



Full wwPDB EM Validation Report ⓘ

Jul 7, 2024 – 12:46 AM JST

PDB ID : 8ZJM
EMDB ID : EMD-60150
Title : Structure of DOCK5/ELMO1/Rac1 core (RhoG/DOCK5/ELMO1/Rac1 dataset, class 5)
Authors : Kukimoto-Niino, M.; Katsura, K.; Ishizuka-Katsura, Y.; Mishima-Tsumagari, C.; Yonemochi, M.; Inoue, M.; Nakagawa, R.; Kaushik, R.; Zhang, K.Y.J.; Shirouzu, M.
Deposited on : 2024-05-15
Resolution : 4.52 Å (reported)
Based on initial model : 7DPA

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

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

A user guide is available at

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

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

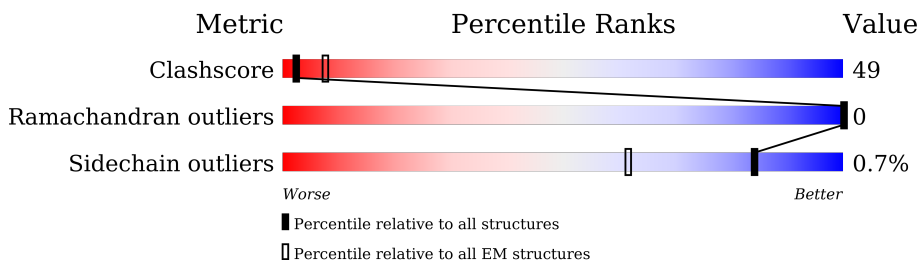
EMDB validation analysis : 0.0.1.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

1 Overall quality at a glance

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

The reported resolution of this entry is 4.52 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 ≥ 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	733	
1	D	733	
2	B	1648	
2	E	1648	
3	C	184	
3	F	184	

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 32858 atoms, of which 0 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 Engulfment and cell motility protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	198	Total	C	N	O	S	0	0
			1608	1018	277	303	10		
1	D	198	Total	C	N	O	S	0	0
			1608	1018	277	303	10		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q92556
A	-4	GLY	-	expression tag	UNP Q92556
A	-3	SER	-	expression tag	UNP Q92556
A	-2	GLY	-	expression tag	UNP Q92556
A	-1	GLY	-	expression tag	UNP Q92556
A	0	SER	-	expression tag	UNP Q92556
D	-5	GLY	-	expression tag	UNP Q92556
D	-4	GLY	-	expression tag	UNP Q92556
D	-3	SER	-	expression tag	UNP Q92556
D	-2	GLY	-	expression tag	UNP Q92556
D	-1	GLY	-	expression tag	UNP Q92556
D	0	SER	-	expression tag	UNP Q92556

- Molecule 2 is a protein called Deducator of cytokinesis protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1642	Total	C	N	O	S	0	0
			13436	8618	2264	2484	70		
2	E	1642	Total	C	N	O	S	0	0
			13436	8618	2264	2484	70		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	GLY	-	expression tag	UNP Q9H7D0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLY	-	expression tag	UNP Q9H7D0
B	-3	SER	-	expression tag	UNP Q9H7D0
B	-2	GLY	-	expression tag	UNP Q9H7D0
B	-1	GLY	-	expression tag	UNP Q9H7D0
B	0	SER	-	expression tag	UNP Q9H7D0
B	1285	ARG	LYS	variant	UNP Q9H7D0
E	-5	GLY	-	expression tag	UNP Q9H7D0
E	-4	GLY	-	expression tag	UNP Q9H7D0
E	-3	SER	-	expression tag	UNP Q9H7D0
E	-2	GLY	-	expression tag	UNP Q9H7D0
E	-1	GLY	-	expression tag	UNP Q9H7D0
E	0	SER	-	expression tag	UNP Q9H7D0
E	1285	ARG	LYS	variant	UNP Q9H7D0

- Molecule 3 is a protein called Ras-related C3 botulinum toxin substrate 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	177	1385	890	228	259	8	0	0
3	F	177	1385	890	228	259	8	0	0

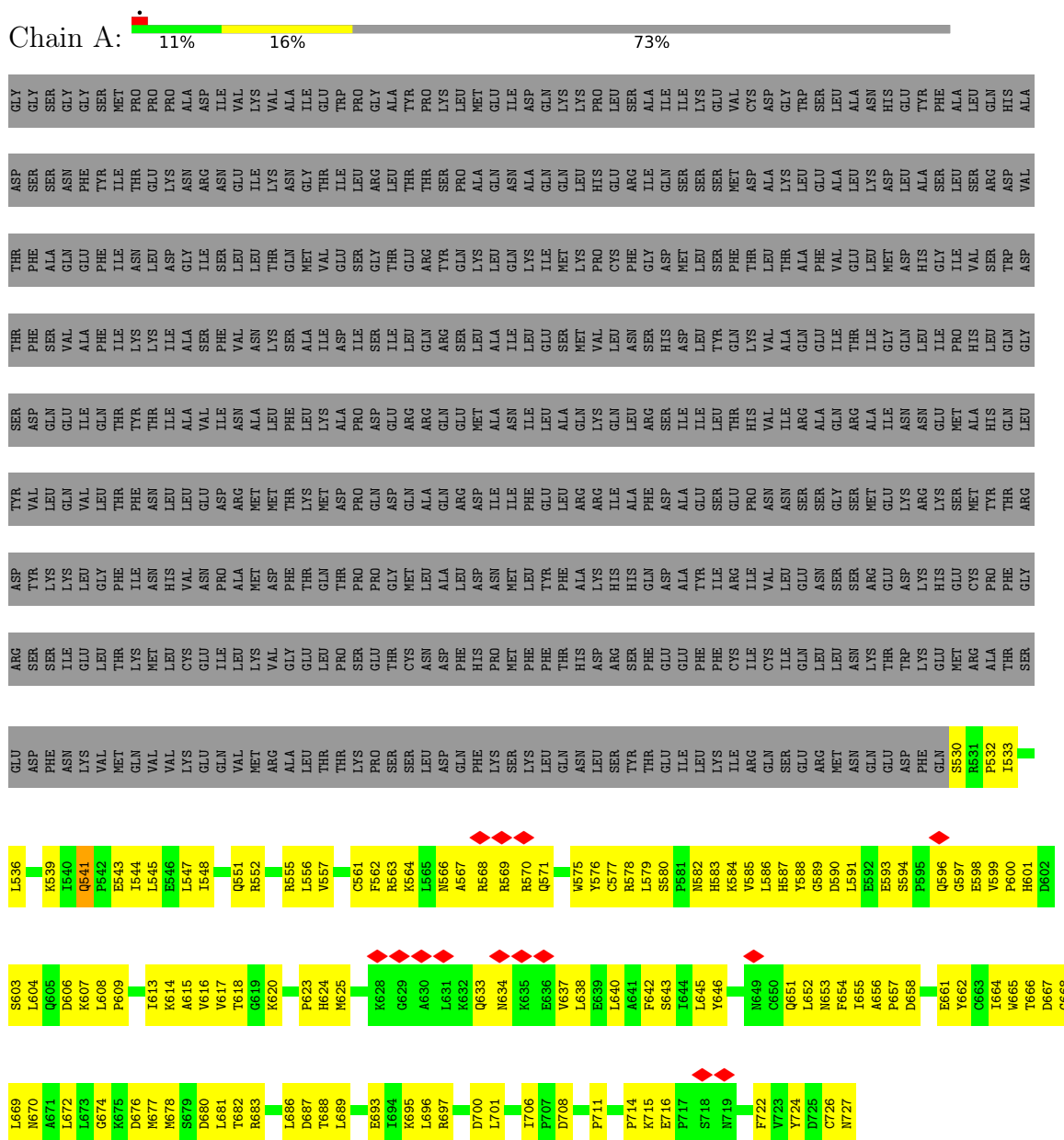
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	GLY	-	expression tag	UNP P63000
C	-5	SER	-	expression tag	UNP P63000
C	-4	SER	-	expression tag	UNP P63000
C	-3	GLY	-	expression tag	UNP P63000
C	-2	SER	-	expression tag	UNP P63000
C	-1	SER	-	expression tag	UNP P63000
C	0	GLY	-	expression tag	UNP P63000
C	15	ALA	GLY	engineered mutation	UNP P63000
F	-6	GLY	-	expression tag	UNP P63000
F	-5	SER	-	expression tag	UNP P63000
F	-4	SER	-	expression tag	UNP P63000
F	-3	GLY	-	expression tag	UNP P63000
F	-2	SER	-	expression tag	UNP P63000
F	-1	SER	-	expression tag	UNP P63000
F	0	GLY	-	expression tag	UNP P63000
F	15	ALA	GLY	engineered mutation	UNP P63000

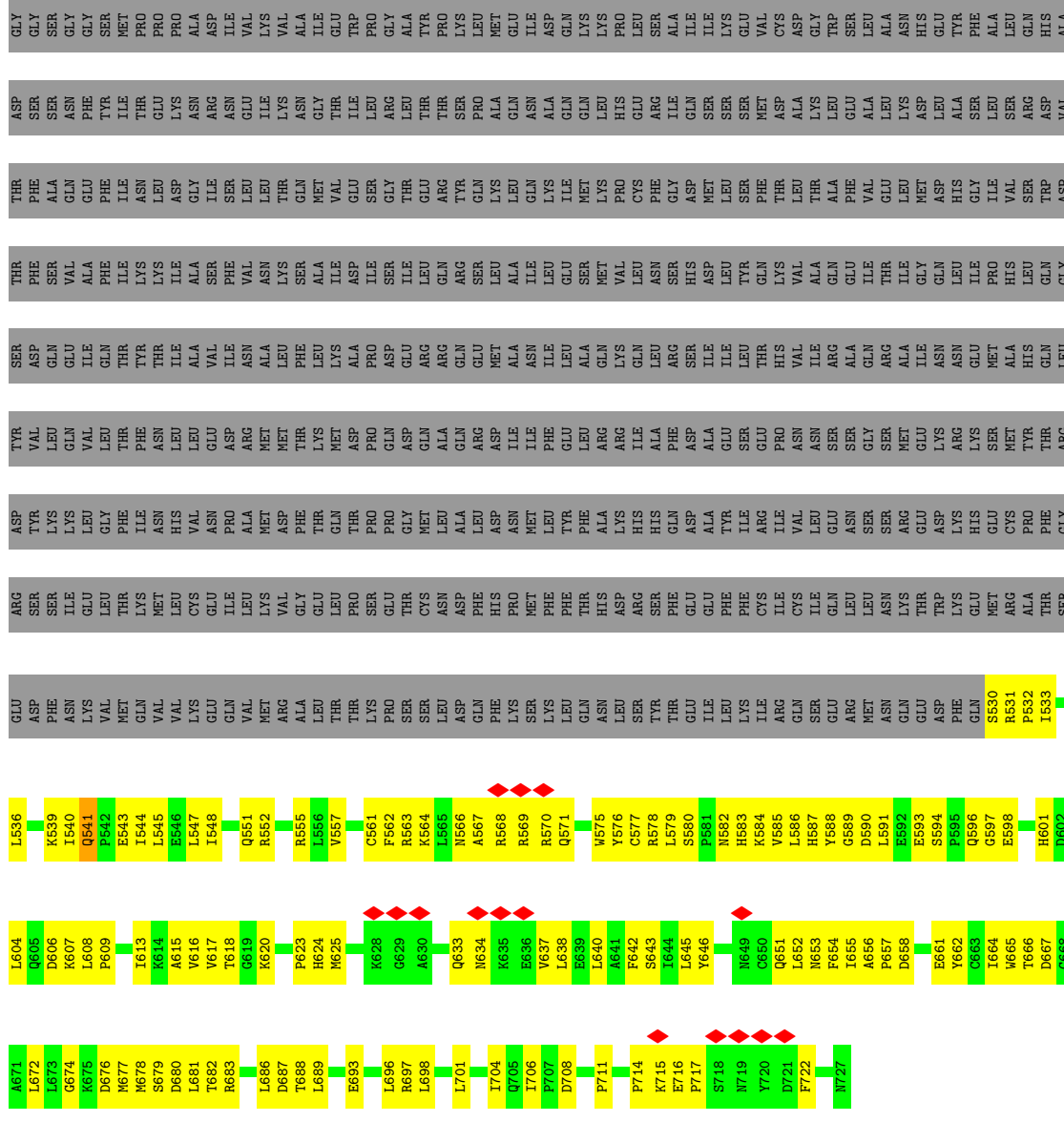
3 Residue-property plots i

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.

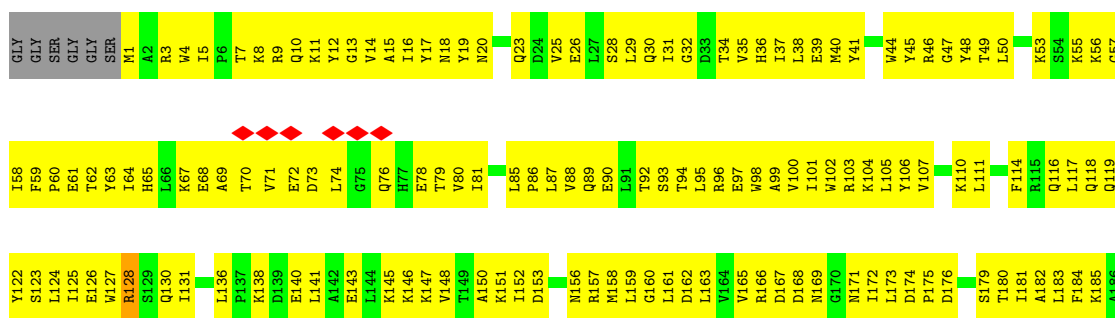
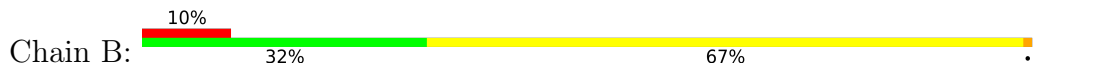
- Molecule 1: Engulfment and cell motility protein 1



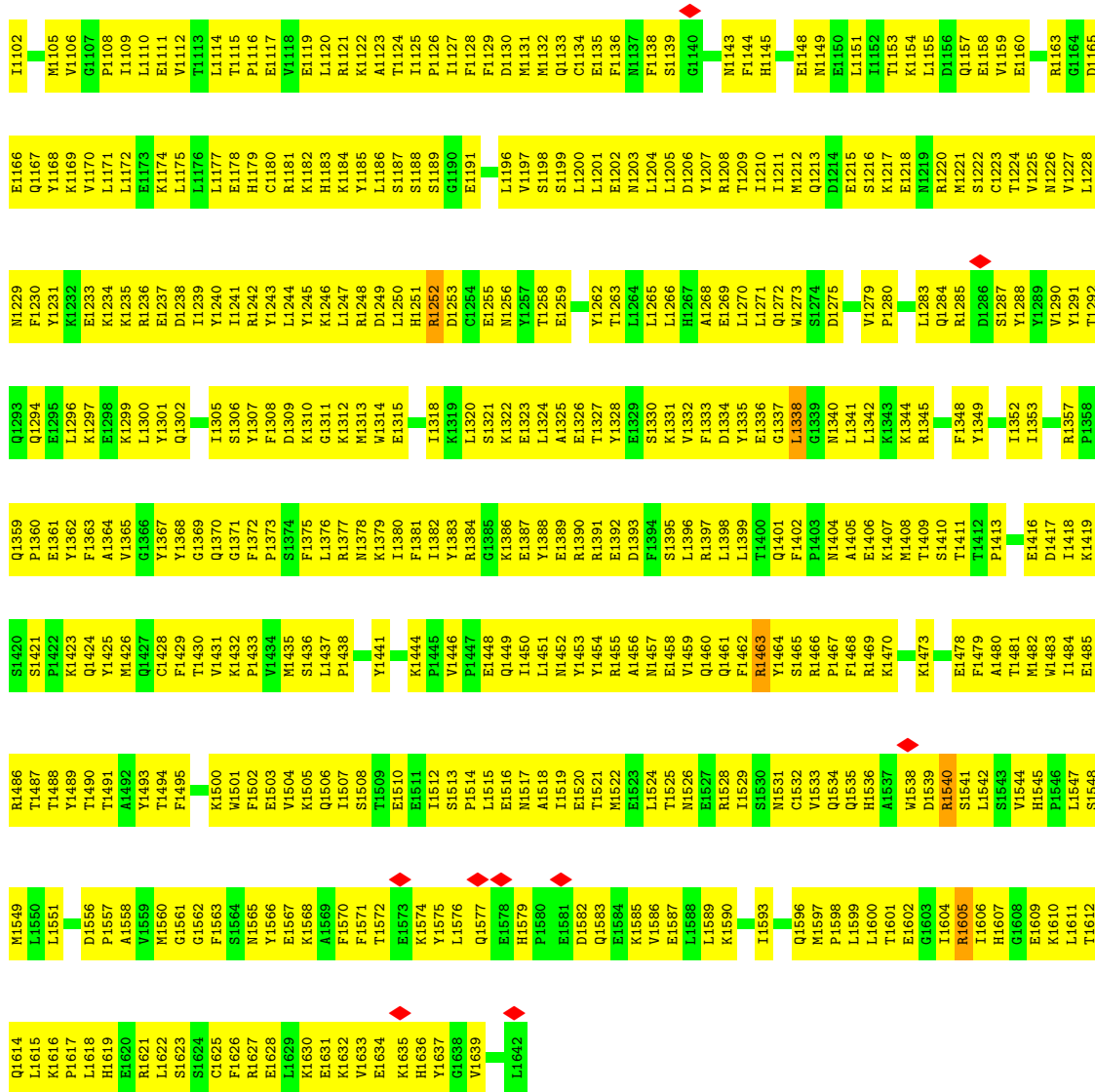
● Molecule 1: Engulfment and cell motility protein 1



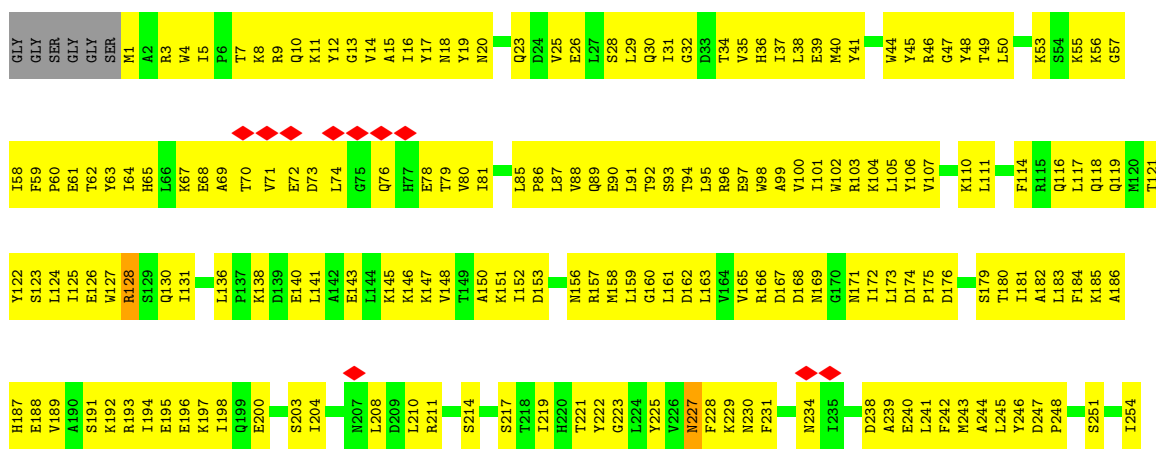
● Molecule 2: Dedicator of cytokinesis protein 5



H187	L390	F322	K390	K459	E520	F584	S645	W715	R776	K842	N908	I973	F1038
E188	L260	V326	E391	K460	E521	Y585	N646	L716	F777	F843	I909	S974	E1039
V189	R261	M327	N392	K461	E522	L586	E717	E717	G778	R844	L910	T975	L1040
S191	G263	M327	N393	T462	T523	T587	Q648	T718	G779	Q845	E911	F976	Q1041
R193	S264	I329	H394	P463	R524	L588	N649	Y719	Q780	S846	N912	K977	L1042
L194	N265	T330	K395	K464	C525	H589	I650	T720	S781	R847	L913	T978	W1043
E196	G266	D331	W400	N465	H526	F589	K651	Y721	F787	Q851	R914	R979	M1044
K197	G266	I332	V401	N466	I527	G590	H652	K722	M788	L852	R915	I982	Y1045
I198	G267	I333	S402	V467	R528	T591	H653	H723	N789	R853	N918	I983	Y1046
E200	P268	I333	L403	V468	F529	K592	L654	F724	N790	R854	N919	D984	H1047
S203	R269	I333	L404	V469	F531	M593	K655	A726	I791	Q855	G919	D985	H1048
I204	K273	I333	K404	T469	R532	M594	L657	L726	R792	Q856	A920	F985	L1049
L208	N275	I333	L406	M470	H533	M595	M658	L728	Q793	L857	T921	L986	L1049
D209	N276	I333	L406	S471	R534	M596	E659	A729	Q793	R858	A922	M987	A1050
R211	L277	I333	T411	H472	R535	E597	V660	K732	F798	R862	Y923	I988	Y1051
G212	L277	I333	Q412	D474	S536	K598	Q662	L733	A797	R863	N924	T989	A1052
Q213	F281	I333	K415	G477	Q537	L600	E664	S734	M800	Y864	H924	F990	F1053
S214	T281	I333	N416	K478	Q538	L606	L665	K735	N809	R865	R925	I991	H1056
S217	T282	I333	F417	L479	T539	L607	T672	W736	M809	R866	E930	F992	E1057
T218	D283	I333	S418	L480	R640	A602	L673	L737	E807	L801	E931	F993	S1058
I219	L284	I333	H419	E481	D541	S603	L669	F738	E808	M802	R932	M992	L1059
H220	S285	I333	L420	K482	K642	R604	L670	N739	A809	R803	L932	F993	L1060
I221	S286	I333	D422	I484	S543	R604	D670	F740	W810	D804	L933	G998	E1062
R222	S287	I333	R423	H485	E544	N605	Q671	Y741	P805	P805	R934	G999	T1063
Y225	D288	I333	S424	G487	A546	I606	Q601	A742	E807	R870	R935	Y1002	Q1065
V226	L289	I333	T425	A488	F547	L606	L607	L742	E808	Q871	N936	Y1006	Q1066
N227	R290	I333	A352	G489	G548	L607	L674	A744	E809	R874	N937	M1007	Q1067
F228	R291	I333	E353	Y490	V549	L607	L675	W745	W810	R875	R938	M1007	Q1068
K229	R292	I333	M554	E491	A550	S612	N680	E751	A815	R876	N939	M1008	Q1069
N230	R293	I333	H431	G492	F551	S612	M681	L752	A816	R877	V940	M1009	Q1070
F231	R294	I333	M431	I493	F552	K613	M681	L753	A817	L817	I941	M1010	Q1071
N234	R296	I333	G482	S494	V552	D614	S684	F754	W819	R818	G942	M1011	Q1072
D238	R297	I333	F433	E495	L554	D614	D685	A755	L820	D884	N943	M1011	Y1076
A239	R299	I333	A435	Y496	M555	T616	P685	A756	R821	R885	N944	D1078	G1077
E240	C298	I333	I436	S498	N556	K617	D690	L757	S822	L886	F953	M1015	M1079
L241	Q299	I333	I437	V499	P557	D618	F691	K758	I823	R889	V954	L1017	K1081
M242	R302	I333	L438	V500	T560	D618	L692	A759	R824	L890	N957	L1018	E1082
A244	V303	I333	D441	Y502	T561	F620	V693	L760	N825	L890	R958	M1019	I1083
L245	G304	I333	V442	Y503	L562	Q621	F694	K761	D826	L890	M957	M1022	G1084
Y246	H305	I333	N444	Q503	G565	L622	A696	T762	N827	N893	N959	Q1023	F1085
D247	E307	I333	D445	V504	L569	L623	F699	F764	K828	S894	A959	A1025	R1086
P248	L308	I333	I446	K505	L625	L626	L700	F766	L829	N895	L961	A1026	D1088
T254	K309	I333	Y447	Q506	V570	C627	I701	F766	F831	K896	Q962	V1027	M1090
S255	E310	I333	V448	W509	V571	SG28	K708	L768	D898	R899	N964	L1028	W1091
E256	E310	I333	T449	Y510	Y572	F629	F709	Q769	F709	H899	D966	T1029	Y1092
N257	G311	I333	L450	E511	Y572	K630	F709	R771	S770	S903	N902	F1031	L1094
M257	K312	I333	I451	T512	G574	L631	Q710	W772	S837	S903	Q904	F1031	H1097
Y258	K313	I333	E454	V513	G574	T632	H711	V773	W838	Q904	Q904	F1031	K1098
	H314	I333	F455	K514	D575	Q633	F712	W773	L839	L905	L906	F1031	I1099
	T315	I333	D456	V515	N576	D636	R713	L774	F840	L906	H971	F1031	K1100
	L318	I333	K457	S516	K577	L637	P714	L775	C841	S907	Y972	F1031	F1101
	R319	I333	K385	A518	K578	L638							
	R320	I333	V386	A518	K578	L639							
	P321	I333	A388	A518	K578	L640							
		I333	A389	A518	K578	L641							
		I333		A518	K578	L642							
		I333		A518	K578	L643							
		I333		A518	K578	L644							



