



## Full wwPDB EM Validation Report ⓘ

Apr 16, 2026 – 04:52 pm BST

PDB ID : 29HB / pdb\_000029hb  
EMDB ID : EMD-57170  
Title : Cryo-EM structure of the ClpE/ClpP degradation complex from E.faecalis  
Authors : Carroni, M.; Mogk, A.  
Deposited on : 2026-03-11  
Resolution : 2.80 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

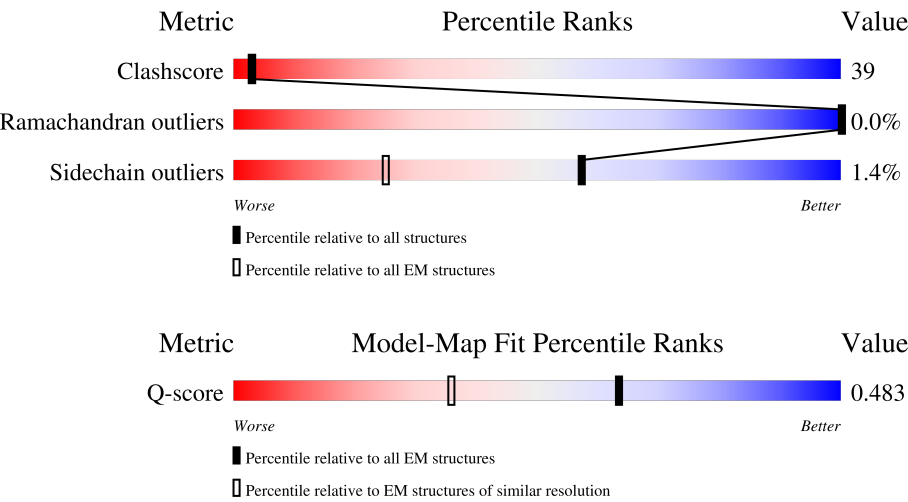
EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
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 i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

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.





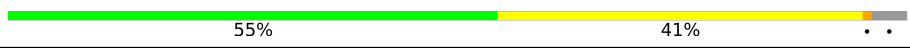

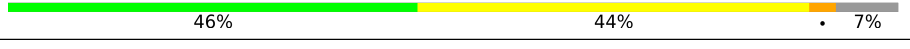


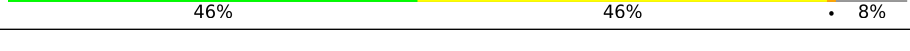
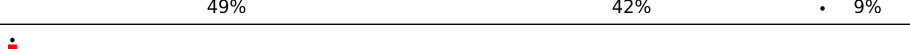
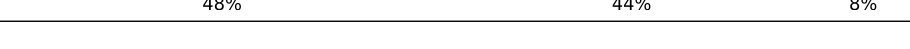
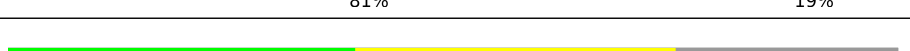
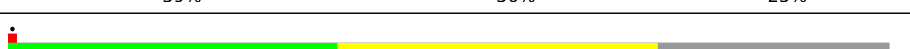
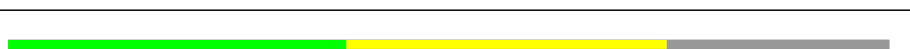
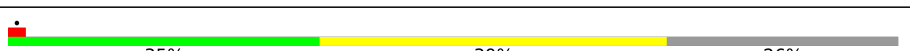
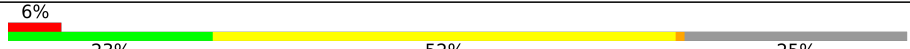
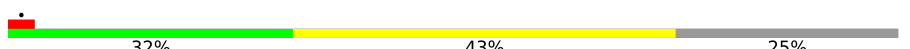

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 ( 2.30 - 3.30 )

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	197	<div><div></div><div>49%</div><div>45%</div><div>..</div></div>
1	B	197	<div><div></div><div>54%</div><div>41%</div><div>..</div></div>
1	C	197	<div><div></div><div>46%</div><div>48%</div><div>..</div></div>
1	D	197	<div><div></div><div>48%</div><div>47%</div><div>..</div></div>

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Mol	Chain	Length	Quality of chain
1	E	197	
1	F	197	
1	G	197	
1	I	197	
1	K	197	
1	L	197	
1	M	197	
1	N	197	
1	S	197	
1	T	197	
2	H	16	
3	a	746	
3	b	746	
3	c	746	
3	d	746	
3	e	746	
3	f	746	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ATP	f	801	-	-	X	-
4	ATP	f	802	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 46198 atoms, of which 28 are hydrogens and 0 are deuteriums.

In the tables below, 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 ATP-dependent Clp protease proteolytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	189	Total	C	N	O	S	0	0
			1449	908	248	286	7		
1	B	189	Total	C	N	O	S	0	0
			1438	900	247	285	6		
1	C	189	Total	C	N	O	S	0	0
			1433	895	244	287	7		
1	D	189	Total	C	N	O	S	0	0
			1443	903	245	288	7		
1	E	189	Total	C	N	O	S	0	0
			1443	900	249	287	7		
1	F	189	Total	C	N	O	S	0	0
			1427	893	243	285	6		
1	G	189	Total	C	N	O	S	0	0
			1430	892	244	287	7		
1	I	185	Total	C	N	O	S	0	0
			1385	868	236	275	6		
1	K	183	Total	C	N	O	S	0	0
			1395	877	236	275	7		
1	L	180	Total	C	N	O	S	0	0
			1367	860	230	270	7		
1	M	181	Total	C	N	O	S	0	0
			1377	865	237	269	6		
1	N	182	Total	C	N	O	S	0	0
			1387	872	235	274	6		
1	S	180	Total	C	N	O	S	0	0
			1363	859	229	269	6		
1	T	181	Total	C	N	O	S	0	0
			1354	847	231	269	7		

- Molecule 2 is a protein called unknown substrate bound to ClpE/ClpP.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	16	Total	C	H	N	O	0	0
			108	48	28	16	16		

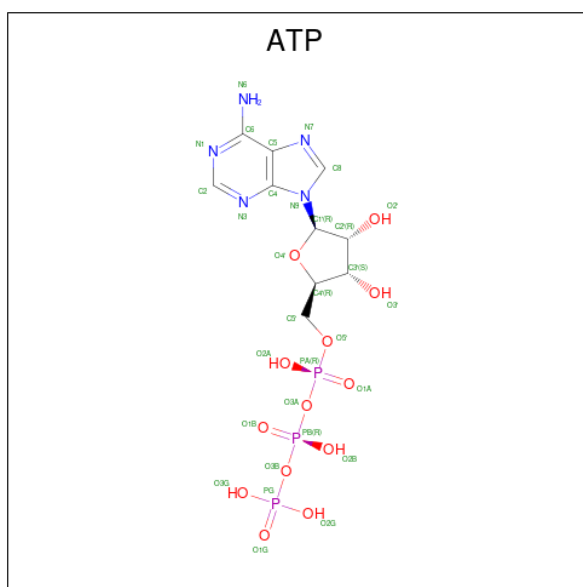
- Molecule 3 is a protein called ATP-dependent Clp protease, ATP-binding subunit ClpE.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	b	553	Total	C	N	O	S	0	0
			4304	2708	747	837	12		
3	c	561	Total	C	N	O	S	0	0
			4360	2744	756	848	12		
3	d	555	Total	C	N	O	S	0	0
			4321	2723	748	838	12		
3	a	563	Total	C	N	O	S	0	0
			4368	2748	758	850	12		
3	e	563	Total	C	N	O	S	0	0
			4368	2748	758	850	12		
3	f	563	Total	C	N	O	S	0	0
			4368	2748	758	850	12		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	550	VAL	ILE	conflict	UNP Q837W9
b	656	SER	GLY	conflict	UNP Q837W9
c	550	VAL	ILE	conflict	UNP Q837W9
c	656	SER	GLY	conflict	UNP Q837W9
d	550	VAL	ILE	conflict	UNP Q837W9
d	656	SER	GLY	conflict	UNP Q837W9
a	550	VAL	ILE	conflict	UNP Q837W9
a	656	SER	GLY	conflict	UNP Q837W9
e	550	VAL	ILE	conflict	UNP Q837W9
e	656	SER	GLY	conflict	UNP Q837W9
f	550	VAL	ILE	conflict	UNP Q837W9
f	656	SER	GLY	conflict	UNP Q837W9

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	b	1	Total 31	C 10	N 5	O 13	P 3	0
4	c	1	Total 31	C 10	N 5	O 13	P 3	0
4	c	1	Total 31	C 10	N 5	O 13	P 3	0
4	d	1	Total 31	C 10	N 5	O 13	P 3	0
4	d	1	Total 31	C 10	N 5	O 13	P 3	0
4	d	1	Total 31	C 10	N 5	O 13	P 3	0
4	a	1	Total 31	C 10	N 5	O 13	P 3	0
4	a	1	Total 31	C 10	N 5	O 13	P 3	0
4	f	1	Total 31	C 10	N 5	O 13	P 3	0
4	f	1	Total 31	C 10	N 5	O 13	P 3	0

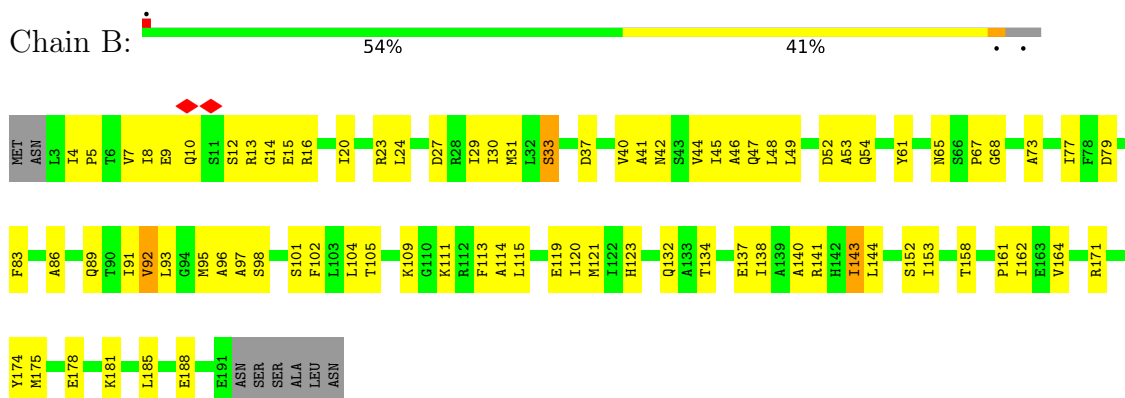
### 3 Residue-property plots [i](#)

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

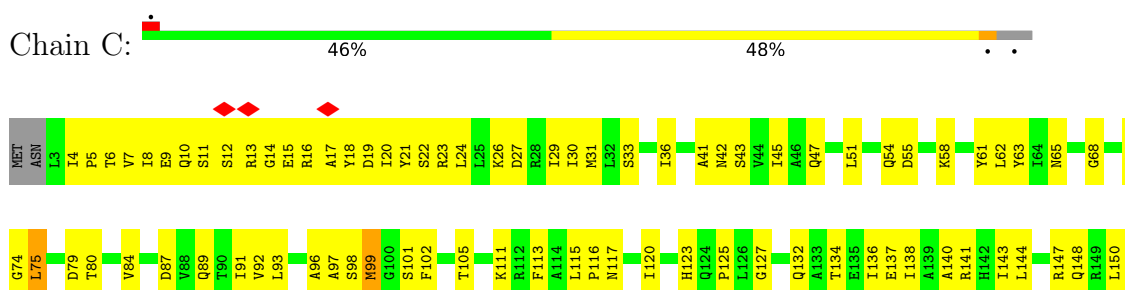
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



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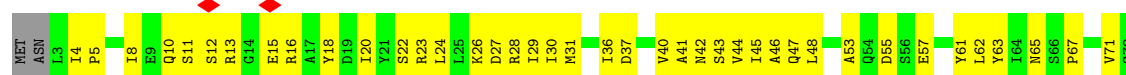


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

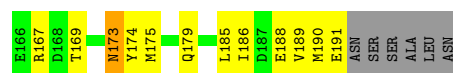




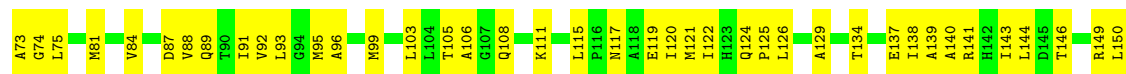
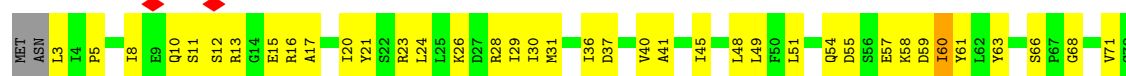
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



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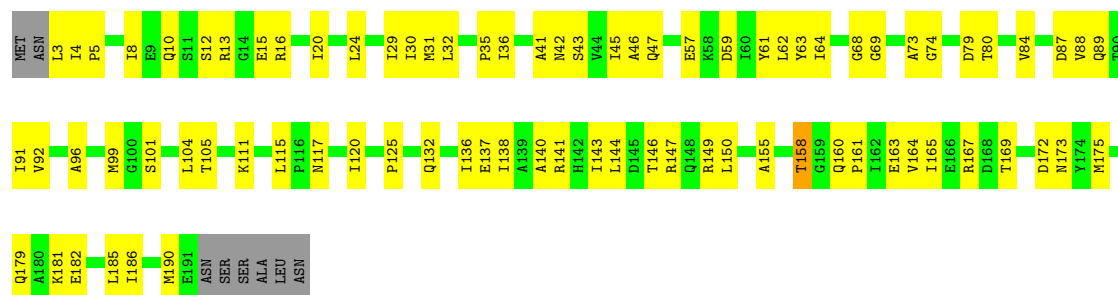
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



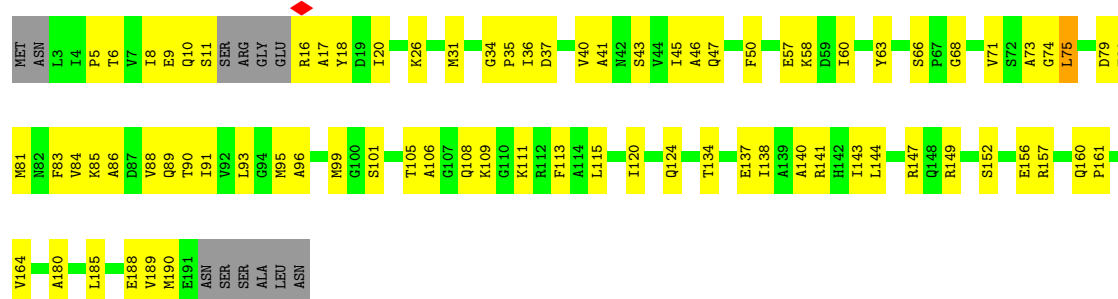
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



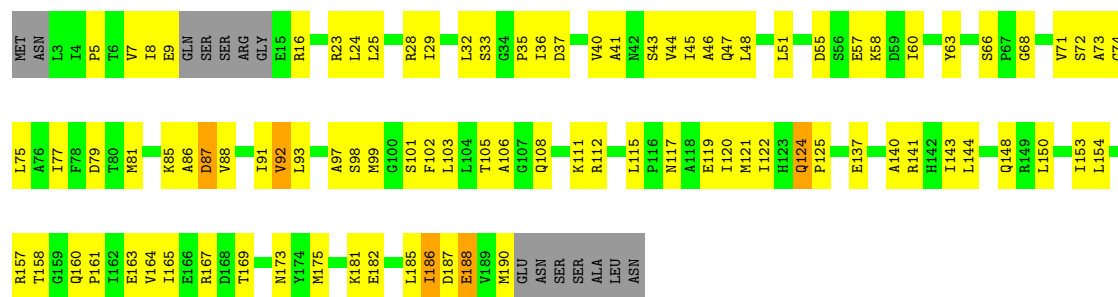




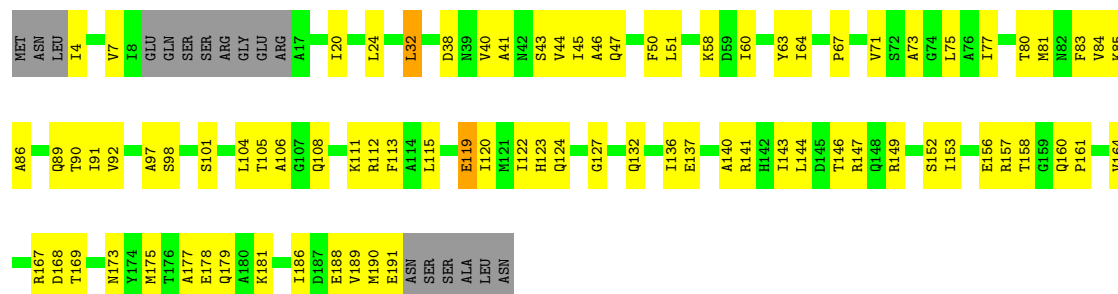
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



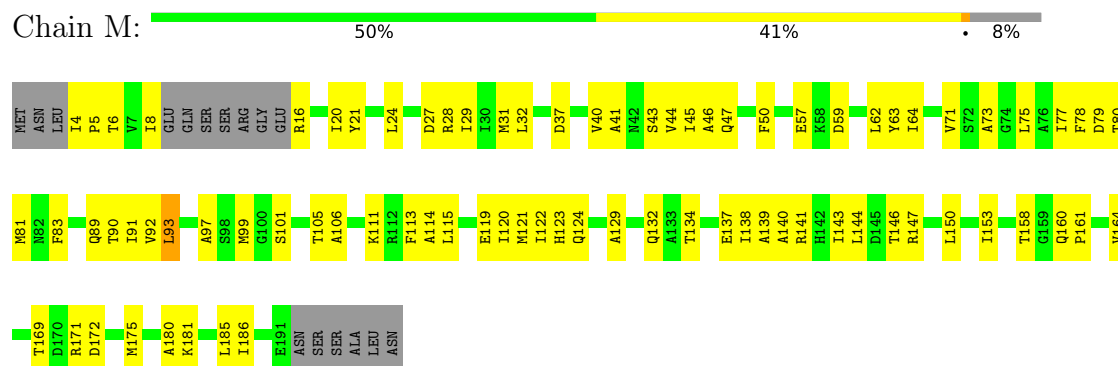
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



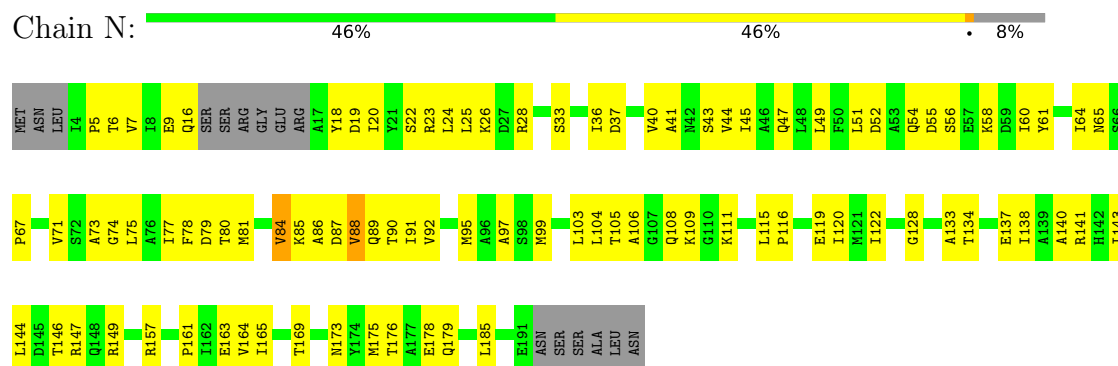
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



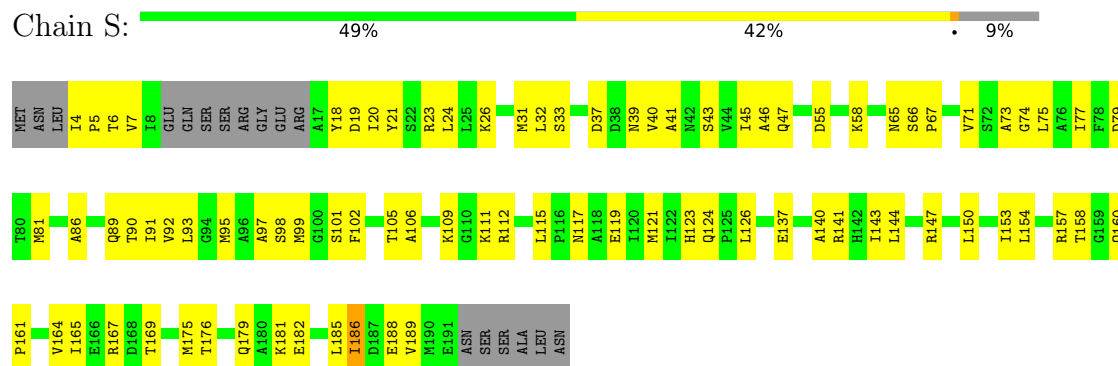
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



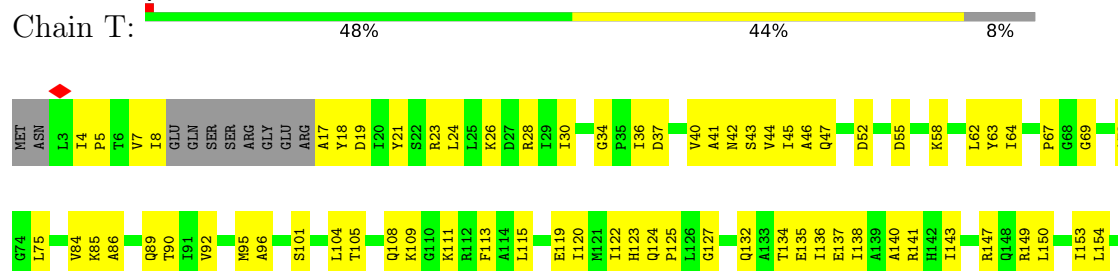
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

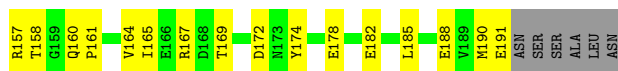


- Molecule 1: ATP-dependent Clp protease proteolytic subunit



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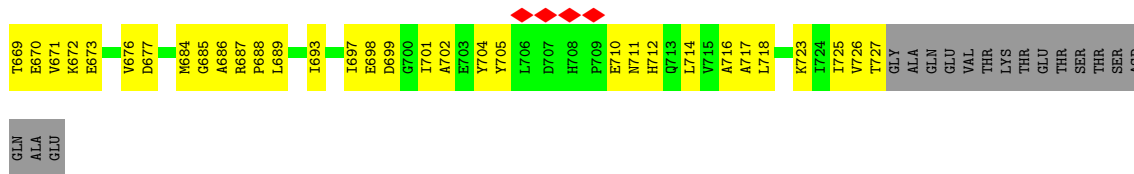
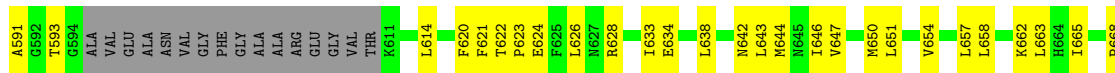
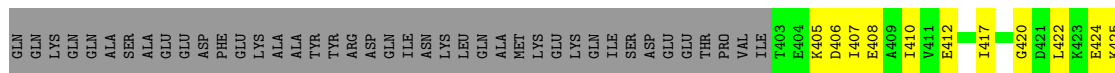
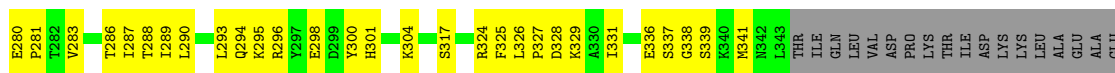
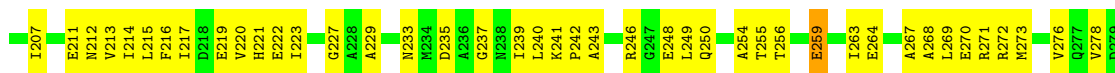
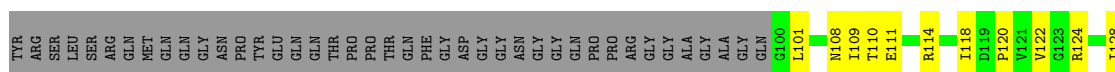
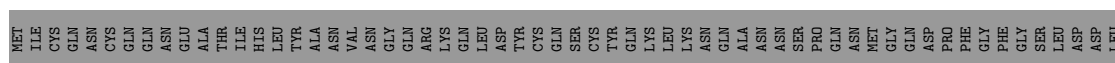
- Molecule 2: unknown substrate bound to ClpE/ClpP

Chain H: 81% 19%



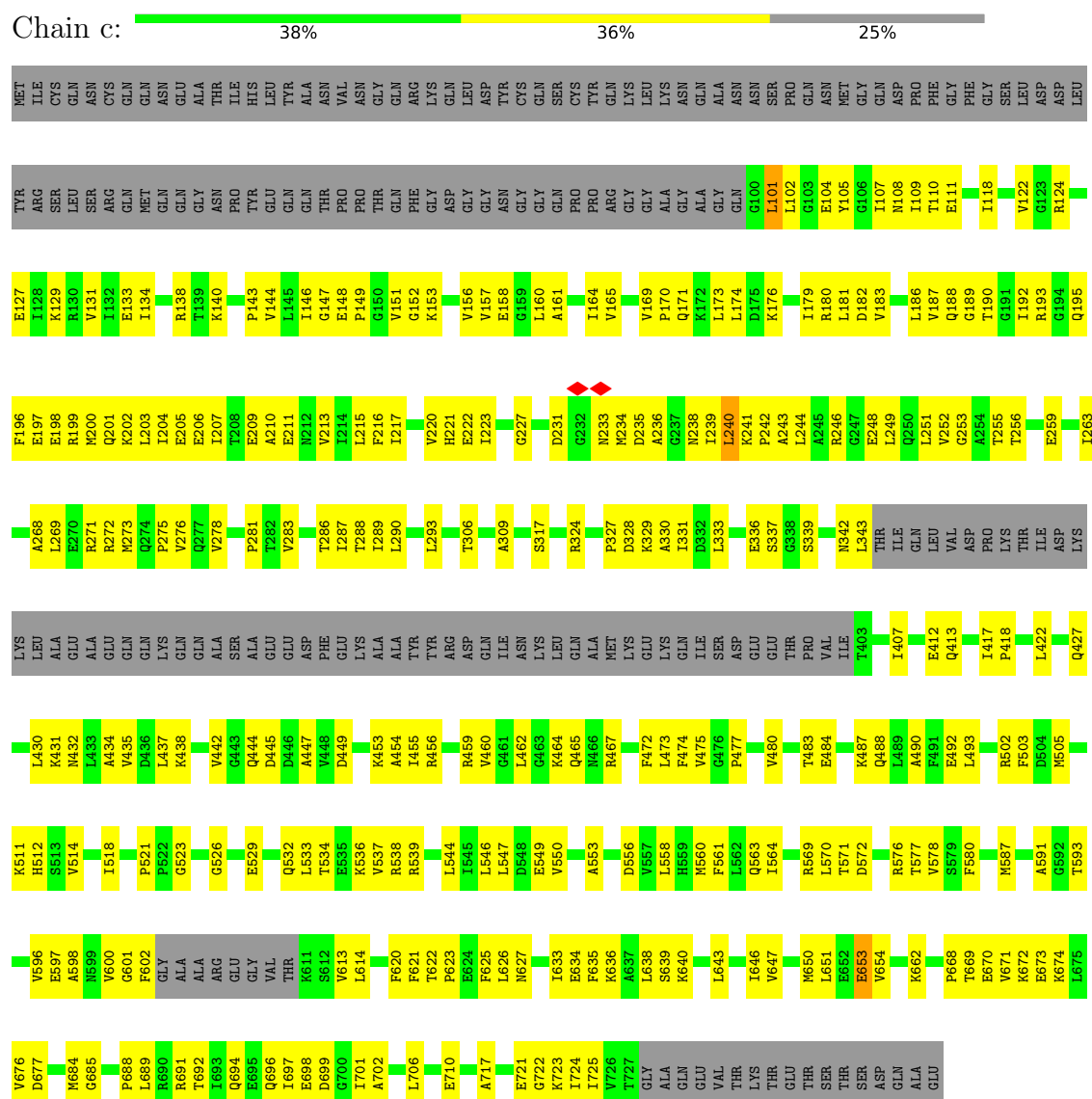
- Molecule 3: ATP-dependent Clp protease, ATP-binding subunit ClpE

Chain b: 37% 36% 26%



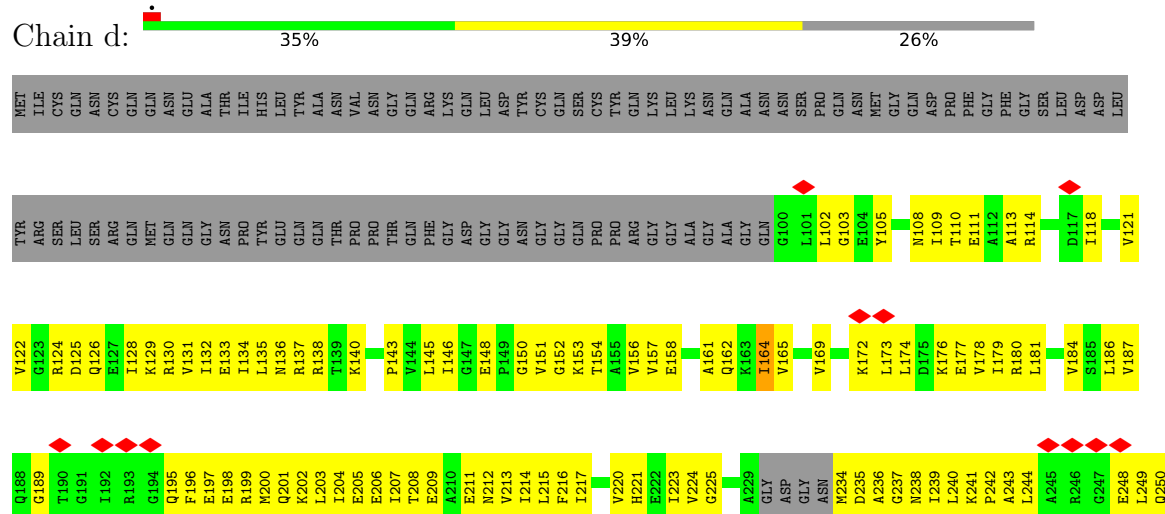
- Molecule 3: ATP-dependent Clp protease, ATP-binding subunit ClpE

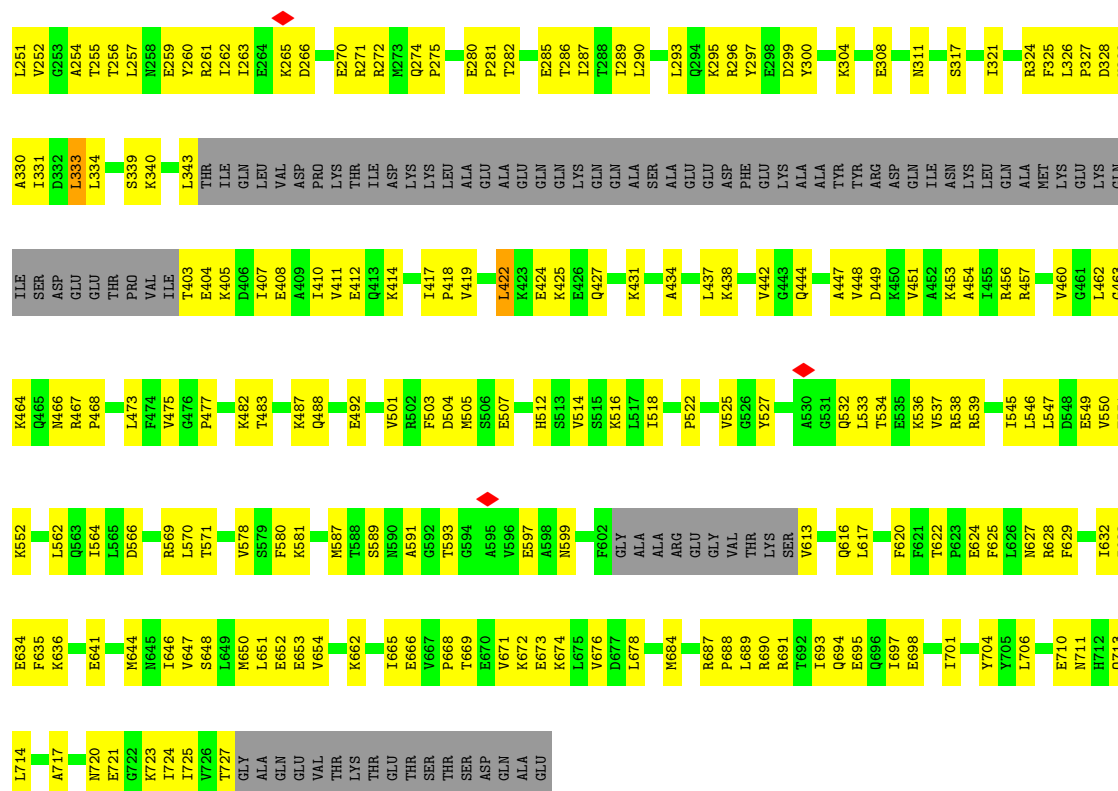
Chain c:



• Molecule 3: ATP-dependent Clp protease, ATP-binding subunit ClpE

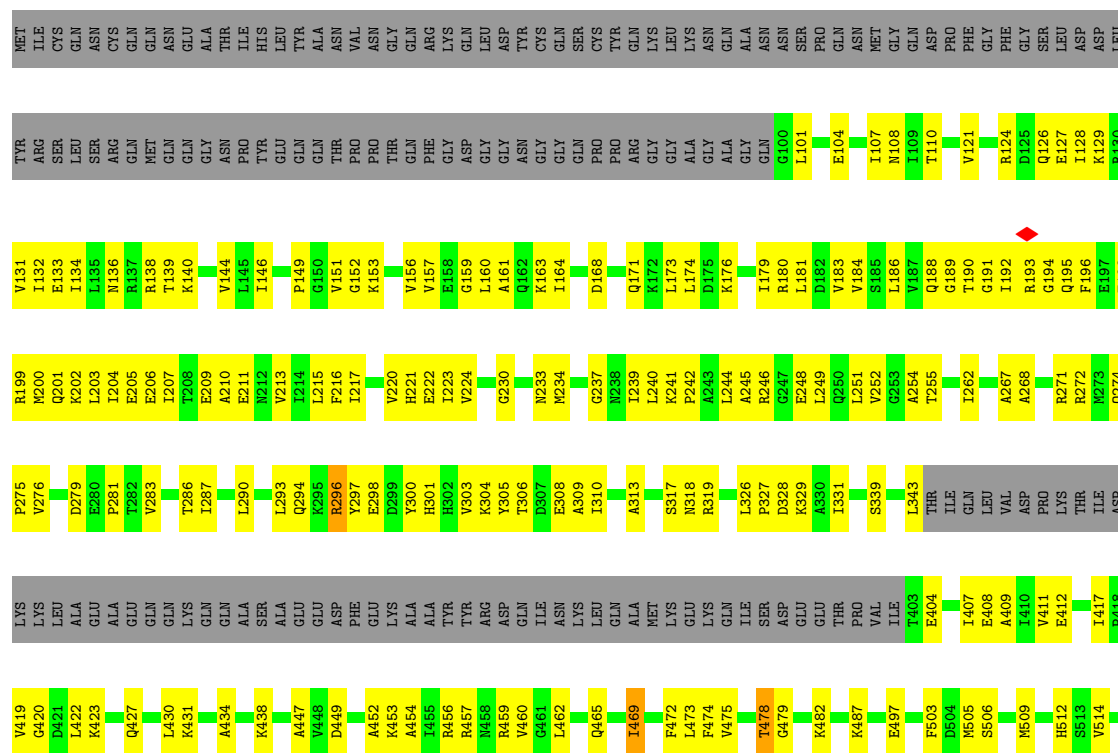
Chain d:

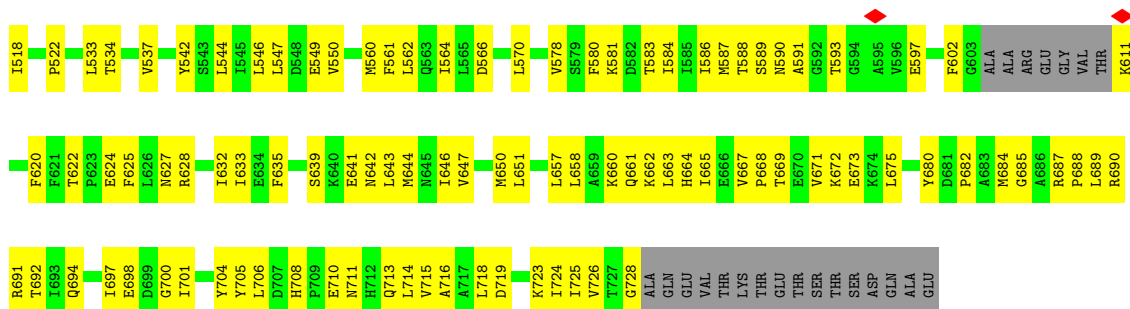




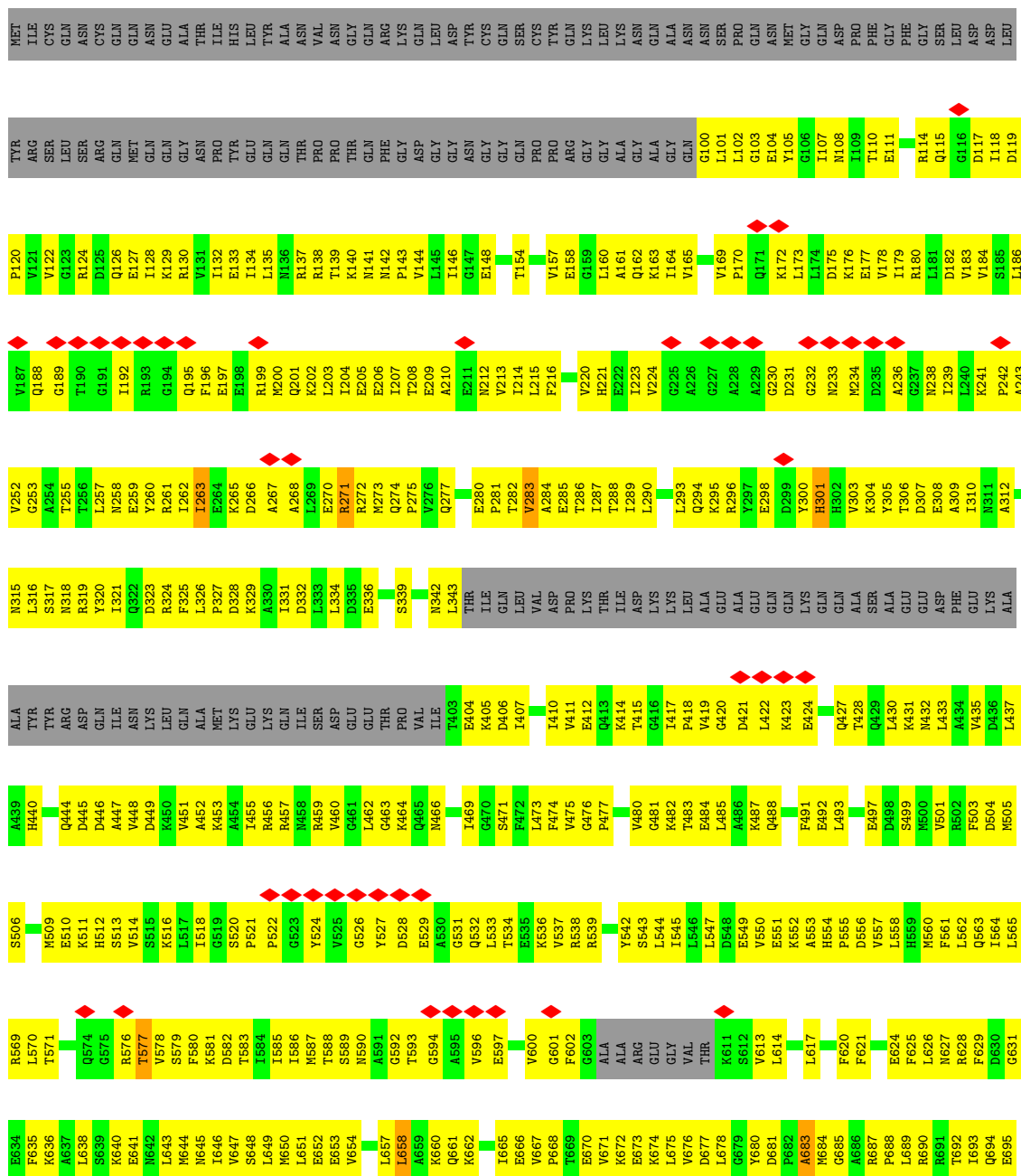
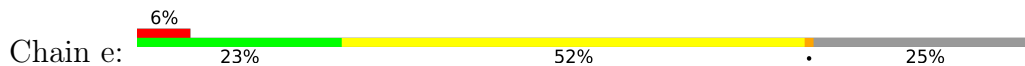
• Molecule 3: ATP-dependent Clp protease, ATP-binding subunit ClpE

Chain a:





• Molecule 3: ATP-dependent Clp protease, ATP-binding subunit ClpE



Q696	Q123	Q124	Q127	Q128	Q129	Q130	Q131	Q132	Q133	Q134	Q135	Q136	Q137	Q138	Q139	Q140	Q143	Q144	Q145	Q146	Q147	Q151	Q152	Q153	Q154	Q155	Q156	Q157	Q158	Q159	Q160	Q161	Q162	Q163	Q164	Q165	Q169	Q170	Q171	Q172	Q173	Q174	Q175	Q176	Q177	Q178	Q179	Q180	Q181	Q182	Q183	Q184	Q185	Q186	Q187	Q188	Q189	Q190	Q191	Q192	Q193	Q194	Q195	Q196	Q197	Q198	Q199	Q200	Q201	Q202	Q203	Q204	Q205	Q206	Q207	Q208	Q209	Q210	Q211	Q212	Q213	Q216	Q217	Q218	Q219	Q220	Q221	Q222	Q223	Q224	Q225	Q226	Q229	Q230	Q231	Q232	Q233	Q234	Q235	Q239	Q240	Q241	Q242	Q243	Q244	Q245	Q246	Q247	Q248	Q249	Q250	Q251	Q256	Q257	Q258	Q259	Q260	Q261	Q262	Q263	Q264	Q267	Q268	Q271	Q272	Q275	Q276	Q277	Q278	Q281	Q282	Q283	Q284	Q285	Q286	Q287	Q288	Q289	Q290	Q291	Q292	Q293	Q294	Q295	Q298	Q299	Q300	Q301	Q302	Q303	Q304	Q305	Q306	Q307	Q308	Q309	Q316	Q317	Q320	Q323	Q324	Q325	Q326	Q327	Q328	Q329	Q330	Q331	Q335	Q336	Q337	Q341	Q342	Q343	Q344	Q345	Q346	Q347	Q348	Q349	Q350	Q351	Q352	Q353	Q354	Q355	Q356	Q357	Q358	Q359	Q360	Q361	Q362	Q363	Q364	Q365	Q366	Q367	Q368	Q369	Q370	Q371	Q372	Q373	Q374	Q375	Q376	Q377	Q378	Q379	Q380	Q381	Q382	Q383	Q384	Q385	Q386	Q387	Q388	Q389	Q390	Q391	Q392	Q393	Q394	Q395	Q396	Q397	Q398	Q399	Q400	Q401	Q402	Q403	Q404	Q405	Q406	Q407	Q408	Q409	Q410	Q411	Q412	Q413	Q414	Q415	Q416	Q417	Q418	Q419	Q420	Q421	Q422	Q423	Q424	Q428	Q429	Q430	Q431	Q432	Q433	Q434	Q435	Q438	Q444	Q445	Q446	Q447	Q448	Q449	Q450	Q451	Q454	Q455	Q456	Q457	Q458	Q459	Q460	Q461	Q462	Q463	Q464	Q465	Q466	Q467	Q468	Q469	Q470	Q471	Q472	Q473	Q474	Q475	Q479	Q482	Q483	Q484	Q488	Q489	Q492	Q493	Q497	Q500	Q501	Q502	Q503	Q504	Q505	Q510	Q511	Q512	Q513	Q514	Q515	Q516	Q517	Q518	Q521	Q522	Q523	Q524	Q525	Q526	Q527	Q528	Q529	Q530	Q533	Q534	Q535	Q536	Q537	Q538	Q539	Q542	Q543	Q544	Q545	Q546	Q547	Q548	Q549	Q550	Q551	Q552	Q553	Q554	Q555	Q556	Q557	Q560	Q561	Q562	Q563	Q564	Q565	Q566	Q569	Q570	Q571	Q572	Q573	Q574	Q575	Q576	Q577	Q578	Q579	Q580	Q581	Q582	Q583	Q584	Q585	Q586	Q587	Q592	Q593	Q594	Q595	Q596	Q597	Q598	Q599	Q600	Q601	Q602	Q603	Q604	Q605	Q606	Q607	Q608	Q609	Q610	Q611	Q612	Q613	Q614	Q615	Q616	Q617	Q620	Q623	Q624	Q625	Q628	Q633	Q634	Q635	Q640	Q641	Q642	Q643	Q644	Q645	Q646	Q647	Q650	Q651	Q652	Q653	Q654	Q655	Q656	Q657	Q658	Q659	Q660	Q661	Q662	Q663	Q664	Q665	Q666	Q667	Q668	Q669	Q670	Q671	Q672	Q673	Q674	Q675	Q678	Q679	Q680	Q684	Q685	Q686	Q687	Q688	Q689	Q690	Q691	Q692	Q693	Q694	Q695	Q696	Q697	Q698	Q699	Q700	Q701	Q702	Q703	Q704	Q705	Q706	Q713	Q714	Q715	Q716	Q717	Q718	Q719	Q720	Q721	Q724	Q725	Q726	Q727	Q728	Q729	Q730	Q731	Q732	Q733	Q734	Q735	Q736	Q737	Q738	Q739	Q740	Q741	Q742	Q743	Q744	Q745	Q746	Q747	Q748	Q749	Q750	Q751	Q752	Q753	Q754	Q755	Q756	Q757	Q758	Q759	Q760	Q761	Q762	Q763	Q764	Q765	Q766	Q767	Q768	Q769	Q770	Q771	Q772	Q773	Q774	Q775	Q776	Q777	Q778	Q779	Q780	Q781	Q782	Q783	Q784	Q785	Q786	Q787	Q788	Q789	Q790	Q791	Q792	Q793	Q794	Q795	Q796	Q797	Q798	Q799	Q800	Q801	Q802	Q803	Q804	Q805	Q806	Q807	Q808	Q809	Q810	Q811	Q812	Q813	Q814	Q815	Q816	Q817	Q818	Q819	Q820	Q821	Q822	Q823	Q824	Q825	Q826	Q827	Q828	Q829	Q830	Q831	Q832	Q833	Q834	Q835	Q836	Q837	Q838	Q839	Q840	Q841	Q842	Q843	Q844	Q845	Q846	Q847	Q848	Q849	Q850	Q851	Q852	Q853	Q854	Q855	Q856	Q857	Q858	Q859	Q860	Q861	Q862	Q863	Q864	Q865	Q866	Q867	Q868	Q869	Q870	Q871	Q872	Q873	Q874	Q875	Q876	Q877	Q878	Q879	Q880	Q881	Q882	Q883	Q884	Q885	Q886	Q887	Q888	Q889	Q890	Q891	Q892	Q893	Q894	Q895	Q896	Q897	Q898	Q899	Q900	Q901	Q902	Q903	Q904	Q905	Q906	Q907	Q908	Q909	Q910	Q911	Q912	Q913	Q914	Q915	Q916	Q917	Q918	Q919	Q920	Q921	Q922	Q923	Q924	Q925	Q926	Q927	Q928	Q929	Q930	Q931	Q932	Q933	Q934	Q935	Q936	Q937	Q938	Q939	Q940	Q941	Q942	Q943	Q944	Q945	Q946	Q947	Q948	Q949	Q950	Q951	Q952	Q953	Q954	Q955	Q956	Q957	Q958	Q959	Q960	Q961	Q962	Q963	Q964	Q965	Q966	Q967	Q968	Q969	Q970	Q971	Q972	Q973	Q974	Q975	Q976	Q977	Q978	Q979	Q980	Q981	Q982	Q983	Q984	Q985	Q986	Q987	Q988	Q989	Q990	Q991	Q992	Q993	Q994	Q995	Q996	Q997	Q998	Q999	Q1000	Q1001	Q1002	Q1003	Q1004	Q1005	Q1006	Q1007	Q1008	Q1009	Q1010	Q1011	Q1012	Q1013	Q1014	Q1015	Q1016	Q1017	Q1018	Q1019	Q1020	Q1021	Q1022	Q1023	Q1024	Q1025	Q1026	Q1027	Q1028	Q1029	Q1030	Q1031	Q1032	Q1033	Q1034	Q1035	Q1036	Q1037	Q1038	Q1039	Q1040	Q1041	Q1042	Q1043	Q1044	Q1045	Q1046	Q1047	Q1048	Q1049	Q1050	Q1051	Q1052	Q1053	Q1054	Q1055	Q1056	Q1057	Q1058	Q1059	Q1060	Q1061	Q1062	Q1063	Q1064	Q1065	Q1066	Q1067	Q1068	Q1069	Q1070	Q1071	Q1072	Q1073	Q1074	Q1075	Q1076	Q1077	Q1078	Q1079	Q1080	Q1081	Q1082	Q1083	Q1084	Q1085	Q1086	Q1087	Q1088	Q1089	Q1090	Q1091	Q1092	Q1093	Q1094	Q1095	Q1096	Q1097	Q1098	Q1099	Q1100	Q1101	Q1102	Q1103	Q1104	Q1105	Q1106	Q1107	Q1108	Q1109	Q1110	Q1111	Q1112	Q1113	Q1114	Q1115	Q1116	Q1117	Q1118	Q1119	Q1120	Q1121	Q1122	Q1123	Q1124	Q1125	Q1126	Q1127	Q1128	Q1129	Q1130	Q1131	Q1132	Q1133	Q1134	Q1135	Q1136	Q1137	Q1138	Q1139	Q1140	Q1141	Q1142	Q1143	Q1144	Q1145	Q1146	Q1147	Q1148	Q1149	Q1150	Q1151	Q1152	Q1153	Q1154	Q1155	Q1156	Q1157	Q1158	Q1159	Q1160	Q1161	Q1162	Q1163	Q1164	Q1165	Q1166	Q1167	Q1168	Q1169	Q1170	Q1171	Q1172	Q1173	Q1174	Q1175	Q1176	Q1177	Q1178	Q1179	Q1180	Q1181	Q1182	Q1183	Q1184	Q1185	Q1186	Q1187	Q1188	Q1189	Q1190	Q1191	Q1192	Q1193	Q1194	Q1195	Q1196	Q1197	Q1198	Q1199	Q1200	Q1201	Q1202	Q1203	Q1204	Q1205	Q1206	Q1207	Q1208	Q1209	Q1210	Q1211	Q1212	Q1213	Q1216	Q1217	Q1218	Q1219	Q1220	Q1221	Q1222	Q1223	Q1224	Q1225	Q1226	Q1229	Q1230	Q1231	Q1232	Q1233	Q1234	Q1235	Q1239	Q1240	Q1241	Q1242	Q1243	Q1244	Q1245	Q1246	Q1247	Q1248	Q1249	Q1250	Q1251	Q1256	Q1257	Q1258	Q1259	Q1260	Q1261	Q1262	Q1263	Q1264	Q1267	Q1268	Q1269	Q1270	Q1271	Q1272	Q1273	Q1274	Q1275	Q1276	Q1277	Q1278	Q1279	Q1280	Q1281	Q1282	Q1283	Q1284	Q1285	Q1286	Q1287	Q1288	Q1289	Q1290	Q1291	Q1292	Q1293	Q1294	Q1295	Q1298	Q1299	Q1300	Q1301	Q1302	Q1303	Q1304	Q1305	Q1306	Q1307	Q1308	Q1309	Q1316	Q1317	Q1320	Q1323	Q1324	Q1325	Q1326	Q1327	Q1328	Q1329	Q1330	Q1331	Q1335	Q1336	Q1337	Q1341	Q1342	Q1343	Q1344	Q1345	Q1346	Q1347	Q1348	Q1349	Q1350	Q1351	Q1352	Q1353	Q1354	Q1355	Q1356	Q1357	Q1358	Q1359	Q1360	Q1361	Q1362	Q1363	Q1364	Q1365	Q1366	Q1367	Q1368	Q1369	Q1370	Q1371	Q1372	Q1373	Q1374	Q1375	Q1376	Q1377	Q1378	Q1379	Q1380	Q1381	Q1382	Q1383	Q1384	Q1385	Q1386	Q1387	Q1388	Q1389	Q1390	Q1391	Q1392	Q1393	Q1394	Q1395	Q1396	Q1397	Q1398	Q1399	Q1400	Q1401	Q1402	Q1403	Q1404	Q1405	Q1406	Q1407	Q1408	Q1409	Q1410	Q1411	Q1412	Q1413	Q1414	Q1415	Q1416	Q1417	Q1418	Q1419	Q1420	Q1421	Q1422	Q1423	Q1424	Q1428	Q1429	Q1430	Q1431	Q1432	Q1433	Q1434	Q1435	Q1438	Q1444	Q1445	Q1446	Q1447	Q1448	Q1449	Q1450	Q1451	Q1454	Q1455	Q1456	Q1457	Q1458	Q1459	Q1460	Q1461	Q1462	Q1463	Q1464	Q1465	Q1466	Q1467	Q1468	Q1469	Q1470	Q1471	Q1472	Q1473	Q1474	Q1475	Q1479	Q1482	Q1483	Q1484	Q1488	Q1489	Q1492	Q1493	Q1497	Q1500	Q1501	Q1502	Q1503	Q1504	Q1505	Q1510	Q1511	Q1512	Q1513	Q1514	Q1515	Q1516	Q1517	Q1518	Q1521	Q1522	Q1523	Q1524	Q1525	Q1526	Q1527	Q1528	Q1529	Q1530	Q1533	Q1534	Q1535	Q1536	Q1537	Q1538	Q1539	Q1542	Q1543	Q1544	Q1545	Q1546	Q1547	Q1548	Q1549	Q1550	Q1551	Q1552	Q1553	Q1554	Q1555	Q1556	Q1557	Q1560	Q1561	Q1562	Q1563	Q1564	Q1565	Q1566	Q1569	Q1570	Q1571	Q1572	Q1573	Q1574	Q1575	Q1576	Q1577	Q1578	Q1579	Q1580	Q1581	Q1582	Q1583	Q1584	Q1585	Q1586	Q1587	Q1592	Q1593	Q1594	Q1595	Q1596	Q1597	Q1598	Q1599	Q1600	Q1601	Q1602	Q1603	Q1604	Q1605	Q1606	Q1607	Q1608	Q1609	Q1610	Q1611	Q1612	Q1613	Q1614	Q1615	Q1616	Q1617	Q1620</
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## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	556680	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	0.471	Depositor
Minimum map value	-0.191	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.063	Depositor
Map size (Å)	396.0, 396.0, 396.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	Depositor



## 5 Model quality

### 5.1 Standard geometry

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

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	0.13	0/1467	0.34	0/1983
1	B	0.13	0/1456	0.40	0/1972
1	C	0.13	0/1451	0.38	0/1965
1	D	0.13	0/1461	0.34	0/1978
1	E	0.14	0/1460	0.38	0/1974
1	F	0.15	0/1444	0.37	0/1956
1	G	0.14	0/1447	0.40	1/1960 (0.1%)
1	I	0.12	0/1401	0.35	0/1897
1	K	0.14	0/1411	0.37	0/1908
1	L	0.12	0/1383	0.35	0/1871
1	M	0.13	0/1393	0.35	0/1884
1	N	0.13	0/1404	0.39	0/1901
1	S	0.13	0/1380	0.34	0/1870
1	T	0.14	0/1368	0.39	0/1852
3	a	0.14	0/4425	0.39	0/5973
3	b	0.13	0/4359	0.38	0/5882
3	c	0.13	0/4416	0.38	0/5960
3	d	0.14	0/4376	0.39	0/5906
3	e	0.15	0/4425	0.46	2/5973 (0.0%)
3	f	0.14	0/4425	0.42	0/5973
All	All	0.14	0/46352	0.39	3/62638 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	e	271	ARG	CA-CB-CG	6.58	127.27	114.10
1	G	158	THR	N-CA-C	-5.30	108.07	114.75
3	e	683	ALA	N-CA-C	-5.12	108.30	114.75

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1449	0	1449	101	0
1	B	1438	0	1422	101	0
1	C	1433	0	1404	131	0
1	D	1443	0	1428	113	0
1	E	1443	0	1434	99	0
1	F	1427	0	1410	117	0
1	G	1430	0	1406	102	0
1	I	1385	0	1358	95	0
1	K	1395	0	1396	111	0
1	L	1367	0	1366	97	0
1	M	1377	0	1379	101	0
1	N	1387	0	1376	113	0
1	S	1363	0	1351	96	0
1	T	1354	0	1331	100	0
2	H	80	28	21	4	0
3	a	4368	0	4414	315	0
3	b	4304	0	4358	327	0
3	c	4360	0	4407	314	0
3	d	4321	0	4372	401	0
3	e	4368	0	4415	580	0
3	f	4368	0	4417	434	0
4	a	62	0	22	1	0
4	b	31	0	12	4	0
4	c	62	0	24	5	0
4	d	93	0	35	12	0
4	f	62	0	24	26	0
All	All	46170	28	46031	3554	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 39.

