2.00	0.43
3:D:34:TYR:CE1	3:D:35:ARG:HG3	2.53	0.43
3:D:185:VAL:CG1	3:D:191:LEU:HD21	2.48	0.43
3:D:521:PRO:O	3:D:525:ARG:HD3	2.19	0.43
3:D:911:LEU:O	3:D:912:LYS:C	2.61	0.43
4:E:57:ASP:H	4:E:58:PRO:HD3	1.83	0.43
5:F:323:ASP:HB3	5:F:325:LYS:HG3	2.00	0.43
5:F:408:LEU:HD13	5:F:411:HIS:HE1	1.83	0.43
1:K:1:MET:O	1:K:6:LEU:HB2	2.18	0.43
2:M:333:ILE:CD1	2:M:467:ILE:HG13	2.48	0.43
2:M:378:LEU:N	8:M:1288:HOH:O	2.51	0.43
2:M:523:ILE:HG23	2:M:523:ILE:O	2.18	0.43
2:M:710:ILE:HD11	2:M:758:ARG:HE	1.83	0.43
2:M:999:HIS:HE1	8:M:1359:HOH:O	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:1002:GLU:H	2:M:1002:GLU:HG3	1.42	0.43
2:M:1018:GLN:NE2	5:P:338:LEU:HD13	2.33	0.43
2:M:1052:MET:HG3	3:N:623:VAL:CG2	2.48	0.43
2:M:1075:ASP:HB2	4:O:31:LEU:HD12	1.99	0.43
3:N:553:ARG:HD2	3:N:570:GLU:CD	2.43	0.43
3:N:660:LYS:HD2	3:N:663:GLU:OE2	2.18	0.43
3:N:1051:GLU:H	3:N:1051:GLU:HG3	1.50	0.43
3:N:1197:ARG:HB3	3:N:1396:GLU:HG3	2.00	0.43
5:P:134:LYS:HE3	5:P:160:ASP:OD2	2.18	0.43
1:A:49:PRO:HB3	1:A:148:VAL:HG22	2.00	0.43
1:A:75:VAL:HA	1:A:78:ILE:HD12	1.99	0.43
1:B:48:ILE:O	1:B:49:PRO:C	2.59	0.43
1:B:101:LEU:HD12	1:B:114:PHE:CD1	2.54	0.43
2:C:127:PHE:CE1	2:C:386:PHE:HE2	2.36	0.43
2:C:289:THR:O	2:C:291:ALA:N	2.52	0.43
2:C:396:ASP:HA	2:C:633:GLN:OE1	2.18	0.43
2:C:401:LEU:HD13	2:C:587:VAL:HG11	1.99	0.43
2:C:1095:LEU:O	2:C:1096:ALA:C	2.61	0.43
3:D:119:SER:H	3:D:123:LEU:CB	2.31	0.43
3:D:369:ALA:HA	8:D:9461:HOH:O	2.19	0.43
3:D:772:PRO:HG3	3:D:1210:SER:OG	2.19	0.43
3:D:805:GLU:OE1	3:D:805:GLU:O	2.37	0.43
3:D:1382:THR:HG21	3:D:1418:LYS:CE	2.48	0.43
3:D:1472:ILE:HG22	3:D:1474:ALA:O	2.19	0.43
5:F:179:GLU:HG3	8:F:503:HOH:O	2.18	0.43
5:F:365:GLU:OE1	5:F:400:ILE:HD12	2.17	0.43
1:K:156:HIS:CD2	1:K:157:GLY:N	2.86	0.43
1:K:175:ARG:HE	1:K:175:ARG:HB2	1.64	0.43
1:K:198:ARG:H	1:K:198:ARG:HG3	1.65	0.43
1:L:101:LEU:HD21	1:L:113:ASP:HB3	1.99	0.43
2:M:15:LEU:HD21	2:M:583:LEU:HD21	2.00	0.43
2:M:196:LEU:O	2:M:199:VAL:HB	2.18	0.43
2:M:572:ILE:HG23	2:M:703:ILE:HD13	1.99	0.43
2:M:1091:GLU:HA	3:N:520:LEU:HD13	2.00	0.43
3:N:89:ARG:NH2	8:N:9103:HOH:O	2.51	0.43
3:N:759:ALA:HA	3:N:763:MET:HE2	2.00	0.43
3:N:789:LEU:O	3:N:792:ILE:HG23	2.18	0.43
3:N:1059:SER:OG	3:N:1065:LEU:HA	2.17	0.43
3:N:1485:GLN:O	4:O:75:PHE:HA	2.19	0.43
1:A:215:VAL:HG11	1:B:225:PHE:CD1	2.53	0.43
1:B:89:PHE:CD1	1:B:120:VAL:HG22	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:ILE:HA	1:B:166:PRO:HD3	1.87	0.43
1:B:223:THR:C	1:B:225:PHE:H	2.26	0.43
2:C:236:ILE:O	2:C:239:PHE:HB2	2.17	0.43
2:C:640:ARG:CB	2:C:640:ARG:HH11	2.32	0.43
2:C:1091:GLU:HG2	3:D:606:ILE:HG21	2.00	0.43
3:D:133:ILE:HD11	8:D:9474:HOH:O	2.18	0.43
3:D:525:ARG:HA	3:D:538:SER:CB	2.49	0.43
3:D:675:ARG:HA	3:D:678:GLU:CD	2.43	0.43
3:D:853:VAL:HA	3:D:858:VAL:O	2.18	0.43
3:D:1029:ARG:NH2	8:D:9488:HOH:O	2.52	0.43
3:D:1087:ARG:HG2	3:D:1087:ARG:HH11	1.83	0.43
3:D:1271:LYS:HE3	3:D:1334:GLN:NE2	2.33	0.43
1:K:229:GLN:HE21	1:K:229:GLN:HB2	1.64	0.43
2:M:186:VAL:HG23	2:M:187:ASN:N	2.26	0.43
2:M:203:ASP:OD1	2:M:206:THR:HG22	2.18	0.43
2:M:220:GLY:HA3	8:M:1170:HOH:O	2.18	0.43
2:M:512:ARG:C	8:M:1203:HOH:O	2.62	0.43
2:M:553:ASP:HA	2:M:881:ASN:HA	1.99	0.43
2:M:1018:GLN:NE2	2:M:1063:ARG:NH2	2.66	0.43
2:M:1019:GLN:OE1	3:N:621:LYS:HA	2.18	0.43
2:M:1051:GLU:CG	2:M:1056:LYS:HE3	2.40	0.43
3:N:47:GLU:HG2	8:N:9894:HOH:O	2.17	0.43
3:N:102:ILE:CG2	3:N:586:ARG:HD3	2.49	0.43
3:N:431:VAL:HG22	8:N:9550:HOH:O	2.18	0.43
3:N:514:LEU:HA	8:N:9079:HOH:O	2.18	0.43
3:N:584:ASN:HB2	3:N:602:SER:OG	2.19	0.43
3:N:657:LEU:HG	3:N:661:MET:HE2	2.00	0.43
3:N:749:VAL:HA	3:N:750:PRO:HD3	1.90	0.43
3:N:924:MET:HE1	4:O:10:PHE:CD1	2.54	0.43
4:O:54:LEU:N	8:O:4983:HOH:O	2.52	0.43
1:A:1:MET:O	1:A:6:LEU:HB2	2.18	0.43
1:A:23:PHE:O	1:A:196:THR:HA	2.18	0.43
1:A:85:LEU:HA	1:A:124:ASN:HD22	1.82	0.43
1:B:49:PRO:HA	8:B:322:HOH:O	2.19	0.43
1:B:101:LEU:HG	1:B:113:ASP:C	2.43	0.43
8:B:441:HOH:O	3:D:821:VAL:HG13	2.18	0.43
2:C:200:LEU:HD13	2:C:300:ASP:OD2	2.18	0.43
2:C:854:PRO:HD2	2:C:857:ASP:OD2	2.18	0.43
2:C:1016:ILE:HD12	3:D:526:PRO:HG2	2.00	0.43
2:C:1042:ALA:HB1	8:D:9123:HOH:O	2.18	0.43
3:D:57:GLU:HG2	3:D:58:CYS:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:606:ILE:O	3:D:613:ARG:HB2	2.18	0.43
3:D:819:GLY:HA2	8:D:9660:HOH:O	2.18	0.43
3:D:820:GLU:HG3	3:D:836:VAL:CG1	2.49	0.43
3:D:838:ARG:HG2	3:D:865:THR:OG1	2.18	0.43
3:D:1102:THR:HG22	3:D:1102:THR:O	2.19	0.43
3:D:1434:TRP:CZ3	3:D:1457:ASP:HB2	2.53	0.43
5:F:313:GLU:H	5:F:313:GLU:HG2	1.42	0.43
1:K:193:ASP:HB2	8:K:3631:HOH:O	2.19	0.43
1:L:19:GLU:O	1:L:200:TRP:HA	2.18	0.43
1:L:142:VAL:HG23	1:L:142:VAL:O	2.19	0.43
2:M:274:ARG:CD	2:M:285:LEU:HB3	2.49	0.43
2:M:654:LEU:HD13	2:M:664:GLY:N	2.33	0.43
3:N:32:ILE:O	5:P:258:ILE:HG23	2.19	0.43
3:N:210:ARG:HD3	8:N:9691:HOH:O	2.18	0.43
3:N:596:SER:OG	3:N:598:ARG:HB3	2.18	0.43
3:N:669:ASN:O	3:N:672:ALA:HB3	2.18	0.43
3:N:694:VAL:HG13	8:N:9146:HOH:O	2.18	0.43
3:N:910:SER:O	3:N:913:ASP:HB2	2.18	0.43
3:N:1237:THR:HB	3:N:1239:ARG:HH21	1.84	0.43
3:N:1425:THR:CG2	3:N:1426:LYS:N	2.82	0.43
5:P:77:THR:O	5:P:81:VAL:HG23	2.17	0.43
5:P:110:MET:HE3	5:P:111:GLU:HG3	2.00	0.43
1:A:24:VAL:HG22	1:A:196:THR:CB	2.46	0.43
2:C:23:VAL:HA	2:C:121:MET:SD	2.59	0.43
2:C:43:GLY:HA2	2:C:341:THR:OG1	2.19	0.43
2:C:588:VAL:HG21	2:C:664:GLY:O	2.17	0.43
2:C:630:ARG:HH22	2:C:707:ARG:CB	2.32	0.43
2:C:816:LYS:O	2:C:819:VAL:HB	2.19	0.43
2:C:915:LYS:O	2:C:968:LEU:HD22	2.19	0.43
2:C:938:LYS:HD3	2:C:939:ARG:NH2	2.33	0.43
2:C:1101:THR:C	2:C:1102:LEU:HD12	2.44	0.43
3:D:106:LYS:HD3	3:D:106:LYS:HA	1.83	0.43
3:D:641:GLN:O	3:D:716:PHE:HD2	2.01	0.43
3:D:677:LEU:HD21	3:D:687:VAL:HG21	2.01	0.43
3:D:699:VAL:CG2	3:D:760:ARG:HB3	2.45	0.43
3:D:965:GLU:HB2	8:D:2028:HOH:O	2.17	0.43
3:D:1106:VAL:HG21	3:D:1474:ALA:HB2	2.00	0.43
3:D:1209:LEU:C	3:D:1211:MET:N	2.76	0.43
5:F:300:ASP:CG	5:F:301:ALA:N	2.77	0.43
1:K:9:PRO:HB3	1:K:25:LEU:CG	2.48	0.43
1:L:137:ARG:HB3	1:L:137:ARG:CZ	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:56:GLU:HB2	2:M:359:MET:SD	2.59	0.43
2:M:139:GLN:NE2	2:M:334:ARG:HH11	2.02	0.43
2:M:267:TYR:O	2:M:288:ARG:HD3	2.17	0.43
2:M:936:VAL:HG22	8:M:1450:HOH:O	2.18	0.43
2:M:1049:LEU:HG	2:M:1049:LEU:O	2.16	0.43
3:N:112:ILE:HD13	3:N:461:ILE:HG21	2.00	0.43
3:N:117:ASP:HB2	3:N:495:ARG:HH21	1.78	0.43
3:N:131:LYS:HE2	3:N:568:ARG:HB3	2.01	0.43
3:N:469:ASP:HB3	8:N:9566:HOH:O	2.18	0.43
3:N:629:SER:OG	3:N:630:VAL:N	2.50	0.43
3:N:698:LYS:HA	3:N:756:GLN:HE21	1.84	0.43
3:N:1124:GLN:HA	3:N:1125:PRO:HD3	1.70	0.43
4:O:9:LEU:HD21	4:O:69:LEU:HG	2.01	0.43
5:P:104:ARG:HD3	8:P:5106:HOH:O	2.18	0.43
5:P:223:ALA:HB2	5:P:242:TRP:CB	2.49	0.43
5:P:343:ASP:O	5:P:346:THR:HB	2.18	0.43
1:A:26:GLU:CB	1:A:194:LYS:HG3	2.49	0.43
1:A:86:VAL:CG1	1:A:124:ASN:HB2	2.49	0.43
1:B:26:GLU:HG2	1:B:27:PRO:CA	2.49	0.43
1:B:143:ARG:CD	1:B:158:ILE:HG21	2.48	0.43
1:B:185:ARG:HG3	1:B:190:THR:HG22	2.01	0.43
1:B:191:ASP:O	1:B:192:LEU:HG	2.19	0.43
2:C:22:GLN:NE2	2:C:121:MET:HE2	2.34	0.43
2:C:98:LEU:HD12	2:C:98:LEU:N	2.33	0.43
2:C:974:LEU:HD11	2:C:989:VAL:HG11	2.01	0.43
3:D:32:ILE:HG22	5:F:258:ILE:HD12	2.00	0.43
3:D:210:ARG:HG3	3:D:398:ALA:N	2.32	0.43
3:D:445:ARG:HG2	3:D:445:ARG:NH1	2.33	0.43
3:D:478:LEU:HD21	3:D:500:ARG:HH22	1.77	0.43
3:D:805:GLU:HA	8:D:9801:HOH:O	2.18	0.43
3:D:907:GLU:OE1	3:D:908:LYS:N	2.52	0.43
4:E:43:GLU:H	4:E:43:GLU:CD	2.25	0.43
1:K:101:LEU:HG	1:K:113:ASP:O	2.18	0.43
1:K:152:PRO:HB3	2:M:832:LYS:NZ	2.34	0.43
1:K:228:PRO:HA	1:L:11:PHE:O	2.19	0.43
2:M:31:GLN:OE1	2:M:38:LYS:HB2	2.18	0.43
2:M:52:PHE:HB3	8:M:1173:HOH:O	2.18	0.43
2:M:89:THR:O	2:M:89:THR:HG23	2.19	0.43
2:M:139:GLN:NE2	2:M:415:PRO:HG2	2.34	0.43
2:M:289:THR:O	2:M:291:ALA:N	2.51	0.43
2:M:309:TYR:CE2	2:M:321:GLU:HB3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:352:ALA:C	2:M:355:VAL:HG12	2.44	0.43
2:M:510:ALA:HB3	2:M:513:VAL:CG2	2.49	0.43
2:M:773:LEU:HA	8:M:1485:HOH:O	2.19	0.43
2:M:925:TYR:C	2:M:925:TYR:HD1	2.26	0.43
2:M:984:GLU:O	3:N:946:GLY:HA3	2.18	0.43
2:M:1050:GLN:NE2	2:M:1079:PRO:HB2	2.33	0.43
2:M:1103:ASP:N	2:M:1107:ASN:O	2.52	0.43
3:N:704:ARG:CD	3:N:705:ALA:H	2.24	0.43
3:N:829:VAL:H	3:N:835:SER:HB2	1.83	0.43
3:N:1009:LYS:HG3	8:N:9857:HOH:O	2.18	0.43
3:N:1124:GLN:HG3	8:N:9303:HOH:O	2.19	0.43
3:N:1274:ILE:HA	8:N:9087:HOH:O	2.19	0.43
3:N:1485:GLN:NE2	4:O:79:LEU:H	2.17	0.43
4:O:41:GLU:HG3	4:O:45:ARG:NH1	2.34	0.43
4:O:67:GLU:OE1	4:O:73:LEU:HD11	2.18	0.43
5:P:337:HIS:CD2	5:P:337:HIS:N	2.86	0.43
5:P:340:SER:O	5:P:342:VAL:N	2.51	0.43
1:B:138:LEU:HB2	8:B:373:HOH:O	2.18	0.43
2:C:10:ARG:HA	2:C:10:ARG:HD3	1.68	0.43
2:C:29:ALA:CB	2:C:337:GLY:HA2	2.49	0.43
2:C:77:PRO:HD2	2:C:91:GLN:O	2.19	0.43
2:C:334:ARG:HB2	2:C:339:LEU:HD11	2.00	0.43
2:C:480:THR:HG22	2:C:482:GLU:N	2.31	0.43
2:C:640:ARG:HA	2:C:641:PRO:HD3	1.90	0.43
2:C:677:MET:HE1	2:C:983:ILE:HD13	2.00	0.43
2:C:680:ASP:HA	8:C:1147:HOH:O	2.18	0.43
2:C:745:ILE:HG13	8:C:1168:HOH:O	2.18	0.43
2:C:1010:THR:HG21	5:F:341:PRO:HB2	2.01	0.43
2:C:1059:ASP:OD2	2:C:1080:SER:N	2.48	0.43
3:D:55:ASP:HB3	3:D:56:TYR:H	1.65	0.43
3:D:1087:ARG:NH1	3:D:1234:THR:O	2.52	0.43
3:D:1144:LEU:O	3:D:1166:LEU:HG	2.18	0.43
3:D:1303:TYR:CD1	3:D:1325:LEU:HD23	2.54	0.43
3:D:1371:VAL:HG12	3:D:1375:MET:HE3	2.00	0.43
5:F:157:GLU:HG3	8:F:479:HOH:O	2.18	0.43
1:L:12:THR:OG1	1:L:24:VAL:HB	2.19	0.43
2:M:6:PHE:CD1	2:M:909:ALA:HB2	2.53	0.43
2:M:443:THR:HA	2:M:444:PRO:HD3	1.80	0.43
2:M:570:PRO:HA	8:M:1348:HOH:O	2.18	0.43
2:M:582:GLY:N	2:M:584:GLU:OE2	2.48	0.43
2:M:794:PRO:HB2	2:M:1027:PHE:CZ	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:1115:LEU:CG	3:N:85:VAL:HG13	2.49	0.43
3:N:87:ARG:HD2	3:N:88:TYR:CE2	2.50	0.43
3:N:185:VAL:HG12	3:N:191:LEU:HD21	2.01	0.43
3:N:397:LYS:HE3	8:N:9313:HOH:O	2.18	0.43
3:N:441:ARG:O	3:N:443:VAL:N	2.52	0.43
3:N:522:PRO:HA	3:N:525:ARG:NH1	2.34	0.43
3:N:760:ARG:HB2	4:O:3:GLU:OE2	2.19	0.43
3:N:781:PRO:HG2	3:N:911:LEU:HD23	2.01	0.43
3:N:898:GLU:HB3	3:N:921:ARG:NH2	2.34	0.43
3:N:1300:SER:HB3	8:N:9965:HOH:O	2.18	0.43
3:N:1413:THR:HG21	8:N:9344:HOH:O	2.18	0.43
1:B:7:LYS:HD3	8:B:328:HOH:O	2.19	0.43
2:C:52:PHE:HB3	8:C:1475:HOH:O	2.18	0.43
2:C:102:HIS:HD2	2:C:365:ASP:OD2	2.02	0.43
2:C:443:THR:HA	2:C:444:PRO:HD3	1.81	0.43
2:C:744:ARG:HA	8:C:1168:HOH:O	2.18	0.43
2:C:975:TYR:N	2:C:975:TYR:CD1	2.86	0.43
3:D:154:THR:HG22	3:D:157:GLU:OE2	2.19	0.43
3:D:421:LEU:HD12	3:D:435:VAL:CG1	2.49	0.43
3:D:427:VAL:CB	3:D:435:VAL:HB	2.49	0.43
3:D:464:LEU:O	3:D:468:LEU:HG	2.19	0.43
3:D:508:ARG:HG2	3:D:508:ARG:HH11	1.84	0.43
3:D:566:ILE:HD13	5:F:217:ASN:HB3	2.01	0.43
3:D:708:LEU:HD23	3:D:708:LEU:HA	1.82	0.43
5:F:225:GLU:HG3	5:F:226:LYS:HG3	2.01	0.43
1:K:48:ILE:HG22	1:K:173:PRO:HD2	2.00	0.43
1:K:112:ARG:HH22	1:K:126:ASP:HB2	1.83	0.43
1:K:212:ASN:O	1:K:215:VAL:HG23	2.19	0.43
1:L:62:LEU:HD22	1:L:63:HIS:HE1	1.83	0.43
2:M:430:VAL:HG13	3:N:1075:HIS:ND1	2.34	0.43
2:M:666:LEU:HD12	2:M:667:ALA:H	1.84	0.43
2:M:1115:LEU:CB	3:N:85:VAL:HG13	2.49	0.43
3:N:493:ARG:NH1	3:N:1390:LEU:N	2.67	0.43
3:N:828:LYS:N	3:N:828:LYS:HD3	2.33	0.43
3:N:1377:LYS:HB3	3:N:1378:TYR:CE1	2.53	0.43
3:N:1476:THR:OG1	4:O:20:THR:HG21	2.19	0.43
5:P:88:ILE:O	5:P:92:PRO:HG3	2.19	0.43
5:P:278:LEU:HB3	5:P:286:PRO:CG	2.48	0.43
1:A:9:PRO:HB3	1:A:25:LEU:HD21	2.01	0.42
1:A:229:GLN:HE21	1:A:229:GLN:HB2	1.58	0.42
1:B:33:GLY:O	1:B:195:LEU:HD22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:ALA:HB3	1:B:124:ASN:O	2.19	0.42
1:B:186:LEU:HD23	1:B:186:LEU:C	2.44	0.42
2:C:103:LYS:HE2	8:C:1421:HOH:O	2.19	0.42
2:C:185:LYS:HE3	8:C:1838:HOH:O	2.19	0.42
2:C:892:LEU:HD12	2:C:892:LEU:O	2.19	0.42
2:C:1083:GLU:O	2:C:1087:VAL:HB	2.19	0.42
8:C:1550:HOH:O	3:D:88:TYR:HB2	2.17	0.42
3:D:28:LYS:O	3:D:43:GLY:HA2	2.19	0.42
3:D:500:ARG:HD2	8:D:9527:HOH:O	2.18	0.42
3:D:1107:VAL:O	3:D:1218:GLY:N	2.49	0.42
4:E:67:GLU:HG3	4:E:67:GLU:H	1.73	0.42
5:F:132:ARG:HG3	8:F:754:HOH:O	2.19	0.42
1:L:23:PHE:CE1	1:L:208:LEU:HD13	2.54	0.42
2:M:34:VAL:CG1	2:M:38:LYS:HG3	2.49	0.42
2:M:68:PHE:HZ	2:M:71:TYR:HB3	1.84	0.42
2:M:106:GLY:C	2:M:107:LEU:HD23	2.43	0.42
2:M:121:MET:HE2	2:M:125:GLY:O	2.19	0.42
2:M:157:ARG:HD3	2:M:158:TYR:N	2.34	0.42
2:M:244:PRO:CD	2:M:245:GLY:N	2.82	0.42
2:M:650:ARG:HB2	8:M:1333:HOH:O	2.17	0.42
2:M:1016:ILE:HD13	2:M:1016:ILE:H	1.83	0.42
2:M:1103:ASP:CG	2:M:1104:GLU:H	2.27	0.42
3:N:104:PHE:HE2	3:N:1448:THR:HA	1.84	0.42
3:N:125:GLN:NE2	8:N:9189:HOH:O	2.50	0.42
3:N:552:ASN:O	3:N:556:LYS:HD3	2.19	0.42
3:N:794:GLN:NE2	3:N:795:VAL:O	2.52	0.42
3:N:1136:LYS:HG3	3:N:1139:ASP:HB2	2.01	0.42
3:N:1435:LEU:HB2	3:N:1457:ASP:OD2	2.19	0.42
1:A:101:LEU:HB2	1:A:114:PHE:CD2	2.54	0.42
1:A:224:TYR:CD2	1:B:9:PRO:HG2	2.54	0.42
2:C:219:GLN:HA	2:C:222:MET:SD	2.58	0.42
2:C:321:GLU:H	2:C:321:GLU:HG2	1.57	0.42
2:C:676:ILE:HG23	2:C:676:ILE:O	2.18	0.42
2:C:834:GLN:HB3	8:C:1816:HOH:O	2.19	0.42
2:C:897:LEU:HD11	2:C:920:GLN:HG2	2.01	0.42
2:C:1105:LYS:C	2:C:1107:ASN:HD22	2.28	0.42
3:D:413:ASP:OD1	3:D:421:LEU:HD22	2.18	0.42
3:D:690:ALA:O	3:D:693:GLU:HB3	2.19	0.42
3:D:828:LYS:HD2	3:D:862:ASP:OD2	2.19	0.42
3:D:1057:VAL:HA	3:D:1069:GLU:HG2	2.00	0.42
3:D:1156:LEU:HG	3:D:1177:ALA:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:84:TYR:CD2	5:F:192:LEU:HD13	2.54	0.42
5:F:309:LYS:O	5:F:312:GLN:HG3	2.19	0.42
5:F:316:SER:HB2	5:F:319:THR:HG1	1.84	0.42
5:F:343:ASP:O	5:F:346:THR:HB	2.18	0.42
5:F:393:THR:O	5:F:397:ILE:HG13	2.19	0.42
1:L:23:PHE:CE1	1:L:208:LEU:HD22	2.55	0.42
2:M:400:PRO:HB3	8:M:1744:HOH:O	2.18	0.42
2:M:595:LEU:HD22	2:M:625:LEU:CD2	2.49	0.42
2:M:822:VAL:HG21	2:M:824:ARG:HH21	1.84	0.42
2:M:1033:GLY:O	2:M:1037:VAL:HG23	2.19	0.42
3:N:134:VAL:HG21	8:N:9491:HOH:O	2.19	0.42
3:N:510:GLU:CD	3:N:510:GLU:H	2.27	0.42
3:N:737:ASN:N	8:N:9095:HOH:O	2.52	0.42
3:N:1241:PHE:H	3:N:1241:PHE:HD1	1.67	0.42
5:P:372:ARG:HA	8:P:3689:HOH:O	2.18	0.42
1:B:58:ILE:HD12	1:B:140:MET:HE3	2.01	0.42
2:C:91:GLN:HA	2:C:119:PRO:HA	2.02	0.42
2:C:238:LEU:HD23	2:C:241:LEU:HB3	2.01	0.42
2:C:254:VAL:O	2:C:257:VAL:HG23	2.18	0.42
2:C:430:VAL:O	2:C:430:VAL:HG13	2.19	0.42
2:C:460:ARG:HH11	2:C:460:ARG:CB	2.26	0.42
2:C:571:LEU:HD21	2:C:700:TYR:HD2	1.84	0.42
2:C:607:ASP:HB3	2:C:610:ARG:H	1.84	0.42
2:C:708:TYR:H	2:C:708:TYR:HD1	1.67	0.42
2:C:1034:GLU:CA	2:C:1037:VAL:HG23	2.49	0.42
3:D:31:THR:HB	3:D:32:ILE:H	1.56	0.42
3:D:34:TYR:O	3:D:35:ARG:C	2.61	0.42
3:D:475:LYS:O	3:D:479:GLU:HG2	2.20	0.42
3:D:561:GLY:HA3	5:F:184:ARG:NH1	2.33	0.42
3:D:759:ALA:O	3:D:763:MET:HB3	2.19	0.42
3:D:917:GLN:NE2	3:D:917:GLN:HA	2.34	0.42
3:D:957:PRO:CD	3:D:1007:VAL:HG12	2.49	0.42
3:D:994:GLN:O	3:D:998:GLU:HG3	2.20	0.42
3:D:1256:LEU:O	3:D:1257:PRO:C	2.61	0.42
4:E:70:THR:HG22	4:E:71:GLY:N	2.34	0.42
5:F:368:VAL:HG13	5:F:388:ALA:O	2.20	0.42
1:L:51:THR:HA	1:L:145:ASP:O	2.19	0.42
1:L:179:PHE:HB2	1:L:195:LEU:HD11	2.00	0.42
2:M:184:MET:HB2	2:M:193:LEU:HD12	2.01	0.42
2:M:287:GLY:O	2:M:288:ARG:C	2.61	0.42
2:M:362:GLY:HA3	2:M:367:LEU:CD2	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:440:PRO:HG2	2:M:441:VAL:HG23	2.00	0.42
2:M:473:ARG:NH2	8:M:1124:HOH:O	2.52	0.42
2:M:732:ALA:O	2:M:735:ARG:HG3	2.19	0.42
2:M:959:PRO:O	2:M:963:LEU:HD23	2.19	0.42
3:N:78:VAL:O	3:N:78:VAL:HG12	2.19	0.42
3:N:168:THR:O	3:N:393:ILE:N	2.52	0.42
3:N:471:GLU:CD	3:N:503:LEU:HD11	2.44	0.42
3:N:675:ARG:O	3:N:678:GLU:HG2	2.19	0.42
3:N:681:ARG:HB3	3:N:681:ARG:HH11	1.84	0.42
3:N:850:LEU:H	3:N:850:LEU:CD1	2.23	0.42
3:N:959:GLU:CD	3:N:959:GLU:H	2.27	0.42
3:N:1047:LYS:HB3	3:N:1048:PRO:HD2	2.01	0.42
3:N:1106:VAL:O	3:N:1108:ARG:HG2	2.20	0.42
3:N:1123:PHE:CD1	3:N:1134:LEU:HA	2.54	0.42
3:N:1145:TYR:CE2	3:N:1168:MET:HB2	2.54	0.42
3:N:1256:LEU:O	3:N:1257:PRO:C	2.62	0.42
3:N:1262:LEU:CD2	3:N:1351:GLU:HG3	2.50	0.42
5:P:419:ARG:O	5:P:421:PHE:N	2.52	0.42
8:B:441:HOH:O	3:D:821:VAL:HG22	2.19	0.42
2:C:437:ARG:HG2	2:C:467:ILE:O	2.20	0.42
2:C:557:ARG:NE	2:C:560:MET:HE1	2.35	0.42
2:C:704:HIS:CG	2:C:831:ARG:HH21	2.37	0.42
2:C:707:ARG:HG3	2:C:826:TYR:CE1	2.54	0.42
2:C:712:ALA:HB1	2:C:820:ARG:NH1	2.33	0.42
2:C:925:TYR:C	2:C:925:TYR:HD1	2.28	0.42
2:C:1094:ALA:HB1	3:D:603:LEU:CD1	2.49	0.42
3:D:145:VAL:HG11	8:D:9724:HOH:O	2.18	0.42
3:D:163:TYR:O	3:D:447:VAL:HG21	2.19	0.42
3:D:164:GLY:O	3:D:165:LYS:C	2.62	0.42
3:D:507:ASN:HA	3:D:507:ASN:HD22	1.65	0.42
3:D:525:ARG:N	3:D:526:PRO:HD3	2.35	0.42
3:D:530:VAL:CG1	3:D:531:ASP:H	2.32	0.42
3:D:556:LYS:HD2	8:D:9348:HOH:O	2.19	0.42
3:D:655:PRO:HA	3:D:658:LEU:HD12	2.01	0.42
3:D:864:VAL:HG23	8:D:9288:HOH:O	2.18	0.42
3:D:1020:LEU:HD21	3:D:1038:LEU:HD13	2.01	0.42
3:D:1199:GLY:N	8:D:9253:HOH:O	2.51	0.42
3:D:1220:ALA:O	3:D:1224:VAL:HG23	2.19	0.42
3:D:1425:THR:CG2	3:D:1426:LYS:N	2.82	0.42
5:F:262:VAL:O	5:F:266:GLU:HG3	2.17	0.42
1:L:161:ARG:HG3	8:L:3450:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:239:PHE:HE1	8:M:1543:HOH:O	2.02	0.42
2:M:549:PHE:CE2	2:M:886:LEU:HD12	2.55	0.42
2:M:652:GLY:HA2	8:M:1180:HOH:O	2.19	0.42
2:M:750:LYS:HG3	2:M:751:PRO:HD2	2.01	0.42
3:N:536:ALA:CA	5:P:315:VAL:O	2.68	0.42
3:N:759:ALA:HA	3:N:763:MET:CE	2.49	0.42
3:N:1007:VAL:CG2	3:N:1008:PHE:N	2.82	0.42
3:N:1112:CYS:CA	3:N:1195:GLN:HE22	2.31	0.42
3:N:1365:ASP:OD2	3:N:1365:ASP:N	2.53	0.42
5:P:113:ILE:HG23	5:P:127:ILE:HG22	2.01	0.42
2:C:1005:MET:HE3	3:D:648:MET:HE3	2.00	0.42
3:D:47:GLU:H	3:D:47:GLU:HG2	1.71	0.42
3:D:112:ILE:HD13	3:D:461:ILE:HG21	2.01	0.42
3:D:129:PHE:CD2	3:D:587:ARG:CZ	3.03	0.42
3:D:421:LEU:HD12	3:D:435:VAL:HG11	2.01	0.42
3:D:669:ASN:O	3:D:672:ALA:HB3	2.19	0.42
3:D:817:GLU:HB2	3:D:839:LEU:CD1	2.50	0.42
3:D:850:LEU:HD22	3:D:884:ARG:NH2	2.33	0.42
3:D:1037:GLN:OE1	3:D:1042:ARG:NE	2.52	0.42
3:D:1120:VAL:HA	3:D:1121:PRO:HD3	1.83	0.42
3:D:1209:LEU:HD23	3:D:1210:SER:H	1.83	0.42
3:D:1432:LYS:HG3	3:D:1433:SER:H	1.83	0.42
5:F:372:ARG:HD3	8:F:635:HOH:O	2.20	0.42
1:L:24:VAL:HG22	1:L:196:THR:OG1	2.20	0.42
2:M:131:GLY:N	8:M:1593:HOH:O	2.53	0.42
2:M:507:ARG:HH11	2:M:507:ARG:CB	2.25	0.42
2:M:572:ILE:HD11	2:M:701:THR:CG2	2.49	0.42
2:M:577:PRO:HA	2:M:993:PHE:HD2	1.83	0.42
2:M:754:ILE:HD13	2:M:791:ARG:HD3	2.01	0.42
2:M:1086:ARG:CB	2:M:1112:PHE:HE2	2.32	0.42
3:N:52:PRO:HG2	3:N:78:VAL:HG13	2.00	0.42
3:N:115:LEU:HD13	3:N:499:VAL:HG22	2.01	0.42
3:N:553:ARG:HD2	3:N:570:GLU:OE2	2.19	0.42
3:N:639:LEU:N	3:N:729:HIS:CD2	2.87	0.42
3:N:700:VAL:HG22	3:N:718:PRO:HG3	2.01	0.42
3:N:888:GLU:HA	3:N:891:GLU:OE1	2.19	0.42
3:N:1142:ALA:HB1	3:N:1365:ASP:OD2	2.19	0.42
3:N:1395:LEU:C	3:N:1395:LEU:HD13	2.45	0.42
3:N:1485:GLN:NE2	4:O:79:LEU:N	2.68	0.42
1:B:13:VAL:HG12	1:B:14:ARG:N	2.34	0.42