● Molecule 2: Dedicator of cytokinesis protein 5



N1083	N1084	P1096	K1097	K1098	I1099	K1100	F1101	I1102	M1105	V1106	G1107	P1108	I1109	L1110	V1046	I1111	V1112	L1113	T1114	T1115	L986	P1116	E1117	V1118	E1119	L1120	R1121	K1122	A1123	T1124	I1125	P1126	I1127	F1128	F1129	D1130	M1131	Q1132	C1133	C1134	E1135	F1136	N1137	F1138	S1139	G1140	N1143	F1144	H1145	E1148	N1149	E1150	L1151	I1152	T1153	K1154	L1155										
T1029	R1030	F1031	M1032	D1033	Q1034	Q1035	A1036	E1039	L1040	Q1041	Q1042	M1043	M1044	M1045	V1046	H1048	H1049	L1049	L1114	V1051	A1051	A1052	F1053	H1056	E1057	S1058	M1059	F1060	Q1060	L1061	E1062	L1063	P1064	S1065	F1128	Q1066	A1067	K1068	M1069	N1070	K1071	E1135	I1072	Y1076	G1077	D1078	M1079	R1080	K1081	E1082	L1083	G1084	F1085	R1086	I1087	L1088	D1089	M1090	M1091	K1154	L1155						
Q963	M964	D966	Y969	S970	H971	Y972	I973	S974	T975	F976	K977	R978	S979	I982	E983	D984	F985	L986	M987	E988	T989	F990	I991	M992	F993	K994	D995	L996	I997	L998	G998	K999	Y1002	M1006	M1007	V1008	M1009	M1010	M1011	T1012	Q1013	M1014	R1015	V1016	F1017	L1018	R1019	N1022	Q1023	F1024	A1025	E1026	M1027	L1028													
B988	H989	S902	S903	Q904	L905	L906	S907	R908	F909	L910	E911	V912	L913	D914	R915	Y918	G919	A920	T921	A922	N923	H924	I925	Q926	R927	F928	M929	E930	R931	L932	L933	R934	R935	I936	R937	R938	T939	V940	I941	G942	H943	R944	R945	Q946	H949	I950	F953	V954	N957	I958	A959	E1026	M1027	L1028													
D832	E835	L836	S837	V838	L839	F840	G841	R842	F843	L844	G845	S846	L847	R851	L852	M853	R854	R855	K856	R857	N858	C859	M860	T861	K862	L863	V864	E865	R866	R867	F868	R869	R870	Q871	C874	R875	E876	H877	L878	L879	F880	L881	L882	T883	D884	O885	L886	Q889	I890	N957	I958	A959	E1026	M1027	L1028												
Q769	S770	R771	V772	L773	V774	L775	R776	F777	G778	G779	S781	D785	E786	F787	M788	M789	S790	I791	R792	Q793	L794	F795	L796	A797	K798	L799	M800	L801	M802	D803	R804	F805	L806	E807	E808	A809	R810	R811	L812	A815	A816	R818	X819	L820	P821	S822	I823	I824	N825	D826	V827	K828	F829	V830	H831												
K708	F709	Q710	H711	F712	N713	P714	V715	L716	E717	T718	L719	L720	V721	K722	H723	F724	S725	A726	T727	L728	A729	V730	L731	M732	S733	S734	K735	V736	L737	E738	N739	L740	V741	N743	D744	V745	D746	K749	T750	L751	F752	L753	F754	A755	A756	L757	K758	A759	L760	K761	V762	L763	F764	R765	F766	L767	I768										
D636	L637	L638	G639	L640	L641	M642	M643	R644	S645	M646	S647	O648	M649	L650	K651	H652	M653	L654	K655	K656	L657	M658	E659	V660	D661	G662	G663	E664	L665	V666	K667	F668	L669	O670	D671	T672	L673	D674	A675	L676	F677	M678	L679	M680	M681	D690	F691	L692	V693	F694	D695	A696	L697	V698	F699	L700	I701										
D575	N576	K577	M578	M579	E580	D581	A582	K583	F584	Y585	L586	T587	L588	P589	G590	T591	K592	M593	E594	M595	E596	E597	K598	E599	L600	Q601	A602	S603	N604	K605	L606	V607	T608	F609	T610	P611	S612	K613	D614	S615	T616	K617	D618	S619	F620	Q621	L622	A623	T624	L625	L626	C627	S628	T629	K630	L631	T632	Q633									
W509	Y510	E511	T512	V513	K514	L517	A518	I519	E520	G458	V522	T523	R524	C525	H526	I527	R528	F529	T530	F531	R532	H533	R534	S535	S536	Q537	H473	D474	E475	F476	G477	K478	L479	L480	K481	K482	A483	I484	H485	P486	A487	A488	G489	Y490	E491	G492	I493	S494	M431	G432	K430	F433	P434	A435	I436	L437	V438	Y501	Y502	Q503	V504	L569	V570	V571	Y572	K573	G574
I446	Y447	V448	L449	L450	I451	F455	D456	K457	G458	K459	K460	K461	T462	P463	K464	M465	V466	V467	V468	M470	G408	D409	L410	I346	P347	F348	Q349	Q350	I351	K415	M353	F417	S418	H419	L420	L421	V421	D422	R423	S424	T425	A426	A428	R429	K430	M431	F433	P434	I368	V369	M306	I372	H371	V372	I373	G374	N376	E377	P378	L379							
C316	R319	R320	P321	F322	V326	A389	K390	E391	L329	T330	D331	I332	I333	K336	V337	D338	D339	E340	E341	K342	Q343	H344	F345	I346	P347	F348	Q349	Q350	I351	M353	E354	T355	V356	L289	I290	R291	P292	Q293	V294	L296	V297	C298	Q299	R302	V303	G304	H305	M306	E307	L308	K309	E310	G311	K312	K313	H314	T315										

D1156	Q1157	M1221	E1158	V1159	E1160	R1163	G1164	D1165	E1166	F1230	Q1167	Y1168	K1169	V1170	L1171	L1172	E1173	K1174	E1237	D1238	L1239	Y1240	I1241	R1242	Y1243	L1244	Y1245	K1182	H1183	K1184	Y1185	D1248	L1250	S1187	S1188	S1189	D1252	D1253	E1255	L1196	V1197	S1198	E1259	A1260	L1200	A1261	E1262	T1203	L1204	L1205	D1206	Y1207	R1208	T1209	L1210	M1211	Q1212	W1213	D1214	S1215	S1216	K1217	E1218	M1219
R1220	M1221	S1222	C1223	T1224	V1225	M1226	V1227	L1228	M1229	F1230	Q1231	K1232	E1233	K1234	K1235	R1236	E1237	D1238	L1239	Y1240	I1241	R1242	Y1243	L1244	Y1245	K1246	L1247	R1248	D1249	L1250	L1251	R1252	D1253	E1255	L1320	M1256	Y1257	T1258	E1259	A1260	A1261	Y1262	T1263	L1264	L1265	L1266	H1267	A1268	E1269	L1270	L1271	Q1272	W1273	D1274	S1275	E1215	S1216	K1217	E1218	M1219				
L1283	Q1284	R1285	D1286	L1287	Y1288	Y1289	V1290	L1291	T1292	Q1293	Q1294	E1295	L1296	K1297	E1298	L1299	L1300	Y1301	Q1302	I1305	Q1306	H1179	Y1307	F1308	D1309	K1310	G1311	L1312	M1313	W1314	E1315	I1316	I1317	I1318	K1319	L1320	S1321	K1322	E1323	L1324	A1325	E1326	T1327	Y1328	E1329	L1330	K1331	V1332	F1333	D1334	Y1335	E1336	G1337	L1338	G1339	M1340	L1341	L1342	K1343	M1344				
R1345	F1346	Y1347	L1348	L1349	R1350	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	
T1409	S1410	T1411	T1412	P1413	E1414	D1417	L1418	L1419	S1420	S1421	E1422	K1423	Q1424	Q1425	A1426	Q1427	C1428	F1429	T1430	V1431	K1432	P1433	V1434	M1435	S1436	L1437	P1438	Y1441	K1444	P1445	P1446	P1447	E1448	Q1449	L1450	L1451	M1452	Y1453	Y1454	R1455	A1456	M1457	E1458	L1459	Q1460	Q1461	F1462	R1463	Y1464	S1465	R1466	P1467	F1468	L1469	K1470	M1408								
K1473	F1479	A1480	S1481	S1482	M1483	L1484	E1485	R1486	L1487	T1488	Y1489	T1490	L1491	A1492	Y1493	L1494	F1495	K1500	W1501	F1502	E1503	E1504	K1505	Q1506	L1507	P1508	T1509	E1510	E1511	L1512	P1513	S1514	L1515	E1516	M1517	A1518	L1519	E1520	Y1521	Y1522	E1523	L1524	T1525	M1526	E1527	R1528	I1529	S1530	M1531	C1532	Y1533	Q1534	R1535	P1536	H1537	W1538	L1539							
R1540	S1541	L1542	S1543	V1544	H1545	P1546	L1547	S1548	M1549	L1550	L1551	D1556	P1557	A1558	G1561	F1562	F1563	S1564	M1565	Y1566	E1567	K1568	A1569	F1570	F1571	L1572	E1573	K1574	Y1575	L1576	Q1577	E1578	H1579	E1580	E1581	D1582	Q1583	E1584	K1585	V1586	E1587	L1588	L1589	K1590	T1593	Q1596	M1597	P1598	L1599	L1600	T1601	E1602	G1603	T1604	R1605									
I1606	H1607	G1608	E1609	K1610	L1611	L1612	E1613	Q1614	L1615	M1616	L1617	L1618	H1619	E1620	L1621	L1622	S1623	S1624	C1625	F1626	R1627	E1628	L1629	E1631	K1632	E1633	E1634	K1635	H1636	L1637	V1639	L1642																																

• Molecule 3: Ras-related C3 botulinum toxin substrate 1

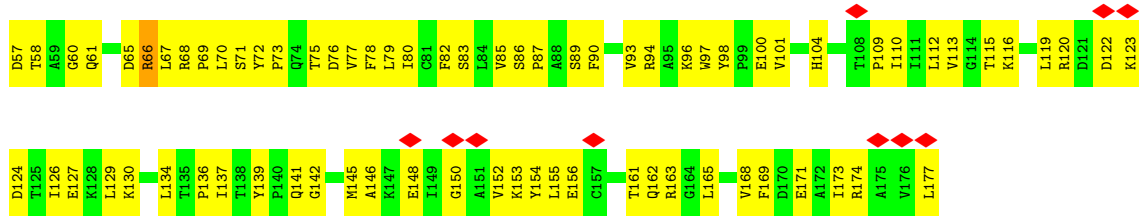


GLY	SER	GLY	SER	SER	GLY	M1	Q2	A3	I4	K5	C6	V7	V8	V9	G10	D11	G12	A13	V14	A15	K16	T17	L20	I21	Y23	T24	T25	N26	A27	F28	P29	R30	G30	E31	Y32	I33	P34	T35	V36	F37	D38	N39	Y40	S41	A42	N43	V44	M45	V46	D47	G48	K49	P50	V51	N52	L53	L53	D122
R56	D57	T58	A59	G60	Q61	D65	R66	L67	R68	P69	L70	S71	Y72	P73	T75	D76	V77	F78	L79	I80	C81	F82	S83	L84	W85	S86	R87	F90	Y93	R94	A95	K96	H97	Y98	P99	E100	V101	H104	M107	T108	P109	L110	I111	L112	L113	G114	T115	K116	L119	R120	D121	D122						
K123	D124	T125	I126	E127	K128	L129	K130	L134	T136	P136	I137	L138	Y139	P140	Q141	G142	L143	A144	M145	A146	K147	E148	L149	G150	A151	V152	K153	Y154	L155	E156	C157	T161	Q162	R163	G164	L165	K166	T167	V168	F169	D170	E171	A172	L173	R174	A175	V176	L177										

• Molecule 3: Ras-related C3 botulinum toxin substrate 1



GLY	SER	GLY	SER	SER	GLY	M1	Q2	A3	I4	K5	C6	V7	V8	V9	G10	D11	G12	A13	V14	A15	K16	T17	L20	I21	Y23	T24	T25	N26	A27	F28	P29	R30	G30	E31	Y32	I33	P34	T35	V36	F37	D38	N39	Y40	S41	A42	N43	V44	M45	V46	K49	P50	V51	N52	L53	L53	W56
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	156585	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.052	Depositor
Minimum map value	-0.015	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	452.2, 452.2, 452.2	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.33, 1.33, 1.33	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.33	0/1641	0.55	0/2218
1	D	0.33	0/1641	0.56	0/2218
2	B	0.36	0/13722	0.54	1/18514 (0.0%)
2	E	0.36	0/13722	0.54	1/18514 (0.0%)
3	C	0.32	0/1415	0.50	0/1924
3	F	0.32	0/1415	0.50	0/1924
All	All	0.35	0/33556	0.54	2/45312 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
2	B	0	1
2	E	0	1
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1338	LEU	CA-CB-CG	5.62	128.24	115.30
2	B	1338	LEU	CA-CB-CG	5.61	128.19	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	541	GLN	Peptide

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Mol	Chain	Res	Type	Group
2	B	1041	GLN	Peptide
1	D	541	GLN	Peptide
2	E	1041	GLN	Peptide

5.2 Too-close contacts [i](#)

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	1608	0	1617	136	0
1	D	1608	0	1617	148	0
2	B	13436	0	13516	1369	0
2	E	13436	0	13516	1393	0
3	C	1385	0	1407	129	0
3	F	1385	0	1407	128	0
All	All	32858	0	33080	3217	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 49.