All (3554) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:89:GLN:HB3	1:F:111:LYS:HB3	1.25	1.14
3:e:538:ARG:HG3	3:e:578:VAL:HG12	1.26	1.13
1:I:11:SER:HB2	1:T:8:ILE:HB	1.24	1.12
1:F:10:GLN:HB3	1:F:15:GLU:HB3	1.17	1.12
3:c:723:LYS:HA	3:c:723:LYS:HE3	1.31	1.11
3:f:341:MET:HA	3:f:341:MET:HE3	1.31	1.10
1:B:53:ALA:HB3	3:f:599:ASN:HB3	1.31	1.10
3:e:715:VAL:H	3:e:728:GLY:HA2	1.17	1.09
3:e:197:GLU:HA	3:e:200:MET:HE2	1.33	1.09
3:e:170:PRO:HG2	3:e:173:LEU:HD13	1.14	1.08
3:a:714:LEU:HD21	3:a:726:VAL:HB	1.34	1.07
3:e:290:LEU:HD22	3:e:334:LEU:HD11	1.38	1.05
1:T:90:THR:HG21	1:T:104:LEU:HA	1.38	1.04
3:a:694:GLN:HA	3:a:698:GLU:HG3	1.35	1.04
3:e:234:MET:HA	3:e:234:MET:HE2	1.34	1.04
3:a:191:GLY:HA2	3:f:192:ILE:HG12	1.39	1.04
1:C:91:ILE:HG22	1:C:113:PHE:HB2	1.38	1.03
1:K:122:ILE:HD12	1:K:169:THR:HG22	1.40	1.03
1:S:109:LYS:HE2	1:S:109:LYS:HA	1.40	1.02
1:F:115:LEU:HD12	1:G:79:ASP:HB3	1.39	1.02
1:N:115:LEU:HD12	1:S:79:ASP:HB3	1.40	1.02
1:G:137:GLU:HG3	1:L:144:LEU:HD11	1.39	1.01
3:b:447:ALA:HB2	3:b:633:ILE:HG21	1.42	1.01
1:I:108:GLN:HE21	1:I:111:LYS:HD2	1.21	1.01
1:T:109:LYS:HA	1:T:109:LYS:HE2	1.41	1.01
3:e:114:ARG:HA	3:e:165:VAL:HG21	1.39	1.00
1:E:92:VAL:HG23	1:E:104:LEU:HD13	1.40	0.99
3:f:686:ALA:HA	3:f:689:LEU:HD23	1.39	0.99
3:a:697:ILE:O	3:a:701:ILE:HD12	1.62	0.99
3:e:132:ILE:HD11	3:e:160:LEU:HD21	1.40	0.99
3:f:714:LEU:HD22	3:f:728:GLY:HA3	1.45	0.99
3:b:267:ALA:HB3	3:c:149:PRO:HG2	1.45	0.98
1:I:8:ILE:HA	1:I:16:ARG:HA	1.42	0.98
3:b:191:GLY:HA2	3:a:192:ILE:HD11	1.42	0.98
1:T:122:ILE:HD12	1:T:169:THR:HG22	1.44	0.98
3:e:636:LYS:HD3	3:e:636:LYS:H	1.28	0.98
3:c:221:HIS:HA	3:c:263:ILE:HD11	1.46	0.98
3:a:662:LYS:HE2	3:a:662:LYS:HA	1.44	0.98
3:e:649:LEU:HA	3:e:652:GLU:HG2	1.43	0.98
1:N:89:GLN:HB3	1:N:111:LYS:HB3	1.42	0.97
1:G:105:THR:HG21	1:G:185:LEU:HD22	1.43	0.97
3:c:207:ILE:HD13	3:c:249:LEU:HB2	1.47	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:e:665:ILE:HD11	3:e:716:ALA:HB2	1.44	0.96
3:d:281:PRO:HG2	3:d:327:PRO:HD3	1.47	0.96
3:e:197:GLU:HG3	3:e:234:MET:HE1	1.47	0.96
3:f:153:LYS:HB2	4:f:802:ATP:O3B	1.65	0.96
1:G:92:VAL:HG23	1:G:104:LEU:HD13	1.44	0.96
3:a:179:ILE:HD13	3:a:213:VAL:HG23	1.46	0.95
3:f:596:VAL:HG22	3:f:616:GLN:HG3	1.45	0.95
3:e:453:LYS:HE2	3:e:457:ARG:HD3	1.49	0.95
3:f:667:VAL:HB	3:f:671:VAL:HG11	1.46	0.94
3:b:519:GLY:HA3	3:b:530:ALA:HB1	1.49	0.94
3:e:192:ILE:HG23	3:e:195:GLN:HB3	1.50	0.94
3:d:265:LYS:HA	3:d:265:LYS:HE2	1.48	0.94
3:a:417:ILE:HG12	3:a:542:TYR:HB2	1.48	0.94
1:M:122:ILE:HD12	1:M:175:MET:HE1	1.50	0.93
1:A:105:THR:HG21	1:A:185:LEU:HD22	1.50	0.93
3:f:154:THR:HG23	4:f:802:ATP:PB	2.09	0.93
3:d:477:PRO:HA	3:d:593:THR:HG21	1.51	0.93
1:C:19:ASP:HB3	1:C:22:SER:HB2	1.50	0.93
1:F:8:ILE:HG12	1:F:17:ALA:HB2	1.51	0.93
1:B:105:THR:HG21	1:B:185:LEU:HD22	1.48	0.92
1:G:89:GLN:HB3	1:G:111:LYS:HB3	1.47	0.92
3:d:181:LEU:HG	3:d:215:LEU:HD11	1.52	0.92
3:b:122:VAL:HG11	3:b:288:THR:HG22	1.52	0.92
3:e:140:LYS:HG2	3:e:274:GLN:NE2	1.84	0.92
1:N:77:ILE:HG21	1:N:103:LEU:HD21	1.49	0.92
1:L:90:THR:HG21	1:L:104:LEU:HA	1.48	0.91
1:B:29:ILE:HD13	1:B:61:TYR:HB2	1.52	0.91
3:f:514:VAL:HG13	3:f:560:MET:HE2	1.52	0.91
1:F:41:ALA:HB2	1:F:73:ALA:HB1	1.51	0.91
3:e:562:LEU:HD11	3:e:625:PHE:HE1	1.35	0.91
3:b:144:VAL:HG21	3:b:273:MET:HB3	1.51	0.91
3:c:717:ALA:HB3	3:c:725:ILE:HD11	1.53	0.91
3:e:674:LYS:HE2	3:e:718:LEU:HD11	1.53	0.91
1:T:34:GLY:HA2	1:T:67:PRO:HD2	1.54	0.90
1:N:75:LEU:HG	1:N:149:ARG:HH21	1.36	0.90
1:T:92:VAL:HG23	1:T:104:LEU:HD13	1.52	0.90
3:e:285:GLU:O	3:e:289:ILE:HG13	1.71	0.89
1:N:92:VAL:HG23	1:N:104:LEU:HD13	1.54	0.89
3:f:697:ILE:O	3:f:701:ILE:HG13	1.73	0.89
3:a:244:LEU:HD23	3:a:249:LEU:HD21	1.54	0.89
3:f:714:LEU:HA	3:f:728:GLY:HA3	1.52	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:456:ARG:HD2	3:e:706:LEU:HD11	1.55	0.88
3:e:318:ASN:HB3	3:e:326:LEU:HD11	1.54	0.88
3:e:298:GLU:OE2	3:e:305:TYR:HB2	1.74	0.88
3:b:701:ILE:HG13	3:b:726:VAL:HG23	1.54	0.88
3:d:244:LEU:HD22	3:d:272:ARG:HE	1.39	0.88
1:D:137:GLU:HG3	1:D:141:ARG:HH22	1.39	0.87
3:e:266:ASP:OD1	3:e:270:GLU:HB2	1.73	0.87
3:a:181:LEU:HD21	3:a:203:LEU:HD11	1.53	0.87
3:e:204:ILE:O	3:e:208:THR:HG23	1.75	0.87
3:e:469:ILE:HG13	3:e:582:ASP:HA	1.54	0.87
1:F:10:GLN:HB3	1:F:15:GLU:CB	2.02	0.87
1:E:175:MET:HB2	1:E:179:GLN:HB2	1.57	0.87
3:b:509:MET:O	3:b:509:MET:HE3	1.75	0.86
3:e:265:LYS:HE2	3:e:265:LYS:HA	1.55	0.86
1:E:29:ILE:HD13	1:E:61:TYR:HB2	1.56	0.86
3:b:723:LYS:HA	3:b:723:LYS:HE2	1.54	0.86
3:e:197:GLU:HA	3:e:200:MET:CE	2.05	0.86
1:N:71:VAL:HG13	1:N:99:MET:HE3	1.58	0.86
1:T:153:ILE:O	1:T:157:ARG:HG2	1.75	0.86
3:a:647:VAL:HG22	3:a:689:LEU:HD11	1.56	0.86
3:f:268:ALA:HB1	3:f:272:ARG:HH21	1.37	0.86
3:f:644:MET:HE1	3:f:673:GLU:HA	1.56	0.86
3:f:684:MET:HA	3:f:684:MET:HE2	1.54	0.86
1:N:92:VAL:HG21	1:N:104:LEU:HD22	1.56	0.86
3:f:154:THR:O	3:f:158:GLU:HG3	1.76	0.86
3:c:122:VAL:HG11	3:c:288:THR:HG22	1.58	0.86
3:a:534:THR:HG23	3:a:578:VAL:HG21	1.58	0.86
1:D:132:GLN:HG2	1:S:124:GLN:HG3	1.57	0.86
3:a:204:ILE:HD11	3:a:240:LEU:HD23	1.58	0.85
3:e:475:VAL:HG21	3:e:617:LEU:HD11	1.58	0.85
3:e:643:LEU:HD13	3:e:689:LEU:HD11	1.56	0.85
3:e:208:THR:HB	3:e:248:GLU:HG3	1.58	0.85
1:E:158:THR:HG23	1:E:160:GLN:H	1.41	0.85
3:a:460:VAL:HG23	3:a:462:LEU:HG	1.58	0.85
3:f:201:GLN:O	3:f:205:GLU:HG2	1.77	0.85
3:a:201:GLN:O	3:a:205:GLU:HG2	1.77	0.85
3:c:668:PRO:HG2	3:c:671:VAL:HG23	1.58	0.85
3:b:281:PRO:HG2	3:b:327:PRO:HG3	1.59	0.84
3:e:650:MET:HE3	3:e:693:ILE:HD12	1.59	0.84
3:d:110:THR:HG23	3:d:178:VAL:HG22	1.60	0.84
1:S:18:TYR:HE2	1:S:23:ARG:HG2	1.40	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:151:VAL:HG13	3:d:281:PRO:HD3	1.59	0.84
3:a:138:ARG:HG2	3:a:139:THR:HG23	1.60	0.84
3:a:188:GLN:HG2	3:a:199:ARG:HH22	1.43	0.84
1:D:105:THR:HG21	1:D:185:LEU:HD22	1.58	0.84
3:d:694:GLN:HA	3:d:698:GLU:HG3	1.59	0.84
1:E:93:LEU:HD12	1:F:45:ILE:HD12	1.58	0.83
1:T:89:GLN:HG3	1:T:111:LYS:HB3	1.60	0.83
3:e:241:LYS:HB2	3:e:242:PRO:HD3	1.59	0.83
1:F:29:ILE:HD12	1:F:63:TYR:HE1	1.43	0.83
1:K:97:ALA:HB1	1:K:121:MET:HE3	1.58	0.83
1:G:8:ILE:HG23	1:G:16:ARG:HG3	1.58	0.83
1:L:51:LEU:HD13	1:L:60:ILE:HD12	1.61	0.83
3:b:110:THR:HG21	3:b:177:GLU:HB3	1.59	0.83
3:d:694:GLN:HA	3:d:698:GLU:CG	2.09	0.83
1:D:144:LEU:HD11	1:S:137:GLU:HG3	1.60	0.83
1:E:190:MET:HE1	3:c:602:PHE:HB3	1.60	0.83
1:F:117:ASN:HB2	1:G:149:ARG:HH11	1.43	0.82
3:e:207:ILE:HG12	3:e:213:VAL:HG11	1.58	0.82
3:d:468:PRO:HA	3:d:581:LYS:HA	1.61	0.82
3:c:434:ALA:O	3:c:438:LYS:HG2	1.77	0.82
3:c:550:VAL:HG21	3:c:587:MET:HB3	1.61	0.82
3:d:176:LYS:HG2	3:d:212:ASN:HA	1.59	0.82
3:d:234:MET:HE3	3:d:236:ALA:H	1.45	0.82
3:e:304:LYS:H	3:e:304:LYS:HD3	1.42	0.82
3:e:565:LEU:HB3	3:e:628:ARG:HH22	1.41	0.82
3:e:537:VAL:HG21	3:e:580:PHE:CZ	2.14	0.82
1:E:92:VAL:HG21	1:E:104:LEU:HD22	1.60	0.81
3:e:110:THR:HG21	3:e:177:GLU:HB2	1.61	0.81
3:f:320:TYR:HE2	3:f:419:VAL:HG13	1.45	0.81
1:B:53:ALA:HB1	3:f:600:VAL:HG22	1.62	0.81
3:b:517:LEU:HD12	3:b:560:MET:HE2	1.62	0.81
1:K:23:ARG:HG3	1:K:23:ARG:HH11	1.44	0.81
3:b:304:LYS:H	3:b:304:LYS:HD3	1.45	0.81
1:L:92:VAL:HG23	1:L:104:LEU:HD13	1.62	0.81
3:f:286:THR:O	3:f:290:LEU:HG	1.81	0.81
1:G:92:VAL:HG21	1:G:104:LEU:HD22	1.63	0.81
1:N:108:GLN:HG3	1:N:111:LYS:HG3	1.62	0.81
3:f:428:THR:HA	3:f:431:LYS:HE2	1.61	0.81
1:D:181:LYS:NZ	1:D:188:GLU:HA	1.96	0.80
3:a:101:LEU:HD11	3:a:199:ARG:HG2	1.62	0.80
3:a:668:PRO:HG2	3:a:671:VAL:HG23	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:e:562:LEU:HD11	3:e:625:PHE:CE1	2.15	0.80
3:b:192:ILE:HB	3:b:195:GLN:HB3	1.62	0.80
3:c:281:PRO:HG2	3:c:327:PRO:HG3	1.63	0.80
3:a:647:VAL:CG2	3:a:689:LEU:HD11	2.11	0.80
1:G:120:ILE:HG23	1:G:175:MET:HG3	1.63	0.80
3:b:219:GLU:HA	3:b:255:THR:HG22	1.63	0.80
3:d:566:ASP:OD1	3:d:628:ARG:HD2	1.80	0.80
3:e:223:ILE:HD12	3:e:224:VAL:HG13	1.64	0.80
1:F:122:ILE:HD13	1:F:169:THR:HG22	1.63	0.80
3:b:687:ARG:HE	4:b:801:ATP:H5'1	1.46	0.80
3:d:260:TYR:OH	3:d:275:PRO:HG3	1.80	0.80
1:C:144:LEU:HD11	1:T:137:GLU:HG3	1.62	0.80
1:E:154:LEU:HD23	1:E:165:ILE:HD11	1.64	0.80
3:d:244:LEU:HD22	3:d:272:ARG:NE	1.96	0.80
3:e:453:LYS:HE2	3:e:457:ARG:CD	2.12	0.80
1:G:146:THR:O	1:G:150:LEU:HD12	1.81	0.80
1:I:10:GLN:HA	1:I:17:ALA:HB3	1.63	0.79
3:b:195:GLN:HG3	3:b:199:ARG:NH2	1.96	0.79
3:c:456:ARG:HD3	3:d:706:LEU:HD11	1.63	0.79
3:a:313:ALA:HB2	3:a:407:ILE:HD13	1.65	0.79
3:b:614:LEU:HD11	3:b:634:GLU:HB2	1.62	0.79
3:c:647:VAL:HG22	3:c:689:LEU:HD21	1.64	0.79
1:B:9:GLU:OE1	1:B:14:GLY:HA3	1.82	0.79
3:e:172:LYS:HG3	3:e:173:LEU:HD12	1.62	0.79
3:a:724:ILE:C	3:a:725:ILE:HD13	2.08	0.79
3:f:128:ILE:HG21	3:f:163:LYS:HD3	1.62	0.79
3:e:122:VAL:HG11	3:e:289:ILE:HA	1.65	0.79
3:e:446:ASP:HA	3:e:449:ASP:OD1	1.82	0.79
3:e:694:GLN:HA	3:e:698:GLU:OE1	1.81	0.79
3:c:202:LYS:O	3:c:206:GLU:HG3	1.83	0.79
3:a:318:ASN:HB2	3:a:326:LEU:HD11	1.64	0.79
3:d:221:HIS:HA	3:d:259:GLU:OE1	1.83	0.78
3:f:716:ALA:HB2	3:f:726:VAL:HG12	1.64	0.78
3:e:154:THR:O	3:e:158:GLU:HG2	1.83	0.78
3:e:207:ILE:CG1	3:e:213:VAL:HG11	2.12	0.78
3:e:241:LYS:HE2	3:e:241:LYS:N	1.98	0.78
3:f:551:GLU:HB2	3:f:620:PHE:HE1	1.47	0.78
3:e:444:GLN:HA	3:e:636:LYS:HZ1	1.48	0.78
3:e:480:VAL:HA	3:e:638:LEU:HD21	1.65	0.78
3:f:128:ILE:O	3:f:132:ILE:HG12	1.82	0.78
1:I:9:GLU:OE2	1:I:26:LYS:HD2	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:202:LYS:O	3:a:206:GLU:HG3	1.84	0.78
3:b:505:MET:HE2	3:b:505:MET:HA	1.66	0.78
3:a:718:LEU:HD12	3:a:723:LYS:O	1.83	0.78
3:e:202:LYS:HA	3:e:205:GLU:CD	2.09	0.78
1:E:125:PRO:HD2	1:E:147:ARG:HG3	1.66	0.78
3:e:544:LEU:HD21	3:e:586:ILE:HD12	1.66	0.78
3:e:290:LEU:CD2	3:e:334:LEU:HD11	2.14	0.77
1:L:98:SER:HB3	1:L:123:HIS:NE2	1.99	0.77
1:N:41:ALA:O	1:N:45:ILE:HG12	1.83	0.77
1:F:105:THR:CG2	1:F:185:LEU:HD13	2.13	0.77
3:f:341:MET:HA	3:f:341:MET:CE	2.12	0.77
3:b:267:ALA:CB	3:c:149:PRO:HG2	2.14	0.77
3:d:260:TYR:HA	3:d:263:ILE:CG1	2.14	0.77
3:f:554:HIS:O	3:f:557:VAL:HG22	1.84	0.77
3:e:183:VAL:HA	3:e:186:LEU:HD23	1.65	0.77
1:C:30:ILE:HD12	1:C:47:GLN:HE21	1.49	0.77
1:N:60:ILE:HB	1:N:88:VAL:HG12	1.66	0.77
1:F:11:SER:O	1:F:15:GLU:HB2	1.83	0.77
3:c:477:PRO:HA	3:c:593:THR:HG21	1.66	0.77
1:L:92:VAL:HG21	1:L:104:LEU:HD22	1.66	0.77
3:b:665:ILE:HD11	3:b:716:ALA:HB2	1.66	0.77
1:E:137:GLU:HG2	1:E:141:ARG:HH22	1.50	0.76
3:f:221:HIS:HA	3:f:263:ILE:HD11	1.67	0.76
3:f:665:ILE:HA	3:f:714:LEU:O	1.85	0.76
1:I:79:ASP:HB3	1:T:115:LEU:HD23	1.67	0.76
3:e:412:GLU:OE1	3:e:419:VAL:HB	1.85	0.76
3:d:199:ARG:HD2	3:d:202:LYS:HD2	1.65	0.76
3:d:340:LYS:HE3	3:d:410:ILE:HD11	1.67	0.76
3:a:153:LYS:HB2	4:f:801:ATP:O2G	1.84	0.76
3:f:725:ILE:CD1	3:f:727:THR:HG23	2.15	0.76
3:e:101:LEU:HD23	3:e:105:TYR:HB3	1.65	0.76
3:f:482:LYS:HA	3:f:635:PHE:HE2	1.50	0.76
1:D:12:SER:O	1:D:13:ARG:HD3	1.84	0.76
1:D:105:THR:O	1:D:157:ARG:HG2	1.83	0.76
1:M:89:GLN:HG2	1:M:111:LYS:HB3	1.68	0.76
3:a:719:ASP:HB3	3:a:723:LYS:H	1.50	0.76
1:F:121:MET:HG3	1:F:174:TYR:CE1	2.20	0.76
1:L:152:SER:O	1:L:156:GLU:HG3	1.86	0.76
1:G:179:GLN:HA	1:G:182:GLU:HG2	1.68	0.76
3:c:643:LEU:O	3:c:647:VAL:HG23	1.86	0.76
3:e:715:VAL:N	3:e:728:GLY:HA2	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:117:ASN:HB2	1:T:149:ARG:NH1	2.00	0.76
3:e:317:SER:HB2	3:e:329:LYS:HG2	1.67	0.76
3:f:186:LEU:HG	3:f:200:MET:HE1	1.68	0.76
1:N:78:PHE:HA	1:N:81:MET:HE2	1.66	0.75
3:d:650:MET:O	3:d:653:GLU:HG3	1.85	0.75
3:f:550:VAL:HG11	3:f:587:MET:HB2	1.65	0.75
1:I:115:LEU:HD23	1:K:79:ASP:HB3	1.67	0.75
3:e:197:GLU:CA	3:e:200:MET:HE2	2.14	0.75
3:d:262:ILE:HD12	3:d:263:ILE:N	2.00	0.75
3:e:701:ILE:HG13	3:e:714:LEU:CD2	2.16	0.75
3:f:179:ILE:HD12	3:f:213:VAL:HG23	1.68	0.75
3:f:234:MET:HA	3:f:234:MET:HE3	1.68	0.75
3:a:723:LYS:C	3:a:724:ILE:HD13	2.12	0.75
1:N:161:PRO:HG2	1:N:164:VAL:HG12	1.69	0.75
3:e:170:PRO:HD3	3:f:343:LEU:CD1	2.17	0.75
3:c:190:THR:HG21	3:c:227:GLY:HA3	1.69	0.75
3:d:562:LEU:HD21	3:d:625:PHE:HD1	1.52	0.75
3:e:438:LYS:HE3	3:e:448:VAL:HB	1.68	0.75
3:f:431:LYS:HD3	3:f:431:LYS:N	2.02	0.75
1:C:8:ILE:HA	1:C:18:TYR:CB	2.17	0.75
1:G:8:ILE:CG2	1:G:16:ARG:HG3	2.17	0.75
3:c:181:LEU:HD21	3:c:186:LEU:HD21	1.68	0.75
3:d:179:ILE:CD1	3:d:213:VAL:HB	2.16	0.75
3:e:670:GLU:HG3	3:e:718:LEU:HD23	1.69	0.75
3:f:650:MET:HE3	3:f:693:ILE:CD1	2.16	0.75
3:a:132:ILE:HD12	3:a:173:LEU:HD11	1.69	0.74
3:a:184:VAL:HG21	3:f:239:ILE:HG13	1.69	0.74
3:e:306:THR:HB	3:e:308:GLU:OE1	1.85	0.74
1:K:97:ALA:CB	1:K:121:MET:HE3	2.17	0.74
3:e:671:VAL:HG23	3:e:718:LEU:HD13	1.68	0.74
1:A:125:PRO:HD2	1:A:147:ARG:HD2	1.67	0.74
1:G:32:LEU:HD11	1:G:36:ILE:HG22	1.69	0.74
3:c:694:GLN:HA	3:c:698:GLU:CG	2.17	0.74
3:d:236:ALA:HA	3:d:239:ILE:HG13	1.69	0.74
3:f:719:ASP:HB2	3:f:725:ILE:HG23	1.69	0.74
1:D:10:GLN:HB3	1:D:13:ARG:O	1.88	0.74
3:b:324:ARG:HB2	3:b:329:LYS:HG2	1.68	0.74
3:d:202:LYS:O	3:d:205:GLU:HG3	1.87	0.74
1:L:45:ILE:HD12	1:L:80:THR:OG1	1.87	0.74
1:M:78:PHE:HE2	1:M:153:ILE:HG21	1.50	0.74
3:a:675:LEU:HD23	3:a:692:THR:HG22	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:41:ALA:O	1:G:45:ILE:HG23	1.88	0.74
1:M:122:ILE:HD12	1:M:175:MET:CE	2.18	0.74
3:e:643:LEU:CD1	3:e:689:LEU:HD11	2.17	0.74
3:e:698:GLU:HA	3:e:701:ILE:HG22	1.68	0.74
3:f:534:THR:HG21	3:f:572:ASP:HB3	1.68	0.74
3:f:686:ALA:CA	3:f:689:LEU:HD23	2.17	0.74
1:A:45:ILE:HD12	1:A:80:THR:OG1	1.86	0.74
3:c:220:VAL:O	3:c:223:ILE:HG12	1.87	0.74
3:e:110:THR:HB	3:e:178:VAL:H	1.53	0.74
3:e:172:LYS:NZ	3:e:173:LEU:HD11	2.01	0.74
3:e:564:ILE:HD11	3:e:580:PHE:HB2	1.70	0.74
1:C:30:ILE:HG23	1:C:47:GLN:NE2	2.03	0.74
1:C:132:GLN:HG2	1:T:124:GLN:HG3	1.67	0.74
1:I:108:GLN:NE2	1:I:111:LYS:HD2	2.00	0.74
3:d:110:THR:OG1	3:d:177:GLU:HB2	1.88	0.74
3:f:285:GLU:O	3:f:288:THR:HG22	1.87	0.74
3:f:464:LYS:HG3	3:f:467:ARG:HG2	1.69	0.74
1:B:83:PHE:HE2	3:f:602:PHE:HE1	1.34	0.74
3:d:449:ASP:O	3:d:453:LYS:HG3	1.87	0.74
3:e:172:LYS:HZ1	3:e:173:LEU:HD11	1.50	0.74
3:b:137:ARG:HD2	3:c:336:GLU:HG2	1.70	0.73
3:a:452:ALA:O	3:a:456:ARG:HG3	1.88	0.73
3:e:102:LEU:HD23	3:e:103:GLY:H	1.53	0.73
3:d:239:ILE:HD12	3:d:240:LEU:N	2.02	0.73
3:a:326:LEU:HD13	3:a:329:LYS:HD2	1.70	0.73
1:T:109:LYS:HA	1:T:109:LYS:CE	2.19	0.73
3:c:674:LYS:HD3	3:c:724:ILE:HD11	1.69	0.73
3:e:719:ASP:HB2	3:e:725:ILE:HG12	1.70	0.73
1:D:167:ARG:NH1	1:D:167:ARG:HB3	2.02	0.73
1:C:18:TYR:CE1	1:C:26:LYS:HD3	2.23	0.73
3:e:513:SER:O	3:e:516:LYS:HG2	1.88	0.73
3:e:569:ARG:HH21	3:e:579:SER:HA	1.53	0.73
3:f:153:LYS:HB2	4:f:802:ATP:PB	2.28	0.73
1:D:8:ILE:HG21	1:E:16:ARG:HE	1.53	0.73
1:F:122:ILE:HD11	1:F:173:ASN:HB3	1.71	0.73
1:K:101:SER:O	1:K:105:THR:HG23	1.87	0.73
3:b:191:GLY:HA2	3:a:192:ILE:CD1	2.18	0.73
3:d:129:LYS:HD2	3:d:130:ARG:N	2.02	0.73
3:d:648:SER:O	3:d:652:GLU:HG3	1.87	0.73
3:c:684:MET:HB3	3:c:688:PRO:HG2	1.70	0.73
3:b:424:GLU:HA	3:b:424:GLU:OE2	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:669:THR:HG22	3:b:673:GLU:OE2	1.89	0.72
3:f:199:ARG:HA	3:f:202:LYS:HG2	1.70	0.72
1:N:55:ASP:OD2	1:N:58:LYS:HD2	1.89	0.72
1:N:106:ALA:HA	1:N:157:ARG:HD3	1.70	0.72
3:a:281:PRO:CG	3:a:327:PRO:HG3	2.19	0.72
3:e:140:LYS:HG2	3:e:274:GLN:HE22	1.53	0.72
3:a:149:PRO:HG2	3:f:267:ALA:HB3	1.71	0.72
3:a:304:LYS:HD3	3:a:304:LYS:H	1.54	0.72
3:e:199:ARG:HA	3:e:202:LYS:HG3	1.71	0.72
1:G:10:GLN:OE1	1:G:10:GLN:HA	1.88	0.72
1:L:45:ILE:HD11	1:L:77:ILE:HA	1.72	0.72
3:b:519:GLY:CA	3:b:530:ALA:HB1	2.19	0.72
3:a:304:LYS:H	3:a:304:LYS:CD	2.03	0.72
3:e:202:LYS:HD2	3:e:202:LYS:C	2.14	0.72
1:K:25:LEU:HD11	1:K:51:LEU:HD21	1.70	0.72
1:T:34:GLY:HA2	1:T:67:PRO:CD	2.18	0.72
3:d:129:LYS:HD2	3:d:129:LYS:C	2.15	0.72
3:d:564:ILE:HD11	3:d:570:LEU:HD22	1.72	0.72
3:e:134:ILE:HB	3:e:143:PRO:HG3	1.70	0.72
3:e:459:ARG:HB3	3:e:459:ARG:NH1	2.05	0.72
3:f:122:VAL:HG12	3:f:289:ILE:HD13	1.70	0.72
1:N:137:GLU:HG2	1:N:141:ARG:HH22	1.55	0.72
3:d:234:MET:HG3	3:d:237:GLY:H	1.53	0.72
3:a:153:LYS:HB2	4:f:801:ATP:PG	2.29	0.72
3:e:101:LEU:HA	3:e:104:GLU:OE2	1.87	0.72
1:A:144:LEU:O	1:A:148:GLN:HG3	1.89	0.72
3:c:477:PRO:HG2	3:c:480:VAL:HG11	1.70	0.72
3:a:132:ILE:HD11	3:a:160:LEU:HD11	1.70	0.72
1:D:63:TYR:HE1	1:D:91:ILE:HD12	1.53	0.72
1:I:160:GLN:HB3	1:I:164:VAL:HG11	1.70	0.72
3:a:550:VAL:HG22	3:a:589:SER:HB2	1.72	0.72
3:f:113:ALA:HB1	3:f:165:VAL:HG11	1.70	0.72
1:E:41:ALA:HB2	1:E:73:ALA:HB1	1.71	0.72
1:G:4:ILE:HG23	1:G:20:ILE:HG22	1.71	0.72
3:d:134:ILE:O	3:d:137:ARG:HG2	1.90	0.72
3:e:645:ASN:O	3:e:649:LEU:HD12	1.89	0.72
3:d:157:VAL:HG21	3:d:216:PHE:CE1	2.25	0.72
3:f:183:VAL:HA	3:f:186:LEU:HD23	1.72	0.72
3:f:417:ILE:H	3:f:417:ILE:HD12	1.55	0.72
1:A:13:ARG:HB3	3:f:555:PRO:HG2	1.72	0.71
1:T:92:VAL:HG21	1:T:104:LEU:HD22	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:475:VAL:HG11	3:d:617:LEU:HD11	1.71	0.71
3:f:500:MET:HE1	3:f:502:ARG:HB2	1.72	0.71
3:a:478:THR:HG23	3:a:684:MET:HA	1.72	0.71
3:e:286:THR:HG21	3:e:326:LEU:HB3	1.70	0.71
3:f:207:ILE:HG23	3:f:213:VAL:CG1	2.20	0.71
3:f:691:ARG:O	3:f:691:ARG:HD3	1.89	0.71
1:G:161:PRO:HG2	1:G:164:VAL:HG12	1.71	0.71
1:N:176:THR:HG23	1:N:179:GLN:NE2	2.05	0.71
1:S:93:LEU:HD12	1:T:45:ILE:HD13	1.73	0.71
3:b:197:GLU:HG3	3:b:229:ALA:HB2	1.70	0.71
3:c:101:LEU:HD11	3:c:203:LEU:HD12	1.70	0.71
1:G:41:ALA:HB2	1:G:73:ALA:HB1	1.73	0.71
1:G:101:SER:O	1:G:105:THR:HG23	1.91	0.71
1:A:98:SER:HB3	1:A:123:HIS:NE2	2.06	0.71
1:C:29:ILE:HB	3:e:602:PHE:HZ	1.55	0.71
1:T:90:THR:HG22	1:T:104:LEU:HD12	1.72	0.71
3:c:140:LYS:HE3	3:c:271:ARG:O	1.91	0.71
3:a:698:GLU:OE2	3:f:462:LEU:HD13	1.90	0.71
3:f:455:ILE:HD13	3:f:493:LEU:HD11	1.71	0.71
1:C:29:ILE:HB	3:e:602:PHE:CZ	2.26	0.71
1:I:137:GLU:HG3	1:I:141:ARG:HH22	1.56	0.71
3:b:144:VAL:CG2	3:b:273:MET:HB3	2.19	0.71
1:A:137:GLU:O	1:A:141:ARG:HG2	1.91	0.71
1:D:93:LEU:HD12	1:D:94:GLY:N	2.06	0.71
1:N:33:SER:HA	1:N:65:ASN:O	1.89	0.71
3:b:111:GLU:HA	3:b:114:ARG:HG2	1.73	0.71
3:c:138:ARG:HD3	3:d:297:TYR:CE2	2.26	0.71
3:e:482:LYS:HE3	3:e:588:THR:HG23	1.73	0.71
1:C:55:ASP:OD1	1:C:58:LYS:HG3	1.91	0.71
1:K:137:GLU:HG2	1:K:141:ARG:HH22	1.55	0.71
3:a:643:LEU:O	3:a:647:VAL:HG23	1.90	0.71
3:e:451:VAL:HG22	3:e:633:ILE:CD1	2.20	0.71
3:e:457:ARG:O	3:e:460:VAL:HG12	1.90	0.71
3:e:565:LEU:HD11	3:e:587:MET:HE3	1.72	0.71
3:f:473:LEU:HD12	3:f:587:MET:O	1.90	0.71
3:f:493:LEU:HD13	3:f:584:ILE:HD11	1.73	0.71
1:I:75:LEU:HD22	1:I:99:MET:HE1	1.73	0.71
1:L:43:SER:O	1:L:47:GLN:HG3	1.91	0.71
1:S:18:TYR:CE2	1:S:23:ARG:HG2	2.24	0.71
3:d:129:LYS:HA	3:d:132:ILE:HG12	1.72	0.71
3:b:195:GLN:OE1	3:c:192:ILE:HG12	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:550:VAL:HG13	3:c:558:LEU:HD21	1.73	0.71
3:f:122:VAL:CG1	3:f:289:ILE:HD13	2.19	0.71
1:C:91:ILE:CG2	1:C:113:PHE:HB2	2.19	0.70
1:S:89:GLN:HG3	1:S:111:LYS:HB3	1.72	0.70
3:a:281:PRO:HG3	3:a:327:PRO:HG3	1.73	0.70
3:e:321:ILE:HB	3:e:329:LYS:HD2	1.73	0.70
3:f:324:ARG:HH11	3:f:324:ARG:HG3	1.56	0.70
1:E:85:LYS:HB2	1:E:85:LYS:NZ	2.06	0.70
1:S:109:LYS:HA	1:S:109:LYS:CE	2.18	0.70
3:d:169:VAL:HG21	3:d:173:LEU:HD11	1.72	0.70
3:d:547:LEU:HD22	3:d:587:MET:HE2	1.73	0.70
1:M:101:SER:O	1:M:105:THR:HG23	1.89	0.70
3:e:516:LYS:O	3:e:531:GLY:HA2	1.91	0.70
3:f:653:GLU:OE1	3:f:653:GLU:HA	1.90	0.70
1:D:105:THR:HG21	1:D:185:LEU:CD2	2.20	0.70
1:F:29:ILE:HD12	1:F:63:TYR:CE1	2.26	0.70
1:S:181:LYS:HA	1:S:186:ILE:HG22	1.71	0.70
3:d:181:LEU:CG	3:d:215:LEU:HD11	2.22	0.70
3:a:171:GLN:HA	3:a:174:LEU:HG	1.74	0.70
3:a:293:LEU:HD21	4:f:801:ATP:H2	1.56	0.70
3:e:216:PHE:HA	3:e:252:VAL:O	1.91	0.70
3:e:453:LYS:O	3:e:457:ARG:HG3	1.90	0.70
3:f:224:VAL:HG11	3:f:262:ILE:HG22	1.73	0.70
1:E:154:LEU:HB3	1:E:165:ILE:CD1	2.21	0.70
3:b:108:ASN:HB3	3:b:111:GLU:HG2	1.73	0.70
3:b:217:ILE:HG23	3:b:220:VAL:HG12	1.73	0.70
3:c:293:LEU:HD12	3:c:331:ILE:HD11	1.74	0.70
3:d:243:ALA:HB2	3:d:248:GLU:OE1	1.90	0.70
3:e:319:ARG:HG3	3:e:320:TYR:CE1	2.27	0.70
3:e:505:MET:HE3	3:e:547:LEU:HD22	1.73	0.70
3:e:636:LYS:H	3:e:636:LYS:CD	2.04	0.70
3:e:698:GLU:HA	3:e:701:ILE:CG2	2.21	0.70
3:b:189:GLY:HA3	3:a:198:GLU:OE2	1.91	0.70
3:b:687:ARG:HB2	3:b:688:PRO:HD3	1.72	0.70
3:e:202:LYS:HA	3:e:205:GLU:OE1	1.91	0.70
3:e:473:LEU:HD12	3:e:587:MET:O	1.90	0.70
1:B:115:LEU:HD13	1:C:79:ASP:HB3	1.73	0.70
1:L:7:VAL:HG21	1:M:50:PHE:CZ	2.27	0.70
1:C:125:PRO:HD2	1:C:147:ARG:HG3	1.74	0.70
1:M:115:LEU:HD23	1:N:79:ASP:HB3	1.74	0.70
3:b:136:ASN:HB3	3:c:339:SER:OG	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:447:ALA:CB	3:b:633:ILE:HG21	2.20	0.70
3:c:200:MET:HE2	3:c:236:ALA:HB1	1.74	0.70
3:d:280:GLU:OE2	3:d:326:LEU:HD23	1.91	0.70
3:e:319:ARG:HD2	3:e:542:TYR:CE1	2.27	0.70
3:e:560:MET:O	3:e:564:ILE:HG22	1.92	0.70
1:C:160:GLN:HB3	1:C:164:VAL:CG1	2.22	0.70
1:G:96:ALA:O	1:G:120:ILE:HD12	1.91	0.70
3:b:478:THR:HG22	3:a:627:ASN:HD22	1.57	0.70
3:d:179:ILE:HD11	3:d:213:VAL:HB	1.72	0.70
3:d:260:TYR:HA	3:d:263:ILE:HG12	1.73	0.70
3:d:462:LEU:CD2	3:e:698:GLU:HB3	2.22	0.70
3:e:294:GLN:O	3:e:298:GLU:HG2	1.90	0.70
1:A:29:ILE:HD13	1:A:61:TYR:HB2	1.72	0.70
1:B:98:SER:HB3	1:B:123:HIS:CE1	2.26	0.70
1:C:6:THR:HG22	1:D:22:SER:OG	1.91	0.70
1:G:141:ARG:CZ	1:G:141:ARG:HB2	2.20	0.70
3:b:249:LEU:HD23	3:b:249:LEU:H	1.57	0.70
3:c:268:ALA:O	3:c:272:ARG:HG2	1.92	0.70
1:C:8:ILE:HA	1:C:18:TYR:HA	1.74	0.69
1:I:75:LEU:HG	1:I:149:ARG:HH21	1.57	0.69
3:b:327:PRO:O	3:b:331:ILE:HD13	1.91	0.69
3:b:622:THR:HG23	3:b:623:PRO:HD2	1.72	0.69
3:e:701:ILE:HG13	3:e:714:LEU:HD21	1.74	0.69
3:c:694:GLN:HA	3:c:698:GLU:HG2	1.74	0.69
3:a:658:LEU:HD21	3:f:462:LEU:CD2	2.22	0.69
3:e:462:LEU:HD21	3:f:702:ALA:HB2	1.72	0.69
3:f:261:ARG:HA	3:f:264:GLU:HG3	1.73	0.69
1:D:10:GLN:HB2	1:D:16:ARG:HG2	1.74	0.69
3:b:110:THR:CG2	3:b:177:GLU:HB3	2.21	0.69
3:d:118:ILE:HD11	3:d:158:GLU:HB3	1.73	0.69
3:a:694:GLN:O	3:a:698:GLU:HB2	1.93	0.69
3:e:208:THR:HB	3:e:248:GLU:CG	2.22	0.69
1:S:160:GLN:HB3	1:S:164:VAL:HG11	1.74	0.69
3:b:647:VAL:CG2	3:b:689:LEU:HD11	2.22	0.69
3:a:482:LYS:HA	3:a:635:PHE:HE2	1.58	0.69
1:S:101:SER:O	1:S:105:THR:HG23	1.90	0.69
3:d:317:SER:HB2	3:d:333:LEU:HD12	1.75	0.69
3:e:440:HIS:HB2	3:e:488:GLN:HG3	1.74	0.69
3:e:545:ILE:HB	3:e:585:ILE:HD13	1.72	0.69
3:f:256:THR:HB	3:f:259:GLU:OE1	1.93	0.69
3:c:483:THR:HB	4:c:801:ATP:O2A	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:134:ILE:CG2	3:d:143:PRO:HG3	2.23	0.69
3:e:650:MET:HE1	3:e:689:LEU:HB3	1.74	0.69
1:F:63:TYR:HD2	1:F:93:LEU:HD21	1.57	0.69
3:b:670:GLU:HA	3:b:673:GLU:OE1	1.93	0.69
3:c:200:MET:HE1	3:c:240:LEU:HD13	1.75	0.69
3:d:223:ILE:HD12	3:d:224:VAL:N	2.08	0.69
3:c:187:VAL:HG13	3:c:190:THR:HG21	1.75	0.69
3:d:434:ALA:O	3:d:438:LYS:HD2	1.92	0.69
3:f:660:LYS:HE2	3:f:660:LYS:N	2.07	0.69
1:E:109:LYS:HE2	1:E:109:LYS:HA	1.75	0.69
1:S:161:PRO:O	1:S:164:VAL:HG12	1.92	0.69
1:T:101:SER:O	1:T:105:THR:HG23	1.93	0.69
3:b:487:LYS:HB3	3:b:497:GLU:HG3	1.74	0.69
3:c:200:MET:HE1	3:c:240:LEU:CD1	2.22	0.69
3:a:662:LYS:HE2	3:a:662:LYS:CA	2.22	0.69
3:a:724:ILE:O	3:a:725:ILE:HD13	1.93	0.69
3:e:565:LEU:HD21	3:e:585:ILE:HG21	1.75	0.69
3:f:193:ARG:NH1	3:f:230:GLY:HA3	2.08	0.69
3:f:283:VAL:O	3:f:286:THR:HG22	1.93	0.69
3:f:492:GLU:OE1	3:f:492:GLU:HA	1.91	0.69
3:c:534:THR:HG23	3:c:578:VAL:HG21	1.75	0.68
3:a:667:VAL:HG12	3:a:716:ALA:HB3	1.74	0.68
3:e:327:PRO:O	3:e:331:ILE:HG12	1.93	0.68
3:f:526:GLY:HA2	3:f:529:GLU:OE2	1.93	0.68
3:f:716:ALA:CB	3:f:726:VAL:HG12	2.23	0.68
1:A:47:GLN:NE2	1:G:5:PRO:HG3	2.07	0.68
1:N:51:LEU:HD23	1:N:60:ILE:HD12	1.73	0.68
3:e:169:VAL:HB	3:e:170:PRO:HD2	1.74	0.68
1:C:8:ILE:HA	1:C:18:TYR:CA	2.23	0.68
1:C:10:GLN:HB2	1:C:15:GLU:H	1.59	0.68
1:N:176:THR:H	1:N:179:GLN:HE21	1.40	0.68
3:f:596:VAL:CG2	3:f:616:GLN:HG3	2.21	0.68
3:f:689:LEU:O	3:f:693:ILE:HG13	1.94	0.68
1:G:89:GLN:CB	1:G:111:LYS:HB3	2.21	0.68
1:N:77:ILE:HD13	1:N:103:LEU:HD23	1.76	0.68
1:S:98:SER:HB3	1:S:123:HIS:CE1	2.27	0.68
3:b:453:LYS:O	3:b:457:ARG:HG3	1.94	0.68
3:c:723:LYS:HE3	3:c:723:LYS:CA	2.13	0.68
3:d:243:ALA:HA	3:d:248:GLU:HB3	1.75	0.68
3:d:668:PRO:HD2	3:d:671:VAL:HG21	1.75	0.68
3:a:184:VAL:CG2	3:f:239:ILE:HG13	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:SER:HA	1:B:162:ILE:HD11	1.75	0.68
3:c:187:VAL:HG13	3:c:227:GLY:HA3	1.76	0.68
3:c:217:ILE:HB	3:c:220:VAL:HG12	1.74	0.68
3:d:403:THR:HG22	3:d:405:LYS:H	1.58	0.68
3:e:724:ILE:C	3:e:725:ILE:HD13	2.18	0.68
1:N:37:ASP:OD1	1:N:40:VAL:HG12	1.93	0.68
1:N:109:LYS:HE2	1:N:109:LYS:HA	1.73	0.68
3:b:220:VAL:O	3:b:223:ILE:HG12	1.93	0.68
3:b:341:MET:HE3	3:b:406:ASP:OD1	1.93	0.68
3:f:309:ALA:HB2	3:f:404:GLU:HA	1.76	0.68
1:B:31:MET:HE1	1:C:45:ILE:HG22	1.75	0.68
1:B:37:ASP:OD1	1:B:40:VAL:HG13	1.93	0.68
3:a:153:LYS:HG3	3:a:254:ALA:HB1	1.76	0.68
3:e:231:ASP:H	3:f:192:ILE:HG22	1.58	0.68
1:B:181:LYS:NZ	1:B:188:GLU:HA	2.09	0.68
3:c:181:LEU:CD2	3:c:203:LEU:HD11	2.24	0.68
3:e:128:ILE:HG21	3:e:163:LYS:HE2	1.74	0.68
3:e:451:VAL:HG22	3:e:633:ILE:HD13	1.76	0.68
3:e:509:MET:O	3:e:554:HIS:HB2	1.92	0.68
1:E:56:SER:HB3	1:E:85:LYS:HD2	1.73	0.68
1:M:172:ASP:O	1:N:138:ILE:HG21	1.94	0.68
1:S:4:ILE:HD13	1:S:21:TYR:HE2	1.59	0.68
3:a:217:ILE:HG22	3:a:251:LEU:HD21	1.75	0.68
3:a:624:GLU:O	3:a:628:ARG:HG3	1.93	0.68
3:f:171:GLN:HA	3:f:174:LEU:HD21	1.75	0.68
1:N:43:SER:O	1:N:47:GLN:HG3	1.94	0.68
3:d:130:ARG:HD2	3:e:414:LYS:HE3	1.76	0.68
3:d:717:ALA:HB3	3:d:725:ILE:HD11	1.76	0.68
3:a:153:LYS:HB2	4:f:801:ATP:O3B	1.92	0.68
3:a:246:ARG:HH11	3:a:246:ARG:HG2	1.59	0.68
3:b:339:SER:OG	3:a:136:ASN:HB3	1.94	0.67
3:e:246:ARG:HB2	3:e:248:GLU:OE1	1.94	0.67
1:C:4:ILE:HD11	1:C:21:TYR:CE1	2.29	0.67
3:c:324:ARG:HB2	3:c:329:LYS:CG	2.24	0.67
3:a:694:GLN:HA	3:a:698:GLU:CG	2.18	0.67
3:f:204:ILE:HD11	3:f:240:LEU:HD21	1.75	0.67
1:F:154:LEU:HB3	1:F:165:ILE:HD11	1.74	0.67
1:S:24:LEU:HD13	1:S:31:MET:HE3	1.76	0.67
3:b:138:ARG:HG3	3:b:139:THR:HG23	1.77	0.67
3:d:148:GLU:HA	3:d:148:GLU:OE2	1.94	0.67
3:f:505:MET:HE2	3:f:547:LEU:HD23	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:f:650:MET:HE3	3:f:693:ILE:HD12	1.76	0.67
1:A:25:LEU:HD11	1:A:51:LEU:HD11	1.75	0.67
1:C:137:GLU:HG3	1:C:141:ARG:HH22	1.60	0.67
1:F:60:ILE:HG13	1:F:88:VAL:HG22	1.75	0.67
3:d:243:ALA:CB	3:d:248:GLU:HB3	2.24	0.67
3:e:565:LEU:HB3	3:e:628:ARG:NH2	2.10	0.67
3:f:294:GLN:O	3:f:298:GLU:HG3	1.94	0.67
1:A:167:ARG:CZ	1:A:167:ARG:HB3	2.23	0.67
1:M:78:PHE:CE2	1:M:153:ILE:HG21	2.29	0.67
3:b:149:PRO:HG2	3:a:267:ALA:HB3	1.75	0.67
1:K:77:ILE:HG21	1:K:103:LEU:HD21	1.75	0.67
3:b:289:ILE:O	3:b:293:LEU:HD12	1.93	0.67
3:c:138:ARG:HD3	3:d:297:TYR:HE2	1.57	0.67
3:c:244:LEU:HD23	3:c:249:LEU:HD21	1.75	0.67
3:e:565:LEU:HD21	3:e:585:ILE:HG13	1.75	0.67
1:C:24:LEU:HB3	1:C:29:ILE:HG21	1.77	0.67
3:b:220:VAL:HG23	3:b:263:ILE:HD11	1.77	0.67
3:e:101:LEU:HD13	3:e:202:LYS:HZ2	1.60	0.67
3:e:670:GLU:HG3	3:e:718:LEU:CD2	2.25	0.67
1:B:158:THR:HG21	1:B:185:LEU:HD23	1.76	0.67
3:e:438:LYS:HE2	3:e:445:ASP:HA	1.76	0.67
1:D:57:GLU:HA	1:D:57:GLU:OE2	1.94	0.67
3:c:462:LEU:HD23	3:d:698:GLU:OE2	1.95	0.67
3:e:424:GLU:O	3:e:428:THR:HG22	1.94	0.67
3:e:560:MET:O	3:e:563:GLN:HG3	1.95	0.67
1:D:181:LYS:HZ1	1:D:188:GLU:HA	1.59	0.67
3:d:503:PHE:HB3	3:d:505:MET:HE1	1.77	0.67
3:a:339:SER:OG	3:f:136:ASN:HB3	1.95	0.67
1:F:154:LEU:HB3	1:F:165:ILE:CD1	2.25	0.66
1:L:41:ALA:O	1:L:45:ILE:HG12	1.95	0.66
1:L:115:LEU:HD13	1:M:79:ASP:HB3	1.77	0.66
3:c:207:ILE:CD1	3:c:249:LEU:HB2	2.23	0.66
1:M:63:TYR:HD1	1:M:91:ILE:HB	1.59	0.66
1:N:45:ILE:HD11	1:N:77:ILE:HA	1.78	0.66
1:T:167:ARG:NH1	1:T:167:ARG:HB3	2.09	0.66
4:c:801:ATP:O1B	4:c:801:ATP:H5'1	1.96	0.66
1:I:79:ASP:CB	1:T:115:LEU:HD23	2.24	0.66
1:M:93:LEU:HD12	1:M:93:LEU:O	1.96	0.66
1:M:115:LEU:HD23	1:N:79:ASP:CB	2.25	0.66
3:c:462:LEU:HD23	3:d:698:GLU:HB3	1.76	0.66
3:d:717:ALA:HB3	3:d:725:ILE:CD1	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:167:ARG:HB3	1:G:167:ARG:NH1	2.10	0.66
1:G:179:GLN:HA	1:G:182:GLU:CG	2.25	0.66
1:I:9:GLU:HB3	1:I:18:TYR:CB	2.25	0.66
3:a:327:PRO:O	3:a:331:ILE:HD13	1.95	0.66
1:F:167:ARG:NH1	1:F:167:ARG:HB3	2.10	0.66
1:C:24:LEU:O	1:C:29:ILE:HG22	1.96	0.66
1:D:37:ASP:OD1	1:D:40:VAL:HG12	1.96	0.66
1:L:124:GLN:HB3	1:L:147:ARG:NH1	2.10	0.66
1:M:63:TYR:CD1	1:M:91:ILE:HB	2.31	0.66
3:b:643:LEU:HD22	3:b:689:LEU:HD12	1.77	0.66
3:a:183:VAL:HG23	3:a:217:ILE:HD11	1.78	0.66
3:f:245:ALA:HB2	3:f:272:ARG:HH11	1.61	0.66
1:M:41:ALA:HB2	1:M:73:ALA:HB1	1.77	0.66
3:b:465:GLN:HA	3:b:465:GLN:OE1	1.93	0.66
3:c:187:VAL:O	3:c:190:THR:HG22	1.96	0.66
3:e:110:THR:HG21	3:e:177:GLU:CB	2.26	0.66
3:e:111:GLU:HA	3:e:114:ARG:NH1	2.11	0.66
3:f:317:SER:HB2	3:f:329:LYS:HD3	1.78	0.66
1:A:120:ILE:HD11	1:A:175:MET:HE3	1.78	0.66
3:c:269:LEU:O	3:c:273:MET:HG3	1.96	0.66
3:d:646:ILE:CG2	3:d:650:MET:HE3	2.25	0.66
3:e:316:LEU:HD21	3:e:421:ASP:CB	2.26	0.66
1:C:11:SER:O	1:C:15:GLU:HG2	1.96	0.66
1:I:161:PRO:O	1:I:164:VAL:HG12	1.96	0.66
1:K:9:GLU:OE1	1:K:9:GLU:HA	1.95	0.66
3:a:665:ILE:HA	3:a:714:LEU:O	1.95	0.66
3:e:162:GLN:O	3:e:165:VAL:HG12	1.96	0.66
3:e:674:LYS:HA	3:e:677:ASP:OD2	1.96	0.66
3:f:679:GLY:O	3:f:688:PRO:HB2	1.96	0.66
3:f:680:TYR:HB2	3:f:689:LEU:HD21	1.77	0.66
1:F:87:ASP:HA	1:F:108:GLN:NE2	2.11	0.65
1:K:105:THR:HG21	1:K:185:LEU:HD22	1.77	0.65
3:d:138:ARG:HB3	3:d:138:ARG:CZ	2.25	0.65
3:f:171:GLN:HA	3:f:174:LEU:CD2	2.26	0.65
1:I:8:ILE:HA	1:I:16:ARG:CA	2.21	0.65
1:L:161:PRO:HD2	1:L:164:VAL:HG11	1.77	0.65
3:e:195:GLN:HG2	3:e:196:PHE:N	2.11	0.65
3:e:270:GLU:OE2	3:e:270:GLU:HA	1.95	0.65
3:f:655:ASN:ND2	3:f:665:ILE:HG23	2.10	0.65
1:E:89:GLN:HB2	1:E:111:LYS:O	1.95	0.65
1:G:105:THR:CG2	1:G:185:LEU:HD22	2.23	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:200:MET:HE2	3:c:236:ALA:CB	2.26	0.65
3:a:514:VAL:O	3:a:518:ILE:HG12	1.96	0.65
3:e:199:ARG:HG3	3:e:202:LYS:HE3	1.78	0.65
3:f:108:ASN:OD1	3:f:110:THR:HG22	1.97	0.65
1:E:101:SER:O	1:E:105:THR:HG23	1.95	0.65
1:M:97:ALA:HB1	1:M:121:MET:HE3	1.76	0.65
1:M:124:GLN:HB3	1:M:147:ARG:NH1	2.12	0.65
1:N:52:ASP:O	1:N:56:SER:HB3	1.96	0.65
3:d:308:GLU:HG3	3:d:404:GLU:HG3	1.79	0.65
3:a:534:THR:HG23	3:a:578:VAL:CG2	2.26	0.65
3:e:685:GLY:O	3:e:688:PRO:HD2	1.96	0.65
3:c:118:ILE:HD12	3:c:158:GLU:HG2	1.78	0.65
3:d:326:LEU:HD23	3:d:326:LEU:H	1.62	0.65
3:a:644:MET:HE2	3:a:644:MET:HA	1.78	0.65
1:D:161:PRO:HD2	1:D:164:VAL:HG11	1.78	0.65
3:f:714:LEU:HA	3:f:728:GLY:CA	2.25	0.65
3:b:198:GLU:HG2	3:b:202:LYS:HZ2	1.62	0.65
3:e:267:ALA:O	3:e:271:ARG:HD2	1.96	0.65
3:c:164:ILE:HD13	3:c:169:VAL:HG11	1.78	0.65
3:d:198:GLU:C	3:d:202:LYS:HE3	2.22	0.65
3:d:411:VAL:CG1	3:d:419:VAL:HG21	2.27	0.65
3:a:646:ILE:O	3:a:650:MET:HG3	1.97	0.65
3:a:680:TYR:CE2	3:a:682:PRO:HG3	2.31	0.65
3:f:547:LEU:HD21	3:f:561:PHE:CZ	2.31	0.65
1:C:160:GLN:HB3	1:C:164:VAL:HG11	1.79	0.65
1:F:117:ASN:HB2	1:G:149:ARG:NH1	2.11	0.65
1:M:105:THR:HG22	1:M:185:LEU:HB2	1.79	0.65
3:b:687:ARG:HG3	3:a:627:ASN:ND2	2.11	0.65
3:e:197:GLU:CG	3:e:234:MET:HE1	2.25	0.65
3:e:224:VAL:HG11	3:e:262:ILE:HG22	1.77	0.65
1:B:105:THR:CG2	1:B:185:LEU:HD22	2.25	0.65
1:B:120:ILE:HG21	1:B:185:LEU:HD12	1.79	0.65
1:F:29:ILE:HD13	1:F:61:TYR:HB2	1.77	0.65
1:S:153:ILE:O	1:S:157:ARG:HG3	1.95	0.65
3:d:208:THR:HG22	3:d:248:GLU:O	1.97	0.65
3:d:477:PRO:CA	3:d:593:THR:HG21	2.26	0.65
3:e:466:ASN:HA	3:e:581:LYS:NZ	2.11	0.65
3:f:320:TYR:CE2	3:f:419:VAL:HG13	2.31	0.65
3:f:529:GLU:HG2	3:f:529:GLU:O	1.97	0.65
3:d:442:VAL:H	4:d:802:ATP:HN62	1.45	0.64
3:e:132:ILE:CD1	3:e:160:LEU:HD21	2.22	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:119:GLU:O	1:F:120:ILE:HD13	1.97	0.64
1:I:41:ALA:HB2	1:I:73:ALA:HB1	1.78	0.64
1:I:93:LEU:HD23	1:I:93:LEU:H	1.60	0.64
1:L:161:PRO:HG2	1:L:164:VAL:HG12	1.78	0.64
1:S:124:GLN:HB3	1:S:147:ARG:NH1	2.12	0.64
3:c:127:GLU:O	3:c:131:VAL:HG23	1.97	0.64
3:d:146:ILE:HG22	3:d:255:THR:HG23	1.79	0.64
3:d:282:THR:HG22	3:d:285:GLU:HG3	1.77	0.64
3:a:644:MET:HE1	3:a:673:GLU:HA	1.78	0.64
3:e:412:GLU:HG3	3:e:417:ILE:O	1.97	0.64