1:B:133:GLU:HG3	1:B:134:GLU:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:135:VAL:N	2:C:393:GLN:O	2.50	0.42
2:C:235:LEU:HD11	8:C:1777:HOH:O	2.20	0.42
2:C:421:GLU:HG3	8:C:1723:HOH:O	2.18	0.42
2:C:710:ILE:HD12	2:C:790:LEU:HB2	2.01	0.42
2:C:751:PRO:HA	2:C:792:VAL:HG12	2.01	0.42
2:C:1115:LEU:HB3	3:D:85:VAL:HG12	2.00	0.42
3:D:49:ILE:HB	3:D:50:PHE:CE1	2.55	0.42
3:D:171:LEU:HD11	3:D:388:HIS:CB	2.50	0.42
3:D:178:LEU:HD11	8:D:9071:HOH:O	2.19	0.42
3:D:183:GLU:HG3	8:D:9600:HOH:O	2.19	0.42
3:D:478:LEU:HD22	3:D:1388:ARG:NH2	2.35	0.42
3:D:502:PHE:CE1	3:D:509:PRO:HB3	2.54	0.42
3:D:650:LEU:HD22	3:D:688:TRP:CH2	2.54	0.42
3:D:678:GLU:HG3	3:D:679:ARG:HG3	2.01	0.42
3:D:817:GLU:HG3	3:D:840:LYS:HZ1	1.85	0.42
3:D:1086:LEU:HB2	8:D:9637:HOH:O	2.20	0.42
3:D:1109:GLU:CG	3:D:1202:GLN:H	2.33	0.42
3:D:1259:VAL:O	3:D:1263:PHE:HD1	2.02	0.42
5:F:113:ILE:HG23	5:F:127:ILE:HG22	2.00	0.42
1:K:19:GLU:CD	1:K:19:GLU:N	2.78	0.42
1:L:134:GLU:HA	8:L:3583:HOH:O	2.20	0.42
1:L:176:ARG:HH12	3:N:884:ARG:HD3	1.84	0.42
2:M:44:ILE:O	2:M:48:PHE:HB2	2.18	0.42
2:M:101:ILE:HG22	2:M:102:HIS:H	1.84	0.42
2:M:183:SER:HB2	2:M:190:LYS:HG2	2.00	0.42
2:M:240:THR:HG23	8:M:1647:HOH:O	2.19	0.42
2:M:345:ARG:HA	2:M:348:LEU:HB2	2.02	0.42
2:M:363:SER:HB3	8:M:1471:HOH:O	2.20	0.42
2:M:511:GLU:H	2:M:511:GLU:HG2	1.63	0.42
2:M:554:ASP:OD2	2:M:556:ASN:HB3	2.19	0.42
2:M:914:ILE:CD1	2:M:918:LEU:HD13	2.48	0.42
2:M:1067:TYR:CE2	5:P:342:VAL:HA	2.55	0.42
3:N:65:ARG:HA	3:N:65:ARG:HD2	1.85	0.42
3:N:860:LEU:HD23	3:N:877:PRO:HB2	2.00	0.42
3:N:1209:LEU:CD2	3:N:1210:SER:H	2.29	0.42
3:N:1478:SER:C	3:N:1480:PHE:N	2.78	0.42
5:P:338:LEU:HG	8:P:2822:HOH:O	2.19	0.42
1:A:216:GLU:O	1:A:220:GLU:HG3	2.20	0.42
1:B:51:THR:HA	1:B:145:ASP:O	2.20	0.42
2:C:7:GLY:HA3	2:C:907:ASP:O	2.20	0.42
2:C:28:ARG:HG3	2:C:40:GLU:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:95:TYR:N	2:C:95:TYR:CD1	2.88	0.42
2:C:347:GLY:HA2	2:C:350:ARG:CD	2.43	0.42
2:C:388:ARG:HA	8:C:1349:HOH:O	2.19	0.42
2:C:437:ARG:NH1	2:C:488:ALA:HA	2.35	0.42
2:C:662:GLU:HB3	8:C:1359:HOH:O	2.19	0.42
3:D:10:ILE:HG13	3:D:1434:TRP:CE2	2.55	0.42
3:D:39:PRO:HB2	8:D:9084:HOH:O	2.19	0.42
3:D:501:ALA:HB1	3:D:1453:ALA:CA	2.47	0.42
3:D:916:TYR:C	3:D:916:TYR:CD2	2.97	0.42
3:D:937:TYR:HE1	8:D:9501:HOH:O	2.02	0.42
3:D:1007:VAL:O	3:D:1010:ASN:HB3	2.20	0.42
3:D:1123:PHE:CE2	3:D:1184:GLN:HA	2.55	0.42
3:D:1205:TYR:CE1	3:D:1221:VAL:CG1	3.02	0.42
5:F:348:SER:OG	5:F:349:LEU:N	2.52	0.42
1:K:41:ARG:HH11	1:K:41:ARG:HG3	1.83	0.42
1:K:46:SER:HB3	2:M:856:GLU:CG	2.49	0.42
1:L:86:VAL:HG13	1:L:86:VAL:O	2.20	0.42
1:L:101:LEU:HG	1:L:113:ASP:C	2.44	0.42
1:L:159:LYS:NZ	8:L:3366:HOH:O	2.53	0.42
2:M:239:PHE:CZ	2:M:254:VAL:HB	2.55	0.42
2:M:367:LEU:HA	2:M:371:LYS:HB2	2.01	0.42
2:M:520:GLU:HA	2:M:521:PRO:HD3	1.90	0.42
2:M:751:PRO:HA	2:M:792:VAL:HB	2.02	0.42
3:N:135:LEU:HA	3:N:453:ASP:O	2.19	0.42
3:N:171:LEU:HB2	3:N:390:PRO:CA	2.46	0.42
3:N:604:THR:C	3:N:606:ILE:N	2.77	0.42
3:N:610:LYS:CG	3:N:611:GLN:HE21	2.26	0.42
3:N:796:ARG:HG2	3:N:861:GLN:O	2.20	0.42
3:N:838:ARG:HD3	3:N:874:GLU:CG	2.50	0.42
3:N:865:THR:N	8:N:9349:HOH:O	2.52	0.42
3:N:948:THR:O	3:N:1019:PRO:CB	2.68	0.42
3:N:1127:GLU:HB3	3:N:1128:VAL:H	1.68	0.42
8:N:9099:HOH:O	4:O:84:ARG:HG2	2.20	0.42
1:A:209:GLU:HA	8:A:418:HOH:O	2.19	0.42
2:C:30:LEU:HD12	2:C:30:LEU:O	2.20	0.42
2:C:147:TYR:HE2	2:C:280:LYS:NZ	2.18	0.42
2:C:724:ARG:HH22	2:C:734:LEU:HB3	1.85	0.42
2:C:1015:LEU:HD13	5:F:334:PRO:O	2.20	0.42
3:D:474:GLU:CD	3:D:500:ARG:HE	2.27	0.42
3:D:591:VAL:CG1	3:D:597:ASP:HA	2.50	0.42
3:D:805:GLU:OE2	3:D:809:PRO:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:848:GLU:HA	3:D:851:LEU:HD12	2.02	0.42
3:D:971:LEU:CD1	3:D:992:ILE:HG23	2.50	0.42
3:D:1047:LYS:HA	3:D:1053:PHE:CZ	2.55	0.42
3:D:1132:LEU:HD12	3:D:1132:LEU:HA	1.80	0.42
3:D:1281:VAL:HG21	3:D:1313:VAL:CG2	2.50	0.42
3:D:1483:PHE:CD1	3:D:1483:PHE:N	2.88	0.42
5:F:213:ILE:HG22	5:F:217:ASN:HD21	1.84	0.42
5:F:401:GLU:HA	8:F:489:HOH:O	2.19	0.42
1:K:111:ALA:HB3	1:K:124:ASN:O	2.20	0.42
1:K:176:ARG:O	1:K:200:TRP:HE3	2.02	0.42
1:K:191:ASP:O	1:K:192:LEU:HD23	2.20	0.42
1:L:111:ALA:HB3	1:L:124:ASN:O	2.20	0.42
1:L:123:MET:HA	8:L:3100:HOH:O	2.20	0.42
1:L:140:MET:HG2	1:L:142:VAL:HG13	2.01	0.42
2:M:54:ILE:HA	8:M:1389:HOH:O	2.19	0.42
2:M:249:LYS:HB2	2:M:249:LYS:NZ	2.35	0.42
2:M:257:VAL:HA	8:M:1429:HOH:O	2.20	0.42
2:M:439:CYS:HB3	2:M:442:GLU:HB2	2.00	0.42
2:M:694:LEU:O	2:M:699:PHE:HB2	2.20	0.42
2:M:910:LYS:N	2:M:910:LYS:HD2	2.35	0.42
2:M:1021:LEU:HD22	5:P:331:ASP:O	2.20	0.42
2:M:1060:ILE:HA	2:M:1063:ARG:HE	1.85	0.42
2:M:1060:ILE:CG1	2:M:1063:ARG:HH21	2.33	0.42
3:N:12:LEU:HD22	3:N:511:TRP:HB3	2.02	0.42
3:N:71:LYS:HE3	8:N:9783:HOH:O	2.19	0.42
3:N:83:SER:N	8:N:9092:HOH:O	2.53	0.42
3:N:161:LEU:CD2	3:N:452:ILE:HG21	2.48	0.42
3:N:408:GLU:HG2	8:N:9502:HOH:O	2.19	0.42
3:N:642:CYS:HA	8:N:9469:HOH:O	2.19	0.42
3:N:1092:GLY:O	3:N:1093:TYR:C	2.63	0.42
3:N:1137:ARG:O	3:N:1138:ALA:C	2.62	0.42
3:N:1221:VAL:O	3:N:1222:GLY:C	2.63	0.42
3:N:1394:VAL:CG1	3:N:1397:LYS:HG3	2.50	0.42
2:C:452:ILE:HG13	2:C:452:ILE:O	2.19	0.42
2:C:498:GLN:CD	3:D:1068:LEU:HD12	2.44	0.42
2:C:708:TYR:HE2	2:C:793:PRO:HD2	1.84	0.42
2:C:1031:ARG:HD3	3:D:619:LEU:HD23	2.02	0.42
2:C:1090:LYS:HD3	2:C:1090:LYS:HA	1.87	0.42
3:D:15:PRO:CB	3:D:19:ARG:HH12	2.32	0.42
3:D:978:TYR:CE1	3:D:985:ASP:HA	2.55	0.42
3:D:1184:GLN:NE2	8:D:9269:HOH:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1382:THR:HA	8:D:9579:HOH:O	2.20	0.42
4:E:26:ARG:HG2	4:E:67:GLU:OE1	2.20	0.42
5:F:82:ARG:HG2	5:F:86:HIS:NE2	2.34	0.42
5:F:166:LEU:HD22	5:F:170:HIS:HB2	2.01	0.42
5:F:181:GLU:O	5:F:184:ARG:HB3	2.19	0.42
1:K:160:ASP:HB2	8:K:3421:HOH:O	2.20	0.42
1:L:108:GLU:HA	8:L:2956:HOH:O	2.20	0.42
2:M:469:THR:HG23	2:M:538:GLN:OE1	2.20	0.42
2:M:503:LEU:HD12	8:M:1190:HOH:O	2.19	0.42
2:M:922:PHE:CD2	2:M:964:LYS:HD3	2.54	0.42
2:M:1086:ARG:HB3	2:M:1112:PHE:HE2	1.84	0.42
3:N:65:ARG:HG3	3:N:66:GLN:HG2	2.00	0.42
3:N:82:LYS:HG2	5:P:337:HIS:HB3	2.01	0.42
3:N:83:SER:O	3:N:86:ARG:N	2.53	0.42
3:N:1465:ASN:HD21	3:N:1470:ARG:HD3	1.85	0.42
3:N:1485:GLN:HE21	4:O:79:LEU:N	2.17	0.42
5:P:197:SER:O	5:P:200:LYS:HB3	2.20	0.42
5:P:273:ARG:O	5:P:276:ARG:HB2	2.20	0.42
5:P:328:PHE:HD2	5:P:328:PHE:HA	1.68	0.42
5:P:329:TYR:C	5:P:331:ASP:N	2.76	0.42
1:A:121:GLU:HG2	1:A:123:MET:SD	2.60	0.42
1:B:11:PHE:C	8:B:493:HOH:O	2.63	0.42
2:C:302:VAL:O	2:C:305:PRO:HD2	2.20	0.42
2:C:346:VAL:O	2:C:350:ARG:HG3	2.20	0.42
2:C:504:GLU:CD	2:C:509:ALA:HB2	2.44	0.42
2:C:783:ARG:C	2:C:785:VAL:H	2.28	0.42
3:D:18:ILE:HD12	3:D:518:PRO:CG	2.49	0.42
3:D:120:ALA:HB1	8:D:9091:HOH:O	2.18	0.42
3:D:154:THR:HG21	3:D:156:GLU:HG2	2.01	0.42
3:D:613:ARG:O	3:D:617:ASN:HB2	2.20	0.42
3:D:671:LYS:CG	5:F:422:LEU:HA	2.46	0.42
3:D:828:LYS:HD3	3:D:828:LYS:N	2.35	0.42
3:D:860:LEU:HA	3:D:860:LEU:HD23	1.93	0.42
3:D:892:ASP:HB3	3:D:895:VAL:HB	2.01	0.42
3:D:1086:LEU:HB3	3:D:1090:ASP:OD1	2.20	0.42
3:D:1241:PHE:HB3	8:D:9758:HOH:O	2.19	0.42
3:D:1369:GLU:O	3:D:1370:ILE:C	2.62	0.42
3:D:1412:LYS:C	3:D:1414:PRO:HD3	2.45	0.42
4:E:42:PRO:HB2	4:E:43:GLU:OE2	2.20	0.42
5:F:96:LEU:HD12	5:F:97:GLU:OE2	2.20	0.42
5:F:291:ILE:HG23	5:F:304:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:26:GLU:N	1:K:26:GLU:OE2	2.53	0.42
1:L:165:ILE:O	1:L:165:ILE:HG13	2.19	0.42
2:M:18:LEU:HB2	2:M:590:ASP:HB3	2.01	0.42
2:M:513:VAL:HG23	8:M:1203:HOH:O	2.19	0.42
2:M:865:THR:HA	2:M:866:PRO:HD3	1.78	0.42
2:M:993:PHE:CE1	2:M:995:MET:HG2	2.54	0.42
2:M:1041:GLU:HG2	3:N:1462:LEU:HD13	2.01	0.42
2:M:1067:TYR:HE2	5:P:342:VAL:HA	1.85	0.42
3:N:142:LEU:HD11	8:N:9478:HOH:O	2.19	0.42
3:N:144:GLY:HA3	8:N:9078:HOH:O	2.19	0.42
3:N:221:ALA:HB1	8:N:9440:HOH:O	2.20	0.42
3:N:482:LYS:HA	3:N:489:ARG:HH21	1.85	0.42
3:N:654:LYS:HD3	3:N:674:ARG:NH2	2.32	0.42
3:N:704:ARG:HD2	3:N:705:ALA:N	2.22	0.42
5:P:133:ALA:HA	5:P:142:ARG:NH2	2.35	0.42
5:P:247:ILE:HG22	5:P:251:ILE:CD1	2.45	0.42
1:A:38:ASN:HB3	1:A:39:PRO:HD3	2.01	0.41
1:B:26:GLU:HG3	1:B:194:LYS:NZ	2.35	0.41
1:B:211:LEU:O	1:B:214:ALA:HB3	2.20	0.41
2:C:110:GLU:OE2	2:C:369:PRO:HG3	2.20	0.41
2:C:142:ARG:NH2	2:C:325:ILE:HD13	2.35	0.41
2:C:216:GLU:HG2	8:C:1241:HOH:O	2.20	0.41
2:C:462:ASP:CG	2:C:463:GLU:H	2.28	0.41
2:C:504:GLU:HG2	2:C:507:ARG:O	2.20	0.41
2:C:543:ASN:ND2	2:C:562:SER:O	2.50	0.41
2:C:864:GLY:C	8:C:1175:HOH:O	2.62	0.41
2:C:901:TYR:CE2	2:C:917:LEU:HD13	2.55	0.41
3:D:3:LYS:CD	3:D:3:LYS:H	2.33	0.41
3:D:470:LEU:HD12	3:D:508:ARG:NH2	2.34	0.41
3:D:628:ARG:HD3	8:D:9382:HOH:O	2.20	0.41
3:D:955:VAL:O	3:D:1039:CYS:HB3	2.20	0.41
3:D:984:THR:HG22	3:D:987:GLU:CD	2.45	0.41
3:D:1221:VAL:O	3:D:1222:GLY:C	2.62	0.41
3:D:1267:ARG:HH21	3:D:1331:ASP:CG	2.28	0.41
1:K:211:LEU:O	1:K:214:ALA:HB3	2.19	0.41
2:M:318:PRO:HD2	2:M:321:GLU:OE1	2.19	0.41
2:M:688:ILE:HD13	2:M:847:GLY:C	2.45	0.41
2:M:881:ASN:HD22	2:M:881:ASN:H	1.68	0.41
3:N:62:LYS:HE2	3:N:75:ARG:HH11	1.84	0.41
3:N:109:PRO:HG2	8:N:9287:HOH:O	2.20	0.41
3:N:123:LEU:HD21	8:N:9865:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:438:ASP:OD1	3:N:440:VAL:HG23	2.20	0.41
3:N:488:ARG:HB3	3:N:488:ARG:CZ	2.50	0.41
3:N:500:ARG:NH1	3:N:1388:ARG:HD2	2.35	0.41
3:N:630:VAL:HG12	3:N:631:ILE:N	2.35	0.41
3:N:972:LEU:HD12	8:N:9750:HOH:O	2.19	0.41
4:O:25:LYS:HA	4:O:28:GLN:CD	2.44	0.41
5:P:132:ARG:CZ	5:P:184:ARG:HH12	2.32	0.41
5:P:278:LEU:HB2	5:P:286:PRO:HG2	2.01	0.41
5:P:336:GLU:HG2	5:P:337:HIS:CD2	2.55	0.41
1:A:127:LEU:HD12	1:A:127:LEU:C	2.44	0.41
1:A:150:TYR:HB3	8:A:460:HOH:O	2.21	0.41
1:B:20:TYR:HD1	8:B:319:HOH:O	2.03	0.41
1:B:151:VAL:HG22	1:B:155:LYS:HZ3	1.84	0.41
2:C:115:LEU:CD2	2:C:373:VAL:HG11	2.50	0.41
2:C:287:GLY:O	2:C:288:ARG:C	2.63	0.41
2:C:412:ALA:HB2	2:C:451:LEU:HB3	2.02	0.41
2:C:862:PRO:HA	2:C:975:TYR:CE1	2.55	0.41
2:C:1115:LEU:HB3	3:D:85:VAL:CG1	2.49	0.41
3:D:50:PHE:CD2	3:D:522:PRO:HG3	2.56	0.41
3:D:447:VAL:HG23	3:D:448:GLU:N	2.35	0.41
3:D:637:LEU:HD11	3:D:642:CYS:N	2.35	0.41
3:D:729:HIS:CE1	3:D:731:LEU:HG	2.56	0.41
3:D:820:GLU:HA	3:D:825:ALA:O	2.20	0.41
3:D:1026:SER:C	3:D:1028:ALA:N	2.78	0.41
3:D:1299:PHE:CD2	3:D:1299:PHE:N	2.88	0.41
5:F:282:LEU:CD1	5:F:286:PRO:HG3	2.47	0.41
1:K:158:ILE:HD11	8:K:4141:HOH:O	2.20	0.41
1:K:173:PRO:HA	1:K:202:ASP:OD1	2.21	0.41
2:M:91:GLN:HB3	2:M:118:ILE:C	2.45	0.41
2:M:172:ILE:HG22	2:M:173:ASP:N	2.35	0.41
2:M:239:PHE:HZ	8:M:1251:HOH:O	2.01	0.41
2:M:352:ALA:HA	2:M:355:VAL:CG1	2.50	0.41
2:M:595:LEU:HD13	2:M:639:GLN:OE1	2.20	0.41
2:M:737:LEU:HD22	2:M:742:VAL:O	2.20	0.41
2:M:964:LYS:O	2:M:968:LEU:HG	2.20	0.41
2:M:984:GLU:OE1	3:N:945:SER:HA	2.20	0.41
3:N:68:PHE:HA	3:N:71:LYS:NZ	2.34	0.41
3:N:223:LEU:N	3:N:365:ASP:O	2.51	0.41
3:N:603:LEU:HA	3:N:606:ILE:HG12	2.02	0.41
3:N:827:ILE:HG23	3:N:837:GLY:HA3	2.02	0.41
3:N:853:VAL:HG22	3:N:858:VAL:HG23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:868:TYR:HB2	3:N:873:LEU:HD13	2.01	0.41
3:N:1058:ARG:HG3	3:N:1058:ARG:NH1	2.30	0.41
3:N:1283:ILE:N	3:N:1315:ASP:OD1	2.53	0.41
3:N:1304:LYS:HB3	8:N:9093:HOH:O	2.20	0.41
4:O:94:PRO:HB3	8:O:4372:HOH:O	2.20	0.41
5:P:371:LEU:O	5:P:375:LEU:HB3	2.21	0.41
1:A:63:HIS:HA	8:A:326:HOH:O	2.19	0.41
1:A:227:ASN:HB2	8:A:473:HOH:O	2.18	0.41
2:C:378:LEU:HG	2:C:382:ILE:HD12	2.03	0.41
2:C:437:ARG:NH2	2:C:469:THR:HG22	2.36	0.41
2:C:565:GLN:OE1	2:C:842:ARG:HG2	2.21	0.41
2:C:569:VAL:HG23	2:C:635:THR:HG22	2.02	0.41
2:C:620:LEU:HD13	2:C:620:LEU:N	2.36	0.41
2:C:643:VAL:HG12	2:C:644:VAL:O	2.21	0.41
2:C:837:ASP:O	2:C:848:VAL:HG13	2.19	0.41
2:C:1005:MET:O	2:C:1005:MET:HG3	2.20	0.41
3:D:156:GLU:HG3	8:D:9239:HOH:O	2.18	0.41
3:D:211:VAL:HG22	3:D:393:ILE:HG23	2.02	0.41
3:D:890:VAL:HG13	3:D:926:LYS:CD	2.50	0.41
3:D:1487:VAL:CG1	3:D:1488:ASP:N	2.84	0.41
5:F:153:PRO:CG	5:F:154:LYS:H	2.33	0.41
5:F:363:GLU:C	5:F:367:MET:HG2	2.45	0.41
5:F:370:LYS:HD2	5:F:370:LYS:O	2.19	0.41
5:F:370:LYS:NZ	5:F:371:LEU:HG	2.35	0.41
1:K:64:GLU:OE2	1:K:76:VAL:HA	2.20	0.41
1:L:81:ASN:ND2	1:L:128:HIS:O	2.53	0.41
2:M:19:THR:HG22	2:M:19:THR:O	2.20	0.41
2:M:132:ALA:HB1	2:M:632:ASN:ND2	2.36	0.41
2:M:371:LYS:HB2	8:M:1183:HOH:O	2.19	0.41
2:M:642:ARG:HG3	2:M:657:ASP:OD2	2.19	0.41
2:M:768:THR:HB	2:M:771:GLU:CB	2.49	0.41
2:M:861:LEU:HD21	2:M:925:TYR:HE2	1.85	0.41
2:M:874:LEU:O	3:N:1029:ARG:HD2	2.20	0.41
2:M:1056:LYS:O	3:N:624:ASP:HB2	2.21	0.41
3:N:30:GLU:N	8:N:9867:HOH:O	2.52	0.41
3:N:421:LEU:HD23	3:N:421:LEU:O	2.20	0.41
3:N:783:ARG:HH21	3:N:1029:ARG:HG3	1.82	0.41
3:N:974:ILE:H	3:N:974:ILE:HG13	1.75	0.41
3:N:1076:GLY:O	3:N:1079:LYS:HG3	2.20	0.41
3:N:1482:ARG:HB2	3:N:1483:PHE:CD1	2.56	0.41
4:O:54:LEU:HA	4:O:58:PRO:CG	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:156:VAL:HG23	5:P:157:GLU:N	2.36	0.41
5:P:340:SER:O	5:P:341:PRO:C	2.63	0.41
5:P:363:GLU:C	5:P:367:MET:HG2	2.44	0.41
1:A:26:GLU:HB2	1:A:194:LYS:HA	2.02	0.41
2:C:9:ILE:HD11	2:C:537:LYS:NZ	2.35	0.41
2:C:52:PHE:CD2	2:C:68:PHE:HB2	2.55	0.41
2:C:69:LEU:HD12	2:C:97:ARG:HB3	2.02	0.41
2:C:198:ARG:CZ	2:C:228:ALA:O	2.68	0.41
2:C:224:GLU:OE1	2:C:226:VAL:HG12	2.20	0.41
2:C:267:TYR:N	2:C:267:TYR:CD2	2.88	0.41
2:C:425:PHE:O	2:C:429:ASP:OD2	2.39	0.41
2:C:451:LEU:H	2:C:451:LEU:HD12	1.86	0.41
2:C:658:GLY:N	2:C:661:SER:OG	2.54	0.41
2:C:679:PHE:CZ	2:C:859:PRO:HD3	2.55	0.41
2:C:713:ARG:HG2	8:C:1811:HOH:O	2.20	0.41
2:C:909:ALA:HB1	2:C:914:ILE:CD1	2.50	0.41
3:D:150:ARG:HG3	3:D:150:ARG:NH1	2.33	0.41
3:D:191:LEU:HD11	8:D:9536:HOH:O	2.19	0.41
3:D:404:GLU:HB3	3:D:414:ARG:CD	2.51	0.41
3:D:434:ARG:HB2	3:D:447:VAL:CG2	2.51	0.41
3:D:521:PRO:HA	3:D:522:PRO:HD3	1.84	0.41
3:D:1145:TYR:HB2	3:D:1168:MET:HE1	2.02	0.41
3:D:1171:VAL:O	3:D:1175:ILE:HG13	2.21	0.41
4:E:29:GLN:CB	4:E:33:HIS:NE2	2.83	0.41
5:F:324:GLU:HA	8:F:663:HOH:O	2.19	0.41
1:K:150:TYR:CD1	2:M:696:LYS:HG2	2.55	0.41
2:M:620:LEU:HG	8:M:1346:HOH:O	2.20	0.41
2:M:821:GLU:HG2	2:M:822:VAL:N	2.35	0.41
2:M:832:LYS:HD2	8:M:1460:HOH:O	2.21	0.41
2:M:1024:LYS:HG3	8:M:1569:HOH:O	2.21	0.41
2:M:1044:GLY:N	3:N:762:GLN:OE1	2.52	0.41
3:N:10:ILE:HG13	3:N:1434:TRP:CE2	2.55	0.41
3:N:404:GLU:HB3	3:N:414:ARG:CZ	2.50	0.41
3:N:592:THR:HA	8:N:9104:HOH:O	2.20	0.41
3:N:659:LYS:O	3:N:663:GLU:HG3	2.21	0.41
3:N:770:LEU:HD12	3:N:775:GLY:O	2.21	0.41
3:N:875:THR:HG22	3:N:879:ARG:HB2	2.03	0.41
3:N:1335:LEU:HD23	3:N:1335:LEU:C	2.45	0.41
5:P:256:ARG:NE	5:P:260:ILE:HD12	2.35	0.41
5:P:392:VAL:HG12	5:P:396:ARG:HB2	2.02	0.41
1:A:29:GLU:HB3	1:A:30:ARG:H	1.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:THR:C	1:A:225:PHE:H	2.29	0.41
1:B:27:PRO:HG2	1:B:186:LEU:CD1	2.50	0.41
2:C:163:ILE:HG13	2:C:171:TRP:CH2	2.55	0.41
2:C:229:MET:HE1	8:C:1174:HOH:O	2.20	0.41
2:C:299:LYS:HD2	8:C:1273:HOH:O	2.20	0.41
2:C:335:THR:HG23	2:C:461:VAL:HG11	2.03	0.41
2:C:525:SER:O	2:C:529:VAL:HG23	2.19	0.41
2:C:557:ARG:CZ	2:C:879:ARG:HG2	2.50	0.41
2:C:693:GLU:HA	2:C:693:GLU:OE1	2.21	0.41
2:C:697:ARG:O	2:C:699:PHE:N	2.53	0.41
3:D:13:ALA:O	3:D:511:TRP:HB3	2.21	0.41
3:D:187:LYS:HD3	3:D:187:LYS:HA	1.78	0.41
3:D:566:ILE:CG1	5:F:192:LEU:HD11	2.50	0.41
3:D:688:TRP:HA	3:D:688:TRP:CE3	2.55	0.41
3:D:786:ILE:HG22	3:D:1026:SER:HB2	2.02	0.41
3:D:817:GLU:HB2	3:D:839:LEU:HD13	2.01	0.41
3:D:1063:GLU:HG3	8:D:9502:HOH:O	2.20	0.41
3:D:1211:MET:HG2	3:D:1213:ARG:H	1.85	0.41
3:D:1364:HIS:ND1	3:D:1365:ASP:N	2.67	0.41
3:D:1423:GLY:HA2	8:D:9248:HOH:O	2.19	0.41
4:E:46:PRO:HD3	8:E:180:HOH:O	2.20	0.41
4:E:93:TYR:HA	4:E:94:PRO:HD3	1.77	0.41
5:F:135:ILE:HD13	5:F:135:ILE:O	2.21	0.41
5:F:244:ARG:NH1	5:F:244:ARG:HG3	2.35	0.41
2:M:205:GLU:OE1	2:M:206:THR:N	2.53	0.41
2:M:327:HIS:O	2:M:330:ASN:HB2	2.20	0.41
2:M:601:GLY:HA3	2:M:615:TYR:HA	2.01	0.41
2:M:691:SER:HA	2:M:858:MET:HE3	2.01	0.41
2:M:909:ALA:C	2:M:910:LYS:HD2	2.45	0.41
2:M:1090:LYS:HG2	2:M:1112:PHE:HZ	1.86	0.41
8:M:1645:HOH:O	3:N:940:THR:HG23	2.21	0.41
3:N:14:SER:H	3:N:17:LYS:HZ1	1.64	0.41
3:N:42:ASP:O	3:N:49:ILE:HD12	2.21	0.41
3:N:50:PHE:CB	3:N:522:PRO:HG2	2.50	0.41
3:N:151:GLN:HE21	3:N:151:GLN:HB2	1.77	0.41
3:N:169:TYR:HA	3:N:392:SER:CB	2.50	0.41
3:N:171:LEU:HD11	3:N:388:HIS:CB	2.50	0.41
3:N:502:PHE:CE1	3:N:509:PRO:HB3	2.56	0.41
3:N:519:VAL:HG13	3:N:544:TYR:CE1	2.55	0.41
3:N:565:ILE:HD12	3:N:565:ILE:N	2.20	0.41
3:N:637:LEU:HD11	3:N:642:CYS:CA	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:702:LEU:HD23	3:N:745:MET:CE	2.51	0.41
3:N:765:SER:C	3:N:767:HIS:H	2.29	0.41
3:N:786:ILE:HD12	3:N:1028:ALA:N	2.35	0.41
3:N:1175:ILE:O	3:N:1179:GLU:HG3	2.21	0.41
5:P:262:VAL:O	5:P:265:VAL:HB	2.21	0.41
1:A:178:ALA:HB3	1:A:198:ARG:HD3	2.03	0.41
1:A:211:LEU:O	1:A:214:ALA:HB3	2.21	0.41
1:B:29:GLU:HB3	1:B:30:ARG:H	1.75	0.41
1:B:42:ARG:HG2	1:B:42:ARG:NH1	2.35	0.41
2:C:162:ILE:CB	2:C:172:ILE:HD13	2.49	0.41
2:C:207:LEU:HD13	2:C:221:LEU:HD13	2.03	0.41
2:C:332:ARG:HH11	2:C:332:ARG:CB	2.15	0.41
2:C:365:ASP:O	2:C:367:LEU:N	2.54	0.41
2:C:710:ILE:HG12	2:C:758:ARG:HE	1.86	0.41
2:C:865:THR:HA	2:C:866:PRO:HD3	1.87	0.41
3:D:397:LYS:HE2	3:D:399:ARG:NE	2.23	0.41
3:D:957:PRO:CG	3:D:1007:VAL:HG12	2.50	0.41
3:D:1106:VAL:HG12	3:D:1107:VAL:N	2.34	0.41
3:D:1208:ASP:OD1	3:D:1209:LEU:O	2.39	0.41
3:D:1262:LEU:HD23	3:D:1352:ILE:HA	2.02	0.41
3:D:1274:ILE:CD1	3:D:1334:GLN:HB3	2.50	0.41
5:F:133:ALA:O	5:F:137:GLY:O	2.38	0.41
5:F:142:ARG:NH1	5:F:150:THR:HG21	2.36	0.41
5:F:362:SER:C	5:F:364:ARG:N	2.79	0.41
1:K:65:PHE:HE1	2:M:799:ILE:HD11	1.85	0.41
1:K:97:VAL:HG12	1:K:99:LEU:HD12	2.01	0.41
1:K:109:VAL:O	1:K:129:ILE:HG12	2.21	0.41
1:L:95:GLN:HE21	1:L:95:GLN:N	2.12	0.41
1:L:100:LEU:HD12	1:L:115:LEU:HD11	2.03	0.41
2:M:139:GLN:HE21	2:M:334:ARG:NH1	2.03	0.41
2:M:305:PRO:HG3	2:M:308:ARG:CZ	2.51	0.41
2:M:383:ARG:NH2	8:M:1405:HOH:O	2.54	0.41
2:M:473:ARG:HE	2:M:531:PHE:HE1	1.67	0.41
2:M:549:PHE:HE2	2:M:887:GLU:N	2.18	0.41
2:M:1034:GLU:HA	2:M:1037:VAL:CG2	2.50	0.41
2:M:1054:THR:HB	2:M:1055:LEU:H	1.57	0.41
3:N:131:LYS:HZ3	3:N:568:ARG:HB2	1.86	0.41
3:N:539:ASP:OD2	3:N:598:ARG:NH2	2.52	0.41
3:N:1105:ILE:HD11	3:N:1374:GLN:CD	2.45	0.41
3:N:1417:TRP:CD1	3:N:1417:TRP:C	2.98	0.41
3:N:1485:GLN:H	3:N:1485:GLN:HG2	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:31:LEU:HD23	4:O:35:PHE:CD1	2.55	0.41
5:P:394:ARG:HA	5:P:397:ILE:CD1	2.37	0.41
1:B:9:PRO:HB3	1:B:25:LEU:HG	2.03	0.41
2:C:30:LEU:HB3	2:C:44:ILE:CD1	2.44	0.41
2:C:123:GLU:HA	8:C:1818:HOH:O	2.21	0.41
2:C:460:ARG:HD2	2:C:485:TYR:CD2	2.56	0.41
2:C:676:ILE:CG2	2:C:988:VAL:HG22	2.50	0.41
2:C:952:LEU:HB3	2:C:966:LEU:HD11	2.02	0.41
2:C:1086:ARG:HD3	3:D:88:TYR:HH	1.84	0.41
3:D:8:VAL:O	3:D:1434:TRP:HH2	2.04	0.41