All (3217) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:929:MET:HA	2:E:933:LEU:HD13	1.43	1.01
1:A:701:LEU:HD23	2:B:31:ILE:HG23	1.43	1.00
2:B:929:MET:HA	2:B:933:LEU:HD13	1.43	0.99
2:E:1545:HIS:HB2	3:F:5:LYS:HE2	1.49	0.95
2:E:657:LEU:HD23	2:E:696:ALA:HB1	1.51	0.93
1:A:711:PRO:HG2	2:B:16:ILE:HG21	1.50	0.92
2:B:657:LEU:HD23	2:B:696:ALA:HB1	1.51	0.92
2:E:1587:GLU:HA	2:E:1590:LYS:HD2	1.53	0.91
2:E:102:TRP:HB2	2:E:114:PHE:HE1	1.36	0.91
2:B:5:ILE:H	2:B:40:MET:H	1.19	0.90
2:E:1484:ILE:HB	2:E:1512:ILE:HD12	1.53	0.90
2:B:657:LEU:HD21	2:B:700:ILE:HD11	1.54	0.90
2:B:1587:GLU:HA	2:B:1590:LYS:HD2	1.53	0.89
2:B:102:TRP:HB2	2:B:114:PHE:HE1	1.36	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:5:ILE:H	2:E:40:MET:H	1.19	0.88
2:B:1526:ASN:HA	2:B:1529:ILE:HD12	1.56	0.88
2:B:1484:ILE:HB	2:B:1512:ILE:HD12	1.53	0.88
2:E:10:GLN:HG3	2:E:37:ILE:HB	1.56	0.87
2:E:1526:ASN:HA	2:E:1529:ILE:HD12	1.56	0.87
2:B:239:ALA:HB3	2:B:262:TRP:HB3	1.57	0.87
2:E:657:LEU:HD21	2:E:700:ILE:HD11	1.54	0.87
2:B:10:GLN:HG3	2:B:37:ILE:HB	1.56	0.85
3:C:87:PRO:HG2	3:C:134:LEU:HB3	1.58	0.85
1:D:580:SER:HA	1:D:587:HIS:HE1	1.41	0.85
2:E:239:ALA:HB3	2:E:262:TRP:HB3	1.57	0.85
2:B:764:PHE:HD2	2:B:767:ILE:HD12	1.41	0.85
2:E:738:ASN:HA	2:E:794:LEU:HD13	1.58	0.85
1:A:580:SER:HA	1:A:587:HIS:HE1	1.42	0.85
2:B:376:ASN:ND2	2:B:502:TYR:O	2.10	0.84
2:B:738:ASN:HA	2:B:794:LEU:HD13	1.59	0.84
3:C:171:GLU:HA	3:C:174:ARG:HG2	1.59	0.83
2:E:677:PHE:HB3	2:E:726:ALA:HB2	1.60	0.83
2:E:764:PHE:HD2	2:E:767:ILE:HD12	1.41	0.83
2:E:166:ARG:NH1	2:E:167:ASP:OD1	2.11	0.83
2:E:376:ASN:ND2	2:E:502:TYR:O	2.11	0.83
3:C:65:ASP:HA	3:C:68:ARG:HG2	1.61	0.83
2:B:166:ARG:NH1	2:B:167:ASP:OD1	2.11	0.83
2:B:1567:GLU:HA	2:B:1571:PHE:HB2	1.61	0.83
3:F:87:PRO:HG2	3:F:134:LEU:HB3	1.58	0.83
2:B:242:PHE:HB2	2:B:299:GLN:HB2	1.61	0.83
2:E:4:TRP:HB3	2:E:39:GLU:HB3	1.61	0.82
2:E:1418:ILE:HG13	2:E:1425:TYR:CD2	2.15	0.82
2:B:1418:ILE:HG13	2:B:1425:TYR:CD2	2.15	0.82
3:C:1:MET:SD	3:C:49:LYS:NZ	2.51	0.82
2:B:677:PHE:HB3	2:B:726:ALA:HB2	1.60	0.82
2:E:242:PHE:HB2	2:E:299:GLN:HB2	1.61	0.82
3:F:65:ASP:HA	3:F:68:ARG:HG2	1.61	0.82
3:F:1:MET:SD	3:F:49:LYS:NZ	2.51	0.82
2:B:1557:PRO:HB2	2:B:1561:GLY:HA2	1.62	0.82
3:C:7:VAL:HA	3:C:56:TRP:HB2	1.61	0.82
2:E:730:TYR:HA	2:E:767:ILE:HG23	1.61	0.82
2:E:1006:TRP:O	2:E:1010:ASN:N	2.12	0.81
3:F:96:LYS:HD2	3:F:100:GLU:HG3	1.62	0.81
2:B:4:TRP:HB3	2:B:39:GLU:HB3	1.61	0.81
2:E:1557:PRO:HB2	2:E:1561:GLY:HA2	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1432:LYS:N	2:B:1463:ARG:O	2.12	0.81
1:D:551:GLN:OE1	1:D:552:ARG:NH2	2.14	0.81
3:C:96:LYS:HD2	3:C:100:GLU:HG3	1.62	0.81
3:F:171:GLU:HA	3:F:174:ARG:HG2	1.59	0.81
2:B:1251:HIS:HB3	2:B:1256:ASN:HB2	1.62	0.81
2:B:1006:TRP:O	2:B:1010:ASN:N	2.12	0.81
2:E:1314:TRP:HB3	2:E:1348:PHE:HB3	1.61	0.81
2:B:1444:LYS:NZ	2:E:1330:SER:O	2.13	0.81
3:F:7:VAL:HA	3:F:56:TRP:HB2	1.61	0.81
2:B:730:TYR:HA	2:B:767:ILE:HG23	1.61	0.81
2:E:1567:GLU:HA	2:E:1571:PHE:HB2	1.61	0.80
1:A:551:GLN:OE1	1:A:552:ARG:NH2	2.14	0.80
2:B:165:VAL:HG23	2:B:175:PRO:HD3	1.62	0.80
2:B:1314:TRP:HB3	2:B:1348:PHE:HB3	1.61	0.80
2:B:241:LEU:HB2	2:B:260:ILE:HB	1.63	0.80
2:E:347:PRO:HB2	2:E:392:VAL:HB	1.64	0.80
2:E:1561:GLY:O	2:E:1565:ASN:N	2.15	0.80
2:E:1251:HIS:HB3	2:E:1256:ASN:HB2	1.62	0.80
2:B:1382:ILE:N	2:B:1502:PHE:O	2.15	0.79
2:E:1488:THR:HB	2:E:1508:SER:HB2	1.64	0.79
2:E:1169:LYS:HA	2:E:1172:LEU:HD12	1.65	0.79
1:A:724:TYR:HB3	2:B:4:TRP:HB2	1.63	0.79
2:E:165:VAL:HG23	2:E:175:PRO:HD3	1.62	0.79
2:E:241:LEU:HB2	2:E:260:ILE:HB	1.63	0.79
2:E:1382:ILE:N	2:E:1502:PHE:O	2.15	0.79
2:E:467:GLU:HB2	2:E:500:VAL:HG22	1.65	0.79
2:E:740:TYR:HA	2:E:749:LYS:HD3	1.65	0.79
2:E:1357:ARG:HH22	2:E:1456:ALA:H	1.31	0.79
2:E:1283:LEU:O	2:E:1285:ARG:NH1	2.16	0.79
3:C:77:VAL:HG12	3:C:109:PRO:HG2	1.65	0.79
2:B:1128:PHE:HA	2:B:1131:MET:SD	2.23	0.79
2:E:1128:PHE:HA	2:E:1131:MET:SD	2.23	0.79
2:B:347:PRO:HB2	2:B:392:VAL:HB	1.64	0.79
2:E:18:ASN:HB3	2:E:28:SER:HB2	1.63	0.78
2:E:1378:ASN:ND2	2:E:1419:LYS:O	2.16	0.78
2:E:889:GLN:OE1	2:E:895:ASN:ND2	2.17	0.78
2:B:1169:LYS:HA	2:B:1172:LEU:HD12	1.65	0.78
2:B:889:GLN:OE1	2:B:895:ASN:ND2	2.17	0.78
2:B:929:MET:HG2	2:B:933:LEU:HD22	1.66	0.78
2:B:1291:TYR:HB3	2:B:1296:LEU:HD21	1.65	0.78
1:A:637:VAL:HG12	1:A:640:LEU:HD12	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:ASN:HB3	2:B:28:SER:HB2	1.63	0.78
1:D:637:VAL:HG12	1:D:640:LEU:HD12	1.65	0.77
2:B:740:TYR:HA	2:B:749:LYS:HD3	1.65	0.77
2:E:46:ARG:HB3	2:E:58:ILE:HG13	1.67	0.77
3:F:77:VAL:HG12	3:F:109:PRO:HG2	1.65	0.77
2:B:1283:LEU:O	2:B:1285:ARG:NH1	2.16	0.77
1:D:640:LEU:HB3	1:D:656:ALA:H	1.49	0.77
2:B:467:GLU:HB2	2:B:500:VAL:HG22	1.65	0.77
2:E:929:MET:HG2	2:E:933:LEU:HD22	1.66	0.77
2:B:1378:ASN:ND2	2:B:1419:LYS:O	2.16	0.77
2:E:1291:TYR:HB3	2:E:1296:LEU:HD21	1.65	0.77
1:D:698:LEU:HA	2:E:31:ILE:HG21	1.66	0.77
2:E:764:PHE:CD2	2:E:767:ILE:HD12	2.20	0.77
2:E:1407:LYS:HG3	2:E:1426:MET:HB2	1.67	0.77
2:E:1056:HIS:ND1	2:E:1057:GLU:OE2	2.17	0.77
2:B:764:PHE:CD2	2:B:767:ILE:HD12	2.20	0.77
2:B:1056:HIS:ND1	2:B:1057:GLU:OE2	2.17	0.77
2:B:1488:THR:HB	2:B:1508:SER:HB2	1.64	0.77
2:E:1524:LEU:HD12	2:E:1528:ARG:HH21	1.49	0.77
1:D:701:LEU:HD11	2:E:16:ILE:HA	1.66	0.77
3:F:2:GLN:HG2	3:F:51:VAL:HG23	1.67	0.77
2:B:1357:ARG:HE	2:B:1453:TYR:HA	1.50	0.76
2:E:37:ILE:HA	2:E:47:GLY:HA3	1.68	0.76
1:A:670:ASN:ND2	1:A:676:ASP:O	2.19	0.76
1:A:640:LEU:HB3	1:A:656:ALA:H	1.50	0.76
2:B:816:ALA:O	2:B:820:LEU:HB2	1.86	0.76
2:B:1028:LEU:HD21	2:B:1042:LEU:HD23	1.68	0.76
2:E:1155:LEU:HD11	2:E:1201:LEU:HD21	1.68	0.76
2:B:904:GLN:O	2:B:908:ASN:ND2	2.19	0.76
2:E:921:THR:O	2:E:925:ILE:N	2.19	0.76
2:B:37:ILE:HA	2:B:47:GLY:HA3	1.68	0.76
2:B:61:GLU:HA	2:B:64:ILE:HB	1.68	0.76
2:B:1524:LEU:HD12	2:B:1528:ARG:HH21	1.49	0.76
2:E:1357:ARG:HE	2:E:1453:TYR:HA	1.50	0.76
2:E:1252:ARG:NH1	2:E:1253:ASP:OD1	2.19	0.76
2:B:676:LEU:HA	2:B:679:ILE:HD12	1.68	0.76
2:B:1407:LYS:HG3	2:B:1426:MET:HB2	1.67	0.76
2:B:921:THR:O	2:B:925:ILE:N	2.19	0.76
2:B:1357:ARG:HH22	2:B:1456:ALA:H	1.31	0.76
2:B:1490:THR:O	2:B:1505:LYS:N	2.19	0.76
2:B:1561:GLY:O	2:B:1565:ASN:N	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:13:GLY:HA3	2:E:35:VAL:HG22	1.67	0.76
2:E:1490:THR:O	2:E:1505:LYS:N	2.19	0.76
2:B:1436:SER:HB3	2:B:1454:TYR:HB3	1.68	0.75
2:E:816:ALA:O	2:E:820:LEU:HB2	1.86	0.75
2:B:1155:LEU:HD11	2:B:1201:LEU:HD21	1.68	0.75
2:E:25:VAL:HG23	2:E:57:GLY:HA2	1.69	0.75
2:B:46:ARG:HB3	2:B:58:ILE:HG13	1.67	0.75
2:E:1028:LEU:HD21	2:E:1042:LEU:HD23	1.68	0.75
2:E:904:GLN:O	2:E:908:ASN:ND2	2.19	0.75
2:B:13:GLY:HA3	2:B:35:VAL:HG22	1.67	0.75
2:B:1252:ARG:NH1	2:B:1253:ASP:OD1	2.19	0.75
3:C:2:GLN:HG2	3:C:51:VAL:HG23	1.67	0.75
2:E:163:LEU:HD21	2:E:194:ILE:HD11	1.69	0.75
2:E:1432:LYS:N	2:E:1463:ARG:O	2.12	0.75
2:B:519:ILE:HG21	2:B:630:LYS:HB3	1.68	0.74
2:E:61:GLU:HA	2:E:64:ILE:HB	1.68	0.74
2:E:519:ILE:HG21	2:E:630:LYS:HB3	1.68	0.74
1:D:530:SER:HA	1:D:533:ILE:HD12	1.69	0.74
2:B:809:ALA:HB1	2:B:812:ILE:HB	1.70	0.74
2:E:676:LEU:HA	2:E:679:ILE:HD12	1.68	0.74
2:E:925:ILE:HA	2:E:928:ILE:HD12	1.69	0.74
2:E:1057:GLU:O	2:E:1080:ARG:NH1	2.21	0.74
2:B:297:VAL:HG22	2:B:326:VAL:HG22	1.69	0.74
2:B:319:ARG:O	2:B:500:VAL:N	2.20	0.74
1:D:670:ASN:ND2	1:D:676:ASP:O	2.19	0.74
2:E:1059:LEU:HD12	2:E:1116:PRO:HB2	1.70	0.74
2:B:288:ASP:HA	2:B:291:ARG:HE	1.52	0.74
2:B:1135:GLU:HA	2:B:1138:PHE:HB3	1.68	0.74
1:D:607:LYS:HG3	1:D:609:PRO:HD3	1.70	0.74
2:E:1586:VAL:HG23	2:E:1589:LEU:HD12	1.69	0.74
2:B:925:ILE:HA	2:B:928:ILE:HD12	1.69	0.74
2:B:1028:LEU:HA	2:B:1032:PHE:HD1	1.52	0.74
2:B:254:ILE:O	2:B:431:MET:N	2.20	0.74
2:B:1114:LEU:HB3	2:B:1163:ARG:HD2	1.70	0.74
2:B:1545:HIS:HB2	3:C:5:LYS:HE2	1.70	0.74
2:B:1567:GLU:HG3	2:B:1636:HIS:HE1	1.53	0.74
1:D:561:CYS:SG	1:D:594:SER:OG	2.46	0.74
2:E:1381:PHE:HA	2:E:1503:GLU:HA	1.69	0.74
2:E:1436:SER:HB3	2:E:1454:TYR:HB3	1.68	0.74
2:E:1521:THR:OG1	2:E:1566:TYR:OH	2.05	0.74
3:F:39:ASN:H	3:F:57:ASP:HB3	1.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:561:CYS:SG	1:A:594:SER:OG	2.46	0.73
2:B:1217:LYS:HD3	2:B:1220:ARG:HH12	1.52	0.73
3:C:93:VAL:HA	3:C:97:TRP:HB2	1.70	0.73
2:E:80:VAL:HG22	2:E:85:LEU:HD11	1.70	0.73
2:E:319:ARG:O	2:E:500:VAL:N	2.20	0.73
2:E:1217:LYS:HD3	2:E:1220:ARG:HH12	1.52	0.73
2:E:1028:LEU:HA	2:E:1032:PHE:HD1	1.52	0.73
2:B:1059:LEU:HD12	2:B:1116:PRO:HB2	1.70	0.73
2:B:1586:VAL:HG23	2:B:1589:LEU:HD12	1.69	0.73
2:E:12:TYR:HB2	2:E:67:LYS:HB2	1.69	0.73
1:A:530:SER:HA	1:A:533:ILE:HD12	1.69	0.73
2:E:256:GLU:OE1	2:E:447:TYR:OH	2.06	0.73
2:E:288:ASP:HA	2:E:291:ARG:HE	1.52	0.73
2:B:12:TYR:HB2	2:B:67:LYS:HB2	1.69	0.73
2:B:1381:PHE:HA	2:B:1503:GLU:HA	1.69	0.73
3:C:39:ASN:H	3:C:57:ASP:HB3	1.53	0.73
2:E:1114:LEU:HB3	2:E:1163:ARG:HD2	1.70	0.73
2:E:1488:THR:N	2:E:1508:SER:O	2.22	0.73
1:D:722:PHE:HE1	2:E:1:MET:HB3	1.52	0.73
2:B:25:VAL:HG23	2:B:57:GLY:HA2	1.69	0.73
2:B:163:LEU:HD21	2:B:194:ILE:HD11	1.69	0.73
2:E:1135:GLU:HA	2:E:1138:PHE:HB3	1.68	0.73
2:B:256:GLU:OE1	2:B:447:TYR:OH	2.06	0.73
2:B:105:LEU:HD22	2:B:110:LYS:HD3	1.71	0.72
2:E:1567:GLU:HG3	2:E:1636:HIS:HE1	1.53	0.72
2:E:225:TYR:HA	2:E:280:VAL:HG22	1.70	0.72
2:E:809:ALA:HB1	2:E:812:ILE:HB	1.70	0.72
3:F:9:VAL:HG21	3:F:101:VAL:HG21	1.71	0.72
1:A:607:LYS:HG3	1:A:609:PRO:HD3	1.70	0.72
2:B:1488:THR:N	2:B:1508:SER:O	2.22	0.72
2:B:1633:VAL:HA	2:B:1637:TYR:HB2	1.71	0.72
2:E:105:LEU:HD22	2:E:110:LYS:HD3	1.71	0.72
2:E:297:VAL:HG22	2:E:326:VAL:HG22	1.69	0.72
2:B:225:TYR:HA	2:B:280:VAL:HG22	1.70	0.72
2:E:1536:HIS:NE2	2:E:1609:GLU:OE2	2.21	0.72
2:B:1057:GLU:O	2:B:1080:ARG:NH1	2.21	0.72
2:E:1633:VAL:HA	2:E:1637:TYR:HB2	1.71	0.72
3:F:93:VAL:HA	3:F:97:TRP:HB2	1.70	0.72
2:B:80:VAL:HG22	2:B:85:LEU:HD11	1.70	0.72
2:B:737:LEU:HD12	2:B:740:TYR:HB2	1.72	0.72
2:E:737:LEU:HD12	2:E:740:TYR:HB2	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:896:LYS:HG3	2:E:897:PRO:HD3	1.71	0.72
2:B:1081:LYS:HE3	2:B:1119:GLU:HB2	1.72	0.72
2:B:771:ARG:NH1	2:B:781:SER:OG	2.23	0.71
3:C:9:VAL:HG21	3:C:101:VAL:HG21	1.72	0.71
2:E:771:ARG:NH1	2:E:781:SER:OG	2.23	0.71
2:B:928:ILE:HA	2:B:932:LEU:HD13	1.72	0.71
2:E:979:ARG:NH2	2:E:1035:GLN:OE1	2.24	0.71
2:E:1110:LEU:HD21	2:E:1151:LEU:HG	1.72	0.71
2:B:482:LYS:HE2	2:B:491:GLU:HG2	1.73	0.71
2:B:1080:ARG:NH2	2:B:1117:GLU:OE2	2.23	0.71
2:E:695:ASP:OD1	2:E:740:TYR:OH	2.08	0.71
2:E:1080:ARG:NH2	2:E:1117:GLU:OE2	2.23	0.71
2:E:1081:LYS:HE3	2:E:1119:GLU:HB2	1.72	0.71
2:B:979:ARG:NH2	2:B:1035:GLN:OE1	2.24	0.71
2:E:1019:ARG:O	2:E:1023:GLN:NE2	2.21	0.71
2:B:1099:ILE:HA	2:B:1102:ILE:HD12	1.72	0.71
2:E:879:LEU:HD23	2:E:927:LEU:HD22	1.73	0.71
2:E:1099:ILE:HA	2:E:1102:ILE:HD12	1.72	0.71
2:B:12:TYR:HA	2:B:34:THR:HG23	1.72	0.71
2:B:1102:ILE:HG12	2:B:1131:MET:HB2	1.73	0.71
2:B:103:ARG:HH12	2:B:104:LYS:HE3	1.55	0.71
2:B:896:LYS:HG3	2:B:897:PRO:HD3	1.71	0.71
2:E:928:ILE:HA	2:E:932:LEU:HD13	1.72	0.70
2:E:1102:ILE:HG12	2:E:1131:MET:HB2	1.73	0.70
2:E:1328:TYR:HB3	2:E:1338:LEU:HD22	1.72	0.70
2:E:1033:MET:SD	2:E:1093:ASN:ND2	2.65	0.70
1:A:701:LEU:HD11	2:B:16:ILE:HA	1.72	0.70
2:B:1059:LEU:O	2:B:1063:THR:OG1	2.09	0.70
2:E:1410:SER:OG	2:E:1413:PRO:O	2.08	0.70
2:B:575:ASP:HB3	2:B:578:LYS:HB2	1.73	0.70
2:B:1328:TYR:HB3	2:B:1338:LEU:HD22	1.72	0.70
2:B:1410:SER:OG	2:B:1413:PRO:O	2.08	0.70
2:E:103:ARG:HH12	2:E:104:LYS:HE3	1.55	0.70
2:E:472:VAL:HG22	2:E:527:ILE:HG12	1.73	0.70
3:F:66:ARG:HG2	3:F:67:LEU:HG	1.74	0.70
3:F:87:PRO:HA	3:F:137:ILE:HD11	1.73	0.70
2:B:964:MET:HG2	2:B:969:TYR:CE1	2.27	0.70
2:B:1110:LEU:HD21	2:B:1151:LEU:HG	1.72	0.70
2:B:1622:LEU:O	2:B:1626:PHE:HB3	1.91	0.70
2:E:12:TYR:HA	2:E:34:THR:HG23	1.72	0.70
2:E:1322:LYS:HD3	2:E:1345:ARG:NH1	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:879:LEU:HD23	2:B:927:LEU:HD22	1.73	0.70
2:E:1622:LEU:O	2:E:1626:PHE:HB3	1.91	0.70
2:E:1630:LYS:O	2:E:1634:GLU:HG2	1.92	0.70
2:E:98:TRP:O	2:E:101:ILE:HG22	1.91	0.70
2:E:254:ILE:O	2:E:431:MET:N	2.20	0.70
2:B:472:VAL:HG22	2:B:527:ILE:HG12	1.73	0.70
2:E:1218:GLU:OE1	2:E:1218:GLU:N	2.25	0.70
2:B:695:ASP:OD1	2:B:740:TYR:OH	2.08	0.70
2:B:1630:LYS:O	2:B:1634:GLU:HG2	1.92	0.70
2:E:451:ILE:HD11	2:E:623:ALA:HB2	1.74	0.70
2:E:575:ASP:HB3	2:E:578:LYS:HB2	1.73	0.70
2:E:1294:GLN:N	2:E:1294:GLN:OE1	2.25	0.70
2:B:451:ILE:HD12	2:B:621:GLN:HG2	1.74	0.69
2:E:482:LYS:HE2	2:E:491:GLU:HG2	1.73	0.69
2:B:775:LEU:HD23	2:B:781:SER:HB2	1.74	0.69
2:B:1231:TYR:O	2:B:1235:LYS:N	2.25	0.69
2:B:1322:LYS:HD3	2:B:1345:ARG:NH1	2.06	0.69
3:C:71:SER:O	3:C:75:THR:OG1	2.09	0.69
2:E:964:MET:HG2	2:E:969:TYR:CE1	2.27	0.69
2:E:1121:ARG:O	2:E:1125:ILE:HD12	1.91	0.69
2:E:1231:TYR:O	2:E:1235:LYS:N	2.25	0.69
2:E:1428:CYS:SG	2:E:1429:PHE:N	2.65	0.69
2:B:1006:TRP:HB3	2:B:1009:MET:HB2	1.73	0.69
2:B:1033:MET:SD	2:B:1093:ASN:ND2	2.65	0.69
2:E:1231:TYR:HD1	2:E:1236:ARG:HB3	1.58	0.69
2:B:1121:ARG:O	2:B:1125:ILE:HD12	1.91	0.69
2:E:451:ILE:HD12	2:E:621:GLN:HG2	1.74	0.69
2:B:98:TRP:O	2:B:101:ILE:HG22	1.92	0.69
2:B:1218:GLU:OE1	2:B:1218:GLU:N	2.25	0.69
3:F:39:ASN:HA	3:F:57:ASP:H	1.57	0.69
2:B:1294:GLN:OE1	2:B:1294:GLN:N	2.24	0.69
2:B:1521:THR:OG1	2:B:1566:TYR:OH	2.06	0.69
2:E:1006:TRP:HB3	2:E:1009:MET:HB2	1.73	0.69
3:C:119:LEU:HA	3:C:122:ASP:HB2	1.75	0.69
2:E:445:ASP:HB3	2:E:447:TYR:HE2	1.58	0.69
2:B:1231:TYR:HD1	2:B:1236:ARG:HB3	1.58	0.69
2:B:1428:CYS:SG	2:B:1429:PHE:N	2.65	0.69
3:C:39:ASN:HA	3:C:57:ASP:H	1.57	0.69
3:C:66:ARG:HG2	3:C:67:LEU:HG	1.73	0.69
1:D:584:LYS:HD2	2:E:1403:PRO:HA	1.74	0.69
2:E:954:VAL:O	2:E:958:ILE:HG12	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:PHE:HE1	2:B:1:MET:HB3	1.56	0.68
2:B:451:ILE:HD11	2:B:623:ALA:HB2	1.74	0.68
3:C:87:PRO:HA	3:C:137:ILE:HD11	1.73	0.68
2:E:41:TYR:HD2	2:E:44:TRP:HB2	1.59	0.68
2:E:474:ASP:HA	2:E:525:CYS:HA	1.75	0.68
2:E:1357:ARG:HH12	2:E:1456:ALA:HB3	1.58	0.68
2:B:928:ILE:HG23	2:B:932:LEU:HD22	1.76	0.68
2:B:1357:ARG:HH12	2:B:1456:ALA:HB3	1.58	0.68
2:E:954:VAL:HA	2:E:957:MET:SD	2.33	0.68
2:E:871:GLN:HE22	2:E:913:LEU:HA	1.58	0.68
2:E:1404:ASN:OD1	2:E:1424:GLN:HB2	1.93	0.68
2:E:36:HIS:N	2:E:48:TYR:O	2.27	0.68
2:E:879:LEU:HD22	2:E:924:HIS:CE1	2.29	0.68
3:F:71:SER:O	3:F:75:THR:OG1	2.09	0.68
2:B:1024:PHE:HA	2:B:1027:VAL:HG12	1.76	0.68
2:E:1307:TYR:O	2:E:1311:GLY:N	2.27	0.68
3:F:119:LEU:HA	3:F:122:ASP:HB2	1.75	0.68
2:E:166:ARG:O	2:E:171:ASN:HA	1.94	0.68
2:E:485:HIS:HB2	2:E:514:LYS:HB3	1.76	0.68
2:B:166:ARG:O	2:B:171:ASN:HA	1.94	0.68
2:B:445:ASP:HB3	2:B:447:TYR:HE2	1.58	0.68
2:E:449:THR:HB	2:E:623:ALA:HB3	1.76	0.68
2:E:1135:GLU:O	2:E:1139:SER:N	2.27	0.68
2:B:871:GLN:HE22	2:B:913:LEU:HA	1.58	0.67
2:B:1404:ASN:OD1	2:B:1424:GLN:HB2	1.93	0.67
2:B:41:TYR:HD2	2:B:44:TRP:HB2	1.59	0.67
2:E:95:LEU:HD21	2:E:124:LEU:HD13	1.75	0.67
2:E:775:LEU:HD23	2:E:781:SER:HB2	1.74	0.67
2:E:1597:MET:HG3	2:E:1600:LEU:HD12	1.76	0.67
2:B:954:VAL:HA	2:B:957:MET:SD	2.34	0.67
2:B:1120:LEU:O	2:B:1124:THR:OG1	2.11	0.67
2:B:1597:MET:HG3	2:B:1600:LEU:HD12	1.76	0.67
3:C:37:PHE:HB2	3:C:40:TYR:HE1	1.60	0.67
2:E:928:ILE:HG23	2:E:932:LEU:HD22	1.76	0.67
2:B:36:HIS:N	2:B:48:TYR:O	2.27	0.67
2:B:471:SER:O	2:B:528:ARG:N	2.27	0.67
2:B:474:ASP:HA	2:B:525:CYS:HA	1.75	0.67
2:B:1333:PHE:HZ	2:E:1444:LYS:HD3	1.60	0.67
2:E:5:ILE:HB	2:E:40:MET:HB2	1.75	0.67
2:E:1059:LEU:O	2:E:1063:THR:OG1	2.09	0.67
3:F:37:PHE:HB2	3:F:40:TYR:HE1	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:613:ILE:HD13	1:A:646:TYR:HB3	1.76	0.67
3:C:130:LYS:HE3	3:C:136:PRO:HD3	1.76	0.67
1:D:613:ILE:HD13	1:D:646:TYR:HB3	1.76	0.67
2:E:471:SER:O	2:E:528:ARG:N	2.27	0.67
2:E:485:HIS:N	2:E:514:LYS:O	2.22	0.67
2:E:1388:TYR:HD2	3:F:45:MET:HE2	1.60	0.67
2:B:4:TRP:CE2	2:B:46:ARG:HD3	2.30	0.67
2:B:240:GLU:OE2	2:B:319:ARG:NE	2.26	0.67
2:B:954:VAL:O	2:B:958:ILE:HG12	1.93	0.67
2:B:1307:TYR:O	2:B:1311:GLY:N	2.27	0.67
2:E:102:TRP:HB2	2:E:114:PHE:CE1	2.27	0.67
2:B:105:LEU:HD13	2:B:110:LYS:HZ2	1.60	0.67
2:E:1364:ALA:HA	2:E:1382:ILE:HA	1.77	0.67
2:B:5:ILE:HB	2:B:40:MET:HB2	1.76	0.67
2:B:879:LEU:HD22	2:B:924:HIS:CE1	2.29	0.67
2:B:1135:GLU:O	2:B:1139:SER:N	2.27	0.67
2:B:1536:HIS:NE2	2:B:1609:GLU:OE2	2.21	0.67
3:C:61:GLN:O	3:C:68:ARG:NH2	2.28	0.67