3:f:102:LEU:HD22	3:f:179:ILE:HG21	1.78	0.64
3:f:671:VAL:HG23	3:f:724:ILE:CD1	2.27	0.64
1:M:62:LEU:HD22	1:M:64:ILE:HD11	1.79	0.64
1:N:77:ILE:HD13	1:N:103:LEU:CD2	2.27	0.64
3:b:621:PHE:HB2	3:b:626:LEU:HD11	1.79	0.64
3:c:256:THR:OG1	3:c:259:GLU:HB2	1.98	0.64
3:d:157:VAL:HG21	3:d:216:PHE:CZ	2.32	0.64
3:d:427:GLN:O	3:d:431:LYS:HG3	1.96	0.64
3:e:323:ASP:HA	3:e:539:ARG:HH22	1.63	0.64
1:I:75:LEU:HD22	1:I:99:MET:CE	2.26	0.64
1:N:122:ILE:HG23	1:N:175:MET:HE1	1.79	0.64
3:c:337:SER:OG	3:c:407:ILE:HD13	1.96	0.64
3:e:289:ILE:O	3:e:293:LEU:HG	1.98	0.64
3:e:290:LEU:HD13	3:e:310:ILE:HG22	1.79	0.64
3:e:668:PRO:HG2	3:e:671:VAL:HG12	1.80	0.64
1:E:33:SER:HA	1:E:65:ASN:O	1.97	0.64
3:b:701:ILE:HG23	3:b:704:TYR:OH	1.96	0.64
3:d:195:GLN:O	3:d:199:ARG:HB2	1.98	0.64
3:e:460:VAL:HG13	3:e:462:LEU:HG	1.80	0.64
3:f:564:ILE:HD11	3:f:570:LEU:HD22	1.79	0.64
1:D:45:ILE:HD12	1:D:80:THR:OG1	1.98	0.64
1:M:57:GLU:HA	1:M:57:GLU:OE2	1.97	0.64
3:b:304:LYS:HD3	3:b:304:LYS:N	2.12	0.64
3:b:537:VAL:HG21	3:b:580:PHE:CE2	2.32	0.64
3:b:643:LEU:O	3:b:647:VAL:HG23	1.96	0.64
3:a:715:VAL:HG12	3:a:728:GLY:HA2	1.77	0.64
3:e:564:ILE:HD11	3:e:580:PHE:CG	2.33	0.64
1:D:41:ALA:HB2	1:D:73:ALA:HB1	1.80	0.64
1:D:67:PRO:HA	1:D:95:MET:HE3	1.80	0.64
1:E:93:LEU:HD12	1:F:45:ILE:CD1	2.28	0.64
1:E:154:LEU:HB3	1:E:165:ILE:HD11	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:93:LEU:HD12	1:K:45:ILE:HG21	1.78	0.64
3:b:462:LEU:HD23	3:c:698:GLU:OE1	1.97	0.64
3:a:188:GLN:O	3:f:198:GLU:HB3	1.96	0.64
3:a:518:ILE:HG23	3:a:560:MET:HE1	1.78	0.64
1:B:7:VAL:HG21	1:B:23:ARG:HG2	1.80	0.64
1:E:4:ILE:CG2	1:E:20:ILE:HG22	2.27	0.64
1:N:84:VAL:HG13	1:N:85:LYS:O	1.98	0.64
3:b:488:GLN:O	3:b:492:GLU:HG2	1.97	0.64
3:d:244:LEU:HD13	3:d:272:ARG:HD3	1.80	0.64
3:a:669:THR:HA	3:a:672:LYS:HE2	1.80	0.64
3:e:658:LEU:HA	3:e:661:GLN:NE2	2.12	0.64
3:e:665:ILE:CD1	3:e:716:ALA:HB2	2.23	0.64
1:B:10:GLN:HG2	1:B:23:ARG:HE	1.62	0.64
1:D:93:LEU:HD12	1:D:94:GLY:H	1.60	0.64
1:N:89:GLN:OE1	1:N:111:LYS:HD2	1.96	0.64
1:S:175:MET:HB2	1:S:179:GLN:HB2	1.79	0.64
1:T:161:PRO:O	1:T:164:VAL:HG12	1.98	0.64
3:b:255:THR:HB	3:b:259:GLU:HG3	1.80	0.64
3:d:505:MET:HE2	3:d:505:MET:N	2.13	0.64
3:e:224:VAL:HG11	3:e:262:ILE:CG2	2.27	0.64
3:e:488:GLN:OE1	3:e:488:GLN:HA	1.96	0.64
1:C:140:ALA:O	1:C:143:ILE:HG22	1.97	0.64
1:E:9:GLU:HG3	1:E:10:GLN:HG3	1.78	0.64
1:T:41:ALA:HB2	1:T:73:ALA:HB1	1.79	0.64
3:b:701:ILE:CG1	3:b:726:VAL:HG23	2.25	0.64
3:c:138:ARG:HB3	3:d:300:TYR:CE2	2.33	0.64
3:d:146:ILE:O	3:d:146:ILE:HD12	1.98	0.64
3:a:149:PRO:HG2	3:f:267:ALA:CB	2.28	0.64
3:e:271:ARG:NH2	4:f:802:ATP:H4'	2.13	0.64
3:e:614:LEU:O	3:e:614:LEU:HD13	1.98	0.64
3:f:554:HIS:CD2	3:f:555:PRO:HD2	2.33	0.64
1:C:74:GLY:HA3	1:C:99:MET:HE2	1.80	0.63
1:K:140:ALA:O	1:K:143:ILE:HG22	1.97	0.63
3:a:469:ILE:HD11	3:a:584:ILE:HG12	1.80	0.63
3:f:510:GLU:HG3	3:f:512:HIS:NE2	2.12	0.63
3:f:687:ARG:HB2	3:f:688:PRO:HD3	1.79	0.63
1:A:120:ILE:HD11	1:A:175:MET:CE	2.28	0.63
3:d:217:ILE:HG22	3:d:251:LEU:HD11	1.79	0.63
3:d:223:ILE:HG12	3:d:263:ILE:HG22	1.79	0.63
3:f:459:ARG:HG2	3:f:459:ARG:HH11	1.62	0.63
3:f:684:MET:HE2	3:f:684:MET:CA	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:67:PRO:C	1:L:97:ALA:HB3	2.24	0.63
3:b:505:MET:HG3	3:b:550:VAL:HA	1.80	0.63
3:a:708:HIS:HB3	3:a:710:GLU:OE2	1.98	0.63
3:e:236:ALA:HA	3:e:239:ILE:HG12	1.80	0.63
3:e:312:ALA:O	3:e:316:LEU:HG	1.98	0.63
1:B:4:ILE:HG23	1:B:20:ILE:HG22	1.81	0.63
1:B:53:ALA:CB	3:f:600:VAL:H	2.12	0.63
1:K:143:ILE:HG23	1:K:144:LEU:HD22	1.81	0.63
1:M:113:PHE:C	1:M:186:ILE:HD11	2.23	0.63
3:c:613:VAL:CG2	3:c:634:GLU:HG3	2.28	0.63
3:a:714:LEU:HD23	3:a:715:VAL:N	2.13	0.63
3:e:280:GLU:OE2	3:e:326:LEU:HD23	1.99	0.63
3:e:423:LYS:O	3:e:427:GLN:HG3	1.98	0.63
3:e:447:ALA:O	3:e:451:VAL:HG23	1.98	0.63
1:E:4:ILE:HG23	1:E:20:ILE:HG22	1.80	0.63
1:E:105:THR:CG2	1:E:185:LEU:HD22	2.28	0.63
1:M:43:SER:O	1:M:47:GLN:HG3	1.99	0.63
3:d:197:GLU:O	3:d:201:GLN:HG2	1.98	0.63
3:a:207:ILE:CD1	3:a:215:LEU:HD22	2.28	0.63
3:e:134:ILE:HG23	3:e:274:GLN:OE1	1.99	0.63
1:D:93:LEU:HA	1:D:115:LEU:HD23	1.81	0.63
1:F:3:LEU:HD23	1:F:3:LEU:O	1.97	0.63
1:G:36:ILE:HD11	1:G:99:MET:CB	2.29	0.63
1:I:101:SER:O	1:I:105:THR:HG23	1.99	0.63
3:d:286:THR:O	3:d:290:LEU:HG	1.98	0.63
3:d:562:LEU:HD21	3:d:625:PHE:CD1	2.34	0.63
3:a:140:LYS:HE3	3:a:271:ARG:O	1.99	0.63
3:e:282:THR:O	3:e:286:THR:HG23	1.98	0.63
3:e:477:PRO:HB2	3:e:480:VAL:CG1	2.27	0.63
3:e:503:PHE:HE1	3:e:533:LEU:HD13	1.63	0.63
1:D:30:ILE:HG23	1:D:47:GLN:OE1	1.99	0.63
3:c:118:ILE:HG23	3:c:158:GLU:HG2	1.79	0.63
3:e:477:PRO:HB2	3:e:480:VAL:HG13	1.79	0.63
3:f:281:PRO:CG	3:f:327:PRO:HG3	2.28	0.63
3:f:611:LYS:HA	3:f:614:LEU:HG	1.80	0.63
1:T:89:GLN:CG	1:T:111:LYS:HB3	2.29	0.63
3:b:658:LEU:HD21	3:a:462:LEU:CD2	2.29	0.63
3:e:554:HIS:CD2	3:e:555:PRO:HD2	2.34	0.63
3:f:406:ASP:O	3:f:410:ILE:HD13	1.99	0.63
1:D:43:SER:O	1:D:47:GLN:HG3	1.99	0.63
3:d:462:LEU:HD23	3:e:698:GLU:HB3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:GLU:CG	1:D:141:ARG:HH22	2.11	0.62
1:N:51:LEU:CD2	1:N:60:ILE:HD12	2.29	0.62
3:b:286:THR:O	3:b:290:LEU:HG	1.98	0.62
3:c:246:ARG:HG3	3:c:248:GLU:OE2	1.99	0.62
3:e:318:ASN:HB3	3:e:326:LEU:CD1	2.26	0.62
3:f:147:GLY:O	3:f:256:THR:HA	1.98	0.62
3:f:455:ILE:CD1	3:f:489:LEU:HD11	2.29	0.62
1:F:54:GLN:HA	3:c:597:GLU:OE2	1.99	0.62
1:K:93:LEU:HD12	1:K:93:LEU:O	1.99	0.62
1:M:180:ALA:HB1	1:M:185:LEU:CD1	2.29	0.62
3:b:716:ALA:C	3:b:717:ALA:HA	2.24	0.62
3:e:521:PRO:HB2	3:e:524:TYR:CE2	2.33	0.62
3:e:564:ILE:HD11	3:e:580:PHE:CB	2.29	0.62
3:e:660:LYS:HB2	3:e:660:LYS:NZ	2.13	0.62
1:A:160:GLN:HB3	1:A:164:VAL:HG11	1.80	0.62
1:C:8:ILE:HA	1:C:18:TYR:HB2	1.79	0.62
1:E:105:THR:HG21	1:E:154:LEU:HD11	1.81	0.62
1:E:105:THR:HG21	1:E:185:LEU:HD22	1.81	0.62
1:M:41:ALA:O	1:M:45:ILE:HD13	1.97	0.62
1:G:4:ILE:CG2	1:G:20:ILE:HG22	2.29	0.62
1:I:36:ILE:HA	1:I:40:VAL:HG21	1.81	0.62
1:M:97:ALA:CB	1:M:121:MET:HE3	2.29	0.62
3:b:145:LEU:HD23	3:b:276:VAL:HB	1.81	0.62
3:d:666:GLU:OE1	3:d:666:GLU:HA	1.99	0.62
3:a:713:GLN:OE1	3:a:713:GLN:HA	1.99	0.62
3:e:411:VAL:O	3:e:415:THR:HG23	1.99	0.62
3:e:514:VAL:O	3:e:518:ILE:HG12	2.00	0.62
3:e:724:ILE:O	3:e:725:ILE:HD13	1.99	0.62
3:f:326:LEU:HD22	3:f:329:LYS:HD2	1.81	0.62
3:f:691:ARG:HG2	3:f:691:ARG:HH11	1.64	0.62
1:D:81:MET:HE3	1:D:88:VAL:HG21	1.79	0.62
1:F:122:ILE:O	1:F:122:ILE:HD12	2.00	0.62
1:N:161:PRO:HD2	1:N:164:VAL:HG11	1.81	0.62
3:d:184:VAL:O	3:d:187:VAL:HG22	1.99	0.62
3:a:328:ASP:OD2	3:f:271:ARG:HD2	1.98	0.62
3:e:138:ARG:HB3	3:f:300:TYR:CE1	2.35	0.62
3:e:640:LYS:HD3	3:e:680:TYR:HE1	1.64	0.62
3:f:151:VAL:HA	3:f:327:PRO:HG2	1.80	0.62
1:F:63:TYR:CD2	1:F:93:LEU:HD21	2.35	0.62
1:N:115:LEU:HD13	1:N:116:PRO:HD3	1.80	0.62
3:b:145:LEU:O	3:b:254:ALA:HB3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:194:GLY:HA2	3:b:197:GLU:HB2	1.82	0.62
3:c:193:ARG:HA	3:c:193:ARG:HH11	1.65	0.62
3:c:662:LYS:HZ3	3:c:662:LYS:HB2	1.63	0.62
3:f:154:THR:HG23	4:f:802:ATP:O1B	2.00	0.62
1:A:3:LEU:HD12	1:A:3:LEU:O	1.99	0.62
1:E:137:GLU:HG3	1:N:144:LEU:HD11	1.82	0.62
1:F:28:ARG:HB3	1:F:60:ILE:HG22	1.79	0.62
1:K:28:ARG:HG2	1:K:51:LEU:HD12	1.82	0.62
3:d:121:VAL:HA	4:d:801:ATP:N1	2.14	0.62
3:d:150:GLY:HA2	4:d:801:ATP:O3A	2.00	0.62
3:f:431:LYS:HD3	3:f:431:LYS:H	1.61	0.62
1:A:67:PRO:O	1:A:97:ALA:HB3	2.00	0.62
3:b:687:ARG:HG3	3:a:627:ASN:HD21	1.64	0.62
3:c:488:GLN:O	3:c:492:GLU:HG2	2.00	0.62
3:c:560:MET:CE	3:d:507:GLU:HA	2.30	0.62
3:d:297:TYR:HE1	3:d:331:ILE:HG23	1.64	0.62
3:e:565:LEU:HD13	3:e:628:ARG:HH12	1.63	0.62
3:f:144:VAL:HG13	3:f:275:PRO:HA	1.81	0.62
3:f:640:LYS:NZ	3:f:640:LYS:HB3	2.15	0.62
1:C:27:ASP:OD2	3:e:600:VAL:HG21	2.00	0.62
1:G:125:PRO:HD2	1:G:147:ARG:HG3	1.81	0.62
1:M:161:PRO:HD2	1:M:164:VAL:HG11	1.81	0.62
3:c:560:MET:HE2	3:d:507:GLU:HA	1.82	0.62
3:d:271:ARG:HG3	3:d:271:ARG:O	1.99	0.62
3:e:719:ASP:HB3	3:e:723:LYS:O	1.98	0.62
1:E:124:GLN:OE1	1:N:133:ALA:HB3	2.00	0.62
1:F:5:PRO:HG3	1:G:47:GLN:NE2	2.15	0.62
1:L:71:VAL:HG12	1:L:75:LEU:HD23	1.82	0.62
1:S:109:LYS:HE3	1:S:112:ARG:HH12	1.63	0.62
3:b:198:GLU:O	3:b:202:LYS:HD2	2.00	0.62
3:b:456:ARG:HD2	3:c:706:LEU:CD1	2.29	0.62
3:d:189:GLY:HA3	3:d:196:PHE:CE2	2.35	0.62
3:d:578:VAL:HG23	3:d:580:PHE:CE1	2.34	0.62
3:e:148:GLU:HG3	3:e:325:PHE:CZ	2.35	0.62
1:B:67:PRO:O	1:B:97:ALA:HB3	2.00	0.61
1:E:144:LEU:HD11	1:N:137:GLU:HG3	1.82	0.61
1:K:165:ILE:O	1:K:169:THR:HG23	2.00	0.61
1:K:167:ARG:CZ	1:K:167:ARG:HB2	2.30	0.61
3:b:457:ARG:HD3	3:c:699:ASP:OD1	2.00	0.61
3:c:293:LEU:HD12	3:c:331:ILE:CD1	2.29	0.61
3:a:157:VAL:HG21	3:a:216:PHE:CE1	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:188:GLN:HG2	3:a:199:ARG:NH2	2.15	0.61
3:e:674:LYS:CE	3:e:718:LEU:HD11	2.28	0.61
1:F:105:THR:HG22	1:F:185:LEU:HD13	1.82	0.61
1:N:176:THR:H	1:N:179:GLN:NE2	1.98	0.61
3:c:272:ARG:HG3	3:c:272:ARG:HH11	1.65	0.61
3:d:128:ILE:HD11	3:d:156:VAL:O	2.00	0.61
3:a:181:LEU:CD2	3:a:203:LEU:HD11	2.28	0.61
3:e:130:ARG:O	3:e:134:ILE:HG12	1.99	0.61
3:e:243:ALA:HA	3:e:248:GLU:OE2	2.00	0.61
1:A:144:LEU:HD11	1:K:137:GLU:HG3	1.81	0.61
1:B:33:SER:HB2	1:C:42:ASN:CG	2.26	0.61
1:B:53:ALA:HB2	3:f:600:VAL:O	2.00	0.61
1:B:109:LYS:HB3	1:B:109:LYS:HZ3	1.65	0.61
1:D:5:PRO:HG2	1:E:47:GLN:OE1	2.00	0.61
1:F:140:ALA:O	1:F:144:LEU:HD23	2.00	0.61
3:b:698:GLU:HA	3:b:726:VAL:HG21	1.80	0.61
3:f:204:ILE:HD11	3:f:240:LEU:CD2	2.29	0.61
1:C:89:GLN:HB3	1:C:111:LYS:CB	2.31	0.61
1:D:108:GLN:HB3	1:D:111:LYS:CB	2.29	0.61
3:d:281:PRO:HG2	3:d:327:PRO:CD	2.25	0.61
3:d:578:VAL:HG23	3:d:580:PHE:HE1	1.65	0.61
3:e:148:GLU:HG3	3:e:325:PHE:CE1	2.35	0.61
3:e:290:LEU:HD13	3:e:310:ILE:CG2	2.31	0.61
3:e:658:LEU:HA	3:e:661:GLN:HE22	1.64	0.61
3:f:686:ALA:HA	3:f:689:LEU:CD2	2.22	0.61
1:F:81:MET:HE1	1:F:106:ALA:HB3	1.82	0.61
1:G:120:ILE:CG2	1:G:175:MET:HG3	2.29	0.61
2:H:5:UNK:N	3:a:193:ARG:HB2	2.14	0.61
1:K:161:PRO:HD2	1:K:164:VAL:HG11	1.80	0.61
3:a:715:VAL:HG12	3:a:728:GLY:CA	2.31	0.61
3:e:122:VAL:CG1	3:e:289:ILE:HG23	2.31	0.61
3:f:714:LEU:HD22	3:f:728:GLY:CA	2.26	0.61
1:B:109:LYS:HB3	1:B:109:LYS:NZ	2.15	0.61
1:F:23:ARG:HD2	1:F:23:ARG:O	2.01	0.61
1:I:43:SER:O	1:I:47:GLN:HG3	2.01	0.61
3:c:447:ALA:CB	3:c:633:ILE:HG21	2.30	0.61
3:d:204:ILE:O	3:d:208:THR:HG23	2.00	0.61
3:d:234:MET:HE3	3:d:235:ASP:HB2	1.81	0.61
3:d:650:MET:O	3:d:654:VAL:HG23	2.00	0.61
3:e:234:MET:HA	3:e:234:MET:CE	2.21	0.61
1:E:27:ASP:HB3	3:c:600:VAL:HG12	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:180:ALA:HB1	1:M:185:LEU:HD11	1.83	0.61
1:N:115:LEU:CD1	1:S:79:ASP:HB3	2.22	0.61
3:b:281:PRO:CG	3:b:327:PRO:HG3	2.30	0.61
3:d:204:ILE:HD12	3:d:207:ILE:CG2	2.29	0.61
1:B:45:ILE:HD11	1:B:77:ILE:HA	1.82	0.61
1:I:9:GLU:O	1:I:17:ALA:HB3	2.01	0.61
1:S:93:LEU:CD1	1:T:45:ILE:HD13	2.30	0.61
1:T:90:THR:CG2	1:T:104:LEU:HD12	2.30	0.61
3:c:206:GLU:O	3:c:209:GLU:HG3	2.00	0.61
3:d:243:ALA:CA	3:d:248:GLU:HB3	2.31	0.61
3:d:265:LYS:HA	3:d:265:LYS:CE	2.27	0.61
3:a:642:ASN:O	3:a:646:ILE:HG13	2.01	0.61
1:A:89:GLN:CB	1:A:111:LYS:HB3	2.30	0.61
1:T:92:VAL:HG23	1:T:104:LEU:CD1	2.28	0.61
1:T:141:ARG:HH11	1:T:141:ARG:HG3	1.66	0.61
3:b:456:ARG:O	3:b:460:VAL:HG23	2.01	0.61
3:b:505:MET:HB3	3:b:553:ALA:HB2	1.82	0.61
3:c:674:LYS:HE2	3:c:722:GLY:O	2.00	0.61
3:d:456:ARG:HD2	3:e:706:LEU:CD1	2.28	0.61
1:F:8:ILE:HG12	1:F:17:ALA:CB	2.27	0.61
3:c:477:PRO:HG2	3:c:480:VAL:CG1	2.30	0.61
3:a:658:LEU:HD21	3:f:462:LEU:HD21	1.82	0.61
3:e:324:ARG:HB2	3:e:329:LYS:HB2	1.83	0.61
3:e:483:THR:HG22	3:e:487:LYS:HE2	1.82	0.61
3:f:695:GLU:HA	3:f:699:ASP:OD2	2.00	0.61
1:C:8:ILE:H	1:C:8:ILE:HD12	1.66	0.60
1:D:29:ILE:HD13	1:D:61:TYR:HB2	1.82	0.60
3:e:499:SER:OG	3:e:543:SER:HA	2.01	0.60
3:e:511:LYS:HA	3:e:554:HIS:ND1	2.16	0.60
3:e:522:PRO:HA	3:e:527:TYR:CD1	2.36	0.60
3:f:546:LEU:HA	3:f:586:ILE:O	2.01	0.60
1:C:16:ARG:HH22	1:D:16:ARG:NH1	1.99	0.60
1:C:18:TYR:HE1	1:C:26:LYS:HD3	1.66	0.60
1:D:23:ARG:O	1:D:26:LYS:HG2	2.00	0.60
1:D:41:ALA:O	1:D:45:ILE:HG12	2.01	0.60
1:E:85:LYS:HB2	1:E:85:LYS:HZ3	1.64	0.60
1:M:37:ASP:OD1	1:M:40:VAL:HG23	2.01	0.60
1:M:160:GLN:HB3	1:M:164:VAL:HG11	1.81	0.60
3:d:483:THR:HB	4:d:802:ATP:O2A	2.01	0.60
3:a:220:VAL:O	3:a:223:ILE:HG12	2.01	0.60
3:a:590:ASN:O	3:a:593:THR:HG22	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:f:101:LEU:O	3:f:105:TYR:HB2	2.01	0.60
3:f:285:GLU:O	3:f:289:ILE:HG12	2.01	0.60
1:A:29:ILE:HD12	1:A:63:TYR:HE2	1.64	0.60
1:A:47:GLN:HE21	1:G:5:PRO:HG3	1.64	0.60
3:b:422:LEU:HD23	3:b:430:LEU:HD12	1.84	0.60
3:c:503:PHE:CE2	3:c:533:LEU:HD13	2.35	0.60
3:d:181:LEU:HD21	3:d:215:LEU:HD21	1.83	0.60
3:f:172:LYS:HZ3	3:f:172:LYS:HB2	1.65	0.60
1:I:46:ALA:HB1	1:T:24:LEU:HD11	1.83	0.60
1:L:140:ALA:O	1:L:143:ILE:HG22	2.01	0.60
3:c:108:ASN:HB3	3:c:111:GLU:HB3	1.83	0.60
3:d:304:LYS:O	3:d:304:LYS:HD3	2.01	0.60
3:e:154:THR:O	3:e:157:VAL:HG12	2.00	0.60
3:f:196:PHE:HA	3:f:199:ARG:HG2	1.81	0.60
3:f:341:MET:HE3	3:f:341:MET:CA	2.19	0.60
1:G:3:LEU:HD13	1:G:4:ILE:N	2.15	0.60
1:I:50:PHE:CE2	1:T:7:VAL:HG21	2.36	0.60
1:K:8:ILE:HA	1:K:16:ARG:O	2.01	0.60
1:M:99:MET:HE1	1:M:150:LEU:HD11	1.84	0.60
1:N:178:GLU:OE2	1:N:178:GLU:HA	2.02	0.60
3:b:171:GLN:O	3:b:172:LYS:HG3	2.01	0.60
3:c:646:ILE:HG22	3:c:650:MET:HE3	1.82	0.60
3:e:683:ALA:HB3	3:e:684:MET:SD	2.42	0.60
1:G:89:GLN:NE2	1:G:111:LYS:HD2	2.16	0.60
1:L:101:SER:O	1:L:105:THR:HG23	2.01	0.60
1:C:68:GLY:N	1:C:97:ALA:HB3	2.16	0.60
1:K:23:ARG:HG3	1:K:23:ARG:NH1	2.10	0.60
1:L:115:LEU:HD13	1:M:79:ASP:CB	2.31	0.60
3:c:694:GLN:O	3:c:698:GLU:HB2	2.01	0.60
3:d:202:LYS:O	3:d:206:GLU:HG2	2.02	0.60
3:a:268:ALA:HB1	3:a:272:ARG:HH12	1.66	0.60
3:e:405:LYS:HA	3:e:405:LYS:HE3	1.82	0.60
3:f:600:VAL:HG23	3:f:601:GLY:O	2.01	0.60
1:S:165:ILE:O	1:S:169:THR:HG23	2.01	0.60
3:c:717:ALA:HB3	3:c:725:ILE:CD1	2.28	0.60
3:d:118:ILE:CD1	3:d:158:GLU:HB3	2.31	0.60
3:d:475:VAL:HG21	3:d:617:LEU:HD21	1.83	0.60
3:a:564:ILE:HD11	3:a:570:LEU:HD22	1.83	0.60
3:e:324:ARG:N	3:e:324:ARG:HD3	2.15	0.60
3:e:420:GLY:HA2	3:e:423:LYS:HE2	1.82	0.60
3:f:503:PHE:HE2	3:f:533:LEU:HD13	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:ILE:HG22	1:B:144:LEU:HD22	1.83	0.60
1:E:155:ALA:HA	1:E:158:THR:HG22	1.84	0.60
1:G:36:ILE:HD11	1:G:99:MET:HB2	1.82	0.60
1:I:120:ILE:HD13	1:I:180:ALA:HB2	1.83	0.60
3:b:202:LYS:HZ2	3:c:189:GLY:HA2	1.67	0.60
3:c:157:VAL:HG21	3:c:216:PHE:CE1	2.36	0.60
3:f:147:GLY:C	3:f:153:LYS:HZ1	2.10	0.60
1:D:37:ASP:H	1:D:40:VAL:HG12	1.67	0.60
1:G:190:MET:HE1	3:a:602:PHE:CZ	2.37	0.60
2:H:4:UNK:HA	3:a:193:ARG:H	1.67	0.60
1:L:98:SER:HB3	1:L:123:HIS:CD2	2.37	0.60
3:b:517:LEU:HD12	3:b:560:MET:CE	2.32	0.60
3:b:698:GLU:CD	3:b:698:GLU:H	2.10	0.60
3:d:178:VAL:HG12	3:d:214:ILE:HB	1.84	0.60
3:d:326:LEU:HB2	3:d:327:PRO:HA	1.84	0.60
3:e:407:ILE:O	3:e:411:VAL:HG23	2.00	0.60
3:e:665:ILE:HD11	3:e:716:ALA:CB	2.25	0.60
3:f:207:ILE:HG23	3:f:213:VAL:HG13	1.83	0.60
3:f:644:MET:HE1	3:f:673:GLU:CA	2.31	0.60
1:C:141:ARG:CZ	1:C:141:ARG:HB2	2.32	0.59
1:L:141:ARG:HB3	1:L:141:ARG:NH1	2.17	0.59
1:M:141:ARG:CZ	1:M:141:ARG:HB2	2.31	0.59
1:N:95:MET:HE3	1:N:119:GLU:HG2	1.84	0.59
1:S:93:LEU:HD23	1:S:93:LEU:H	1.66	0.59
3:d:262:ILE:HD12	3:d:262:ILE:C	2.27	0.59
3:a:675:LEU:CD2	3:a:692:THR:HG22	2.31	0.59
3:e:501:VAL:CG2	3:e:545:ILE:HD13	2.32	0.59
1:A:152:SER:HA	1:A:162:ILE:HD11	1.82	0.59
1:D:160:GLN:HB3	1:D:164:VAL:HG11	1.83	0.59
1:N:58:LYS:O	1:N:86:ALA:HB1	2.02	0.59
1:S:141:ARG:CZ	1:S:141:ARG:HB2	2.31	0.59
3:b:152:GLY:O	3:b:156:VAL:HG23	2.01	0.59
3:e:101:LEU:O	3:e:105:TYR:HB3	2.02	0.59
3:e:431:LYS:HE2	3:e:431:LYS:N	2.17	0.59
3:f:514:VAL:HG13	3:f:560:MET:CE	2.29	0.59
1:A:43:SER:O	1:A:47:GLN:HG3	2.02	0.59
1:C:24:LEU:HD11	1:D:46:ALA:HB1	1.84	0.59
1:K:153:ILE:O	1:K:157:ARG:HG2	2.03	0.59
3:d:169:VAL:HG21	3:d:173:LEU:CD1	2.31	0.59
3:d:261:ARG:HG2	3:d:261:ARG:HH11	1.67	0.59
3:e:336:GLU:OE1	3:e:410:ILE:HG21	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:e:554:HIS:O	3:e:557:VAL:HG12	2.02	0.59
3:e:661:GLN:OE1	3:e:661:GLN:N	2.34	0.59
1:K:140:ALA:O	1:K:144:LEU:HD23	2.02	0.59
3:c:183:VAL:HG21	3:c:222:GLU:HB3	1.83	0.59
3:c:190:THR:HA	3:c:196:PHE:HB2	1.83	0.59
3:a:159:GLY:O	3:a:163:LYS:HG3	2.03	0.59
3:e:451:VAL:CG2	3:e:633:ILE:HD13	2.33	0.59
1:C:16:ARG:HG2	1:C:17:ALA:O	2.01	0.59
1:L:40:VAL:O	1:L:44:VAL:HG23	2.02	0.59
3:a:664:HIS:HB3	3:a:713:GLN:OE1	2.01	0.59
3:e:336:GLU:OE1	3:e:410:ILE:HG12	2.03	0.59
3:e:614:LEU:HA	3:e:617:LEU:CD2	2.33	0.59
1:I:85:LYS:O	1:I:86:ALA:HB3	2.02	0.59
1:N:45:ILE:CD1	1:N:77:ILE:HA	2.32	0.59
3:d:129:LYS:HA	3:d:132:ILE:CD1	2.33	0.59
3:e:241:LYS:HE2	3:e:241:LYS:CA	2.33	0.59
3:e:319:ARG:HD2	3:e:542:TYR:HE1	1.65	0.59
3:e:558:LEU:HD23	3:e:562:LEU:HD13	1.85	0.59
3:f:202:LYS:O	3:f:206:GLU:HG3	2.02	0.59
1:M:122:ILE:HD11	1:M:185:LEU:CD2	2.33	0.59
1:S:140:ALA:O	1:S:143:ILE:HG22	2.03	0.59
3:c:521:PRO:HG2	3:d:512:HIS:CD2	2.37	0.59
3:d:221:HIS:HA	3:d:259:GLU:CD	2.27	0.59
3:d:221:HIS:CD2	3:d:259:GLU:HB2	2.37	0.59
3:d:240:LEU:O	3:d:244:LEU:HG	2.03	0.59
1:A:10:GLN:HB3	3:f:620:PHE:HE2	1.66	0.59
1:A:33:SER:HA	1:A:65:ASN:O	2.02	0.59
1:C:93:LEU:HD13	1:D:45:ILE:HG21	1.85	0.59
1:F:161:PRO:HD2	1:F:164:VAL:HG11	1.85	0.59
3:b:157:VAL:HG21	3:b:216:PHE:CE1	2.38	0.59
3:b:215:LEU:O	3:b:215:LEU:HG	2.02	0.59
3:b:271:ARG:HD2	3:c:328:ASP:OD2	2.02	0.59
3:c:418:PRO:HB2	3:c:459:ARG:NH1	2.18	0.59
3:c:710:GLU:HA	3:c:710:GLU:OE2	2.03	0.59
3:d:189:GLY:HA3	3:d:196:PHE:CZ	2.38	0.59
3:d:464:LYS:HB2	3:d:467:ARG:HB2	1.85	0.59
1:F:152:SER:O	1:F:156:GLU:HG3	2.02	0.59
3:b:190:THR:O	3:a:192:ILE:HD11	2.03	0.59
3:d:110:THR:HG23	3:d:178:VAL:H	1.67	0.59
3:d:113:ALA:HA	3:d:118:ILE:CG2	2.33	0.59
3:d:223:ILE:HG12	3:d:263:ILE:CG2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:101:LEU:O	3:a:101:LEU:HD23	2.03	0.59
3:a:469:ILE:HD11	3:a:584:ILE:CG1	2.32	0.59
3:e:102:LEU:HD23	3:e:103:GLY:N	2.17	0.59
3:f:505:MET:CE	3:f:547:LEU:HD23	2.32	0.59
3:f:570:LEU:O	3:f:578:VAL:HG22	2.02	0.59
3:f:654:VAL:O	3:f:658:LEU:HG	2.02	0.59
3:f:671:VAL:HG23	3:f:724:ILE:HD12	1.85	0.59
1:C:63:TYR:CE2	1:C:91:ILE:HD11	2.38	0.59
1:F:74:GLY:HA3	1:F:99:MET:HG2	1.85	0.59
1:I:143:ILE:HG23	1:I:144:LEU:HD22	1.84	0.59
3:b:110:THR:HG21	3:b:177:GLU:OE1	2.03	0.59
3:e:260:TYR:OH	3:e:275:PRO:HD3	2.03	0.59
3:f:646:ILE:O	3:f:650:MET:HG3	2.02	0.59
1:C:12:SER:HB2	1:C:15:GLU:HG2	1.85	0.58
1:D:85:LYS:HD3	1:D:85:LYS:N	2.17	0.58
1:E:109:LYS:NZ	1:E:109:LYS:HB3	2.18	0.58
1:K:32:LEU:HD22	1:K:66:SER:OG	2.03	0.58
3:e:210:ALA:HB1	3:e:212:ASN:OD1	2.03	0.58
3:f:235:ASP:O	3:f:239:ILE:HD13	2.02	0.58
3:f:474:PHE:HE1	3:f:633:ILE:HD12	1.68	0.58
1:I:93:LEU:CD1	1:K:45:ILE:HG21	2.33	0.58
1:K:43:SER:O	1:K:47:GLN:HG3	2.03	0.58
1:K:141:ARG:CZ	1:K:141:ARG:HB2	2.33	0.58
1:N:75:LEU:HG	1:N:149:ARG:NH2	2.14	0.58
3:b:434:ALA:HB1	3:b:438:LYS:NZ	2.18	0.58
3:a:161:ALA:O	3:a:164:ILE:HG22	2.02	0.58
3:e:304:LYS:H	3:e:304:LYS:CD	2.15	0.58
3:e:640:LYS:HD3	3:e:680:TYR:CE1	2.37	0.58
3:f:193:ARG:HH11	3:f:230:GLY:HA3	1.67	0.58
1:E:121:MET:HG3	1:E:174:TYR:CE1	2.38	0.58
1:F:122:ILE:CD1	1:F:173:ASN:HB3	2.33	0.58
1:G:181:LYS:HA	1:G:186:ILE:O	2.03	0.58
1:L:51:LEU:CD1	1:L:60:ILE:HD12	2.34	0.58
3:b:647:VAL:HG22	3:b:689:LEU:HD11	1.84	0.58
3:a:512:HIS:O	3:f:521:PRO:HG3	2.04	0.58
3:e:462:LEU:HD21	3:f:702:ALA:CA	2.33	0.58
3:e:503:PHE:CE1	3:e:533:LEU:HD13	2.38	0.58
3:e:650:MET:HE1	3:e:689:LEU:CB	2.33	0.58
3:e:652:GLU:HA	3:e:652:GLU:OE2	2.04	0.58
3:f:450:LYS:NZ	3:f:450:LYS:HB3	2.18	0.58
1:D:155:ALA:HB2	1:D:162:ILE:HD13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:141:ARG:HB2	1:I:141:ARG:CZ	2.33	0.58
1:K:161:PRO:HG2	1:K:164:VAL:HG12	1.86	0.58
3:b:478:THR:CG2	3:a:627:ASN:HD22	2.14	0.58
3:d:710:GLU:OE1	3:d:710:GLU:N	2.36	0.58
3:a:224:VAL:HG21	3:a:262:ILE:HG22	1.84	0.58
3:f:651:LEU:HA	3:f:654:VAL:HG12	1.85	0.58
1:B:24:LEU:HB3	1:B:29:ILE:HB	1.86	0.58
1:B:93:LEU:HD23	1:B:93:LEU:H	1.68	0.58
1:B:161:PRO:HG2	1:B:164:VAL:HG23	1.86	0.58
1:D:181:LYS:HZ3	1:D:188:GLU:HA	1.68	0.58
1:E:141:ARG:CZ	1:E:141:ARG:HB2	2.32	0.58
1:L:167:ARG:HB2	1:L:167:ARG:CZ	2.34	0.58
3:e:192:ILE:CG2	3:e:195:GLN:HB3	2.27	0.58
3:e:281:PRO:CG	3:e:327:PRO:HG3	2.33	0.58
3:f:281:PRO:CD	3:f:327:PRO:HG3	2.32	0.58
3:f:306:THR:HG23	3:f:403:THR:N	2.19	0.58
1:M:62:LEU:HD22	1:M:64:ILE:CD1	2.33	0.58
1:T:62:LEU:HD22	1:T:64:ILE:CD1	2.33	0.58
3:b:140:LYS:HD2	3:b:272:ARG:HA	1.84	0.58
3:c:697:ILE:O	3:c:701:ILE:HG13	2.04	0.58
3:d:173:LEU:HB2	3:d:176:LYS:HD3	1.85	0.58
3:e:643:LEU:O	3:e:647:VAL:HG23	2.04	0.58
3:f:596:VAL:HG13	3:f:616:GLN:HG3	1.84	0.58
1:F:41:ALA:CB	1:F:73:ALA:HB1	2.31	0.58
1:G:140:ALA:O	1:G:144:LEU:HD13	2.04	0.58
1:K:108:GLN:O	1:K:111:LYS:HB2	2.03	0.58
3:b:268:ALA:HB1	3:b:272:ARG:NH1	2.18	0.58
3:d:110:THR:HG21	3:d:177:GLU:HA	1.85	0.58
3:d:176:LYS:HA	3:d:212:ASN:O	2.04	0.58
3:d:616:GLN:OE1	3:d:616:GLN:N	2.35	0.58
3:a:479:GLY:HA2	4:a:802:ATP:O2A	2.04	0.58
3:e:203:LEU:HD23	3:e:203:LEU:O	2.03	0.58
3:e:565:LEU:CD2	3:e:585:ILE:HG13	2.34	0.58
3:f:475:VAL:HG21	3:f:617:LEU:HD21	1.85	0.58
3:f:668:PRO:O	3:f:671:VAL:HG12	2.03	0.58
1:A:153:ILE:O	1:A:157:ARG:HG2	2.04	0.58
1:K:25:LEU:CD1	1:K:51:LEU:HD21	2.34	0.58
3:b:101:LEU:HD11	3:b:203:LEU:CD1	2.33	0.58
3:c:622:THR:OG1	3:c:623:PRO:HD2	2.04	0.58
3:d:181:LEU:HD12	3:d:181:LEU:O	2.02	0.58
3:e:124:ARG:O	3:e:128:ILE:HG12	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:e:433:LEU:HD22	3:e:452:ALA:CB	2.34	0.58
3:e:460:VAL:CG1	3:e:462:LEU:HG	2.34	0.58
1:N:44:VAL:HG11	1:N:77:ILE:CD1	2.33	0.58
1:T:140:ALA:O	1:T:143:ILE:HG22	2.04	0.58
3:c:571:THR:HG22	3:c:577:THR:HB	1.86	0.58
3:d:109:ILE:HB	3:d:178:VAL:HG23	1.84	0.58
3:a:408:GLU:OE2	3:a:420:GLY:HA3	2.03	0.58
3:f:553:ALA:HB1	3:f:557:VAL:HG21	1.86	0.58
1:N:137:GLU:HG2	1:N:141:ARG:NH2	2.18	0.58
1:N:140:ALA:O	1:N:143:ILE:HG22	2.04	0.58
1:S:7:VAL:HG21	1:S:23:ARG:HG3	1.85	0.58
3:d:126:GLN:O	3:d:129:LYS:HE3	2.03	0.58
3:d:641:GLU:OE1	3:d:641:GLU:N	2.34	0.58
3:a:482:LYS:HD2	3:a:588:THR:HG23	1.85	0.58
3:a:663:LEU:HD21	3:a:705:TYR:CD1	2.39	0.58
3:e:650:MET:O	3:e:654:VAL:HG23	2.04	0.58
3:e:714:LEU:HD12	3:e:715:VAL:N	2.19	0.58
1:C:43:SER:O	1:C:47:GLN:HG3	2.04	0.57
1:K:120:ILE:O	1:K:175:MET:HG2	2.04	0.57
1:K:137:GLU:HG2	1:K:141:ARG:NH2	2.18	0.57
1:N:47:GLN:O	1:N:51:LEU:HD13	2.04	0.57
1:N:109:LYS:HB3	1:N:109:LYS:NZ	2.19	0.57
3:c:200:MET:HE3	3:c:239:ILE:HB	1.86	0.57
3:d:422:LEU:O	3:d:422:LEU:HD12	2.04	0.57
3:a:171:GLN:N	3:a:171:GLN:OE1	2.37	0.57
3:e:114:ARG:CA	3:e:165:VAL:HG21	2.25	0.57
3:e:231:ASP:O	3:f:195:GLN:HB3	2.04	0.57
3:e:580:PHE:HD1	3:e:583:THR:HG21	1.69	0.57
3:e:590:ASN:OD1	3:e:594:GLY:HA3	2.03	0.57
3:e:665:ILE:HA	3:e:714:LEU:O	2.04	0.57
3:f:482:LYS:HG2	3:f:635:PHE:CD2	2.39	0.57
1:C:13:ARG:NE	1:C:13:ARG:HA	2.19	0.57
1:I:81:MET:HG2	1:I:88:VAL:HG11	1.85	0.57
1:M:71:VAL:HG12	1:M:75:LEU:HD23	1.85	0.57
1:N:92:VAL:HG23	1:N:104:LEU:CD1	2.31	0.57
3:d:130:ARG:O	3:d:134:ILE:HG13	2.04	0.57
3:a:308:GLU:HG2	3:a:404:GLU:OE2	2.04	0.57
3:e:342:ASN:O	3:e:343:LEU:HD23	2.04	0.57
3:e:697:ILE:O	3:e:701:ILE:HG22	2.04	0.57
3:f:169:VAL:HG23	3:f:174:LEU:HD13	1.86	0.57
3:f:611:LYS:HG2	3:f:614:LEU:HD11	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:516:LYS:HG2	3:a:522:PRO:HD3	1.84	0.57
3:c:195:GLN:HG2	3:c:196:PHE:H	1.68	0.57
3:d:243:ALA:HB1	3:d:249:LEU:H	1.68	0.57
3:a:245:ALA:HB2	3:a:272:ARG:HE	1.70	0.57
3:e:670:GLU:HA	3:e:673:GLU:OE1	2.03	0.57
3:f:283:VAL:O	3:f:287:ILE:HG13	2.04	0.57
1:C:19:ASP:CB	1:C:22:SER:HB2	2.29	0.57
1:E:137:GLU:CG	1:E:141:ARG:HH22	2.17	0.57
1:N:99:MET:O	1:N:103:LEU:HD13	2.05	0.57
3:b:192:ILE:CG2	3:c:192:ILE:HD13	2.35	0.57
3:b:336:GLU:HB3	3:b:410:ILE:HD13	1.87	0.57
3:b:714:LEU:HA	3:b:727:THR:C	2.30	0.57
3:d:234:MET:HE3	3:d:236:ALA:N	2.18	0.57
3:d:243:ALA:HB1	3:d:249:LEU:N	2.19	0.57
3:e:170:PRO:HD3	3:f:343:LEU:HD11	1.87	0.57
3:f:430:LEU:HG	3:f:431:LYS:HD3	1.86	0.57
3:f:560:MET:O	3:f:563:GLN:HG2	2.04	0.57
3:f:670:GLU:O	3:f:670:GLU:OE2	2.23	0.57
1:B:152:SER:HA	1:B:162:ILE:CD1	2.34	0.57
1:T:84:VAL:HG13	1:T:85:LYS:O	2.04	0.57
1:T:160:GLN:HB3	1:T:164:VAL:HG11	1.85	0.57
3:a:101:LEU:HD11	3:a:199:ARG:CG	2.33	0.57
3:e:671:VAL:CG2	3:e:718:LEU:HD13	2.33	0.57
3:f:459:ARG:O	3:f:459:ARG:HD3	2.05	0.57
1:A:89:GLN:HB2	1:A:111:LYS:O	2.03	0.57
1:B:140:ALA:O	1:B:144:LEU:HD23	2.05	0.57
1:L:112:ARG:HB3	1:L:186:ILE:HD12	1.86	0.57
3:b:180:ARG:HA	3:b:216:PHE:O	2.04	0.57
3:f:551:GLU:HB2	3:f:620:PHE:CE1	2.36	0.57
1:B:121:MET:HG3	1:B:174:TYR:CE2	2.40	0.57
1:D:190:MET:HE3	1:E:83:PHE:CE1	2.40	0.57
1:L:181:LYS:HA	1:L:186:ILE:HG22	1.86	0.57
3:d:234:MET:CE	3:d:235:ASP:HB2	2.34	0.57
3:a:221:HIS:O	3:a:224:VAL:HG22	2.05	0.57
3:e:161:ALA:HA	3:e:164:ILE:HG22	1.86	0.57
3:f:249:LEU:HD23	3:f:250:GLN:N	2.19	0.57
3:f:657:LEU:O	3:f:657:LEU:HD13	2.05	0.57
1:A:41:ALA:HB2	1:A:73:ALA:HB1	1.87	0.57
1:B:45:ILE:O	1:B:49:LEU:HG	2.05	0.57
1:B:141:ARG:CZ	1:B:141:ARG:HB2	2.35	0.57
1:F:29:ILE:HG23	1:F:63:TYR:CE1	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:101:LEU:HD23	3:b:101:LEU:O	2.04	0.57
3:b:222:GLU:OE1	3:a:234:MET:HE1	2.04	0.57
3:b:662:LYS:HB3	3:b:710:GLU:HB3	1.86	0.57
3:c:725:ILE:HD12	3:c:725:ILE:O	2.05	0.57
3:a:283:VAL:O	3:a:287:ILE:HG13	2.05	0.57
3:e:671:VAL:N	3:e:718:LEU:HD22	2.19	0.57
1:A:89:GLN:HB3	1:A:111:LYS:HB3	1.87	0.57
1:C:115:LEU:HD23	1:D:79:ASP:CB	2.34	0.57
1:F:49:LEU:HD22	3:c:601:GLY:HA3	1.85	0.57
3:b:237:GLY:O	3:b:241:LYS:HG3	2.04	0.57
3:b:505:MET:HE2	3:b:505:MET:CA	2.35	0.57
3:b:668:PRO:HD2	3:b:671:VAL:HG21	1.87	0.57
3:e:319:ARG:HG3	3:e:320:TYR:CD1	2.38	0.57
3:e:428:THR:O	3:e:431:LYS:HG2	2.05	0.57
3:e:533:LEU:O	3:e:537:VAL:HG23	2.04	0.57
3:e:565:LEU:HD21	3:e:585:ILE:CB	2.35	0.57
1:D:89:GLN:HG2	1:D:111:LYS:CB	2.35	0.57
1:F:154:LEU:HD23	1:F:165:ILE:HD11	1.87	0.57
1:G:43:SER:O	1:G:47:GLN:HG3	2.04	0.57
1:K:58:LYS:O	1:K:86:ALA:HB1	2.05	0.57
3:c:537:VAL:HG21	3:c:580:PHE:CE2	2.40	0.57
3:c:627:ASN:ND2	3:d:687:ARG:HH11	2.02	0.57
3:a:153:LYS:CB	4:f:801:ATP:O3B	2.52	0.57
3:a:647:VAL:O	3:a:651:LEU:HD23	2.05	0.57
3:e:316:LEU:HD21	3:e:421:ASP:HB3	1.85	0.57
3:f:493:LEU:HD13	3:f:584:ILE:CD1	2.33	0.57
1:F:92:VAL:HG21	1:F:120:ILE:HD11	1.87	0.56
1:N:5:PRO:HG3	1:S:47:GLN:NE2	2.20	0.56
3:c:324:ARG:HB2	3:c:329:LYS:HG2	1.87	0.56
3:a:164:ILE:CD1	3:a:176:LYS:HB2	2.35	0.56
3:e:597:GLU:CD	3:e:597:GLU:H	2.13	0.56
3:f:643:LEU:O	3:f:647:VAL:HG23	2.04	0.56
1:A:13:ARG:HH11	1:A:14:GLY:H	1.53	0.56
1:K:51:LEU:HG	1:K:60:ILE:HD12	1.87	0.56
3:c:200:MET:HE2	3:c:236:ALA:CA	2.35	0.56
3:d:148:GLU:HG3	3:d:325:PHE:CE1	2.40	0.56
3:a:580:PHE:O	3:a:583:THR:HG22	2.06	0.56
3:e:503:PHE:HB2	3:e:547:LEU:HD23	1.87	0.56
3:e:708:HIS:HB3	3:e:710:GLU:OE2	2.05	0.56
1:B:95:MET:HG2	1:B:96:ALA:N	2.20	0.56
1:C:8:ILE:HG13	1:C:19:ASP:N	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:ALA:HB2	1:C:73:ALA:HB1	1.87	0.56
1:C:134:THR:O	1:C:138:ILE:HG13	2.05	0.56
1:C:154:LEU:O	1:C:158:THR:HB	2.05	0.56
1:E:43:SER:O	1:E:47:GLN:HG3	2.05	0.56
1:E:175:MET:HB2	1:E:179:GLN:CB	2.34	0.56
1:F:162:ILE:HA	1:F:165:ILE:HG22	1.86	0.56
1:I:152:SER:O	1:I:156:GLU:HG3	2.05	0.56
1:K:51:LEU:HB3	1:K:60:ILE:HD11	1.87	0.56
1:L:92:VAL:CG2	1:L:104:LEU:HD22	2.32	0.56
1:M:134:THR:O	1:M:138:ILE:HG12	2.05	0.56
1:M:137:GLU:CD	1:M:141:ARG:HH22	2.12	0.56
1:M:140:ALA:O	1:M:144:LEU:HD23	2.05	0.56
3:b:647:VAL:HG21	3:b:676:VAL:HG22	1.85	0.56
3:b:701:ILE:HG23	3:b:704:TYR:CZ	2.40	0.56
3:c:462:LEU:CD2	3:d:698:GLU:HB3	2.35	0.56
3:d:129:LYS:HA	3:d:132:ILE:CG1	2.35	0.56
3:d:206:GLU:HA	3:d:209:GLU:HG3	1.85	0.56
3:d:522:PRO:HA	3:d:527:TYR:CD2	2.41	0.56
3:d:694:GLN:HA	3:d:698:GLU:HG2	1.84	0.56
3:a:301:HIS:O	3:a:303:VAL:HG23	2.06	0.56
3:e:644:MET:SD	3:e:672:LYS:HB3	2.45	0.56
3:e:650:MET:HE3	3:e:693:ILE:CD1	2.32	0.56
3:f:616:GLN:OE1	3:f:616:GLN:C	2.48	0.56
3:f:715:VAL:H	3:f:728:GLY:HA2	1.70	0.56
3:b:658:LEU:HD21	3:a:462:LEU:HD21	1.87	0.56
3:c:289:ILE:O	3:c:293:LEU:HG	2.06	0.56
3:c:550:VAL:CG2	3:c:587:MET:HB3	2.32	0.56
3:d:324:ARG:O	3:d:329:LYS:HD3	2.04	0.56
4:d:803:ATP:N1	3:e:122:VAL:HG12	2.20	0.56
3:a:417:ILE:O	3:a:419:VAL:HG23	2.05	0.56
3:a:566:ASP:HB2	3:a:628:ARG:HE	1.69	0.56
3:e:122:VAL:HG12	3:e:289:ILE:HG23	1.87	0.56
3:e:462:LEU:HD21	3:f:702:ALA:CB	2.34	0.56
3:e:482:LYS:CE	3:e:588:THR:HG23	2.35	0.56
3:e:698:GLU:CA	3:e:701:ILE:HG22	2.35	0.56
3:f:140:LYS:HE3	3:f:271:ARG:O	2.06	0.56
3:f:298:GLU:HG2	3:f:305:TYR:HD1	1.70	0.56
3:f:511:LYS:HE2	3:f:556:ASP:OD2	2.05	0.56
1:C:116:PRO:HA	1:C:189:VAL:HG11	1.86	0.56
1:C:158:THR:HG23	1:C:183:TYR:O	2.06	0.56
1:N:77:ILE:CG2	1:N:103:LEU:HD21	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:105:THR:HG22	1:N:185:LEU:HA	1.87	0.56
1:T:43:SER:O	1:T:47:GLN:HG3	2.05	0.56
3:b:118:ILE:CG2	3:b:158:GLU:HB3	2.35	0.56
3:b:179:ILE:HG12	3:b:213:VAL:HB	1.88	0.56
3:b:503:PHE:CE2	3:b:533:LEU:HD13	2.41	0.56
3:c:538:ARG:HD2	3:c:576:ARG:HD3	1.88	0.56
3:d:646:ILE:O	3:d:650:MET:HG3	2.05	0.56
3:d:672:LYS:O	3:d:676:VAL:HG23	2.06	0.56
3:d:713:GLN:C	3:d:714:LEU:HD12	2.30	0.56
3:a:173:LEU:H	3:a:173:LEU:HD23	1.70	0.56
3:e:621:PHE:HB2	3:e:626:LEU:HD21	1.86	0.56
1:G:59:ASP:OD1	1:G:87:ASP:HB3	2.06	0.56
3:b:417:ILE:HD13	3:b:582:ASP:OD1	2.06	0.56
3:d:198:GLU:O	3:d:202:LYS:HG3	2.06	0.56
3:d:204:ILE:HA	3:d:207:ILE:HG22	1.86	0.56
3:e:316:LEU:HD21	3:e:421:ASP:HB2	1.86	0.56
3:f:138:ARG:HG3	3:f:139:THR:HG23	1.88	0.56
3:f:432:ASN:O	3:f:435:VAL:HG22	2.06	0.56
3:f:500:MET:CE	3:f:502:ARG:HB2	2.35	0.56
1:A:45:ILE:HD11	1:A:77:ILE:HA	1.88	0.56
1:E:108:GLN:HB3	1:E:111:LYS:CB	2.35	0.56
1:G:92:VAL:CG2	1:G:104:LEU:HD22	2.33	0.56
1:I:140:ALA:O	1:I:143:ILE:HG22	2.05	0.56
1:S:4:ILE:HD13	1:S:21:TYR:CE2	2.41	0.56
3:d:181:LEU:CD2	3:d:215:LEU:HD11	2.36	0.56
3:d:488:GLN:O	3:d:492:GLU:HG2	2.06	0.56
3:a:482:LYS:HA	3:a:635:PHE:CE2	2.39	0.56
3:e:456:ARG:CZ	3:f:706:LEU:HD21	2.36	0.56
3:f:467:ARG:NH1	3:f:566:ASP:HA	2.21	0.56
1:I:140:ALA:O	1:I:144:LEU:HD23	2.06	0.56
1:K:28:ARG:NH2	1:K:60:ILE:HD11	2.20	0.56
1:N:92:VAL:CG2	1:N:104:LEU:HD13	2.32	0.56
3:b:122:VAL:CG1	3:b:288:THR:HG22	2.29	0.56
3:b:324:ARG:CB	3:b:329:LYS:HG2	2.34	0.56
3:c:422:LEU:HD21	3:c:430:LEU:HD12	1.88	0.56
3:d:169:VAL:O	3:d:174:LEU:HD12	2.05	0.56
3:a:244:LEU:HD23	3:a:249:LEU:CD2	2.32	0.56
3:f:145:LEU:HD13	3:f:156:VAL:CG2	2.36	0.56
1:B:181:LYS:HZ3	1:B:188:GLU:HA	1.71	0.56
1:F:89:GLN:CB	1:F:111:LYS:HB3	2.18	0.56
1:L:32:LEU:HD12	1:L:64:ILE:CD1	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:141:ARG:HB2	1:S:141:ARG:NH1	2.20	0.56
3:c:422:LEU:CD2	3:c:430:LEU:HD12	2.36	0.56
3:c:646:ILE:CG2	3:c:650:MET:HE3	2.35	0.56
3:a:317:SER:OG	3:a:329:LYS:HB2	2.06	0.56
3:e:257:LEU:HG	3:e:258:ASN:N	2.21	0.56
3:e:272:ARG:HH22	4:f:802:ATP:H8	1.53	0.56
3:e:466:ASN:O	3:e:581:LYS:HE2	2.05	0.56
1:C:20:ILE:O	1:C:24:LEU:HG	2.06	0.56
1:C:36:ILE:HG22	1:C:73:ALA:HB3	1.86	0.56
1:C:41:ALA:O	1:C:45:ILE:HD13	2.06	0.56
1:D:167:ARG:HB3	1:D:167:ARG:CZ	2.36	0.56
1:E:123:HIS:C	1:E:169:THR:HG23	2.31	0.56
1:F:21:TYR:HE2	1:F:31:MET:HE3	1.69	0.56
1:F:137:GLU:CG	1:F:141:ARG:HH22	2.19	0.56
1:K:99:MET:HE3	1:K:102:PHE:CD2	2.41	0.56
1:M:141:ARG:HB2	1:M:141:ARG:NH1	2.20	0.56
3:d:591:ALA:HB1	3:d:620:PHE:CG	2.41	0.56
3:a:173:LEU:HB2	3:a:176:LYS:HG3	1.87	0.56
3:a:224:VAL:HG21	3:a:262:ILE:CG2	2.35	0.56
3:e:570:LEU:O	3:e:577:THR:HA	2.05	0.56
1:D:12:SER:C	1:D:13:ARG:HD3	2.30	0.55
1:F:137:GLU:HG3	1:F:141:ARG:HH22	1.71	0.55
1:G:104:LEU:HD21	1:G:186:ILE:HD11	1.88	0.55
1:T:4:ILE:HD12	1:T:21:TYR:CE2	2.40	0.55
3:c:447:ALA:HB2	3:c:633:ILE:HG21	1.88	0.55
3:e:207:ILE:CD1	3:e:215:LEU:HD13	2.36	0.55
3:f:650:MET:HE1	3:f:689:LEU:HB3	1.86	0.55
1:D:80:THR:O	1:D:84:VAL:HG13	2.06	0.55
1:K:119:GLU:OE1	1:K:119:GLU:HA	2.05	0.55