3:D:86:ARG:O	3:D:86:ARG:HG3	2.20	0.41
3:D:587:ARG:HG2	8:D:9367:HOH:O	2.21	0.41
3:D:639:LEU:HD22	3:D:766:ALA:CA	2.50	0.41
3:D:806:PHE:O	3:D:806:PHE:CG	2.74	0.41
3:D:893:GLU:O	3:D:896:ALA:HB3	2.21	0.41
3:D:1136:LYS:HE3	3:D:1139:ASP:OD2	2.21	0.41
3:D:1353:GLN:HB3	3:D:1357:ARG:NE	2.36	0.41
3:D:1467:ILE:HD12	3:D:1467:ILE:H	1.86	0.41
5:F:113:ILE:O	5:F:116:LEU:HB2	2.21	0.41
5:F:329:TYR:HE1	8:F:541:HOH:O	2.02	0.41
1:K:85:LEU:HB2	1:K:127:LEU:HD21	2.01	0.41
1:K:197:LEU:HD23	1:K:197:LEU:N	2.33	0.41
1:L:2:LEU:HD13	1:L:3:ASP:OD1	2.21	0.41
1:L:51:THR:HG22	1:L:89:PHE:CZ	2.56	0.41
1:L:101:LEU:HD12	1:L:114:PHE:CE1	2.55	0.41
1:L:105:GLY:HA2	8:L:3583:HOH:O	2.19	0.41
2:M:86:LYS:HG3	2:M:813:VAL:HG12	2.03	0.41
2:M:425:PHE:HZ	3:N:1079:LYS:HB2	1.86	0.41
2:M:612:VAL:HG22	2:M:622:GLU:HG3	2.03	0.41
2:M:671:ASN:ND2	2:M:671:ASN:N	2.69	0.41
3:N:500:ARG:HH22	3:N:1388:ARG:HD3	1.85	0.41
3:N:783:ARG:CZ	3:N:783:ARG:HB3	2.50	0.41
3:N:1310:ARG:H	3:N:1310:ARG:HG2	1.61	0.41
5:P:142:ARG:H	5:P:142:ARG:HG2	1.63	0.41
5:P:303:ARG:NH2	8:P:3667:HOH:O	2.52	0.41
1:B:72:LYS:HB3	1:B:131:THR:OG1	2.21	0.41
2:C:25:SER:OG	2:C:337:GLY:N	2.50	0.41
2:C:34:VAL:HA	2:C:35:PRO:HD3	1.96	0.41
2:C:416:GLY:HA3	8:C:1572:HOH:O	2.21	0.41
2:C:547:ILE:HA	2:C:548:PRO:HD3	1.97	0.41
2:C:592:LEU:HD23	2:C:592:LEU:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:860:HIS:N	8:C:1448:HOH:O	2.42	0.41
2:C:873:PRO:HG2	3:D:947:ILE:O	2.20	0.41
2:C:1109:VAL:CG2	3:D:3:LYS:HG2	2.49	0.41
3:D:143:ASN:ND2	3:D:145:VAL:HG12	2.18	0.41
3:D:729:HIS:ND1	3:D:730:PRO:N	2.68	0.41
3:D:761:ILE:HD13	4:E:20:THR:HA	2.02	0.41
3:D:794:GLN:HE21	3:D:794:GLN:HB3	1.50	0.41
3:D:907:GLU:N	3:D:910:SER:OG	2.53	0.41
3:D:965:GLU:HA	3:D:968:ASP:OD2	2.21	0.41
3:D:1472:ILE:HG22	3:D:1474:ALA:N	2.35	0.41
5:F:95:THR:HG22	5:F:96:LEU:HD23	2.03	0.41
5:F:151:LEU:HB2	5:F:155:THR:OG1	2.21	0.41
5:F:192:LEU:O	5:F:192:LEU:HD23	2.21	0.41
5:F:292:ALA:HB1	5:F:299:TRP:O	2.21	0.41
1:L:51:THR:HG23	8:L:4444:HOH:O	2.20	0.41
2:M:87:ASP:HA	8:M:1593:HOH:O	2.20	0.41
2:M:137:VAL:HG22	2:M:391:LEU:O	2.20	0.41
2:M:253:ALA:O	2:M:256:TYR:HB2	2.21	0.41
2:M:899:GLN:HG3	2:M:901:TYR:OH	2.21	0.41
2:M:964:LYS:HD3	8:M:1484:HOH:O	2.20	0.41
2:M:1013:TYR:HB2	5:P:335:ASP:OD2	2.21	0.41
3:N:36:THR:O	3:N:38:LYS:N	2.51	0.41
3:N:107:ASP:O	3:N:108:VAL:C	2.64	0.41
3:N:131:LYS:HZ3	3:N:456:MET:HE3	1.85	0.41
3:N:206:ARG:O	3:N:206:ARG:HD3	2.19	0.41
3:N:600:LEU:O	3:N:601:ARG:C	2.62	0.41
3:N:704:ARG:HD3	3:N:738:ALA:HB2	2.03	0.41
3:N:820:GLU:HB2	3:N:836:VAL:HG11	2.01	0.41
3:N:826:PRO:HD2	3:N:829:VAL:HG13	2.03	0.41
3:N:960:LYS:O	3:N:964:LEU:HD12	2.20	0.41
3:N:1465:ASN:OD1	3:N:1473:PRO:HG3	2.20	0.41
4:O:5:GLY:HA2	8:O:3467:HOH:O	2.20	0.41
5:P:140:ARG:O	5:P:144:ILE:HG13	2.20	0.41
5:P:372:ARG:HA	8:P:4564:HOH:O	2.20	0.41
1:A:79:ILE:O	1:A:83:LYS:HG3	2.20	0.41
1:A:101:LEU:HG	1:A:113:ASP:C	2.46	0.41
8:B:347:HOH:O	3:D:688:TRP:HB3	2.19	0.41
2:C:166:PRO:HD3	2:C:265:ARG:NE	2.33	0.41
2:C:325:ILE:HA	8:C:1441:HOH:O	2.21	0.41
2:C:366:SER:O	2:C:371:LYS:HE3	2.20	0.41
2:C:479:VAL:HG22	2:C:508:ILE:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:881:ASN:ND2	8:C:1494:HOH:O	2.41	0.41
2:C:895:TYR:HD1	2:C:991:GLN:NE2	2.16	0.41
2:C:919:ALA:HA	8:C:1456:HOH:O	2.19	0.41
2:C:1101:THR:OG1	2:C:1109:VAL:HG12	2.21	0.41
3:D:45:PHE:O	3:D:46:ASP:C	2.64	0.41
3:D:65:ARG:CG	3:D:66:GLN:H	2.24	0.41
3:D:107:ASP:O	3:D:108:VAL:C	2.63	0.41
3:D:114:THR:HG21	3:D:498:VAL:HG11	2.01	0.41
3:D:127:LEU:CD1	3:D:461:ILE:HD11	2.42	0.41
3:D:411:THR:HG23	8:D:9458:HOH:O	2.20	0.41
3:D:461:ILE:O	3:D:465:LEU:HB2	2.19	0.41
3:D:463:GLN:O	3:D:467:GLU:HG3	2.21	0.41
3:D:470:LEU:HD22	3:D:499:VAL:HG13	2.01	0.41
3:D:569:ASN:O	3:D:573:MET:SD	2.78	0.41
3:D:619:LEU:HD23	3:D:619:LEU:C	2.45	0.41
3:D:631:ILE:HG21	3:D:745:MET:CG	2.51	0.41
3:D:667:ALA:HB2	3:D:676:MET:CE	2.38	0.41
3:D:710:ARG:NE	8:D:9123:HOH:O	2.54	0.41
3:D:762:GLN:HE21	4:E:20:THR:CB	2.33	0.41
3:D:783:ARG:NE	3:D:1029:ARG:NE	2.64	0.41
3:D:827:ILE:HB	3:D:828:LYS:HD3	2.01	0.41
3:D:916:TYR:C	3:D:916:TYR:HD2	2.28	0.41
3:D:996:TRP:CE2	3:D:1056:PRO:HG2	2.56	0.41
3:D:999:THR:O	3:D:1003:VAL:HG13	2.21	0.41
3:D:1023:MET:O	3:D:1028:ALA:HB3	2.21	0.41
3:D:1101:VAL:HG12	3:D:1374:GLN:HB3	2.03	0.41
3:D:1263:PHE:HD2	3:D:1375:MET:HE1	1.86	0.41
3:D:1300:SER:HB3	8:D:9222:HOH:O	2.20	0.41
3:D:1314:LYS:HZ1	3:D:1317:ASP:HB2	1.86	0.41
3:D:1352:ILE:HG21	3:D:1368:ILE:CG2	2.48	0.41
3:D:1353:GLN:OE1	3:D:1368:ILE:HD11	2.21	0.41
3:D:1365:ASP:O	3:D:1368:ILE:HG13	2.21	0.41
3:D:1462:LEU:HD22	3:D:1473:PRO:HD2	2.03	0.41
4:E:33:HIS:HD2	4:E:89:MET:HE2	1.86	0.41
4:E:70:THR:HG21	4:E:72:ARG:NH2	2.36	0.41
5:F:74:LYS:HD3	5:F:74:LYS:HA	1.93	0.41
5:F:84:TYR:O	5:F:88:ILE:HG13	2.20	0.41
5:F:96:LEU:HB2	5:F:97:GLU:OE2	2.21	0.41
5:F:109:GLY:O	5:F:113:ILE:HG13	2.21	0.41
5:F:352:GLU:O	5:F:356:LYS:HG3	2.21	0.41
1:K:14:ARG:CG	1:K:22:GLU:HB2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:100:LEU:HD12	8:K:3405:HOH:O	2.20	0.41
1:K:132:LEU:HD12	1:K:132:LEU:N	2.36	0.41
1:L:71:VAL:HG22	1:L:132:LEU:CD1	2.51	0.41
2:M:116:GLY:N	8:M:1773:HOH:O	2.54	0.41
2:M:144:PRO:HB2	2:M:267:TYR:HE1	1.86	0.41
2:M:340:MET:SD	2:M:344:PHE:HB2	2.61	0.41
2:M:353:ARG:HE	2:M:353:ARG:HB2	1.66	0.41
2:M:414:GLY:C	2:M:416:GLY:N	2.79	0.41
2:M:556:ASN:O	2:M:559:LEU:HB3	2.21	0.41
2:M:593:ALA:HB2	8:M:1744:HOH:O	2.20	0.41
2:M:682:TYR:HB3	2:M:689:VAL:HG22	2.02	0.41
2:M:769:PRO:HB2	3:N:65:ARG:NH1	2.36	0.41
2:M:772:ARG:HG3	2:M:773:LEU:N	2.36	0.41
2:M:807:ARG:HB3	8:M:1400:HOH:O	2.21	0.41
2:M:833:LEU:CD1	2:M:837:ASP:HB2	2.51	0.41
2:M:975:TYR:N	2:M:975:TYR:CD1	2.88	0.41
2:M:1083:GLU:O	2:M:1087:VAL:HB	2.19	0.41
2:M:1087:VAL:HG23	3:N:524:LEU:HD21	2.03	0.41
2:M:1097:LEU:HD22	2:M:1097:LEU:N	2.35	0.41
2:M:1109:VAL:CG1	3:N:5:VAL:HG22	2.51	0.41
2:M:1118:LYS:HA	3:N:23:TYR:OH	2.21	0.41
3:N:33:ASN:O	3:N:36:THR:O	2.39	0.41
3:N:110:SER:OG	3:N:113:GLY:N	2.51	0.41
3:N:112:ILE:O	3:N:116:LEU:HB2	2.21	0.41
3:N:172:PRO:HA	3:N:173:PRO:HD3	1.67	0.41
3:N:212:ARG:HD3	3:N:445:ARG:NH1	2.24	0.41
3:N:243:ALA:HB3	8:N:9487:HOH:O	2.20	0.41
3:N:443:VAL:HG12	3:N:445:ARG:HD2	2.02	0.41
3:N:638:LYS:C	3:N:729:HIS:HD2	2.29	0.41
3:N:705:ALA:CB	3:N:706:PRO:HD3	2.50	0.41
3:N:728:LEU:HD22	3:N:745:MET:CE	2.47	0.41
3:N:774:SER:HB3	3:N:1362:LYS:O	2.21	0.41
3:N:881:LEU:HD12	3:N:881:LEU:O	2.21	0.41
3:N:891:GLU:N	8:N:9462:HOH:O	2.54	0.41
3:N:948:THR:HG22	3:N:949:ILE:N	2.27	0.41
3:N:1107:VAL:HA	3:N:1200:VAL:O	2.21	0.41
3:N:1148:VAL:HG13	3:N:1163:GLY:O	2.20	0.41
3:N:1292:VAL:O	3:N:1303:TYR:HB2	2.21	0.41
3:N:1330:ILE:HD13	3:N:1347:TYR:OH	2.21	0.41
3:N:1380:GLU:HB3	3:N:1418:LYS:HB2	2.02	0.41
3:N:1437:ALA:O	3:N:1446:VAL:HG21	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:35:PHE:HZ	4:O:60:ALA:HA	1.86	0.41
4:O:47:LYS:C	4:O:54:LEU:HD13	2.45	0.41
5:P:261:PRO:HA	8:P:3364:HOH:O	2.20	0.41
5:P:338:LEU:HA	5:P:339:PRO:HD3	1.89	0.41
5:P:367:MET:N	5:P:367:MET:SD	2.94	0.41
1:A:64:GLU:OE2	1:A:76:VAL:HG13	2.21	0.41
1:B:73:GLU:HB3	1:B:77:GLU:HG2	1.98	0.41
2:C:41:ASN:ND2	2:C:41:ASN:N	2.57	0.41
2:C:101:ILE:HG23	2:C:107:LEU:CD2	2.45	0.41
2:C:137:VAL:O	2:C:391:LEU:HD11	2.21	0.41
2:C:139:GLN:HE22	2:C:415:PRO:HD3	1.86	0.41
2:C:308:ARG:HH11	2:C:308:ARG:HG2	1.85	0.41
2:C:313:LEU:HB2	2:C:321:GLU:HG3	2.03	0.41
2:C:328:LEU:H	2:C:433:THR:HG21	1.86	0.41
2:C:474:VAL:HG23	2:C:478:VAL:O	2.21	0.41
2:C:668:LEU:O	2:C:669:GLY:C	2.61	0.41
2:C:759:THR:HB	2:C:785:VAL:CG2	2.50	0.41
2:C:885:ILE:HD12	3:D:949:ILE:HB	2.02	0.41
2:C:1037:VAL:O	2:C:1041:GLU:HG3	2.20	0.41
2:C:1092:LEU:HD22	2:C:1099:VAL:CG2	2.51	0.41
3:D:120:ALA:HA	8:D:9188:HOH:O	2.20	0.41
3:D:135:LEU:HD11	3:D:139:GLY:HA3	2.02	0.41
3:D:393:ILE:HD12	3:D:393:ILE:N	2.32	0.41
3:D:573:MET:HE1	5:F:214:GLN:HG3	2.02	0.41
3:D:804:LEU:N	8:D:9497:HOH:O	2.53	0.41
3:D:1133:ARG:HG2	3:D:1134:LEU:N	2.35	0.41
3:D:1155:VAL:HG11	3:D:1177:ALA:CB	2.51	0.41
3:D:1168:MET:HA	3:D:1168:MET:HE3	2.03	0.41
3:D:1208:ASP:HB3	8:D:2063:HOH:O	2.21	0.41
3:D:1209:LEU:HB3	3:D:1211:MET:HE2	2.03	0.41
3:D:1272:ALA:CB	3:D:1326:THR:HB	2.51	0.41
3:D:1342:GLU:HA	3:D:1346:ARG:NH2	2.36	0.41
3:D:1480:PHE:HD1	3:D:1480:PHE:O	2.02	0.41
5:F:160:ASP:O	5:F:163:LEU:HB2	2.22	0.41
5:F:192:LEU:O	5:F:196:VAL:HG23	2.21	0.41
5:F:287:THR:HG22	5:F:290:GLU:OE1	2.20	0.41
1:K:100:LEU:O	1:K:115:LEU:HG	2.21	0.41
1:K:150:TYR:HA	1:K:169:ALA:O	2.21	0.41
1:L:150:TYR:HA	1:L:169:ALA:O	2.21	0.41
2:M:261:ILE:HG22	2:M:262:ALA:N	2.36	0.41
2:M:304:LEU:HG	2:M:305:PRO:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:401:LEU:HD21	2:M:565:GLN:HE21	1.86	0.41
2:M:430:VAL:CG1	3:N:1075:HIS:HA	2.51	0.41
2:M:525:SER:O	2:M:529:VAL:HG23	2.21	0.41
2:M:592:LEU:HD23	2:M:592:LEU:HA	1.85	0.41
2:M:755:LEU:HD11	2:M:792:VAL:HG22	2.03	0.41
2:M:918:LEU:HD23	2:M:968:LEU:C	2.45	0.41
3:N:501:ALA:HA	3:N:504:ASP:HB2	2.03	0.41
3:N:575:GLN:O	3:N:576:GLU:C	2.64	0.41
3:N:787:LEU:HD21	3:N:947:ILE:CD1	2.51	0.41
3:N:1173:LEU:HA	8:N:9311:HOH:O	2.21	0.41
3:N:1301:LYS:HA	3:N:1301:LYS:HD2	1.89	0.41
4:O:49:GLN:HA	4:O:51:LEU:O	2.21	0.41
1:A:95:GLN:CG	1:A:146:ARG:HH22	2.19	0.40
1:B:55:SER:OG	1:B:158:ILE:HB	2.21	0.40
1:B:106:PRO:HG3	1:B:133:GLU:O	2.22	0.40
2:C:13:ILE:HG13	2:C:458:TYR:HE2	1.86	0.40
2:C:124:ASP:OD1	2:C:126:SER:N	2.48	0.40
2:C:722:ILE:HD12	2:C:805:ARG:NH2	2.36	0.40
2:C:897:LEU:HD21	2:C:920:GLN:HB3	2.02	0.40
2:C:1018:GLN:HE21	2:C:1060:ILE:CD1	2.34	0.40
3:D:613:ARG:HA	3:D:613:ARG:HD2	1.83	0.40
3:D:900:ILE:HD12	3:D:900:ILE:O	2.21	0.40
3:D:936:TYR:HD1	8:D:9501:HOH:O	2.03	0.40
3:D:988:ARG:O	3:D:992:ILE:HG13	2.20	0.40
3:D:1047:LYS:HE3	3:D:1051:GLU:HB2	2.03	0.40
3:D:1066:THR:CG2	3:D:1069:GLU:H	2.18	0.40
3:D:1068:LEU:HD23	3:D:1068:LEU:O	2.21	0.40
3:D:1243:THR:HG22	3:D:1244:GLY:H	1.87	0.40
3:D:1330:ILE:HD12	3:D:1347:TYR:HE1	1.86	0.40
5:F:115:LYS:HG3	5:F:173:TYR:CE2	2.56	0.40
5:F:272:SER:O	5:F:276:ARG:HG3	2.21	0.40
5:F:339:PRO:HB3	5:F:343:ASP:HB2	2.02	0.40
1:L:38:ASN:C	1:L:38:ASN:HD22	2.29	0.40
1:L:48:ILE:HA	1:L:49:PRO:HD3	1.85	0.40
1:L:73:GLU:CD	1:L:73:GLU:H	2.28	0.40
1:L:145:ASP:O	1:L:171:PHE:HE1	2.05	0.40
1:L:152:PRO:HD2	1:L:155:LYS:CD	2.47	0.40
2:M:133:ASP:OD2	2:M:133:ASP:N	2.54	0.40
2:M:299:LYS:HG3	8:M:1137:HOH:O	2.21	0.40
2:M:415:PRO:HB2	2:M:418:LEU:CD1	2.52	0.40
2:M:419:THR:HA	2:M:420:ARG:NH1	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:510:ALA:CB	8:M:1203:HOH:O	2.67	0.40
2:M:575:GLN:HG2	2:M:662:GLU:OE2	2.21	0.40
2:M:753:ASP:O	2:M:792:VAL:HG23	2.20	0.40
2:M:920:GLN:HG3	8:M:1705:HOH:O	2.21	0.40
2:M:1043:TYR:HA	3:N:710:ARG:NH1	2.35	0.40
2:M:1115:LEU:N	2:M:1115:LEU:CD1	2.78	0.40
3:N:122:GLU:OE1	3:N:126:VAL:HG23	2.21	0.40
3:N:558:LEU:HB2	8:N:9625:HOH:O	2.21	0.40
3:N:650:LEU:CD1	3:N:691:LEU:HD22	2.51	0.40
3:N:866:VAL:CG1	3:N:867:ARG:N	2.84	0.40
3:N:1426:LYS:NZ	3:N:1430:SER:OG	2.54	0.40
3:N:1475:GLY:C	3:N:1477:GLY:N	2.78	0.40
1:A:63:HIS:HB3	2:C:746:GLY:CA	2.44	0.40
2:C:367:LEU:CA	2:C:371:LYS:HB2	2.52	0.40
2:C:536:PRO:HD2	2:C:537:LYS:HD2	2.03	0.40
2:C:668:LEU:O	2:C:993:PHE:CZ	2.74	0.40
2:C:707:ARG:O	2:C:707:ARG:HG2	2.20	0.40
2:C:971:LYS:HB3	2:C:988:VAL:N	2.36	0.40
2:C:987:ILE:HD12	2:C:987:ILE:N	2.36	0.40
2:C:1020:PRO:O	3:D:622:ARG:HD2	2.20	0.40
3:D:10:ILE:CD1	3:D:1434:TRP:NE1	2.84	0.40
3:D:90:MET:HE2	3:D:90:MET:HB3	1.84	0.40
3:D:118:LEU:CB	3:D:123:LEU:HD22	2.38	0.40
3:D:592:THR:H	3:D:600:LEU:HD21	1.86	0.40
3:D:613:ARG:HG3	8:D:9002:HOH:O	2.21	0.40
3:D:637:LEU:HD21	3:D:642:CYS:CA	2.47	0.40
3:D:1047:LYS:HE3	3:D:1051:GLU:O	2.22	0.40
3:D:1057:VAL:HA	3:D:1069:GLU:CD	2.46	0.40
5:F:124:PRO:O	5:F:128:ARG:HB2	2.21	0.40
5:F:278:LEU:HB2	5:F:286:PRO:HG2	2.02	0.40
1:K:51:THR:HA	1:K:145:ASP:O	2.20	0.40
1:K:59:GLU:HG3	1:K:139:ASN:O	2.21	0.40
1:L:91:ASN:O	1:L:94:LEU:HD12	2.20	0.40
1:L:101:LEU:HG	1:L:113:ASP:O	2.21	0.40
1:L:180:GLN:HB2	1:L:198:ARG:NH2	2.22	0.40
1:L:211:LEU:O	1:L:214:ALA:HB3	2.21	0.40
2:M:250:ARG:HG2	2:M:253:ALA:CB	2.46	0.40
2:M:455:LEU:O	2:M:541:SER:HB2	2.21	0.40
2:M:602:GLU:HG2	2:M:603:VAL:H	1.86	0.40
2:M:880:MET:HE3	2:M:880:MET:HB2	1.97	0.40
2:M:904:PRO:HG3	8:M:1508:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:931:GLY:C	2:M:933:GLY:N	2.77	0.40
2:M:988:VAL:HG11	3:N:949:ILE:O	2.21	0.40
2:M:1031:ARG:HD3	8:M:1668:HOH:O	2.21	0.40
2:M:1049:LEU:HG	2:M:1053:LEU:CD1	2.51	0.40
8:M:1148:HOH:O	5:P:276:ARG:HD3	2.19	0.40
3:N:13:ALA:O	3:N:511:TRP:HB3	2.21	0.40
3:N:138:LYS:HE3	3:N:138:LYS:HB2	1.87	0.40
3:N:156:GLU:O	3:N:159:ARG:HB3	2.21	0.40
3:N:432:TYR:HA	3:N:448:GLU:O	2.22	0.40
3:N:948:THR:HB	8:N:9352:HOH:O	2.20	0.40
3:N:1026:SER:C	3:N:1028:ALA:N	2.79	0.40
3:N:1236:LEU:HD11	3:N:1356:TYR:CE1	2.57	0.40
3:N:1280:VAL:HG13	3:N:1316:GLY:O	2.21	0.40
3:N:1314:LYS:NZ	3:N:1317:ASP:HB2	2.35	0.40
3:N:1422:MET:CE	3:N:1426:LYS:HG3	2.50	0.40
3:N:1480:PHE:O	4:O:18:ARG:NH2	2.55	0.40
5:P:220:LEU:HB2	5:P:243:ILE:HD11	2.03	0.40
5:P:361:LEU:HD13	5:P:366:ALA:HB1	2.03	0.40
1:B:39:PRO:O	1:B:43:ILE:HG12	2.21	0.40
1:B:218:LEU:O	1:B:222:LEU:HG	2.21	0.40
2:C:9:ILE:HD11	2:C:537:LYS:HZ1	1.86	0.40
2:C:75:GLU:HA	2:C:76:PRO:HD3	1.89	0.40
2:C:440:PRO:HG2	2:C:441:VAL:HG23	2.02	0.40
2:C:1001:VAL:HG23	8:C:1823:HOH:O	2.21	0.40
3:D:27:GLU:O	3:D:28:LYS:HD2	2.21	0.40
3:D:105:VAL:HG21	3:D:128:TYR:HE2	1.86	0.40
3:D:150:ARG:O	3:D:150:ARG:HG2	2.20	0.40
3:D:455:ARG:HH22	5:F:140:ARG:HD3	1.86	0.40
3:D:646:LYS:HD3	8:D:2059:HOH:O	2.22	0.40
3:D:884:ARG:O	3:D:888:GLU:N	2.53	0.40
3:D:1123:PHE:CZ	3:D:1178:ALA:HB1	2.57	0.40
3:D:1167:SER:N	3:D:1170:ASP:OD2	2.48	0.40
3:D:1293:PHE:HD2	8:D:9222:HOH:O	2.03	0.40
3:D:1320:GLU:HG2	3:D:1339:LYS:NZ	2.36	0.40
3:D:1497:GLU:OE1	3:D:1500:LYS:HD2	2.21	0.40
5:F:312:GLN:NE2	8:F:455:HOH:O	2.48	0.40
1:K:67:THR:OG1	2:M:627:ARG:NH2	2.53	0.40
1:L:100:LEU:HB2	1:L:115:LEU:CD2	2.49	0.40
2:M:167:LYS:HD2	2:M:168:ARG:NH1	2.35	0.40
2:M:207:LEU:HD22	2:M:221:LEU:CD2	2.51	0.40
2:M:621:VAL:HG13	8:M:1199:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:863:ASP:CG	2:M:865:THR:HG22	2.47	0.40
3:N:85:VAL:HG12	3:N:89:ARG:CZ	2.51	0.40
3:N:396:VAL:CG1	3:N:447:VAL:HA	2.52	0.40
3:N:461:ILE:O	3:N:465:LEU:HB2	2.22	0.40
3:N:608:SER:O	3:N:615:ARG:NH1	2.54	0.40
3:N:868:TYR:HB3	8:N:9527:HOH:O	2.20	0.40
3:N:875:THR:CG2	3:N:879:ARG:HE	2.33	0.40
3:N:951:ILE:HD12	3:N:1062:ARG:NE	2.37	0.40
3:N:1209:LEU:HD23	3:N:1210:SER:N	2.28	0.40
3:N:1266:ARG:NH2	8:N:9590:HOH:O	2.54	0.40
4:O:59:ASN:HB3	4:O:62:THR:OG1	2.22	0.40
5:P:76:SER:O	5:P:80:PRO:CD	2.66	0.40
5:P:109:GLY:O	5:P:112:ALA:HB3	2.21	0.40
5:P:249:ARG:NH2	8:P:2663:HOH:O	2.52	0.40
5:P:273:ARG:HG3	8:P:2904:HOH:O	2.20	0.40
5:P:323:ASP:C	5:P:325:LYS:N	2.79	0.40
1:A:229:GLN:C	1:B:13:VAL:H	2.30	0.40
1:B:54:THR:CG2	1:B:158:ILE:HG13	2.50	0.40
1:B:123:MET:O	1:B:125:PRO:HD3	2.21	0.40
1:B:180:GLN:HG3	1:B:196:THR:OG1	2.21	0.40
2:C:150:PRO:HB2	8:C:1325:HOH:O	2.21	0.40
2:C:199:VAL:HG13	2:C:235:LEU:CD2	2.51	0.40
2:C:329:GLY:HA3	8:C:1467:HOH:O	2.21	0.40
2:C:367:LEU:HA	2:C:371:LYS:HB2	2.02	0.40
2:C:432:ARG:NE	2:C:519:GLY:HA3	2.37	0.40
2:C:730:SER:N	8:C:1699:HOH:O	2.54	0.40
2:C:787:ASP:OD1	2:C:787:ASP:C	2.64	0.40
2:C:871:LEU:HD23	2:C:871:LEU:HA	1.79	0.40
3:D:53:ILE:HG12	3:D:53:ILE:O	2.22	0.40
3:D:191:LEU:HB2	3:D:211:VAL:CG2	2.51	0.40
3:D:216:VAL:HG11	8:D:9324:HOH:O	2.22	0.40
3:D:430:ASP:CG	3:D:431:VAL:N	2.75	0.40
3:D:500:ARG:HD3	3:D:500:ARG:HA	1.86	0.40
3:D:602:SER:O	3:D:603:LEU:C	2.65	0.40
3:D:639:LEU:CD1	3:D:640:HIS:H	2.35	0.40
3:D:755:ALA:HA	3:D:758:GLU:OE2	2.21	0.40
3:D:961:LYS:HG2	3:D:962:GLN:N	2.35	0.40
3:D:1136:LYS:C	3:D:1138:ALA:N	2.80	0.40
4:E:57:ASP:N	4:E:58:PRO:HD3	2.37	0.40
5:F:225:GLU:OE1	5:F:226:LYS:HG2	2.21	0.40
5:F:325:LYS:HB2	8:F:519:HOH:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:44:LEU:O	1:L:174:VAL:HG21	2.20	0.40
2:M:331:ARG:HG3	8:M:1502:HOH:O	2.22	0.40
2:M:478:VAL:HG13	2:M:506:ASN:ND2	2.36	0.40
2:M:496:ILE:HD12	2:M:496:ILE:N	2.36	0.40
2:M:507:ARG:NH1	8:M:1728:HOH:O	2.53	0.40
2:M:614:ARG:HG2	8:M:1443:HOH:O	2.20	0.40
2:M:666:LEU:HD12	2:M:667:ALA:N	2.35	0.40
2:M:724:ARG:O	2:M:734:LEU:HD11	2.22	0.40
2:M:1098:ASP:OD1	2:M:1098:ASP:C	2.64	0.40
3:N:159:ARG:HB2	3:N:159:ARG:NH1	2.36	0.40
3:N:164:GLY:O	3:N:165:LYS:C	2.65	0.40
3:N:474:GLU:OE1	3:N:500:ARG:NE	2.54	0.40
3:N:583:ASP:HB2	3:N:604:THR:OG1	2.21	0.40
3:N:817:GLU:CD	3:N:839:LEU:HD22	2.46	0.40
3:N:951:ILE:HD12	3:N:1062:ARG:HE	1.85	0.40
3:N:970:LYS:O	3:N:974:ILE:HG13	2.21	0.40
3:N:1103:HIS:CG	3:N:1104:GLU:N	2.90	0.40
3:N:1114:THR:HG22	3:N:1195:GLN:HB3	2.02	0.40
5:P:401:GLU:O	5:P:405:LEU:HD13	2.21	0.40
1:A:111:ALA:HB3	1:A:124:ASN:O	2.21	0.40
1:B:61:VAL:HG11	1:B:75:VAL:HG21	2.03	0.40
1:B:117:VAL:HG11	8:B:346:HOH:O	2.21	0.40
1:B:150:TYR:HA	1:B:169:ALA:O	2.21	0.40
2:C:585:GLU:HG2	2:C:665:PHE:HD2	1.87	0.40
2:C:693:GLU:OE1	2:C:696:LYS:HG3	2.22	0.40
2:C:966:LEU:HD12	2:C:966:LEU:HA	1.96	0.40
3:D:101:HIS:CE1	3:D:582:LEU:HD22	2.57	0.40
3:D:417:PRO:HB2	8:D:9616:HOH:O	2.21	0.40
3:D:602:SER:O	3:D:606:ILE:HG12	2.22	0.40
3:D:1161:GLU:H	3:D:1161:GLU:HG2	1.67	0.40
3:D:1320:GLU:HG3	8:D:9376:HOH:O	2.20	0.40
1:K:26:GLU:HB2	1:K:27:PRO:HA	2.04	0.40
1:K:57:TYR:CD2	1:K:161:ARG:NH1	2.90	0.40
1:K:64:GLU:OE2	1:K:76:VAL:HG22	2.22	0.40
2:M:28:ARG:HG3	2:M:40:GLU:OE1	2.22	0.40
2:M:211:LEU:HD21	2:M:311:PHE:HE1	1.87	0.40
2:M:480:THR:HG22	2:M:481:ASP:H	1.86	0.40
2:M:513:VAL:HG12	8:M:1272:HOH:O	2.21	0.40
2:M:1008:ARG:NH2	2:M:1020:PRO:HB3	2.37	0.40
3:N:8:VAL:C	3:N:1434:TRP:HH2	2.30	0.40
3:N:14:SER:O	3:N:17:LYS:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:602:SER:O	3:N:603:LEU:C	2.63	0.40
3:N:789:LEU:HA	3:N:789:LEU:HD23	1.84	0.40
3:N:960:LYS:HG2	3:N:964:LEU:HD12	2.04	0.40
3:N:1102:THR:HG22	3:N:1102:THR:O	2.21	0.40
5:P:315:VAL:HA	8:P:4638:HOH:O	2.21	0.40
5:P:348:SER:N	8:P:4815:HOH:O	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	227/315 (72%)	202 (89%)	21 (9%)	4 (2%)	6	23
1	B	227/315 (72%)	202 (89%)	21 (9%)	4 (2%)	6	23
1	K	227/315 (72%)	200 (88%)	23 (10%)	4 (2%)	6	23
1	L	227/315 (72%)	204 (90%)	19 (8%)	4 (2%)	6	23
2	C	1117/1119 (100%)	917 (82%)	150 (13%)	50 (4%)	2	7
2	M	1117/1119 (100%)	907 (81%)	159 (14%)	51 (5%)	2	6
3	D	1388/1524 (91%)	1123 (81%)	191 (14%)	74 (5%)	1	5
3	N	1388/1524 (91%)	1110 (80%)	195 (14%)	83 (6%)	1	3
4	E	93/99 (94%)	74 (80%)	16 (17%)	3 (3%)	3	11
4	O	93/99 (94%)	75 (81%)	15 (16%)	3 (3%)	3	11
5	F	341/423 (81%)	283 (83%)	42 (12%)	16 (5%)	2	6
5	P	341/423 (81%)	285 (84%)	40 (12%)	16 (5%)	2	6
All	All	6786/7590 (89%)	5582 (82%)	892 (13%)	312 (5%)	2	6