2:E:890:LEU:HD12	2:E:935:ARG:HG3	1.77	0.67
2:E:972:TYR:OH	2:E:977:LYS:NZ	2.27	0.67
1:A:567:ALA:HA	1:A:571:GLN:HB2	1.78	0.66
2:B:95:LEU:HD21	2:B:124:LEU:HD13	1.75	0.66
2:B:485:HIS:HB2	2:B:514:LYS:HB3	1.76	0.66
2:B:1491:THR:HG22	2:B:1493:TYR:H	1.59	0.66
2:B:1536:HIS:HD2	2:B:1606:ILE:HB	1.60	0.66
2:E:1120:LEU:O	2:E:1124:THR:OG1	2.11	0.66
2:B:96:ARG:NH1	2:B:97:GLU:OE2	2.28	0.66
2:E:79:THR:HA	2:E:85:LEU:HD22	1.78	0.66
2:E:95:LEU:HA	2:E:98:TRP:HD1	1.60	0.66
2:E:172:ILE:HA	2:E:175:PRO:HG2	1.77	0.66
3:F:61:GLN:O	3:F:68:ARG:NH2	2.28	0.66
2:B:172:ILE:HA	2:B:175:PRO:HG2	1.77	0.66
2:B:860:MET:HA	2:B:863:ILE:HD12	1.76	0.66
2:B:890:LEU:HD12	2:B:935:ARG:HG3	1.77	0.66
3:C:100:GLU:O	3:C:104:HIS:ND1	2.27	0.66
2:E:938:ARG:HA	2:E:941:ILE:HD12	1.78	0.66
2:E:946:GLN:HA	2:E:950:ILE:HG21	1.77	0.66
2:B:449:THR:HB	2:B:623:ALA:HB3	1.76	0.66
2:B:1364:ALA:HA	2:B:1382:ILE:HA	1.77	0.66
2:B:95:LEU:HA	2:B:98:TRP:HD1	1.60	0.66
2:E:860:MET:HA	2:E:863:ILE:HD12	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1491:THR:HG22	2:E:1493:TYR:H	1.59	0.66
3:F:100:GLU:O	3:F:104:HIS:ND1	2.27	0.66
3:F:130:LYS:HE3	3:F:136:PRO:HD3	1.76	0.66
2:B:450:LEU:O	2:B:510:TYR:N	2.28	0.66
2:B:938:ARG:HA	2:B:941:ILE:HD12	1.78	0.66
2:E:1536:HIS:HD2	2:E:1606:ILE:HB	1.60	0.66
1:D:578:ARG:HB3	1:D:587:HIS:HB2	1.77	0.66
2:E:96:ARG:NH1	2:E:97:GLU:OE2	2.28	0.66
1:A:615:ALA:HB3	1:A:645:LEU:HD12	1.78	0.66
2:B:1631:GLU:OE1	2:B:1635:LYS:NZ	2.28	0.66
2:E:1024:PHE:HA	2:E:1027:VAL:HG12	1.76	0.66
2:B:35:VAL:HG12	2:B:49:THR:HA	1.77	0.66
2:B:561:THR:HG21	2:B:631:LEU:HB3	1.77	0.66
2:B:1314:TRP:HB2	2:B:1352:ILE:HD11	1.78	0.66
2:B:1596:GLN:O	2:B:1600:LEU:N	2.26	0.66
2:E:561:THR:HG21	2:E:631:LEU:HB3	1.77	0.66
2:B:946:GLN:HA	2:B:950:ILE:HG21	1.77	0.65
2:B:1369:GLY:N	2:B:1418:ILE:O	2.30	0.65
3:C:4:ILE:HG13	3:C:76:ASP:HB2	1.76	0.65
2:E:35:VAL:HG12	2:E:49:THR:HA	1.77	0.65
2:E:757:LEU:HD23	2:E:760:LEU:HD11	1.79	0.65
2:E:1369:GLY:N	2:E:1418:ILE:O	2.30	0.65
2:E:1631:GLU:OE1	2:E:1635:LYS:NZ	2.28	0.65
1:A:578:ARG:HB3	1:A:587:HIS:HB2	1.77	0.65
1:D:567:ALA:HA	1:D:571:GLN:HB2	1.77	0.65
2:E:136:LEU:HD12	2:E:140:GLU:HG2	1.78	0.65
3:F:4:ILE:HG13	3:F:76:ASP:HB2	1.77	0.65
2:B:79:THR:HG22	2:B:85:LEU:HB2	1.77	0.65
2:B:204:ILE:HG13	2:B:211:ARG:HB3	1.79	0.65
2:E:1367:TYR:O	2:E:1378:ASN:N	2.27	0.65
2:B:94:THR:HG21	2:B:152:ILE:HG12	1.79	0.65
2:B:1586:VAL:HA	2:B:1589:LEU:HG	1.79	0.65
2:E:4:TRP:CE2	2:E:46:ARG:HD3	2.30	0.65
2:E:450:LEU:O	2:E:510:TYR:N	2.28	0.65
2:B:136:LEU:HD12	2:B:140:GLU:HG2	1.78	0.65
2:B:1124:THR:HG23	2:B:1127:ILE:HD12	1.79	0.65
2:B:1372:PHE:O	2:B:1377:ARG:NH2	2.28	0.65
3:C:23:TYR:HB2	3:C:165:LEU:HD21	1.79	0.65
1:D:615:ALA:HB3	1:D:645:LEU:HD12	1.78	0.65
2:E:79:THR:HG22	2:E:85:LEU:HB2	1.77	0.65
2:B:79:THR:HA	2:B:85:LEU:HD22	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1248:ARG:NH1	2:B:1249:ASP:OD1	2.30	0.65
2:E:157:ARG:NH1	2:E:157:ARG:O	2.29	0.65
2:E:243:MET:HG3	2:E:281:PHE:HZ	1.62	0.65
2:E:1314:TRP:HB2	2:E:1352:ILE:HD11	1.78	0.65
2:E:1579:HIS:HB3	2:E:1582:ASP:OD1	1.96	0.65
2:E:204:ILE:HG13	2:E:211:ARG:HB3	1.79	0.65
2:B:1463:ARG:HA	2:B:1487:THR:O	1.96	0.65
2:E:821:PRO:HG3	2:E:863:ILE:HG13	1.79	0.65
2:E:1057:GLU:HA	2:E:1061:LEU:HD13	1.79	0.65
1:A:624:HIS:HD2	1:A:633:GLN:HG3	1.62	0.65
2:B:481:GLU:OE1	2:B:494:SER:OG	2.13	0.65
2:B:1315:GLU:OE1	2:B:1315:GLU:N	2.28	0.65
2:E:1124:THR:HG23	2:E:1127:ILE:HD12	1.79	0.65
2:E:1353:ILE:HA	2:E:1449:GLN:HG2	1.79	0.65
2:E:1463:ARG:HA	2:E:1487:THR:O	1.96	0.65
1:D:576:TYR:HB2	1:D:598:GLU:HG2	1.79	0.65
2:E:1533:VAL:HA	2:E:1606:ILE:HD13	1.79	0.65
2:B:1167:GLN:OE1	2:B:1167:GLN:N	2.31	0.64
2:B:302:ARG:HD3	2:B:322:PHE:HD1	1.61	0.64
2:B:1579:HIS:HB3	2:B:1582:ASP:OD1	1.96	0.64
2:E:302:ARG:HD3	2:E:322:PHE:HD1	1.61	0.64
3:F:12:GLY:H	3:F:60:GLY:HA3	1.62	0.64
3:F:80:ILE:HG23	3:F:112:LEU:HA	1.79	0.64
2:B:102:TRP:HB2	2:B:114:PHE:CE1	2.27	0.64
3:F:23:TYR:HB2	3:F:165:LEU:HD21	1.79	0.64
1:D:667:ASP:OD1	1:D:678:MET:N	2.31	0.64
2:E:1197:VAL:O	2:E:1201:LEU:HG	1.98	0.64
2:E:256:GLU:HB3	2:E:431:MET:HE3	1.80	0.64
2:B:187:HIS:CE1	2:B:1006:TRP:HA	2.33	0.64
2:B:430:LYS:NZ	2:B:433:PHE:O	2.28	0.64
3:C:80:ILE:HG23	3:C:112:LEU:HA	1.79	0.64
2:E:268:PRO:HG2	2:E:274:LEU:HB2	1.80	0.64
2:B:757:LEU:HD23	2:B:760:LEU:HD11	1.79	0.64
1:D:624:HIS:HD2	1:D:633:GLN:HG3	1.62	0.64
2:E:166:ARG:O	2:E:171:ASN:ND2	2.28	0.64
2:E:187:HIS:CE1	2:E:1006:TRP:HA	2.33	0.64
2:E:1586:VAL:HA	2:E:1589:LEU:HG	1.79	0.64
2:B:268:PRO:HG2	2:B:274:LEU:HB2	1.80	0.64
2:B:1336:GLU:OE1	2:B:1336:GLU:N	2.19	0.64
2:E:821:PRO:HB2	2:E:862:LYS:HB3	1.80	0.64
2:B:757:LEU:HD13	2:B:815:ALA:HB3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1390:ARG:NH2	3:C:26:ASN:OD1	2.30	0.64
2:E:1596:GLN:O	2:E:1600:LEU:N	2.26	0.64
3:C:12:GLY:H	3:C:60:GLY:HA3	1.62	0.64
1:D:584:LYS:HG3	1:D:585:VAL:HG13	1.80	0.64
2:E:225:TYR:N	2:E:404:LYS:O	2.28	0.64
2:E:481:GLU:OE1	2:E:494:SER:OG	2.13	0.64
2:B:821:PRO:HB2	2:B:862:LYS:HB3	1.80	0.63
2:B:1353:ILE:HA	2:B:1449:GLN:HG2	1.79	0.63
3:C:116:LYS:HD2	3:C:119:LEU:HD12	1.80	0.63
2:E:187:HIS:NE2	2:E:1006:TRP:HA	2.12	0.63
2:E:1248:ARG:NH1	2:E:1249:ASP:OD1	2.30	0.63
2:E:1495:PHE:HE1	2:E:1502:PHE:HD2	1.45	0.63
3:F:146:ALA:O	3:F:150:GLY:N	2.30	0.63
1:A:667:ASP:OD1	1:A:678:MET:N	2.31	0.63
2:B:821:PRO:HG3	2:B:863:ILE:HG13	1.79	0.63
2:B:1197:VAL:O	2:B:1201:LEU:HG	1.98	0.63
2:E:1280:PRO:HA	2:E:1283:LEU:HB2	1.80	0.63
1:A:576:TYR:HB2	1:A:598:GLU:HG2	1.79	0.63
2:B:243:MET:HG3	2:B:281:PHE:HZ	1.62	0.63
2:B:244:ALA:HB2	2:B:257:ASN:HA	1.80	0.63
2:B:857:LEU:HD22	2:B:905:LEU:HD11	1.80	0.63
2:E:1315:GLU:OE1	2:E:1315:GLU:N	2.29	0.63
1:A:584:LYS:HG3	1:A:585:VAL:HG13	1.80	0.63
2:B:1135:GLU:OE1	2:B:1144:PHE:HA	1.99	0.63
2:B:1361:GLU:OE1	2:B:1361:GLU:N	2.30	0.63
2:B:1533:VAL:HA	2:B:1606:ILE:HD13	1.79	0.63
2:E:569:LEU:N	2:E:620:PHE:O	2.32	0.63
2:E:676:LEU:HB3	2:E:693:VAL:HG13	1.80	0.63
2:B:1057:GLU:HA	2:B:1061:LEU:HD13	1.79	0.63
2:B:1221:MET:HA	2:B:1224:THR:HG22	1.81	0.63
2:E:105:LEU:HD13	2:E:110:LYS:HZ2	1.63	0.63
2:B:182:ALA:HA	2:B:185:LYS:NZ	2.14	0.63
2:B:256:GLU:HB3	2:B:431:MET:HE3	1.79	0.63
2:B:839:LEU:HA	2:B:842:LYS:HD2	1.81	0.63
2:B:1019:ARG:O	2:B:1023:GLN:NE2	2.21	0.63
2:B:1241:ILE:HA	2:B:1244:LEU:HD12	1.81	0.63
2:E:69:ALA:HB2	2:E:78:GLU:HG2	1.81	0.63
2:E:1135:GLU:OE1	2:E:1144:PHE:HA	1.99	0.63
1:A:722:PHE:CE1	2:B:1:MET:HB3	2.33	0.63
2:B:225:TYR:N	2:B:404:LYS:O	2.28	0.63
2:B:973:ILE:HA	2:B:976:PHE:CE2	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1368:TYR:O	2:B:1425:TYR:N	2.31	0.63
2:B:1571:PHE:HA	2:B:1586:VAL:HG21	1.81	0.63
2:E:94:THR:HG21	2:E:152:ILE:HG12	1.79	0.63
2:E:746:ASP:O	2:E:750:THR:OG1	2.10	0.63
2:E:1167:GLN:OE1	2:E:1167:GLN:N	2.31	0.63
2:E:1221:MET:HA	2:E:1224:THR:HG22	1.81	0.63
2:B:285:SER:N	2:B:288:ASP:OD2	2.32	0.63
3:C:21:ILE:HD13	3:C:34:PRO:HA	1.80	0.63
1:D:548:ILE:HG21	1:D:682:THR:HG23	1.81	0.63
2:E:182:ALA:HA	2:E:185:LYS:NZ	2.14	0.63
2:E:760:LEU:HB3	2:E:823:ILE:HG21	1.80	0.63
2:B:187:HIS:NE2	2:B:1006:TRP:HA	2.13	0.63
2:B:569:LEU:N	2:B:620:PHE:O	2.32	0.63
2:B:761:LYS:HB2	2:B:822:SER:HB2	1.80	0.63
2:B:1126:PRO:HB3	2:B:1179:HIS:CE1	2.34	0.63
1:D:551:GLN:HG3	2:E:106:TYR:CE2	2.34	0.63
2:E:244:ALA:HB2	2:E:257:ASN:HA	1.80	0.63
2:E:798:PHE:O	2:E:802:MET:HG3	1.99	0.63
2:E:973:ILE:HA	2:E:976:PHE:CE2	2.34	0.63
2:B:719:TYR:CD1	2:B:723:HIS:HB2	2.34	0.62
2:B:798:PHE:O	2:B:802:MET:HG3	1.99	0.62
2:B:1280:PRO:HA	2:B:1283:LEU:HB2	1.80	0.62
2:E:719:TYR:CD1	2:E:723:HIS:HB2	2.34	0.62
2:E:1336:GLU:OE1	2:E:1336:GLU:N	2.18	0.62
2:E:757:LEU:HD13	2:E:815:ALA:HB3	1.80	0.62
2:E:1126:PRO:HB3	2:E:1179:HIS:CE1	2.34	0.62
2:E:1372:PHE:O	2:E:1377:ARG:NH2	2.28	0.62
2:E:1571:PHE:HA	2:E:1586:VAL:HG21	1.81	0.62
3:F:171:GLU:HG3	3:F:174:ARG:HH11	1.64	0.62
2:B:69:ALA:HB2	2:B:78:GLU:HG2	1.81	0.62
2:B:70:THR:HG22	2:B:71:VAL:H	1.64	0.62
2:E:1361:GLU:OE1	2:E:1361:GLU:N	2.30	0.62
3:F:21:ILE:HD13	3:F:34:PRO:HA	1.81	0.62
1:A:716:GLU:HG3	2:B:44:TRP:CZ2	2.34	0.62
2:B:1495:PHE:HE1	2:B:1502:PHE:HD2	1.45	0.62
2:E:761:LYS:HB2	2:E:822:SER:HB2	1.81	0.62
2:B:243:MET:O	2:B:258:TYR:N	2.23	0.62
2:B:1247:LEU:HA	2:B:1250:LEU:HD12	1.81	0.62
2:B:1367:TYR:O	2:B:1378:ASN:N	2.27	0.62
2:E:243:MET:O	2:E:258:TYR:N	2.24	0.62
2:E:839:LEU:HA	2:E:842:LYS:HD2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:LEU:HA	2:B:98:TRP:CD1	2.34	0.62
2:B:166:ARG:HD3	2:B:173:LEU:HB2	1.82	0.62
2:B:1330:SER:O	2:E:1444:LYS:NZ	2.26	0.62
1:D:536:LEU:HD21	2:E:17:TYR:HB2	1.80	0.62
2:E:15:ALA:HA	2:E:59:PHE:CE2	2.35	0.62
2:E:95:LEU:HA	2:E:98:TRP:CD1	2.34	0.62
2:E:138:LYS:HA	2:E:141:LEU:HB2	1.81	0.62
2:E:493:ILE:HD11	2:E:496:TYR:HD1	1.65	0.62
2:E:285:SER:N	2:E:288:ASP:OD2	2.32	0.62
2:E:866:SER:O	2:E:868:LEU:N	2.32	0.62
2:E:1247:LEU:HA	2:E:1250:LEU:HD12	1.81	0.62
3:F:116:LYS:HD2	3:F:119:LEU:HD12	1.80	0.62
2:B:157:ARG:NH1	2:B:157:ARG:O	2.29	0.62
2:B:496:TYR:CZ	2:B:513:VAL:HG11	2.35	0.62
2:B:972:TYR:OH	2:B:977:LYS:NZ	2.27	0.62
2:E:1122:LYS:HD3	2:E:1175:LEU:HD21	1.82	0.62
2:B:5:ILE:H	2:B:40:MET:N	1.95	0.62
2:B:509:TRP:HB3	2:B:511:GLU:HG3	1.82	0.62
2:B:1016:VAL:HG23	2:B:1017:PHE:HD1	1.65	0.62
2:B:1372:PHE:CE2	2:B:1424:GLN:HB3	2.34	0.62
2:E:1372:PHE:CE2	2:E:1424:GLN:HB3	2.34	0.62
2:E:1463:ARG:NE	2:E:1486:ARG:HE	1.98	0.62
2:B:443:ARG:HG3	2:B:628:SER:HA	1.82	0.62
2:E:857:LEU:HD22	2:E:905:LEU:HD11	1.80	0.62
2:E:879:LEU:HG	2:E:931:ARG:HH21	1.65	0.62
2:E:1016:VAL:HG23	2:E:1017:PHE:HD1	1.65	0.62
2:B:180:THR:O	2:B:184:PHE:N	2.33	0.61
2:B:760:LEU:HB3	2:B:823:ILE:HG21	1.80	0.61
2:E:240:GLU:OE2	2:E:319:ARG:NE	2.26	0.61
2:E:1241:ILE:HA	2:E:1244:LEU:HD12	1.81	0.61
2:E:1375:PHE:CE2	2:E:1376:LEU:HG	2.35	0.61
1:A:617:VAL:HG13	1:A:645:LEU:HD21	1.81	0.61
2:B:15:ALA:HA	2:B:59:PHE:CE2	2.35	0.61
2:B:1463:ARG:NE	2:B:1486:ARG:HE	1.98	0.61
2:E:1170:VAL:HG12	2:E:1174:LYS:HE2	1.82	0.61
2:E:1227:VAL:HA	2:E:1230:PHE:CD2	2.35	0.61
2:E:1238:ASP:OD1	2:E:1239:ILE:N	2.31	0.61
2:E:1532:CYS:O	2:E:1535:GLN:NE2	2.30	0.61
2:B:719:TYR:HA	2:B:723:HIS:HD2	1.66	0.61
2:B:1122:LYS:HD3	2:B:1175:LEU:HD21	1.82	0.61
3:C:171:GLU:HG3	3:C:174:ARG:HH11	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:496:TYR:CZ	2:E:513:VAL:HG11	2.35	0.61
2:E:936:ILE:HD12	2:E:939:THR:HB	1.82	0.61
2:E:1065:SER:O	2:E:1069:ARG:NH1	2.34	0.61
2:E:1080:ARG:HA	2:E:1083:ILE:HD12	1.82	0.61
2:B:138:LYS:HA	2:B:141:LEU:HB2	1.81	0.61
2:B:1231:TYR:HH	2:B:1243:TYR:HE1	1.47	0.61
1:D:701:LEU:HD23	2:E:31:ILE:HG23	1.82	0.61
2:B:166:ARG:O	2:B:171:ASN:ND2	2.28	0.61
2:B:1065:SER:O	2:B:1069:ARG:NH1	2.34	0.61
1:D:580:SER:HA	1:D:587:HIS:CE1	2.30	0.61
2:B:676:LEU:HB3	2:B:693:VAL:HG13	1.80	0.61
2:B:879:LEU:HG	2:B:931:ARG:HH21	1.65	0.61
2:E:100:VAL:HA	2:E:103:ARG:HG2	1.83	0.61
2:B:523:THR:HA	2:B:555:MET:SD	2.40	0.61
2:B:979:ARG:HD3	2:B:1039:GLU:OE2	2.01	0.61
1:A:726:CYS:HA	2:B:46:ARG:NH2	2.15	0.61
2:B:493:ILE:HD11	2:B:496:TYR:HD1	1.65	0.61
2:E:1125:ILE:HG12	2:E:1172:LEU:HA	1.83	0.61
1:A:548:ILE:HG21	1:A:682:THR:HG23	1.81	0.61
2:B:936:ILE:HD12	2:B:939:THR:HB	1.82	0.61
2:B:970:SER:O	2:B:974:SER:OG	2.15	0.61
3:C:42:ALA:HB3	3:C:53:LEU:HD11	1.82	0.61
2:E:166:ARG:HD3	2:E:173:LEU:HB2	1.81	0.61
2:E:443:ARG:HG3	2:E:628:SER:HA	1.82	0.61
2:E:523:THR:HA	2:E:555:MET:SD	2.41	0.61
2:B:1227:VAL:HA	2:B:1230:PHE:CD2	2.35	0.61
2:E:843:PHE:O	2:E:846:SER:OG	2.19	0.61
2:B:326:VAL:HB	2:B:386:VAL:HG12	1.83	0.60
2:B:1480:ALA:HA	2:B:1514:PRO:HB3	1.83	0.60
3:C:94:ARG:CZ	3:C:145:MET:HG2	2.31	0.60
1:D:697:ARG:NH1	2:E:30:GLN:HG3	2.16	0.60
2:E:70:THR:HG22	2:E:71:VAL:H	1.64	0.60
2:E:1243:TYR:HA	2:E:1246:LYS:HG2	1.83	0.60
3:F:7:VAL:HG21	3:F:71:SER:HB3	1.83	0.60
1:D:711:PRO:O	2:E:63:TYR:OH	2.06	0.60
2:E:701:ILE:HG21	2:E:763:LEU:HD21	1.83	0.60
2:E:857:LEU:HB3	2:E:905:LEU:HD21	1.83	0.60
2:E:961:LEU:O	2:E:969:TYR:OH	2.19	0.60
2:B:882:LEU:O	2:B:885:GLN:HG2	2.02	0.60
2:B:1170:VAL:HG12	2:B:1174:LYS:HE2	1.83	0.60
2:B:1375:PHE:CE2	2:B:1376:LEU:HG	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:326:VAL:HB	2:E:386:VAL:HG12	1.83	0.60
2:E:719:TYR:HA	2:E:723:HIS:HD2	1.65	0.60
3:F:94:ARG:CZ	3:F:145:MET:HG2	2.31	0.60
2:B:485:HIS:N	2:B:514:LYS:O	2.22	0.60
2:B:1243:TYR:HA	2:B:1246:LYS:HG2	1.83	0.60
2:B:1532:CYS:O	2:B:1535:GLN:NE2	2.30	0.60
2:E:1258:THR:HG22	2:E:1262:TYR:CE2	2.36	0.60
2:E:1459:VAL:HG23	2:E:1495:PHE:HB2	1.84	0.60
2:B:85:LEU:O	2:B:88:VAL:HG22	2.02	0.60
2:B:565:GLY:N	2:B:624:THR:O	2.34	0.60
2:B:866:SER:O	2:B:868:LEU:N	2.33	0.60
2:B:1006:TRP:HE3	2:B:1009:MET:HG3	1.67	0.60
2:B:1080:ARG:HA	2:B:1083:ILE:HD12	1.82	0.60
2:B:1206:ASP:O	2:B:1209:THR:HG22	2.02	0.60
2:B:1258:THR:HG22	2:B:1262:TYR:CE2	2.37	0.60
2:E:467:GLU:OE2	2:E:534:ARG:NH1	2.35	0.60
2:B:94:THR:HG22	2:B:98:TRP:NE1	2.16	0.60
2:B:857:LEU:HB3	2:B:905:LEU:HD21	1.83	0.60
2:B:961:LEU:O	2:B:969:TYR:OH	2.19	0.60
2:B:964:MET:O	2:B:1019:ARG:NH2	2.34	0.60
3:C:11:ASP:OD1	3:C:16:LYS:NZ	2.35	0.60
1:D:617:VAL:HG13	1:D:645:LEU:HD21	1.81	0.60
1:D:711:PRO:HG2	2:E:16:ILE:HG21	1.82	0.60
2:E:34:THR:HB	2:E:50:LEU:HD12	1.83	0.60
2:E:94:THR:HG22	2:E:98:TRP:NE1	2.16	0.60
1:A:580:SER:HB3	1:A:584:LYS:H	1.67	0.60
2:B:256:GLU:HG3	2:B:488:ALA:HB2	1.83	0.60
2:B:701:ILE:HG21	2:B:763:LEU:HD21	1.83	0.60
2:B:911:GLU:O	2:B:915:ARG:N	2.34	0.60
2:E:565:GLY:N	2:E:624:THR:O	2.34	0.60
2:E:937:ASN:HA	2:E:940:VAL:HG12	1.84	0.60
2:B:1357:ARG:HH21	2:B:1453:TYR:C	2.05	0.60
2:E:90:GLU:O	2:E:94:THR:OG1	2.13	0.60
2:E:509:TRP:HB3	2:E:511:GLU:HG3	1.82	0.60
2:E:964:MET:O	2:E:1019:ARG:NH2	2.34	0.60
2:E:1059:LEU:HA	2:E:1062:GLU:HG2	1.84	0.60
2:E:1067:ALA:O	2:E:1071:LYS:N	2.23	0.60
2:E:1206:ASP:O	2:E:1209:THR:HG22	2.02	0.60
2:E:1368:TYR:O	2:E:1425:TYR:N	2.31	0.60
3:F:42:ALA:HB3	3:F:53:LEU:HD11	1.83	0.60
2:B:470:MET:HG3	2:B:484:ILE:HD13	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1367:TYR:HE1	2:B:1398:LEU:HD23	1.67	0.60
2:B:1408:MET:N	2:B:1426:MET:O	2.33	0.60
1:D:562:PHE:N	1:D:575:TRP:O	2.35	0.60
1:D:580:SER:HB3	1:D:584:LYS:H	1.67	0.60
2:E:99:ALA:HA	2:E:102:TRP:NE1	2.17	0.60
2:E:911:GLU:O	2:E:915:ARG:N	2.34	0.60
1:A:580:SER:HA	1:A:587:HIS:CE1	2.30	0.59
3:C:146:ALA:O	3:C:150:GLY:N	2.30	0.59
1:D:643:SER:HB3	1:D:651:GLN:HB3	1.84	0.59
2:E:430:LYS:NZ	2:E:433:PHE:O	2.28	0.59
2:B:843:PHE:O	2:B:846:SER:OG	2.19	0.59
2:B:1313:MET:HA	2:B:1453:TYR:OH	2.02	0.59
2:B:1321:SER:O	2:B:1345:ARG:NH2	2.35	0.59
3:C:82:PHE:O	3:C:115:THR:N	2.24	0.59
1:D:601:HIS:CE1	1:D:603:SER:HA	2.38	0.59
2:E:36:HIS:O	2:E:48:TYR:N	2.35	0.59
2:E:85:LEU:O	2:E:88:VAL:HG22	2.02	0.59
2:E:166:ARG:NH1	2:E:168:ASP:H	2.00	0.59
2:E:166:ARG:HH21	2:E:169:ASN:HD21	1.49	0.59
2:E:1357:ARG:HH21	2:E:1453:TYR:C	2.05	0.59
3:F:11:ASP:OD1	3:F:16:LYS:NZ	2.35	0.59
1:A:562:PHE:N	1:A:575:TRP:O	2.35	0.59
1:A:580:SER:HB2	1:A:585:VAL:HG22	1.83	0.59
1:A:601:HIS:CE1	1:A:603:SER:HA	2.38	0.59
2:B:1067:ALA:O	2:B:1071:LYS:N	2.23	0.59
2:E:757:LEU:HA	2:E:760:LEU:HG	1.84	0.59
2:E:882:LEU:O	2:E:885:GLN:HG2	2.02	0.59
2:B:1183:HIS:CG	2:B:1184:LYS:H	2.21	0.59
2:E:1006:TRP:HE3	2:E:1009:MET:HG3	1.67	0.59
2:E:1321:SER:O	2:E:1345:ARG:NH2	2.35	0.59
2:E:1367:TYR:HE1	2:E:1398:LEU:HD23	1.67	0.59
2:E:1462:PHE:O	2:E:1489:TYR:N	2.33	0.59
2:E:1480:ALA:HA	2:E:1514:PRO:HB3	1.83	0.59
1:A:617:VAL:HG21	1:A:623:PRO:HD3	1.84	0.59
2:B:467:GLU:OE2	2:B:534:ARG:NH1	2.35	0.59
2:B:1125:ILE:HG12	2:B:1172:LEU:HA	1.83	0.59
2:B:1466:ARG:NH1	3:C:31:GLU:OE2	2.35	0.59
2:E:256:GLU:HG3	2:E:488:ALA:HB2	1.83	0.59
2:E:392:VAL:O	2:E:394:HIS:ND1	2.35	0.59
2:E:569:LEU:HD12	2:E:620:PHE:HD2	1.68	0.59
2:E:879:LEU:HG	2:E:931:ARG:NH2	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:34:THR:HB	2:B:50:LEU:HD12	1.83	0.59
2:B:99:ALA:HA	2:B:102:TRP:NE1	2.17	0.59
2:B:879:LEU:HG	2:B:931:ARG:NH2	2.18	0.59
2:B:937:ASN:HA	2:B:940:VAL:HG12	1.84	0.59
2:B:1381:PHE:HB2	2:B:1383:TYR:HE1	1.66	0.59
1:D:580:SER:HB2	1:D:585:VAL:HG22	1.83	0.59
1:D:617:VAL:HG21	1:D:623:PRO:HD3	1.84	0.59
2:E:37:ILE:HD13	2:E:45:TYR:HB3	1.85	0.59
2:E:197:LYS:HA	2:E:200:GLU:HG2	1.84	0.59
2:E:470:MET:HG3	2:E:484:ILE:HD13	1.84	0.59
2:E:789:ASN:O	2:E:792:ARG:N	2.36	0.59
2:E:1183:HIS:CG	2:E:1184:LYS:H	2.21	0.59
2:E:1381:PHE:HB2	2:E:1383:TYR:HE1	1.66	0.59