1:T:52:ASP:HB2	1:T:84:VAL:HG21	1.88	0.55
3:e:189:GLY:O	3:e:195:GLN:HG3	2.06	0.55
3:e:200:MET:HE1	3:e:234:MET:SD	2.46	0.55
3:e:444:GLN:HA	3:e:636:LYS:NZ	2.20	0.55
3:e:462:LEU:HD12	3:e:463:GLY:N	2.21	0.55
3:e:501:VAL:HG21	3:e:545:ILE:HD13	1.89	0.55
3:f:180:ARG:NH1	3:f:216:PHE:HE2	2.04	0.55
1:E:167:ARG:HH11	1:E:167:ARG:HG3	1.72	0.55
1:F:55:ASP:CG	1:F:58:LYS:HG2	2.31	0.55
1:K:24:LEU:HD11	1:L:46:ALA:HB1	1.88	0.55
1:L:92:VAL:HG23	1:L:104:LEU:CD1	2.34	0.55
1:M:45:ILE:HG13	1:M:80:THR:OG1	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:143:ILE:HG23	1:M:144:LEU:HD22	1.89	0.55
3:b:693:ILE:O	3:b:697:ILE:HG23	2.05	0.55
3:d:162:GLN:O	3:d:165:VAL:HG12	2.05	0.55
3:d:239:ILE:HD12	3:d:239:ILE:C	2.31	0.55
3:a:661:GLN:HA	3:a:661:GLN:OE1	2.05	0.55
3:e:309:ALA:HB2	3:e:404:GLU:HA	1.87	0.55
3:f:245:ALA:HB2	3:f:272:ARG:NH1	2.20	0.55
1:F:59:ASP:HB3	1:F:87:ASP:HB2	1.89	0.55
3:c:164:ILE:HD13	3:c:169:VAL:HG21	1.89	0.55
3:c:455:ILE:HD13	3:c:493:LEU:HD11	1.88	0.55
3:d:241:LYS:HD2	3:e:184:VAL:HG21	1.88	0.55
3:f:611:LYS:HA	3:f:614:LEU:CG	2.36	0.55
1:C:29:ILE:HA	1:C:61:TYR:O	2.07	0.55
1:C:105:THR:OG1	1:C:185:LEU:HD22	2.05	0.55
1:D:36:ILE:HG22	1:D:73:ALA:HB3	1.89	0.55
1:F:13:ARG:O	1:F:15:GLU:HG3	2.06	0.55
1:F:54:GLN:HA	3:c:597:GLU:CD	2.31	0.55
1:I:83:PHE:CE1	1:T:190:MET:HG2	2.41	0.55
1:K:74:GLY:HA3	1:K:99:MET:HG2	1.88	0.55
1:M:119:GLU:C	1:M:120:ILE:HD12	2.31	0.55
3:c:456:ARG:O	3:c:460:VAL:HG23	2.06	0.55
3:c:723:LYS:HA	3:c:723:LYS:CE	2.20	0.55
3:d:259:GLU:O	3:d:262:ILE:HG13	2.06	0.55
3:d:405:LYS:HA	3:d:408:GLU:OE1	2.07	0.55
1:C:5:PRO:HG2	1:D:47:GLN:NE2	2.21	0.55
1:I:161:PRO:HD2	1:I:164:VAL:HG11	1.87	0.55
1:T:141:ARG:HB2	1:T:141:ARG:CZ	2.36	0.55
3:b:101:LEU:HD11	3:b:203:LEU:HD12	1.88	0.55
3:b:647:VAL:HG22	3:b:689:LEU:HD21	1.88	0.55
3:c:283:VAL:O	3:c:287:ILE:HG13	2.06	0.55
3:d:201:GLN:O	3:d:204:ILE:HG22	2.07	0.55
3:d:725:ILE:O	3:d:725:ILE:HD12	2.07	0.55
3:a:716:ALA:HB2	3:a:726:VAL:HG12	1.88	0.55
3:e:177:GLU:OE2	3:e:179:ILE:HG23	2.06	0.55
3:e:518:ILE:C	3:e:531:GLY:HA3	2.32	0.55
1:S:43:SER:O	1:S:47:GLN:HG3	2.06	0.55
3:d:289:ILE:O	3:d:293:LEU:HG	2.07	0.55
3:d:411:VAL:HG13	3:d:419:VAL:HG21	1.88	0.55
3:d:668:PRO:HD2	3:d:671:VAL:CG2	2.36	0.55
3:d:704:TYR:CE2	3:d:727:THR:HA	2.42	0.55
3:f:144:VAL:CG1	3:f:275:PRO:HA	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ALA:HB2	1:A:162:ILE:HD13	1.87	0.55
1:E:16:ARG:CZ	1:E:26:LYS:HD3	2.36	0.55
1:I:58:LYS:O	1:I:86:ALA:HB1	2.07	0.55
1:S:181:LYS:CA	1:S:186:ILE:HG22	2.37	0.55
3:b:118:ILE:HD12	3:b:158:GLU:OE2	2.06	0.55
3:b:192:ILE:HG21	3:c:192:ILE:HD13	1.88	0.55
3:b:195:GLN:HG3	3:b:199:ARG:HH22	1.68	0.55
3:b:197:GLU:OE1	3:b:197:GLU:HA	2.06	0.55
3:b:723:LYS:HA	3:b:723:LYS:CE	2.30	0.55
3:d:146:ILE:HA	3:d:255:THR:O	2.06	0.55
3:d:317:SER:HB2	3:d:333:LEU:CD1	2.37	0.55
3:a:164:ILE:HD11	3:a:176:LYS:HB2	1.87	0.55
3:f:324:ARG:HG3	3:f:324:ARG:NH1	2.21	0.55
1:M:4:ILE:HD11	1:M:21:TYR:CE1	2.42	0.55
1:T:154:LEU:O	1:T:158:THR:HG23	2.07	0.55
3:b:521:PRO:HG2	3:c:512:HIS:CD2	2.41	0.55
3:b:571:THR:HG22	3:b:577:THR:OG1	2.06	0.55
3:c:647:VAL:CG2	3:c:689:LEU:HD11	2.37	0.55
3:d:647:VAL:O	3:d:651:LEU:HD23	2.06	0.55
3:a:191:GLY:CA	3:f:192:ILE:HG12	2.24	0.55
3:a:404:GLU:O	3:a:408:GLU:HG3	2.07	0.55
3:a:422:LEU:HD23	3:a:430:LEU:HD12	1.89	0.55
3:e:230:GLY:HA2	3:f:191:GLY:CA	2.37	0.55
3:e:464:LYS:H	3:e:464:LYS:CD	2.20	0.55
3:f:651:LEU:HA	3:f:654:VAL:CG1	2.37	0.55
1:F:162:ILE:HA	1:F:165:ILE:CG2	2.37	0.55
1:L:24:LEU:HD11	1:M:46:ALA:HB1	1.89	0.55
1:S:41:ALA:HB2	1:S:73:ALA:HB1	1.89	0.55
3:c:183:VAL:O	3:c:187:VAL:HG23	2.07	0.55
3:c:238:ASN:O	3:c:242:PRO:HD3	2.07	0.55
3:d:177:GLU:OE2	3:d:213:VAL:HG12	2.07	0.55
3:d:444:GLN:O	3:d:448:VAL:HG23	2.07	0.55
3:d:549:GLU:CB	3:d:552:LYS:HD3	2.37	0.55
1:A:29:ILE:HG23	1:A:63:TYR:CE2	2.41	0.54
1:B:178:GLU:H	1:B:178:GLU:CD	2.14	0.54
1:L:113:PHE:CE1	1:L:188:GLU:HG2	2.42	0.54
1:T:178:GLU:O	1:T:182:GLU:HG2	2.07	0.54
3:b:108:ASN:HD22	3:b:179:ILE:CD1	2.20	0.54
3:b:295:LYS:HB2	3:b:295:LYS:HZ1	1.71	0.54
3:d:297:TYR:CE1	3:d:331:ILE:HG23	2.42	0.54
3:d:454:ALA:HA	3:d:457:ARG:NH1	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:591:ALA:HB1	3:d:620:PHE:CD2	2.42	0.54
3:a:144:VAL:HG13	3:a:275:PRO:HA	1.88	0.54
3:e:140:LYS:HZ1	3:e:271:ARG:C	2.15	0.54
3:e:654:VAL:O	3:e:658:LEU:HD22	2.07	0.54
3:f:246:ARG:HH22	4:f:801:ATP:H3'	1.72	0.54
1:L:122:ILE:HG13	1:L:169:THR:HG22	1.88	0.54
1:L:167:ARG:HB2	1:L:167:ARG:NH1	2.22	0.54
3:b:129:LYS:O	3:b:133:GLU:HG3	2.08	0.54
3:c:456:ARG:HD3	3:d:706:LEU:CD1	2.37	0.54
3:a:534:THR:CG2	3:a:578:VAL:HG21	2.35	0.54
3:e:690:ARG:HA	3:e:690:ARG:HH11	1.73	0.54
3:f:220:VAL:O	3:f:223:ILE:HG12	2.07	0.54
3:f:487:LYS:HD2	3:f:497:GLU:OE2	2.07	0.54
1:D:152:SER:HA	1:D:162:ILE:HD11	1.89	0.54
1:E:10:GLN:OE1	1:E:11:SER:HB3	2.07	0.54
1:K:40:VAL:O	1:K:44:VAL:HG23	2.07	0.54
1:S:7:VAL:CG2	1:S:23:ARG:HG3	2.37	0.54
3:c:196:PHE:HZ	3:c:236:ALA:HB2	1.73	0.54
3:c:243:ALA:HB1	3:c:249:LEU:HD22	1.88	0.54
3:c:271:ARG:HH12	3:d:150:GLY:HA3	1.72	0.54
3:c:561:PHE:CD1	3:c:564:ILE:HD12	2.43	0.54
3:a:687:ARG:HH21	3:f:628:ARG:CZ	2.21	0.54
3:f:410:ILE:O	3:f:414:LYS:HB2	2.07	0.54
1:A:5:PRO:HG2	1:B:47:GLN:OE1	2.08	0.54
1:K:35:PRO:HA	1:K:68:GLY:O	2.08	0.54
1:M:147:ARG:HH12	1:M:169:THR:HG22	1.73	0.54
3:c:138:ARG:HB3	3:d:300:TYR:CD2	2.43	0.54
3:c:281:PRO:CG	3:c:327:PRO:HG3	2.35	0.54
3:c:684:MET:HB3	3:c:688:PRO:CG	2.37	0.54
3:a:318:ASN:CB	3:a:326:LEU:HD11	2.35	0.54
3:e:231:ASP:N	3:f:192:ILE:HG22	2.21	0.54
3:e:480:VAL:HA	3:e:638:LEU:CD2	2.34	0.54
3:e:521:PRO:HB2	3:e:524:TYR:CD2	2.42	0.54
3:f:674:LYS:HD2	3:f:675:LEU:N	2.21	0.54
1:G:120:ILE:HG23	1:G:175:MET:CG	2.35	0.54
1:I:41:ALA:O	1:I:45:ILE:HD13	2.07	0.54
1:L:81:MET:HE1	1:L:106:ALA:CB	2.38	0.54
1:N:141:ARG:HB2	1:N:141:ARG:CZ	2.38	0.54
3:b:477:PRO:HG2	3:b:480:VAL:CG1	2.37	0.54
3:b:647:VAL:O	3:b:651:LEU:HD23	2.06	0.54
3:c:181:LEU:HD21	3:c:203:LEU:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:217:ILE:HG13	3:c:251:LEU:HD11	1.89	0.54
3:e:295:LYS:HD2	3:e:296:ARG:N	2.22	0.54
3:f:725:ILE:HD13	3:f:727:THR:HG23	1.88	0.54
1:G:161:PRO:HG2	1:G:164:VAL:CG1	2.37	0.54
1:S:55:ASP:HB3	1:S:58:LYS:HD2	1.90	0.54
3:b:221:HIS:ND1	3:b:255:THR:HG21	2.22	0.54
3:c:721:GLU:OE2	3:c:721:GLU:N	2.41	0.54
3:a:706:LEU:HD21	3:f:430:LEU:HD11	1.90	0.54
3:e:175:ASP:OD2	3:e:175:ASP:C	2.51	0.54
3:f:320:TYR:CE2	3:f:419:VAL:HG22	2.43	0.54
1:G:30:ILE:HG23	1:G:47:GLN:OE1	2.07	0.54
1:K:77:ILE:HG22	1:K:103:LEU:HD11	1.89	0.54
3:e:119:ASP:C	3:e:119:ASP:OD1	2.50	0.54
3:e:146:ILE:HD11	3:e:260:TYR:CD2	2.42	0.54
3:f:458:ASN:HD21	3:f:469:ILE:HD13	1.73	0.54
1:L:175:MET:HB2	1:L:179:GLN:HB2	1.90	0.54
1:N:41:ALA:HB2	1:N:73:ALA:HB1	1.90	0.54
1:N:137:GLU:CG	1:N:141:ARG:HH22	2.21	0.54
1:T:161:PRO:HD2	1:T:164:VAL:HG11	1.88	0.54
3:b:294:GLN:O	3:b:298:GLU:HG3	2.07	0.54
3:b:566:ASP:HB2	3:b:628:ARG:HH11	1.72	0.54
3:c:215:LEU:O	3:c:251:LEU:HD12	2.07	0.54
3:d:282:THR:CG2	3:d:285:GLU:HG3	2.38	0.54
1:C:30:ILE:HD11	1:C:51:LEU:CD1	2.38	0.54
1:F:49:LEU:HD22	3:c:601:GLY:CA	2.38	0.54
1:G:35:PRO:HA	1:G:68:GLY:O	2.07	0.54
1:I:10:GLN:HA	1:I:17:ALA:CB	2.34	0.54
1:M:32:LEU:HD12	1:M:62:LEU:HD21	1.89	0.54
1:N:71:VAL:HG12	1:N:75:LEU:HD23	1.89	0.54
3:b:149:PRO:HG2	3:a:267:ALA:CB	2.38	0.54
3:d:131:VAL:O	3:d:135:LEU:HG	2.06	0.54
1:K:41:ALA:HB2	1:K:73:ALA:HB1	1.90	0.54
1:N:44:VAL:HG11	1:N:77:ILE:HD12	1.88	0.54
1:T:75:LEU:HD13	1:T:149:ARG:NH1	2.23	0.54
3:b:192:ILE:HB	3:b:195:GLN:CB	2.36	0.54
3:d:243:ALA:HB2	3:d:248:GLU:HB3	1.89	0.54
3:e:336:GLU:CD	3:e:410:ILE:HG12	2.33	0.54
3:e:701:ILE:HG13	3:e:714:LEU:HD23	1.89	0.54
3:f:181:LEU:HD11	3:f:203:LEU:HD11	1.90	0.54
3:f:434:ALA:O	3:f:438:LYS:HG3	2.08	0.54
3:f:484:GLU:O	3:f:488:GLN:HG2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ASP:HB3	1:G:115:LEU:HD23	1.90	0.53
1:A:141:ARG:NH2	1:A:144:LEU:HD12	2.23	0.53
1:A:177:ALA:O	1:A:186:ILE:HD11	2.07	0.53
1:E:93:LEU:HD23	1:E:93:LEU:H	1.74	0.53
1:G:120:ILE:HG22	1:G:175:MET:O	2.08	0.53
1:I:105:THR:HG21	1:I:185:LEU:HD22	1.90	0.53
1:L:85:LYS:HB2	1:L:85:LYS:NZ	2.24	0.53
3:c:220:VAL:HG22	3:c:255:THR:HG23	1.90	0.53
3:d:169:VAL:HG13	3:d:174:LEU:HG	1.90	0.53
3:a:297:TYR:CE1	3:f:138:ARG:HD3	2.42	0.53
3:e:580:PHE:CD1	3:e:583:THR:HG21	2.42	0.53
3:f:424:GLU:HB2	3:f:428:THR:OG1	2.08	0.53
1:F:125:PRO:HG3	1:F:150:LEU:HD12	1.90	0.53
1:M:5:PRO:HG3	1:N:47:GLN:NE2	2.23	0.53
3:d:238:ASN:O	3:d:242:PRO:HD2	2.08	0.53
3:e:101:LEU:HD23	3:e:105:TYR:CB	2.38	0.53
3:e:172:LYS:HG3	3:e:173:LEU:CD1	2.34	0.53
1:A:92:VAL:HG12	1:A:114:ALA:HA	1.90	0.53
1:B:12:SER:O	1:B:13:ARG:HG2	2.08	0.53
1:E:89:GLN:HB3	1:E:111:LYS:CB	2.38	0.53
1:G:42:ASN:O	1:G:45:ILE:HG13	2.07	0.53
1:T:4:ILE:HD12	1:T:21:TYR:HE2	1.73	0.53
3:e:627:ASN:C	3:e:627:ASN:OD1	2.52	0.53
1:F:91:ILE:HG22	1:F:93:LEU:HD23	1.90	0.53
1:T:30:ILE:HD12	1:T:47:GLN:OE1	2.08	0.53
3:b:417:ILE:HD11	3:b:541:PRO:HB2	1.90	0.53
3:d:140:LYS:HG3	3:d:271:ARG:O	2.07	0.53
3:d:262:ILE:CD1	3:d:263:ILE:HG23	2.38	0.53
3:d:597:GLU:OE1	3:d:597:GLU:N	2.42	0.53
3:d:644:MET:O	3:d:647:VAL:HG12	2.07	0.53
3:a:161:ALA:HA	3:a:164:ILE:HG22	1.90	0.53
3:e:100:GLY:O	3:e:104:GLU:HG3	2.08	0.53
3:e:532:GLN:N	3:e:532:GLN:OE1	2.40	0.53
3:f:146:ILE:O	3:f:278:VAL:HG12	2.08	0.53
1:A:105:THR:CG2	1:A:185:LEU:HD22	2.33	0.53
1:A:149:ARG:HH11	1:G:117:ASN:HB3	1.73	0.53
1:I:47:GLN:NE2	1:T:5:PRO:HG3	2.24	0.53
1:I:81:MET:HE1	1:I:106:ALA:HB3	1.90	0.53
1:T:7:VAL:O	1:T:18:TYR:HB2	2.08	0.53
1:T:92:VAL:CG2	1:T:104:LEU:HD22	2.38	0.53
3:d:113:ALA:HA	3:d:118:ILE:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:246:ARG:HH11	3:a:246:ARG:CG	2.21	0.53
3:e:234:MET:HE2	3:e:234:MET:CA	2.21	0.53
3:e:624:GLU:C	3:e:624:GLU:OE1	2.52	0.53
3:e:668:PRO:HG2	3:e:671:VAL:CG1	2.38	0.53
3:f:224:VAL:HG11	3:f:262:ILE:CG2	2.37	0.53
1:C:30:ILE:O	1:C:62:LEU:HD12	2.08	0.53
1:D:63:TYR:CE1	1:D:91:ILE:HD12	2.41	0.53
1:D:140:ALA:O	1:D:143:ILE:HG22	2.08	0.53
1:I:137:GLU:CG	1:I:141:ARG:HH22	2.20	0.53
1:K:28:ARG:HG2	1:K:51:LEU:CD1	2.38	0.53
1:L:45:ILE:CD1	1:L:77:ILE:HA	2.38	0.53
3:d:249:LEU:HD13	3:d:250:GLN:N	2.24	0.53
3:a:144:VAL:CG1	3:a:275:PRO:HA	2.38	0.53
3:e:431:LYS:NZ	3:f:706:LEU:HD11	2.24	0.53
3:f:161:ALA:O	3:f:164:ILE:HG22	2.08	0.53
3:f:695:GLU:C	3:f:695:GLU:OE1	2.52	0.53
1:C:24:LEU:HB3	1:C:29:ILE:CG2	2.38	0.53
1:I:63:TYR:CD1	1:I:91:ILE:HB	2.44	0.53
1:M:20:ILE:O	1:M:24:LEU:HD23	2.08	0.53
1:T:167:ARG:HB3	1:T:167:ARG:CZ	2.38	0.53
3:c:422:LEU:HD21	3:c:430:LEU:CD1	2.39	0.53
3:c:534:THR:HG23	3:c:578:VAL:CG2	2.39	0.53
3:d:154:THR:O	3:d:158:GLU:HG2	2.09	0.53
3:a:286:THR:O	3:a:290:LEU:HG	2.09	0.53
3:e:238:ASN:O	3:e:241:LYS:HG2	2.08	0.53
3:e:323:ASP:CA	3:e:539:ARG:HH22	2.22	0.53
3:f:124:ARG:HD2	3:f:156:VAL:HG12	1.90	0.53
3:f:411:VAL:O	3:f:415:THR:HG23	2.08	0.53
3:f:446:ASP:O	3:f:450:LYS:HG3	2.08	0.53
3:f:539:ARG:CB	3:f:539:ARG:HH11	2.22	0.53
3:f:663:LEU:HD21	3:f:705:TYR:CD1	2.43	0.53
1:C:115:LEU:HD23	1:D:79:ASP:HB2	1.90	0.53
1:E:120:ILE:HD12	1:E:120:ILE:N	2.24	0.53
1:T:41:ALA:O	1:T:45:ILE:HD12	2.08	0.53
3:b:193:ARG:HG3	3:b:194:GLY:H	1.74	0.53
3:c:647:VAL:O	3:c:651:LEU:HD23	2.09	0.53
3:d:425:LYS:HB2	3:d:425:LYS:NZ	2.24	0.53
3:a:319:ARG:HD2	3:a:319:ARG:O	2.09	0.53
3:a:518:ILE:CG2	3:a:560:MET:HE1	2.38	0.53
3:e:438:LYS:HE2	3:e:445:ASP:CA	2.38	0.53
3:e:532:GLN:HG2	3:e:536:LYS:NZ	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:f:718:LEU:HD12	3:f:719:ASP:H	1.73	0.53
1:A:16:ARG:HG3	1:A:18:TYR:CE2	2.43	0.53
1:B:53:ALA:HB3	3:f:600:VAL:H	1.73	0.53
1:C:30:ILE:HB	1:C:62:LEU:HD13	1.89	0.53
1:C:161:PRO:HD2	1:C:164:VAL:HG11	1.90	0.53
1:D:29:ILE:CD1	1:D:61:TYR:HB2	2.39	0.53
1:E:140:ALA:O	1:E:143:ILE:HG22	2.08	0.53
1:K:55:ASP:OD1	1:K:58:LYS:HB2	2.09	0.53
1:L:164:VAL:O	1:L:168:ASP:HB2	2.09	0.53
1:M:40:VAL:O	1:M:44:VAL:HG23	2.09	0.53
1:M:171:ARG:HA	1:M:171:ARG:HE	1.73	0.53
3:b:202:LYS:NZ	3:c:189:GLY:HA2	2.24	0.53
3:d:140:LYS:HE2	3:e:332:ASP:OD2	2.08	0.53
3:d:297:TYR:HD1	3:d:334:LEU:HD23	1.74	0.53
3:a:547:LEU:HD21	3:a:561:PHE:CZ	2.44	0.53
3:a:587:MET:HE1	3:a:625:PHE:CZ	2.44	0.53
3:a:668:PRO:HD2	3:a:671:VAL:HG21	1.89	0.53
3:e:277:GLN:N	3:e:277:GLN:OE1	2.42	0.53
3:e:459:ARG:HB3	3:e:459:ARG:HH11	1.74	0.53
3:e:480:VAL:CA	3:e:638:LEU:HD21	2.36	0.53
3:e:649:LEU:HD12	3:e:649:LEU:H	1.74	0.53
3:f:670:GLU:HG3	3:f:718:LEU:HD22	1.91	0.53
3:f:714:LEU:HD13	3:f:715:VAL:N	2.23	0.53
1:A:55:ASP:OD1	1:A:58:LYS:HE3	2.09	0.53
1:B:12:SER:O	1:B:15:GLU:HG2	2.09	0.53
1:G:74:GLY:HA3	1:G:99:MET:HE3	1.91	0.53
1:K:158:THR:HG22	1:K:185:LEU:HD23	1.91	0.53
3:c:464:LYS:HD3	3:c:467:ARG:HD3	1.91	0.53
3:c:550:VAL:HG13	3:c:558:LEU:CD2	2.37	0.53
3:d:215:LEU:O	3:d:251:LEU:HD22	2.08	0.53
3:a:691:ARG:NH1	3:a:691:ARG:HG2	2.23	0.53
3:e:170:PRO:HD3	3:f:343:LEU:HD12	1.91	0.53
3:e:232:GLY:N	3:f:188:GLN:HB3	2.24	0.53
3:e:444:GLN:CA	3:e:636:LYS:HZ1	2.18	0.53
3:e:487:LYS:HD2	3:e:497:GLU:OE2	2.10	0.53
3:e:678:LEU:HD12	3:e:678:LEU:O	2.09	0.53
3:f:412:GLU:OE1	3:f:418:PRO:HA	2.08	0.53
3:f:596:VAL:O	3:f:596:VAL:HG12	2.08	0.53
1:B:53:ALA:HA	3:f:603:GLY:HA2	1.91	0.52
1:G:146:THR:HG22	1:G:150:LEU:HD11	1.91	0.52
1:T:37:ASP:OD1	1:T:40:VAL:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:684:MET:HG2	3:a:627:ASN:CG	2.33	0.52
3:d:134:ILE:HB	3:d:143:PRO:HG3	1.89	0.52
3:d:234:MET:HG3	3:d:237:GLY:N	2.23	0.52
1:B:8:ILE:O	1:B:9:GLU:HB2	2.09	0.52
1:S:92:VAL:O	1:S:115:LEU:HD23	2.08	0.52
1:T:165:ILE:O	1:T:169:THR:HG23	2.09	0.52
3:b:446:ASP:O	3:b:450:LYS:HG3	2.09	0.52
3:c:241:LYS:HD3	3:c:269:LEU:HG	1.90	0.52
3:d:122:VAL:H	4:d:801:ATP:HN62	1.57	0.52
3:a:129:LYS:O	3:a:133:GLU:HG3	2.09	0.52
3:e:558:LEU:O	3:e:562:LEU:HD13	2.09	0.52
1:S:158:THR:HG22	1:S:185:LEU:HD23	1.91	0.52
1:T:96:ALA:HB3	1:T:120:ILE:HD13	1.89	0.52
1:T:125:PRO:HG3	1:T:150:LEU:HD12	1.90	0.52
3:b:269:LEU:O	3:b:273:MET:HG3	2.09	0.52
3:d:569:ARG:NH1	3:d:569:ARG:HB2	2.25	0.52
3:a:308:GLU:OE1	3:a:308:GLU:N	2.43	0.52
3:e:565:LEU:HD21	3:e:585:ILE:CG2	2.38	0.52
3:f:475:VAL:HG11	3:f:617:LEU:HD11	1.90	0.52
3:f:657:LEU:O	3:f:660:LYS:HG2	2.09	0.52
1:A:154:LEU:O	1:A:158:THR:HG23	2.10	0.52
1:B:10:GLN:HE22	1:C:54:GLN:HE22	1.55	0.52
1:C:10:GLN:CG	1:C:14:GLY:HA2	2.40	0.52
1:I:57:GLU:O	1:I:58:LYS:HG3	2.09	0.52
1:K:124:GLN:O	1:K:124:GLN:HG2	2.10	0.52
1:N:140:ALA:HA	1:N:143:ILE:HG22	1.91	0.52
3:b:233:ASN:CG	3:b:233:ASN:O	2.52	0.52
3:b:246:ARG:HB3	3:b:248:GLU:OE1	2.10	0.52
3:b:460:VAL:HG12	3:b:462:LEU:HD13	1.91	0.52
3:b:697:ILE:HG13	3:b:699:ASP:OD1	2.10	0.52
3:d:134:ILE:HD13	3:d:274:GLN:HG2	1.91	0.52
3:e:419:VAL:HG22	3:e:420:GLY:N	2.25	0.52
3:f:456:ARG:O	3:f:460:VAL:HG13	2.10	0.52
1:K:75:LEU:HD22	1:K:99:MET:CE	2.40	0.52
1:M:161:PRO:O	1:M:164:VAL:HG12	2.08	0.52
3:b:644:MET:SD	3:b:676:VAL:HG21	2.49	0.52
3:c:622:THR:HG23	3:c:625:PHE:H	1.74	0.52
3:a:190:THR:O	3:f:192:ILE:HD11	2.10	0.52
3:a:205:GLU:O	3:a:209:GLU:HG3	2.09	0.52
1:B:158:THR:CG2	1:B:185:LEU:HD23	2.39	0.52
1:D:134:THR:O	1:D:138:ILE:HG13	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:119:GLU:C	1:E:120:ILE:HD12	2.34	0.52
1:S:5:PRO:HG3	1:T:47:GLN:NE2	2.25	0.52
1:S:141:ARG:HG3	1:S:141:ARG:HH11	1.74	0.52
3:b:193:ARG:HH12	3:c:231:ASP:N	2.07	0.52
3:c:215:LEU:HD12	3:c:251:LEU:CD1	2.40	0.52
3:e:545:ILE:HB	3:e:585:ILE:CD1	2.37	0.52
3:e:671:VAL:CA	3:e:718:LEU:HD22	2.40	0.52
1:B:10:GLN:NE2	1:C:54:GLN:HE22	2.07	0.52
1:B:119:GLU:C	1:B:120:ILE:HD12	2.35	0.52
1:G:36:ILE:CG1	1:G:69:GLY:HA3	2.39	0.52
1:K:57:GLU:OE1	1:K:57:GLU:N	2.41	0.52
1:N:55:ASP:CG	1:N:58:LYS:HD2	2.35	0.52
3:c:650:MET:O	3:c:654:VAL:HG23	2.09	0.52
3:d:424:GLU:OE2	3:d:424:GLU:N	2.43	0.52
3:d:463:GLY:O	3:d:464:LYS:HD2	2.10	0.52
3:e:101:LEU:HD23	3:e:101:LEU:O	2.10	0.52
3:f:684:MET:HA	3:f:684:MET:CE	2.34	0.52
1:A:10:GLN:HA	1:A:10:GLN:OE1	2.09	0.52
1:B:33:SER:HB2	1:C:42:ASN:ND2	2.25	0.52
1:G:63:TYR:CE1	1:G:91:ILE:HD13	2.45	0.52
1:S:137:GLU:CD	1:S:141:ARG:HH22	2.17	0.52
1:T:141:ARG:HH11	1:T:141:ARG:CG	2.23	0.52
3:c:473:LEU:HD22	3:c:475:VAL:HG23	1.91	0.52
3:d:501:VAL:HG13	3:d:536:LYS:HD2	1.90	0.52
3:a:153:LYS:HB3	4:f:801:ATP:O2B	2.10	0.52
3:a:691:ARG:HG2	3:a:691:ARG:HH11	1.74	0.52
3:e:101:LEU:HD23	3:e:101:LEU:C	2.35	0.52
3:f:652:GLU:C	3:f:652:GLU:OE1	2.53	0.52
3:f:703:GLU:OE1	3:f:703:GLU:C	2.52	0.52
3:f:715:VAL:H	3:f:728:GLY:CA	2.22	0.52
1:C:12:SER:HB2	1:C:15:GLU:CG	2.39	0.52
1:E:122:ILE:HG13	1:E:122:ILE:O	2.09	0.52
1:I:11:SER:HB2	1:T:8:ILE:CB	2.17	0.52
1:K:37:ASP:OD1	1:K:40:VAL:HG23	2.10	0.52
1:M:158:THR:HG22	1:M:160:GLN:HG2	1.92	0.52
3:c:464:LYS:HB3	3:c:464:LYS:NZ	2.24	0.52
3:d:442:VAL:N	4:d:802:ATP:HN62	2.07	0.52
3:a:447:ALA:CB	3:a:633:ILE:HG21	2.39	0.52
3:e:255:THR:OG1	3:e:259:GLU:HB2	2.10	0.52
3:e:520:SER:HB2	3:e:526:GLY:C	2.34	0.52
3:e:596:VAL:HG21	3:e:620:PHE:CE1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:e:723:LYS:C	3:e:724:ILE:HD12	2.34	0.52
3:f:596:VAL:HG13	3:f:616:GLN:CG	2.39	0.52
3:f:662:LYS:HB2	3:f:662:LYS:NZ	2.23	0.52
3:f:701:ILE:HG23	3:f:714:LEU:HG	1.91	0.52
1:A:45:ILE:HD12	1:A:80:THR:CB	2.40	0.52
1:A:89:GLN:HB2	1:A:111:LYS:HB3	1.92	0.52
1:S:20:ILE:CD1	1:T:47:GLN:HA	2.40	0.52
3:c:199:ARG:O	3:c:202:LYS:HG2	2.09	0.52
3:d:211:GLU:OE1	3:d:211:GLU:O	2.28	0.52
3:a:152:GLY:O	3:a:156:VAL:HG23	2.09	0.52
3:a:192:ILE:HG13	3:a:195:GLN:HB2	1.92	0.52
3:f:674:LYS:CE	3:f:724:ILE:HD12	2.40	0.52
1:A:23:ARG:HH21	1:A:26:LYS:CG	2.23	0.51
1:G:167:ARG:HB3	1:G:167:ARG:CZ	2.40	0.51
1:S:24:LEU:HD11	1:T:46:ALA:HB1	1.91	0.51
3:c:244:LEU:HD23	3:c:249:LEU:CD2	2.39	0.51
3:c:444:GLN:HG3	3:c:635:PHE:CD2	2.44	0.51
3:c:564:ILE:HG23	3:c:580:PHE:CG	2.45	0.51
3:d:161:ALA:O	3:d:164:ILE:HG22	2.11	0.51
3:d:220:VAL:HG22	3:d:255:THR:HB	1.91	0.51
3:d:327:PRO:O	3:d:331:ILE:HG13	2.11	0.51
3:e:173:LEU:HD12	3:e:173:LEU:N	2.25	0.51
3:e:565:LEU:HD21	3:e:585:ILE:CG1	2.39	0.51
3:f:181:LEU:CD1	3:f:203:LEU:HD11	2.40	0.51
3:f:514:VAL:O	3:f:518:ILE:HG12	2.10	0.51
3:f:713:GLN:OE1	3:f:713:GLN:HA	2.10	0.51
1:F:29:ILE:HG23	1:F:63:TYR:CD1	2.44	0.51
1:L:81:MET:HE1	1:L:106:ALA:HB3	1.91	0.51
1:S:58:LYS:O	1:S:86:ALA:HB1	2.10	0.51
1:S:71:VAL:HG12	1:S:75:LEU:HD23	1.93	0.51
3:b:204:ILE:HA	3:b:207:ILE:HG22	1.92	0.51
3:b:437:LEU:CD2	3:b:492:GLU:HG3	2.40	0.51
3:c:129:LYS:O	3:c:133:GLU:HG3	2.10	0.51
3:c:144:VAL:CG1	3:c:275:PRO:HA	2.40	0.51
3:a:449:ASP:O	3:a:453:LYS:HG3	2.11	0.51
3:a:723:LYS:O	3:a:724:ILE:HD13	2.10	0.51
3:e:201:GLN:OE1	3:e:201:GLN:O	2.28	0.51
3:e:430:LEU:C	3:e:431:LYS:HE2	2.35	0.51
1:A:10:GLN:HE22	1:B:16:ARG:NH2	2.07	0.51
1:A:55:ASP:OD1	1:A:58:LYS:HG2	2.10	0.51
1:F:171:ARG:O	1:G:138:ILE:HD13	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:105:THR:CG2	1:K:185:LEU:HD22	2.39	0.51
3:b:204:ILE:HG21	3:b:239:ILE:HG21	1.92	0.51
3:b:295:LYS:HB2	3:b:295:LYS:NZ	2.23	0.51
3:b:725:ILE:HD12	3:b:725:ILE:O	2.10	0.51
3:d:447:ALA:HB1	3:d:633:ILE:HG21	1.92	0.51
3:a:108:ASN:OD1	3:a:110:THR:HG22	2.10	0.51
3:e:570:LEU:HB3	3:e:578:VAL:CG2	2.40	0.51
3:f:451:VAL:HG22	3:f:633:ILE:CD1	2.40	0.51
3:f:464:LYS:CG	3:f:467:ARG:HG2	2.40	0.51
1:F:12:SER:O	1:F:13:ARG:HB3	2.10	0.51
1:M:8:ILE:HD12	1:M:8:ILE:O	2.11	0.51
1:N:163:GLU:N	1:N:163:GLU:OE2	2.41	0.51
3:b:227:GLY:O	3:b:235:ASP:HA	2.11	0.51
3:b:468:PRO:HB3	3:b:580:PHE:O	2.09	0.51
3:b:487:LYS:HB3	3:b:497:GLU:CG	2.40	0.51
3:c:327:PRO:O	3:c:331:ILE:HG12	2.11	0.51
3:d:289:ILE:HG23	4:d:801:ATP:C2	2.46	0.51
3:e:430:LEU:HD11	3:e:459:ARG:NH1	2.26	0.51
3:f:154:THR:HG1	4:f:802:ATP:C5'	2.23	0.51
3:f:256:THR:HG22	3:f:257:LEU:N	2.26	0.51
3:f:553:ALA:HB1	3:f:557:VAL:CG2	2.40	0.51
3:f:642:ASN:O	3:f:646:ILE:HG13	2.10	0.51
1:M:90:THR:HG21	1:M:106:ALA:O	2.10	0.51
1:T:137:GLU:HG2	1:T:141:ARG:NH2	2.26	0.51
3:b:144:VAL:HG21	3:b:273:MET:CB	2.32	0.51
3:b:417:ILE:HG12	3:b:542:TYR:HB2	1.93	0.51
3:b:461:GLY:C	3:b:462:LEU:HD12	2.35	0.51
3:b:468:PRO:HA	3:b:581:LYS:O	2.10	0.51
3:c:692:THR:O	3:c:696:GLN:HG2	2.10	0.51
3:a:662:LYS:HA	3:a:662:LYS:CE	2.30	0.51
3:e:464:LYS:H	3:e:464:LYS:HD3	1.75	0.51
3:f:186:LEU:CG	3:f:200:MET:HE1	2.39	0.51
3:f:204:ILE:O	3:f:208:THR:HG23	2.11	0.51
3:f:466:ASN:HA	3:f:581:LYS:NZ	2.25	0.51
3:f:592:GLY:HA3	3:f:613:VAL:HG13	1.92	0.51
3:f:678:LEU:HD23	3:f:678:LEU:H	1.75	0.51
1:G:91:ILE:CG2	1:G:190:MET:HE2	2.41	0.51
1:M:59:ASP:OD2	1:M:111:LYS:HE2	2.11	0.51
3:b:280:GLU:OE2	3:b:326:LEU:HD23	2.11	0.51
3:b:647:VAL:HG23	3:b:689:LEU:HD11	1.91	0.51
3:b:658:LEU:HD11	3:b:698:GLU:OE2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:503:PHE:HE2	3:c:533:LEU:HD13	1.76	0.51
3:c:639:SER:O	3:c:643:LEU:HD13	2.10	0.51
3:d:198:GLU:O	3:d:202:LYS:HE3	2.10	0.51
3:e:453:LYS:HE2	3:e:457:ARG:NE	2.24	0.51
3:e:510:GLU:OE1	3:e:512:HIS:ND1	2.43	0.51
3:f:145:LEU:HD13	3:f:156:VAL:HG21	1.93	0.51
3:f:239:ILE:O	3:f:242:PRO:HD2	2.11	0.51
3:f:679:GLY:O	3:f:689:LEU:HD22	2.11	0.51
1:A:181:LYS:HD2	1:A:188:GLU:HA	1.93	0.51
1:C:7:VAL:HB	1:C:16:ARG:HD2	1.92	0.51
1:I:89:GLN:HG2	1:I:111:LYS:HD3	1.93	0.51
1:L:4:ILE:CD1	1:L:20:ILE:HG22	2.41	0.51
1:T:134:THR:O	1:T:138:ILE:HG13	2.11	0.51
3:c:455:ILE:CD1	3:c:493:LEU:HD11	2.41	0.51
3:a:186:LEU:HD21	3:a:203:LEU:CD1	2.40	0.51
3:a:308:GLU:HG2	3:a:404:GLU:CD	2.36	0.51
3:e:220:VAL:O	3:e:223:ILE:HG13	2.11	0.51
3:e:476:GLY:CA	3:e:593:THR:HG21	2.41	0.51
3:e:488:GLN:OE1	3:e:491:PHE:HB3	2.11	0.51
3:e:564:ILE:HD11	3:e:580:PHE:CD2	2.45	0.51
3:f:200:MET:O	3:f:204:ILE:HD13	2.11	0.51
3:f:660:LYS:N	3:f:660:LYS:CE	2.73	0.51
1:I:10:GLN:CD	1:I:10:GLN:N	2.69	0.51
1:L:90:THR:CG2	1:L:104:LEU:HD12	2.41	0.51
1:S:161:PRO:HD2	1:S:164:VAL:HG11	1.91	0.51
1:T:62:LEU:HD22	1:T:64:ILE:HD11	1.91	0.51
3:b:449:ASP:O	3:b:453:LYS:HG3	2.11	0.51
3:c:148:GLU:O	3:c:151:VAL:HG22	2.11	0.51
3:d:537:VAL:HG21	3:d:580:PHE:CE2	2.45	0.51
3:e:124:ARG:HH22	3:e:281:PRO:HD3	1.76	0.51
3:e:471:SER:HB3	3:e:629:PHE:HD1	1.75	0.51
3:e:647:VAL:HG21	3:e:676:VAL:HG22	1.93	0.51
1:B:5:PRO:HG3	1:C:47:GLN:OE1	2.11	0.51
1:F:167:ARG:HB3	1:F:167:ARG:CZ	2.40	0.51
1:G:12:SER:O	1:G:13:ARG:HD3	2.10	0.51
1:I:90:THR:C	1:I:91:ILE:HD12	2.36	0.51
1:K:125:PRO:HG3	1:K:150:LEU:HD12	1.93	0.51
1:M:180:ALA:C	1:M:186:ILE:HG22	2.36	0.51
1:S:140:ALA:O	1:S:144:LEU:HD23	2.10	0.51
3:b:716:ALA:O	3:b:717:ALA:HA	2.11	0.51
3:c:152:GLY:O	3:c:156:VAL:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:706:LEU:CD1	3:f:456:ARG:HH11	2.24	0.51
3:e:241:LYS:HB2	3:e:242:PRO:CD	2.38	0.51
3:e:446:ASP:OD2	3:e:446:ASP:N	2.44	0.51
3:e:561:PHE:HA	3:e:564:ILE:CG2	2.40	0.51
3:e:643:LEU:HD12	3:e:689:LEU:HD21	1.92	0.51
1:K:47:GLN:O	1:K:51:LEU:HD23	2.11	0.51
1:L:177:ALA:HB1	1:L:189:VAL:HG22	1.93	0.51
1:N:81:MET:HE1	1:N:106:ALA:HB3	1.92	0.51
1:N:92:VAL:CG2	1:N:104:LEU:HD22	2.35	0.51
3:c:109:ILE:HG22	3:c:161:ALA:CB	2.41	0.51
3:c:670:GLU:O	3:c:670:GLU:OE2	2.27	0.51
3:d:721:GLU:HG2	3:d:723:LYS:NZ	2.26	0.51
3:a:657:LEU:HD23	3:a:657:LEU:O	2.11	0.51
3:f:562:LEU:HD22	3:f:628:ARG:HG3	1.93	0.51
1:B:4:ILE:CG2	1:B:20:ILE:HG22	2.41	0.50
1:D:45:ILE:HD11	1:D:77:ILE:HA	1.92	0.50
1:D:132:GLN:CD	1:S:124:GLN:HE21	2.19	0.50
3:b:450:LYS:NZ	3:b:450:LYS:HB3	2.26	0.50
3:d:569:ARG:CB	3:d:569:ARG:HH11	2.24	0.50
3:d:689:LEU:O	3:d:689:LEU:HD22	2.11	0.50
3:d:697:ILE:O	3:d:701:ILE:HG13	2.11	0.50
3:a:293:LEU:HD21	4:f:801:ATP:C2	2.43	0.50
3:e:304:LYS:HD3	3:e:304:LYS:N	2.20	0.50
1:L:45:ILE:HD12	1:L:80:THR:CB	2.41	0.50
1:S:188:GLU:HG2	1:S:189:VAL:N	2.26	0.50
1:T:4:ILE:HG22	1:T:19:ASP:OD2	2.11	0.50
3:b:198:GLU:HG3	3:c:190:THR:N	2.27	0.50
3:c:235:ASP:OD1	3:c:238:ASN:HB2	2.11	0.50
3:d:483:THR:HG23	3:d:546:LEU:HD21	1.93	0.50
3:d:671:VAL:HG13	3:d:724:ILE:HD13	1.93	0.50
3:a:132:ILE:HD11	3:a:160:LEU:CD1	2.41	0.50
3:e:481:GLY:HA2	3:e:484:GLU:OE1	2.11	0.50
1:B:23:ARG:HH12	1:B:27:ASP:CG	2.19	0.50
1:B:41:ALA:HB2	1:B:73:ALA:HB1	1.93	0.50
1:D:37:ASP:H	1:D:40:VAL:CG1	2.23	0.50
1:F:10:GLN:CB	1:F:15:GLU:HB3	2.12	0.50
1:G:36:ILE:HG12	1:G:69:GLY:HA3	1.92	0.50
3:d:153:LYS:HZ1	3:d:256:THR:HA	1.76	0.50
3:d:259:GLU:O	3:d:263:ILE:HG12	2.11	0.50
3:e:475:VAL:HA	3:e:589:SER:O	2.11	0.50
3:e:580:PHE:O	3:e:583:THR:HG22	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:e:692:THR:O	3:e:696:GLN:HG2	2.11	0.50
3:e:717:ALA:HB3	3:e:725:ILE:O	2.11	0.50
3:f:725:ILE:C	3:f:725:ILE:HD12	2.36	0.50
1:B:8:ILE:HG21	1:C:10:GLN:HE22	1.76	0.50
1:G:137:GLU:HG2	1:G:141:ARG:NH2	2.26	0.50
3:b:509:MET:HE3	3:b:509:MET:C	2.36	0.50
3:c:546:LEU:C	3:c:547:LEU:HD23	2.37	0.50
3:e:134:ILE:CG2	3:e:143:PRO:HG3	2.41	0.50
3:e:660:LYS:HB2	3:e:660:LYS:HZ3	1.77	0.50
3:f:174:LEU:H	3:f:174:LEU:HD22	1.77	0.50
1:D:87:ASP:OD2	1:D:108:GLN:HB2	2.12	0.50
1:F:36:ILE:HD12	1:F:68:GLY:O	2.12	0.50
1:L:137:GLU:O	1:L:141:ARG:HG3	2.11	0.50
1:S:33:SER:HA	1:S:65:ASN:O	2.11	0.50
3:b:110:THR:HG21	3:b:177:GLU:CB	2.37	0.50
3:b:662:LYS:O	3:b:663:LEU:HD12	2.12	0.50
3:b:718:LEU:HD23	3:b:723:LYS:O	2.12	0.50
3:d:340:LYS:CE	3:d:410:ILE:HD11	2.39	0.50
3:d:473:LEU:HD22	3:d:629:PHE:HE2	1.76	0.50
3:d:483:THR:O	3:d:487:LYS:HG3	2.12	0.50
3:f:113:ALA:HB1	3:f:165:VAL:CG1	2.40	0.50
1:A:30:ILE:HG23	1:A:47:GLN:OE1	2.11	0.50
1:A:101:SER:O	1:A:105:THR:HG23	2.10	0.50
1:F:54:GLN:HA	3:c:597:GLU:OE1	2.11	0.50
1:L:141:ARG:HB3	1:L:141:ARG:HH11	1.76	0.50
3:b:281:PRO:HD2	3:b:327:PRO:HD3	1.94	0.50
3:b:521:PRO:HG2	3:c:512:HIS:HD2	1.76	0.50
3:d:251:LEU:HD13	3:d:252:VAL:N	2.26	0.50
3:d:669:THR:O	3:d:673:GLU:HG2	2.12	0.50
3:e:206:GLU:O	3:e:209:GLU:HG3	2.12	0.50
3:f:447:ALA:O	3:f:451:VAL:HG23	2.11	0.50
3:f:530:ALA:HB3	3:f:535:GLU:OE2	2.11	0.50
1:A:23:ARG:HH21	1:A:26:LYS:HD3	1.76	0.50
1:L:41:ALA:HB2	1:L:73:ALA:HB1	1.94	0.50
1:L:153:ILE:O	1:L:157:ARG:HG3	2.11	0.50
3:b:118:ILE:HG23	3:b:158:GLU:HB3	1.93	0.50
3:b:673:GLU:O	3:b:677:ASP:OD1	2.30	0.50
3:c:164:ILE:HD12	3:c:173:LEU:O	2.12	0.50
3:d:266:ASP:O	3:d:270:GLU:HB2	2.11	0.50
3:d:462:LEU:HD12	3:d:462:LEU:N	2.27	0.50
3:a:591:ALA:HB1	3:a:620:PHE:CG	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:e:188:GLN:NE2	3:e:196:PHE:HB3	2.26	0.50
3:e:563:GLN:NE2	3:e:570:LEU:HD12	2.26	0.50
3:f:281:PRO:HD2	3:f:327:PRO:HG3	1.93	0.50
3:c:243:ALA:HA	3:c:248:GLU:OE1	2.12	0.50
3:c:621:PHE:HB2	3:c:626:LEU:HD11	1.93	0.50
3:c:646:ILE:O	3:c:650:MET:HG3	2.12	0.50
3:d:238:ASN:OD1	3:d:238:ASN:N	2.45	0.50
3:d:262:ILE:HD12	3:d:263:ILE:HG23	1.91	0.50
3:d:324:ARG:C	3:d:329:LYS:HD3	2.36	0.50
3:e:286:THR:CG2	3:e:326:LEU:HB3	2.39	0.50
3:f:596:VAL:HG22	3:f:616:GLN:CG	2.30	0.50
1:K:81:MET:HE1	1:K:106:ALA:HB3	1.94	0.50
1:N:71:VAL:HG12	1:N:75:LEU:CD2	2.41	0.50
3:b:148:GLU:HB2	3:b:151:VAL:CG2	2.42	0.50
3:b:561:PHE:CD1	3:b:564:ILE:HD12	2.47	0.50
3:b:622:THR:O	3:b:626:LEU:HD12	2.12	0.50
3:d:241:LYS:HE2	3:e:182:ASP:HB2	1.94	0.50
3:e:433:LEU:HD11	3:e:493:LEU:HD21	1.94	0.50
3:e:474:PHE:HB3	3:e:482:LYS:NZ	2.27	0.50
3:e:694:GLN:HA	3:e:698:GLU:CD	2.37	0.50
3:f:246:ARG:NH2	4:f:801:ATP:H3'	2.26	0.50
1:B:134:THR:O	1:B:138:ILE:HG13	2.11	0.49
1:E:161:PRO:HG2	1:E:164:VAL:CG2	2.42	0.49
1:L:32:LEU:HD12	1:L:64:ILE:HD13	1.93	0.49
1:M:123:HIS:C	1:M:169:THR:HG23	2.37	0.49
3:b:184:VAL:HG12	3:a:234:MET:HE2	1.94	0.49
3:b:296:ARG:HG2	3:b:296:ARG:HH11	1.77	0.49
3:c:220:VAL:HG11	3:c:253:GLY:HA3	1.92	0.49
3:c:477:PRO:CA	3:c:593:THR:HG21	2.38	0.49
3:d:265:LYS:HE2	3:d:265:LYS:CA	2.31	0.49
3:e:284:ALA:O	3:e:288:THR:HG23	2.12	0.49
3:e:704:TYR:CE2	3:e:714:LEU:HD13	2.47	0.49
3:f:650:MET:HE3	3:f:693:ILE:HD11	1.92	0.49
1:F:134:THR:O	1:F:138:ILE:HG13	2.11	0.49
1:S:41:ALA:O	1:S:45:ILE:HD13	2.12	0.49
3:b:109:ILE:HD11	3:b:180:ARG:HB2	1.94	0.49
3:b:697:ILE:HD12	3:a:462:LEU:HD13	1.94	0.49
3:c:437:LEU:CD2	3:c:492:GLU:HG3	2.43	0.49
3:c:465:GLN:OE1	3:c:465:GLN:HA	2.10	0.49
3:d:134:ILE:HG22	3:d:143:PRO:HG3	1.92	0.49
3:d:206:GLU:HA	3:d:209:GLU:CG	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:173:LEU:HB2	3:a:176:LYS:CG	2.43	0.49
3:e:538:ARG:NE	3:e:576:ARG:HE	2.10	0.49
3:f:159:GLY:O	3:f:163:LYS:HG3	2.13	0.49
3:f:244:LEU:O	3:f:272:ARG:HG2	2.12	0.49
1:I:63:TYR:HD1	1:I:91:ILE:HB	1.77	0.49
1:M:4:ILE:O	1:M:4:ILE:CG2	2.60	0.49
1:T:23:ARG:HH11	1:T:26:LYS:HD2	1.77	0.49
1:T:167:ARG:NH1	1:T:167:ARG:CB	2.75	0.49
3:b:200:MET:HE2	3:b:227:GLY:HA3	1.93	0.49
3:b:702:ALA:HA	3:b:705:TYR:CD1	2.47	0.49
3:c:449:ASP:HB3	3:c:453:LYS:NZ	2.27	0.49
3:d:108:ASN:HB3	3:d:111:GLU:CG	2.42	0.49
3:e:592:GLY:O	3:e:597:GLU:HB3	2.12	0.49
3:f:337:SER:OG	3:f:407:ILE:HD13	2.11	0.49
1:A:23:ARG:HE	1:A:26:LYS:CD	2.26	0.49
1:E:188:GLU:HG3	1:E:189:VAL:N	2.27	0.49
1:G:15:GLU:C	1:G:16:ARG:HD2	2.37	0.49
1:N:24:LEU:HD11	1:S:46:ALA:HB1	1.93	0.49
1:N:71:VAL:O	1:N:75:LEU:HD23	2.12	0.49
1:T:95:MET:HE1	1:T:174:TYR:HE1	1.78	0.49
3:c:200:MET:HE2	3:c:236:ALA:HA	1.94	0.49
3:a:126:GLN:HA	3:a:126:GLN:OE1	2.12	0.49
3:e:134:ILE:CB	3:e:143:PRO:HG3	2.39	0.49
3:f:196:PHE:HA	3:f:199:ARG:CG	2.43	0.49
1:D:175:MET:HB3	1:D:179:GLN:HB2	1.94	0.49
1:E:29:ILE:HD13	1:E:61:TYR:CB	2.37	0.49
1:K:9:GLU:HB2	1:K:16:ARG:CB	2.42	0.49
1:N:25:LEU:HD21	1:N:51:LEU:HD11	1.93	0.49
1:T:58:LYS:O	1:T:86:ALA:HB1	2.12	0.49
3:c:241:LYS:HD2	3:c:268:ALA:HB3	1.92	0.49
3:d:130:ARG:HD3	3:d:133:GLU:OE2	2.13	0.49
3:d:308:GLU:CG	3:d:404:GLU:HG3	2.41	0.49
3:e:265:LYS:HA	3:e:265:LYS:CE	2.33	0.49
3:e:328:ASP:C	3:e:328:ASP:OD2	2.55	0.49
3:e:684:MET:CE	3:e:688:PRO:HG3	2.42	0.49
1:C:29:ILE:HD12	1:C:63:TYR:CZ	2.47	0.49
1:C:175:MET:HE1	1:C:185:LEU:HD12	1.93	0.49
1:E:41:ALA:O	1:E:45:ILE:HD13	2.13	0.49
3:b:120:PRO:HD3	3:b:296:ARG:NE	2.27	0.49
3:b:672:LYS:O	3:b:676:VAL:HG23	2.13	0.49
3:d:504:ASP:C	3:d:505:MET:HE2	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:408:GLU:O	3:a:412:GLU:HG2	2.13	0.49
3:a:537:VAL:HG21	3:a:580:PHE:CE1	2.48	0.49
3:a:680:TYR:CZ	3:a:682:PRO:HG3	2.47	0.49
3:e:455:ILE:O	3:e:459:ARG:HG3	2.11	0.49
3:e:641:GLU:N	3:e:641:GLU:OE1	2.45	0.49
3:f:101:LEU:O	3:f:101:LEU:HD13	2.11	0.49
3:f:179:ILE:HD12	3:f:213:VAL:CG2	2.38	0.49
3:f:691:ARG:HG2	3:f:691:ARG:NH1	2.28	0.49
1:D:8:ILE:CG2	1:E:16:ARG:HE	2.23	0.49
1:D:140:ALA:HA	1:D:143:ILE:HG22	1.94	0.49
1:L:122:ILE:HG12	1:L:173:ASN:HB3	1.94	0.49
1:M:140:ALA:O	1:M:143:ILE:HG22	2.13	0.49
3:b:336:GLU:CB	3:b:410:ILE:HD13	2.43	0.49
3:c:203:LEU:O	3:c:207:ILE:HG22	2.13	0.49
3:d:110:THR:O	3:d:114:ARG:HG3	2.12	0.49
3:d:146:ILE:HG21	3:d:260:TYR:HB2	1.95	0.49
3:a:622:THR:HG23	3:a:625:PHE:H	1.77	0.49
3:a:663:LEU:HD21	3:a:705:TYR:HD1	1.76	0.49
3:e:272:ARG:O	3:e:272:ARG:HG3	2.13	0.49
3:e:554:HIS:CD2	3:e:556:ASP:H	2.30	0.49
3:f:307:ASP:C	3:f:307:ASP:OD1	2.55	0.49
1:A:36:ILE:HB	1:A:69:GLY:HA3	1.93	0.49
1:D:16:ARG:O	1:D:16:ARG:HG3	2.12	0.49
1:D:140:ALA:O	1:D:144:LEU:HG	2.13	0.49
1:D:141:ARG:HB2	1:D:141:ARG:CZ	2.42	0.49
1:F:99:MET:O	1:F:103:LEU:HD13	2.13	0.49
1:K:167:ARG:HB2	1:K:167:ARG:NH1	2.28	0.49
1:S:105:THR:HG21	1:S:154:LEU:HD11	1.93	0.49
3:b:135:LEU:HD22	3:b:250:GLN:HB3	1.95	0.49
3:c:271:ARG:NH1	3:d:150:GLY:HA3	2.28	0.49
3:d:172:LYS:HD2	3:d:173:LEU:N	2.28	0.49
3:d:412:GLU:OE2	3:d:418:PRO:HA	2.13	0.49
3:a:191:GLY:HA2	3:f:192:ILE:CG1	2.26	0.49
3:a:546:LEU:HA	3:a:586:ILE:O	2.13	0.49
3:e:176:LYS:HB3	3:e:214:ILE:HG12	1.94	0.49
3:f:157:VAL:HG21	3:f:216:PHE:CE1	2.47	0.49
3:f:459:ARG:HG2	3:f:459:ARG:NH1	2.26	0.49
1:C:153:ILE:O	1:C:157:ARG:HG3	2.13	0.49
2:H:6:UNK:CB	3:f:193:ARG:HB2	2.43	0.49
1:I:108:GLN:HA	1:I:109:LYS:NZ	2.28	0.49
1:M:45:ILE:HD11	1:M:77:ILE:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:87:ASP:OD2	1:N:108:GLN:HG2	2.13	0.49
3:b:128:ILE:O	3:b:132:ILE:HG12	2.13	0.49
3:a:128:ILE:HG21	3:a:163:LYS:HD3	1.95	0.49
3:a:506:SER:O	3:a:509:MET:HG3	2.12	0.49
3:e:120:PRO:HD3	3:e:295:LYS:NZ	2.27	0.49
1:B:89:GLN:HB3	1:B:111:LYS:HB2	1.95	0.49
1:B:161:PRO:HG2	1:B:164:VAL:CG2	2.43	0.49
1:D:132:GLN:HG2	1:S:124:GLN:CG	2.36	0.49
1:F:21:TYR:CE2	1:F:31:MET:HE3	2.47	0.49