All (312) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	B	29	GLU
1	B	48	ILE
2	C	152	PRO
2	C	178	PRO
2	C	231	PRO
2	C	244	PRO
2	C	261	ILE
2	C	262	ALA
2	C	288	ARG
2	C	369	PRO
2	C	425	PHE
2	C	462	ASP
2	C	465	GLY
2	C	548	PRO
2	C	680	ASP
2	C	864	GLY
2	C	908	GLY
2	C	1004	LYS
2	C	1106	ASP
3	D	40	GLU
3	D	43	GLY
3	D	55	ASP
3	D	82	LYS
3	D	137	PRO
3	D	208	PRO
3	D	209	ARG
3	D	238	PRO
3	D	246	PRO
3	D	370	ALA
3	D	373	PRO
3	D	385	VAL
3	D	440	VAL
3	D	451	ASP
3	D	504	ASP
3	D	832	ARG
3	D	844	ALA
3	D	1028	ALA
3	D	1129	THR
3	D	1208	ASP
3	D	1213	ARG
3	D	1243	THR
3	D	1441	GLN

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Mol	Chain	Res	Type
4	E	42	PRO
4	E	58	PRO
5	F	147	LEU
5	F	153	PRO
5	F	324	GLU
5	F	326	ASP
5	F	341	PRO
5	F	390	PHE
1	K	29	GLU
1	L	29	GLU
2	M	152	PRO
2	M	178	PRO
2	M	231	PRO
2	M	244	PRO
2	M	261	ILE
2	M	262	ALA
2	M	288	ARG
2	M	369	PRO
2	M	425	PHE
2	M	462	ASP
2	M	465	GLY
2	M	548	PRO
2	M	680	ASP
2	M	864	GLY
2	M	908	GLY
2	M	1106	ASP
3	N	31	THR
3	N	40	GLU
3	N	43	GLY
3	N	55	ASP
3	N	82	LYS
3	N	137	PRO
3	N	208	PRO
3	N	209	ARG
3	N	217	LYS
3	N	238	PRO
3	N	246	PRO
3	N	370	ALA
3	N	373	PRO
3	N	385	VAL
3	N	440	VAL
3	N	504	ASP