1:A:693:GLU:HA	1:A:696:LEU:HG	1.85	0.59
2:B:100:VAL:HA	2:B:103:ARG:HG2	1.83	0.59
2:B:789:ASN:O	2:B:792:ARG:N	2.36	0.59
2:E:802:MET:SD	2:E:846:SER:OG	2.58	0.59
2:E:970:SER:O	2:E:974:SER:OG	2.15	0.59
2:E:979:ARG:HD3	2:E:1039:GLU:OE2	2.01	0.59
2:E:1313:MET:HA	2:E:1453:TYR:OH	2.02	0.59
2:E:1390:ARG:NH1	3:F:26:ASN:OD1	2.36	0.59
1:A:711:PRO:CG	2:B:16:ILE:HG21	2.28	0.59
2:B:166:ARG:HH21	2:B:169:ASN:HD21	1.49	0.59
2:B:392:VAL:O	2:B:394:HIS:ND1	2.35	0.59
2:B:945:ARG:NH1	2:B:946:GLN:HB2	2.18	0.59
2:B:1238:ASP:OD1	2:B:1239:ILE:N	2.31	0.59
2:E:1438:PRO:HB2	2:E:1441:TYR:HB2	1.85	0.59
2:B:1256:ASN:HB3	2:B:1259:GLU:HB2	1.85	0.59
2:B:1468:PHE:CE2	2:B:1470:LYS:HB2	2.38	0.59
3:C:7:VAL:HG21	3:C:71:SER:HB3	1.83	0.59
2:E:1115:THR:HB	2:E:1120:LEU:HD11	1.85	0.59
2:E:1275:ASP:O	2:E:1292:THR:OG1	2.21	0.59
2:E:1362:TYR:O	2:E:1431:VAL:N	2.32	0.59
2:E:1468:PHE:CE2	2:E:1470:LYS:HB2	2.38	0.59
1:A:576:TYR:O	1:A:588:TYR:HA	2.03	0.59
2:B:187:HIS:CD2	2:B:1009:MET:HG2	2.38	0.59
2:B:1270:LEU:O	2:B:1272:GLN:NE2	2.36	0.59
2:B:1467:PRO:HG2	3:C:31:GLU:O	2.03	0.59
2:E:181:ILE:HA	2:E:184:PHE:HB3	1.85	0.59
2:E:1217:LYS:HA	2:E:1220:ARG:CZ	2.33	0.59
2:B:958:ILE:HD12	2:B:1016:VAL:HG21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1459:VAL:HG23	2:B:1495:PHE:HB2	1.84	0.58
3:C:80:ILE:HD11	3:C:97:TRP:HB3	1.84	0.58
2:E:921:THR:HG23	2:E:925:ILE:HG13	1.84	0.58
2:E:958:ILE:HD12	2:E:1016:VAL:HG21	1.85	0.58
2:E:1259:GLU:OE1	2:E:1259:GLU:N	2.35	0.58
2:B:36:HIS:O	2:B:48:TYR:N	2.35	0.58
2:B:757:LEU:HA	2:B:760:LEU:HG	1.84	0.58
2:B:1115:THR:HB	2:B:1120:LEU:HD11	1.85	0.58
2:B:1479:PHE:HB3	2:B:1482:MET:HE2	1.84	0.58
2:B:181:ILE:HA	2:B:184:PHE:HB3	1.85	0.58
2:B:554:LEU:O	2:B:562:LEU:N	2.36	0.58
2:B:921:THR:HG23	2:B:925:ILE:HG13	1.84	0.58
2:B:1102:ILE:HD13	2:B:1135:GLU:HG3	1.85	0.58
2:B:1397:ARG:O	2:B:1401:GLN:N	2.35	0.58
2:B:1515:LEU:HG	2:B:1575:TYR:CE2	2.39	0.58
2:E:1262:TYR:O	2:E:1266:LEU:HG	2.03	0.58
2:E:1515:LEU:HG	2:E:1575:TYR:CE2	2.39	0.58
2:B:569:LEU:HD12	2:B:620:PHE:HD2	1.68	0.58
2:B:1059:LEU:HA	2:B:1062:GLU:HG2	1.84	0.58
2:B:1197:VAL:O	2:B:1200:LEU:HB3	2.03	0.58
2:B:1462:PHE:O	2:B:1489:TYR:N	2.33	0.58
2:E:180:THR:O	2:E:184:PHE:N	2.33	0.58
2:E:1265:LEU:O	2:E:1269:GLU:N	2.30	0.58
2:B:166:ARG:NH1	2:B:168:ASP:H	2.00	0.58
2:B:1438:PRO:HB2	2:B:1441:TYR:HB2	1.85	0.58
2:B:1539:ASP:OD1	2:B:1540:ARG:N	2.36	0.58
3:C:43:ASN:ND2	3:C:52:ASN:OD1	2.36	0.58
2:E:1357:ARG:NH2	2:E:1456:ALA:H	1.99	0.58
2:B:792:ARG:O	2:B:795:PHE:HB2	2.03	0.58
2:B:817:LEU:HB3	2:B:859:CYS:HB2	1.86	0.58
2:E:1379:LYS:HZ2	2:E:1503:GLU:HB2	1.69	0.58
3:F:80:ILE:HD11	3:F:97:TRP:HB3	1.84	0.58
3:F:82:PHE:O	3:F:115:THR:N	2.24	0.58
2:B:1111:GLU:OE2	2:B:1163:ARG:NH2	2.32	0.58
2:B:1262:TYR:O	2:B:1266:LEU:HG	2.03	0.58
2:B:1526:ASN:O	2:B:1599:LEU:HD21	2.04	0.58
2:E:1470:LYS:HB3	2:E:1483:TRP:CD1	2.39	0.58
2:E:1485:GLU:OE1	2:E:1485:GLU:N	2.36	0.58
3:F:43:ASN:ND2	3:F:52:ASN:OD1	2.36	0.58
2:B:1259:GLU:HA	2:B:1262:TYR:HD2	1.68	0.58
2:B:1485:GLU:OE1	2:B:1485:GLU:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:522:VAL:HG23	2:E:554:LEU:HD13	1.85	0.58
2:E:1197:VAL:O	2:E:1200:LEU:HB3	2.03	0.58
2:B:1217:LYS:HA	2:B:1220:ARG:CZ	2.33	0.58
2:B:1470:LYS:HB3	2:B:1483:TRP:CD1	2.39	0.58
2:E:81:ILE:HG21	2:E:141:LEU:HD21	1.85	0.58
2:E:189:VAL:HG13	2:E:193:ARG:NH1	2.19	0.58
2:E:450:LEU:HB3	2:E:620:PHE:HZ	1.69	0.58
2:E:945:ARG:NH1	2:E:946:GLN:HB2	2.18	0.58
2:E:1256:ASN:HB3	2:E:1259:GLU:HB2	1.85	0.58
2:E:1518:ALA:HA	2:E:1566:TYR:OH	2.04	0.58
2:E:1557:PRO:HA	3:F:36:VAL:CG1	2.33	0.58
2:B:189:VAL:HG13	2:B:193:ARG:NH1	2.19	0.58
2:B:450:LEU:HB3	2:B:620:PHE:HZ	1.69	0.58
1:D:711:PRO:HB2	2:E:63:TYR:CE1	2.39	0.58
2:E:187:HIS:CD2	2:E:1009:MET:HG2	2.38	0.58
2:E:1397:ARG:O	2:E:1401:GLN:N	2.35	0.58
2:B:1259:GLU:HA	2:B:1262:TYR:CD2	2.39	0.57
1:D:693:GLU:HA	1:D:696:LEU:HG	1.85	0.57
2:E:5:ILE:H	2:E:40:MET:N	1.95	0.57
3:F:90:PHE:CD1	3:F:137:ILE:HG12	2.40	0.57
2:B:1367:TYR:CE2	2:B:1402:PHE:HE2	2.21	0.57
1:D:576:TYR:O	1:D:588:TYR:HA	2.03	0.57
2:E:554:LEU:O	2:E:562:LEU:N	2.36	0.57
2:E:677:PHE:O	2:E:681:MET:HG2	2.04	0.57
2:E:874:CYS:HA	2:E:877:VAL:HG12	1.87	0.57
2:E:1539:ASP:OD1	2:E:1540:ARG:N	2.36	0.57
2:B:81:ILE:HG21	2:B:141:LEU:HD21	1.85	0.57
2:B:556:ASN:ND2	2:B:561:THR:O	2.37	0.57
2:B:643:TRP:CE2	2:B:679:ILE:HG13	2.40	0.57
2:B:1518:ALA:HA	2:B:1566:TYR:OH	2.04	0.57
2:E:1479:PHE:HB3	2:E:1482:MET:HE2	1.86	0.57
1:A:594:SER:HB2	1:A:596:GLN:HE21	1.69	0.57
2:B:197:LYS:HA	2:B:200:GLU:HG2	1.84	0.57
2:B:303:VAL:HG22	2:B:319:ARG:HG2	1.86	0.57
2:B:1275:ASP:O	2:B:1292:THR:OG1	2.21	0.57
2:E:520:GLU:O	2:E:523:THR:OG1	2.15	0.57
2:E:643:TRP:CE2	2:E:679:ILE:HG13	2.40	0.57
2:E:1359:GLN:HB3	2:E:1456:ALA:HB2	1.87	0.57
1:A:643:SER:HB3	1:A:651:GLN:HB3	1.85	0.57
2:B:1256:ASN:HD21	2:B:1500:LYS:HE2	1.70	0.57
2:E:719:TYR:HA	2:E:723:HIS:CD2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:ILE:HD13	2:B:45:TYR:HB3	1.85	0.57
2:B:677:PHE:O	2:B:681:MET:HG2	2.05	0.57
2:B:765:ARG:NE	2:B:826:ASP:OD1	2.36	0.57
2:B:910:LEU:HB3	2:B:963:GLN:HE22	1.70	0.57
2:B:1099:ILE:HG13	2:B:1134:CYS:HB3	1.87	0.57
2:B:1515:LEU:HD13	2:B:1585:LYS:HB2	1.87	0.57
2:E:166:ARG:NH2	2:E:168:ASP:HB2	2.20	0.57
2:E:792:ARG:O	2:E:795:PHE:HB2	2.03	0.57
2:E:1099:ILE:HG13	2:E:1134:CYS:HB3	1.86	0.57
2:E:1165:ASP:HB2	2:E:1167:GLN:HE22	1.69	0.57
2:E:1242:ARG:HG2	2:E:1246:LYS:NZ	2.20	0.57
3:C:161:THR:O	3:C:163:ARG:NH1	2.37	0.57
1:D:693:GLU:O	1:D:697:ARG:HG2	2.05	0.57
2:E:556:ASN:ND2	2:E:561:THR:O	2.37	0.57
2:E:1205:LEU:HA	2:E:1208:ARG:HH21	1.70	0.57
2:E:1367:TYR:CE2	2:E:1402:PHE:HE2	2.21	0.57
3:F:8:VAL:O	3:F:58:THR:OG1	2.23	0.57
1:A:568:ARG:NH2	1:A:634:ASN:OD1	2.38	0.57
2:B:179:SER:OG	2:B:182:ALA:HB3	2.05	0.57
2:B:772:VAL:HA	2:B:775:LEU:HD12	1.86	0.57
2:B:838:VAL:HG12	2:B:877:VAL:HG21	1.87	0.57
2:B:1098:LYS:O	2:B:1102:ILE:HG13	2.05	0.57
2:B:1109:ILE:HA	2:B:1112:VAL:HG22	1.86	0.57
2:B:1242:ARG:HG2	2:B:1246:LYS:NZ	2.20	0.57
2:B:1284:GLN:NE2	2:B:1287:SER:O	2.37	0.57
3:C:7:VAL:HG23	3:C:75:THR:HG21	1.86	0.57
3:C:90:PHE:CD1	3:C:137:ILE:HG12	2.39	0.57
2:E:727:THR:HA	2:E:773:LEU:HD22	1.87	0.57
2:E:1102:ILE:HD13	2:E:1135:GLU:HG3	1.85	0.57
2:B:522:VAL:HG23	2:B:554:LEU:HD13	1.85	0.57
2:B:719:TYR:HA	2:B:723:HIS:CD2	2.40	0.57
2:B:828:LYS:HZ3	2:B:867:THR:HA	1.69	0.57
2:B:1259:GLU:OE1	2:B:1259:GLU:N	2.35	0.57
2:E:772:VAL:HA	2:E:775:LEU:HD12	1.87	0.57
2:E:1259:GLU:HA	2:E:1262:TYR:HD2	1.68	0.57
2:E:1259:GLU:HA	2:E:1262:TYR:CD2	2.39	0.57
2:E:1335:TYR:HA	2:E:1338:LEU:HD23	1.86	0.57
3:F:161:THR:O	3:F:163:ARG:NH1	2.37	0.57
2:B:1379:LYS:HZ2	2:B:1503:GLU:HB2	1.70	0.57
2:E:1526:ASN:O	2:E:1599:LEU:HD21	2.04	0.57
3:F:7:VAL:HG23	3:F:75:THR:HG21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:8:VAL:HG22	3:F:79:LEU:HD12	1.87	0.57
1:A:541:GLN:O	1:A:544:ILE:HG22	2.04	0.56
2:B:874:CYS:HA	2:B:877:VAL:HG12	1.86	0.56
3:C:8:VAL:O	3:C:58:THR:OG1	2.23	0.56
1:D:568:ARG:NH2	1:D:634:ASN:OD1	2.38	0.56
2:E:1109:ILE:HA	2:E:1112:VAL:HG22	1.86	0.56
2:E:1284:GLN:NE2	2:E:1287:SER:O	2.37	0.56
2:B:727:THR:HA	2:B:773:LEU:HD22	1.87	0.56
2:B:1362:TYR:O	2:B:1431:VAL:N	2.32	0.56
2:B:1388:TYR:CE2	3:C:50:PRO:HG3	2.40	0.56
2:E:73:ASP:O	2:E:79:THR:N	2.38	0.56
2:E:760:LEU:HD12	2:E:819:TYR:HB2	1.87	0.56
2:E:817:LEU:HB3	2:E:859:CYS:HB2	1.86	0.56
2:E:1034:ASP:OD1	2:E:1097:HIS:NE2	2.38	0.56
2:E:1452:ASN:OD1	2:E:1453:TYR:N	2.38	0.56
2:B:73:ASP:O	2:B:79:THR:N	2.38	0.56
2:B:143:GLU:O	2:B:147:LYS:HG2	2.05	0.56
2:B:772:VAL:HG13	2:B:776:ARG:HH12	1.71	0.56
2:B:1207:TYR:O	2:B:1211:ILE:HG12	2.05	0.56
2:B:1235:LYS:O	2:B:1237:GLU:N	2.39	0.56
2:B:1359:GLN:HB3	2:B:1456:ALA:HB2	1.87	0.56
2:B:1452:ASN:OD1	2:B:1453:TYR:N	2.38	0.56
2:E:59:PHE:HD2	2:E:64:ILE:HG12	1.70	0.56
2:E:903:SER:HB3	2:E:953:PHE:CE2	2.40	0.56
2:E:914:ASP:CG	2:E:963:GLN:HG2	2.26	0.56
2:E:1207:TYR:O	2:E:1211:ILE:HG12	2.06	0.56
2:E:1240:TYR:O	2:E:1244:LEU:HG	2.05	0.56
2:E:1391:ARG:HG3	2:E:1429:PHE:HA	1.87	0.56
2:B:1034:ASP:OD1	2:B:1097:HIS:NE2	2.38	0.56
2:B:1088:ARG:HG3	2:B:1127:ILE:HD11	1.87	0.56
2:B:1325:ALA:HB2	2:B:1341:LEU:HD23	1.87	0.56
2:B:1448:GLU:OE1	2:B:1452:ASN:ND2	2.38	0.56
3:C:8:VAL:HG22	3:C:79:LEU:HD12	1.87	0.56
2:E:772:VAL:HG13	2:E:776:ARG:HH12	1.71	0.56
2:E:1408:MET:N	2:E:1426:MET:O	2.33	0.56
2:E:1525:THR:HA	2:E:1528:ARG:NH2	2.21	0.56
2:B:19:TYR:CG	2:B:59:PHE:HE1	2.24	0.56
2:B:208:LEU:HA	2:B:211:ARG:HD3	1.86	0.56
2:B:1167:GLN:O	2:B:1171:LEU:HG	2.05	0.56
1:D:541:GLN:O	1:D:544:ILE:HG22	2.04	0.56
1:D:586:LEU:HB2	1:D:608:LEU:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:594:SER:HB2	1:D:596:GLN:HE21	1.69	0.56
2:E:196:GLU:O	2:E:200:GLU:HB3	2.05	0.56
2:E:1072:ILE:O	2:E:1076:TYR:N	2.37	0.56
2:E:1098:LYS:O	2:E:1102:ILE:HG13	2.05	0.56
2:E:1325:ALA:HB2	2:E:1341:LEU:HD23	1.87	0.56
1:A:714:PRO:HG3	2:B:60:PRO:HB3	1.88	0.56
2:B:1165:ASP:HB2	2:B:1167:GLN:HE22	1.69	0.56
1:D:708:ASP:OD1	1:D:708:ASP:N	2.39	0.56
2:E:303:VAL:HG22	2:E:319:ARG:HG2	1.86	0.56
2:E:838:VAL:HG12	2:E:877:VAL:HG21	1.87	0.56
2:E:1178:GLU:HA	2:E:1181:ARG:HD3	1.88	0.56
2:E:1270:LEU:O	2:E:1272:GLN:NE2	2.36	0.56
1:A:580:SER:HB2	1:A:585:VAL:H	1.71	0.56
1:A:596:GLN:NE2	1:A:597:GLY:O	2.39	0.56
2:B:1178:GLU:HA	2:B:1181:ARG:HD3	1.88	0.56
2:B:1240:TYR:O	2:B:1244:LEU:HG	2.05	0.56
1:D:711:PRO:HB2	2:E:63:TYR:HE1	1.70	0.56
2:E:143:GLU:O	2:E:147:LYS:HG2	2.05	0.56
2:E:910:LEU:HB3	2:E:963:GLN:HE22	1.70	0.56
3:F:27:ALA:O	3:F:162:GLN:NE2	2.38	0.56
1:A:677:MET:CB	1:A:682:THR:HG21	2.36	0.56
2:B:899:HIS:CD2	2:B:943:MET:HG2	2.41	0.56
2:B:1205:LEU:HA	2:B:1208:ARG:HH21	1.70	0.56
2:B:1357:ARG:NH2	2:B:1456:ALA:H	1.99	0.56
3:C:27:ALA:O	3:C:162:GLN:NE2	2.38	0.56
1:D:677:MET:CB	1:D:682:THR:HG21	2.36	0.56
2:E:484:ILE:O	2:E:493:ILE:N	2.39	0.56
2:E:1167:GLN:O	2:E:1171:LEU:HG	2.05	0.56
2:E:1371:GLY:C	2:E:1424:GLN:HE21	2.09	0.56
2:E:1484:ILE:H	2:E:1512:ILE:HB	1.71	0.56
2:E:1515:LEU:HD13	2:E:1585:LYS:HB2	1.87	0.56
2:B:166:ARG:NH2	2:B:168:ASP:HB2	2.20	0.56
2:B:261:ARG:HD3	2:B:269:LYS:HD3	1.88	0.56
2:B:1371:GLY:C	2:B:1424:GLN:HE21	2.09	0.56
1:D:711:PRO:HG2	2:E:16:ILE:HD13	1.88	0.56
2:E:208:LEU:HA	2:E:211:ARG:HD3	1.86	0.56
2:E:473:HIS:HB2	2:E:526:HIS:CE1	2.41	0.56
2:E:979:ARG:NH2	2:E:1031:PHE:O	2.39	0.56
2:B:484:ILE:O	2:B:493:ILE:N	2.39	0.56
2:B:903:SER:HB3	2:B:953:PHE:CE2	2.40	0.56
2:B:914:ASP:CG	2:B:963:GLN:HG2	2.26	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1041:GLN:NE2	2:B:1044:ASN:OD1	2.39	0.56
2:B:1072:ILE:O	2:B:1076:TYR:N	2.37	0.56
2:E:1041:GLN:NE2	2:E:1044:ASN:OD1	2.39	0.56
2:E:1256:ASN:HD21	2:E:1500:LYS:HE2	1.70	0.56
1:A:562:PHE:CE1	1:A:577:CYS:HB3	2.41	0.55
1:A:693:GLU:O	1:A:697:ARG:HG2	2.05	0.55
2:B:933:LEU:H	2:B:935:ARG:HH21	1.53	0.55
2:B:979:ARG:NH2	2:B:1031:PHE:O	2.39	0.55
2:B:1441:TYR:CD2	2:B:1450:ILE:HG21	2.41	0.55
2:B:1484:ILE:H	2:B:1512:ILE:HB	1.71	0.55
2:B:1525:THR:HA	2:B:1528:ARG:NH2	2.21	0.55
3:C:137:ILE:HG23	3:C:141:GLN:HB2	1.88	0.55
2:E:761:LYS:O	2:E:765:ARG:HG2	2.06	0.55
2:E:1615:LEU:O	2:E:1619:HIS:N	2.29	0.55
2:B:273:LYS:HD3	2:B:277:LEU:HD23	1.88	0.55
2:B:760:LEU:HD12	2:B:819:TYR:HB2	1.87	0.55
2:B:828:LYS:NZ	2:B:867:THR:HA	2.21	0.55
2:B:855:GLN:OE1	2:B:855:GLN:N	2.39	0.55
2:B:1045:ASN:O	2:B:1049:LEU:HB3	2.06	0.55
2:B:1335:TYR:HA	2:B:1338:LEU:HD23	1.86	0.55
2:B:1391:ARG:HG3	2:B:1429:PHE:HA	1.87	0.55
1:D:596:GLN:NE2	1:D:597:GLY:O	2.39	0.55
2:E:828:LYS:NZ	2:E:867:THR:HA	2.21	0.55
2:E:1029:THR:HA	2:E:1033:MET:HB2	1.87	0.55
2:E:1235:LYS:O	2:E:1237:GLU:N	2.39	0.55
2:E:1441:TYR:CD2	2:E:1450:ILE:HG21	2.41	0.55
2:B:59:PHE:HD2	2:B:64:ILE:HG12	1.70	0.55
2:B:196:GLU:O	2:B:200:GLU:HB3	2.05	0.55
2:B:825:ASN:ND2	2:B:866:SER:HB2	2.22	0.55
2:B:896:LYS:CG	2:B:897:PRO:HD3	2.35	0.55
2:B:1198:SER:HA	2:B:1201:LEU:HD12	1.89	0.55
2:B:1340:ASN:OD1	2:B:1341:LEU:N	2.40	0.55
1:D:578:ARG:HB2	1:D:598:GLU:OE1	2.07	0.55
1:D:580:SER:HB2	1:D:585:VAL:H	1.71	0.55
2:E:435:GLU:HA	2:E:708:LYS:NZ	2.21	0.55
2:E:1467:PRO:HG2	3:F:31:GLU:O	2.07	0.55
2:B:761:LYS:O	2:B:765:ARG:HG2	2.06	0.55
2:B:1242:ARG:HG2	2:B:1246:LYS:HZ1	1.72	0.55
3:C:126:ILE:HD12	3:C:136:PRO:HB3	1.88	0.55
2:E:273:LYS:HD3	2:E:277:LEU:HD23	1.88	0.55
2:E:1340:ASN:OD1	2:E:1341:LEU:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1571:PHE:CE2	2:E:1590:LYS:HG3	2.42	0.55
3:F:137:ILE:HG23	3:F:141:GLN:HB2	1.88	0.55
2:B:156:ASN:O	2:B:160:GLY:N	2.40	0.55
2:E:19:TYR:CG	2:E:59:PHE:HE1	2.24	0.55
2:B:17:TYR:OH	2:B:20:ASN:OD1	2.23	0.55
2:B:473:HIS:HB2	2:B:526:HIS:CE1	2.41	0.55
1:D:557:VAL:HA	1:D:579:LEU:HB3	1.89	0.55
2:E:17:TYR:OH	2:E:20:ASN:OD1	2.23	0.55
2:E:156:ASN:O	2:E:160:GLY:N	2.40	0.55
2:E:1045:ASN:O	2:E:1049:LEU:HB3	2.06	0.55
2:E:1159:VAL:O	2:E:1208:ARG:NH1	2.40	0.55
2:E:1328:TYR:HB3	2:E:1338:LEU:CD2	2.37	0.55
2:E:1460:GLN:O	2:E:1491:THR:N	2.39	0.55
3:F:126:ILE:HD12	3:F:136:PRO:HB3	1.88	0.55
1:A:669:LEU:HA	1:A:672:LEU:HD12	1.89	0.55
2:B:746:ASP:O	2:B:750:THR:OG1	2.10	0.55
2:B:856:LYS:HD2	2:B:857:LEU:HD23	1.89	0.55
2:B:965:ASP:OD1	2:B:966:ASP:N	2.40	0.55
2:B:1601:THR:HG22	2:B:1605:ARG:NE	2.21	0.55
2:E:179:SER:OG	2:E:182:ALA:HB3	2.05	0.55
2:E:1028:LEU:HD23	2:E:1032:PHE:CD1	2.42	0.55
2:E:1328:TYR:HA	2:E:1332:VAL:HG12	1.89	0.55
2:E:1601:THR:HG22	2:E:1605:ARG:NE	2.21	0.55
1:A:557:VAL:HA	1:A:579:LEU:HB3	1.89	0.55
2:B:435:GLU:HA	2:B:708:LYS:NZ	2.21	0.55
2:B:1029:THR:HA	2:B:1033:MET:HB2	1.87	0.55
2:B:1109:ILE:HG23	2:B:1128:PHE:HE1	1.72	0.55
2:B:1345:ARG:HA	2:B:1348:PHE:CD2	2.42	0.55
2:E:48:TYR:HB3	2:E:53:LYS:HD2	1.88	0.55
2:E:1012:THR:HA	2:E:1015:ARG:NH1	2.21	0.55
2:E:1043:TRP:CD1	2:E:1094:LEU:HD21	2.42	0.55
2:E:1448:GLU:OE1	2:E:1452:ASN:ND2	2.38	0.55
2:B:76:GLN:NE2	2:B:78:GLU:OE1	2.36	0.55
2:B:958:ILE:HB	2:B:1016:VAL:HG21	1.89	0.55
2:B:1506:GLN:NE2	2:B:1507:ILE:O	2.40	0.55
1:D:562:PHE:CE1	1:D:577:CYS:HB3	2.41	0.55
2:E:45:TYR:O	2:E:59:PHE:N	2.31	0.55
2:E:714:PRO:HA	2:E:717:GLU:HG2	1.89	0.55
2:E:1483:TRP:CZ2	2:E:1514:PRO:HD3	2.42	0.55
2:B:19:TYR:O	2:B:28:SER:HA	2.07	0.55
2:B:1251:HIS:O	2:B:1255:GLU:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1458:GLU:N	2:B:1495:PHE:O	2.40	0.55
2:B:1615:LEU:HA	2:B:1618:LEU:HB2	1.89	0.55
2:E:1088:ARG:HG3	2:E:1127:ILE:HD11	1.88	0.55
2:E:1458:GLU:N	2:E:1495:PHE:O	2.40	0.55
3:F:83:SER:HB3	3:F:86:SER:HB3	1.89	0.55
2:B:562:LEU:O	2:B:633:GLN:NE2	2.40	0.54
2:B:1159:VAL:O	2:B:1208:ARG:NH1	2.40	0.54
2:E:283:ASP:HB2	2:E:430:LYS:HB3	1.89	0.54
2:E:1251:HIS:O	2:E:1255:GLU:N	2.39	0.54
2:E:1506:GLN:NE2	2:E:1507:ILE:O	2.40	0.54
2:B:48:TYR:HB3	2:B:53:LYS:HD2	1.88	0.54
2:B:958:ILE:HA	2:B:961:LEU:HD12	1.89	0.54
2:B:1328:TYR:HA	2:B:1332:VAL:HG12	1.89	0.54
2:B:1571:PHE:CE2	2:B:1590:LYS:HG3	2.42	0.54
3:C:83:SER:HB3	3:C:86:SER:HB3	1.89	0.54
3:C:85:VAL:HG11	3:C:119:LEU:HB2	1.89	0.54
2:E:832:ASP:OD2	2:E:835:GLU:N	2.24	0.54
2:E:1216:SER:O	2:E:1220:ARG:NH1	2.41	0.54
1:A:586:LEU:HB2	1:A:608:LEU:HB3	1.88	0.54
2:B:105:LEU:HD13	2:B:110:LYS:NZ	2.22	0.54
2:B:832:ASP:OD2	2:B:835:GLU:N	2.24	0.54
2:B:880:PRO:HA	2:B:931:ARG:HH12	1.73	0.54
1:D:669:LEU:HA	1:D:672:LEU:HD12	1.89	0.54
2:E:958:ILE:HA	2:E:961:LEU:HD12	1.89	0.54
3:F:68:ARG:HG3	3:F:72:TYR:CE1	2.43	0.54
2:B:1535:GLN:HE22	2:B:1542:LEU:HD21	1.71	0.54
2:E:76:GLN:NE2	2:E:78:GLU:OE1	2.36	0.54
2:E:261:ARG:HD3	2:E:269:LYS:HD3	1.88	0.54
2:E:795:PHE:CD1	2:E:839:LEU:HB3	2.43	0.54
2:E:825:ASN:ND2	2:E:866:SER:HB2	2.22	0.54
2:E:899:HIS:CD2	2:E:943:MET:HG2	2.41	0.54
2:E:958:ILE:HB	2:E:1016:VAL:HG21	1.89	0.54
2:E:1418:ILE:HA	2:E:1421:SER:HB3	1.89	0.54
2:E:1545:HIS:O	2:E:1548:SER:OG	2.21	0.54
2:E:1615:LEU:HA	2:E:1618:LEU:HB2	1.89	0.54
1:A:708:ASP:N	1:A:708:ASP:OD1	2.39	0.54
2:B:97:GLU:OE2	2:B:1065:SER:HB2	2.08	0.54
2:B:1216:SER:O	2:B:1220:ARG:NH1	2.41	0.54
2:E:562:LEU:O	2:E:633:GLN:NE2	2.40	0.54
2:E:1109:ILE:HG23	2:E:1128:PHE:HE1	1.72	0.54
2:E:1111:GLU:OE2	2:E:1163:ARG:NH2	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1165:ASP:O	2:B:1168:TYR:HB3	2.08	0.54
2:B:1409:THR:HA	3:C:28:PHE:HZ	1.72	0.54
2:B:1557:PRO:HB2	2:B:1561:GLY:CA	2.36	0.54
2:E:11:LYS:HZ1	2:E:36:HIS:HB2	1.72	0.54
2:E:933:LEU:H	2:E:935:ARG:HH21	1.54	0.54
2:B:11:LYS:HZ1	2:B:36:HIS:HB2	1.73	0.54