1:I:46:ALA:CB	1:T:24:LEU:HD11	2.43	0.49
1:I:71:VAL:HG12	1:I:75:LEU:HD23	1.95	0.49
1:K:102:PHE:HD1	1:K:154:LEU:HD13	1.78	0.49
1:M:181:LYS:HA	1:M:186:ILE:HG22	1.95	0.49
3:b:178:VAL:HA	3:b:214:ILE:HB	1.95	0.49
3:b:301:HIS:ND1	3:b:338:GLY:HA3	2.28	0.49
3:b:578:VAL:HG23	3:b:580:PHE:CE1	2.47	0.49
3:c:534:THR:HG21	3:c:572:ASP:HB3	1.94	0.49
3:d:613:VAL:HG22	3:d:634:GLU:OE2	2.13	0.49
1:C:125:PRO:CD	1:C:147:ARG:HG3	2.42	0.48
1:D:40:VAL:O	1:D:44:VAL:HG23	2.13	0.48
1:E:114:ALA:HB3	1:E:186:ILE:HD13	1.95	0.48
1:S:37:ASP:OD2	1:S:40:VAL:HG23	2.13	0.48
1:S:98:SER:HB3	1:S:123:HIS:ND1	2.28	0.48
3:b:202:LYS:HD2	3:c:188:GLN:O	2.13	0.48
3:c:198:GLU:OE2	3:c:198:GLU:N	2.38	0.48
3:c:204:ILE:HA	3:c:207:ILE:HG22	1.95	0.48
3:c:442:VAL:HG21	3:c:646:ILE:HG13	1.94	0.48
3:a:427:GLN:O	3:a:431:LYS:HG3	2.13	0.48
3:e:471:SER:HB3	3:e:629:PHE:CD1	2.47	0.48
3:f:202:LYS:NZ	3:f:202:LYS:HB3	2.28	0.48
1:E:7:VAL:HG21	1:E:23:ARG:HG2	1.94	0.48
1:F:96:ALA:HB3	1:F:120:ILE:HD12	1.95	0.48
1:L:89:GLN:HG2	1:L:111:LYS:CD	2.43	0.48
1:M:78:PHE:HE2	1:M:153:ILE:CG2	2.23	0.48
1:S:6:THR:HA	1:S:19:ASP:HA	1.95	0.48
1:S:20:ILE:HD11	1:T:47:GLN:HA	1.95	0.48
3:b:702:ALA:HB1	3:b:705:TYR:CE1	2.48	0.48
3:c:449:ASP:O	3:c:453:LYS:HG3	2.12	0.48
3:c:638:LEU:HD13	3:c:646:ILE:CD1	2.44	0.48
3:a:465:GLN:O	3:a:581:LYS:HD3	2.13	0.48
3:a:685:GLY:O	3:a:688:PRO:HD2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:e:556:ASP:OD2	3:e:556:ASP:C	2.55	0.48
1:A:123:HIS:C	1:A:169:THR:HG23	2.38	0.48
1:B:44:VAL:O	1:B:48:LEU:HG	2.14	0.48
1:C:10:GLN:HB3	1:C:16:ARG:O	2.14	0.48
1:C:31:MET:HE2	1:C:31:MET:HB2	1.73	0.48
1:D:71:VAL:HG11	1:D:146:THR:CG2	2.43	0.48
1:F:167:ARG:NH1	1:F:167:ARG:CB	2.76	0.48
1:G:31:MET:HE2	1:G:31:MET:HB2	1.81	0.48
1:G:143:ILE:HG23	1:G:144:LEU:HD12	1.94	0.48
1:G:167:ARG:NH1	1:G:167:ARG:CB	2.76	0.48
1:I:134:THR:O	1:I:138:ILE:HG12	2.13	0.48
1:L:80:THR:O	1:L:84:VAL:HG22	2.13	0.48
1:S:175:MET:HE2	1:S:175:MET:HB3	1.76	0.48
3:b:111:GLU:O	3:b:114:ARG:HG2	2.13	0.48
3:d:134:ILE:CB	3:d:143:PRO:HG3	2.43	0.48
3:a:107:ILE:HD12	3:a:107:ILE:N	2.27	0.48
3:e:101:LEU:CD1	3:e:202:LYS:HZ2	2.26	0.48
3:e:315:ASN:C	3:e:315:ASN:OD1	2.56	0.48
3:e:592:GLY:H	3:e:596:VAL:CG2	2.26	0.48
3:f:134:ILE:CG2	3:f:143:PRO:HG3	2.44	0.48
3:f:611:LYS:HD2	3:f:611:LYS:O	2.13	0.48
1:B:12:SER:HB3	1:B:16:ARG:NH2	2.28	0.48
1:C:16:ARG:CG	1:C:17:ALA:N	2.77	0.48
1:D:92:VAL:O	1:D:115:LEU:HD23	2.13	0.48
1:I:34:GLY:O	1:I:66:SER:HB2	2.13	0.48
1:K:44:VAL:O	1:K:48:LEU:HD23	2.13	0.48
1:K:112:ARG:HB3	1:K:186:ILE:HD12	1.94	0.48
3:c:483:THR:HB	4:c:801:ATP:PA	2.54	0.48
3:c:596:VAL:O	3:c:597:GLU:HB3	2.13	0.48
3:d:225:GLY:HA2	3:d:234:MET:SD	2.53	0.48
3:d:690:ARG:HH11	3:d:694:GLN:HG3	1.79	0.48
3:a:249:LEU:O	3:a:249:LEU:HD23	2.13	0.48
3:a:487:LYS:HB3	3:a:497:GLU:OE1	2.13	0.48
3:e:649:LEU:CA	3:e:652:GLU:HG2	2.27	0.48
3:f:667:VAL:HB	3:f:671:VAL:CG1	2.29	0.48
1:B:30:ILE:HG23	1:B:47:GLN:HE22	1.79	0.48
1:C:144:LEU:O	1:C:148:GLN:HG3	2.13	0.48
1:D:129:ALA:HB2	1:D:139:ALA:HB3	1.95	0.48
1:D:161:PRO:HD2	1:D:164:VAL:CG1	2.42	0.48
1:K:190:MET:HE2	1:L:83:PHE:CZ	2.49	0.48
1:S:141:ARG:HH11	1:S:141:ARG:CG	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:110:THR:HG21	3:d:177:GLU:CA	2.43	0.48
3:d:204:ILE:HA	3:d:207:ILE:CG2	2.43	0.48
3:a:151:VAL:HA	3:a:327:PRO:HG2	1.95	0.48
3:e:213:VAL:C	3:e:214:ILE:HD13	2.38	0.48
3:e:283:VAL:O	3:e:287:ILE:HG13	2.14	0.48
3:e:417:ILE:HG23	3:e:418:PRO:HD2	1.96	0.48
3:f:128:ILE:HG21	3:f:163:LYS:CD	2.38	0.48
3:f:153:LYS:CB	4:f:802:ATP:PB	3.02	0.48
3:f:522:PRO:HA	3:f:527:TYR:CD1	2.49	0.48
1:E:134:THR:O	1:E:138:ILE:HG13	2.13	0.48
1:K:93:LEU:HB3	1:K:115:LEU:HD23	1.96	0.48
1:N:90:THR:C	1:N:91:ILE:HD12	2.39	0.48
1:N:141:ARG:HG2	1:N:141:ARG:HH11	1.78	0.48
3:d:137:ARG:HD3	3:d:140:LYS:O	2.13	0.48
3:e:140:LYS:HG2	3:e:140:LYS:O	2.14	0.48
3:e:675:LEU:CD2	3:e:692:THR:HG22	2.43	0.48
3:f:415:THR:OG1	3:f:417:ILE:HD12	2.14	0.48
1:F:23:ARG:O	1:F:26:LYS:HG3	2.13	0.48
1:F:51:LEU:HD13	1:F:60:ILE:CG2	2.44	0.48
1:K:144:LEU:O	1:K:148:GLN:HG3	2.14	0.48
1:T:108:GLN:CB	1:T:111:LYS:HG3	2.42	0.48
1:T:123:HIS:HB3	1:T:172:ASP:HA	1.95	0.48
3:b:221:HIS:H	3:b:255:THR:HG21	1.78	0.48
3:c:173:LEU:HA	3:c:176:LYS:HG2	1.95	0.48
3:c:278:VAL:HG23	3:c:278:VAL:O	2.14	0.48
3:d:249:LEU:CD1	3:d:251:LEU:HB2	2.44	0.48
3:a:306:THR:O	3:a:309:ALA:HB3	2.13	0.48
3:e:271:ARG:CZ	4:f:802:ATP:H4'	2.43	0.48
3:e:466:ASN:HA	3:e:581:LYS:CE	2.43	0.48
3:e:666:GLU:O	3:e:716:ALA:HB3	2.13	0.48
1:D:20:ILE:O	1:D:24:LEU:HD13	2.14	0.48
3:b:132:ILE:HD11	3:b:160:LEU:HD11	1.94	0.48
3:b:714:LEU:HD23	3:b:714:LEU:H	1.78	0.48
3:c:427:GLN:O	3:c:431:LYS:HG3	2.14	0.48
3:d:148:GLU:OE2	3:d:148:GLU:CA	2.62	0.48
3:d:482:LYS:HE3	3:d:589:SER:O	2.13	0.48
3:d:665:ILE:HD12	3:d:701:ILE:HD11	1.95	0.48
3:a:127:GLU:O	3:a:131:VAL:HG23	2.14	0.48
3:e:142:ASN:ND2	3:e:272:ARG:HG3	2.29	0.48
3:e:203:LEU:O	3:e:207:ILE:HG22	2.13	0.48
1:E:10:GLN:OE1	1:E:10:GLN:C	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:71:VAL:HG11	1:F:146:THR:CG2	2.43	0.48
1:F:141:ARG:HB2	1:F:141:ARG:CZ	2.44	0.48
1:K:91:ILE:N	1:K:91:ILE:HD12	2.29	0.48
1:K:92:VAL:O	1:K:115:LEU:HD23	2.13	0.48
1:L:113:PHE:CD1	1:L:188:GLU:HG2	2.49	0.48
1:M:129:ALA:HB2	1:M:139:ALA:CB	2.43	0.48
1:S:167:ARG:CB	1:S:167:ARG:NH1	2.77	0.48
3:b:647:VAL:HG21	3:b:676:VAL:CG2	2.43	0.48
3:c:484:GLU:O	3:c:488:GLN:HG2	2.14	0.48
3:d:124:ARG:HG3	3:d:156:VAL:HG22	1.96	0.48
3:d:244:LEU:HB3	3:d:272:ARG:CZ	2.44	0.48
3:d:636:LYS:HE3	3:d:636:LYS:HB2	1.74	0.48
3:d:695:GLU:OE1	3:d:695:GLU:O	2.32	0.48
3:a:343:LEU:HD11	3:f:133:GLU:HG2	1.95	0.48
3:a:697:ILE:HG22	3:a:701:ILE:HD11	1.96	0.48
3:e:309:ALA:HA	3:e:404:GLU:HG2	1.95	0.48
3:e:315:ASN:HD21	3:e:422:LEU:HG	1.79	0.48
3:e:671:VAL:CB	3:e:718:LEU:HD13	2.44	0.48
1:B:53:ALA:HB1	3:f:600:VAL:CG2	2.38	0.48
1:L:113:PHE:O	1:L:186:ILE:HD11	2.13	0.48
3:b:154:THR:O	3:b:158:GLU:HG2	2.14	0.48
3:b:204:ILE:HG21	3:b:239:ILE:CG2	2.43	0.48
3:d:282:THR:HG22	3:d:285:GLU:CG	2.43	0.48
3:d:295:LYS:HE2	3:d:299:ASP:OD2	2.13	0.48
3:d:534:THR:O	3:d:538:ARG:HG2	2.14	0.48
3:f:537:VAL:HG21	3:f:580:PHE:CE2	2.49	0.48
1:C:115:LEU:HD23	1:D:79:ASP:HB3	1.96	0.47
1:K:137:GLU:CG	1:K:141:ARG:HH22	2.22	0.47
3:b:591:ALA:HB1	3:b:620:PHE:CG	2.49	0.47
3:c:151:VAL:HG21	3:c:278:VAL:HG23	1.95	0.47
3:c:691:ARG:HA	3:c:694:GLN:HG2	1.96	0.47
3:d:462:LEU:HD23	3:e:698:GLU:HG2	1.95	0.47
3:e:110:THR:HG21	3:e:177:GLU:CA	2.44	0.47
3:e:238:ASN:HD21	3:f:185:SER:HA	1.79	0.47
1:B:83:PHE:CE2	3:f:602:PHE:HE1	2.23	0.47
1:C:63:TYR:CZ	1:C:91:ILE:HD11	2.49	0.47
1:E:55:ASP:OD2	1:E:58:LYS:HG3	2.14	0.47
1:G:89:GLN:HB2	1:G:111:LYS:O	2.14	0.47
3:b:412:GLU:HG3	3:b:417:ILE:O	2.14	0.47
3:b:425:LYS:HB2	3:b:425:LYS:NZ	2.29	0.47
3:c:107:ILE:HD13	3:c:180:ARG:CZ	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:668:PRO:HG2	3:c:671:VAL:CG2	2.38	0.47
4:d:802:ATP:O1B	4:d:802:ATP:H5'1	2.14	0.47
3:a:657:LEU:HD21	3:f:461:GLY:O	2.15	0.47
3:e:233:ASN:ND2	3:e:238:ASN:HD22	2.12	0.47
3:e:241:LYS:N	3:e:241:LYS:CE	2.75	0.47
3:e:662:LYS:HB3	3:e:712:HIS:CE1	2.48	0.47
3:f:234:MET:HE2	3:f:239:ILE:HD11	1.96	0.47
1:D:27:ASP:OD2	3:d:599:ASN:HB3	2.15	0.47
1:E:190:MET:HE1	3:c:602:PHE:CB	2.38	0.47
1:M:140:ALA:HA	1:M:143:ILE:HG22	1.97	0.47
3:b:478:THR:HG23	4:b:801:ATP:O3G	2.14	0.47
3:b:481:GLY:HA2	4:b:801:ATP:O1A	2.14	0.47
3:c:104:GLU:OE1	3:c:104:GLU:N	2.33	0.47
3:c:215:LEU:HD12	3:c:251:LEU:HD13	1.96	0.47
3:c:221:HIS:HA	3:c:263:ILE:CD1	2.30	0.47
3:c:483:THR:HG22	3:c:487:LYS:HE3	1.96	0.47
3:d:234:MET:HE3	3:d:235:ASP:N	2.29	0.47
3:a:189:GLY:HA2	3:f:197:GLU:OE1	2.14	0.47
3:e:232:GLY:O	3:f:188:GLN:HG2	2.13	0.47
3:e:419:VAL:HG22	3:e:420:GLY:H	1.78	0.47
3:f:221:HIS:CE1	3:f:259:GLU:HG2	2.49	0.47
3:f:674:LYS:NZ	3:f:724:ILE:HD12	2.29	0.47
1:B:54:GLN:HB2	3:f:599:ASN:OD1	2.15	0.47
1:E:92:VAL:CG2	1:E:104:LEU:HD22	2.37	0.47
1:F:20:ILE:O	1:F:24:LEU:HD13	2.13	0.47
1:F:75:LEU:HD13	1:F:149:ARG:NH1	2.29	0.47
1:I:50:PHE:CZ	1:T:7:VAL:HG21	2.49	0.47
1:K:119:GLU:C	1:K:120:ILE:HD12	2.39	0.47
3:b:130:ARG:HG2	3:c:413:GLN:NE2	2.29	0.47
3:c:514:VAL:O	3:c:518:ILE:HG12	2.14	0.47
3:d:148:GLU:HG3	3:d:325:PHE:CZ	2.49	0.47
3:d:261:ARG:HG2	3:d:261:ARG:NH1	2.27	0.47
3:e:501:VAL:HG11	3:e:536:LYS:HD3	1.95	0.47
1:D:167:ARG:NH1	1:D:167:ARG:CB	2.76	0.47
1:E:8:ILE:HG22	1:E:15:GLU:HG2	1.96	0.47
1:M:141:ARG:HH11	1:M:141:ARG:HG3	1.78	0.47
3:b:505:MET:HB2	3:b:549:GLU:O	2.14	0.47
3:d:285:GLU:O	3:d:289:ILE:HG13	2.15	0.47
3:a:469:ILE:HG23	3:a:583:THR:H	1.78	0.47
1:A:29:ILE:CD1	1:A:61:TYR:HB2	2.43	0.47
1:I:105:THR:O	1:I:157:ARG:HD3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:120:ILE:HD12	1:K:120:ILE:N	2.30	0.47
1:K:187:ASP:O	1:K:188:GLU:HG2	2.14	0.47
1:L:58:LYS:O	1:L:86:ALA:HB1	2.14	0.47
1:N:90:THR:OG1	1:N:104:LEU:HD12	2.15	0.47
3:b:477:PRO:O	3:b:480:VAL:HG22	2.15	0.47
3:b:622:THR:CG2	3:b:623:PRO:HD2	2.43	0.47
3:d:134:ILE:HG21	3:d:274:GLN:HG2	1.97	0.47
3:d:136:ASN:OD1	3:e:339:SER:HA	2.15	0.47
3:d:173:LEU:CB	3:d:176:LYS:HD3	2.44	0.47
3:d:321:ILE:CD1	3:d:414:LYS:HD2	2.44	0.47
3:a:210:ALA:O	3:a:211:GLU:HB2	2.13	0.47
3:e:197:GLU:HG3	3:e:234:MET:CE	2.33	0.47
3:e:202:LYS:C	3:e:202:LYS:CD	2.87	0.47
3:e:318:ASN:HA	3:e:329:LYS:NZ	2.30	0.47
3:f:451:VAL:CG2	3:f:633:ILE:HD13	2.45	0.47
1:A:47:GLN:O	1:A:51:LEU:HD13	2.14	0.47
1:C:33:SER:HA	1:C:65:ASN:O	2.15	0.47
1:C:136:ILE:HD11	1:T:127:GLY:O	2.15	0.47
1:E:152:SER:HA	1:E:162:ILE:HD11	1.96	0.47
1:E:161:PRO:HG2	1:E:164:VAL:HB	1.95	0.47
1:F:23:ARG:HD2	1:F:23:ARG:C	2.40	0.47
1:F:124:GLN:HG2	1:F:169:THR:O	2.15	0.47
1:F:126:LEU:HD21	1:M:132:GLN:HG2	1.97	0.47
1:L:4:ILE:HD11	1:L:20:ILE:HG22	1.95	0.47
1:N:45:ILE:HD11	1:N:77:ILE:CA	2.44	0.47
1:S:74:GLY:HA3	1:S:99:MET:HE2	1.97	0.47
1:T:96:ALA:HB3	1:T:120:ILE:CD1	2.45	0.47
3:c:101:LEU:CD1	3:c:203:LEU:HD12	2.41	0.47
3:c:118:ILE:CG2	3:c:158:GLU:HG2	2.45	0.47
3:c:473:LEU:HD22	3:c:475:VAL:CG2	2.45	0.47
3:d:217:ILE:HG23	3:d:220:VAL:HG12	1.95	0.47
3:d:622:THR:HB	3:d:624:GLU:OE1	2.14	0.47
3:a:639:SER:O	3:a:643:LEU:HD13	2.15	0.47
3:a:706:LEU:HD12	3:f:456:ARG:HH11	1.79	0.47
3:e:197:GLU:O	3:e:200:MET:HG2	2.15	0.47
3:e:433:LEU:HD21	3:e:437:LEU:HD11	1.95	0.47
3:e:544:LEU:HD21	3:e:586:ILE:CD1	2.42	0.47
3:e:551:GLU:OE1	3:e:551:GLU:N	2.37	0.47
3:e:554:HIS:HD2	3:e:555:PRO:HD2	1.79	0.47
3:e:631:GLY:C	3:e:632:ILE:HD12	2.39	0.47
3:f:651:LEU:O	3:f:655:ASN:OD1	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:VAL:HG13	1:B:114:ALA:HA	1.95	0.47
1:E:80:THR:O	1:E:84:VAL:HG13	2.14	0.47
1:K:7:VAL:HG11	1:L:50:PHE:CZ	2.50	0.47
3:b:144:VAL:HG22	3:b:273:MET:HE2	1.97	0.47
3:c:134:ILE:HB	3:c:143:PRO:HG3	1.96	0.47
3:c:211:GLU:O	3:c:211:GLU:CD	2.57	0.47
3:c:216:PHE:HD1	3:c:252:VAL:HG13	1.79	0.47
3:c:526:GLY:HA2	3:c:529:GLU:OE2	2.15	0.47
3:d:243:ALA:HA	3:d:248:GLU:CB	2.43	0.47
3:d:466:ASN:OD1	3:d:466:ASN:N	2.47	0.47
3:d:647:VAL:HG22	3:d:651:LEU:HD23	1.97	0.47
3:d:689:LEU:O	3:d:693:ILE:HG13	2.15	0.47
3:a:124:ARG:O	3:a:128:ILE:HG12	2.14	0.47
3:a:168:ASP:OD1	3:a:168:ASP:O	2.33	0.47
3:a:487:LYS:HB3	3:a:497:GLU:HG3	1.96	0.47
3:e:115:GLN:HB2	3:e:117:ASP:OD1	2.15	0.47
3:e:144:VAL:O	3:e:275:PRO:HA	2.15	0.47
3:e:230:GLY:HA2	3:f:191:GLY:HA3	1.97	0.47
3:e:684:MET:HB2	3:e:688:PRO:HD3	1.97	0.47
3:f:542:TYR:HE1	3:f:582:ASP:OD2	1.97	0.47
1:B:68:GLY:HA3	1:B:98:SER:OG	2.15	0.47
1:E:9:GLU:O	1:E:10:GLN:HB3	2.15	0.47
1:F:57:GLU:OE1	1:F:57:GLU:HA	2.14	0.47
1:M:6:THR:O	1:N:22:SER:HB3	2.15	0.47
3:b:500:MET:HE3	3:b:546:LEU:HD23	1.97	0.47
3:d:105:TYR:OH	3:d:203:LEU:HD13	2.15	0.47
3:d:326:LEU:H	3:d:326:LEU:CD2	2.27	0.47
3:d:505:MET:HE2	3:d:505:MET:CA	2.45	0.47
3:a:192:ILE:CG1	3:a:195:GLN:HB2	2.45	0.47
3:a:675:LEU:HD23	3:a:692:THR:CG2	2.41	0.47
3:f:488:GLN:OE1	3:f:488:GLN:HA	2.15	0.47
3:f:671:VAL:HG13	3:f:672:LYS:N	2.30	0.47
1:A:138:ILE:HG21	1:G:172:ASP:O	2.15	0.47
1:B:89:GLN:HB2	1:B:111:LYS:O	2.15	0.47
1:E:130:GLN:HB3	1:N:128:GLY:HA2	1.96	0.47
1:K:185:LEU:O	1:K:186:ILE:HD13	2.15	0.47
1:N:36:ILE:HA	1:N:40:VAL:HG11	1.96	0.47
3:b:317:SER:OG	3:b:329:LYS:HB3	2.14	0.47
3:b:570:LEU:O	3:b:578:VAL:HG22	2.15	0.47
3:d:260:TYR:CZ	3:d:275:PRO:HG3	2.49	0.47
3:d:321:ILE:HD11	3:d:414:LYS:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:222:GLU:OE1	3:f:234:MET:HE1	2.14	0.47
3:e:101:LEU:HD21	3:e:105:TYR:CG	2.50	0.47
3:e:142:ASN:HD22	3:e:272:ARG:HG3	1.79	0.47
3:e:474:PHE:C	3:e:482:LYS:HZ1	2.23	0.47
1:D:4:ILE:CG2	1:D:20:ILE:HG22	2.44	0.46
1:D:160:GLN:HB3	1:D:164:VAL:CG1	2.44	0.46
1:G:32:LEU:HD23	1:G:64:ILE:CD1	2.46	0.46
1:G:140:ALA:O	1:G:143:ILE:HG22	2.15	0.46
1:K:33:SER:OG	1:L:38:ASP:HB3	2.15	0.46
1:S:90:THR:HG21	1:S:106:ALA:O	2.15	0.46
3:c:146:ILE:HA	3:c:255:THR:O	2.15	0.46
3:d:152:GLY:O	3:d:156:VAL:HG23	2.15	0.46
3:a:587:MET:HE1	3:a:625:PHE:HZ	1.79	0.46
3:a:632:ILE:HD12	3:a:632:ILE:N	2.30	0.46
3:a:697:ILE:HG22	3:a:701:ILE:CD1	2.45	0.46
3:e:307:ASP:OD1	3:e:307:ASP:C	2.57	0.46
3:e:536:LYS:HB3	3:e:536:LYS:HE3	1.62	0.46
3:e:714:LEU:HD12	3:e:714:LEU:C	2.40	0.46
3:f:127:GLU:O	3:f:131:VAL:HG23	2.15	0.46
1:A:8:ILE:HG23	1:A:15:GLU:OE2	2.15	0.46
1:A:11:SER:HB2	1:A:14:GLY:O	2.15	0.46
1:D:4:ILE:HG23	1:D:20:ILE:HG22	1.96	0.46
1:F:59:ASP:HB2	1:F:87:ASP:O	2.15	0.46
1:T:124:GLN:HB3	1:T:147:ARG:NH1	2.30	0.46
3:b:514:VAL:HG12	3:b:557:VAL:HG22	1.96	0.46
3:b:723:LYS:NZ	3:b:723:LYS:HB3	2.29	0.46
3:c:217:ILE:O	3:c:220:VAL:HG13	2.15	0.46
3:a:196:PHE:CD2	3:a:200:MET:HE3	2.49	0.46
3:a:246:ARG:HD2	3:a:248:GLU:OE1	2.16	0.46
3:e:272:ARG:NH2	4:f:802:ATP:H1'	2.30	0.46
3:e:569:ARG:HH12	3:e:581:LYS:HE3	1.80	0.46
3:f:581:LYS:HB2	3:f:581:LYS:HE2	1.66	0.46
1:A:95:MET:HA	1:A:119:GLU:O	2.15	0.46
1:E:11:SER:O	1:E:15:GLU:HG3	2.16	0.46
1:F:126:LEU:CD2	1:M:132:GLN:HG2	2.45	0.46
1:G:105:THR:HG22	1:G:185:LEU:HB3	1.98	0.46
1:I:37:ASP:H	1:I:40:VAL:HG22	1.79	0.46
3:b:178:VAL:C	3:b:179:ILE:HD13	2.41	0.46
3:b:529:GLU:O	3:b:529:GLU:HG2	2.15	0.46
3:b:670:GLU:HG2	3:b:671:VAL:N	2.30	0.46
3:d:326:LEU:HA	3:d:328:ASP:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:190:THR:HG22	3:f:194:GLY:O	2.15	0.46
3:a:419:VAL:HG12	3:a:420:GLY:N	2.30	0.46
3:a:724:ILE:HD13	3:a:724:ILE:N	2.28	0.46
3:e:565:LEU:CD1	3:e:587:MET:HE3	2.42	0.46
3:f:671:VAL:HG23	3:f:674:LYS:HE3	1.98	0.46
1:D:18:TYR:HB3	1:D:22:SER:HB2	1.97	0.46
1:F:137:GLU:HB2	1:M:144:LEU:HD21	1.96	0.46
3:c:183:VAL:HG21	3:c:222:GLU:CB	2.45	0.46
3:d:111:GLU:HA	3:d:114:ARG:HB2	1.97	0.46
3:d:169:VAL:CG1	3:d:174:LEU:HG	2.45	0.46
3:d:444:GLN:HG3	3:d:635:PHE:HD2	1.80	0.46
3:e:485:LEU:HD23	3:e:635:PHE:HZ	1.80	0.46
3:f:671:VAL:CG2	3:f:724:ILE:HD11	2.45	0.46
1:A:161:PRO:O	1:A:164:VAL:HG12	2.16	0.46
1:C:29:ILE:HD11	1:C:63:TYR:CD1	2.50	0.46
1:F:81:MET:O	1:F:84:VAL:HG22	2.16	0.46
1:F:93:LEU:HD13	1:G:45:ILE:HD13	1.98	0.46
1:G:80:THR:O	1:G:84:VAL:HG13	2.15	0.46
1:M:64:ILE:HD12	1:M:64:ILE:N	2.31	0.46
1:M:141:ARG:HH11	1:M:141:ARG:CG	2.28	0.46
1:T:34:GLY:CA	1:T:67:PRO:HD2	2.35	0.46
3:a:152:GLY:HA2	4:f:801:ATP:H8	1.80	0.46
3:a:180:ARG:HA	3:a:216:PHE:O	2.16	0.46
3:e:342:ASN:C	3:e:342:ASN:OD1	2.59	0.46
3:f:569:ARG:HH11	3:f:569:ARG:HB2	1.81	0.46
1:G:158:THR:HG22	1:G:160:GLN:HG3	1.98	0.46
1:I:74:GLY:HA3	1:I:99:MET:HG2	1.97	0.46
1:I:80:THR:O	1:I:84:VAL:HG13	2.16	0.46
3:b:422:LEU:H	3:b:422:LEU:HD12	1.80	0.46
3:c:187:VAL:O	3:c:187:VAL:HG12	2.16	0.46
3:d:110:THR:CG2	3:d:178:VAL:H	2.27	0.46
3:a:195:GLN:O	3:a:198:GLU:OE1	2.33	0.46
3:a:246:ARG:CG	3:a:246:ARG:NH1	2.79	0.46
3:f:169:VAL:HB	3:f:173:LEU:HB2	1.98	0.46
1:D:65:ASN:HB2	1:D:93:LEU:CD1	2.46	0.46
1:E:63:TYR:CE1	1:E:91:ILE:HD13	2.50	0.46
1:F:10:GLN:HB2	1:F:16:ARG:O	2.14	0.46
1:I:113:PHE:CD2	1:I:188:GLU:HB3	2.50	0.46
1:N:120:ILE:HG21	1:N:185:LEU:HD13	1.97	0.46
1:S:143:ILE:HG23	1:S:144:LEU:HD22	1.98	0.46
3:b:283:VAL:O	3:b:287:ILE:HG13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:455:ILE:HD13	3:b:493:LEU:HD11	1.98	0.46
3:b:460:VAL:HG12	3:b:462:LEU:CD1	2.46	0.46
3:d:199:ARG:HD2	3:d:199:ARG:HA	1.61	0.46
3:a:101:LEU:HA	3:a:104:GLU:CG	2.46	0.46
3:a:246:ARG:HB2	3:a:248:GLU:OE1	2.16	0.46
3:a:698:GLU:HB3	3:f:457:ARG:HD2	1.97	0.46
3:e:124:ARG:HA	3:e:127:GLU:OE1	2.15	0.46
3:e:464:LYS:H	3:e:464:LYS:CE	2.28	0.46
3:e:506:SER:HA	3:e:552:LYS:HE2	1.96	0.46
3:e:553:ALA:HB1	3:e:557:VAL:HG13	1.97	0.46
3:f:298:GLU:HG2	3:f:305:TYR:CD1	2.50	0.46
3:f:444:GLN:O	3:f:448:VAL:HG23	2.16	0.46
1:A:120:ILE:O	1:A:120:ILE:HG13	2.15	0.46
1:A:124:GLN:N	1:A:169:THR:HG23	2.31	0.46
1:C:10:GLN:HG3	1:C:14:GLY:HA2	1.97	0.46
1:D:67:PRO:O	1:D:97:ALA:HB3	2.16	0.46
1:F:91:ILE:HD12	1:F:91:ILE:N	2.31	0.46
1:F:171:ARG:HH12	1:G:132:GLN:NE2	2.14	0.46
1:L:51:LEU:HB3	1:L:60:ILE:HD11	1.98	0.46
1:S:74:GLY:HA3	1:S:99:MET:CE	2.45	0.46
3:b:108:ASN:HB3	3:b:111:GLU:CG	2.42	0.46
3:b:124:ARG:O	3:b:128:ILE:HG12	2.16	0.46
3:b:337:SER:OG	3:b:410:ILE:HD12	2.16	0.46
3:b:432:ASN:O	3:b:435:VAL:HG22	2.16	0.46
3:b:503:PHE:HB3	3:b:505:MET:CE	2.45	0.46
3:c:211:GLU:HA	3:c:211:GLU:OE2	2.16	0.46
3:a:294:GLN:O	3:a:298:GLU:HG3	2.14	0.46
3:a:662:LYS:C	3:a:663:LEU:HD12	2.40	0.46
3:e:230:GLY:HA2	3:f:191:GLY:C	2.41	0.46
3:e:300:TYR:CE1	3:e:301:HIS:CD2	3.04	0.46
3:e:510:GLU:OE2	3:e:511:LYS:N	2.48	0.46
3:f:450:LYS:HB3	3:f:450:LYS:HZ1	1.81	0.46
1:A:24:LEU:HD11	1:B:46:ALA:HB1	1.98	0.46
1:B:12:SER:HB3	1:B:16:ARG:HH22	1.80	0.46
1:B:29:ILE:HD13	1:B:61:TYR:CB	2.36	0.46
1:E:161:PRO:HG2	1:E:164:VAL:HG23	1.97	0.46
1:F:161:PRO:HG2	1:F:164:VAL:HG12	1.97	0.46
1:M:75:LEU:HD22	1:M:99:MET:HE2	1.97	0.46
3:b:171:GLN:OE1	3:b:171:GLN:N	2.36	0.46
3:b:198:GLU:HG3	3:c:190:THR:O	2.15	0.46
3:a:101:LEU:HD23	3:a:101:LEU:C	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:457:ARG:HG2	3:a:462:LEU:HB2	1.97	0.46
3:e:417:ILE:CG2	3:e:418:PRO:HD2	2.46	0.46
3:e:488:GLN:O	3:e:492:GLU:HG3	2.16	0.46
3:e:675:LEU:HD23	3:e:692:THR:HG22	1.98	0.46
3:f:650:MET:O	3:f:654:VAL:HG12	2.15	0.46
1:C:105:THR:CG2	1:C:157:ARG:HB2	2.46	0.46
1:F:51:LEU:HD13	1:F:60:ILE:HG21	1.97	0.46
1:G:91:ILE:HG23	1:G:190:MET:HE2	1.97	0.46
1:G:155:ALA:HB2	1:G:165:ILE:HD12	1.98	0.46
1:L:71:VAL:O	1:L:75:LEU:HD23	2.16	0.46
1:S:95:MET:HE2	1:S:95:MET:HB2	1.79	0.46
3:b:192:ILE:HG22	3:c:192:ILE:HG21	1.97	0.46
3:b:243:ALA:HB1	3:b:249:LEU:HD22	1.98	0.46
3:b:524:TYR:CZ	3:c:512:HIS:HB2	2.51	0.46
3:c:195:GLN:O	3:c:196:PHE:HB3	2.16	0.46
3:a:434:ALA:O	3:a:438:LYS:HG3	2.15	0.46
3:e:406:ASP:O	3:e:410:ILE:HG22	2.16	0.46
3:e:503:PHE:HB2	3:e:547:LEU:CD2	2.45	0.46
1:A:71:VAL:HG11	1:A:146:THR:CG2	2.46	0.45
1:A:152:SER:HA	1:A:162:ILE:CD1	2.46	0.45
1:A:160:GLN:HB3	1:A:164:VAL:CG1	2.46	0.45
1:E:130:GLN:HB3	1:N:128:GLY:CA	2.46	0.45
3:b:502:ARG:HG3	3:b:546:LEU:HD23	1.97	0.45
3:b:705:TYR:HB2	3:b:711:ASN:HB2	1.97	0.45
3:e:200:MET:HE1	3:e:234:MET:CE	2.46	0.45
3:e:632:ILE:HD12	3:e:632:ILE:N	2.31	0.45
3:e:652:GLU:OE2	3:e:652:GLU:CA	2.64	0.45
3:e:695:GLU:HA	3:e:699:ASP:OD1	2.16	0.45
3:e:719:ASP:OD2	3:e:721:GLU:HB2	2.16	0.45
3:f:146:ILE:HG21	3:f:257:LEU:HD12	1.98	0.45
1:A:33:SER:HB2	1:B:42:ASN:ND2	2.32	0.45
1:C:7:VAL:O	1:C:17:ALA:O	2.34	0.45
1:E:154:LEU:O	1:E:158:THR:HG22	2.16	0.45
1:F:37:ASP:OD1	1:F:40:VAL:HG23	2.16	0.45
1:L:58:LYS:NZ	1:L:60:ILE:HD11	2.31	0.45
1:L:63:TYR:CD1	1:L:91:ILE:HB	2.50	0.45
1:M:180:ALA:CB	1:M:185:LEU:HD11	2.47	0.45
1:N:87:ASP:HB2	1:N:108:GLN:HB2	1.98	0.45
1:N:91:ILE:HD12	1:N:91:ILE:N	2.31	0.45
3:b:219:GLU:HA	3:b:255:THR:CG2	2.42	0.45
3:b:550:VAL:HG22	3:b:589:SER:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:197:GLU:HB3	3:c:233:ASN:HD22	1.82	0.45
3:c:221:HIS:CA	3:c:263:ILE:HD11	2.33	0.45
3:c:462:LEU:N	3:c:462:LEU:HD12	2.31	0.45
3:a:101:LEU:HA	3:a:104:GLU:HG2	1.98	0.45
3:a:206:GLU:O	3:a:209:GLU:OE1	2.34	0.45
3:a:409:ALA:HA	3:a:412:GLU:HG2	1.99	0.45
3:f:417:ILE:CG2	3:f:418:PRO:HD2	2.46	0.45
1:A:55:ASP:OD2	1:A:55:ASP:C	2.58	0.45
1:C:101:SER:HB3	1:C:120:ILE:HG23	1.96	0.45
1:D:105:THR:HG22	1:D:185:LEU:O	2.17	0.45
1:I:11:SER:O	1:T:8:ILE:HD13	2.15	0.45
1:M:91:ILE:CD1	1:M:113:PHE:HB2	2.46	0.45
1:N:61:TYR:HE2	1:N:89:GLN:NE2	2.14	0.45
1:N:67:PRO:O	1:N:97:ALA:HB3	2.15	0.45
1:S:186:ILE:HD12	1:S:186:ILE:HA	1.87	0.45
3:b:173:LEU:HB2	3:b:176:LYS:HD3	1.98	0.45
3:c:201:GLN:O	3:c:205:GLU:HG3	2.15	0.45
3:d:196:PHE:O	3:d:200:MET:HG3	2.15	0.45
3:d:714:LEU:HD12	3:d:714:LEU:N	2.32	0.45
3:e:501:VAL:HG22	3:e:544:LEU:O	2.15	0.45
3:e:513:SER:HA	3:e:516:LYS:HD3	1.98	0.45
3:f:147:GLY:HA3	3:f:278:VAL:CG1	2.46	0.45
3:f:169:VAL:CG2	3:f:174:LEU:HD13	2.45	0.45
3:f:210:ALA:O	3:f:211:GLU:HB2	2.17	0.45
3:f:417:ILE:HG22	3:f:418:PRO:HD2	1.98	0.45
3:f:479:GLY:HA2	3:f:687:ARG:NE	2.32	0.45
3:f:655:ASN:ND2	3:f:665:ILE:O	2.48	0.45
3:f:662:LYS:HB2	3:f:662:LYS:HZ3	1.82	0.45
1:A:28:ARG:HA	1:A:51:LEU:HD21	1.97	0.45
1:A:92:VAL:O	1:A:92:VAL:HG13	2.16	0.45
1:D:112:ARG:HB2	1:D:187:ASP:OD1	2.17	0.45
1:G:29:ILE:HG12	1:G:61:TYR:HB2	1.98	0.45
1:I:91:ILE:HD12	1:I:91:ILE:N	2.31	0.45
1:M:81:MET:HE2	1:M:81:MET:HB2	1.78	0.45
1:S:140:ALA:HA	1:S:143:ILE:HG22	1.99	0.45
3:b:176:LYS:NZ	3:b:212:ASN:HA	2.31	0.45
3:b:337:SER:HA	3:b:410:ILE:HD11	1.97	0.45
3:b:447:ALA:HB2	3:b:633:ILE:CG2	2.30	0.45
3:b:638:LEU:HD13	3:b:646:ILE:CD1	2.46	0.45
3:c:153:LYS:HG2	3:c:278:VAL:HG21	1.97	0.45
3:c:521:PRO:HG2	3:d:512:HIS:HD2	1.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:591:ALA:HB1	3:c:620:PHE:CD2	2.51	0.45
3:d:255:THR:OG1	3:d:259:GLU:HG2	2.17	0.45
3:d:324:ARG:HB2	3:d:329:LYS:HG2	1.99	0.45
3:d:483:THR:HG22	3:d:487:LYS:HE3	1.99	0.45
3:a:305:TYR:HB3	3:a:310:ILE:HD11	1.98	0.45
1:A:25:LEU:CD1	1:A:51:LEU:HD11	2.45	0.45
1:B:9:GLU:HB2	1:B:10:GLN:OE1	2.16	0.45
1:B:92:VAL:HG12	1:B:113:PHE:O	2.16	0.45
1:E:113:PHE:CD1	1:E:188:GLU:HB3	2.51	0.45
1:E:190:MET:O	1:E:191:GLU:HB3	2.16	0.45
1:I:96:ALA:O	1:I:120:ILE:HA	2.16	0.45
1:L:178:GLU:HA	1:L:178:GLU:OE2	2.15	0.45
3:b:712:HIS:HD1	3:b:712:HIS:C	2.25	0.45
3:d:176:LYS:HG2	3:d:212:ASN:CA	2.39	0.45
3:d:180:ARG:HA	3:d:216:PHE:O	2.16	0.45
3:a:475:VAL:HA	3:a:589:SER:O	2.16	0.45
3:a:662:LYS:CA	3:a:662:LYS:CE	2.92	0.45
3:e:101:LEU:HD21	3:e:105:TYR:CD2	2.51	0.45
3:e:308:GLU:H	3:e:308:GLU:CD	2.25	0.45
3:e:681:ASP:OD1	3:e:681:ASP:C	2.60	0.45
4:f:801:ATP:O1B	4:f:801:ATP:H5'1	2.17	0.45
1:E:154:LEU:HD23	1:E:165:ILE:CD1	2.43	0.45
1:K:161:PRO:O	1:K:164:VAL:HG12	2.17	0.45
1:N:95:MET:CE	1:N:119:GLU:HG2	2.46	0.45
1:S:102:PHE:CE1	1:S:150:LEU:HD23	2.51	0.45
1:T:132:GLN:HB2	1:T:135:GLU:HG3	1.99	0.45
3:c:613:VAL:HG21	3:c:634:GLU:HG3	1.99	0.45
3:a:186:LEU:HD21	3:a:203:LEU:HD13	1.98	0.45
3:a:587:MET:CE	3:a:625:PHE:HZ	2.29	0.45
3:e:203:LEU:HD23	3:e:203:LEU:C	2.42	0.45
3:e:204:ILE:O	3:e:207:ILE:HG22	2.17	0.45
3:e:336:GLU:OE2	3:e:336:GLU:C	2.59	0.45
3:e:647:VAL:HG13	3:e:693:ILE:HD11	1.98	0.45
3:f:672:LYS:NZ	3:f:672:LYS:HB3	2.32	0.45
1:B:33:SER:HA	1:B:65:ASN:O	2.17	0.45
1:C:30:ILE:HD11	1:C:51:LEU:HD12	1.98	0.45
1:E:71:VAL:HG11	1:E:146:THR:CG2	2.46	0.45
1:K:108:GLN:CB	1:K:111:LYS:HG3	2.47	0.45
1:L:89:GLN:HG2	1:L:111:LYS:HD3	1.99	0.45
1:N:45:ILE:O	1:N:49:LEU:HD23	2.16	0.45
3:b:151:VAL:HG12	3:b:278:VAL:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:256:THR:OG1	3:b:259:GLU:HG2	2.16	0.45
3:b:477:PRO:HG2	3:b:480:VAL:HG11	1.98	0.45
3:c:685:GLY:O	3:c:688:PRO:HD2	2.16	0.45
3:a:193:ARG:HH12	3:a:230:GLY:HA3	1.82	0.45
3:a:487:LYS:HB3	3:a:497:GLU:CG	2.47	0.45
3:e:477:PRO:O	3:e:482:LYS:HD2	2.17	0.45
3:e:668:PRO:O	3:e:671:VAL:HG12	2.16	0.45
1:B:24:LEU:HD23	1:B:29:ILE:HG21	1.98	0.45
1:B:141:ARG:HB2	1:B:141:ARG:NH1	2.31	0.45
1:C:80:THR:O	1:C:84:VAL:HG13	2.17	0.45
1:C:167:ARG:HH11	1:C:167:ARG:HG3	1.81	0.45
1:D:42:ASN:HD22	1:D:42:ASN:N	2.15	0.45
1:K:154:LEU:O	1:K:158:THR:HG23	2.17	0.45
1:M:143:ILE:HA	1:M:146:THR:HG22	1.98	0.45
1:M:161:PRO:HD2	1:M:164:VAL:CG1	2.45	0.45
1:N:175:MET:HE3	1:N:175:MET:HB2	1.75	0.45
1:S:32:LEU:HD22	1:S:66:SER:HB3	1.98	0.45
3:b:138:ARG:CG	3:b:139:THR:HG23	2.45	0.45
3:c:627:ASN:HB2	3:d:684:MET:SD	2.57	0.45
3:d:151:VAL:O	3:d:151:VAL:HG12	2.17	0.45
3:d:720:ASN:OD1	3:d:721:GLU:OE1	2.35	0.45
3:a:624:GLU:HG2	3:a:625:PHE:N	2.32	0.45
3:e:140:LYS:O	3:e:140:LYS:CG	2.65	0.45
3:e:272:ARG:HB3	3:e:273:MET:HE3	1.99	0.45
3:f:132:ILE:CD1	3:f:160:LEU:HD13	2.47	0.45
3:f:592:GLY:C	3:f:596:VAL:HG21	2.42	0.45
3:f:671:VAL:HG23	3:f:724:ILE:HD11	1.99	0.45
3:b:193:ARG:HE	3:c:192:ILE:HG22	1.81	0.45
3:b:434:ALA:O	3:b:438:LYS:HG3	2.16	0.45
3:c:144:VAL:HG13	3:c:275:PRO:HA	1.99	0.45
3:c:317:SER:OG	3:c:333:LEU:HD12	2.17	0.45
3:d:437:LEU:CD2	3:d:492:GLU:HG3	2.47	0.45
3:d:545:ILE:HG22	3:d:547:LEU:CD1	2.46	0.45
3:a:684:MET:HE1	3:f:623:PRO:HB2	1.99	0.45
3:e:239:ILE:HD13	3:e:239:ILE:N	2.31	0.45
3:e:268:ALA:HB2	3:f:218:ASP:HB3	1.99	0.45
3:e:488:GLN:OE1	3:e:488:GLN:CA	2.64	0.45
3:e:564:ILE:HD13	3:e:570:LEU:HB2	1.99	0.45
3:e:647:VAL:O	3:e:651:LEU:HD23	2.16	0.45
3:f:138:ARG:HG3	3:f:139:THR:N	2.31	0.45
1:C:30:ILE:HD11	1:C:51:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:GLU:HB2	1:D:83:PHE:CD1	2.52	0.45
1:G:141:ARG:HB2	1:G:141:ARG:NH1	2.31	0.45
1:I:106:ALA:HA	1:I:157:ARG:HD3	1.99	0.45
1:K:141:ARG:HG2	1:K:141:ARG:HH11	1.82	0.45
1:N:52:ASP:HB2	1:N:84:VAL:HG21	1.99	0.45
1:T:36:ILE:HB	1:T:69:GLY:HA3	1.98	0.45
3:c:672:LYS:O	3:c:676:VAL:HG23	2.16	0.45
3:d:505:MET:HB2	3:d:549:GLU:O	2.17	0.45
3:a:300:TYR:CD2	3:f:138:ARG:HB3	2.52	0.45
3:e:107:ILE:N	3:e:107:ILE:HD12	2.32	0.45
3:e:565:LEU:HD13	3:e:628:ARG:NH1	2.32	0.45
3:e:571:THR:HG22	3:e:577:THR:OG1	2.17	0.45
3:e:625:PHE:O	3:e:628:ARG:HG2	2.17	0.45
3:e:667:VAL:HG23	3:e:672:LYS:NZ	2.31	0.45
3:f:324:ARG:HB2	3:f:329:LYS:HE2	1.99	0.45
3:f:412:GLU:HA	3:f:419:VAL:HG23	1.97	0.45
3:f:424:GLU:HB2	3:f:428:THR:CG2	2.47	0.45
3:f:687:ARG:N	3:f:687:ARG:HD3	2.32	0.45
1:A:23:ARG:HE	1:A:26:LYS:HD3	1.82	0.44
1:B:132:GLN:HB3	1:I:124:GLN:OE1	2.17	0.44
1:C:4:ILE:HD11	1:C:21:TYR:HE1	1.78	0.44
1:C:29:ILE:HG21	3:e:602:PHE:HE1	1.83	0.44
1:C:98:SER:HB3	1:C:123:HIS:CE1	2.51	0.44
1:G:169:THR:O	1:G:169:THR:CG2	2.65	0.44
1:K:75:LEU:HD22	1:K:99:MET:HE1	1.99	0.44
1:L:160:GLN:HB3	1:L:164:VAL:CG1	2.47	0.44
1:N:40:VAL:O	1:N:44:VAL:HG23	2.16	0.44
1:S:91:ILE:N	1:S:91:ILE:HD12	2.32	0.44
3:b:193:ARG:HH12	3:c:231:ASP:H	1.65	0.44
3:b:462:LEU:HB3	3:c:698:GLU:OE1	2.17	0.44
3:b:471:SER:HB2	3:b:565:LEU:HD22	1.98	0.44
3:b:642:ASN:O	3:b:646:ILE:HG13	2.18	0.44
3:c:171:GLN:HA	3:c:174:LEU:CD2	2.47	0.44
3:c:179:ILE:HG12	3:c:213:VAL:HG23	2.00	0.44
3:c:444:GLN:HG3	3:c:635:PHE:HD2	1.82	0.44
3:a:152:GLY:HA2	4:f:801:ATP:C8	2.51	0.44
3:e:220:VAL:HG11	3:e:253:GLY:HA3	2.00	0.44
3:e:405:LYS:HA	3:e:405:LYS:CE	2.47	0.44
3:e:537:VAL:HG11	3:e:580:PHE:CE2	2.52	0.44
3:f:147:GLY:HA3	3:f:278:VAL:HG13	1.99	0.44
1:A:169:THR:O	1:A:169:THR:CG2	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:ILE:HG22	1:B:9:GLU:N	2.33	0.44
1:B:91:ILE:HD12	1:B:91:ILE:N	2.32	0.44
1:C:16:ARG:HH22	1:D:16:ARG:HH12	1.65	0.44
1:E:105:THR:HG22	1:E:185:LEU:HD22	1.98	0.44
1:E:162:ILE:HA	1:E:165:ILE:HG22	1.98	0.44
1:F:160:GLN:HB3	1:F:164:VAL:HG11	1.99	0.44
1:K:29:ILE:HG23	1:K:63:TYR:CE2	2.52	0.44
1:K:29:ILE:HG23	1:K:63:TYR:HE2	1.82	0.44
1:S:158:THR:CG2	1:S:185:LEU:HD23	2.47	0.44
3:b:120:PRO:HD3	3:b:296:ARG:CD	2.47	0.44
3:b:198:GLU:HG2	3:b:202:LYS:NZ	2.30	0.44
3:c:239:ILE:O	3:c:242:PRO:HD2	2.17	0.44
3:c:539:ARG:HD3	3:c:539:ARG:HA	1.75	0.44
3:a:668:PRO:HG2	3:a:671:VAL:CG2	2.41	0.44
3:e:281:PRO:HG3	3:e:327:PRO:HG3	1.98	0.44
3:e:294:GLN:HE21	3:e:305:TYR:HB2	1.83	0.44
3:f:458:ASN:HD21	3:f:469:ILE:CD1	2.30	0.44
1:C:117:ASN:HB2	1:D:79:ASP:OD2	2.16	0.44
1:C:141:ARG:HB2	1:C:141:ARG:NH1	2.32	0.44
1:C:169:THR:HG22	1:C:169:THR:O	2.16	0.44
1:F:81:MET:HE1	1:F:106:ALA:CB	2.45	0.44
1:F:89:GLN:NE2	1:F:111:LYS:HD2	2.33	0.44
1:F:161:PRO:HD2	1:F:164:VAL:CG1	2.47	0.44
1:F:188:GLU:N	1:F:188:GLU:OE2	2.50	0.44
1:G:36:ILE:O	1:G:36:ILE:HG13	2.16	0.44
1:G:175:MET:HE2	1:G:175:MET:HB3	1.83	0.44
3:b:157:VAL:HG11	3:b:216:PHE:CG	2.53	0.44
3:b:281:PRO:CD	3:b:327:PRO:HG3	2.47	0.44
3:d:129:LYS:CA	3:d:132:ILE:HG12	2.43	0.44
3:d:203:LEU:HA	3:d:206:GLU:OE2	2.17	0.44
3:d:241:LYS:HD2	3:e:184:VAL:CG2	2.45	0.44
3:d:404:GLU:O	3:d:408:GLU:OE1	2.36	0.44
3:a:132:ILE:CD1	3:a:173:LEU:HD11	2.42	0.44
3:e:474:PHE:HB3	3:e:482:LYS:HZ2	1.82	0.44
3:e:649:LEU:O	3:e:653:GLU:OE2	2.36	0.44
3:f:117:ASP:C	3:f:117:ASP:OD2	2.61	0.44
3:f:129:LYS:O	3:f:133:GLU:HG3	2.18	0.44
3:f:186:LEU:CB	3:f:200:MET:HE1	2.48	0.44
3:f:248:GLU:OE1	3:f:248:GLU:HA	2.18	0.44
1:E:4:ILE:HG23	1:E:20:ILE:CG2	2.47	0.44
1:I:108:GLN:H	1:I:108:GLN:CD	2.19	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:140:ALA:HA	1:I:143:ILE:HG22	1.98	0.44
1:L:191:GLU:HG3	1:M:83:PHE:HD1	1.83	0.44
1:T:23:ARG:NH1	1:T:26:LYS:HD2	2.32	0.44
3:b:240:LEU:HD22	3:b:249:LEU:HD11	1.98	0.44
3:b:300:TYR:HD2	3:b:301:HIS:CD2	2.35	0.44
3:d:505:MET:HG3	3:d:550:VAL:HA	2.00	0.44
3:d:620:PHE:N	3:d:620:PHE:CD1	2.86	0.44
3:a:217:ILE:CG2	3:a:251:LEU:HD21	2.45	0.44
3:a:241:LYS:HB2	3:a:242:PRO:HD3	2.00	0.44
3:a:469:ILE:CD1	3:a:584:ILE:HG12	2.46	0.44
3:a:474:PHE:HE1	3:a:633:ILE:HD12	1.82	0.44
3:e:105:TYR:CD1	3:e:105:TYR:C	2.95	0.44
3:e:568:GLY:O	3:e:580:PHE:HB2	2.18	0.44
3:e:638:LEU:HB3	3:e:643:LEU:CD2	2.47	0.44
1:A:181:LYS:HD2	1:A:187:ASP:O	2.17	0.44
1:C:16:ARG:HG3	1:C:17:ALA:N	2.33	0.44
1:I:105:THR:CG2	1:I:185:LEU:HD22	2.47	0.44
1:L:24:LEU:HD11	1:M:46:ALA:CB	2.47	0.44
1:L:91:ILE:HG13	1:L:113:PHE:HB2	2.00	0.44
1:L:177:ALA:HB1	1:L:189:VAL:CG2	2.48	0.44
1:S:45:ILE:HD11	1:S:77:ILE:HA	2.00	0.44
1:S:154:LEU:O	1:S:158:THR:HG23	2.16	0.44
1:T:113:PHE:CE2	1:T:188:GLU:HG2	2.53	0.44
3:b:184:VAL:CG1	3:a:234:MET:HE2	2.47	0.44
3:b:193:ARG:O	3:b:197:GLU:HG2	2.17	0.44
3:b:712:HIS:O	3:b:714:LEU:HD23	2.17	0.44
3:c:101:LEU:HD13	3:c:101:LEU:C	2.42	0.44
3:c:160:LEU:O	3:c:164:ILE:HG12	2.17	0.44
3:d:411:VAL:HG11	3:d:419:VAL:HG21	1.99	0.44
3:d:417:ILE:HD12	3:d:417:ILE:N	2.32	0.44
3:a:237:GLY:O	3:a:241:LYS:HG3	2.17	0.44
3:e:316:LEU:HD23	3:e:316:LEU:N	2.32	0.44
3:f:640:LYS:HB3	3:f:640:LYS:HZ3	1.81	0.44
1:A:182:GLU:H	1:A:182:GLU:HG2	1.67	0.44
1:F:143:ILE:HD12	1:F:143:ILE:HA	1.90	0.44
1:I:189:VAL:HG12	1:I:190:MET:N	2.32	0.44
1:K:41:ALA:O	1:K:45:ILE:CD1	2.66	0.44
1:L:45:ILE:HD11	1:L:77:ILE:CA	2.46	0.44
1:L:119:GLU:OE1	1:L:119:GLU:N	2.50	0.44
1:M:169:THR:HG22	1:M:169:THR:O	2.18	0.44
1:N:9:GLU:OE2	1:N:16:GLN:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:108:GLN:OE1	1:N:109:LYS:N	2.51	0.44
1:S:67:PRO:C	1:S:97:ALA:HB3	2.43	0.44
1:S:167:ARG:HB3	1:S:167:ARG:CZ	2.46	0.44
1:T:105:THR:CG2	1:T:185:LEU:HD22	2.47	0.44
3:b:437:LEU:HD21	3:b:492:GLU:HG3	1.98	0.44
3:b:487:LYS:HD3	3:b:497:GLU:OE2	2.18	0.44
3:b:702:ALA:HB1	3:b:705:TYR:HE1	1.82	0.44
3:c:101:LEU:O	3:c:105:TYR:HB2	2.18	0.44
3:d:125:ASP:OD1	3:d:125:ASP:C	2.60	0.44
3:d:134:ILE:HD13	3:d:274:GLN:CG	2.47	0.44
3:e:324:ARG:HH11	3:e:324:ARG:HG3	1.83	0.44
3:e:501:VAL:HG21	3:e:545:ILE:CD1	2.47	0.44
3:f:640:LYS:HA	3:f:640:LYS:HE2	1.99	0.44
1:B:73:ALA:O	1:B:77:ILE:HG13	2.17	0.44
1:C:91:ILE:HA	1:C:113:PHE:O	2.17	0.44
2:H:5:UNK:O	3:a:193:ARG:HB2	2.17	0.44
1:S:24:LEU:HD11	1:T:46:ALA:CB	2.47	0.44
3:c:124:ARG:HA	3:c:127:GLU:OE1	2.17	0.44
3:c:241:LYS:HB2	3:c:241:LYS:HE2	1.74	0.44
3:c:464:LYS:HD3	3:c:467:ARG:CD	2.47	0.44
3:c:490:ALA:HB2	3:c:544:LEU:HD23	2.00	0.44
3:d:108:ASN:HB3	3:d:111:GLU:HG2	1.98	0.44
3:d:216:PHE:HA	3:d:252:VAL:O	2.17	0.44
3:d:249:LEU:HD11	3:d:251:LEU:HB2	1.98	0.44
3:d:444:GLN:HG3	3:d:635:PHE:CD2	2.53	0.44
3:a:193:ARG:NH1	3:a:230:GLY:HA3	2.32	0.44
3:a:198:GLU:H	3:a:198:GLU:CD	2.25	0.44
3:e:261:ARG:HH11	3:e:261:ARG:HG3	1.83	0.44
3:e:440:HIS:CD2	3:e:488:GLN:HE21	2.35	0.44
3:e:476:GLY:HA2	3:e:593:THR:HG21	2.00	0.44