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Mol	Chain	Res	Type
3	N	832	ARG
3	N	844	ALA
3	N	1028	ALA
3	N	1125	PRO
3	N	1129	THR
3	N	1208	ASP
3	N	1213	ARG
3	N	1243	THR
3	N	1441	GLN
4	O	42	PRO
4	O	58	PRO
5	P	147	LEU
5	P	153	PRO
5	P	324	GLU
5	P	326	ASP
5	P	390	PHE
1	A	187	GLY
1	B	187	GLY
2	C	59	LYS
2	C	156	GLY
2	C	170	PRO
2	C	290	LEU
2	C	363	SER
2	C	517	ARG
2	C	626	ARG
2	C	627	ARG
3	D	31	THR
3	D	96	ALA
3	D	120	ALA
3	D	231	VAL
3	D	381	ALA
3	D	415	VAL
3	D	417	PRO
3	D	594	PRO
3	D	609	GLY
3	D	766	ALA
3	D	783	ARG
3	D	803	GLY
3	D	822	ALA
3	D	1389	LEU
4	E	53	GLY
5	F	393	THR

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Mol	Chain	Res	Type
5	F	420	ASP
1	K	187	GLY
1	L	187	GLY
2	M	59	LYS
2	M	156	GLY
2	M	170	PRO
2	M	290	LEU
2	M	363	SER
2	M	517	ARG
2	M	626	ARG
2	M	781	LYS
3	N	96	ALA
3	N	231	VAL
3	N	381	ALA
3	N	415	VAL
3	N	417	PRO
3	N	451	ASP
3	N	594	PRO
3	N	609	GLY
3	N	803	GLY
3	N	822	ALA
3	N	1342	GLU
4	O	53	GLY
5	P	288	TYR
5	P	341	PRO
1	A	106	PRO
1	B	106	PRO
2	C	18	LEU
2	C	40	GLU
2	C	164	PRO
2	C	419	THR
2	C	727	PRO
2	C	781	LYS
3	D	37	LEU
3	D	98	PRO
3	D	161	LEU
3	D	165	LYS
3	D	170	PRO
3	D	424	GLY
3	D	1388	ARG
5	F	97	GLU
5	F	286	PRO