2:B:732:LYS:O	2:B:736:VAL:HG23	2.08	0.54
2:B:1012:THR:HA	2:B:1015:ARG:NH1	2.21	0.54
2:B:1328:TYR:HB3	2:B:1338:LEU:CD2	2.37	0.54
2:E:473:HIS:ND1	2:E:477:GLY:O	2.41	0.54
2:E:896:LYS:CG	2:E:897:PRO:HD3	2.36	0.54
2:E:965:ASP:OD1	2:E:966:ASP:N	2.40	0.54
2:E:1217:LYS:HD3	2:E:1220:ARG:NH1	2.22	0.54
2:E:1535:GLN:HE22	2:E:1542:LEU:HD21	1.71	0.54
2:E:1593:ILE:HA	2:E:1596:GLN:HB3	1.90	0.54
1:A:578:ARG:HB2	1:A:598:GLU:OE1	2.07	0.54
2:E:93:SER:O	2:E:96:ARG:HB3	2.08	0.54
2:E:105:LEU:HD13	2:E:110:LYS:NZ	2.22	0.54
2:E:940:VAL:HG13	2:E:992:MET:CE	2.37	0.54
2:E:1623:SER:HA	2:E:1627:ARG:NH1	2.23	0.54
2:B:283:ASP:HB2	2:B:430:LYS:HB3	1.89	0.54
2:B:899:HIS:HB3	2:B:949:HIS:NE2	2.23	0.54
2:B:940:VAL:HG13	2:B:992:MET:CE	2.37	0.54
2:B:1028:LEU:HD23	2:B:1032:PHE:CD1	2.42	0.54
2:B:1065:SER:OG	2:B:1068:LYS:HB2	2.08	0.54
3:C:68:ARG:HG3	3:C:72:TYR:CE1	2.43	0.54
2:E:97:GLU:OE2	2:E:1065:SER:HB2	2.08	0.54
2:E:662:GLY:HA2	2:E:665:ILE:HB	1.90	0.54
2:E:855:GLN:OE1	2:E:855:GLN:N	2.39	0.54
2:E:1212:MET:HA	2:E:1215:GLU:OE2	2.08	0.54
2:E:1242:ARG:HG2	2:E:1246:LYS:HZ1	1.73	0.54
3:F:85:VAL:HG11	3:F:119:LEU:HB2	1.89	0.54
2:B:818:LYS:HZ3	2:B:858:ASN:HB3	1.73	0.54
2:B:1460:GLN:O	2:B:1491:THR:N	2.39	0.54
2:B:1483:TRP:CZ2	2:B:1514:PRO:HD3	2.42	0.54
2:E:19:TYR:HB3	2:E:29:LEU:H	1.73	0.54
2:E:1065:SER:OG	2:E:1068:LYS:HB2	2.08	0.54
2:E:1198:SER:HA	2:E:1201:LEU:HD12	1.88	0.54
2:E:1345:ARG:HA	2:E:1348:PHE:CD2	2.42	0.54
2:B:561:THR:HB	2:B:631:LEU:HD22	1.90	0.53
2:B:938:ARG:O	2:B:941:ILE:HB	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1043:TRP:CD1	2:B:1094:LEU:HD21	2.42	0.53
2:B:1449:GLN:HA	2:B:1452:ASN:ND2	2.24	0.53
2:E:19:TYR:O	2:E:28:SER:HA	2.07	0.53
2:E:23:GLN:HG2	2:E:58:ILE:HD13	1.89	0.53
2:E:649:ASN:OD1	2:E:652:HIS:HB3	2.08	0.53
2:E:732:LYS:O	2:E:736:VAL:HG23	2.08	0.53
2:B:4:TRP:CZ3	2:B:46:ARG:HG2	2.43	0.53
2:B:23:GLN:HG2	2:B:58:ILE:HD13	1.89	0.53
2:B:649:ASN:OD1	2:B:652:HIS:HB3	2.08	0.53
2:B:662:GLY:HA2	2:B:665:ILE:HB	1.90	0.53
2:B:714:PRO:HA	2:B:717:GLU:HG2	1.89	0.53
2:B:934:ARG:HB3	2:B:935:ARG:NH1	2.24	0.53
2:B:1418:ILE:HA	2:B:1421:SER:HB3	1.90	0.53
3:C:6:CYS:SG	3:C:79:LEU:HG	2.48	0.53
1:D:618:THR:HB	1:D:662:TYR:OH	2.08	0.53
1:D:670:ASN:O	1:D:674:GLY:N	2.41	0.53
2:E:856:LYS:HD2	2:E:857:LEU:HD23	1.89	0.53
2:E:992:MET:O	2:E:996:LEU:HD23	2.08	0.53
2:E:1363:PHE:O	2:E:1383:TYR:N	2.31	0.53
2:E:1579:HIS:O	2:E:1583:GLN:NE2	2.37	0.53
2:B:1091:TRP:CH2	2:B:1131:MET:HB3	2.44	0.53
2:B:1623:SER:HA	2:B:1627:ARG:NH1	2.23	0.53
2:E:4:TRP:CZ3	2:E:46:ARG:HG2	2.42	0.53
2:E:122:TYR:HA	2:E:125:ILE:HG12	1.91	0.53
2:E:899:HIS:HB3	2:E:949:HIS:NE2	2.23	0.53
2:B:1395:SER:O	2:B:1399:LEU:HG	2.09	0.53
2:B:1463:ARG:HH21	2:B:1484:ILE:HG21	1.73	0.53
2:B:1518:ALA:HB2	2:B:1570:PHE:CE2	2.44	0.53
1:D:704:ILE:HD11	2:E:65:HIS:CG	2.43	0.53
2:E:46:ARG:HA	2:E:57:GLY:O	2.09	0.53
2:E:820:LEU:O	2:E:823:ILE:HG12	2.09	0.53
2:E:1006:TRP:CD1	2:E:1006:TRP:N	2.77	0.53
3:F:41:SER:OG	3:F:53:LEU:O	2.15	0.53
3:F:142:GLY:HA3	3:F:154:TYR:CZ	2.44	0.53
2:B:473:HIS:ND1	2:B:477:GLY:O	2.41	0.53
2:B:795:PHE:CD1	2:B:839:LEU:HB3	2.43	0.53
2:B:824:ILE:O	2:B:828:LYS:HG2	2.09	0.53
2:B:831:PHE:HD2	2:B:836:LEU:HB2	1.74	0.53
2:B:886:LEU:HD13	2:B:932:LEU:HD23	1.90	0.53
2:B:1228:LEU:HD13	2:B:1244:LEU:HD23	1.90	0.53
2:E:938:ARG:O	2:E:941:ILE:HB	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1228:LEU:HD13	2:E:1244:LEU:HD23	1.90	0.53
2:E:1399:LEU:HD13	2:E:1405:ALA:HB1	1.90	0.53
2:E:1632:LYS:O	2:E:1636:HIS:N	2.41	0.53
3:F:69:PRO:HA	3:F:72:TYR:HD1	1.74	0.53
2:B:929:MET:HA	2:B:933:LEU:CD1	2.29	0.53
2:B:1212:MET:HA	2:B:1215:GLU:OE2	2.08	0.53
2:E:7:THR:O	2:E:10:GLN:NE2	2.42	0.53
2:E:281:PHE:HD1	2:E:428:ALA:HB3	1.74	0.53
2:E:886:LEU:HD13	2:E:932:LEU:HD23	1.90	0.53
2:E:1626:PHE:HD2	2:E:1627:ARG:HD2	1.74	0.53
3:F:6:CYS:SG	3:F:79:LEU:HG	2.48	0.53
1:A:670:ASN:O	1:A:674:GLY:N	2.41	0.53
2:B:296:LEU:HD23	2:B:346:ILE:HD11	1.90	0.53
2:B:820:LEU:O	2:B:823:ILE:HG12	2.09	0.53
2:B:1272:GLN:C	2:B:1297:LYS:HD2	2.29	0.53
3:C:69:PRO:HA	3:C:72:TYR:HD1	1.74	0.53
2:E:730:TYR:CD1	2:E:771:ARG:HD3	2.44	0.53
2:E:929:MET:HA	2:E:933:LEU:CD1	2.29	0.53
2:E:1348:PHE:O	2:E:1352:ILE:HG12	2.09	0.53
3:F:72:TYR:CE2	3:F:101:VAL:HG22	2.44	0.53
1:A:618:THR:HB	1:A:662:TYR:OH	2.08	0.53
2:B:19:TYR:HB3	2:B:29:LEU:H	1.73	0.53
2:B:46:ARG:HA	2:B:57:GLY:O	2.09	0.53
2:B:90:GLU:O	2:B:94:THR:OG1	2.13	0.53
2:B:320:ARG:NH1	2:B:375:GLU:OE1	2.42	0.53
2:B:992:MET:O	2:B:996:LEU:HD23	2.08	0.53
2:B:1391:ARG:NH2	2:B:1392:GLU:OE2	2.42	0.53
2:B:1399:LEU:HD13	2:B:1405:ALA:HB1	1.89	0.53
2:E:102:TRP:HA	2:E:105:LEU:HG	1.90	0.53
2:E:880:PRO:HA	2:E:931:ARG:HH12	1.73	0.53
2:E:940:VAL:HG13	2:E:992:MET:HE1	1.91	0.53
2:E:945:ARG:HH12	2:E:946:GLN:HB2	1.73	0.53
2:B:73:ASP:O	2:B:78:GLU:N	2.42	0.53
2:B:122:TYR:HA	2:B:125:ILE:HG12	1.90	0.53
2:B:1321:SER:OG	2:B:1345:ARG:NH2	2.42	0.53
2:B:1495:PHE:CE1	2:B:1502:PHE:HD2	2.26	0.53
3:C:66:ARG:NH1	3:C:67:LEU:HB2	2.24	0.53
2:E:881:LEU:O	2:E:884:ASP:HB2	2.09	0.53
2:E:997:ILE:HG21	2:E:1053:PHE:HB2	1.90	0.53
1:A:536:LEU:HA	1:A:539:LYS:HE3	1.91	0.53
2:B:93:SER:O	2:B:96:ARG:HB3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:243:MET:HG3	2:B:281:PHE:CZ	2.44	0.53
2:B:294:VAL:HG11	2:B:333:ILE:HD12	1.91	0.53
2:B:990:PHE:HB3	2:B:1045:ASN:CG	2.30	0.53
2:B:1006:TRP:N	2:B:1006:TRP:CD1	2.77	0.53
2:B:1203:ASN:O	2:B:1207:TYR:HB3	2.09	0.53
2:B:1407:LYS:HA	2:B:1426:MET:H	1.74	0.53
2:B:1545:HIS:O	2:B:1548:SER:OG	2.21	0.53
3:C:68:ARG:HG2	3:C:69:PRO:HD3	1.91	0.53
2:E:189:VAL:HA	2:E:192:LYS:HE2	1.91	0.53
2:E:222:TYR:CZ	2:E:289:LEU:HD11	2.44	0.53
2:E:561:THR:HB	2:E:631:LEU:HD22	1.90	0.53
2:E:765:ARG:NE	2:E:826:ASP:OD1	2.35	0.53
2:E:1091:TRP:CH2	2:E:1131:MET:HB3	2.44	0.53
2:E:1386:LYS:H	2:E:1389:GLU:HG3	1.74	0.53
2:E:1398:LEU:HA	2:E:1401:GLN:HB3	1.91	0.53
2:E:1518:ALA:HB2	2:E:1570:PHE:CE2	2.44	0.53
2:B:730:TYR:CZ	2:B:731:VAL:HG23	2.43	0.52
2:B:789:ASN:HA	2:B:792:ARG:HD2	1.91	0.52
2:B:881:LEU:O	2:B:884:ASP:HB2	2.09	0.52
2:B:1600:LEU:O	2:B:1604:ILE:HG12	2.09	0.52
2:E:14:VAL:HB	2:E:65:HIS:HB3	1.91	0.52
2:E:828:LYS:HZ3	2:E:867:THR:HA	1.75	0.52
2:E:1391:ARG:NH2	2:E:1392:GLU:OE2	2.42	0.52
2:E:1407:LYS:HA	2:E:1426:MET:H	1.74	0.52
1:A:576:TYR:HE1	1:A:591:LEU:HG	1.75	0.52
2:B:30:GLN:NE2	2:B:32:GLY:H	2.08	0.52
2:B:102:TRP:HA	2:B:105:LEU:HG	1.90	0.52
2:B:281:PHE:HD1	2:B:428:ALA:HB3	1.74	0.52
2:B:570:VAL:HG22	2:B:592:LYS:HZ2	1.74	0.52
2:B:570:VAL:HA	2:B:592:LYS:HZ2	1.73	0.52
2:B:945:ARG:HH12	2:B:946:GLN:HB2	1.74	0.52
2:B:997:ILE:HG21	2:B:1053:PHE:HB2	1.90	0.52
2:B:1027:VAL:HG22	2:B:1032:PHE:CE1	2.44	0.52
2:B:1207:TYR:HD2	2:B:1208:ARG:HG3	1.74	0.52
2:B:1348:PHE:O	2:B:1352:ILE:HG12	2.09	0.52
2:B:1404:ASN:HB2	2:B:1406:GLU:OE2	2.09	0.52
2:B:1626:PHE:CD2	2:B:1627:ARG:HD2	2.45	0.52
1:D:536:LEU:HD21	2:E:17:TYR:HA	1.91	0.52
2:E:46:ARG:HD2	2:E:58:ILE:HG13	1.91	0.52
2:E:99:ALA:HA	2:E:102:TRP:HE1	1.75	0.52
2:E:296:LEU:HD23	2:E:346:ILE:HD11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:320:ARG:NH1	2:E:375:GLU:OE1	2.42	0.52
2:E:533:HIS:CE1	2:E:535:SER:HB3	2.44	0.52
2:E:730:TYR:CZ	2:E:731:VAL:HG23	2.43	0.52
2:E:1165:ASP:O	2:E:1168:TYR:HB3	2.08	0.52
2:E:1233:GLU:O	2:E:1235:LYS:NZ	2.22	0.52
2:E:1370:GLN:N	2:E:1421:SER:O	2.40	0.52
2:E:1395:SER:O	2:E:1399:LEU:HG	2.09	0.52
2:B:1363:PHE:O	2:B:1383:TYR:N	2.30	0.52
2:B:1386:LYS:H	2:B:1389:GLU:HG3	1.74	0.52
2:B:1626:PHE:HD2	2:B:1627:ARG:HD2	1.74	0.52
2:E:528:ARG:HA	2:E:551:PHE:HA	1.92	0.52
2:E:831:PHE:HD2	2:E:836:LEU:HB2	1.74	0.52
2:E:1027:VAL:HG22	2:E:1032:PHE:CE1	2.44	0.52
2:E:1203:ASN:O	2:E:1207:TYR:HB3	2.09	0.52
2:E:1463:ARG:HH21	2:E:1484:ILE:HG21	1.73	0.52
2:E:1521:THR:O	2:E:1524:LEU:HG	2.09	0.52
2:E:1522:MET:HG3	2:E:1566:TYR:HE2	1.75	0.52
3:F:68:ARG:HG2	3:F:69:PRO:HD3	1.91	0.52
1:A:544:ILE:O	1:A:547:LEU:HG	2.09	0.52
2:B:44:TRP:CE3	2:B:58:ILE:HG22	2.45	0.52
2:B:871:GLN:HG2	2:B:875:ARG:HD3	1.91	0.52
2:B:1398:LEU:HA	2:B:1401:GLN:HB3	1.92	0.52
3:C:72:TYR:CE2	3:C:101:VAL:HG22	2.44	0.52
1:D:536:LEU:HA	1:D:539:LYS:HE3	1.91	0.52
2:E:871:GLN:HG2	2:E:875:ARG:HD3	1.91	0.52
2:E:1058:SER:O	2:E:1062:GLU:HG2	2.09	0.52
2:E:1593:ILE:HB	2:E:1597:MET:HE1	1.92	0.52
2:B:646:ASN:HD21	2:B:649:ASN:HD22	1.57	0.52
2:B:853:VAL:O	2:B:856:LYS:HG3	2.10	0.52
2:B:1265:LEU:O	2:B:1269:GLU:N	2.30	0.52
2:B:1593:ILE:HA	2:B:1596:GLN:HB3	1.90	0.52
2:B:1615:LEU:O	2:B:1619:HIS:N	2.29	0.52
3:C:12:GLY:N	3:C:60:GLY:HA3	2.25	0.52
2:E:200:GLU:HA	2:E:203:SER:HB3	1.91	0.52
2:E:262:TRP:CZ3	2:E:268:PRO:HG3	2.44	0.52
2:E:789:ASN:HA	2:E:792:ARG:HD2	1.91	0.52
2:E:1249:ASP:HA	2:E:1252:ARG:NE	2.25	0.52
2:E:1404:ASN:HB2	2:E:1406:GLU:OE2	2.09	0.52
2:E:1626:PHE:CD2	2:E:1627:ARG:HD2	2.45	0.52
2:B:94:THR:HG22	2:B:98:TRP:HE1	1.74	0.52
2:B:730:TYR:CD1	2:B:771:ARG:HD3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:589:GLY:O	1:D:591:LEU:N	2.42	0.52
2:E:570:VAL:HG22	2:E:592:LYS:HZ2	1.74	0.52
2:E:570:VAL:HA	2:E:592:LYS:HZ2	1.73	0.52
2:E:889:GLN:HA	2:E:895:ASN:HD21	1.75	0.52
2:E:934:ARG:HB3	2:E:935:ARG:NH1	2.24	0.52
2:E:990:PHE:HB3	2:E:1045:ASN:CG	2.30	0.52
3:F:2:GLN:NE2	3:F:50:PRO:O	2.42	0.52
2:B:105:LEU:HD11	2:B:117:LEU:HD13	1.91	0.52
2:B:860:MET:SD	2:B:905:LEU:HD22	2.50	0.52
2:B:929:MET:CA	2:B:933:LEU:HD13	2.30	0.52
2:B:1129:PHE:CG	2:B:1179:HIS:HB3	2.45	0.52
2:B:1249:ASP:HA	2:B:1252:ARG:NE	2.25	0.52
2:B:1373:PRO:HG2	2:B:1376:LEU:HD12	1.91	0.52
1:D:536:LEU:HD21	2:E:17:TYR:CB	2.38	0.52
1:D:544:ILE:O	1:D:547:LEU:HG	2.09	0.52
3:F:82:PHE:HE1	3:F:154:TYR:HE1	1.58	0.52
2:B:182:ALA:HA	2:B:185:LYS:HZ2	1.73	0.52
2:B:222:TYR:CE1	2:B:289:LEU:HD11	2.45	0.52
2:B:528:ARG:HA	2:B:551:PHE:HA	1.92	0.52
2:B:1129:PHE:HA	2:B:1132:MET:HG3	1.92	0.52
3:C:2:GLN:NE2	3:C:50:PRO:O	2.42	0.52
2:E:94:THR:HG22	2:E:98:TRP:HE1	1.75	0.52
2:E:105:LEU:HD11	2:E:117:LEU:HD13	1.91	0.52
2:E:166:ARG:HH22	2:E:168:ASP:HB2	1.75	0.52
2:E:421:VAL:HG13	2:E:425:THR:HG21	1.92	0.52
2:E:853:VAL:O	2:E:856:LYS:HG3	2.10	0.52
2:E:860:MET:SD	2:E:905:LEU:HD22	2.50	0.52
2:E:984:ASP:O	2:E:988:GLU:HG3	2.09	0.52
2:E:1102:ILE:CG1	2:E:1131:MET:HB2	2.39	0.52
2:E:1207:TYR:HD2	2:E:1208:ARG:HG3	1.74	0.52
2:E:1359:GLN:NE2	2:E:1455:ARG:HB2	2.25	0.52
2:E:1449:GLN:HA	2:E:1452:ASN:ND2	2.23	0.52
2:E:1618:LEU:HD22	2:E:1621:ARG:HH21	1.75	0.52
3:F:12:GLY:N	3:F:60:GLY:HA3	2.25	0.52
1:A:700:ASP:HB2	2:B:32:GLY:HA2	1.92	0.52
2:B:1058:SER:O	2:B:1062:GLU:HG2	2.09	0.52
2:B:1370:GLN:N	2:B:1421:SER:O	2.40	0.52
3:C:2:GLN:OE1	3:C:2:GLN:N	2.43	0.52
3:C:53:LEU:HD22	3:C:169:PHE:CE1	2.45	0.52
3:C:174:ARG:HA	3:C:177:LEU:HD12	1.92	0.52
2:E:32:GLY:O	2:E:50:LEU:HD13	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:824:ILE:O	2:E:828:LYS:HG2	2.09	0.52
2:B:189:VAL:HA	2:B:192:LYS:HE2	1.91	0.52
2:B:222:TYR:CZ	2:B:289:LEU:HD11	2.44	0.52
2:B:228:PHE:HB3	2:B:277:LEU:HB3	1.92	0.52
2:B:889:GLN:HA	2:B:895:ASN:HD21	1.75	0.52
2:B:902:SER:O	2:B:906:LEU:HG	2.10	0.52
2:B:984:ASP:O	2:B:988:GLU:HG3	2.10	0.52
2:B:1490:THR:OG1	2:B:1506:GLN:N	2.43	0.52
2:B:1521:THR:O	2:B:1524:LEU:HG	2.09	0.52
1:D:584:LYS:HZ1	2:E:1405:ALA:HB2	1.74	0.52
2:E:228:PHE:HB3	2:E:277:LEU:HB3	1.92	0.52
2:E:681:MET:SD	2:E:726:ALA:HB1	2.50	0.52
2:E:741:VAL:HG11	2:E:798:PHE:HD1	1.75	0.52
2:E:795:PHE:O	2:E:798:PHE:HB2	2.10	0.52
2:E:934:ARG:NH1	2:E:938:ARG:HB2	2.25	0.52
2:E:1129:PHE:CG	2:E:1179:HIS:HB3	2.45	0.52
2:E:1544:VAL:HG13	2:E:1547:LEU:HD22	1.92	0.52
3:F:2:GLN:OE1	3:F:2:GLN:N	2.43	0.52
3:F:66:ARG:NH1	3:F:67:LEU:HB2	2.24	0.52
2:B:1153:THR:O	2:B:1157:GLN:NE2	2.43	0.51
1:D:711:PRO:HD2	2:E:17:TYR:CE1	2.45	0.51
2:E:646:ASN:HD21	2:E:649:ASN:HD22	1.57	0.51
2:E:1536:HIS:CD2	2:E:1606:ILE:HB	2.43	0.51
1:A:578:ARG:HH22	1:A:601:HIS:H	1.58	0.51
2:B:7:THR:O	2:B:10:GLN:NE2	2.42	0.51
2:B:60:PRO:O	2:B:64:ILE:N	2.37	0.51
2:B:555:MET:HE2	2:B:561:THR:HA	1.92	0.51
2:B:1079:MET:N	2:B:1079:MET:SD	2.83	0.51
3:C:142:GLY:HA3	3:C:154:TYR:CZ	2.44	0.51
2:E:294:VAL:HG11	2:E:333:ILE:HD12	1.91	0.51
2:E:902:SER:O	2:E:906:LEU:HG	2.10	0.51
2:B:32:GLY:O	2:B:50:LEU:HD13	2.09	0.51
2:B:1306:SER:O	2:B:1310:LYS:HG2	2.11	0.51
2:B:1322:LYS:HD3	2:B:1345:ARG:HH11	1.74	0.51
2:E:44:TRP:CE3	2:E:58:ILE:HG22	2.45	0.51
2:E:222:TYR:CE1	2:E:289:LEU:HD11	2.45	0.51
2:E:637:LEU:O	2:E:641:LEU:HG	2.11	0.51
2:E:1153:THR:O	2:E:1157:GLN:NE2	2.43	0.51
2:E:1600:LEU:O	2:E:1604:ILE:HG12	2.09	0.51
2:B:173:LEU:O	2:B:176:ASP:HB2	2.11	0.51
2:B:262:TRP:CZ3	2:B:268:PRO:HG3	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:295:SER:HB2	2:B:326:VAL:HG13	1.93	0.51
2:B:533:HIS:CE1	2:B:535:SER:HB3	2.44	0.51
2:B:741:VAL:HG11	2:B:798:PHE:HD1	1.75	0.51
2:B:1145:HIS:O	2:B:1149:ASN:ND2	2.44	0.51
2:B:1359:GLN:NE2	2:B:1455:ARG:HB2	2.25	0.51
2:B:1379:LYS:NZ	2:B:1504:VAL:O	2.36	0.51
2:B:1574:LYS:O	2:B:1577:GLN:HB2	2.11	0.51
1:D:576:TYR:CE1	1:D:591:LEU:HG	2.46	0.51
2:E:555:MET:HE2	2:E:561:THR:HA	1.93	0.51
2:E:929:MET:CA	2:E:933:LEU:HD13	2.30	0.51
2:E:1322:LYS:HD3	2:E:1345:ARG:HH11	1.74	0.51
2:E:1557:PRO:HB2	2:E:1561:GLY:CA	2.36	0.51
1:A:532:PRO:HG3	1:A:708:ASP:HA	1.93	0.51
1:A:576:TYR:CE1	1:A:591:LEU:HG	2.46	0.51
2:B:192:LYS:O	2:B:195:GLU:HG2	2.10	0.51
2:B:637:LEU:O	2:B:641:LEU:HG	2.11	0.51
2:B:795:PHE:O	2:B:798:PHE:HB2	2.11	0.51
3:C:82:PHE:HE1	3:C:154:TYR:HE1	1.58	0.51
2:E:73:ASP:O	2:E:78:GLU:N	2.42	0.51
2:E:295:SER:HB2	2:E:326:VAL:HG13	1.93	0.51
2:E:673:LEU:HD13	2:E:719:TYR:CG	2.45	0.51
1:A:551:GLN:NE2	1:A:555:ARG:HD3	2.25	0.51
2:B:219:ILE:O	2:B:222:TYR:OH	2.21	0.51
2:B:1308:PHE:CD1	2:B:1313:MET:HB2	2.46	0.51
2:B:1438:PRO:HB2	2:B:1441:TYR:CD2	2.46	0.51
1:D:582:ASN:HB2	1:D:584:LYS:HG2	1.91	0.51
2:E:25:VAL:HG21	2:E:56:LYS:HG3	1.93	0.51
2:E:243:MET:HG3	2:E:281:PHE:CZ	2.44	0.51
2:E:1079:MET:N	2:E:1079:MET:SD	2.83	0.51
2:E:1129:PHE:HA	2:E:1132:MET:HG3	1.92	0.51
2:E:1145:HIS:O	2:E:1149:ASN:ND2	2.44	0.51
2:E:1490:THR:OG1	2:E:1506:GLN:N	2.44	0.51
3:F:53:LEU:HD22	3:F:169:PHE:CE1	2.45	0.51
2:B:451:ILE:HG23	2:B:510:TYR:CZ	2.46	0.51
2:B:472:VAL:HA	2:B:527:ILE:HA	1.93	0.51
2:B:681:MET:SD	2:B:726:ALA:HB1	2.51	0.51
2:B:880:PRO:HA	2:B:931:ARG:NH1	2.25	0.51
2:B:1478:GLU:OE1	3:C:34:PRO:HG2	2.11	0.51
2:E:30:GLN:NE2	2:E:32:GLY:H	2.08	0.51
2:E:88:VAL:HB	2:E:128:ARG:NH2	2.26	0.51
2:E:179:SER:H	2:E:183:LEU:HD13	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:730:TYR:CE1	2:E:731:VAL:HG23	2.46	0.51
2:E:979:ARG:HG3	2:E:1032:PHE:HE2	1.76	0.51
2:E:1272:GLN:C	2:E:1297:LYS:HD2	2.29	0.51
2:E:1321:SER:OG	2:E:1345:ARG:NH2	2.42	0.51
1:A:544:ILE:HD11	1:A:686:LEU:O	2.10	0.51
1:A:582:ASN:HB2	1:A:584:LYS:HG2	1.91	0.51
2:B:46:ARG:HD2	2:B:58:ILE:HG13	1.91	0.51
2:B:166:ARG:HH22	2:B:168:ASP:HB2	1.75	0.51
1:D:532:PRO:HG3	1:D:708:ASP:HA	1.93	0.51
1:D:578:ARG:HH22	1:D:601:HIS:H	1.58	0.51
2:E:195:GLU:HA	2:E:198:ILE:HG22	1.92	0.51
2:E:880:PRO:HA	2:E:931:ARG:NH1	2.25	0.51
2:E:958:ILE:HG21	2:E:1017:PHE:CE1	2.46	0.51
2:E:1441:TYR:CE2	2:E:1450:ILE:HD13	2.46	0.51
1:A:677:MET:O	1:A:683:ARG:NH1	2.44	0.51
2:B:116:GLN:HA	2:B:119:GLN:HG3	1.93	0.51
2:B:421:VAL:HG13	2:B:425:THR:HG21	1.92	0.51
2:B:934:ARG:NH1	2:B:938:ARG:HB2	2.25	0.51
2:B:1032:PHE:HA	2:B:1036:ALA:HB2	1.93	0.51
2:B:1362:TYR:OH	2:B:1456:ALA:O	2.20	0.51
1:D:576:TYR:HE1	1:D:591:LEU:HG	1.75	0.51
1:D:677:MET:O	1:D:683:ARG:NH1	2.44	0.51
2:E:192:LYS:O	2:E:195:GLU:HG2	2.10	0.51
2:E:203:SER:OG	2:E:210:LEU:HD22	2.11	0.51
2:E:1308:PHE:CD1	2:E:1313:MET:HB2	2.46	0.51
2:E:1373:PRO:HG2	2:E:1376:LEU:HD12	1.91	0.51
2:E:1438:PRO:HB2	2:E:1441:TYR:CD2	2.46	0.51
2:E:1488:THR:O	2:E:1508:SER:N	2.39	0.51
2:B:14:VAL:HB	2:B:65:HIS:HB3	1.91	0.51
2:B:520:GLU:O	2:B:523:THR:OG1	2.15	0.51
2:B:1334:ASP:O	2:B:1338:LEU:N	2.33	0.51
2:B:1563:PHE:HB3	2:B:1637:TYR:OH	2.11	0.51
2:B:1593:ILE:HB	2:B:1597:MET:HE1	1.93	0.51
2:E:46:ARG:HD2	2:E:58:ILE:CG1	2.41	0.51
2:E:238:ASP:O	2:E:303:VAL:N	2.36	0.51
2:E:966:ASP:HA	2:E:969:TYR:CD2	2.46	0.51
2:E:1166:GLU:O	2:E:1169:LYS:HG2	2.10	0.51
2:E:1411:THR:HB	3:F:28:PHE:CZ	2.46	0.51
2:E:1495:PHE:CE1	2:E:1502:PHE:HD2	2.26	0.51
2:E:1614:GLN:HG2	3:F:70:LEU:HD22	1.93	0.51
3:F:174:ARG:HA	3:F:177:LEU:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:179:SER:H	2:B:183:LEU:HD13	1.76	0.50