3:e:687:ARG:HB2	3:e:688:PRO:HD3	1.99	0.44
3:f:304:LYS:CD	3:f:304:LYS:H	2.30	0.44
1:A:60:ILE:HB	1:A:88:VAL:HG22	2.00	0.44
1:B:92:VAL:CG1	1:B:114:ALA:HA	2.47	0.44
1:C:5:PRO:HG2	1:D:47:GLN:HE21	1.83	0.44
1:C:137:GLU:CG	1:C:141:ARG:HH22	2.28	0.44
1:E:30:ILE:HG23	1:E:47:GLN:NE2	2.33	0.44
1:K:87:ASP:O	1:K:88:VAL:HG23	2.17	0.44
1:M:115:LEU:HD23	1:N:79:ASP:HB2	1.97	0.44
3:b:184:VAL:HG11	3:a:239:ILE:HG12	2.00	0.44
3:b:516:LYS:HG2	3:a:522:PRO:CD	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:342:ASN:O	3:c:343:LEU:HB2	2.18	0.44
3:c:596:VAL:HG23	3:c:598:ALA:H	1.83	0.44
3:d:407:ILE:O	3:d:411:VAL:HG12	2.18	0.44
3:e:163:LYS:HB3	3:e:163:LYS:HE3	1.62	0.44
3:e:223:ILE:HD11	3:e:263:ILE:CG2	2.48	0.44
3:f:308:GLU:OE1	3:f:404:GLU:HG2	2.18	0.44
3:f:309:ALA:CB	3:f:404:GLU:HA	2.46	0.44
3:f:691:ARG:HD3	3:f:691:ARG:C	2.41	0.44
1:A:25:LEU:HD11	1:A:51:LEU:CD1	2.46	0.44
1:G:20:ILE:O	1:G:24:LEU:HD13	2.18	0.44
1:I:108:GLN:OE1	1:I:108:GLN:N	2.31	0.44
3:b:531:GLY:HA3	3:b:534:THR:OG1	2.18	0.44
3:b:547:LEU:HB2	3:b:587:MET:HG2	2.00	0.44
3:b:687:ARG:HE	4:b:801:ATP:C5'	2.24	0.44
3:c:206:GLU:HA	3:c:209:GLU:HG3	2.00	0.44
3:c:286:THR:O	3:c:290:LEU:HG	2.17	0.44
3:a:505:MET:HG3	3:a:550:VAL:HA	2.00	0.44
3:e:671:VAL:HB	3:e:718:LEU:HB2	1.98	0.44
3:f:510:GLU:HG3	3:f:512:HIS:CD2	2.53	0.44
1:B:20:ILE:O	1:B:24:LEU:HD13	2.18	0.43
1:B:49:LEU:HB3	3:f:603:GLY:H	1.83	0.43
1:G:74:GLY:HA3	1:G:99:MET:CE	2.48	0.43
1:N:54:GLN:HG3	1:N:54:GLN:O	2.17	0.43
1:N:122:ILE:HG12	1:N:173:ASN:HB3	2.00	0.43
1:T:62:LEU:HD23	1:T:63:TYR:N	2.32	0.43
3:c:187:VAL:HG13	3:c:227:GLY:CA	2.45	0.43
3:c:200:MET:HE1	3:c:240:LEU:HD12	1.95	0.43
3:d:129:LYS:O	3:d:132:ILE:HG12	2.17	0.43
3:d:260:TYR:HA	3:d:263:ILE:CD1	2.48	0.43
3:d:408:GLU:HA	3:d:411:VAL:HG12	2.00	0.43
3:a:153:LYS:CB	4:f:801:ATP:PB	3.06	0.43
3:a:641:GLU:OE2	3:a:641:GLU:N	2.51	0.43
3:e:437:LEU:HD23	3:e:492:GLU:CD	2.43	0.43
1:A:18:TYR:OH	1:A:26:LYS:HE3	2.18	0.43
1:A:23:ARG:NH2	1:A:26:LYS:HD3	2.33	0.43
1:E:169:THR:O	1:E:169:THR:CG2	2.65	0.43
1:I:89:GLN:NE2	1:I:111:LYS:HD3	2.34	0.43
1:T:8:ILE:HD13	1:T:17:ALA:HB3	2.00	0.43
3:b:198:GLU:HG2	3:c:189:GLY:HA2	2.00	0.43
3:b:456:ARG:HD2	3:c:706:LEU:HD12	2.00	0.43
3:b:566:ASP:CB	3:b:628:ARG:HH11	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:668:PRO:HG2	3:b:717:ALA:HB1	2.00	0.43
3:c:271:ARG:HH12	3:d:150:GLY:CA	2.31	0.43
3:a:704:TYR:HE2	3:a:711:ASN:HB3	1.83	0.43
3:e:221:HIS:CD2	3:e:259:GLU:HG3	2.53	0.43
3:e:261:ARG:O	3:e:265:LYS:HG2	2.19	0.43
3:e:433:LEU:HD22	3:e:452:ALA:HB2	2.00	0.43
3:f:457:ARG:O	3:f:460:VAL:HG22	2.19	0.43
1:B:137:GLU:HB2	1:I:144:LEU:HD21	2.00	0.43
1:B:175:MET:HE2	1:B:175:MET:HB2	1.77	0.43
1:C:33:SER:HB2	1:D:42:ASN:OD1	2.18	0.43
1:D:20:ILE:HG13	1:E:46:ALA:HB1	2.01	0.43
1:I:5:PRO:HG3	1:K:47:GLN:NE2	2.33	0.43
1:I:89:GLN:HE21	1:I:111:LYS:HD3	1.83	0.43
1:L:90:THR:HG22	1:L:104:LEU:HD12	1.99	0.43
1:M:4:ILE:O	1:M:4:ILE:HG23	2.18	0.43
1:N:176:THR:HG23	1:N:179:GLN:HE21	1.81	0.43
1:S:71:VAL:O	1:S:75:LEU:HD23	2.17	0.43
1:S:95:MET:CE	1:S:119:GLU:HB2	2.48	0.43
3:b:177:GLU:O	3:b:214:ILE:HG12	2.18	0.43
3:c:432:ASN:O	3:c:435:VAL:HG22	2.18	0.43
3:d:138:ARG:CG	3:e:300:TYR:CE1	3.01	0.43
3:d:308:GLU:HG3	3:d:404:GLU:CG	2.46	0.43
3:d:721:GLU:HG2	3:d:723:LYS:HZ2	1.82	0.43
3:e:154:THR:HG22	3:e:158:GLU:OE2	2.18	0.43
3:e:592:GLY:H	3:e:596:VAL:HG23	1.82	0.43
3:e:600:VAL:HG22	3:e:602:PHE:HB2	2.00	0.43
1:D:36:ILE:HD12	1:D:36:ILE:N	2.33	0.43
1:D:36:ILE:HA	1:D:40:VAL:HG11	2.00	0.43
1:E:20:ILE:O	1:E:24:LEU:HD13	2.18	0.43
1:E:35:PRO:HA	1:E:68:GLY:O	2.18	0.43
1:M:147:ARG:HH12	1:M:169:THR:CG2	2.31	0.43
1:N:74:GLY:O	1:N:77:ILE:HG22	2.18	0.43
1:S:121:MET:HE1	1:S:123:HIS:CE1	2.53	0.43
1:T:190:MET:O	1:T:191:GLU:HB2	2.19	0.43
3:b:211:GLU:HG3	3:b:212:ASN:OD1	2.18	0.43
3:b:663:LEU:HD11	3:b:705:TYR:CD2	2.53	0.43
3:c:102:LEU:HD23	3:c:102:LEU:C	2.42	0.43
3:d:108:ASN:OD1	3:d:111:GLU:HG3	2.18	0.43
3:d:460:VAL:HB	3:d:462:LEU:HD13	2.00	0.43
3:d:503:PHE:CE2	3:d:533:LEU:HD13	2.53	0.43
3:d:514:VAL:O	3:d:518:ILE:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:646:ILE:HG22	3:d:650:MET:HE3	2.01	0.43
3:d:698:GLU:HG2	3:d:698:GLU:H	1.60	0.43
3:e:108:ASN:CG	3:e:111:GLU:HG3	2.44	0.43
3:e:309:ALA:CA	3:e:404:GLU:HG2	2.49	0.43
3:f:134:ILE:HD12	3:f:276:VAL:CG2	2.48	0.43
1:C:4:ILE:HD11	1:C:21:TYR:CD1	2.53	0.43
1:E:154:LEU:CD2	1:E:165:ILE:HD11	2.43	0.43
1:F:30:ILE:HD12	1:F:48:LEU:HD23	2.00	0.43
1:F:163:GLU:O	1:F:167:ARG:HG3	2.18	0.43
1:I:31:MET:HB3	1:I:31:MET:HE3	1.74	0.43
1:T:105:THR:HG21	1:T:185:LEU:HD22	2.00	0.43
3:b:532:GLN:O	3:b:536:LYS:HG3	2.18	0.43
3:d:105:TYR:CD2	3:d:105:TYR:C	2.96	0.43
3:d:632:ILE:HD12	3:d:632:ILE:N	2.33	0.43
3:e:505:MET:HG3	3:e:550:VAL:HA	1.99	0.43
3:e:704:TYR:CD2	3:e:714:LEU:HD13	2.54	0.43
3:f:544:LEU:HG	3:f:584:ILE:HB	2.00	0.43
1:C:154:LEU:HB3	1:C:165:ILE:HD13	2.01	0.43
1:D:12:SER:HB3	1:D:13:ARG:HE	1.82	0.43
1:G:8:ILE:HD13	1:G:16:ARG:CG	2.48	0.43
1:I:75:LEU:CD2	1:I:99:MET:HE1	2.46	0.43
1:I:108:GLN:HA	1:I:109:LYS:HZ2	1.84	0.43
1:K:36:ILE:N	1:K:36:ILE:HD12	2.34	0.43
1:L:63:TYR:HD1	1:L:91:ILE:HB	1.84	0.43
1:L:161:PRO:HD2	1:L:164:VAL:CG1	2.47	0.43
3:b:650:MET:HE1	3:b:686:ALA:O	2.18	0.43
3:c:614:LEU:HD22	3:c:614:LEU:H	1.84	0.43
3:d:169:VAL:O	3:d:169:VAL:HG13	2.19	0.43
3:d:217:ILE:CG2	3:d:251:LEU:HD11	2.47	0.43
3:d:674:LYS:O	3:d:678:LEU:HB2	2.19	0.43
3:a:647:VAL:HG23	3:a:689:LEU:HD11	1.94	0.43
3:f:497:GLU:HG2	3:f:497:GLU:O	2.19	0.43
3:f:697:ILE:CG2	3:f:701:ILE:HD11	2.48	0.43
1:A:10:GLN:HB3	3:f:620:PHE:CE2	2.50	0.43
1:A:13:ARG:H	1:A:13:ARG:HD3	1.83	0.43
1:D:31:MET:HE2	1:D:31:MET:HB2	1.82	0.43
1:D:175:MET:HE1	1:D:185:LEU:CD1	2.48	0.43
1:F:93:LEU:CD1	1:G:45:ILE:HD13	2.47	0.43
1:G:62:LEU:HD22	1:G:64:ILE:HD11	2.01	0.43
1:I:160:GLN:HB3	1:I:164:VAL:CG1	2.45	0.43
1:K:122:ILE:HG13	1:K:173:ASN:OD1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:158:THR:HG22	1:L:160:GLN:OE1	2.18	0.43
1:M:16:ARG:HE	1:M:16:ARG:HB2	1.62	0.43
1:N:64:ILE:HD12	1:N:64:ILE:N	2.33	0.43
1:S:71:VAL:HG12	1:S:75:LEU:CD2	2.48	0.43
3:b:408:GLU:OE1	3:b:420:GLY:HA3	2.19	0.43
3:b:476:GLY:C	3:b:593:THR:HG21	2.44	0.43
3:b:698:GLU:OE1	3:b:698:GLU:N	2.41	0.43
3:d:462:LEU:HD23	3:e:698:GLU:CB	2.48	0.43
3:a:473:LEU:HD12	3:a:587:MET:O	2.18	0.43
3:e:140:LYS:HA	3:e:272:ARG:O	2.18	0.43
3:e:617:LEU:H	3:e:617:LEU:HD22	1.83	0.43
3:e:674:LYS:HE3	3:e:722:GLY:O	2.19	0.43
3:f:596:VAL:CG1	3:f:616:GLN:HG3	2.49	0.43
1:D:30:ILE:HD12	1:D:48:LEU:HD23	2.01	0.43
1:K:71:VAL:HG12	1:K:75:LEU:HD23	2.00	0.43
1:M:89:GLN:HG2	1:M:111:LYS:HD3	2.00	0.43
1:N:161:PRO:CG	1:N:164:VAL:HG12	2.45	0.43
3:c:306:THR:O	3:c:309:ALA:HB3	2.19	0.43
3:c:564:ILE:HD11	3:c:570:LEU:HD22	2.00	0.43
3:d:546:LEU:C	3:d:547:LEU:HD12	2.43	0.43
3:a:207:ILE:HD13	3:a:215:LEU:HD22	2.00	0.43
3:a:306:THR:HB	3:a:308:GLU:OE1	2.18	0.43
3:a:700:GLY:C	3:a:726:VAL:HG21	2.44	0.43
3:e:554:HIS:HD2	3:e:555:PRO:CD	2.32	0.43
3:e:613:VAL:O	3:e:617:LEU:HD22	2.19	0.43
3:e:666:GLU:OE1	3:e:666:GLU:C	2.62	0.43
3:f:115:GLN:N	3:f:115:GLN:OE1	2.52	0.43
3:f:154:THR:HG23	4:f:802:ATP:O2B	2.19	0.43
3:f:671:VAL:CG2	3:f:724:ILE:CD1	2.97	0.43
1:D:28:ARG:NH1	1:D:55:ASP:HB3	2.34	0.43
1:D:112:ARG:NH1	1:D:157:ARG:HG3	2.34	0.43
1:D:121:MET:HG3	1:D:174:TYR:CE1	2.54	0.43
1:D:137:GLU:HB2	1:S:144:LEU:HD21	2.00	0.43
1:F:141:ARG:HG2	1:F:141:ARG:HH11	1.83	0.43
1:G:158:THR:HG22	1:G:160:GLN:CG	2.49	0.43
1:I:36:ILE:HD12	1:I:36:ILE:N	2.34	0.43
1:I:95:MET:HB2	1:K:72:SER:OG	2.19	0.43
1:S:137:GLU:HG2	1:S:141:ARG:HH22	1.84	0.43
3:b:264:GLU:HG2	3:b:270:GLU:HG3	2.01	0.43
3:d:234:MET:SD	3:d:235:ASP:N	2.92	0.43
3:a:173:LEU:HD23	3:a:173:LEU:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:e:129:LYS:O	3:e:133:GLU:HG3	2.19	0.43
3:e:620:PHE:CD2	3:e:620:PHE:N	2.87	0.43
3:e:654:VAL:O	3:e:658:LEU:CD2	2.67	0.43
3:e:684:MET:SD	3:e:684:MET:N	2.92	0.43
3:f:111:GLU:OE1	3:f:111:GLU:C	2.61	0.43
3:f:124:ARG:HD2	3:f:156:VAL:CG1	2.49	0.43
1:B:30:ILE:HG23	1:B:47:GLN:NE2	2.34	0.43
1:D:161:PRO:HG2	1:D:164:VAL:HG12	2.00	0.43
1:E:143:ILE:HD12	1:E:143:ILE:HA	1.81	0.43
1:E:190:MET:HE3	3:c:602:PHE:CD1	2.54	0.43
1:I:35:PRO:HA	1:I:68:GLY:O	2.18	0.43
1:K:190:MET:HE2	1:L:83:PHE:HZ	1.83	0.43
1:M:8:ILE:HD12	1:M:8:ILE:C	2.44	0.43
1:M:105:THR:HG22	1:M:185:LEU:CB	2.49	0.43
1:T:40:VAL:O	1:T:44:VAL:HG23	2.19	0.43
1:T:141:ARG:CG	1:T:141:ARG:NH1	2.81	0.43
3:b:422:LEU:HD12	3:b:422:LEU:N	2.34	0.43
3:c:215:LEU:CD1	3:c:217:ILE:HG13	2.48	0.43
3:c:460:VAL:O	3:c:460:VAL:HG12	2.19	0.43
3:d:211:GLU:O	3:d:211:GLU:CG	2.66	0.43
3:a:146:ILE:HA	3:a:255:THR:O	2.19	0.43
3:e:405:LYS:O	3:e:405:LYS:HD3	2.19	0.43
3:e:466:ASN:HA	3:e:581:LYS:HZ3	1.80	0.43
3:e:518:ILE:HG21	3:e:560:MET:HE2	2.00	0.43
3:f:309:ALA:HB2	3:f:404:GLU:CA	2.47	0.43
1:A:143:ILE:HD12	1:A:143:ILE:HA	1.92	0.42
1:C:175:MET:HE2	1:C:175:MET:HB2	1.83	0.42
1:G:92:VAL:HG23	1:G:104:LEU:CD1	2.31	0.42
1:I:10:GLN:CD	1:I:10:GLN:H	2.26	0.42
1:K:161:PRO:HD2	1:K:164:VAL:CG1	2.48	0.42
1:M:143:ILE:O	1:M:146:THR:HG22	2.19	0.42
1:N:105:THR:O	1:N:157:ARG:HG2	2.19	0.42
3:b:189:GLY:HA2	3:a:194:GLY:O	2.19	0.42
3:c:206:GLU:HA	3:c:209:GLU:CG	2.49	0.42
3:c:571:THR:HG22	3:c:577:THR:CB	2.47	0.42
3:e:107:ILE:HB	3:e:180:ARG:HB3	2.01	0.42
3:e:142:ASN:O	3:e:273:MET:CB	2.66	0.42
3:e:459:ARG:HB3	3:e:459:ARG:CZ	2.49	0.42
3:e:528:ASP:OD1	3:e:529:GLU:OE1	2.37	0.42
3:f:248:GLU:OE1	3:f:248:GLU:CA	2.66	0.42
3:f:320:TYR:N	3:f:320:TYR:CD1	2.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:f:696:GLN:C	3:f:697:ILE:HD12	2.44	0.42
1:G:161:PRO:O	1:G:164:VAL:HG12	2.19	0.42
1:T:52:ASP:HB2	1:T:84:VAL:CG2	2.49	0.42
3:b:172:LYS:C	3:b:173:LEU:HG	2.44	0.42
3:b:624:GLU:O	3:b:628:ARG:HG3	2.19	0.42
3:c:216:PHE:HA	3:c:252:VAL:HG13	2.00	0.42
3:c:437:LEU:HD21	3:c:492:GLU:HG3	2.01	0.42
3:c:532:GLN:O	3:c:536:LYS:HG3	2.19	0.42
3:d:105:TYR:OH	3:d:186:LEU:HD21	2.19	0.42
3:d:201:GLN:HA	3:d:204:ILE:HG22	2.01	0.42
3:d:217:ILE:HG23	3:d:217:ILE:O	2.19	0.42
3:d:239:ILE:C	3:d:239:ILE:CD1	2.92	0.42
3:d:462:LEU:HD22	3:e:698:GLU:HB3	1.96	0.42
3:a:140:LYS:HE2	3:a:274:GLN:NE2	2.34	0.42
3:a:447:ALA:HB2	3:a:633:ILE:HG21	2.01	0.42
3:e:444:GLN:HG3	3:e:636:LYS:HZ3	1.84	0.42
3:e:561:PHE:HA	3:e:564:ILE:HG22	2.01	0.42
3:f:222:GLU:O	3:f:226:ALA:HB2	2.19	0.42
1:A:33:SER:HB2	1:B:42:ASN:OD1	2.18	0.42
1:C:92:VAL:HG21	1:C:96:ALA:HB2	2.00	0.42
1:C:123:HIS:C	1:C:169:THR:HG23	2.44	0.42
1:D:11:SER:O	1:D:12:SER:HB3	2.19	0.42
1:G:136:ILE:HD11	1:L:127:GLY:O	2.19	0.42
1:G:163:GLU:O	1:G:167:ARG:HG3	2.18	0.42
1:I:20:ILE:HD11	1:K:46:ALA:C	2.43	0.42
1:I:60:ILE:O	1:I:88:VAL:HA	2.18	0.42
1:K:81:MET:HE1	1:K:106:ALA:CB	2.50	0.42
1:L:132:GLN:O	1:L:136:ILE:HG13	2.18	0.42
3:c:272:ARG:HG3	3:c:272:ARG:NH1	2.32	0.42
3:c:505:MET:HB2	3:c:549:GLU:O	2.19	0.42
3:d:180:ARG:HG2	3:d:180:ARG:HH11	1.85	0.42
3:d:569:ARG:NH1	3:d:569:ARG:CB	2.82	0.42
3:a:469:ILE:CG1	3:a:584:ILE:HG12	2.50	0.42
3:e:432:ASN:HB2	3:e:435:VAL:CG1	2.49	0.42
3:e:704:TYR:HB2	3:e:726:VAL:HG23	2.01	0.42
1:A:134:THR:O	1:A:138:ILE:HG13	2.19	0.42
1:D:67:PRO:CA	1:D:95:MET:HE3	2.48	0.42
1:F:161:PRO:O	1:F:164:VAL:HG12	2.19	0.42
1:L:91:ILE:HD12	1:L:91:ILE:N	2.34	0.42
1:L:108:GLN:O	1:L:111:LYS:HB2	2.19	0.42
1:M:124:GLN:HB3	1:M:147:ARG:HH11	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:28:ARG:HA	1:N:51:LEU:HD21	2.02	0.42
3:b:203:LEU:HD12	3:b:203:LEU:HA	1.81	0.42
3:c:289:ILE:HG23	4:c:802:ATP:C2	2.54	0.42
3:d:121:VAL:HG13	4:d:801:ATP:C6	2.54	0.42
3:d:447:ALA:O	3:d:451:VAL:HG23	2.18	0.42
3:d:711:ASN:C	3:d:711:ASN:OD1	2.63	0.42
3:a:179:ILE:N	3:a:179:ILE:HD12	2.34	0.42
3:a:423:LYS:H	3:a:423:LYS:HG2	1.71	0.42
3:e:101:LEU:CD1	3:e:202:LYS:NZ	2.83	0.42
3:e:308:GLU:OE1	3:e:308:GLU:N	2.48	0.42
3:f:317:SER:HB2	3:f:329:LYS:CD	2.46	0.42
1:B:115:LEU:HD13	1:C:79:ASP:CB	2.44	0.42
1:C:30:ILE:HB	1:C:62:LEU:CD1	2.49	0.42
1:D:20:ILE:HD12	1:D:20:ILE:HA	1.82	0.42
1:F:146:THR:O	1:F:150:LEU:HG	2.19	0.42
1:G:101:SER:CB	1:G:120:ILE:HD11	2.50	0.42
1:I:81:MET:HE2	1:I:81:MET:HB2	1.81	0.42
1:L:186:ILE:HD12	1:L:186:ILE:HA	1.83	0.42
1:M:92:VAL:HG13	1:M:114:ALA:HA	2.02	0.42
1:S:77:ILE:O	1:S:81:MET:HG3	2.19	0.42
3:b:477:PRO:HG2	3:b:480:VAL:HG13	2.01	0.42
3:c:505:MET:HE3	3:c:553:ALA:HB2	2.01	0.42
3:d:105:TYR:OH	3:d:186:LEU:HD11	2.20	0.42
3:d:456:ARG:O	3:d:460:VAL:HG23	2.19	0.42
3:a:251:LEU:HD23	3:a:252:VAL:N	2.34	0.42
3:a:296:ARG:H	3:a:296:ARG:HG2	1.67	0.42
3:a:304:LYS:CD	3:a:304:LYS:N	2.76	0.42
3:e:118:ILE:H	3:e:118:ILE:HG13	1.64	0.42
3:e:178:VAL:HG22	3:e:214:ILE:HB	2.00	0.42
3:f:186:LEU:O	3:f:199:ARG:HD3	2.20	0.42
3:f:234:MET:HE2	3:f:239:ILE:CD1	2.49	0.42
3:f:465:GLN:O	3:f:581:LYS:HG3	2.19	0.42
1:A:92:VAL:HG12	1:A:114:ALA:CB	2.49	0.42
1:G:173:ASN:OD1	1:G:173:ASN:O	2.38	0.42
1:I:109:LYS:HA	1:I:109:LYS:HD3	1.91	0.42
1:L:190:MET:O	1:L:191:GLU:HB2	2.18	0.42
1:M:27:ASP:C	1:M:28:ARG:HG3	2.45	0.42
1:M:92:VAL:CG1	1:M:114:ALA:HA	2.49	0.42
1:N:6:THR:HA	1:N:19:ASP:HA	2.02	0.42
1:N:165:ILE:O	1:N:169:THR:HG23	2.19	0.42
3:b:221:HIS:ND1	3:b:255:THR:CG2	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:233:ASN:O	3:b:233:ASN:OD1	2.37	0.42
3:c:523:GLY:H	3:d:525:VAL:HG13	1.84	0.42
3:d:516:LYS:O	3:d:532:GLN:HG3	2.19	0.42
3:e:241:LYS:HE2	3:e:241:LYS:HA	2.01	0.42
3:f:327:PRO:O	3:f:331:ILE:HG12	2.20	0.42
3:f:454:ALA:O	3:f:457:ARG:HB3	2.20	0.42
3:f:505:MET:HB2	3:f:549:GLU:O	2.19	0.42
3:f:719:ASP:OD2	3:f:721:GLU:HB2	2.19	0.42
1:A:151:ASN:HD22	1:A:165:ILE:HG22	1.85	0.42
1:B:12:SER:OG	1:B:13:ARG:HD3	2.20	0.42
1:B:83:PHE:HE2	3:f:602:PHE:CE1	2.25	0.42
1:C:127:GLY:O	1:T:136:ILE:HD11	2.20	0.42
1:M:91:ILE:HD12	1:M:113:PHE:HB2	2.00	0.42
3:b:633:ILE:HD12	3:b:633:ILE:N	2.34	0.42
3:d:135:LEU:HD23	3:d:143:PRO:CD	2.50	0.42
3:d:197:GLU:HG2	3:d:198:GLU:N	2.35	0.42
3:d:539:ARG:HD2	3:d:539:ARG:HA	1.93	0.42
3:a:217:ILE:HG23	3:a:217:ILE:O	2.19	0.42
3:e:323:ASP:C	3:e:324:ARG:HD3	2.44	0.42
3:e:668:PRO:HD2	3:e:671:VAL:HG11	2.02	0.42
1:E:91:ILE:HA	1:E:113:PHE:O	2.20	0.42
1:F:13:ARG:O	1:F:13:ARG:NH1	2.34	0.42
1:G:96:ALA:HB3	1:G:120:ILE:CD1	2.49	0.42
1:G:182:GLU:HG2	1:G:182:GLU:H	1.67	0.42
1:N:122:ILE:CG2	1:N:175:MET:HE1	2.49	0.42
1:N:141:ARG:HH11	1:N:141:ARG:CG	2.33	0.42
1:S:176:THR:OG1	1:S:179:GLN:HG3	2.19	0.42
1:T:90:THR:HG22	1:T:104:LEU:CD1	2.43	0.42
3:b:328:ASP:OD2	3:a:271:ARG:HD2	2.19	0.42
3:c:702:ALA:O	3:c:706:LEU:HG	2.20	0.42
3:d:483:THR:HB	4:d:802:ATP:PA	2.59	0.42
3:e:126:GLN:O	3:e:130:ARG:HG2	2.19	0.42
3:e:177:GLU:OE2	3:e:177:GLU:C	2.62	0.42
3:e:290:LEU:HD23	3:e:293:LEU:HD11	2.01	0.42
3:e:295:LYS:HZ3	3:e:296:ARG:HD3	1.85	0.42
3:e:590:ASN:HB2	3:e:593:THR:HG23	2.02	0.42
3:e:690:ARG:HH11	3:e:690:ARG:CA	2.33	0.42
3:f:295:LYS:HD2	3:f:295:LYS:O	2.19	0.42
3:f:641:GLU:O	3:f:644:MET:HB2	2.19	0.42
1:A:62:LEU:HG	1:A:64:ILE:HD11	2.02	0.42
1:A:141:ARG:HG2	1:A:141:ARG:HH11	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:SER:OG	1:B:120:ILE:HG23	2.19	0.42
1:C:89:GLN:HB2	1:C:111:LYS:O	2.20	0.42
1:E:93:LEU:HG	1:E:93:LEU:O	2.19	0.42
1:F:125:PRO:HG3	1:F:150:LEU:CD1	2.48	0.42
1:F:181:LYS:HB3	1:F:181:LYS:HE2	1.75	0.42
1:K:25:LEU:HD11	1:K:51:LEU:CD2	2.45	0.42
1:L:4:ILE:HG23	1:L:4:ILE:O	2.19	0.42
1:L:120:ILE:HD12	1:L:120:ILE:N	2.35	0.42
1:M:120:ILE:HD12	1:M:120:ILE:N	2.35	0.42
1:S:18:TYR:OH	1:S:26:LYS:HE3	2.20	0.42
1:T:120:ILE:HG21	1:T:185:LEU:HD13	2.01	0.42
3:b:494:PHE:CE2	3:b:544:LEU:HB2	2.55	0.42
3:b:569:ARG:NH1	3:c:502:ARG:HD3	2.34	0.42
3:c:662:LYS:HB2	3:c:662:LYS:NZ	2.34	0.42
3:c:673:GLU:O	3:c:677:ASP:OD2	2.38	0.42
3:c:694:GLN:HA	3:c:698:GLU:HG3	1.98	0.42
3:d:234:MET:HE3	3:d:235:ASP:CB	2.48	0.42
3:a:124:ARG:HA	3:a:127:GLU:OE1	2.20	0.42
3:a:641:GLU:H	3:a:641:GLU:CD	2.28	0.42
3:e:160:LEU:C	3:e:160:LEU:HD13	2.44	0.42
3:e:260:TYR:CD2	3:e:263:ILE:HD11	2.55	0.42
1:A:20:ILE:O	1:A:24:LEU:HG	2.19	0.42
1:C:8:ILE:HG22	1:C:9:GLU:N	2.34	0.42
1:C:18:TYR:O	1:C:23:ARG:N	2.53	0.42
1:C:102:PHE:CZ	1:C:153:ILE:HG21	2.55	0.42
1:F:167:ARG:CB	1:F:167:ARG:HH11	2.33	0.42
1:S:33:SER:HB2	1:T:42:ASN:ND2	2.35	0.42
3:b:204:ILE:HA	3:b:207:ILE:CG2	2.50	0.42
3:c:546:LEU:O	3:c:547:LEU:HD23	2.20	0.42
3:d:562:LEU:HD23	3:d:562:LEU:HA	1.78	0.42
3:d:662:LYS:HE2	3:d:662:LYS:HA	2.01	0.42
3:d:721:GLU:H	3:d:721:GLU:CD	2.25	0.42
3:a:241:LYS:HD2	3:a:272:ARG:NH1	2.35	0.42
3:a:562:LEU:HD22	3:a:628:ARG:HD2	2.02	0.42
3:e:534:THR:HG22	3:e:570:LEU:HD23	2.01	0.42
3:e:653:GLU:OE2	3:e:653:GLU:N	2.38	0.42
3:f:104:GLU:O	3:f:105:TYR:HD1	2.03	0.42
3:f:224:VAL:HA	3:f:235:ASP:OD2	2.19	0.42
3:f:281:PRO:HD2	3:f:327:PRO:CG	2.50	0.42
3:f:569:ARG:HB2	3:f:569:ARG:NH1	2.35	0.42
1:B:98:SER:HB3	1:B:123:HIS:HE1	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:PHE:CZ	1:B:153:ILE:HG21	2.55	0.41
1:B:181:LYS:HZ2	1:B:188:GLU:HA	1.84	0.41
1:C:10:GLN:HB2	1:C:16:ARG:H	1.85	0.41
1:G:158:THR:CG2	1:G:160:GLN:HG3	2.49	0.41
1:I:6:THR:HG22	1:I:16:ARG:CB	2.50	0.41
1:I:93:LEU:HD23	1:I:93:LEU:N	2.32	0.41
1:K:51:LEU:HB3	1:K:60:ILE:CD1	2.50	0.41
1:K:71:VAL:O	1:K:75:LEU:HD23	2.20	0.41
1:K:93:LEU:HB3	1:K:115:LEU:CD2	2.50	0.41
1:K:157:ARG:HG2	1:K:157:ARG:H	1.62	0.41
1:M:57:GLU:OE2	1:M:57:GLU:CA	2.63	0.41
1:S:141:ARG:NH1	1:S:141:ARG:CG	2.83	0.41
3:b:108:ASN:HD21	3:b:177:GLU:HB3	1.84	0.41
3:b:130:ARG:HD3	3:c:413:GLN:CD	2.45	0.41
3:b:203:LEU:O	3:b:207:ILE:HG22	2.19	0.41
3:b:211:GLU:HG3	3:b:212:ASN:N	2.35	0.41
3:c:248:GLU:OE2	3:c:248:GLU:N	2.53	0.41
3:d:223:ILE:HD12	3:d:224:VAL:HG23	2.02	0.41
3:d:339:SER:O	3:d:343:LEU:HG	2.19	0.41
3:e:170:PRO:CG	3:e:173:LEU:HD13	2.10	0.41
3:e:505:MET:HB2	3:e:549:GLU:O	2.20	0.41
3:e:638:LEU:HB3	3:e:643:LEU:HD23	2.02	0.41
3:f:146:ILE:HG21	3:f:257:LEU:CD1	2.49	0.41
3:f:290:LEU:HD22	3:f:331:ILE:HD13	2.03	0.41
3:f:458:ASN:ND2	3:f:469:ILE:HD13	2.35	0.41
1:C:181:LYS:HA	1:C:186:ILE:HD12	2.01	0.41
1:M:75:LEU:HD22	1:M:99:MET:CE	2.49	0.41
1:M:181:LYS:HA	1:M:186:ILE:CG2	2.49	0.41
1:N:23:ARG:O	1:N:26:LYS:HG2	2.19	0.41
1:T:28:ARG:NH1	1:T:55:ASP:HB3	2.35	0.41
3:b:240:LEU:CD2	3:b:249:LEU:HD11	2.50	0.41
3:b:241:LYS:HB2	3:b:242:PRO:HD3	2.02	0.41
3:c:204:ILE:HA	3:c:207:ILE:CG2	2.49	0.41
3:c:636:LYS:HE2	3:c:636:LYS:HB2	1.91	0.41
3:a:153:LYS:CB	4:f:801:ATP:O2B	2.68	0.41
3:a:660:LYS:H	3:a:660:LYS:HG2	1.61	0.41
3:e:201:GLN:HA	3:e:239:ILE:HG21	2.01	0.41
3:e:646:ILE:HA	3:e:649:LEU:CD1	2.50	0.41
3:f:234:MET:HA	3:f:234:MET:CE	2.46	0.41
3:f:562:LEU:HD21	3:f:625:PHE:HD1	1.84	0.41
1:A:121:MET:HG2	1:A:122:ILE:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:ILE:HD12	1:B:120:ILE:N	2.35	0.41
1:C:7:VAL:C	1:C:18:TYR:HA	2.45	0.41
1:D:13:ARG:HB3	1:D:15:GLU:OE2	2.20	0.41
1:D:168:ASP:OD2	1:D:183:TYR:HE2	2.03	0.41
1:I:26:LYS:NZ	1:I:26:LYS:HB3	2.35	0.41
1:N:109:LYS:HB3	1:N:109:LYS:HZ3	1.85	0.41
1:S:65:ASN:HB2	1:S:93:LEU:O	2.20	0.41
1:S:105:THR:CG2	1:S:185:LEU:HD22	2.51	0.41
1:S:167:ARG:HH11	1:S:167:ARG:HB2	1.85	0.41
3:b:503:PHE:HE2	3:b:533:LEU:HD13	1.83	0.41
3:c:412:GLU:HG3	3:c:417:ILE:O	2.20	0.41
3:c:597:GLU:HG3	3:c:597:GLU:O	2.21	0.41
3:a:121:VAL:HG21	3:a:159:GLY:CA	2.50	0.41
3:a:134:ILE:HD12	3:a:276:VAL:CG2	2.50	0.41
3:a:503:PHE:CE2	3:a:533:LEU:HD13	2.54	0.41
3:e:556:ASP:OD2	3:e:557:VAL:N	2.53	0.41
3:f:278:VAL:HG13	3:f:278:VAL:O	2.20	0.41
1:A:13:ARG:HG2	1:A:14:GLY:N	2.35	0.41
1:D:53:ALA:HA	3:e:601:GLY:H	1.86	0.41
1:F:175:MET:HE2	1:F:175:MET:HB3	1.74	0.41
1:G:4:ILE:HG23	1:G:20:ILE:CG2	2.47	0.41
1:I:20:ILE:HD11	1:K:47:GLN:HA	2.01	0.41
1:K:117:ASN:HB2	1:L:149:ARG:CZ	2.51	0.41
1:L:119:GLU:C	1:L:120:ILE:HD12	2.45	0.41
1:L:122:ILE:CG1	1:L:169:THR:HG22	2.50	0.41
1:L:175:MET:HE2	1:L:175:MET:HB3	1.73	0.41
1:L:181:LYS:CA	1:L:186:ILE:HG22	2.50	0.41
1:N:7:VAL:O	1:N:18:TYR:HB2	2.21	0.41
1:S:123:HIS:NE2	1:S:126:LEU:HD21	2.34	0.41
3:b:183:VAL:HG21	3:b:222:GLU:HB2	2.03	0.41
3:c:613:VAL:HG22	3:c:634:GLU:HG3	1.99	0.41
3:e:128:ILE:CG2	3:e:163:LYS:HE2	2.45	0.41
3:e:521:PRO:HB2	3:e:524:TYR:HE2	1.81	0.41
3:f:161:ALA:HA	3:f:164:ILE:HG22	2.01	0.41
3:f:251:LEU:HD23	3:f:251:LEU:C	2.45	0.41
3:f:301:HIS:O	3:f:303:VAL:HG23	2.20	0.41
1:C:75:LEU:HD13	1:C:75:LEU:HA	1.90	0.41
1:K:5:PRO:HG2	1:L:47:GLN:NE2	2.34	0.41
1:L:71:VAL:HG11	1:L:146:THR:CG2	2.51	0.41
1:L:81:MET:HE2	1:L:81:MET:HB2	1.81	0.41
3:b:108:ASN:O	3:b:111:GLU:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:132:ILE:HD11	3:b:160:LEU:CD1	2.51	0.41
3:b:246:ARG:HG3	3:b:246:ARG:HH11	1.85	0.41
3:b:459:ARG:HD2	3:b:459:ARG:HA	1.52	0.41
3:c:484:GLU:HB2	4:c:801:ATP:PA	2.53	0.41
3:e:137:ARG:HB2	3:e:141:ASN:HB3	2.02	0.41
3:e:257:LEU:HG	3:e:258:ASN:OD1	2.20	0.41
3:e:485:LEU:HD23	3:e:635:PHE:CZ	2.56	0.41
3:f:224:VAL:HG13	3:f:224:VAL:O	2.20	0.41
3:f:534:THR:HG22	3:f:578:VAL:HG11	2.01	0.41
1:C:161:PRO:O	1:C:164:VAL:HG12	2.21	0.41
1:D:30:ILE:O	1:D:62:LEU:HD12	2.20	0.41
1:E:26:LYS:HB2	1:E:26:LYS:NZ	2.35	0.41
1:F:57:GLU:OE1	1:F:57:GLU:CA	2.69	0.41
1:M:24:LEU:HD12	1:M:29:ILE:HD12	2.02	0.41
3:b:214:ILE:O	3:b:250:GLN:O	2.39	0.41
3:b:405:LYS:HA	3:b:405:LYS:HD3	1.74	0.41
3:b:685:GLY:C	3:b:687:ARG:H	2.29	0.41
3:c:122:VAL:CG1	3:c:288:THR:HG22	2.40	0.41
3:c:447:ALA:HB2	3:c:633:ILE:CG2	2.50	0.41
3:d:145:LEU:HD12	3:d:145:LEU:N	2.36	0.41
3:d:290:LEU:HD11	3:d:330:ALA:HB1	2.01	0.41
3:d:296:ARG:HB2	3:d:296:ARG:CZ	2.51	0.41
3:a:591:ALA:HB1	3:a:620:PHE:CD2	2.55	0.41
3:e:295:LYS:H	3:e:295:LYS:HG3	1.71	0.41
3:e:647:VAL:HG22	3:e:689:LEU:HD13	2.02	0.41
3:f:465:GLN:HG2	3:f:466:ASN:N	2.36	0.41
3:f:725:ILE:HD12	3:f:726:VAL:N	2.35	0.41
1:A:4:ILE:HD12	1:A:21:TYR:CE2	2.56	0.41
1:A:16:ARG:HG3	1:A:18:TYR:CZ	2.55	0.41
1:B:9:GLU:HA	1:B:14:GLY:HA2	2.02	0.41
1:B:92:VAL:HB	1:B:104:LEU:HD13	2.02	0.41
1:C:36:ILE:HD12	1:C:36:ILE:N	2.36	0.41
1:C:125:PRO:HG3	1:C:150:LEU:HD12	2.01	0.41
1:D:61:TYR:CD1	1:D:61:TYR:N	2.88	0.41
1:G:144:LEU:HD11	1:L:137:GLU:HB2	2.02	0.41
1:K:160:GLN:HB3	1:K:164:VAL:HG11	2.01	0.41
3:b:455:ILE:CD1	3:b:493:LEU:HD11	2.51	0.41
3:c:110:THR:HG23	3:c:165:VAL:CG2	2.50	0.41
3:d:145:LEU:O	3:d:254:ALA:HA	2.20	0.41
3:d:202:LYS:HA	3:d:205:GLU:HG3	2.03	0.41
3:d:297:TYR:HD2	3:d:297:TYR:HA	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:308:GLU:HG3	3:d:404:GLU:HB2	2.02	0.41
3:a:298:GLU:HG2	3:a:305:TYR:HD2	1.86	0.41
3:a:469:ILE:HD11	3:a:584:ILE:HD11	2.02	0.41
3:e:323:ASP:HA	3:e:539:ARG:NH2	2.31	0.41
3:e:672:LYS:O	3:e:676:VAL:HG23	2.20	0.41
3:f:246:ARG:HH22	4:f:801:ATP:PA	2.44	0.41
3:f:668:PRO:HD2	3:f:671:VAL:HG11	2.02	0.41
3:f:675:LEU:HD11	3:f:697:ILE:HD11	2.02	0.41
1:A:105:THR:HG21	1:A:185:LEU:CD2	2.36	0.41
1:D:190:MET:HE3	1:D:190:MET:HB3	1.78	0.41
1:F:63:TYR:CD2	1:F:93:LEU:HD11	2.56	0.41
1:K:124:GLN:HE21	1:K:124:GLN:H	1.67	0.41
1:T:8:ILE:CD1	1:T:17:ALA:HB3	2.51	0.41
3:b:145:LEU:N	3:b:254:ALA:HB3	2.36	0.41
3:b:621:PHE:CB	3:b:626:LEU:HD11	2.50	0.41
3:c:249:LEU:O	3:c:249:LEU:HG	2.20	0.41
3:d:146:ILE:HG22	3:d:255:THR:CG2	2.49	0.41
3:d:164:ILE:CD1	3:d:169:VAL:HG12	2.51	0.41
3:d:199:ARG:O	3:d:203:LEU:HG	2.21	0.41
3:d:206:GLU:HG2	3:d:206:GLU:H	1.74	0.41
3:d:425:LYS:HB2	3:d:425:LYS:HZ3	1.84	0.41
3:a:297:TYR:CD1	3:f:138:ARG:HD3	2.56	0.41
3:e:433:LEU:O	3:e:437:LEU:HG	2.21	0.41
3:e:684:MET:HE2	3:e:688:PRO:HG3	2.02	0.41
3:f:170:PRO:O	3:f:174:LEU:HD22	2.20	0.41
3:f:221:HIS:CG	3:f:259:GLU:HB3	2.56	0.41
1:A:20:ILE:HD12	1:A:20:ILE:HA	1.89	0.41
1:B:53:ALA:CB	3:f:600:VAL:O	2.67	0.41
1:C:92:VAL:O	1:C:92:VAL:HG13	2.20	0.41
1:D:114:ALA:HB2	1:D:186:ILE:HG21	2.03	0.41
1:E:10:GLN:OE1	1:E:11:SER:CB	2.68	0.41
1:E:141:ARG:HB2	1:E:141:ARG:NH1	2.36	0.41
1:E:152:SER:HA	1:E:162:ILE:CD1	2.51	0.41
1:F:24:LEU:O	1:F:29:ILE:HB	2.21	0.41
1:G:167:ARG:CB	1:G:167:ARG:HH11	2.34	0.41
1:I:141:ARG:HB2	1:I:141:ARG:NH1	2.36	0.41
1:K:75:LEU:HD22	1:K:99:MET:HE2	2.03	0.41
1:L:140:ALA:HA	1:L:143:ILE:HG22	2.02	0.41
1:M:31:MET:HE2	1:M:31:MET:HB3	1.89	0.41
1:N:45:ILE:HD12	1:N:80:THR:OG1	2.21	0.41
3:b:337:SER:OG	3:b:407:ILE:HD13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:567:ASP:CG	3:c:502:ARG:HH22	2.29	0.41
3:c:147:GLY:N	3:c:153:LYS:HD3	2.36	0.41
3:c:181:LEU:HD22	3:c:203:LEU:HD11	2.02	0.41
3:c:650:MET:O	3:c:653:GLU:HG2	2.21	0.41
3:d:204:ILE:HG13	3:d:248:GLU:OE2	2.21	0.41
3:d:260:TYR:HA	3:d:263:ILE:HD11	2.02	0.41
3:d:538:ARG:HB3	3:d:578:VAL:CG1	2.51	0.41
3:d:550:VAL:HG12	3:d:589:SER:HB2	2.02	0.41
3:d:662:LYS:N	3:d:662:LYS:HD2	2.35	0.41
3:a:697:ILE:N	3:a:697:ILE:HD13	2.36	0.41
3:a:706:LEU:HD23	3:a:706:LEU:HA	1.87	0.41
3:e:231:ASP:H	3:f:192:ILE:CG2	2.29	0.41
3:e:469:ILE:HG13	3:e:582:ASP:CA	2.39	0.41
3:e:645:ASN:O	3:e:648:SER:HB2	2.21	0.41
3:e:657:LEU:O	3:e:660:LYS:NZ	2.54	0.41
3:f:134:ILE:HG22	3:f:143:PRO:HG3	2.03	0.41
3:f:200:MET:HE3	3:f:200:MET:HB2	2.00	0.41
3:f:465:GLN:O	3:f:581:LYS:CG	2.69	0.41
3:f:611:LYS:HA	3:f:614:LEU:CD2	2.50	0.41
3:f:665:ILE:CG1	3:f:666:GLU:N	2.84	0.41
3:f:695:GLU:OE2	3:f:696:GLN:HG2	2.21	0.41
1:A:23:ARG:HH21	1:A:26:LYS:CD	2.34	0.41
1:A:33:SER:HB2	1:B:42:ASN:CG	2.46	0.41
1:C:8:ILE:O	1:C:9:GLU:HB3	2.21	0.41
1:D:167:ARG:CB	1:D:167:ARG:HH11	2.34	0.41
1:F:162:ILE:CA	1:F:165:ILE:HG22	2.51	0.41
1:F:171:ARG:HH12	1:G:132:GLN:HE21	1.69	0.41
1:I:79:ASP:HB2	1:T:115:LEU:HD23	2.01	0.41
1:K:28:ARG:CZ	1:K:58:LYS:HB3	2.51	0.41
1:K:85:LYS:HB2	1:K:85:LYS:NZ	2.35	0.41
1:K:163:GLU:HB3	1:K:167:ARG:HH22	1.86	0.41
1:K:182:GLU:H	1:K:182:GLU:HG2	1.66	0.41
1:M:141:ARG:CZ	1:M:141:ARG:CB	2.99	0.41
1:N:77:ILE:O	1:N:81:MET:HG3	2.21	0.41
3:b:547:LEU:HD21	3:b:561:PHE:CZ	2.55	0.41
3:c:109:ILE:HG22	3:c:161:ALA:HB2	2.03	0.41
3:c:134:ILE:HD12	3:c:276:VAL:CG2	2.51	0.41
3:c:290:LEU:HD11	3:c:330:ALA:HB1	2.03	0.41
3:c:454:ALA:CB	3:c:472:PHE:HZ	2.33	0.41
3:c:474:PHE:HE1	3:c:633:ILE:HD12	1.86	0.41
3:c:669:THR:O	3:c:673:GLU:OE2	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:154:THR:HB	4:d:801:ATP:O1B	2.20	0.41
3:d:181:LEU:HD12	3:d:217:ILE:HD13	2.03	0.41
3:d:287:ILE:HD13	3:d:311:ASN:HD22	1.86	0.41
3:d:624:GLU:HG3	3:e:504:ASP:OD2	2.21	0.41
3:d:688:PRO:O	3:d:691:ARG:HG2	2.21	0.41
3:d:721:GLU:CG	3:d:723:LYS:NZ	2.84	0.41
3:a:196:PHE:CE2	3:a:200:MET:HE3	2.56	0.41
3:a:544:LEU:C	3:a:544:LEU:HD23	2.46	0.41
3:e:554:HIS:HD2	3:e:555:PRO:N	2.19	0.41
3:f:207:ILE:HG23	3:f:213:VAL:HG11	2.00	0.41
3:f:474:PHE:CE2	3:f:586:ILE:HG21	2.56	0.41
3:f:611:LYS:CA	3:f:614:LEU:HG	2.49	0.41
1:E:97:ALA:CB	1:E:121:MET:HB3	2.51	0.40
1:F:175:MET:HB2	1:F:179:GLN:HB2	2.02	0.40
1:M:71:VAL:O	1:M:75:LEU:HD23	2.21	0.40
1:N:134:THR:O	1:N:138:ILE:HG13	2.21	0.40
1:N:161:PRO:HD2	1:N:164:VAL:CG1	2.50	0.40
1:T:161:PRO:HG2	1:T:164:VAL:HG12	2.03	0.40
1:T:167:ARG:CB	1:T:167:ARG:HH11	2.33	0.40
3:b:148:GLU:HB3	3:b:325:PHE:CE1	2.55	0.40
3:b:217:ILE:HG23	3:b:220:VAL:CG1	2.48	0.40
3:d:102:LEU:HD12	3:d:103:GLY:N	2.35	0.40
3:d:551:GLU:HG2	3:d:552:LYS:HD2	2.03	0.40
3:a:459:ARG:HH11	3:a:459:ARG:HA	1.85	0.40
3:a:697:ILE:CD1	3:a:724:ILE:HG21	2.52	0.40
3:e:137:ARG:HB3	3:f:335:ASP:OD2	2.21	0.40
3:e:301:HIS:O	3:e:303:VAL:HG23	2.21	0.40
3:e:331:ILE:N	3:e:331:ILE:HD13	2.36	0.40
3:e:569:ARG:HH21	3:e:579:SER:CA	2.27	0.40
3:f:316:LEU:HD12	3:f:407:ILE:HG22	2.02	0.40
3:f:421:ASP:HB2	3:f:423:LYS:HG3	2.03	0.40
3:f:550:VAL:CG1	3:f:587:MET:HB2	2.44	0.40
1:K:97:ALA:HB1	1:K:121:MET:CE	2.40	0.40
1:S:182:GLU:H	1:S:182:GLU:HG3	1.73	0.40
3:b:144:VAL:HG13	3:b:254:ALA:HB2	2.03	0.40
3:b:460:VAL:CG1	3:b:462:LEU:HD13	2.50	0.40
3:c:725:ILE:HD12	3:c:725:ILE:C	2.46	0.40
3:a:611:LYS:HE3	3:a:611:LYS:HB3	1.93	0.40
3:e:135:LEU:HD23	3:e:143:PRO:HD3	2.03	0.40
3:e:139:THR:O	3:e:140:LYS:HB3	2.21	0.40
3:e:511:LYS:HB2	3:e:554:HIS:HE1	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:f:186:LEU:HD22	3:f:186:LEU:N	2.36	0.40
3:f:455:ILE:HD11	3:f:489:LEU:HD11	2.02	0.40
3:f:686:ALA:C	3:f:689:LEU:HD23	2.47	0.40
1:B:52:ASP:OD1	1:B:86:ALA:HB2	2.22	0.40
1:C:169:THR:O	1:C:169:THR:CG2	2.68	0.40
1:C:175:MET:HE1	1:C:185:LEU:CD1	2.51	0.40
1:E:93:LEU:HD23	1:E:93:LEU:N	2.37	0.40
1:E:122:ILE:HG12	1:E:173:ASN:HB3	2.03	0.40
1:F:66:SER:C	1:F:95:MET:HE3	2.46	0.40
1:F:137:GLU:HG3	1:F:141:ARG:NH2	2.35	0.40
1:G:45:ILE:HG13	1:G:46:ALA:N	2.37	0.40
1:K:9:GLU:H	1:K:16:ARG:CB	2.35	0.40
1:N:143:ILE:O	1:N:146:THR:HG22	2.21	0.40
3:b:204:ILE:O	3:b:207:ILE:HG22	2.22	0.40
3:b:537:VAL:HG21	3:b:580:PHE:HE2	1.82	0.40
3:c:438:LYS:HD2	3:c:445:ASP:OD2	2.21	0.40
3:c:534:THR:CG2	3:c:578:VAL:HG21	2.48	0.40
3:d:125:ASP:OD1	3:d:126:GLN:N	2.54	0.40
3:d:241:LYS:HB2	3:d:242:PRO:CD	2.51	0.40
3:a:454:ALA:CB	3:a:472:PHE:HZ	2.35	0.40
3:e:234:MET:CE	3:e:234:MET:CA	2.93	0.40
3:e:453:LYS:HE2	3:e:457:ARG:HE	1.86	0.40
3:e:516:LYS:O	3:e:532:GLN:OE1	2.39	0.40
3:f:466:ASN:HA	3:f:581:LYS:HZ2	1.85	0.40
1:A:13:ARG:HD3	1:A:13:ARG:N	2.37	0.40
1:A:115:LEU:HD23	1:B:79:ASP:HB3	2.03	0.40
1:B:93:LEU:HD23	1:B:93:LEU:N	2.34	0.40
1:C:120:ILE:HD12	1:C:120:ILE:N	2.37	0.40
1:D:45:ILE:HD12	1:D:80:THR:CB	2.50	0.40
1:K:68:GLY:CA	1:K:98:SER:HB3	2.51	0.40
1:K:112:ARG:HB3	1:K:186:ILE:CD1	2.52	0.40
1:K:125:PRO:HG3	1:K:150:LEU:CD1	2.51	0.40
1:S:119:GLU:OE2	1:T:149:ARG:NH2	2.49	0.40
3:b:268:ALA:HB1	3:b:272:ARG:HH12	1.87	0.40
3:c:170:PRO:O	3:c:174:LEU:HD22	2.21	0.40
3:c:210:ALA:O	3:c:211:GLU:HB3	2.21	0.40
3:c:640:LYS:HD3	3:c:676:VAL:HG12	2.03	0.40
3:c:724:ILE:N	3:c:724:ILE:HD12	2.36	0.40
3:d:122:VAL:CG1	3:d:289:ILE:HG12	2.51	0.40
3:d:257:LEU:H	3:d:257:LEU:HD12	1.85	0.40
3:d:462:LEU:HD23	3:e:698:GLU:CG	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:300:TYR:CE2	3:f:138:ARG:HB3	2.56	0.40
3:a:407:ILE:O	3:a:411:VAL:HG23	2.21	0.40
3:a:505:MET:HB2	3:a:549:GLU:O	2.21	0.40
3:a:644:MET:HE2	3:a:644:MET:CA	2.46	0.40
3:a:690:ARG:HD2	3:a:690:ARG:C	2.46	0.40
3:e:110:THR:HG21	3:e:177:GLU:HA	2.03	0.40
3:e:221:HIS:O	3:e:224:VAL:HG22	2.19	0.40
3:e:271:ARG:O	3:e:271:ARG:NH1	2.54	0.40
3:e:431:LYS:HE2	3:e:431:LYS:CA	2.51	0.40
3:e:650:MET:HA	3:e:653:GLU:OE1	2.21	0.40
3:f:293:LEU:HD12	3:f:293:LEU:N	2.36	0.40
3:f:516:LYS:HB3	3:f:516:LYS:NZ	2.36	0.40
1:C:8:ILE:CA	1:C:18:TYR:HA	2.47	0.40
1:F:129:ALA:HB2	1:F:139:ALA:HB3	2.03	0.40
1:G:57:GLU:HA	1:G:57:GLU:OE1	2.21	0.40
1:I:93:LEU:HG	1:I:93:LEU:O	2.21	0.40
1:S:55:ASP:O	1:S:58:LYS:HG2	2.21	0.40
1:S:137:GLU:CG	1:S:141:ARG:HH22	2.35	0.40
1:T:182:GLU:HG2	1:T:182:GLU:H	1.75	0.40
3:b:654:VAL:O	3:b:657:LEU:HG	2.22	0.40
3:c:241:LYS:HB3	3:c:242:PRO:HD3	2.03	0.40
3:c:511:LYS:HD3	3:c:556:ASP:OD2	2.21	0.40
3:d:633:ILE:HG22	3:d:635:PHE:CE1	2.57	0.40
3:a:512:HIS:HB2	3:f:524:TYR:CZ	2.57	0.40
3:a:597:GLU:H	3:a:597:GLU:CD	2.30	0.40
3:e:270:GLU:OE2	3:e:270:GLU:CA	2.67	0.40
3:e:587:MET:HG3	3:e:629:PHE:CZ	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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	187/197 (95%)	180 (96%)	7 (4%)	0	100	100
1	B	187/197 (95%)	181 (97%)	6 (3%)	0	100	100
1	C	187/197 (95%)	174 (93%)	13 (7%)	0	100	100
1	D	187/197 (95%)	180 (96%)	7 (4%)	0	100	100
1	E	187/197 (95%)	179 (96%)	8 (4%)	0	100	100
1	F	187/197 (95%)	176 (94%)	11 (6%)	0	100	100
1	G	187/197 (95%)	180 (96%)	7 (4%)	0	100	100
1	I	181/197 (92%)	173 (96%)	8 (4%)	0	100	100
1	K	179/197 (91%)	174 (97%)	4 (2%)	1 (1%)	21	51
1	L	176/197 (89%)	172 (98%)	4 (2%)	0	100	100
1	M	177/197 (90%)	175 (99%)	2 (1%)	0	100	100
1	N	178/197 (90%)	170 (96%)	8 (4%)	0	100	100
1	S	176/197 (89%)	174 (99%)	2 (1%)	0	100	100
1	T	175/197 (89%)	167 (95%)	8 (5%)	0	100	100
3	a	557/746 (75%)	541 (97%)	16 (3%)	0	100	100
3	b	545/746 (73%)	524 (96%)	21 (4%)	0	100	100
3	c	553/746 (74%)	539 (98%)	13 (2%)	1 (0%)	43	72
3	d	545/746 (73%)	528 (97%)	17 (3%)	0	100	100
3	e	557/746 (75%)	532 (96%)	25 (4%)	0	100	100
3	f	557/746 (75%)	534 (96%)	23 (4%)	0	100	100
All	All	5865/7234 (81%)	5653 (96%)	210 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	87	ASP
3	c	101	LEU