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Mol	Chain	Res	Type
5	F	288	TYR
1	K	106	PRO
2	M	40	GLU
2	M	164	PRO
2	M	419	THR
2	M	455	LEU
2	M	627	ARG
2	M	727	PRO
2	M	1004	LYS
3	N	37	LEU
3	N	98	PRO
3	N	120	ALA
3	N	161	LEU
3	N	165	LYS
3	N	170	PRO
3	N	424	GLY
3	N	533	GLY
3	N	705	ALA
3	N	766	ALA
3	N	783	ARG
3	N	1341	PRO
3	N	1349	VAL
3	N	1385	GLY
3	N	1389	LEU
5	P	97	GLU
5	P	232	ARG
5	P	286	PRO
5	P	393	THR
1	A	188	GLN
2	C	74	GLY
2	C	144	PRO
2	C	180	GLY
2	C	400	PRO
2	C	529	VAL
2	C	905	ILE
3	D	220	ARG
3	D	416	ALA
3	D	522	PRO
3	D	696	HIS
3	D	705	ALA
3	D	808	THR
3	D	1020	LEU

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Mol	Chain	Res	Type
3	D	1137	ARG
3	D	1366	LYS
3	D	1385	GLY
3	D	1446	VAL
5	F	232	ARG
1	K	188	GLN
1	L	106	PRO
2	M	74	GLY
2	M	180	GLY
2	M	413	LEU
2	M	529	VAL
3	N	24	GLY
3	N	110	SER
3	N	220	ARG
3	N	416	ALA
3	N	526	PRO
3	N	530	VAL
3	N	808	THR
3	N	1019	PRO
3	N	1366	LYS
3	N	1388	ARG
5	P	420	ASP
2	C	251	ASP
2	C	272	ALA
2	C	420	ARG
2	C	422	ARG
2	C	1097	LEU
3	D	521	PRO
3	D	526	PRO
3	D	530	VAL
3	D	615	ARG
3	D	924	MET
3	D	1019	PRO
3	D	1390	LEU
5	F	184	ARG
5	F	360	LYS
1	L	188	GLN
2	M	223	ASP
2	M	272	ALA
2	M	574	ALA
2	M	705	ILE
2	M	905	ILE

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Mol	Chain	Res	Type
2	M	1097	LEU
3	N	34	TYR
3	N	407	VAL
3	N	522	PRO
3	N	1137	ARG
3	N	1390	LEU
3	N	1432	LYS
3	N	1446	VAL
2	C	779	GLY
2	C	784	ASP
3	D	24	GLY
3	D	136	ASP
3	D	368	VAL
3	D	1248	GLY
3	D	1306	PRO
5	F	297	PRO
2	M	144	PRO
2	M	251	ASP
2	M	779	GLY
3	N	615	ARG
3	N	833	GLU
3	N	1226	ALA
3	N	1268	PRO
5	P	360	LYS
2	C	53	PRO
2	C	270	GLY
2	C	336	VAL
3	D	407	VAL
2	M	53	PRO
2	M	270	GLY
3	N	670	VAL
3	N	1248	GLY
3	N	1306	PRO
5	P	297	PRO
2	C	79	PRO
3	D	425	GLY
3	D	1064	GLY
3	D	1349	VAL
5	F	167	PRO
3	N	1064	GLY
5	P	167	PRO
2	C	273	GLY

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Mol	Chain	Res	Type
3	D	670	VAL
3	D	1050	GLY
3	D	1379	VAL
2	M	424	GLY
2	M	1079	PRO
3	N	173	PRO
3	N	425	GLY
5	P	314	PRO
2	M	79	PRO
2	M	273	GLY
2	M	336	VAL
3	N	136	ASP
3	N	368	VAL
3	N	521	PRO
3	N	1050	GLY
3	N	509	PRO
2	C	166	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	202/273 (74%)	147 (73%)	55 (27%)	0	1
1	B	202/273 (74%)	161 (80%)	41 (20%)	1	4
1	K	202/273 (74%)	155 (77%)	47 (23%)	1	3
1	L	202/273 (74%)	155 (77%)	47 (23%)	1	3
2	C	941/941 (100%)	724 (77%)	217 (23%)	1	3
2	M	941/941 (100%)	723 (77%)	218 (23%)	1	3
3	D	1123/1279 (88%)	832 (74%)	291 (26%)	0	2
3	N	1123/1279 (88%)	842 (75%)	281 (25%)	0	2
4	E	83/87 (95%)	61 (74%)	22 (26%)	0	2
4	O	83/87 (95%)	61 (74%)	22 (26%)	0	2
5	F	295/370 (80%)	224 (76%)	71 (24%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	P	295/370 (80%)	250 (85%)	45 (15%)	3 10
All	All	5692/6446 (88%)	4335 (76%)	1357 (24%)	1 3

All (1357) 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	19	GLU
1	A	26	GLU
1	A	28	LEU
1	A	32	PHE
1	A	34	VAL
1	A	44	LEU
1	A	47	SER
1	A	54	THR
1	A	62	LEU
1	A	66	SER
1	A	73	GLU
1	A	74	ASP
1	A	76	VAL
1	A	77	GLU
1	A	84	GLU
1	A	87	VAL
1	A	88	ARG
1	A	89	PHE
1	A	96	THR
1	A	101	LEU
1	A	104	GLU
1	A	120	VAL
1	A	123	MET
1	A	127	LEU
1	A	137	ARG
1	A	139	ASN
1	A	142	VAL
1	A	161	ARG
1	A	163	ASN
1	A	165	ILE
1	A	166	PRO

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Mol	Chain	Res	Type
1	A	167	VAL
1	A	170	VAL
1	A	176	ARG
1	A	180	GLN
1	A	183	ASP
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	201	THR
1	A	205	VAL
1	A	206	THR
1	A	211	LEU
1	A	216	GLU
1	A	227	ASN
1	A	229	GLN
1	B	1	MET
1	B	5	LYS
1	B	26	GLU
1	B	62	LEU
1	B	65	PHE
1	B	68	ILE
1	B	73	GLU
1	B	77	GLU
1	B	80	LEU
1	B	81	ASN
1	B	83	LYS
1	B	87	VAL
1	B	89	PHE
1	B	92	PRO
1	B	94	LEU
1	B	95	GLN
1	B	96	THR
1	B	99	LEU
1	B	101	LEU
1	B	110	LYS
1	B	112	ARG
1	B	119	ASP
1	B	121	GLU