2:B:228:PHE:HB3	2:B:277:LEU:CB	2.41	0.50
2:B:680:MET:HG3	2:B:681:MET:HE3	1.93	0.50
2:B:1102:ILE:CD1	2:B:1131:MET:HB2	2.41	0.50
2:B:1166:GLU:O	2:B:1169:LYS:HG2	2.10	0.50
2:B:1544:VAL:HG13	2:B:1547:LEU:HD22	1.91	0.50
1:A:577:CYS:SG	1:A:586:LEU:HD12	2.51	0.50
2:B:98:TRP:O	2:B:102:TRP:HD1	1.94	0.50
2:B:1522:MET:HG3	2:B:1566:TYR:HE2	1.75	0.50
1:D:697:ARG:HA	2:E:30:GLN:HE21	1.76	0.50
2:E:121:THR:HA	2:E:124:LEU:HG	1.93	0.50
2:E:1032:PHE:HA	2:E:1036:ALA:HB2	1.93	0.50
2:E:1563:PHE:HB3	2:E:1637:TYR:OH	2.11	0.50
2:E:1633:VAL:HG12	2:E:1637:TYR:CG	2.46	0.50
2:B:45:TYR:O	2:B:59:PHE:N	2.31	0.50
2:B:45:TYR:HD2	2:B:64:ILE:HG13	1.77	0.50
2:B:200:GLU:HA	2:B:203:SER:HB3	1.91	0.50
2:B:589:PRO:HB3	2:B:594:GLU:HB3	1.94	0.50
2:B:757:LEU:HB3	2:B:815:ALA:HB1	1.94	0.50
2:B:958:ILE:HG21	2:B:1017:PHE:CE1	2.46	0.50
2:B:1336:GLU:H	2:B:1336:GLU:CD	2.11	0.50
2:E:98:TRP:O	2:E:102:TRP:HD1	1.94	0.50
2:E:644:ARG:NH2	2:E:678:ASN:OD1	2.43	0.50
1:A:584:LYS:CE	2:B:1405:ALA:HB2	2.41	0.50
1:A:677:MET:HB2	1:A:682:THR:HG21	1.93	0.50
2:B:99:ALA:HA	2:B:102:TRP:HE1	1.75	0.50
2:B:332:ILE:HD13	2:B:403:LEU:HB2	1.94	0.50
2:B:836:LEU:HG	2:B:840:PHE:HE2	1.76	0.50
2:B:1051:VAL:HG11	2:B:1108:PRO:HB3	1.93	0.50
2:B:1618:LEU:HD22	2:B:1621:ARG:HH21	1.75	0.50
1:D:551:GLN:NE2	1:D:555:ARG:HD3	2.26	0.50
1:D:577:CYS:SG	1:D:586:LEU:HD12	2.51	0.50
1:D:584:LYS:NZ	2:E:1399:LEU:O	2.42	0.50
2:E:768:ILE:HG21	2:E:829:LEU:HB2	1.94	0.50
2:E:876:GLU:OE1	2:E:876:GLU:N	2.40	0.50
2:E:1180:CYS:HB3	2:E:1187:SER:HB3	1.94	0.50
2:E:1334:ASP:O	2:E:1338:LEU:N	2.33	0.50
3:F:14:VAL:HG13	3:F:116:LYS:NZ	2.27	0.50
1:A:696:LEU:HD12	1:A:697:ARG:NE	2.26	0.50
2:B:121:THR:HA	2:B:124:LEU:HG	1.93	0.50
2:B:673:LEU:HD13	2:B:719:TYR:CG	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:740:TYR:CE2	2:B:752:LEU:HB3	2.46	0.50
2:B:979:ARG:HG3	2:B:1032:PHE:HE2	1.76	0.50
2:B:1207:TYR:CD2	2:B:1208:ARG:HG3	2.47	0.50
2:B:1632:LYS:O	2:B:1636:HIS:N	2.41	0.50
2:E:321:PRO:HB2	2:E:351:ILE:HD11	1.93	0.50
2:E:757:LEU:HB3	2:E:815:ALA:HB1	1.94	0.50
2:E:931:ARG:HB3	2:E:932:LEU:HD12	1.94	0.50
2:E:1574:LYS:O	2:E:1577:GLN:HB2	2.11	0.50
2:B:195:GLU:HA	2:B:198:ILE:HG22	1.92	0.50
2:B:444:ASN:ND2	2:B:517:ILE:O	2.45	0.50
2:B:644:ARG:NH2	2:B:678:ASN:OD1	2.43	0.50
2:B:730:TYR:CE1	2:B:731:VAL:HG23	2.46	0.50
2:B:966:ASP:HA	2:B:969:TYR:CD2	2.46	0.50
2:B:1102:ILE:CG1	2:B:1131:MET:HB2	2.40	0.50
2:B:1418:ILE:HG13	2:B:1425:TYR:CE2	2.47	0.50
2:B:1602:GLU:N	2:B:1605:ARG:HH21	2.10	0.50
1:D:677:MET:HB2	1:D:682:THR:HG21	1.94	0.50
1:D:696:LEU:HD12	1:D:697:ARG:NE	2.26	0.50
2:E:37:ILE:HG21	2:E:45:TYR:HB3	1.94	0.50
2:E:836:LEU:HG	2:E:840:PHE:HE2	1.76	0.50
2:E:1482:MET:HG3	2:E:1517:ASN:HB3	1.93	0.50
3:F:25:THR:HG21	3:F:32:TYR:HA	1.93	0.50
2:B:1441:TYR:CE2	2:B:1450:ILE:HD13	2.46	0.50
2:B:1444:LYS:HD3	2:E:1333:PHE:HZ	1.77	0.50
1:D:544:ILE:HD11	1:D:686:LEU:O	2.10	0.50
2:E:116:GLN:HA	2:E:119:GLN:HG3	1.93	0.50
2:E:1046:TYR:OH	2:E:1090:MET:HG3	2.11	0.50
2:E:1306:SER:O	2:E:1310:LYS:HG2	2.11	0.50
2:E:1602:GLU:N	2:E:1605:ARG:HH21	2.10	0.50
2:B:88:VAL:HB	2:B:128:ARG:NH2	2.26	0.50
2:B:468:VAL:HB	2:B:498:SER:HB3	1.94	0.50
2:B:871:GLN:OE1	2:B:918:VAL:HG12	2.12	0.50
2:B:931:ARG:HB3	2:B:932:LEU:HD12	1.94	0.50
2:B:1062:GLU:O	2:B:1068:LYS:HB3	2.12	0.50
2:B:1362:TYR:C	2:B:1431:VAL:HG22	2.32	0.50
2:B:1378:ASN:HB3	2:B:1419:LYS:HD3	1.94	0.50
2:B:1562:GLY:HA2	2:B:1565:ASN:HB2	1.94	0.50
2:E:451:ILE:HG23	2:E:510:TYR:CZ	2.46	0.50
2:E:468:VAL:HB	2:E:498:SER:HB3	1.94	0.50
2:E:1102:ILE:CD1	2:E:1131:MET:HB2	2.41	0.50
2:E:1102:ILE:O	2:E:1106:VAL:HG23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1126:PRO:HD3	2:E:1175:LEU:HD12	1.94	0.50
2:E:1463:ARG:HG2	2:E:1487:THR:H	1.77	0.50
2:B:1008:VAL:O	2:B:1012:THR:HG23	2.12	0.50
2:B:1598:PRO:O	2:B:1601:THR:HB	2.12	0.50
1:D:717:PRO:HB2	2:E:1:MET:N	2.27	0.50
2:E:45:TYR:HD2	2:E:64:ILE:HG13	1.77	0.50
2:E:173:LEU:O	2:E:176:ASP:HB2	2.11	0.50
2:E:319:ARG:HB2	2:E:499:VAL:HA	1.94	0.50
2:E:472:VAL:HA	2:E:527:ILE:HA	1.93	0.50
2:E:589:PRO:HB3	2:E:594:GLU:HB3	1.94	0.50
2:E:899:HIS:HB3	2:E:949:HIS:CE1	2.46	0.50
2:E:1062:GLU:O	2:E:1068:LYS:HB3	2.12	0.50
2:E:1200:LEU:O	2:E:1204:LEU:HG	2.12	0.50
2:B:25:VAL:CG2	2:B:57:GLY:HA2	2.40	0.49
2:B:46:ARG:HD2	2:B:58:ILE:CG1	2.41	0.49
2:B:450:LEU:HD21	2:B:470:MET:SD	2.52	0.49
2:B:945:ARG:HH11	2:B:946:GLN:H	1.60	0.49
2:B:1180:CYS:HB3	2:B:1187:SER:HB3	1.93	0.49
2:B:1299:LYS:HE2	2:B:1302:GLN:OE1	2.12	0.49
1:D:570:ARG:HH22	1:D:593:GLU:HG3	1.77	0.49
2:E:228:PHE:HB3	2:E:277:LEU:CB	2.41	0.49
2:E:818:LYS:HZ3	2:E:858:ASN:HB3	1.76	0.49
2:E:1063:THR:HA	2:E:1069:ARG:HH11	1.77	0.49
1:A:552:ARG:HE	1:A:664:ILE:HG23	1.77	0.49
2:B:741:VAL:HG11	2:B:798:PHE:CD1	2.47	0.49
2:B:1046:TYR:OH	2:B:1090:MET:HG3	2.11	0.49
2:B:1619:HIS:HA	2:B:1622:LEU:HG	1.93	0.49
2:E:150:ALA:HB1	2:E:197:LYS:NZ	2.27	0.49
2:E:444:ASN:ND2	2:E:517:ILE:O	2.45	0.49
2:E:741:VAL:HG21	2:E:798:PHE:HE1	1.78	0.49
2:E:1028:LEU:HD23	2:E:1032:PHE:HD1	1.77	0.49
2:E:1388:TYR:CD2	3:F:45:MET:HE2	2.44	0.49
2:E:1619:HIS:HA	2:E:1622:LEU:HG	1.93	0.49
2:B:25:VAL:HG21	2:B:56:LYS:HG3	1.93	0.49
2:B:95:LEU:HD13	2:B:98:TRP:CD1	2.47	0.49
2:B:1633:VAL:HG12	2:B:1637:TYR:CG	2.46	0.49
2:E:417:PHE:HA	2:E:419:HIS:CE1	2.48	0.49
2:E:740:TYR:CE2	2:E:752:LEU:HB3	2.46	0.49
2:E:1483:TRP:CE2	2:E:1514:PRO:HD3	2.47	0.49
2:B:156:ASN:HD22	2:B:161:LEU:HD12	1.77	0.49
2:B:1611:LEU:HD21	2:B:1616:LYS:NZ	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:25:VAL:CG2	2:E:57:GLY:HA2	2.40	0.49
2:E:754:PHE:CZ	2:E:812:ILE:HG13	2.48	0.49
2:B:130:GLN:HG3	2:B:131:ILE:HG12	1.95	0.49
2:B:203:SER:OG	2:B:210:LEU:HD22	2.11	0.49
2:B:321:PRO:HB2	2:B:351:ILE:HD11	1.93	0.49
2:B:436:ILE:HG22	2:B:438:LEU:HD22	1.95	0.49
2:B:768:ILE:HG21	2:B:829:LEU:HB2	1.94	0.49
2:B:899:HIS:HB3	2:B:949:HIS:CE1	2.46	0.49
2:B:1196:LEU:O	2:B:1199:SER:OG	2.26	0.49
2:B:1463:ARG:HG2	2:B:1487:THR:H	1.77	0.49
2:B:1468:PHE:HE2	2:B:1470:LYS:HB2	1.78	0.49
3:C:14:VAL:HG13	3:C:116:LYS:NZ	2.27	0.49
2:E:95:LEU:HD13	2:E:98:TRP:CD1	2.47	0.49
2:E:332:ILE:HD13	2:E:403:LEU:HB2	1.94	0.49
2:E:436:ILE:HG22	2:E:438:LEU:HD22	1.95	0.49
2:E:945:ARG:HH11	2:E:946:GLN:H	1.60	0.49
2:E:1207:TYR:CD2	2:E:1208:ARG:HG3	2.47	0.49
2:E:1451:LEU:O	2:E:1455:ARG:HG3	2.12	0.49
2:E:1515:LEU:HG	2:E:1575:TYR:HE2	1.77	0.49
2:E:1562:GLY:HA2	2:E:1565:ASN:HB2	1.94	0.49
2:E:1611:LEU:HD21	2:E:1616:LYS:NZ	2.27	0.49
1:A:570:ARG:HH22	1:A:593:GLU:HG3	1.77	0.49
2:B:1483:TRP:CE2	2:B:1514:PRO:HD3	2.47	0.49
2:B:1536:HIS:CD2	2:B:1606:ILE:HB	2.43	0.49
2:B:1597:MET:HA	2:B:1600:LEU:HB2	1.94	0.49
2:B:1613:GLU:OE2	2:B:1614:GLN:HG3	2.13	0.49
1:D:680:ASP:OD1	1:D:681:LEU:N	2.45	0.49
2:E:529:PHE:O	2:E:550:ALA:N	2.41	0.49
2:E:1597:MET:HA	2:E:1600:LEU:HB2	1.94	0.49
3:F:129:LEU:HB3	3:F:134:LEU:O	2.13	0.49
2:B:19:TYR:CE2	2:B:26:GLU:HB3	2.48	0.49
2:B:444:ASN:HB2	2:B:519:ILE:HG12	1.95	0.49
2:B:1102:ILE:O	2:B:1106:VAL:HG23	2.12	0.49
3:C:7:VAL:HB	3:C:78:PHE:CE1	2.48	0.49
3:C:25:THR:HG21	3:C:32:TYR:HA	1.94	0.49
2:E:1008:VAL:O	2:E:1012:THR:HG23	2.12	0.49
2:E:1202:GLU:HA	2:E:1205:LEU:HB2	1.95	0.49
2:B:417:PHE:HA	2:B:419:HIS:CE1	2.48	0.49
2:B:647:SER:HA	2:B:650:ILE:HG13	1.94	0.49
3:C:41:SER:OG	3:C:53:LEU:O	2.15	0.49
2:E:19:TYR:CE2	2:E:26:GLU:HB3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:187:HIS:HB3	2:E:1006:TRP:CZ3	2.48	0.49
2:E:741:VAL:HG11	2:E:798:PHE:CD1	2.47	0.49
2:E:1242:ARG:NH1	2:E:1246:LYS:HZ1	2.10	0.49
1:A:589:GLY:O	1:A:591:LEU:N	2.42	0.49
2:B:940:VAL:HG13	2:B:992:MET:HE1	1.95	0.49
1:D:564:LYS:NZ	1:D:590:ASP:OD1	2.40	0.49
2:E:552:VAL:HB	2:E:569:LEU:HD22	1.95	0.49
2:E:646:ASN:ND2	2:E:649:ASN:HD22	2.11	0.49
2:E:871:GLN:OE1	2:E:918:VAL:HG12	2.12	0.49
2:E:1291:TYR:CB	2:E:1296:LEU:HD21	2.40	0.49
2:E:1388:TYR:HD2	3:F:45:MET:CE	2.24	0.49
2:E:1598:PRO:O	2:E:1601:THR:HB	2.12	0.49
1:A:680:ASP:OD1	1:A:681:LEU:N	2.45	0.49
2:B:4:TRP:CD2	2:B:46:ARG:HD3	2.47	0.49
2:B:552:VAL:HB	2:B:569:LEU:HD22	1.95	0.49
2:B:716:LEU:O	2:B:720:ILE:HG13	2.13	0.49
2:B:741:VAL:HG21	2:B:798:PHE:HE1	1.78	0.49
2:B:932:LEU:N	2:B:935:ARG:HH21	2.11	0.49
2:B:1114:LEU:CB	2:B:1163:ARG:HD2	2.41	0.49
2:B:1217:LYS:HD3	2:B:1220:ARG:NH1	2.22	0.49
2:B:1222:SER:O	2:B:1225:VAL:HG22	2.13	0.49
2:B:1359:GLN:HE21	2:B:1455:ARG:HB2	1.77	0.49
2:B:1451:LEU:O	2:B:1455:ARG:HG3	2.13	0.49
2:B:1623:SER:O	2:B:1627:ARG:HD3	2.13	0.49
3:C:60:GLY:HA2	3:C:97:TRP:HZ2	1.78	0.49
3:C:129:LEU:HB3	3:C:134:LEU:O	2.13	0.49
1:D:557:VAL:O	1:D:578:ARG:HG3	2.13	0.49
2:E:46:ARG:HB3	2:E:58:ILE:HA	1.95	0.49
2:E:444:ASN:HB2	2:E:519:ILE:HG12	1.95	0.49
2:E:730:TYR:HD1	2:E:787:PHE:CG	2.31	0.49
2:E:764:PHE:O	2:E:768:ILE:HG12	2.13	0.49
2:E:883:THR:HG21	2:E:931:ARG:HG2	1.95	0.49
2:E:1051:VAL:HG11	2:E:1108:PRO:HB3	1.93	0.49
2:E:1186:LEU:HD12	2:E:1189:SER:HB2	1.95	0.49
2:E:1378:ASN:HB3	2:E:1419:LYS:HD3	1.94	0.49
2:B:319:ARG:HB2	2:B:499:VAL:HA	1.94	0.48
2:B:526:HIS:HB2	2:B:552:VAL:O	2.13	0.48
2:B:1126:PRO:HD3	2:B:1175:LEU:HD12	1.94	0.48
2:B:1390:ARG:HD3	3:C:44:VAL:CG1	2.42	0.48
2:B:1463:ARG:HG3	2:B:1486:ARG:HB3	1.95	0.48
1:D:552:ARG:HE	1:D:664:ILE:HG23	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:166:ARG:HG2	2:E:173:LEU:H	1.77	0.48
2:E:471:SER:HB3	2:E:495:GLU:HG2	1.95	0.48
2:E:560:THR:HG22	2:E:638:LEU:HD23	1.95	0.48
2:E:643:TRP:CD1	2:E:675:ALA:HB1	2.48	0.48
2:E:647:SER:HA	2:E:650:ILE:HG13	1.93	0.48
2:E:759:ALA:O	2:E:763:LEU:HG	2.13	0.48
2:E:1299:LYS:HE2	2:E:1302:GLN:OE1	2.12	0.48
2:E:1379:LYS:HZ3	2:E:1504:VAL:HG12	1.78	0.48
1:A:584:LYS:NZ	2:B:1405:ALA:HB2	2.28	0.48
2:B:111:LEU:HD13	2:B:114:PHE:HD2	1.78	0.48
2:B:646:ASN:ND2	2:B:649:ASN:HD22	2.11	0.48
2:B:670:GLN:HG3	2:B:719:TYR:HD1	1.78	0.48
2:B:759:ALA:O	2:B:763:LEU:HG	2.13	0.48
2:B:1057:GLU:O	2:B:1080:ARG:HD3	2.12	0.48
2:B:1063:THR:HA	2:B:1069:ARG:HH11	1.77	0.48
2:B:1233:GLU:O	2:B:1235:LYS:NZ	2.22	0.48
2:B:1452:ASN:HA	2:B:1455:ARG:CZ	2.43	0.48
2:E:4:TRP:CD2	2:E:46:ARG:HD3	2.47	0.48
2:E:182:ALA:HA	2:E:185:LYS:HZ2	1.78	0.48
2:E:245:LEU:HB3	2:E:254:ILE:HD12	1.95	0.48
2:E:532:ARG:HB3	2:E:534:ARG:HD3	1.95	0.48
2:E:716:LEU:O	2:E:720:ILE:HG13	2.13	0.48
2:E:743:ASN:HB2	2:E:749:LYS:HD2	1.95	0.48
2:E:932:LEU:N	2:E:935:ARG:HH21	2.11	0.48
2:E:1362:TYR:C	2:E:1431:VAL:HG22	2.32	0.48
2:E:1623:SER:O	2:E:1627:ARG:HD3	2.13	0.48
3:F:94:ARG:HA	3:F:98:TYR:HB3	1.95	0.48
1:A:557:VAL:O	1:A:578:ARG:HG3	2.13	0.48
2:B:734:SER:HB3	2:B:787:PHE:HE1	1.79	0.48
2:B:929:MET:CE	2:B:972:TYR:HB3	2.43	0.48
2:B:1186:LEU:HD12	2:B:1189:SER:HB2	1.95	0.48
2:B:1200:LEU:O	2:B:1204:LEU:HG	2.12	0.48
2:E:182:ALA:HA	2:E:185:LYS:HZ3	1.77	0.48
2:E:450:LEU:HD21	2:E:470:MET:SD	2.52	0.48
2:B:150:ALA:HB1	2:B:197:LYS:NZ	2.27	0.48
2:B:238:ASP:O	2:B:303:VAL:N	2.36	0.48
2:B:242:PHE:HB3	2:B:257:ASN:HB3	1.96	0.48
2:B:643:TRP:CD1	2:B:675:ALA:HB1	2.48	0.48
2:B:730:TYR:HD1	2:B:787:PHE:CG	2.31	0.48
2:B:743:ASN:HB2	2:B:749:LYS:HD2	1.95	0.48
2:B:754:PHE:CZ	2:B:812:ILE:HG13	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1202:GLU:HA	2:B:1205:LEU:HB2	1.95	0.48
2:B:1242:ARG:NH1	2:B:1246:LYS:HZ1	2.11	0.48
2:B:1470:LYS:N	2:B:1481:THR:O	2.37	0.48
2:B:1596:GLN:O	2:B:1600:LEU:HG	2.13	0.48
3:C:2:GLN:HE22	3:C:49:LYS:HG3	1.78	0.48
3:C:58:THR:HB	3:C:68:ARG:HH12	1.78	0.48
3:C:94:ARG:HA	3:C:98:TYR:HB3	1.95	0.48
1:D:539:LYS:HE3	2:E:18:ASN:OD1	2.13	0.48
2:E:156:ASN:HD22	2:E:161:LEU:HD12	1.77	0.48
2:E:680:MET:HG3	2:E:681:MET:HE3	1.94	0.48
2:E:921:THR:OG1	2:E:924:HIS:HB3	2.14	0.48
2:E:1057:GLU:O	2:E:1080:ARG:HD3	2.12	0.48
2:E:1145:HIS:HA	2:E:1148:GLU:HG3	1.96	0.48
2:E:1362:TYR:CE2	2:E:1459:VAL:HG21	2.49	0.48
2:E:1383:TYR:CD2	2:E:1501:TRP:HB3	2.49	0.48
2:E:1596:GLN:O	2:E:1600:LEU:HG	2.13	0.48
2:E:1618:LEU:HD22	2:E:1621:ARG:NH2	2.28	0.48
3:F:39:ASN:OD1	3:F:57:ASP:N	2.47	0.48
2:B:72:GLU:HG3	2:B:74:LEU:H	1.79	0.48
2:B:187:HIS:HB3	2:B:1006:TRP:CZ3	2.48	0.48
2:B:764:PHE:O	2:B:768:ILE:HG12	2.13	0.48
2:B:987:MET:CE	2:B:1042:LEU:HD13	2.44	0.48
2:B:1481:THR:O	2:B:1483:TRP:HD1	1.97	0.48
3:C:6:CYS:SG	3:C:77:VAL:HG23	2.54	0.48
3:C:39:ASN:OD1	3:C:57:ASP:N	2.47	0.48
1:D:584:LYS:CD	2:E:1403:PRO:HA	2.43	0.48
2:E:4:TRP:HZ3	2:E:45:TYR:HA	1.78	0.48
2:E:734:SER:HB3	2:E:787:PHE:HE1	1.78	0.48
2:E:1196:LEU:HD22	2:E:1234:LYS:HD2	1.95	0.48
2:E:1275:ASP:OD2	2:E:1275:ASP:N	2.45	0.48
2:E:1383:TYR:CG	2:E:1501:TRP:HB3	2.49	0.48
2:E:1463:ARG:HG3	2:E:1486:ARG:HB3	1.95	0.48
2:E:1539:ASP:OD1	2:E:1541:SER:N	2.47	0.48
3:F:7:VAL:HB	3:F:78:PHE:CE1	2.48	0.48
2:B:98:TRP:HA	2:B:101:ILE:HG22	1.96	0.48
2:B:273:LYS:O	2:B:277:LEU:HG	2.14	0.48
2:B:471:SER:HB3	2:B:495:GLU:HG2	1.95	0.48
2:B:883:THR:HG21	2:B:931:ARG:HG2	1.95	0.48
2:B:1256:ASN:HB3	2:B:1259:GLU:OE1	2.14	0.48
2:B:1379:LYS:HZ3	2:B:1504:VAL:HG12	1.78	0.48
2:B:1460:GLN:OE1	2:B:1494:THR:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1482:MET:HG3	2:B:1517:ASN:HB3	1.94	0.48
2:B:1517:ASN:O	2:B:1520:GLU:HG3	2.14	0.48
2:B:1557:PRO:O	2:B:1561:GLY:HA2	2.14	0.48
2:B:1618:LEU:HD22	2:B:1621:ARG:NH2	2.28	0.48
1:D:569:ARG:NH2	1:D:571:GLN:OE1	2.47	0.48
1:D:697:ARG:HD3	2:E:30:GLN:HG2	1.95	0.48
2:E:98:TRP:O	2:E:102:TRP:CD1	2.67	0.48
2:E:191:SER:HA	2:E:194:ILE:HD12	1.96	0.48
2:E:248:PRO:HD2	2:E:293:ARG:HG3	1.96	0.48
2:E:728:LEU:HA	2:E:730:TYR:CE2	2.49	0.48
2:E:915:ARG:HA	2:E:915:ARG:HH11	1.79	0.48
2:E:1359:GLN:HE21	2:E:1455:ARG:HB2	1.77	0.48
2:E:1618:LEU:O	2:E:1622:LEU:HG	2.14	0.48
3:F:58:THR:HB	3:F:68:ARG:HH12	1.78	0.48
2:B:669:LEU:HD11	2:B:716:LEU:HD13	1.95	0.48
2:B:915:ARG:HA	2:B:915:ARG:HH11	1.78	0.48
2:B:1028:LEU:HD23	2:B:1032:PHE:HD1	1.77	0.48
2:B:1098:LYS:HD2	2:B:1134:CYS:SG	2.54	0.48
2:B:1185:TYR:O	2:B:1188:SER:OG	2.18	0.48
2:B:1357:ARG:NH1	2:B:1456:ALA:HB3	2.28	0.48
2:E:72:GLU:HG3	2:E:74:LEU:H	1.79	0.48
2:E:230:ASN:HA	2:E:274:LEU:HD11	1.96	0.48
2:E:751:GLU:OE2	2:E:751:GLU:N	2.38	0.48
2:E:792:ARG:HA	2:E:795:PHE:HD2	1.78	0.48
2:E:1006:TRP:CE3	2:E:1009:MET:HG3	2.49	0.48
2:E:1372:PHE:HE1	2:E:1402:PHE:CD2	2.32	0.48
2:B:4:TRP:HZ3	2:B:45:TYR:HA	1.78	0.48
2:B:37:ILE:HG21	2:B:45:TYR:HB3	1.94	0.48
2:B:98:TRP:O	2:B:102:TRP:CD1	2.67	0.48
2:B:166:ARG:HG2	2:B:173:LEU:H	1.77	0.48
2:B:191:SER:HA	2:B:194:ILE:HD12	1.96	0.48
2:B:230:ASN:HA	2:B:274:LEU:HD11	1.96	0.48
2:B:529:PHE:O	2:B:550:ALA:N	2.41	0.48
2:B:532:ARG:HB3	2:B:534:ARG:HD3	1.95	0.48
2:B:728:LEU:O	2:B:732:LYS:HG2	2.14	0.48
2:B:737:LEU:HD23	2:B:764:PHE:CZ	2.49	0.48
2:B:983:ILE:HD11	2:B:1032:PHE:CD2	2.48	0.48
2:E:130:GLN:HG3	2:E:131:ILE:HG12	1.95	0.48
2:E:584:PHE:O	2:E:588:LEU:HG	2.14	0.48
2:E:670:GLN:HG3	2:E:719:TYR:HD1	1.78	0.48
2:E:1222:SER:O	2:E:1225:VAL:HG22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1408:MET:HB3	2:E:1410:SER:HB3	1.96	0.48
3:F:110:ILE:O	3:F:152:VAL:HG12	2.14	0.48
3:F:145:MET:O	3:F:148:GLU:HB3	2.14	0.48
2:B:248:PRO:HD2	2:B:293:ARG:HG3	1.96	0.48
2:B:257:ASN:O	2:B:487:GLY:HA3	2.14	0.48
2:B:1078:ASP:OD1	2:B:1081:LYS:HG2	2.13	0.48
2:B:1145:HIS:HA	2:B:1148:GLU:HG3	1.96	0.48
2:B:1468:PHE:N	2:B:1483:TRP:O	2.47	0.48
2:B:1633:VAL:O	2:B:1639:VAL:HG22	2.14	0.48
1:D:536:LEU:HD21	2:E:17:TYR:CA	2.43	0.48
2:E:118:GLN:HB3	2:E:122:TYR:CZ	2.49	0.48
2:E:242:PHE:HB3	2:E:257:ASN:HB3	1.96	0.48
2:E:983:ILE:HD11	2:E:1032:PHE:CD2	2.48	0.48
2:E:1452:ASN:HA	2:E:1455:ARG:CZ	2.43	0.48
2:B:72:GLU:OE1	2:B:86:PRO:HG3	2.14	0.48
2:B:302:ARG:HD3	2:B:322:PHE:CD1	2.47	0.48
2:B:839:LEU:HG	2:B:842:LYS:HZ1	1.79	0.48
2:B:1387:GLU:HG2	2:B:1388:TYR:N	2.28	0.48
1:D:687:ASP:OD1	1:D:688:THR:N	2.47	0.48
1:D:716:GLU:HG3	2:E:44:TRP:CZ2	2.48	0.48
2:E:111:LEU:HD13	2:E:114:PHE:HD2	1.78	0.48
2:E:556:ASN:N	2:E:560:THR:O	2.41	0.48
2:E:728:LEU:O	2:E:732:LYS:HG2	2.14	0.48
2:E:754:PHE:CZ	2:E:811:LYS:HB2	2.49	0.48
2:E:754:PHE:HZ	2:E:811:LYS:HB2	1.78	0.48
2:E:1114:LEU:CB	2:E:1163:ARG:HD2	2.41	0.48
2:E:1344:LYS:HB3	2:E:1348:PHE:CZ	2.49	0.48
2:E:1468:PHE:N	2:E:1483:TRP:O	2.47	0.48
1:A:544:ILE:HG12	1:A:686:LEU:HG	1.95	0.47
2:B:754:PHE:CZ	2:B:811:LYS:HB2	2.49	0.47
2:B:792:ARG:HA	2:B:795:PHE:HD2	1.78	0.47
2:B:1133:GLN:NE2	2:B:1133:GLN:O	2.47	0.47
2:B:1362:TYR:CE2	2:B:1459:VAL:HG21	2.49	0.47
2:B:1368:TYR:CE2	2:B:1419:LYS:HE3	2.49	0.47
2:B:1408:MET:HB3	2:B:1410:SER:HB3	1.96	0.47