### 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 PDB entries followed by that with respect to all EM entries.

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	154/163 (94%)	151 (98%)	3 (2%)	50	81
1	B	151/163 (93%)	147 (97%)	4 (3%)	40	75
1	C	150/163 (92%)	146 (97%)	4 (3%)	39	74
1	D	153/163 (94%)	150 (98%)	3 (2%)	48	80
1	E	153/163 (94%)	149 (97%)	4 (3%)	40	75
1	F	150/163 (92%)	148 (99%)	2 (1%)	61	86
1	G	150/163 (92%)	149 (99%)	1 (1%)	76	91
1	I	143/163 (88%)	141 (99%)	2 (1%)	59	85
1	K	148/163 (91%)	143 (97%)	5 (3%)	32	68
1	L	145/163 (89%)	143 (99%)	2 (1%)	59	85
1	M	145/163 (89%)	144 (99%)	1 (1%)	76	91
1	N	146/163 (90%)	142 (97%)	4 (3%)	39	74
1	S	143/163 (88%)	141 (99%)	2 (1%)	59	85
1	T	140/163 (86%)	139 (99%)	1 (1%)	76	91
3	a	471/625 (75%)	466 (99%)	5 (1%)	65	87
3	b	466/625 (75%)	461 (99%)	5 (1%)	65	87
3	c	471/625 (75%)	465 (99%)	6 (1%)	61	86
3	d	467/625 (75%)	462 (99%)	5 (1%)	65	87
3	e	471/625 (75%)	466 (99%)	5 (1%)	65	87
3	f	471/625 (75%)	467 (99%)	4 (1%)	73	90
All	All	4888/6032 (81%)	4820 (99%)	68 (1%)	57	85

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	120	ILE
1	A	169	THR
1	B	33	SER
1	B	92	VAL
1	B	143	ILE
1	B	171	ARG
1	C	75	LEU
1	C	87	ASP
1	C	99	MET
1	C	158	THR

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Mol	Chain	Res	Type
1	D	92	VAL
1	D	93	LEU
1	D	130	GLN
1	E	40	VAL
1	E	92	VAL
1	E	130	GLN
1	E	173	ASN
1	F	60	ILE
1	F	182	GLU
1	G	88	VAL
1	I	75	LEU
1	I	147	ARG
1	K	92	VAL
1	K	124	GLN
1	K	181	LYS
1	K	186	ILE
1	K	188	GLU
1	L	32	LEU
1	L	119	GLU
1	M	93	LEU
1	N	20	ILE
1	N	84	VAL
1	N	88	VAL
1	N	147	ARG
1	S	39	ASN
1	S	186	ILE
1	T	119	GLU
3	b	138	ARG
3	b	181	LEU
3	b	259	GLU
3	b	539	ARG
3	b	560	MET
3	c	182	ASP
3	c	234	MET
3	c	240	LEU
3	c	563	GLN
3	c	569	ARG
3	c	653	GLU
3	d	164	ILE
3	d	333	LEU
3	d	422	LEU
3	d	571	THR

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Mol	Chain	Res	Type
3	d	627	ASN
3	a	233	ASN
3	a	279	ASP
3	a	296	ARG
3	a	469	ILE
3	a	478	THR
3	e	263	ILE
3	e	283	VAL
3	e	301	HIS
3	e	577	THR
3	e	658	LEU
3	f	181	LEU
3	f	199	ARG
3	f	233	ASN
3	f	657	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	ASN
1	B	47	GLN
1	B	54	GLN
1	C	47	GLN
1	C	54	GLN
1	C	173	ASN
1	D	65	ASN
1	E	47	GLN
1	G	89	GLN
1	G	124	GLN
1	K	42	ASN
1	K	124	GLN
1	N	124	GLN
1	N	179	GLN
1	S	42	ASN
1	S	124	GLN
1	T	42	ASN
1	T	117	ASN
1	T	151	ASN
1	T	173	ASN
1	T	179	GLN
3	b	233	ASN
3	b	619	ASN

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Mol	Chain	Res	Type
3	b	664	HIS
3	c	413	GLN
3	c	563	GLN
3	c	711	ASN
3	a	136	ASN
3	a	427	GLN
3	a	574	GLN
3	a	645	ASN
3	a	694	GLN
3	a	711	ASN
3	e	221	HIS
3	e	238	ASN
3	e	294	GLN
3	e	315	ASN
3	e	440	HIS
3	e	554	HIS
3	e	711	ASN
3	e	712	HIS
3	f	274	GLN
3	f	342	ASN
3	f	458	ASN
3	f	540	ASN
3	f	554	HIS
3	f	655	ASN
3	f	694	GLN
3	f	720	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.



## 5.6 Ligand geometry

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	ATP	d	803	-	29,33,33	0.28	0	44,52,52	0.53	1 (2%)
4	ATP	f	801	-	29,33,33	0.37	0	44,52,52	0.51	1 (2%)
4	ATP	d	802	-	29,33,33	0.26	0	44,52,52	0.50	1 (2%)
4	ATP	d	801	-	29,33,33	0.29	0	44,52,52	0.52	1 (2%)
4	ATP	a	802	-	29,33,33	0.29	0	44,52,52	0.52	1 (2%)
4	ATP	c	801	-	29,33,33	0.27	0	44,52,52	0.50	0
4	ATP	c	802	-	29,33,33	0.29	0	44,52,52	0.49	1 (2%)
4	ATP	b	801	-	29,33,33	0.28	0	44,52,52	0.48	1 (2%)
4	ATP	a	801	-	29,33,33	0.28	0	44,52,52	0.51	1 (2%)
4	ATP	f	802	-	29,33,33	0.28	0	44,52,52	0.49	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	d	803	-	-	6/22/38/38	0/3/3/3
4	ATP	f	801	-	-	11/22/38/38	0/3/3/3
4	ATP	d	802	-	-	3/22/38/38	0/3/3/3
4	ATP	d	801	-	-	4/22/38/38	0/3/3/3
4	ATP	a	802	-	-	7/22/38/38	0/3/3/3
4	ATP	c	801	-	-	1/22/38/38	0/3/3/3
4	ATP	c	802	-	-	0/22/38/38	0/3/3/3
4	ATP	b	801	-	-	6/22/38/38	0/3/3/3
4	ATP	a	801	-	-	5/22/38/38	0/3/3/3
4	ATP	f	802	-	-	11/22/38/38	0/3/3/3

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	f	802	ATP	PB-O3B-PG	2.11	140.07	132.83
4	f	801	ATP	PB-O3B-PG	2.10	140.05	132.83
4	d	801	ATP	PB-O3B-PG	2.07	139.92	132.83
4	d	803	ATP	PB-O3B-PG	2.07	139.92	132.83
4	a	801	ATP	PB-O3B-PG	2.06	139.90	132.83
4	a	802	ATP	PB-O3B-PG	2.04	139.82	132.83
4	b	801	ATP	PB-O3B-PG	2.03	139.78	132.83
4	d	802	ATP	PB-O3B-PG	2.02	139.77	132.83
4	c	802	ATP	PB-O3B-PG	2.02	139.76	132.83

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	b	801	ATP	PB-O3B-PG-O2G
4	b	801	ATP	PB-O3B-PG-O3G
4	d	801	ATP	O4'-C4'-C5'-O5'
4	d	801	ATP	C3'-C4'-C5'-O5'
4	d	802	ATP	PB-O3B-PG-O2G
4	d	802	ATP	PB-O3A-PA-O5'
4	d	803	ATP	PB-O3B-PG-O2G
4	a	801	ATP	C4'-C5'-O5'-PA
4	a	802	ATP	PB-O3B-PG-O2G
4	a	802	ATP	C5'-O5'-PA-O2A
4	f	801	ATP	PB-O3B-PG-O3G
4	f	802	ATP	O4'-C1'-N9-C8
4	f	802	ATP	O4'-C1'-N9-C4
4	d	803	ATP	O4'-C4'-C5'-O5'
4	f	801	ATP	O4'-C4'-C5'-O5'
4	f	801	ATP	C3'-C4'-C5'-O5'
4	d	801	ATP	PB-O3A-PA-O1A
4	f	802	ATP	PA-O3A-PB-O1B
4	f	802	ATP	C4'-C5'-O5'-PA
4	f	801	ATP	PB-O3A-PA-O5'
4	d	802	ATP	PB-O3B-PG-O1G
4	f	802	ATP	PB-O3B-PG-O1G
4	a	802	ATP	C5'-O5'-PA-O3A
4	d	803	ATP	C3'-C4'-C5'-O5'
4	a	801	ATP	C2'-C1'-N9-C4
4	a	802	ATP	C5'-O5'-PA-O1A

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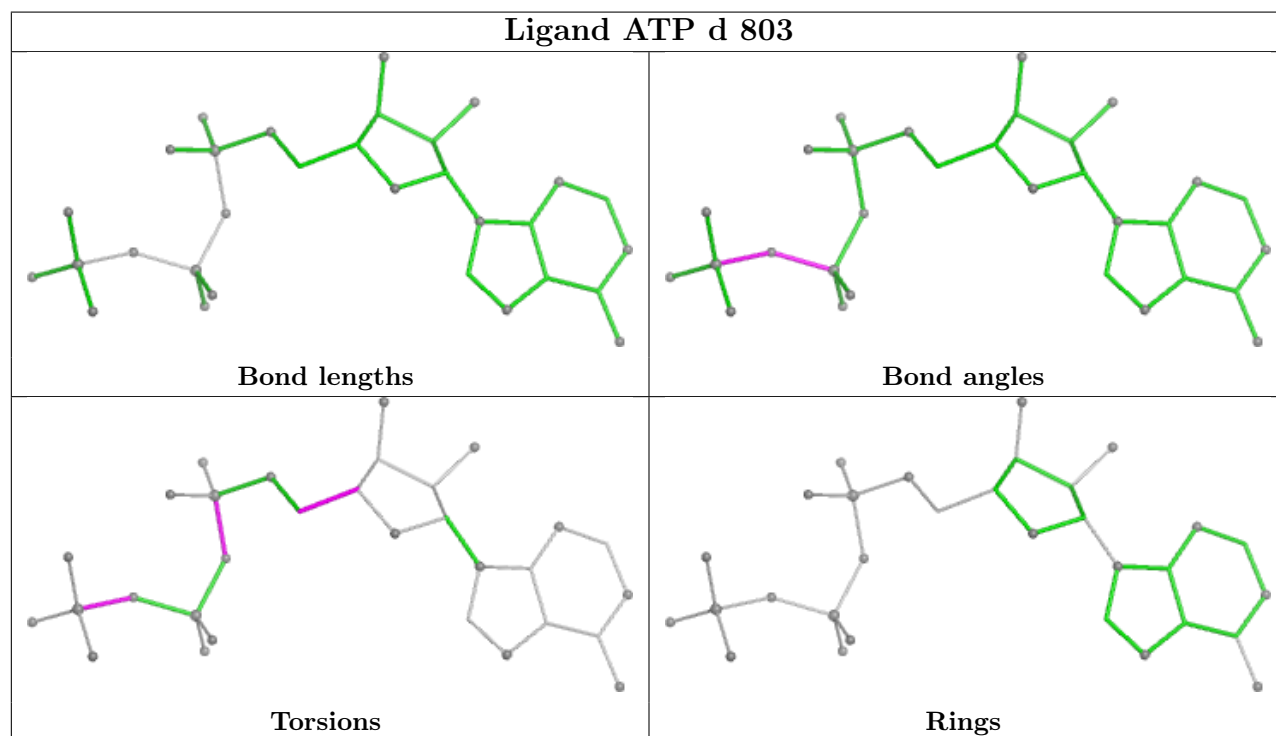
Mol	Chain	Res	Type	Atoms
4	f	801	ATP	C5'-O5'-PA-O1A
4	f	802	ATP	C5'-O5'-PA-O2A
4	a	801	ATP	C2'-C1'-N9-C8
4	a	802	ATP	PG-O3B-PB-O3A
4	c	801	ATP	PG-O3B-PB-O2B
4	a	802	ATP	C4'-C5'-O5'-PA
4	d	803	ATP	PB-O3A-PA-O1A
4	d	803	ATP	PB-O3A-PA-O2A
4	f	801	ATP	PB-O3A-PA-O1A
4	f	802	ATP	PA-O3A-PB-O2B
4	b	801	ATP	O4'-C4'-C5'-O5'
4	f	802	ATP	O4'-C4'-C5'-O5'
4	a	801	ATP	O4'-C4'-C5'-O5'
4	d	803	ATP	PB-O3B-PG-O1G
4	f	801	ATP	PB-O3B-PG-O1G
4	a	801	ATP	C3'-C4'-C5'-O5'
4	f	802	ATP	PB-O3B-PG-O2G
4	f	802	ATP	PB-O3B-PG-O3G
4	f	801	ATP	C5'-O5'-PA-O3A
4	f	802	ATP	C5'-O5'-PA-O3A
4	b	801	ATP	C3'-C4'-C5'-O5'
4	b	801	ATP	PB-O3A-PA-O1A
4	b	801	ATP	PB-O3A-PA-O2A
4	d	801	ATP	PB-O3A-PA-O2A
4	a	802	ATP	PG-O3B-PB-O1B
4	f	801	ATP	PG-O3B-PB-O2B
4	f	801	ATP	PA-O3A-PB-O2B
4	f	801	ATP	C5'-O5'-PA-O2A

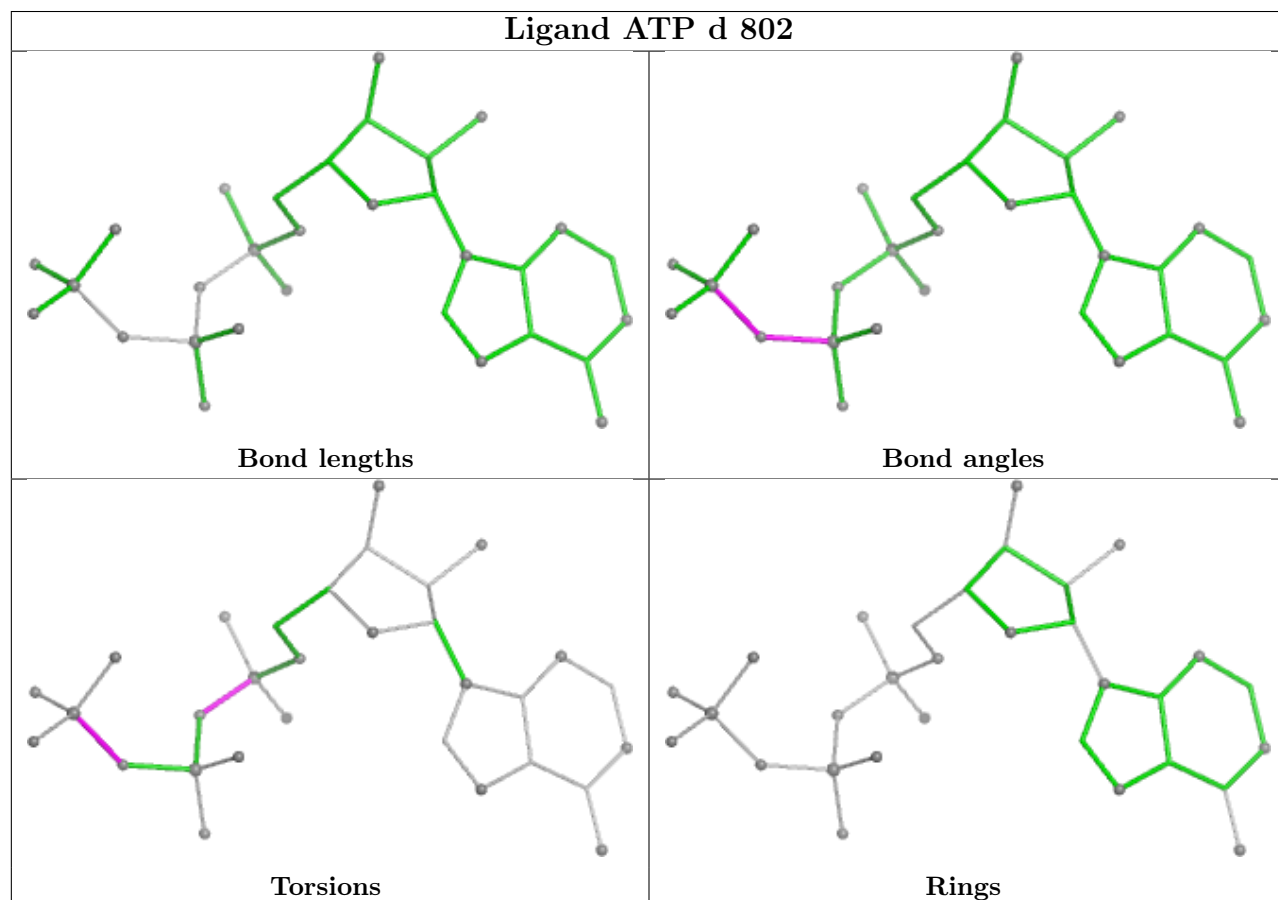
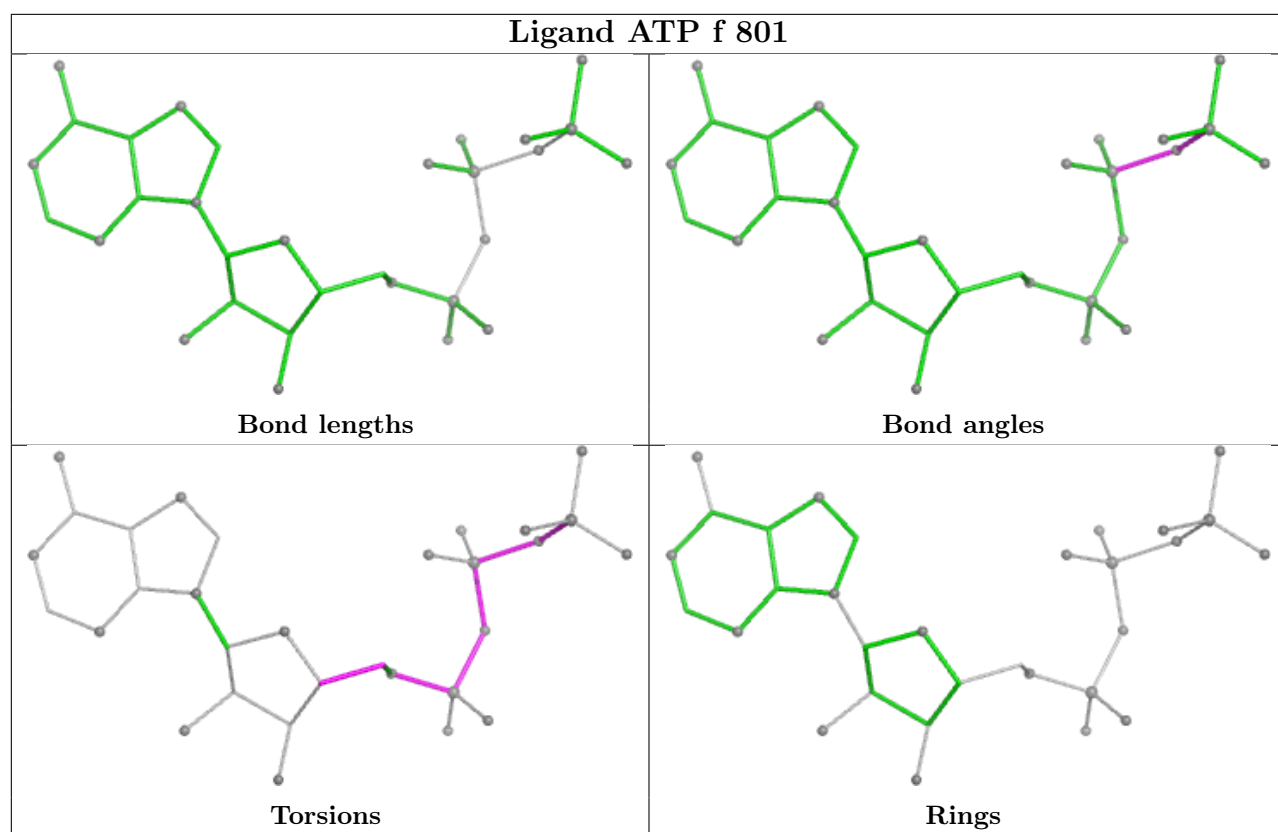
There are no ring outliers.

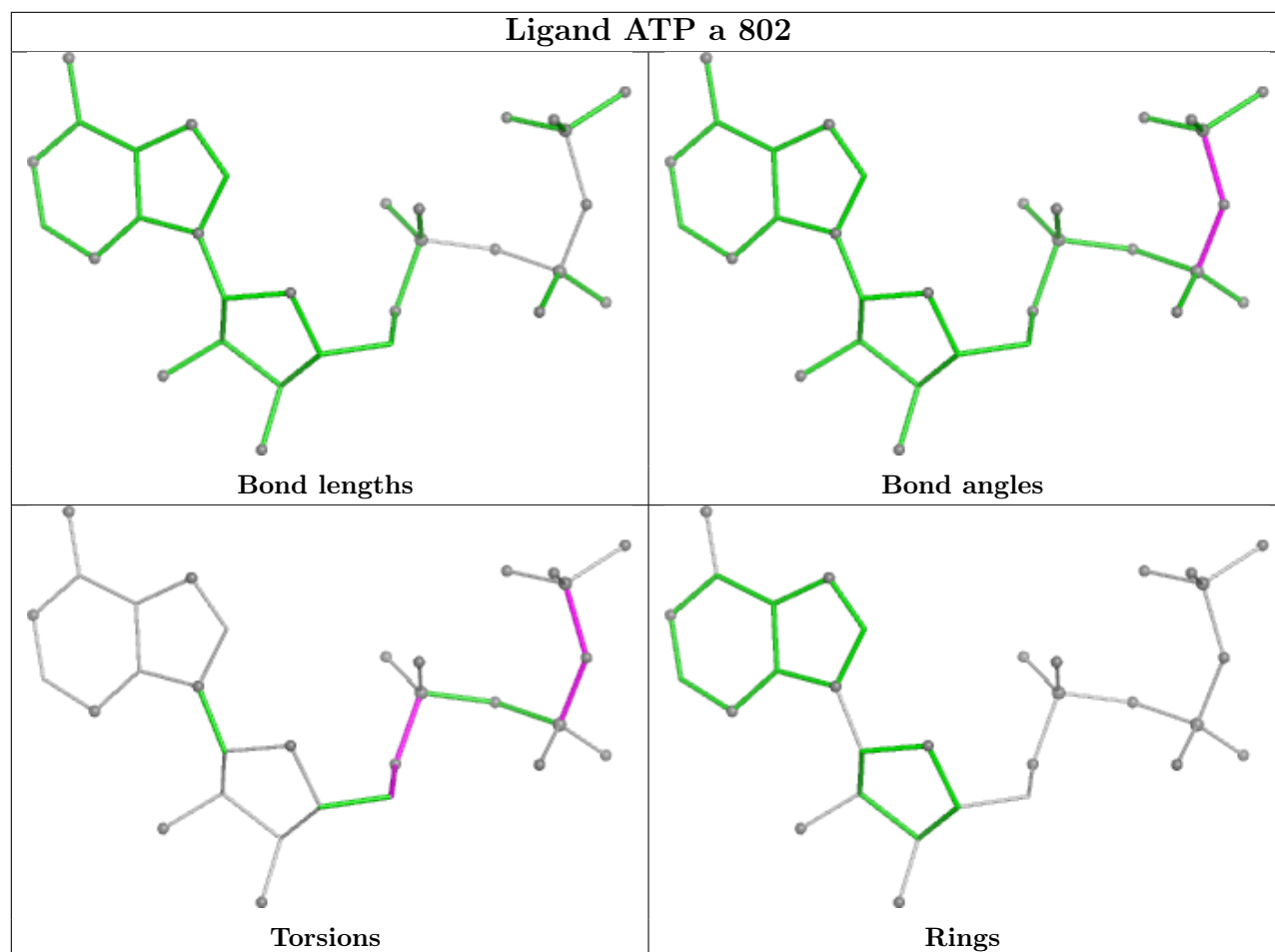
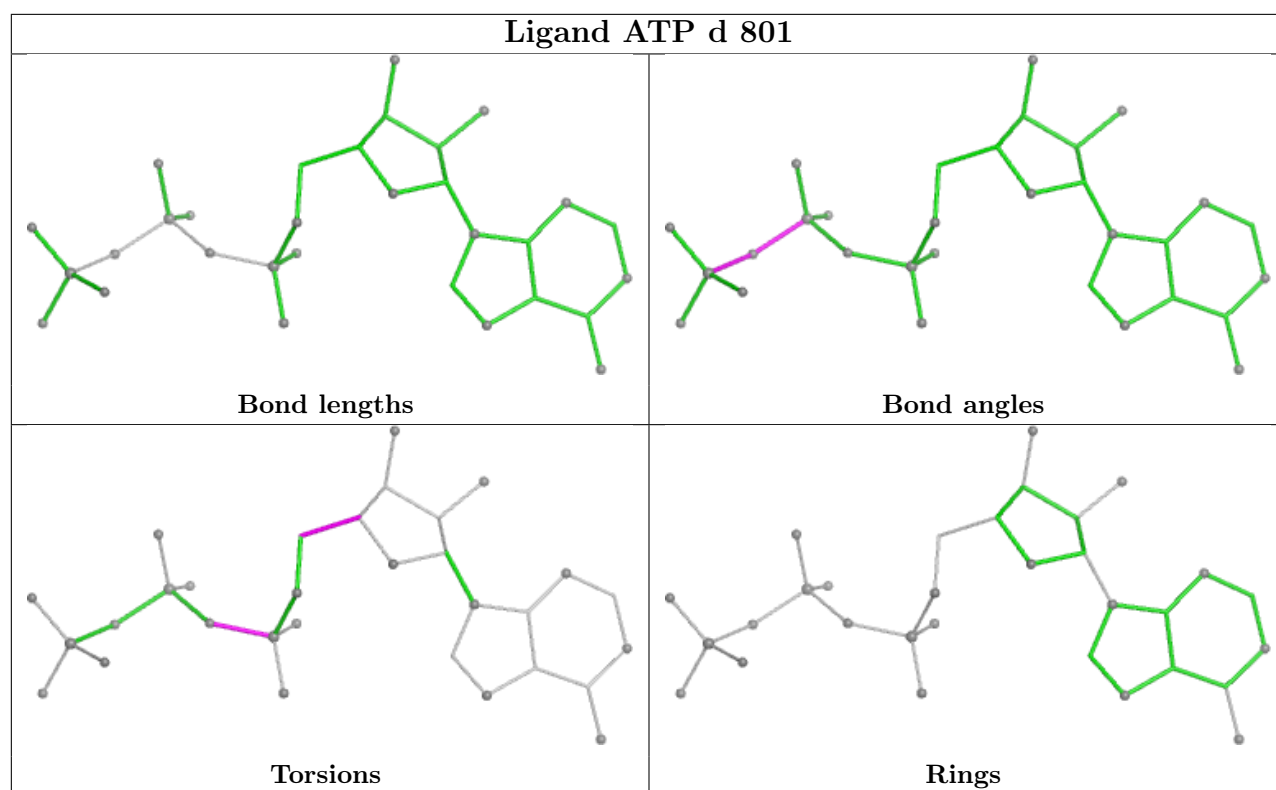
9 monomers are involved in 48 short contacts:

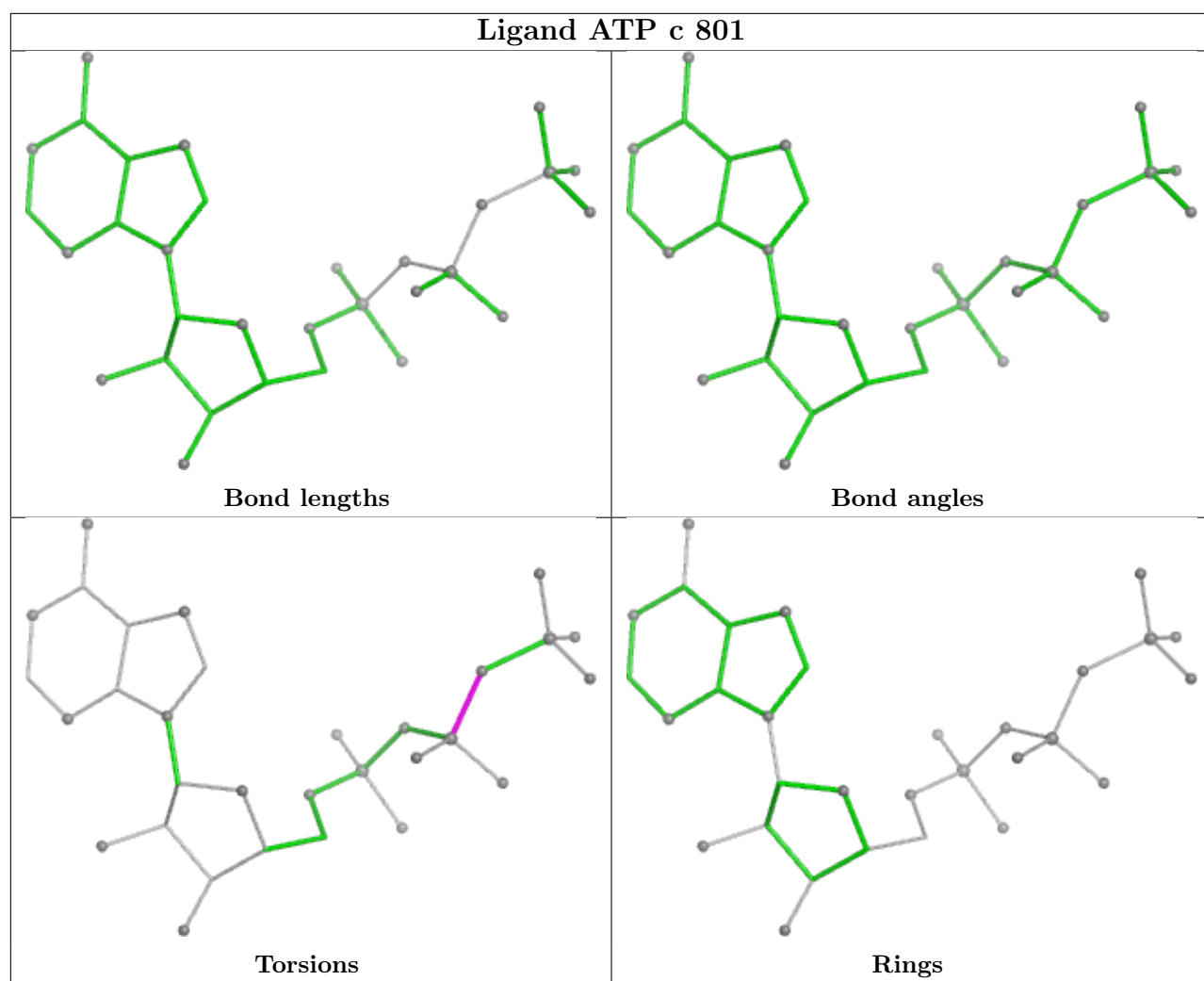
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	d	803	ATP	1	0
4	f	801	ATP	15	0
4	d	802	ATP	5	0
4	d	801	ATP	6	0
4	a	802	ATP	1	0
4	c	801	ATP	4	0
4	c	802	ATP	1	0
4	b	801	ATP	4	0
4	f	802	ATP	11	0