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Mol	Chain	Res	Type
1	B	128	HIS
1	B	133	GLU
1	B	140	MET
1	B	159	LYS
1	B	162	ILE
1	B	176	ARG
1	B	180	GLN
1	B	192	LEU
1	B	196	THR
1	B	197	LEU
1	B	200	TRP
1	B	201	THR
1	B	206	THR
1	B	208	LEU
1	B	209	GLU
1	B	213	GLN
1	B	220	GLU
1	B	224	TYR
2	C	5	ARG
2	C	9	ILE
2	C	10	ARG
2	C	12	VAL
2	C	15	LEU
2	C	20	GLU
2	C	22	GLN
2	C	26	TYR
2	C	30	LEU
2	C	31	GLN
2	C	34	VAL
2	C	41	ASN
2	C	48	PHE
2	C	49	ARG
2	C	51	THR
2	C	71	TYR
2	C	72	ARG
2	C	73	LEU
2	C	89	THR
2	C	95	TYR
2	C	98	LEU
2	C	100	LEU
2	C	104	ASP
2	C	108	ILE

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Mol	Chain	Res	Type
2	C	110	GLU
2	C	111	ASP
2	C	114	PHE
2	C	115	LEU
2	C	140	ILE
2	C	149	THR
2	C	152	PRO
2	C	157	ARG
2	C	158	TYR
2	C	163	ILE
2	C	168	ARG
2	C	170	PRO
2	C	172	ILE
2	C	177	GLU
2	C	178	PRO
2	C	182	VAL
2	C	193	LEU
2	C	198	ARG
2	C	205	GLU
2	C	209	ARG
2	C	216	GLU
2	C	218	VAL
2	C	221	LEU
2	C	222	MET
2	C	224	GLU
2	C	229	MET
2	C	237	ARG
2	C	238	LEU
2	C	243	ARG
2	C	252	LYS
2	C	254	VAL
2	C	257	VAL
2	C	267	TYR
2	C	279	GLU
2	C	281	LEU
2	C	285	LEU
2	C	288	ARG
2	C	290	LEU
2	C	303	PHE
2	C	304	LEU
2	C	321	GLU
2	C	332	ARG

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Mol	Chain	Res	Type
2	C	334	ARG
2	C	340	MET
2	C	342	ASP
2	C	343	GLN
2	C	350	ARG
2	C	351	LEU
2	C	357	GLU
2	C	359	MET
2	C	360	LEU
2	C	368	THR
2	C	371	LYS
2	C	373	VAL
2	C	384	GLU
2	C	392	SER
2	C	393	GLN
2	C	394	PHE
2	C	399	ASN
2	C	400	PRO
2	C	409	ARG
2	C	413	LEU
2	C	420	ARG
2	C	425	PHE
2	C	427	VAL
2	C	432	ARG
2	C	449	ILE
2	C	451	LEU
2	C	453	THR
2	C	460	ARG
2	C	474	VAL
2	C	479	VAL
2	C	481	ASP
2	C	487	THR
2	C	496	ILE
2	C	500	ASN
2	C	503	LEU
2	C	504	GLU
2	C	508	ILE
2	C	513	VAL
2	C	523	ILE
2	C	524	VAL
2	C	527	GLU
2	C	532	MET

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Mol	Chain	Res	Type
2	C	533	ASP
2	C	542	VAL
2	C	543	ASN
2	C	548	PRO
2	C	559	LEU
2	C	563	ASN
2	C	564	MET
2	C	566	THR
2	C	575	GLN
2	C	584	GLU
2	C	589	ARG
2	C	605	LYS
2	C	611	ILE
2	C	620	LEU
2	C	622	GLU
2	C	637	LEU
2	C	639	GLN
2	C	640	ARG
2	C	645	VAL
2	C	650	ARG
2	C	655	LEU
2	C	657	ASP
2	C	663	ASN
2	C	668	LEU
2	C	671	ASN
2	C	672	VAL
2	C	679	PHE
2	C	690	ILE
2	C	691	SER
2	C	693	GLU
2	C	697	ARG
2	C	699	PHE
2	C	701	THR
2	C	715	THR
2	C	722	ILE
2	C	724	ARG
2	C	727	PRO
2	C	729	LEU
2	C	737	LEU
2	C	740	GLU
2	C	749	VAL
2	C	764	GLU

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Mol	Chain	Res	Type
2	C	785	VAL
2	C	791	ARG
2	C	799	ILE
2	C	803	THR
2	C	804	VAL
2	C	814	GLU
2	C	821	GLU
2	C	832	LYS
2	C	839	LEU
2	C	841	ASN
2	C	853	LEU
2	C	858	MET
2	C	862	PRO
2	C	863	ASP
2	C	870	ILE
2	C	878	SER
2	C	881	ASN
2	C	882	LEU
2	C	886	LEU
2	C	900	ARG
2	C	901	TYR
2	C	904	PRO
2	C	905	ILE
2	C	907	ASP
2	C	923	GLU
2	C	925	TYR
2	C	934	PHE
2	C	945	ARG
2	C	948	GLU
2	C	950	LEU
2	C	953	VAL
2	C	959	PRO
2	C	966	LEU
2	C	969	GLN
2	C	971	LYS
2	C	972	VAL
2	C	975	TYR
2	C	978	ARG
2	C	981	GLU
2	C	982	PRO
2	C	984	GLU
2	C	988	VAL

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Mol	Chain	Res	Type
2	C	995	MET
2	C	1006	HIS
2	C	1008	ARG
2	C	1016	ILE
2	C	1017	THR
2	C	1019	GLN
2	C	1020	PRO
2	C	1021	LEU
2	C	1035	MET
2	C	1040	LEU
2	C	1052	MET
2	C	1054	THR
2	C	1076	VAL
2	C	1079	PRO
2	C	1081	VAL
2	C	1087	VAL
2	C	1092	LEU
2	C	1095	LEU
2	C	1097	LEU
2	C	1098	ASP
2	C	1103	ASP
2	C	1104	GLU
2	C	1106	ASP
2	C	1109	VAL
2	C	1115	LEU
3	D	3	LYS
3	D	6	ARG
3	D	12	LEU
3	D	17	LYS
3	D	25	GLU
3	D	27	GLU
3	D	29	PRO
3	D	30	GLU
3	D	32	ILE
3	D	41	ARG
3	D	42	ASP
3	D	47	GLU
3	D	56	TYR
3	D	58	CYS
3	D	62	LYS
3	D	71	LYS
3	D	74	GLU

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Mol	Chain	Res	Type
3	D	76	CYS
3	D	80	VAL
3	D	82	LYS
3	D	85	VAL
3	D	86	ARG
3	D	90	MET
3	D	97	THR
3	D	98	PRO
3	D	101	HIS
3	D	102	ILE
3	D	103	TRP
3	D	107	ASP
3	D	112	ILE
3	D	115	LEU
3	D	117	ASP
3	D	118	LEU
3	D	121	THR
3	D	133	ILE
3	D	145	VAL
3	D	148	GLU
3	D	153	LEU
3	D	155	ASP
3	D	156	GLU
3	D	162	ARG
3	D	170	PRO
3	D	171	LEU
3	D	175	VAL
3	D	185	VAL
3	D	199	LEU
3	D	204	LEU
3	D	205	TYR
3	D	208	PRO
3	D	209	ARG
3	D	210	ARG
3	D	211	VAL
3	D	389	GLU
3	D	394	LEU
3	D	395	VAL
3	D	411	THR
3	D	413	ASP
3	D	421	LEU
3	D	427	VAL

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Mol	Chain	Res	Type
3	D	432	TYR
3	D	444	VAL
3	D	445	ARG
3	D	447	VAL
3	D	451	ASP
3	D	452	ILE
3	D	456	MET
3	D	465	LEU
3	D	466	LYS
3	D	469	ASP
3	D	479	GLU
3	D	481	MET
3	D	483	HIS
3	D	485	SER
3	D	489	ARG
3	D	491	LYS
3	D	493	ARG
3	D	497	GLU
3	D	503	LEU
3	D	507	ASN
3	D	513	ILE
3	D	521	PRO
3	D	525	ARG
3	D	528	VAL
3	D	529	GLN
3	D	540	LEU
3	D	548	ILE
3	D	549	ASN
3	D	554	LEU
3	D	565	ILE
3	D	573	MET
3	D	590	PRO
3	D	594	PRO
3	D	597	ASP
3	D	598	ARG
3	D	600	LEU
3	D	615	ARG
3	D	616	GLN
3	D	624	ASP
3	D	632	VAL
3	D	636	GLN
3	D	638	LYS

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Mol	Chain	Res	Type
3	D	639	LEU
3	D	641	GLN
3	D	651	GLU
3	D	652	LEU
3	D	653	PHE
3	D	655	PRO
3	D	659	LYS
3	D	660	LYS
3	D	666	ILE
3	D	675	ARG
3	D	676	MET
3	D	687	VAL
3	D	688	TRP
3	D	692	GLU
3	D	695	ILE
3	D	702	LEU
3	D	704	ARG
3	D	710	ARG
3	D	713	ILE
3	D	717	GLN
3	D	719	VAL
3	D	724	GLN
3	D	725	SER
3	D	739	ASP
3	D	749	VAL
3	D	762	GLN
3	D	763	MET
3	D	765	SER
3	D	768	ASN
3	D	778	LEU
3	D	794	GLN
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	833	GLU
3	D	836	VAL

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Mol	Chain	Res	Type
3	D	838	ARG
3	D	839	LEU
3	D	847	ASP
3	D	858	VAL
3	D	859	ASP
3	D	862	ASP
3	D	863	VAL
3	D	864	VAL
3	D	865	THR
3	D	867	ARG
3	D	879	ARG
3	D	880	ILE
3	D	884	ARG
3	D	888	GLU
3	D	891	GLU
3	D	897	TRP
3	D	898	GLU
3	D	902	LEU
3	D	907	GLU
3	D	910	SER
3	D	911	LEU
3	D	914	LEU
3	D	915	VAL
3	D	922	LEU
3	D	926	LYS
3	D	944	THR
3	D	959	GLU
3	D	961	LYS
3	D	964	LEU
3	D	969	ARG
3	D	970	LYS
3	D	972	LEU
3	D	985	ASP
3	D	987	GLU
3	D	988	ARG
3	D	997	THR
3	D	999	THR
3	D	1000	THR
3	D	1001	GLU
3	D	1003	VAL
3	D	1032	PRO
3	D	1033	GLN

Continued on next page...

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Mol	Chain	Res	Type
3	D	1038	LEU
3	D	1039	CYS
3	D	1042	ARG
3	D	1049	SER
3	D	1051	GLU
3	D	1058	ARG
3	D	1060	SER
3	D	1062	ARG
3	D	1068	LEU
3	D	1083	ASP
3	D	1087	ARG
3	D	1093	TYR
3	D	1095	THR
3	D	1096	ARG
3	D	1099	VAL
3	D	1104	GLU
3	D	1109	GLU
3	D	1112	CYS
3	D	1116	ASN
3	D	1124	GLN
3	D	1129	THR
3	D	1134	LEU
3	D	1144	LEU
3	D	1160	LEU
3	D	1161	GLU
3	D	1164	ARG
3	D	1166	LEU
3	D	1176	LYS
3	D	1182	GLU
3	D	1183	ILE
3	D	1188	VAL
3	D	1190	SER
3	D	1191	PRO
3	D	1195	GLN
3	D	1207	TYR
3	D	1210	SER
3	D	1211	MET
3	D	1213	ARG
3	D	1223	ILE
3	D	1236	LEU
3	D	1238	MET
3	D	1243	THR

Continued on next page...

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Mol	Chain	Res	Type
3	D	1252	ILE
3	D	1258	ARG
3	D	1259	VAL
3	D	1260	ILE
3	D	1262	LEU
3	D	1267	ARG
3	D	1269	LYS
3	D	1280	VAL
3	D	1290	LEU
3	D	1295	GLU
3	D	1299	PHE
3	D	1302	GLU
3	D	1304	LYS
3	D	1305	LEU
3	D	1306	PRO
3	D	1307	LYS
3	D	1310	ARG
3	D	1314	LYS
3	D	1317	ASP
3	D	1331	ASP
3	D	1332	PRO
3	D	1336	LEU
3	D	1337	GLU
3	D	1339	LYS
3	D	1344	VAL
3	D	1346	ARG
3	D	1348	LEU
3	D	1352	ILE
3	D	1359	GLN
3	D	1363	LEU
3	D	1368	ILE
3	D	1382	THR
3	D	1395	LEU
3	D	1401	GLU
3	D	1403	LEU
3	D	1406	ARG
3	D	1407	LEU
3	D	1410	GLU
3	D	1415	VAL
3	D	1419	PRO
3	D	1420	LEU
3	D	1421	LEU

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Mol	Chain	Res	Type
3	D	1424	VAL
3	D	1425	THR
3	D	1433	SER
3	D	1435	LEU
3	D	1439	SER
3	D	1440	PHE
3	D	1444	THR
3	D	1447	LEU
3	D	1455	LYS
3	D	1456	LYS
3	D	1460	ILE
3	D	1462	LEU
3	D	1464	GLU
3	D	1465	ASN
3	D	1466	VAL
3	D	1470	ARG
3	D	1481	VAL
3	D	1483	PHE
3	D	1485	GLN
3	D	1488	ASP
3	D	1496	GLU
3	D	1501	GLU
4	E	7	ASP
4	E	12	MET
4	E	14	ASP
4	E	15	SER
4	E	20	THR
4	E	28	GLN
4	E	29	GLN
4	E	30	LEU
4	E	31	LEU
4	E	33	HIS
4	E	40	LEU
4	E	42	PRO
4	E	45	ARG
4	E	51	LEU
4	E	57	ASP
4	E	58	PRO
4	E	59	ASN
4	E	61	GLU
4	E	66	LYS
4	E	67	GLU

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Mol	Chain	Res	Type
4	E	81	PRO
4	E	89	MET
5	F	80	PRO
5	F	83	GLN
5	F	84	TYR
5	F	87	GLU
5	F	91	VAL
5	F	96	LEU
5	F	101	GLU
5	F	117	SER
5	F	120	THR
5	F	124	PRO
5	F	125	ASP
5	F	127	ILE
5	F	135	ILE
5	F	136	LEU
5	F	142	ARG
5	F	149	GLU
5	F	169	GLU
5	F	170	HIS
5	F	174	LEU
5	F	176	ILE
5	F	181	GLU
5	F	185	GLN
5	F	186	HIS
5	F	192	LEU
5	F	194	LEU
5	F	208	SER
5	F	220	LEU
5	F	225	GLU
5	F	228	GLU
5	F	233	PHE
5	F	236	SER
5	F	240	THR
5	F	245	GLN
5	F	260	ILE
5	F	262	VAL
5	F	264	MET
5	F	269	ASN
5	F	273	ARG
5	F	282	LEU
5	F	285	GLU

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Mol	Chain	Res	Type
5	F	288	TYR
5	F	289	GLU
5	F	295	MET
5	F	302	LYS
5	F	313	GLU
5	F	317	LEU
5	F	328	PHE
5	F	331	ASP
5	F	335	ASP
5	F	336	GLU
5	F	340	SER
5	F	341	PRO
5	F	342	VAL
5	F	347	GLN
5	F	349	LEU
5	F	350	LEU
5	F	353	GLU
5	F	355	GLU
5	F	361	LEU
5	F	365	GLU
5	F	370	LYS
5	F	392	VAL
5	F	393	THR
5	F	398	ARG
5	F	399	GLN
5	F	403	LYS
5	F	410	TYR
5	F	412	GLU
5	F	414	ARG
5	F	420	ASP
5	F	422	LEU
1	K	5	LYS
1	K	9	PRO
1	K	12	THR
1	K	14	ARG
1	K	15	THR
1	K	18	ARG
1	K	34	VAL
1	K	44	LEU
1	K	45	LEU
1	K	62	LEU
1	K	66	SER

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Mol	Chain	Res	Type
1	K	71	VAL
1	K	80	LEU
1	K	88	ARG
1	K	92	PRO
1	K	94	LEU
1	K	96	THR
1	K	100	LEU
1	K	101	LEU
1	K	108	GLU
1	K	113	ASP
1	K	116	PRO
1	K	119	ASP
1	K	120	VAL
1	K	121	GLU
1	K	127	LEU
1	K	131	THR
1	K	133	GLU
1	K	138	LEU
1	K	142	VAL
1	K	154	GLU
1	K	165	ILE
1	K	167	VAL
1	K	170	VAL
1	K	180	GLN
1	K	184	THR
1	K	185	ARG
1	K	186	LEU
1	K	190	THR
1	K	191	ASP
1	K	196	THR
1	K	198	ARG
1	K	206	THR
1	K	211	LEU
1	K	219	ARG
1	K	223	THR
1	K	227	ASN
1	L	1	MET
1	L	3	ASP
1	L	5	LYS
1	L	7	LYS
1	L	9	PRO
1	L	25	LEU

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Mol	Chain	Res	Type
1	L	29	GLU
1	L	30	ARG
1	L	47	SER
1	L	55	SER
1	L	62	LEU
1	L	63	HIS
1	L	64	GLU
1	L	65	PHE
1	L	67	THR
1	L	73	GLU
1	L	77	GLU
1	L	80	LEU
1	L	81	ASN
1	L	83	LYS
1	L	88	ARG
1	L	89	PHE
1	L	91	ASN
1	L	92	PRO
1	L	94	LEU
1	L	95	GLN
1	L	99	LEU
1	L	101	LEU
1	L	110	LYS
1	L	115	LEU
1	L	121	GLU
1	L	134	GLU
1	L	138	LEU
1	L	141	GLU
1	L	151	VAL
1	L	159	LYS
1	L	167	VAL
1	L	177	VAL
1	L	184	THR
1	L	197	LEU
1	L	201	THR
1	L	206	THR
1	L	213	GLN
1	L	216	GLU
1	L	219	ARG
1	L	220	GLU
1	L	229	GLN
2	M	5	ARG

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Mol	Chain	Res	Type
2	M	9	ILE
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	39	ARG
2	M	42	VAL
2	M	48	PHE
2	M	49	ARG
2	M	51	THR
2	M	71	TYR
2	M	81	ASP
2	M	91	GLN
2	M	94	LEU
2	M	95	TYR
2	M	98	LEU
2	M	99	GLN
2	M	100	LEU
2	M	105	THR
2	M	107	LEU
2	M	108	ILE
2	M	114	PHE
2	M	115	LEU
2	M	118	ILE
2	M	133	ASP
2	M	140	ILE
2	M	149	THR
2	M	152	PRO
2	M	157	ARG
2	M	158	TYR
2	M	163	ILE
2	M	175	GLU
2	M	177	GLU
2	M	178	PRO
2	M	182	VAL
2	M	184	MET
2	M	185	LYS
2	M	193	LEU
2	M	196	LEU

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Mol	Chain	Res	Type
2	M	198	ARG
2	M	205	GLU
2	M	209	ARG
2	M	211	LEU
2	M	218	VAL
2	M	221	LEU
2	M	223	ASP
2	M	229	MET
2	M	230	ARG
2	M	235	LEU
2	M	239	PHE
2	M	241	LEU
2	M	242	LEU
2	M	246	ASP
2	M	249	LYS
2	M	252	LYS
2	M	254	VAL
2	M	257	VAL
2	M	260	LEU
2	M	267	TYR
2	M	268	ASP
2	M	279	GLU
2	M	285	LEU
2	M	290	LEU
2	M	297	GLU
2	M	304	LEU
2	M	313	LEU
2	M	321	GLU
2	M	322	VAL
2	M	327	HIS
2	M	328	LEU
2	M	332	ARG
2	M	335	THR
2	M	341	THR
2	M	343	GLN
2	M	345	ARG
2	M	348	LEU
2	M	359	MET
2	M	367	LEU
2	M	371	LYS
2	M	379	GLU
2	M	383	ARG

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Mol	Chain	Res	Type
2	M	392	SER
2	M	397	GLU
2	M	400	PRO
2	M	405	ARG
2	M	408	ARG
2	M	425	PHE
2	M	426	ASP
2	M	427	VAL
2	M	443	THR
2	M	448	ASN
2	M	451	LEU
2	M	455	LEU
2	M	460	ARG
2	M	468	ARG
2	M	469	THR
2	M	470	PRO
2	M	474	VAL
2	M	475	VAL
2	M	479	VAL
2	M	480	THR
2	M	496	ILE
2	M	502	PRO
2	M	503	LEU
2	M	507	ARG
2	M	511	GLU
2	M	517	ARG
2	M	524	VAL
2	M	527	GLU
2	M	528	GLU
2	M	533	ASP
2	M	544	THR
2	M	554	ASP
2	M	559	LEU
2	M	564	MET
2	M	571	LEU
2	M	575	GLN
2	M	579	VAL
2	M	581	THR
2	M	584	GLU
2	M	585	GLU
2	M	588	VAL
2	M	589	ARG

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Mol	Chain	Res	Type
2	M	595	LEU
2	M	607	ASP
2	M	614	ARG
2	M	620	LEU
2	M	627	ARG
2	M	632	ASN
2	M	633	GLN
2	M	635	THR
2	M	637	LEU
2	M	640	ARG
2	M	654	LEU
2	M	663	ASN
2	M	668	LEU
2	M	670	GLN
2	M	672	VAL
2	M	676	ILE
2	M	697	ARG
2	M	699	PHE
2	M	705	ILE
2	M	715	THR
2	M	717	LEU
2	M	725	ASP
2	M	727	PRO
2	M	728	HIS
2	M	729	LEU
2	M	737	LEU
2	M	748	GLU
2	M	750	LYS
2	M	762	LYS
2	M	772	ARG
2	M	780	GLU
2	M	785	VAL
2	M	788	THR
2	M	799	ILE
2	M	807	ARG
2	M	808	ARG
2	M	821	GLU
2	M	829	GLN
2	M	834	GLN
2	M	839	LEU
2	M	841	ASN
2	M	853	LEU

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Mol	Chain	Res	Type
2	M	861	LEU
2	M	862	PRO
2	M	870	ILE
2	M	881	ASN
2	M	886	LEU
2	M	897	LEU
2	M	900	ARG
2	M	907	ASP
2	M	910	LYS
2	M	911	GLU
2	M	914	ILE
2	M	916	GLU
2	M	917	LEU
2	M	918	LEU
2	M	923	GLU
2	M	925	TYR
2	M	938	LYS
2	M	950	LEU
2	M	975	TYR
2	M	981	GLU
2	M	984	GLU
2	M	988	VAL
2	M	991	GLN
2	M	999	HIS
2	M	1000	MET
2	M	1002	GLU
2	M	1003	ASP
2	M	1008	ARG
2	M	1016	ILE
2	M	1017	THR
2	M	1035	MET
2	M	1041	GLU
2	M	1053	LEU
2	M	1054	THR
2	M	1058	ASP
2	M	1060	ILE
2	M	1074	GLU
2	M	1076	VAL
2	M	1079	PRO
2	M	1081	VAL
2	M	1087	VAL
2	M	1088	LEU

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Mol	Chain	Res	Type
2	M	1091	GLU
2	M	1092	LEU
2	M	1097	LEU
2	M	1098	ASP
2	M	1099	VAL
2	M	1100	GLN
2	M	1111	ILE
3	N	2	LYS
3	N	3	LYS
3	N	6	ARG
3	N	12	LEU
3	N	15	PRO
3	N	17	LYS
3	N	27	GLU
3	N	34	TYR
3	N	36	THR
3	N	41	ARG
3	N	52	PRO
3	N	53	ILE
3	N	56	TYR
3	N	71	LYS
3	N	76	CYS
3	N	78	VAL
3	N	80	VAL
3	N	82	LYS
3	N	85	VAL
3	N	86	ARG
3	N	87	ARG
3	N	97	THR
3	N	101	HIS
3	N	102	ILE
3	N	107	ASP
3	N	108	VAL
3	N	111	LYS
3	N	112	ILE
3	N	114	THR
3	N	117	ASP
3	N	118	LEU
3	N	123	LEU
3	N	128	TYR
3	N	133	ILE
3	N	145	VAL

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Mol	Chain	Res	Type
3	N	147	VAL
3	N	148	GLU
3	N	151	GLN
3	N	152	LEU
3	N	153	LEU
3	N	160	GLU
3	N	162	ARG
3	N	165	LYS
3	N	169	TYR
3	N	170	PRO
3	N	171	LEU
3	N	172	PRO
3	N	185	VAL
3	N	199	LEU
3	N	200	ASP
3	N	205	TYR
3	N	208	PRO
3	N	389	GLU
3	N	394	LEU
3	N	395	VAL
3	N	405	ASP
3	N	411	THR
3	N	413	ASP
3	N	414	ARG
3	N	419	ASP
3	N	427	VAL
3	N	430	ASP
3	N	432	TYR
3	N	442	ASN
3	N	444	VAL
3	N	447	VAL
3	N	448	GLU
3	N	449	SER
3	N	456	MET
3	N	459	GLU
3	N	463	GLN
3	N	465	LEU
3	N	470	LEU
3	N	473	LEU
3	N	475	LYS
3	N	481	MET
3	N	488	ARG

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Mol	Chain	Res	Type
3	N	493	ARG
3	N	498	VAL
3	N	503	LEU
3	N	512	MET
3	N	513	ILE
3	N	518	PRO
3	N	521	PRO
3	N	528	VAL
3	N	530	VAL
3	N	534	ARG
3	N	535	PHE
3	N	549	ASN
3	N	554	LEU
3	N	560	GLN
3	N	565	ILE
3	N	567	ILE
3	N	569	ASN
3	N	571	LYS
3	N	581	LEU
3	N	590	PRO
3	N	592	THR
3	N	594	PRO
3	N	596	SER
3	N	601	ARG
3	N	602	SER
3	N	613	ARG
3	N	624	ASP
3	N	629	SER
3	N	632	VAL
3	N	635	PRO
3	N	636	GLN
3	N	639	LEU
3	N	641	GLN
3	N	651	GLU
3	N	666	ILE
3	N	676	MET
3	N	677	LEU
3	N	681	ARG
3	N	688	TRP
3	N	689	ASP
3	N	695	ILE
3	N	704	ARG

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Mol	Chain	Res	Type
3	N	709	HIS
3	N	710	ARG
3	N	713	ILE
3	N	717	GLN
3	N	719	VAL
3	N	721	VAL
3	N	725	SER
3	N	732	VAL
3	N	734	GLU
3	N	736	PHE
3	N	739	ASP
3	N	744	GLN
3	N	770	LEU
3	N	780	LYS
3	N	781	PRO
3	N	786	ILE
3	N	787	LEU
3	N	792	ILE
3	N	794	GLN
3	N	796	ARG
3	N	797	LYS
3	N	799	LYS
3	N	800	LYS
3	N	804	LEU
3	N	823	LEU
3	N	828	LYS
3	N	829	VAL
3	N	832	ARG
3	N	836	VAL
3	N	839	LEU
3	N	846	PRO
3	N	847	ASP
3	N	850	LEU
3	N	858	VAL
3	N	863	VAL
3	N	864	VAL
3	N	865	THR
3	N	867	ARG
3	N	876	SER
3	N	880	ILE
3	N	888	GLU
3	N	899	LEU

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Mol	Chain	Res	Type
3	N	901	GLN
3	N	914	LEU
3	N	917	GLN
3	N	947	ILE
3	N	951	ILE
3	N	952	ASP
3	N	959	GLU
3	N	961	LYS
3	N	970	LYS
3	N	972	LEU
3	N	975	GLU
3	N	980	MET
3	N	984	THR
3	N	994	GLN
3	N	1005	GLN
3	N	1029	ARG
3	N	1031	ASN
3	N	1033	GLN
3	N	1042	ARG
3	N	1051	GLU
3	N	1052	THR
3	N	1058	ARG
3	N	1059	SER
3	N	1065	LEU
3	N	1066	THR
3	N	1068	LEU
3	N	1079	LYS
3	N	1087	ARG
3	N	1090	ASP
3	N	1095	THR
3	N	1096	ARG
3	N	1109	GLU
3	N	1112	CYS
3	N	1127	GLU
3	N	1129	THR
3	N	1133	ARG
3	N	1134	LEU
3	N	1137	ARG
3	N	1144	LEU
3	N	1162	GLU
3	N	1166	LEU
3	N	1173	LEU

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Mol	Chain	Res	Type
3	N	1176	LYS
3	N	1182	GLU
3	N	1183	ILE
3	N	1185	GLU
3	N	1195	GLN
3	N	1202	GLN
3	N	1207	TYR
3	N	1211	MET
3	N	1219	GLU
3	N	1223	ILE
3	N	1231	GLU
3	N	1238	MET
3	N	1243	THR
3	N	1252	ILE
3	N	1254	GLN
3	N	1257	PRO
3	N	1259	VAL
3	N	1260	ILE
3	N	1262	LEU
3	N	1264	GLU
3	N	1267	ARG
3	N	1274	ILE
3	N	1278	ASP
3	N	1285	GLU
3	N	1295	GLU
3	N	1297	GLU
3	N	1299	PHE
3	N	1305	LEU
3	N	1306	PRO
3	N	1314	LYS
3	N	1331	ASP
3	N	1337	GLU
3	N	1342	GLU
3	N	1344	VAL
3	N	1346	ARG
3	N	1348	LEU
3	N	1350	GLU
3	N	1353	GLN
3	N	1355	VAL
3	N	1357	ARG
3	N	1359	GLN
3	N	1363	LEU

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Mol	Chain	Res	Type
3	N	1365	ASP
3	N	1368	ILE
3	N	1380	GLU
3	N	1382	THR
3	N	1383	ASP
3	N	1388	ARG
3	N	1390	LEU
3	N	1391	GLU
3	N	1396	GLU
3	N	1401	GLU
3	N	1410	GLU
3	N	1412	LYS
3	N	1415	VAL
3	N	1419	PRO
3	N	1424	VAL
3	N	1432	LYS
3	N	1433	SER
3	N	1435	LEU
3	N	1440	PHE
3	N	1441	GLN
3	N	1452	ILE
3	N	1455	LYS
3	N	1456	LYS
3	N	1460	ILE
3	N	1463	LYS
3	N	1465	ASN
3	N	1466	VAL
3	N	1467	ILE
3	N	1468	LEU
3	N	1481	VAL
3	N	1485	GLN
3	N	1487	VAL
3	N	1488	ASP
3	N	1493	LYS
3	N	1496	GLU
3	N	1501	GLU
4	O	12	MET
4	O	17	TYR
4	O	20	THR
4	O	21	VAL
4	O	30	LEU
4	O	32	ARG

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Mol	Chain	Res	Type
4	O	42	PRO
4	O	43	GLU
4	O	45	ARG
4	O	47	LYS
4	O	51	LEU
4	O	57	ASP
4	O	59	ASN
4	O	61	GLU
4	O	66	LYS
4	O	69	LEU
4	O	70	THR
4	O	74	VAL
4	O	77	GLU
4	O	85	LEU
4	O	86	GLN
4	O	89	MET
5	P	83	GLN
5	P	84	TYR
5	P	85	LEU
5	P	91	VAL
5	P	96	LEU
5	P	101	GLU
5	P	108	GLU
5	P	125	ASP
5	P	126	LEU
5	P	131	VAL
5	P	135	ILE
5	P	136	LEU
5	P	138	SER
5	P	142	ARG
5	P	144	ILE
5	P	149	GLU
5	P	150	THR
5	P	164	LYS
5	P	174	LEU
5	P	176	ILE
5	P	181	GLU
5	P	186	HIS
5	P	214	GLN
5	P	221	ILE
5	P	262	VAL
5	P	280	GLN

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Mol	Chain	Res	Type
5	P	289	GLU
5	P	295	MET
5	P	318	GLU
5	P	328	PHE
5	P	337	HIS
5	P	338	LEU
5	P	341	PRO
5	P	347	GLN
5	P	350	LEU
5	P	353	GLU
5	P	365	GLU
5	P	370	LYS
5	P	393	THR
5	P	394	ARG
5	P	399	GLN
5	P	403	LYS
5	P	410	TYR
5	P	419	ARG
5	P	420	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (197) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	38	ASN
1	A	63	HIS
1	A	128	HIS
1	A	139	ASN
1	A	156	HIS
1	A	163	ASN
1	A	188	GLN
1	A	227	ASN
1	A	229	GLN
1	B	95	GLN
1	B	128	HIS
1	B	163	ASN
2	C	22	GLN
2	C	31	GLN
2	C	41	ASN
2	C	117	HIS
2	C	130	ASN
2	C	187	ASN

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Mol	Chain	Res	Type
2	C	327	HIS
2	C	343	GLN
2	C	374	ASN
2	C	393	GLN
2	C	399	ASN
2	C	431	HIS
2	C	434	HIS
2	C	538	GLN
2	C	545	ASN
2	C	563	ASN
2	C	567	GLN
2	C	609	ASN
2	C	633	GLN
2	C	639	GLN
2	C	663	ASN
2	C	834	GLN
2	C	841	ASN
2	C	843	HIS
2	C	881	ASN
2	C	899	GLN
2	C	920	GLN
2	C	991	GLN
2	C	999	HIS
2	C	1018	GLN
2	C	1047	HIS
2	C	1100	GLN
2	C	1107	ASN
3	D	66	GLN
3	D	143	ASN
3	D	151	GLN
3	D	166	GLN
3	D	507	ASN
3	D	541	ASN
3	D	549	ASN
3	D	552	ASN
3	D	560	GLN
3	D	575	GLN
3	D	611	GLN
3	D	640	HIS
3	D	669	ASN
3	D	703	ASN
3	D	717	GLN

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Mol	Chain	Res	Type
3	D	748	HIS
3	D	756	GLN
3	D	762	GLN
3	D	768	ASN
3	D	794	GLN
3	D	824	ASN
3	D	855	HIS
3	D	906	GLN
3	D	909	ASN
3	D	917	GLN
3	D	1033	GLN
3	D	1075	HIS
3	D	1116	ASN
3	D	1202	GLN
3	D	1242	HIS
3	D	1323	GLN
3	D	1333	HIS
3	D	1353	GLN
3	D	1359	GLN
3	D	1367	HIS
3	D	1404	ASN
3	D	1465	ASN
4	E	28	GLN
4	E	37	ASN
4	E	86	GLN
5	F	161	GLN
5	F	218	GLN
5	F	254	GLN
5	F	399	GLN
5	F	402	ASN
1	K	63	HIS
1	K	124	ASN
1	K	156	HIS
1	K	212	ASN
1	K	213	GLN
1	K	221	HIS
1	K	227	ASN
1	K	229	GLN
1	L	16	GLN
1	L	38	ASN
1	L	81	ASN
1	L	95	GLN

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Mol	Chain	Res	Type
1	L	124	ASN
1	L	163	ASN
1	L	180	GLN
1	L	212	ASN
2	M	22	GLN
2	M	91	GLN
2	M	99	GLN
2	M	117	HIS
2	M	139	GLN
2	M	187	ASN
2	M	204	GLN
2	M	343	GLN
2	M	390	GLN
2	M	393	GLN
2	M	431	HIS
2	M	506	ASN
2	M	538	GLN
2	M	543	ASN
2	M	545	ASN
2	M	565	GLN
2	M	567	GLN
2	M	609	ASN
2	M	639	GLN
2	M	663	ASN
2	M	671	ASN
2	M	704	HIS
2	M	829	GLN
2	M	834	GLN
2	M	841	ASN
2	M	843	HIS
2	M	860	HIS
2	M	872	ASN
2	M	881	ASN
2	M	884	GLN
2	M	889	HIS
2	M	920	GLN
2	M	969	GLN
2	M	991	GLN
2	M	999	HIS
2	M	1018	GLN
2	M	1050	GLN
2	M	1100	GLN

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Mol	Chain	Res	Type
2	M	1107	ASN
3	N	125	GLN
3	N	151	GLN
3	N	166	GLN
3	N	463	GLN
3	N	507	ASN
3	N	552	ASN
3	N	560	GLN
3	N	703	ASN
3	N	724	GLN
3	N	756	GLN
3	N	768	ASN
3	N	794	GLN
3	N	855	HIS
3	N	909	ASN
3	N	962	GLN
3	N	976	GLN
3	N	991	GLN
3	N	1005	GLN
3	N	1010	ASN
3	N	1014	ASN
3	N	1033	GLN
3	N	1034	GLN
3	N	1103	HIS
3	N	1116	ASN
3	N	1172	HIS
3	N	1202	GLN
3	N	1235	GLN
3	N	1333	HIS
3	N	1334	GLN
3	N	1353	GLN
3	N	1359	GLN
3	N	1374	GLN
3	N	1404	ASN
3	N	1441	GLN
3	N	1442	ASN
3	N	1465	ASN
3	N	1485	GLN
4	O	28	GLN
4	O	29	GLN
4	O	33	HIS
4	O	59	ASN

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Mol	Chain	Res	Type
5	P	186	HIS
5	P	191	ASN
5	P	214	GLN
5	P	217	ASN
5	P	218	GLN
5	P	245	GLN
5	P	269	ASN
5	P	279	GLN
5	P	337	HIS
5	P	399	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	229/315 (72%)	-1.72	0 100 100	38, 65, 92, 117	0
1	B	229/315 (72%)	-1.66	0 100 100	53, 95, 115, 121	0
1	K	229/315 (72%)	-1.75	0 100 100	41, 66, 93, 122	0
1	L	229/315 (72%)	-1.70	0 100 100	52, 94, 114, 127	0
2	C	1119/1119 (100%)	-1.70	0 100 100	23, 81, 110, 119	0
2	M	1119/1119 (100%)	-1.72	0 100 100	27, 79, 109, 122	0
3	D	1392/1524 (91%)	-1.71	0 100 100	17, 68, 113, 130	0
3	N	1392/1524 (91%)	-1.72	0 100 100	27, 69, 110, 138	0
4	E	95/99 (95%)	-1.64	0 100 100	47, 85, 115, 133	0
4	O	95/99 (95%)	-1.76	0 100 100	40, 76, 97, 111	0
5	F	345/423 (81%)	-1.69	0 100 100	46, 84, 112, 131	0
5	P	345/423 (81%)	-1.69	0 100 100	54, 87, 112, 125	0
All	All	6818/7590 (89%)	-1.71	0 100 100	17, 77, 111, 138	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	MG	N	9002	1/1	0.99	0.02	64,64,64,64	0
6	ZN	D	7112	1/1	1.00	0.01	75,75,75,75	0
6	ZN	N	7059	1/1	1.00	0.01	100,100,100,100	0
6	ZN	N	7113	1/1	1.00	0.01	87,87,87,87	0
7	MG	D	9001	1/1	1.00	0.01	67,67,67,67	0
6	ZN	D	7058	1/1	1.00	0.03	109,109,109,109	0

6.5 Other polymers [i](#)

There are no such residues in this entry.