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

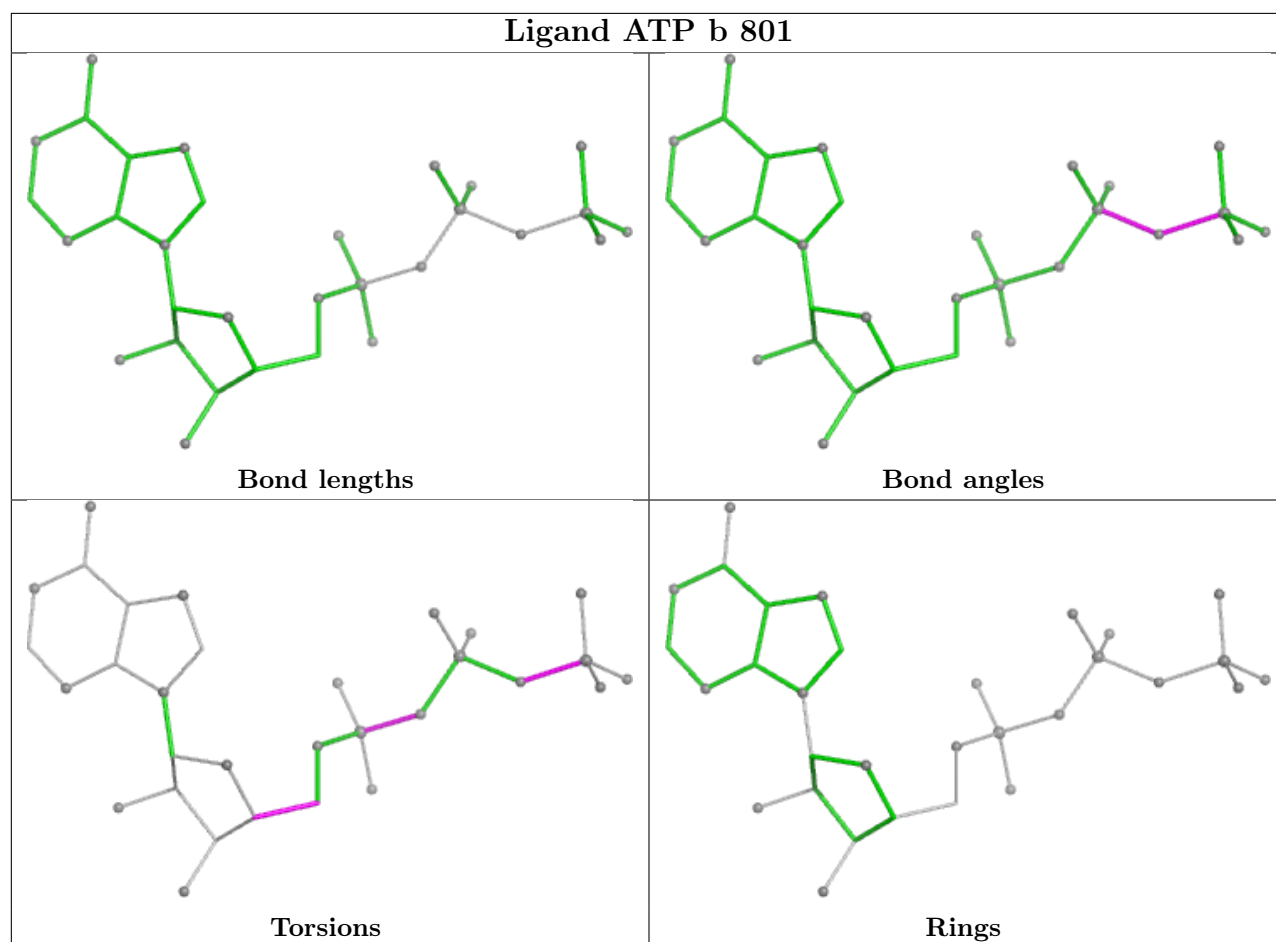
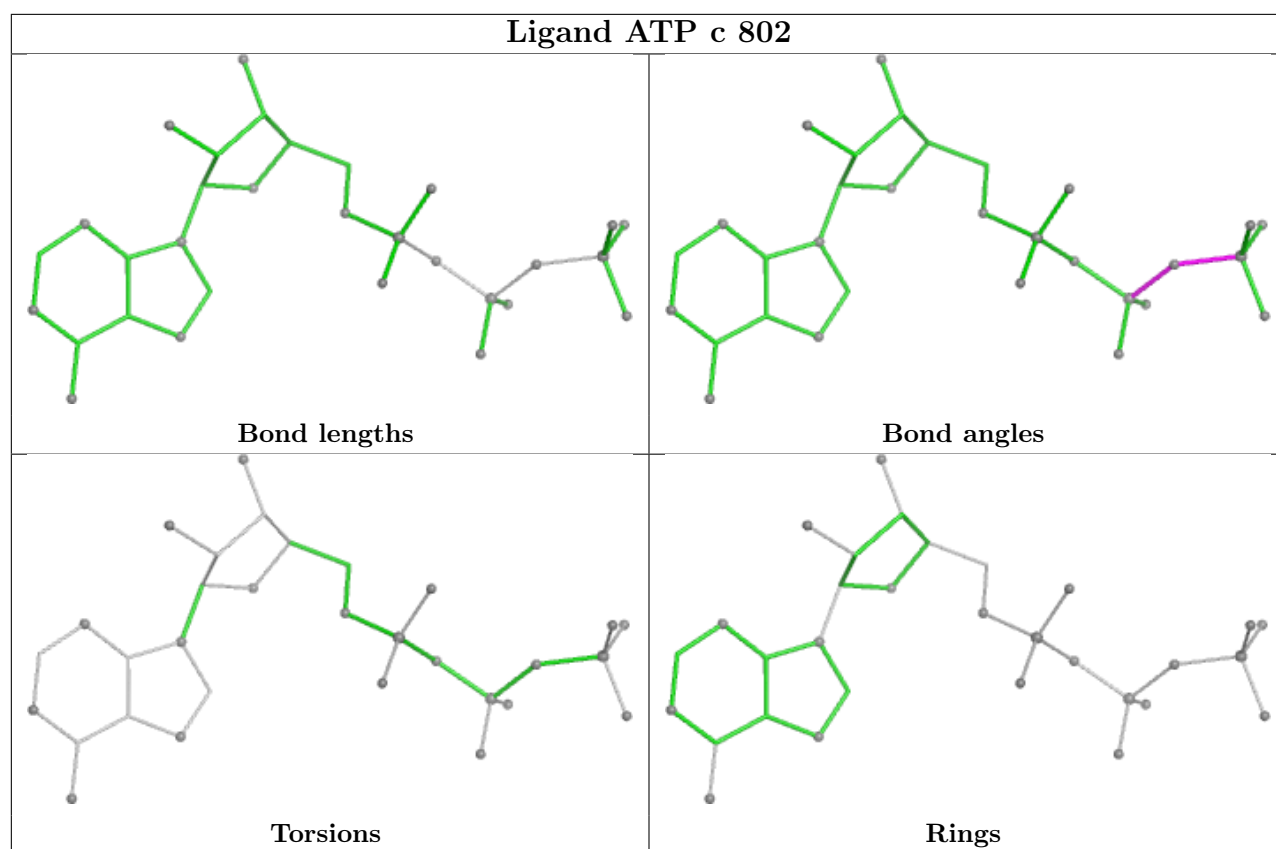


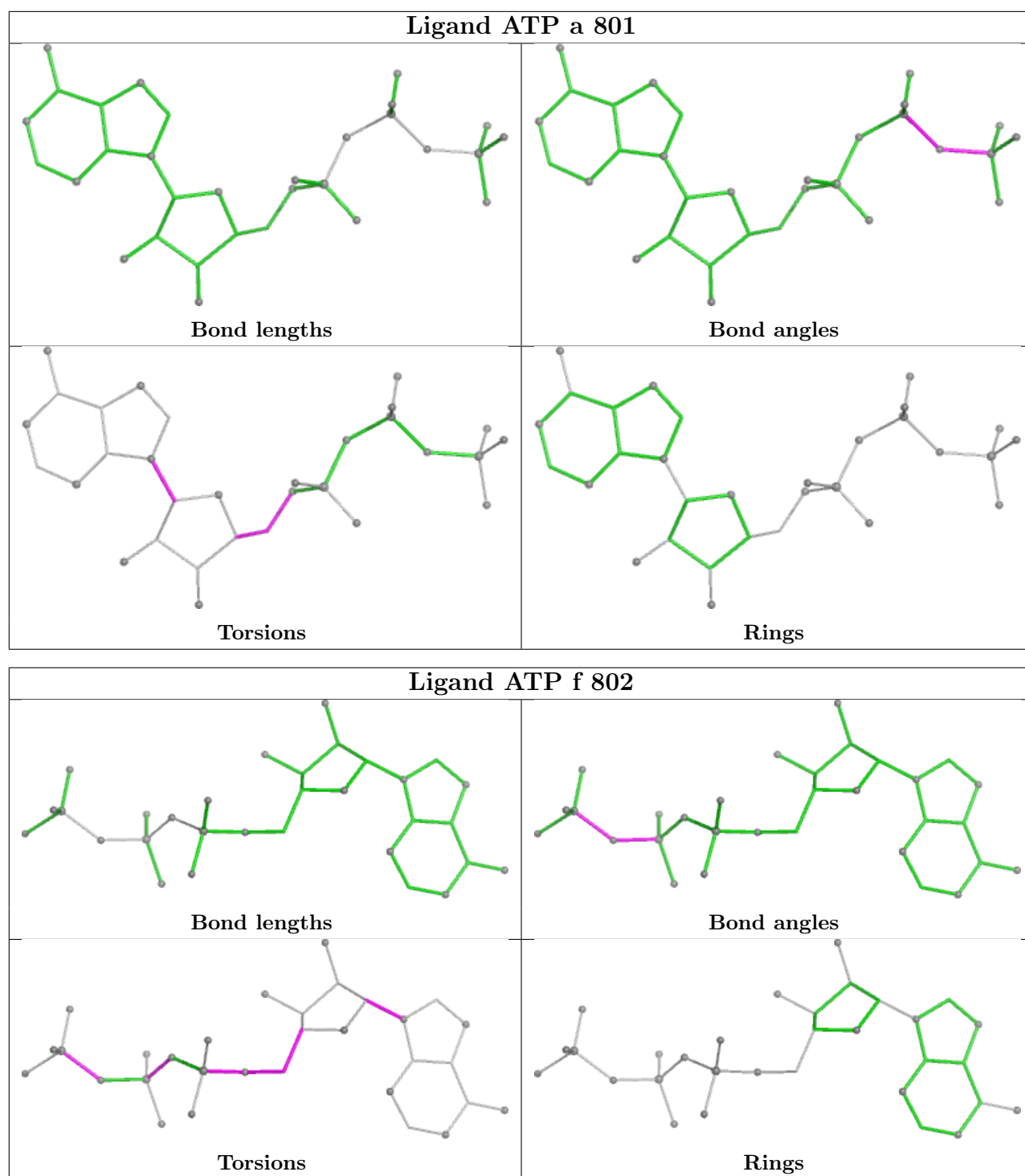












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	N	1
3	c	1
3	b	1
1	T	1
3	d	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	9:GLU	C	16:GLN	N	6.47
1	c	718:LEU	C	719:ASP	N	5.42
1	b	716:ALA	C	717:ALA	N	4.15
1	T	34:GLY	C	35:PRO	N	3.13
1	d	711:ASN	C	712:HIS	N	3.12

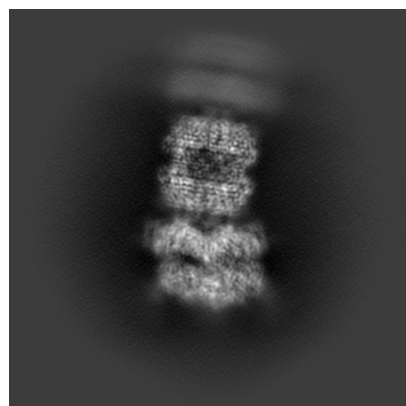
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-57170. These allow visual inspection of the internal detail of the map and identification of artifacts.

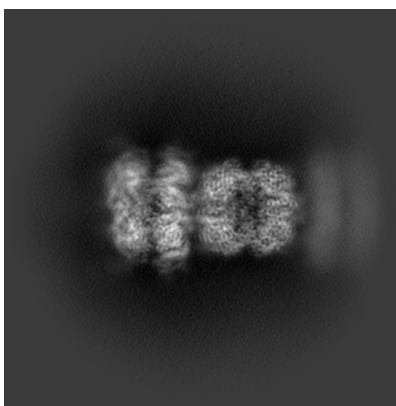
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

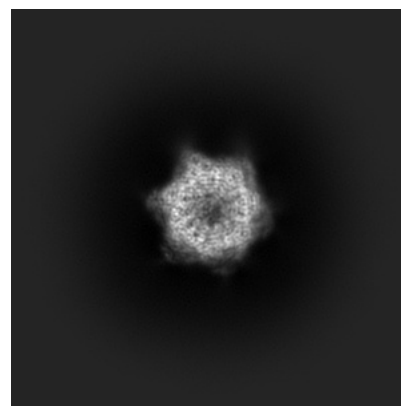
#### 6.1.1 Primary map



X

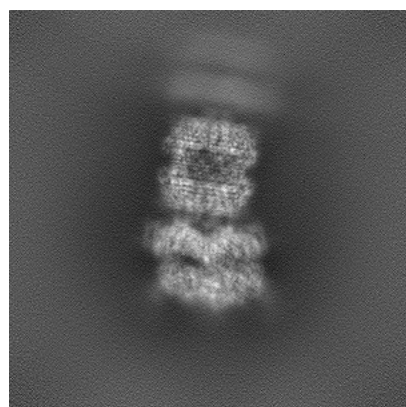


Y

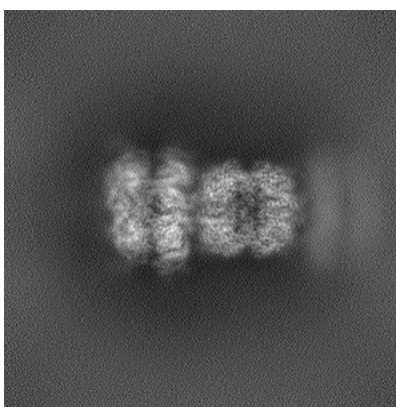


Z

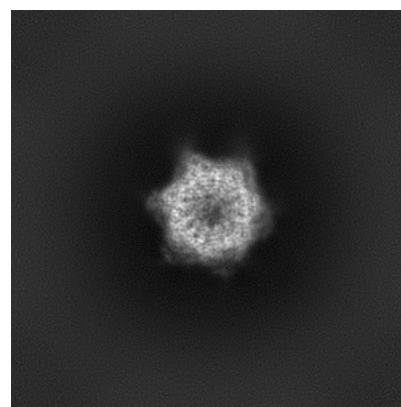
#### 6.1.2 Raw map



X



Y

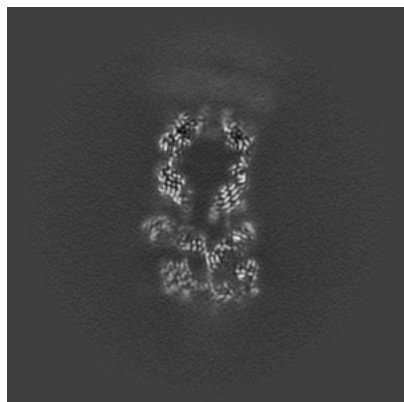


Z

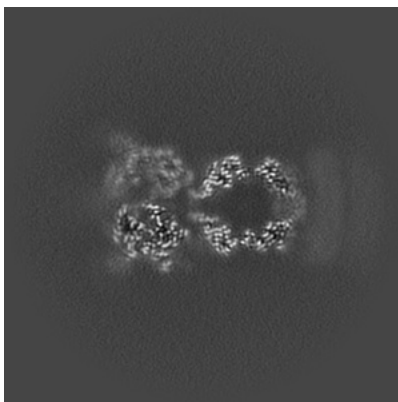
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

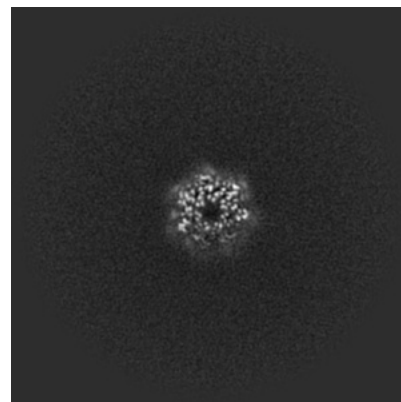
### 6.2.1 Primary map



X Index: 240

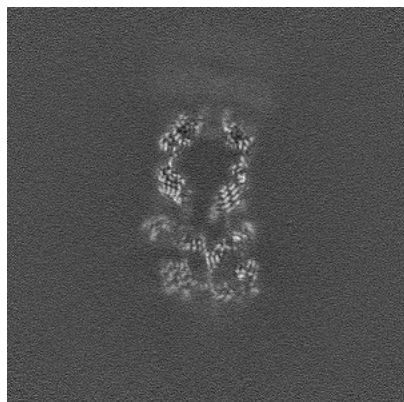


Y Index: 240

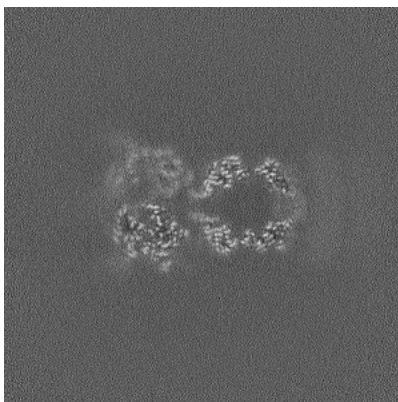


Z Index: 240

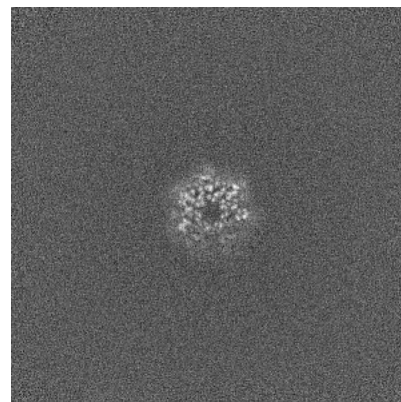
### 6.2.2 Raw map



X Index: 240



Y Index: 240

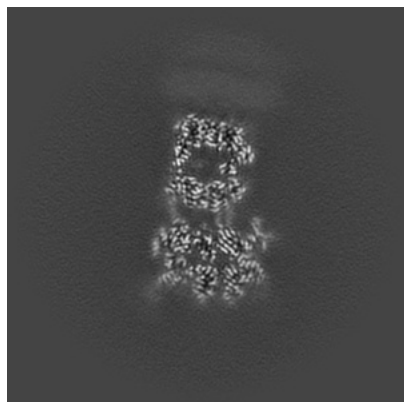


Z Index: 240

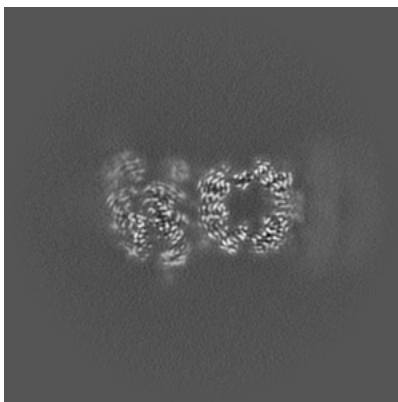
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

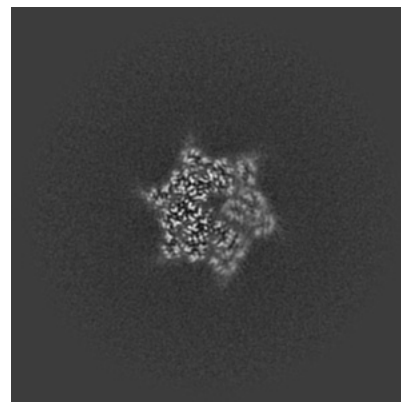
### 6.3.1 Primary map



X Index: 214

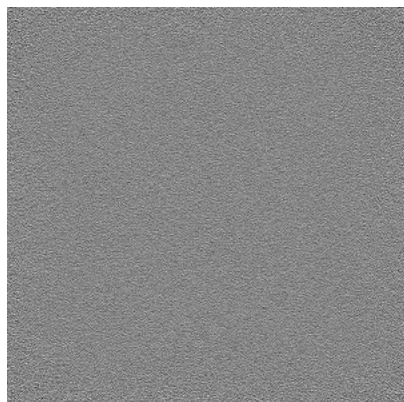


Y Index: 260

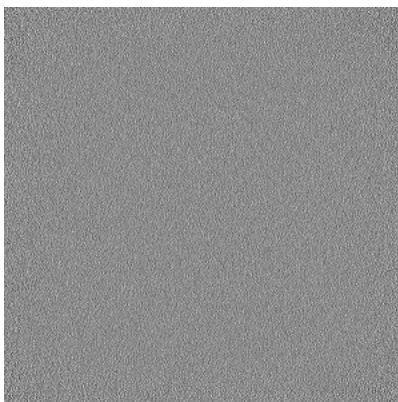


Z Index: 201

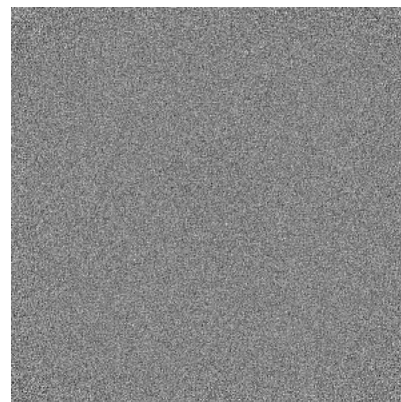
### 6.3.2 Raw map



X Index: 0



Y Index: 0



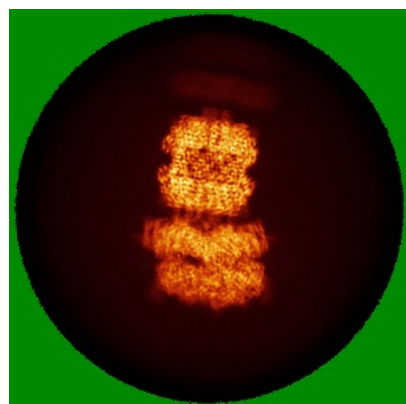
Z Index: 0

The images above show the largest variance slices of the map in three orthogonal directions.

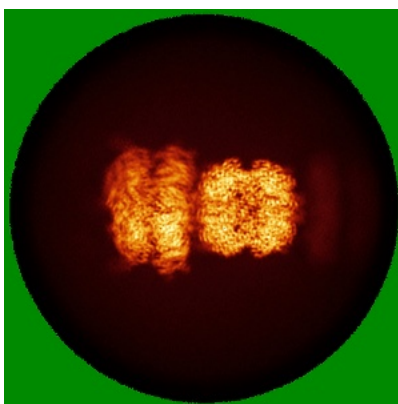


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

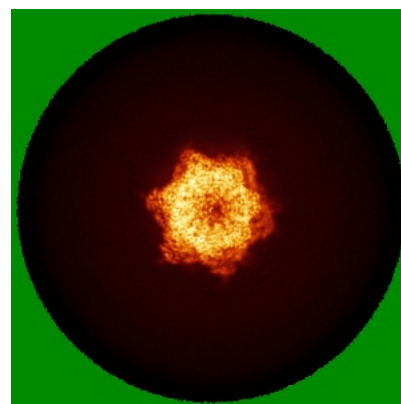
### 6.4.1 Primary map



X

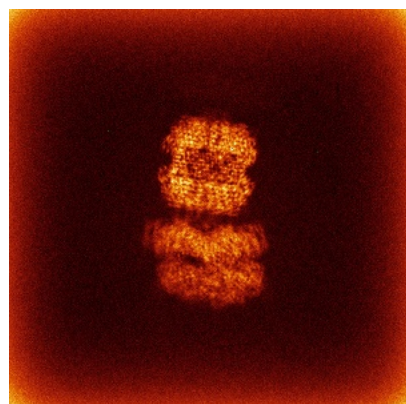


Y

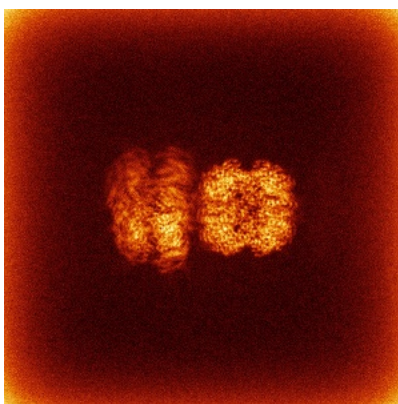


Z

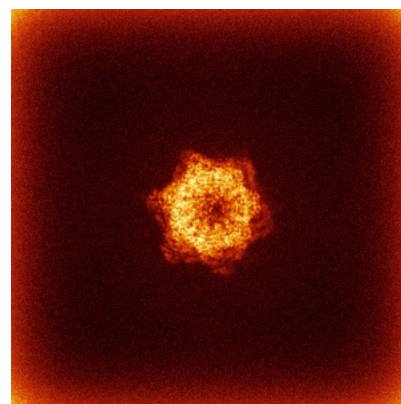
### 6.4.2 Raw map



X



Y



Z

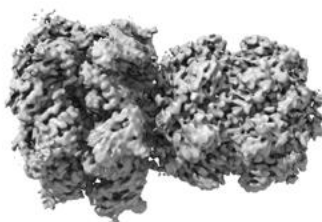
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

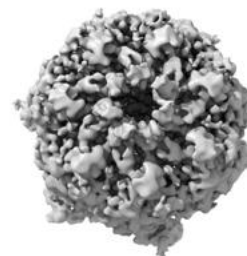
### 6.5.1 Primary map



X



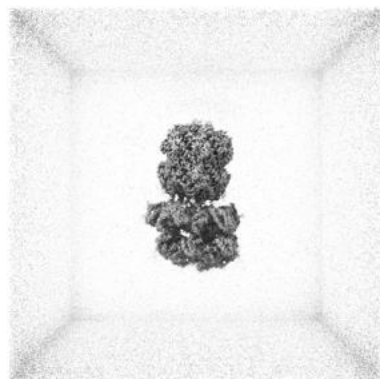
Y



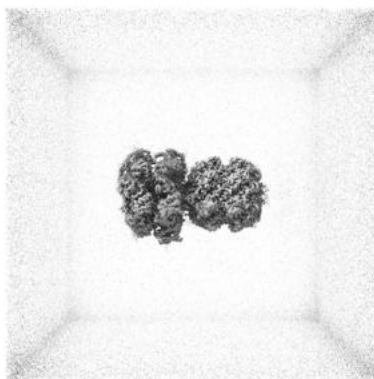
Z

The images above show the 3D surface view of the map at the recommended contour level 0.063. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

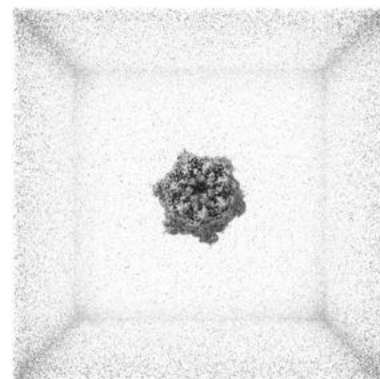
### 6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.



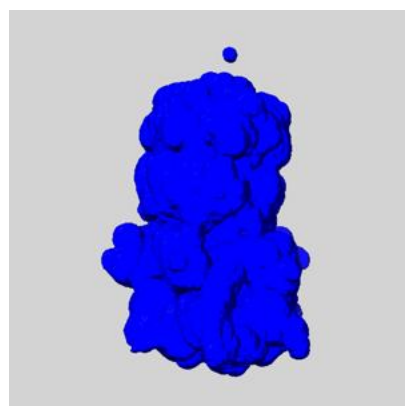
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

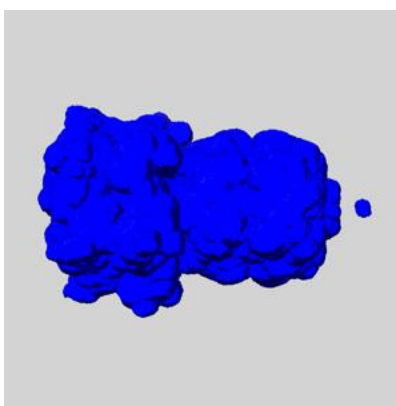
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

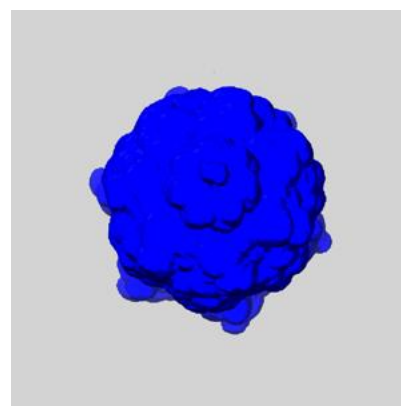
### 6.6.1 emd\_57170\_msk\_1.map [i](#)



X



Y

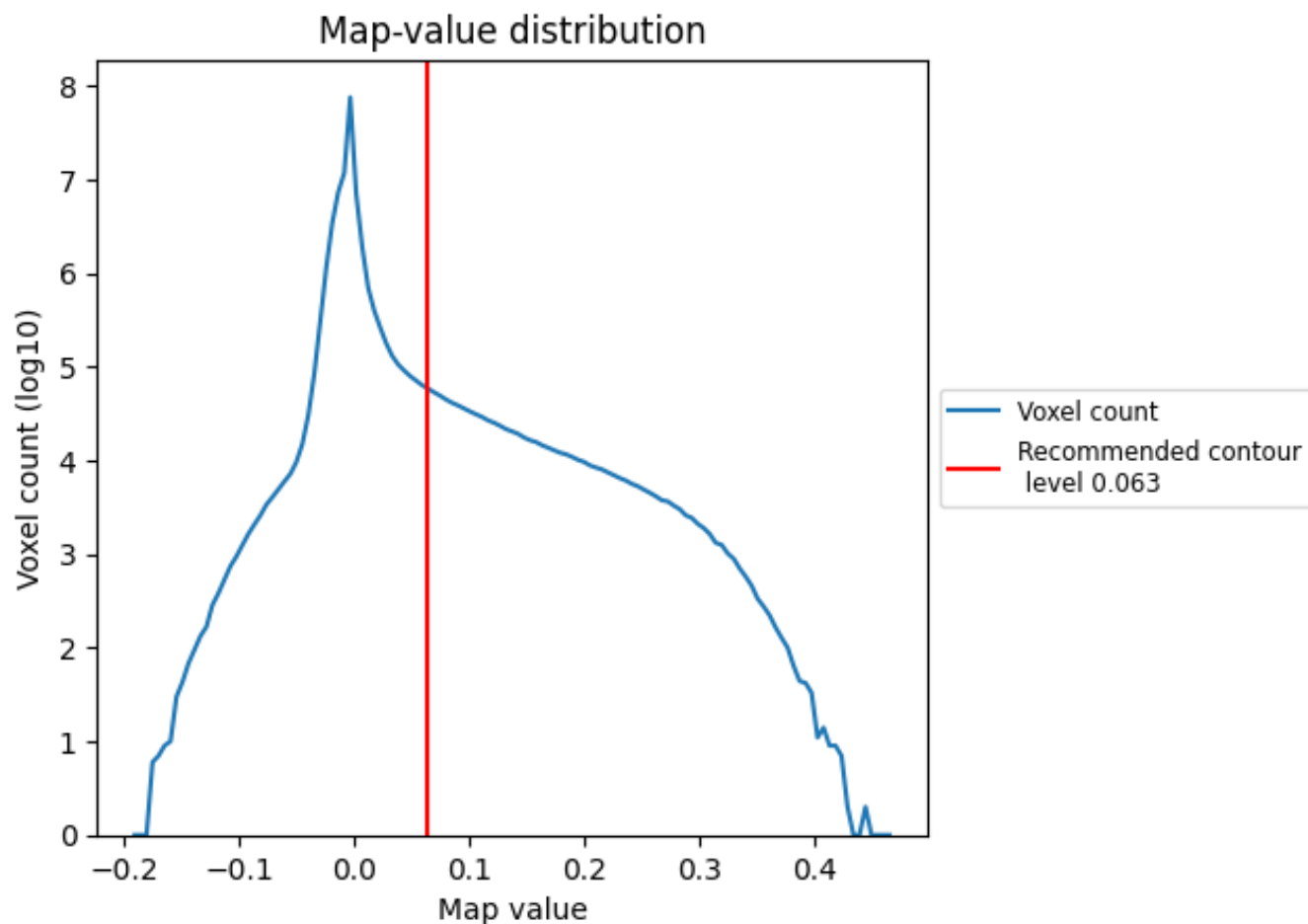


Z

## 7 Map analysis [i](#)

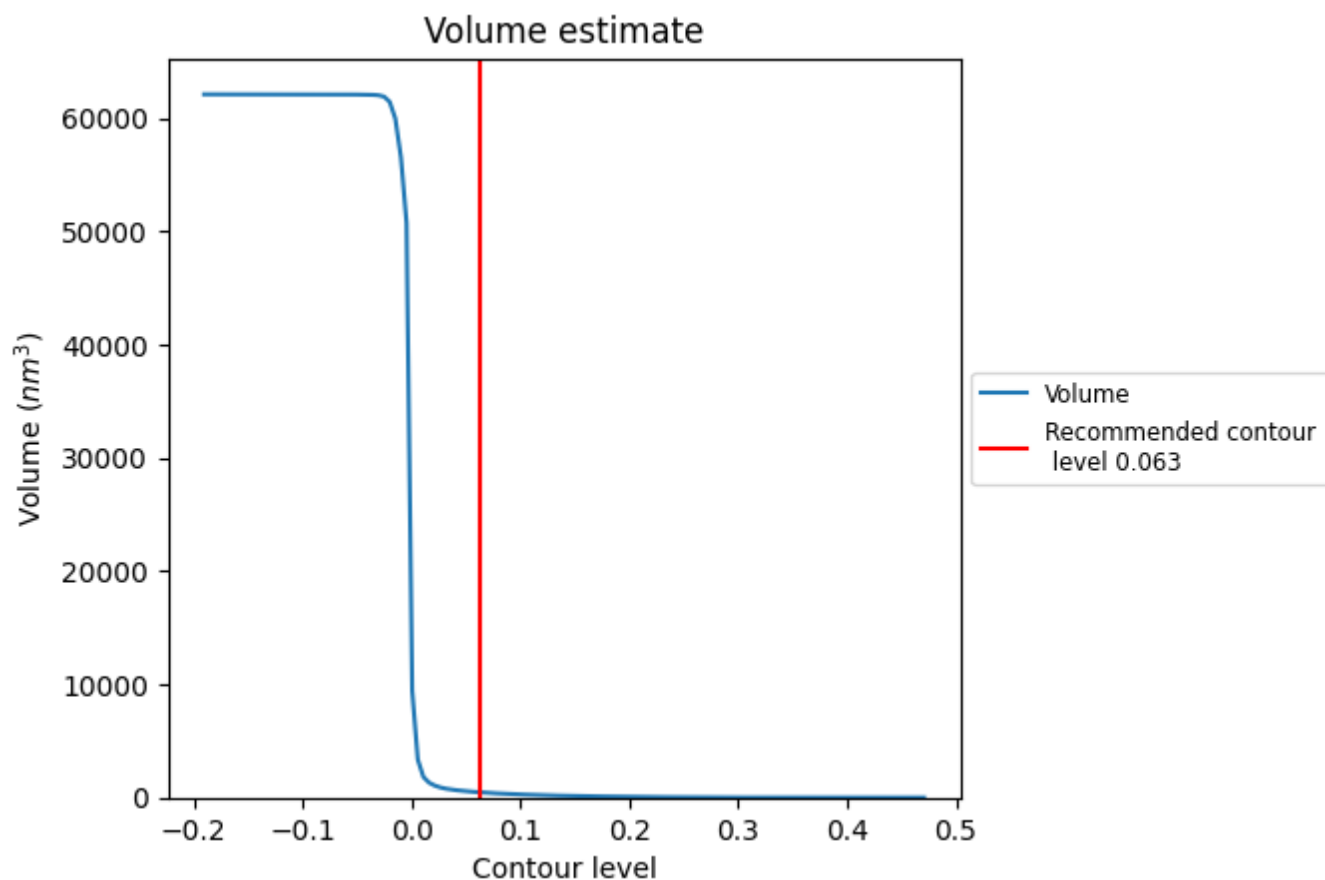
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

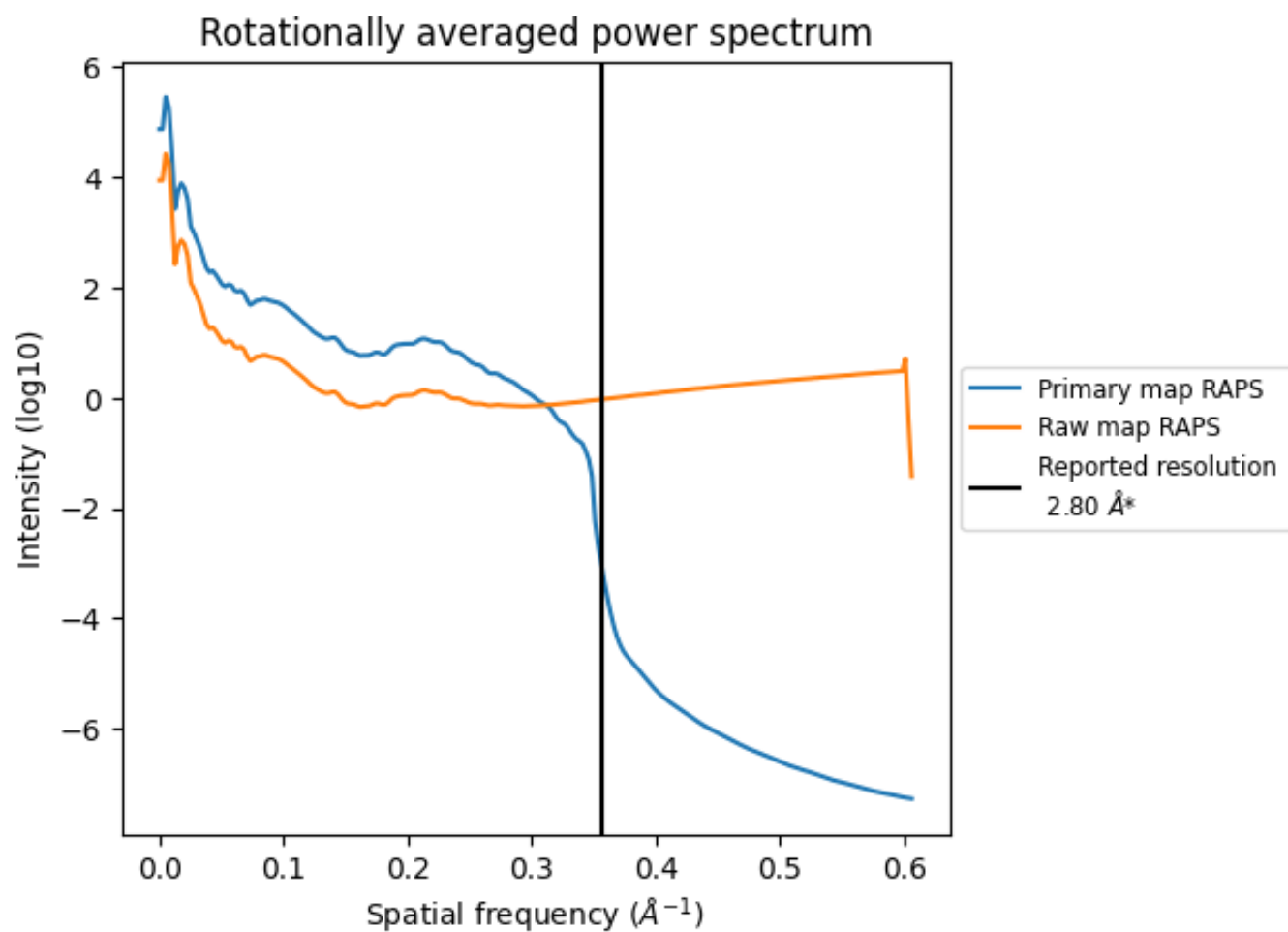
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 460  $\text{nm}^3$ ; this corresponds to an approximate mass of 416 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

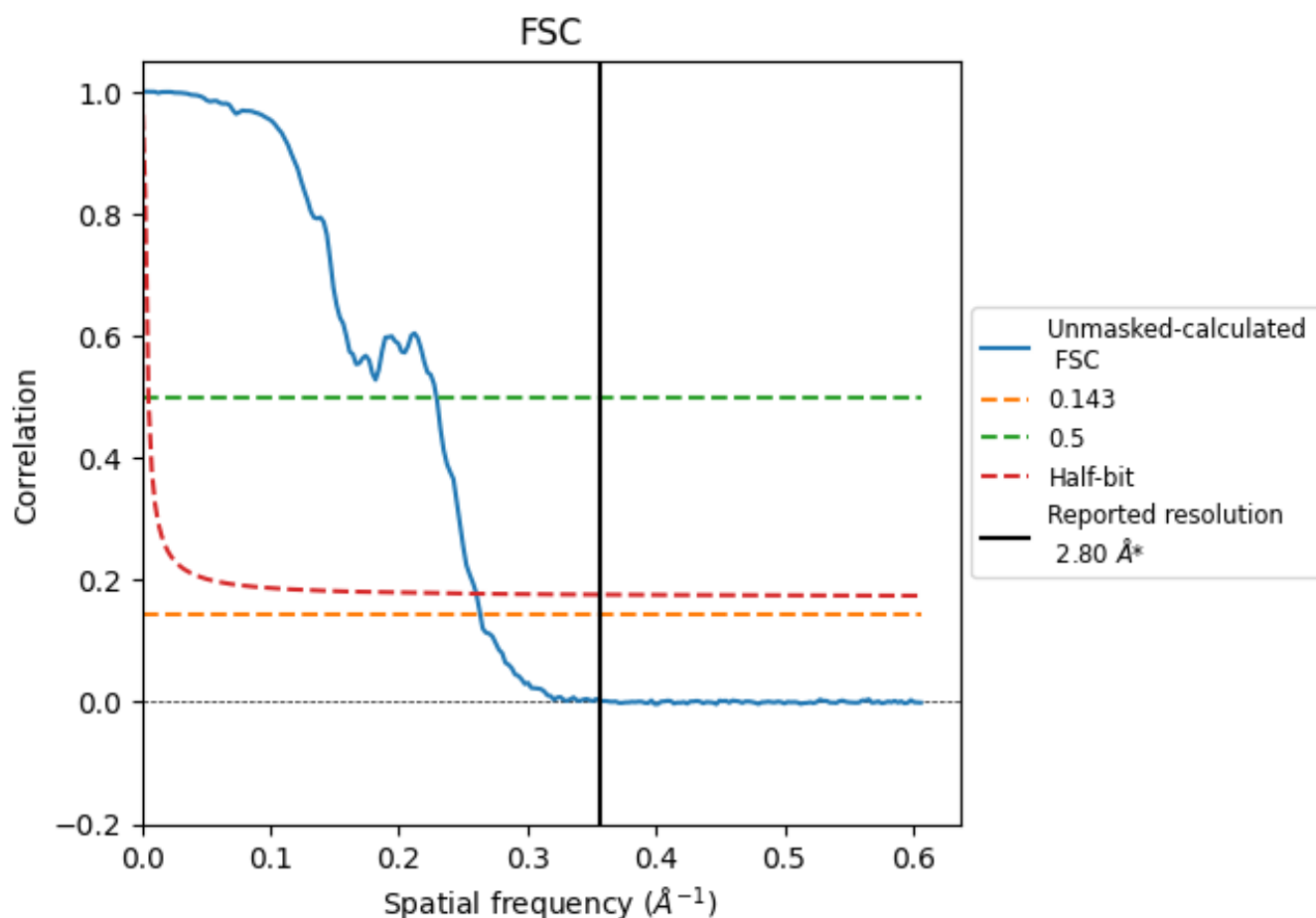


\*Reported resolution corresponds to spatial frequency of 0.357 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.357 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

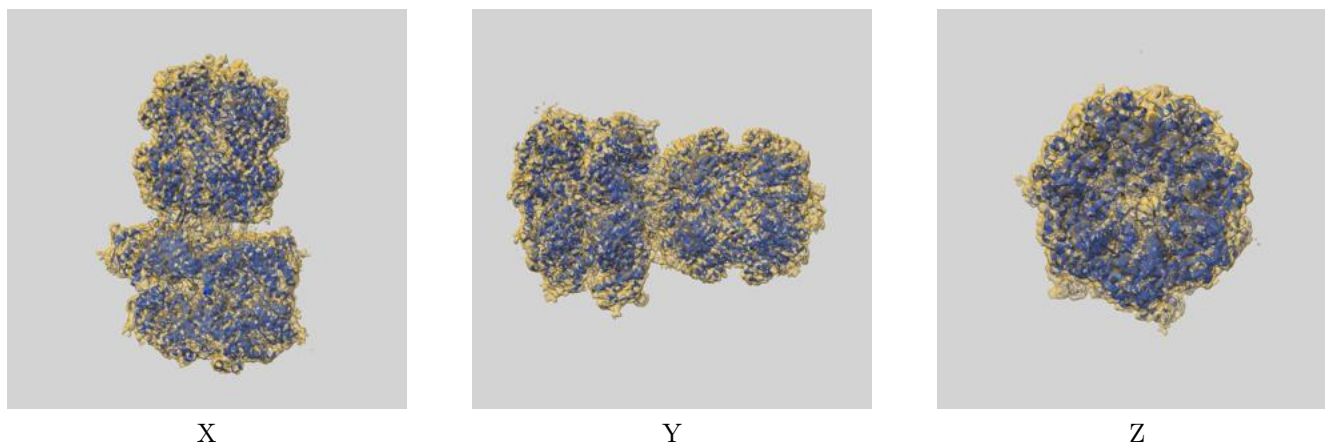
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.80	4.36	3.84

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.80 differs from the reported value 2.8 by more than 10 %

## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-57170 and PDB model 29HB. Per-residue inclusion information can be found in section [3](#) on page [7](#).

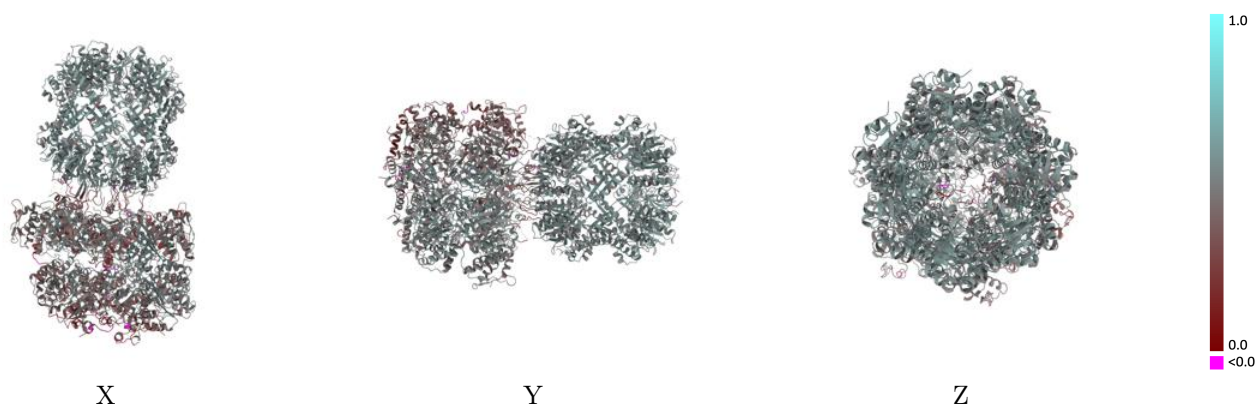
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.063 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

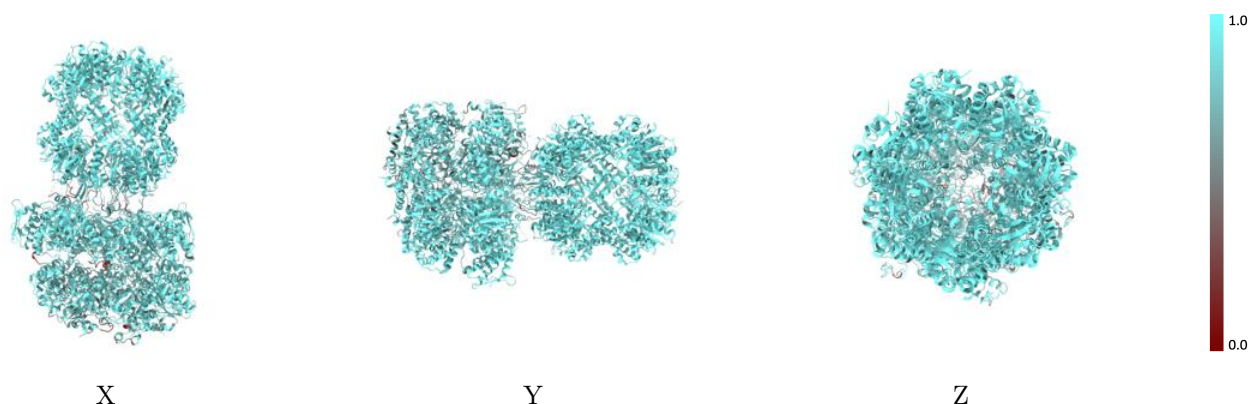


## 9.2 Q-score mapped to coordinate model [i](#)



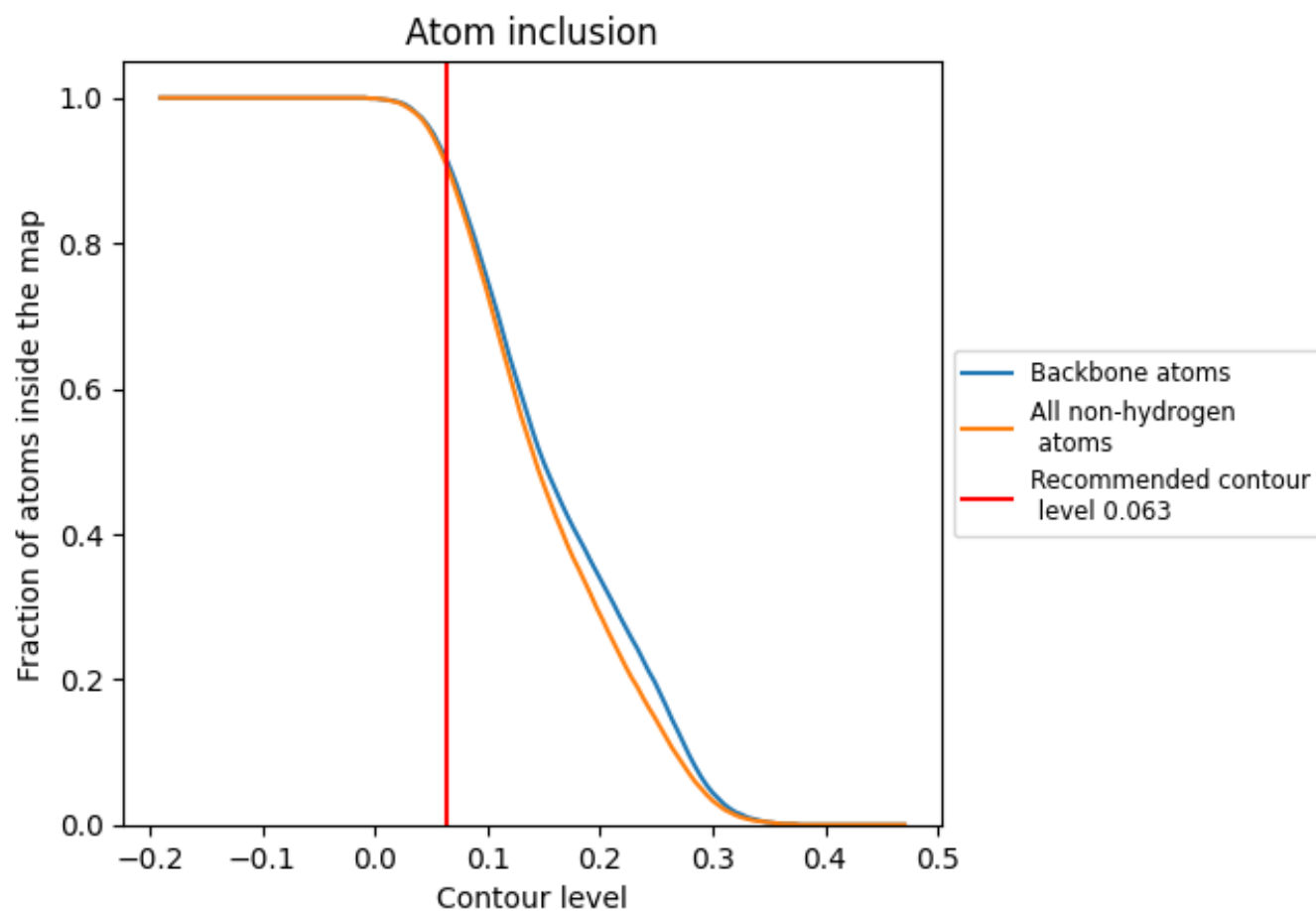
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.063).













































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.063) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9090	 0.4830
A	 0.9680	 0.5320
B	 0.9550	 0.5200
C	 0.9490	 0.5170
D	 0.9530	 0.5130
E	 0.9540	 0.5080
F	 0.9480	 0.5090
G	 0.9530	 0.5230
H	 0.9380	 0.5030
I	 0.9460	 0.5200
K	 0.9510	 0.5300
L	 0.9640	 0.5400
M	 0.9630	 0.5360
N	 0.9560	 0.5340
S	 0.9610	 0.5340
T	 0.9520	 0.5290
a	 0.9190	 0.4910
b	 0.9220	 0.4990
c	 0.9200	 0.4980
d	 0.8730	 0.4360
e	 0.7840	 0.3570
f	 0.8560	 0.4330