2:B:1483:TRP:CZ2	2:B:1513:SER:HA	2.49	0.47
2:B:1539:ASP:OD1	2:B:1541:SER:N	2.47	0.47
2:B:1560:MET:HG3	3:C:36:VAL:HG22	1.95	0.47
2:B:1622:LEU:O	2:B:1626:PHE:CB	2.61	0.47
2:E:1196:LEU:O	2:E:1199:SER:OG	2.26	0.47
2:E:1206:ASP:HA	2:E:1209:THR:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1256:ASN:HB3	2:E:1259:GLU:OE1	2.14	0.47
2:E:1460:GLN:OE1	2:E:1494:THR:HA	2.13	0.47
2:E:1517:ASN:O	2:E:1520:GLU:HG3	2.14	0.47
2:E:1557:PRO:O	2:E:1561:GLY:HA2	2.14	0.47
2:E:1613:GLU:OE2	2:E:1614:GLN:HG3	2.13	0.47
3:F:43:ASN:HA	3:F:51:VAL:O	2.14	0.47
3:F:155:LEU:HD13	3:F:168:VAL:HG22	1.95	0.47
2:B:179:SER:HA	2:B:962:GLN:HE22	1.79	0.47
2:B:893:ASN:O	2:B:896:LYS:NZ	2.47	0.47
2:B:1196:LEU:HD22	2:B:1234:LYS:HD2	1.94	0.47
3:C:120:ARG:HH12	3:C:139:TYR:HB2	1.79	0.47
2:E:724:PHE:CZ	2:E:726:ALA:HB3	2.49	0.47
2:E:929:MET:HB2	2:E:964:MET:CE	2.44	0.47
2:E:1123:ALA:O	2:E:1126:PRO:HG2	2.14	0.47
2:E:1125:ILE:CG1	2:E:1172:LEU:HD23	2.44	0.47
2:E:1280:PRO:HA	2:E:1283:LEU:HD23	1.96	0.47
2:E:1318:ILE:HD11	2:E:1348:PHE:HB2	1.97	0.47
2:E:1401:GLN:HG3	2:E:1402:PHE:CE2	2.49	0.47
2:E:1418:ILE:HG13	2:E:1425:TYR:CE2	2.47	0.47
3:F:120:ARG:HH12	3:F:139:TYR:HB2	1.79	0.47
1:A:642:PHE:HB3	1:A:662:TYR:HE1	1.79	0.47
1:A:687:ASP:OD1	1:A:688:THR:N	2.47	0.47
2:B:118:GLN:HB3	2:B:122:TYR:CZ	2.49	0.47
2:B:728:LEU:HA	2:B:730:TYR:CE2	2.49	0.47
2:B:921:THR:OG1	2:B:924:HIS:HB3	2.14	0.47
2:B:997:ILE:HG13	2:B:998:GLY:H	1.79	0.47
2:B:1515:LEU:HD23	2:B:1589:LEU:HD11	1.96	0.47
2:E:188:GLU:HG3	2:E:192:LYS:NZ	2.29	0.47
2:E:273:LYS:O	2:E:277:LEU:HG	2.14	0.47
2:E:893:ASN:O	2:E:896:LYS:NZ	2.47	0.47
2:E:929:MET:CE	2:E:972:TYR:HB3	2.43	0.47
2:E:1078:ASP:OD1	2:E:1081:LYS:HG2	2.13	0.47
2:E:1416:GLU:O	2:E:1419:LYS:HB2	2.15	0.47
3:F:60:GLY:HA2	3:F:97:TRP:HZ2	1.78	0.47
1:A:643:SER:HA	1:A:652:LEU:O	2.15	0.47
2:B:39:GLU:CD	2:B:46:ARG:HE	2.17	0.47
2:B:473:HIS:HB3	2:B:477:GLY:HA2	1.96	0.47
2:B:751:GLU:OE2	2:B:751:GLU:N	2.38	0.47
2:B:802:MET:HG2	2:B:843:PHE:HE1	1.79	0.47
2:B:928:ILE:O	2:B:932:LEU:HB2	2.15	0.47
2:B:1123:ALA:O	2:B:1126:PRO:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1583:GLN:HG3	2:B:1586:VAL:HG12	1.97	0.47
2:B:1590:LYS:HB3	2:B:1639:VAL:HG12	1.97	0.47
3:C:155:LEU:HD13	3:C:168:VAL:HG22	1.95	0.47
1:D:563:ARG:HB2	1:D:655:ILE:O	2.14	0.47
1:D:585:VAL:HG12	1:D:607:LYS:HD2	1.96	0.47
2:E:257:ASN:O	2:E:487:GLY:HA3	2.14	0.47
2:E:288:ASP:OD1	2:E:291:ARG:NH2	2.47	0.47
2:E:526:HIS:HB2	2:E:552:VAL:O	2.13	0.47
2:E:669:LEU:HD11	2:E:716:LEU:HD13	1.95	0.47
2:E:737:LEU:HD23	2:E:764:PHE:CZ	2.49	0.47
2:E:795:PHE:HZ	2:E:836:LEU:HD12	1.79	0.47
2:E:1387:GLU:HG2	2:E:1388:TYR:N	2.28	0.47
2:E:1607:HIS:NE2	2:E:1619:HIS:HB2	2.29	0.47
3:F:2:GLN:HE22	3:F:49:LYS:HG3	1.79	0.47
3:F:6:CYS:SG	3:F:77:VAL:HG23	2.54	0.47
2:B:902:SER:HA	2:B:905:LEU:HD12	1.96	0.47
2:B:1122:LYS:HE2	2:B:1171:LEU:HD22	1.97	0.47
2:B:1280:PRO:HA	2:B:1283:LEU:HD23	1.96	0.47
2:B:1301:TYR:O	2:B:1305:ILE:HG12	2.15	0.47
2:B:1383:TYR:CD2	2:B:1501:TRP:HB3	2.49	0.47
2:B:1384:ARG:HE	2:B:1495:PHE:HB3	1.80	0.47
2:B:1601:THR:HG1	2:B:1626:PHE:HZ	1.63	0.47
3:C:43:ASN:HA	3:C:51:VAL:O	2.14	0.47
2:E:802:MET:HG2	2:E:843:PHE:HE1	1.79	0.47
2:E:909:ILE:HA	2:E:912:VAL:HG22	1.97	0.47
2:E:1468:PHE:HE2	2:E:1470:LYS:HB2	1.78	0.47
2:E:1515:LEU:HD23	2:E:1589:LEU:HD11	1.96	0.47
2:E:1534:GLN:HB3	2:E:1538:TRP:HZ3	1.80	0.47
2:E:1562:GLY:HA3	3:F:36:VAL:HG21	1.96	0.47
3:F:24:THR:HG21	3:F:40:TYR:HB3	1.97	0.47
1:A:625:MET:HE3	1:A:637:VAL:O	2.13	0.47
2:B:46:ARG:HB3	2:B:58:ILE:HA	1.95	0.47
2:B:1044:ASN:HA	2:B:1101:PHE:HZ	1.80	0.47
2:B:1169:LYS:HE3	2:B:1202:GLU:HB3	1.97	0.47
2:B:1383:TYR:CG	2:B:1501:TRP:HB3	2.49	0.47
2:B:1614:GLN:O	2:B:1618:LEU:HD23	2.15	0.47
1:D:642:PHE:HB3	1:D:662:TYR:HE1	1.79	0.47
2:E:902:SER:HA	2:E:905:LEU:HD12	1.96	0.47
2:E:1098:LYS:HD2	2:E:1134:CYS:SG	2.54	0.47
2:E:1570:PHE:HA	2:E:1575:TYR:CG	2.50	0.47
2:E:1590:LYS:HB3	2:E:1639:VAL:HG12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:153:LYS:NZ	3:F:154:TYR:O	2.37	0.47
1:A:585:VAL:HG12	1:A:607:LYS:HD2	1.96	0.47
2:B:48:TYR:HB3	2:B:53:LYS:HA	1.96	0.47
2:B:105:LEU:CD1	2:B:117:LEU:HD13	2.45	0.47
2:B:166:ARG:HB2	2:B:174:ASP:H	1.79	0.47
2:B:188:GLU:HG3	2:B:192:LYS:HZ3	1.79	0.47
2:B:245:LEU:HB3	2:B:254:ILE:HD12	1.95	0.47
2:B:560:THR:HG22	2:B:638:LEU:HD23	1.95	0.47
2:B:584:PHE:O	2:B:588:LEU:HG	2.14	0.47
2:B:737:LEU:HD23	2:B:764:PHE:HZ	1.80	0.47
2:B:771:ARG:CZ	2:B:787:PHE:HB3	2.44	0.47
2:B:801:LEU:HA	2:B:804:ARG:NE	2.30	0.47
2:B:856:LYS:HZ3	2:B:885:GLN:HB2	1.78	0.47
2:B:868:LEU:HD11	2:B:871:GLN:HG3	1.97	0.47
2:B:909:ILE:HA	2:B:912:VAL:HG22	1.97	0.47
2:B:1249:ASP:HA	2:B:1252:ARG:CD	2.45	0.47
2:B:1323:GLU:HA	2:B:1326:GLU:HB3	1.97	0.47
2:B:1372:PHE:HE1	2:B:1402:PHE:CD2	2.32	0.47
2:B:1401:GLN:HG3	2:B:1402:PHE:CE2	2.49	0.47
2:B:1545:HIS:CB	3:C:5:LYS:HE2	2.43	0.47
2:B:1576:LEU:HG	2:B:1583:GLN:HG2	1.97	0.47
2:B:1599:LEU:HA	2:B:1602:GLU:OE1	2.15	0.47
2:B:1609:GLU:O	2:B:1610:LYS:HD2	2.15	0.47
2:B:1618:LEU:O	2:B:1622:LEU:HG	2.14	0.47
3:C:82:PHE:CE1	3:C:154:TYR:HE1	2.32	0.47
3:C:110:ILE:O	3:C:152:VAL:HG12	2.14	0.47
1:D:714:PRO:HD3	2:E:62:THR:HG21	1.96	0.47
2:E:60:PRO:O	2:E:64:ILE:N	2.37	0.47
2:E:98:TRP:HA	2:E:101:ILE:HG22	1.96	0.47
2:E:179:SER:HA	2:E:962:GLN:HE22	1.79	0.47
2:E:737:LEU:HD23	2:E:764:PHE:HZ	1.79	0.47
2:E:792:ARG:O	2:E:796:LEU:HG	2.15	0.47
2:E:895:ASN:O	2:E:899:HIS:N	2.48	0.47
2:E:979:ARG:HG3	2:E:1032:PHE:CE2	2.50	0.47
2:E:987:MET:O	2:E:991:ILE:HG12	2.15	0.47
2:E:997:ILE:HG13	2:E:998:GLY:H	1.79	0.47
2:E:1061:LEU:HA	2:E:1064:PHE:CE1	2.50	0.47
2:E:1368:TYR:HB2	2:E:1408:MET:HE1	1.97	0.47
2:E:1406:GLU:OE2	2:E:1423:LYS:HG3	2.14	0.47
2:E:1599:LEU:HA	2:E:1602:GLU:OE1	2.15	0.47
2:E:1622:LEU:O	2:E:1626:PHE:CB	2.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:563:ARG:HB2	1:A:655:ILE:O	2.14	0.47
1:A:569:ARG:NH2	1:A:571:GLN:OE1	2.47	0.47
2:B:26:GLU:OE1	2:B:29:LEU:HD11	2.14	0.47
2:B:222:TYR:CD1	2:B:289:LEU:HD21	2.50	0.47
2:B:331:ASP:HB3	2:B:336:LYS:HB2	1.97	0.47
2:B:450:LEU:O	2:B:509:TRP:HB2	2.15	0.47
2:B:720:ILE:HG12	2:B:766:PHE:CZ	2.50	0.47
2:B:754:PHE:HZ	2:B:811:LYS:HB2	1.78	0.47
2:B:1133:GLN:O	2:B:1136:PHE:HB3	2.15	0.47
2:B:1291:TYR:CB	2:B:1296:LEU:HD21	2.40	0.47
2:B:1318:ILE:HD11	2:B:1348:PHE:HB2	1.97	0.47
2:B:1406:GLU:C	2:B:1407:LYS:HD3	2.36	0.47
2:B:1570:PHE:HA	2:B:1575:TYR:CG	2.50	0.47
1:D:544:ILE:HG12	1:D:686:LEU:HG	1.95	0.47
2:E:26:GLU:OE1	2:E:29:LEU:HD11	2.14	0.47
2:E:39:GLU:CD	2:E:46:ARG:HE	2.17	0.47
2:E:45:TYR:N	2:E:59:PHE:O	2.48	0.47
2:E:166:ARG:HB2	2:E:174:ASP:H	1.79	0.47
2:E:1028:LEU:HD22	2:E:1043:TRP:CH2	2.50	0.47
2:E:1633:VAL:O	2:E:1639:VAL:HG22	2.14	0.47
1:A:584:LYS:HZ1	2:B:1405:ALA:HB2	1.78	0.47
2:B:724:PHE:CZ	2:B:726:ALA:HB3	2.49	0.47
2:B:802:MET:SD	2:B:846:SER:OG	2.58	0.47
2:B:1221:MET:O	2:B:1225:VAL:HG13	2.15	0.47
2:B:1570:PHE:HA	2:B:1575:TYR:CD2	2.50	0.47
2:E:95:LEU:HD21	2:E:124:LEU:CD1	2.45	0.47
2:E:163:LEU:HD22	2:E:187:HIS:HE1	1.80	0.47
2:E:1283:LEU:HD11	2:E:1291:TYR:HB2	1.97	0.47
2:E:1370:GLN:OE1	2:E:1377:ARG:NH1	2.48	0.47
2:E:1609:GLU:O	2:E:1610:LYS:HD2	2.15	0.47
3:F:7:VAL:CG2	3:F:71:SER:HB3	2.45	0.47
2:B:45:TYR:N	2:B:59:PHE:O	2.48	0.47
2:B:150:ALA:HB1	2:B:197:LYS:HZ1	1.79	0.47
2:B:157:ARG:HH21	2:B:198:ILE:HG12	1.80	0.47
2:B:225:TYR:CZ	2:B:227:ASN:HB2	2.50	0.47
2:B:531:PHE:CE2	2:B:571:VAL:HG22	2.50	0.47
2:B:869:PHE:HA	2:B:918:VAL:HA	1.97	0.47
2:B:929:MET:HB2	2:B:964:MET:CE	2.44	0.47
2:B:1007:MET:O	2:B:1011:MET:HG2	2.15	0.47
2:B:1344:LYS:HB3	2:B:1348:PHE:CZ	2.49	0.47
2:B:1406:GLU:OE2	2:B:1423:LYS:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:145:MET:O	3:C:148:GLU:HB3	2.14	0.47
1:D:625:MET:HE3	1:D:637:VAL:O	2.15	0.47
2:E:890:LEU:CD1	2:E:935:ARG:HA	2.45	0.47
2:E:928:ILE:O	2:E:932:LEU:HB2	2.15	0.47
2:E:986:LEU:HB3	2:E:1042:LEU:HD21	1.97	0.47
2:E:1308:PHE:HD1	2:E:1313:MET:HB2	1.79	0.47
2:E:1399:LEU:HD22	2:E:1405:ALA:HA	1.97	0.47
2:E:1481:THR:O	2:E:1483:TRP:HD1	1.97	0.47
3:F:113:VAL:HA	3:F:155:LEU:O	2.15	0.47
3:F:163:ARG:C	3:F:165:LEU:H	2.19	0.47
1:A:591:LEU:HD22	1:A:604:LEU:HD23	1.97	0.46
2:B:143:GLU:HA	2:B:146:LYS:HE2	1.97	0.46
2:B:188:GLU:HG3	2:B:192:LYS:NZ	2.29	0.46
2:B:521:GLU:HG3	2:B:524:ARG:CZ	2.45	0.46
2:B:876:GLU:OE1	2:B:876:GLU:N	2.40	0.46
2:B:890:LEU:CD1	2:B:935:ARG:HA	2.45	0.46
2:B:1308:PHE:HD1	2:B:1313:MET:HB2	1.79	0.46
3:C:113:VAL:HA	3:C:155:LEU:O	2.15	0.46
2:E:72:GLU:OE1	2:E:86:PRO:HG3	2.14	0.46
2:E:105:LEU:CD1	2:E:117:LEU:HD13	2.45	0.46
2:E:479:LEU:HD11	2:E:494:SER:HB3	1.97	0.46
2:E:800:MET:CE	2:E:804:ARG:HH21	2.28	0.46
2:E:869:PHE:HA	2:E:918:VAL:HA	1.97	0.46
2:E:1169:LYS:HE3	2:E:1202:GLU:HB3	1.97	0.46
2:E:1249:ASP:HA	2:E:1252:ARG:CD	2.45	0.46
2:E:1273:TRP:CD2	2:E:1297:LYS:HD3	2.50	0.46
2:E:1323:GLU:HA	2:E:1326:GLU:HB3	1.97	0.46
2:E:1601:THR:C	2:E:1605:ARG:HE	2.15	0.46
2:B:479:LEU:HD11	2:B:494:SER:HB3	1.97	0.46
2:B:485:HIS:O	2:B:514:LYS:N	2.48	0.46
2:B:640:LEU:HD21	2:B:676:LEU:HD21	1.97	0.46
2:E:179:SER:H	2:E:183:LEU:CD1	2.28	0.46
2:E:450:LEU:O	2:E:509:TRP:HB2	2.15	0.46
2:E:521:GLU:HG3	2:E:524:ARG:CZ	2.45	0.46
2:E:720:ILE:HG12	2:E:766:PHE:CZ	2.50	0.46
2:E:1337:GLY:HA2	2:E:1340:ASN:HD21	1.80	0.46
2:E:1432:LYS:HD3	2:E:1433:PRO:HD2	1.98	0.46
3:F:82:PHE:CE1	3:F:154:TYR:HE1	2.33	0.46
2:B:45:TYR:HE2	2:B:61:GLU:HG3	1.81	0.46
2:B:124:LEU:HD12	2:B:125:ILE:N	2.31	0.46
2:B:166:ARG:HB3	2:B:171:ASN:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:530:THR:HA	2:B:549:VAL:HG22	1.96	0.46
2:B:1028:LEU:HD22	2:B:1043:TRP:CH2	2.50	0.46
2:B:1127:ILE:HA	2:B:1130:ASP:OD2	2.15	0.46
2:B:1136:PHE:HD1	2:B:1186:LEU:HD23	1.80	0.46
2:B:1399:LEU:HD22	2:B:1405:ALA:HA	1.97	0.46
3:C:24:THR:HG21	3:C:40:TYR:HB3	1.97	0.46
2:E:225:TYR:CZ	2:E:227:ASN:HB2	2.50	0.46
2:E:526:HIS:CE1	2:E:586:LEU:HD21	2.50	0.46
2:E:771:ARG:CZ	2:E:787:PHE:HB3	2.44	0.46
2:E:823:ILE:O	2:E:827:VAL:HG23	2.16	0.46
2:E:868:LEU:HD11	2:E:871:GLN:HG3	1.97	0.46
2:E:987:MET:CE	2:E:1042:LEU:HD13	2.44	0.46
2:E:1127:ILE:HA	2:E:1130:ASP:OD2	2.15	0.46
2:E:1133:GLN:NE2	2:E:1133:GLN:O	2.47	0.46
2:E:1362:TYR:OH	2:E:1456:ALA:O	2.20	0.46
2:E:1470:LYS:N	2:E:1481:THR:O	2.37	0.46
2:E:1563:PHE:O	2:E:1567:GLU:HG2	2.16	0.46
2:E:1576:LEU:HG	2:E:1583:GLN:HG2	1.97	0.46
2:E:1583:GLN:HG3	2:E:1586:VAL:HG12	1.97	0.46
2:E:1614:GLN:O	2:E:1618:LEU:HD23	2.15	0.46
3:F:53:LEU:HD22	3:F:169:PHE:HE1	1.80	0.46
3:F:122:ASP:O	3:F:126:ILE:HG12	2.16	0.46
1:A:566:ASN:OD1	1:A:633:GLN:NE2	2.49	0.46
1:A:624:HIS:HB3	1:A:653:ASN:HB3	1.97	0.46
1:A:727:ASN:H	2:B:46:ARG:HH21	1.62	0.46
2:B:62:THR:HG23	2:B:63:TYR:CD1	2.50	0.46
2:B:296:LEU:HB2	2:B:329:ILE:HG21	1.97	0.46
2:B:1515:LEU:HG	2:B:1575:TYR:HE2	1.76	0.46
3:C:21:ILE:HB	3:C:40:TYR:CE2	2.51	0.46
1:D:617:VAL:O	1:D:642:PHE:HA	2.15	0.46
1:D:643:SER:HA	1:D:652:LEU:O	2.15	0.46
2:E:124:LEU:HD12	2:E:125:ILE:N	2.31	0.46
2:E:296:LEU:HB2	2:E:329:ILE:HG21	1.97	0.46
2:E:473:HIS:HB3	2:E:477:GLY:HA2	1.96	0.46
2:E:640:LEU:HD21	2:E:676:LEU:HD21	1.97	0.46
2:E:802:MET:HG2	2:E:843:PHE:CE1	2.51	0.46
2:E:1057:GLU:HA	2:E:1061:LEU:HD22	1.98	0.46
2:E:1221:MET:O	2:E:1225:VAL:HG13	2.15	0.46
2:E:1231:TYR:HH	2:E:1243:TYR:HE1	1.62	0.46
2:E:1406:GLU:C	2:E:1407:LYS:HD3	2.35	0.46
2:E:1483:TRP:CZ2	2:E:1513:SER:HA	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1491:THR:HG21	2:E:1495:PHE:CE1	2.51	0.46
2:B:526:HIS:HE1	2:B:585:TYR:OH	1.99	0.46
2:B:840:PHE:O	2:B:844:ILE:HG13	2.16	0.46
2:B:895:ASN:O	2:B:899:HIS:N	2.48	0.46
2:B:979:ARG:HG3	2:B:1032:PHE:CE2	2.50	0.46
2:B:1061:LEU:HA	2:B:1064:PHE:CE1	2.50	0.46
2:B:1125:ILE:CG1	2:B:1172:LEU:HD23	2.44	0.46
2:B:1129:PHE:HZ	2:B:1183:HIS:HB2	1.81	0.46
2:B:1353:ILE:HG23	2:E:1335:TYR:CD2	2.51	0.46
2:B:1362:TYR:CE1	2:B:1384:ARG:HG3	2.50	0.46
2:B:1607:HIS:NE2	2:B:1619:HIS:HB2	2.29	0.46
3:C:7:VAL:CG2	3:C:71:SER:HB3	2.45	0.46
2:E:7:THR:HG22	2:E:9:ARG:H	1.80	0.46
2:E:820:LEU:HD12	2:E:823:ILE:HD11	1.98	0.46
2:E:958:ILE:HG21	2:E:1017:PHE:HE1	1.81	0.46
2:E:1007:MET:O	2:E:1011:MET:HG2	2.15	0.46
2:E:1133:GLN:O	2:E:1136:PHE:HB3	2.15	0.46
2:E:1362:TYR:CE1	2:E:1384:ARG:HG3	2.51	0.46
2:E:1368:TYR:CE2	2:E:1419:LYS:HE3	2.49	0.46
2:B:820:LEU:HD12	2:B:823:ILE:HD11	1.98	0.46
2:B:986:LEU:HB3	2:B:1042:LEU:HD21	1.97	0.46
2:B:1012:THR:O	2:B:1016:VAL:HG22	2.16	0.46
2:B:1057:GLU:HA	2:B:1061:LEU:HD22	1.98	0.46
2:B:1125:ILE:HA	2:B:1128:PHE:CD2	2.51	0.46
2:B:1181:ARG:C	2:B:1183:HIS:H	2.19	0.46
2:B:1206:ASP:HA	2:B:1209:THR:HG22	1.96	0.46
3:C:53:LEU:HD22	3:C:169:PHE:HE1	1.80	0.46
3:C:153:LYS:NZ	3:C:154:TYR:O	2.37	0.46
1:D:566:ASN:OD1	1:D:633:GLN:NE2	2.49	0.46
2:E:45:TYR:HE2	2:E:61:GLU:HG3	1.81	0.46
2:E:62:THR:HG23	2:E:63:TYR:CD1	2.50	0.46
2:E:157:ARG:HH21	2:E:198:ILE:HG12	1.80	0.46
2:E:485:HIS:O	2:E:514:LYS:N	2.48	0.46
2:E:529:PHE:HE2	2:E:552:VAL:HG12	1.81	0.46
2:E:801:LEU:HA	2:E:804:ARG:NE	2.30	0.46
2:E:907:SER:OG	2:E:908:ASN:N	2.49	0.46
2:E:1007:MET:HE3	2:E:1007:MET:H	1.81	0.46
2:E:1122:LYS:HE2	2:E:1171:LEU:HD22	1.97	0.46
2:E:1129:PHE:HZ	2:E:1183:HIS:HB2	1.81	0.46
2:E:1203:ASN:O	2:E:1207:TYR:CB	2.64	0.46
2:E:1249:ASP:O	2:E:1252:ARG:HD3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1383:TYR:HA	2:E:1501:TRP:HA	1.98	0.46
2:E:1486:ARG:HB2	2:E:1510:GLU:HB2	1.98	0.46
2:E:1623:SER:HA	2:E:1627:ARG:HH11	1.81	0.46
3:F:21:ILE:HB	3:F:40:TYR:CE2	2.51	0.46
1:A:543:GLU:OE1	1:A:543:GLU:N	2.48	0.46
2:B:81:ILE:HD11	2:B:138:LYS:HE2	1.98	0.46
2:B:871:GLN:HB2	2:B:918:VAL:O	2.16	0.46
2:B:1139:SER:OG	2:B:1143:ASN:HA	2.16	0.46
2:B:1390:ARG:HD3	3:C:44:VAL:HG13	1.96	0.46
2:B:1486:ARG:HB2	2:B:1510:GLU:HB2	1.98	0.46
2:B:1563:PHE:O	2:B:1567:GLU:HG2	2.16	0.46
3:C:122:ASP:O	3:C:126:ILE:HG12	2.16	0.46
1:D:544:ILE:HD11	1:D:689:LEU:HB2	1.98	0.46
2:E:222:TYR:CD1	2:E:289:LEU:HD21	2.50	0.46
2:E:932:LEU:CA	2:E:935:ARG:HE	2.29	0.46
2:E:1125:ILE:HA	2:E:1128:PHE:CD2	2.51	0.46
2:B:95:LEU:HD21	2:B:124:LEU:CD1	2.45	0.46
2:B:98:TRP:CE3	2:B:101:ILE:HG21	2.51	0.46
2:B:245:LEU:HB2	2:B:254:ILE:HB	1.98	0.46
2:B:792:ARG:O	2:B:796:LEU:HG	2.15	0.46
2:B:856:LYS:NZ	2:B:885:GLN:HB2	2.31	0.46
2:B:929:MET:HG3	2:B:964:MET:HE1	1.98	0.46
2:B:932:LEU:CA	2:B:935:ARG:HE	2.29	0.46
2:B:990:PHE:HB3	2:B:1045:ASN:OD1	2.16	0.46
2:B:1111:GLU:HA	2:B:1114:LEU:HD12	1.98	0.46
2:B:1283:LEU:HD11	2:B:1291:TYR:HB2	1.97	0.46
2:B:1416:GLU:O	2:B:1419:LYS:HB2	2.15	0.46
2:B:1467:PRO:HA	2:B:1484:ILE:HD13	1.98	0.46
2:B:1491:THR:HG21	2:B:1495:PHE:CE1	2.51	0.46
2:E:245:LEU:HB2	2:E:254:ILE:HB	1.98	0.46
2:E:530:THR:HA	2:E:549:VAL:HG22	1.96	0.46
2:E:744:ALA:HB1	2:E:812:ILE:HD13	1.98	0.46
2:E:1044:ASN:HA	2:E:1101:PHE:HZ	1.80	0.46
2:E:1066:GLN:HA	2:E:1069:ARG:NH2	2.31	0.46
2:E:1404:ASN:HB3	2:E:1423:LYS:HD2	1.98	0.46
2:E:1570:PHE:HA	2:E:1575:TYR:CD2	2.50	0.46
2:E:1601:THR:HG22	2:E:1605:ARG:CZ	2.46	0.46
3:F:80:ILE:CD1	3:F:97:TRP:HB3	2.46	0.46
2:B:7:THR:HG22	2:B:9:ARG:H	1.80	0.46
2:B:677:PHE:HD1	2:B:680:MET:HE2	1.81	0.46
2:B:823:ILE:HA	2:B:826:ASP:OD2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1203:ASN:O	2:B:1207:TYR:CB	2.64	0.46
2:B:1206:ASP:OD1	2:B:1207:TYR:N	2.49	0.46
3:C:80:ILE:CD1	3:C:97:TRP:HB3	2.46	0.46
2:E:48:TYR:HB3	2:E:53:LYS:HA	1.96	0.46
2:E:840:PHE:O	2:E:844:ILE:HG13	2.16	0.46
2:E:866:SER:C	2:E:868:LEU:H	2.19	0.46
2:E:933:LEU:H	2:E:935:ARG:NH2	2.14	0.46
2:E:1139:SER:OG	2:E:1143:ASN:HA	2.16	0.46
2:E:1379:LYS:NZ	2:E:1504:VAL:O	2.36	0.46
2:E:1457:ASN:O	2:E:1459:VAL:HG13	2.16	0.46
2:E:1466:ARG:O	2:E:1484:ILE:HA	2.16	0.46
3:F:53:LEU:HD22	3:F:173:ILE:HD11	1.97	0.46
2:B:526:HIS:CE1	2:B:586:LEU:HD21	2.50	0.46
2:B:578:LYS:HD3	2:B:584:PHE:CZ	2.51	0.46
2:B:802:MET:HE2	2:B:847:ILE:HD13	1.97	0.46
2:B:1062:GLU:OE2	2:B:1080:ARG:NH1	2.49	0.46
2:B:1370:GLN:OE1	2:B:1377:ARG:NH1	2.48	0.46
2:B:1566:TYR:HB3	2:B:1571:PHE:CE1	2.51	0.46
2:B:1606:ILE:HG13	2:B:1607:HIS:N	2.31	0.46
2:B:1623:SER:HA	2:B:1627:ARG:HH11	1.80	0.46
3:C:60:GLY:HA2	3:C:97:TRP:CZ2	2.51	0.46
2:E:554:LEU:HA	2:E:562:LEU:HB2	1.97	0.46
2:E:1002:TYR:OH	2:E:1013:GLN:HB2	2.16	0.46
2:E:1136:PHE:HD1	2:E:1186:LEU:HD23	1.80	0.46
2:E:1301:TYR:O	2:E:1305:ILE:HG12	2.15	0.46
2:E:1467:PRO:HA	2:E:1484:ILE:HD13	1.98	0.46
2:B:456:ASP:HB3	2:B:573:LYS:NZ	2.32	0.45
2:B:800:MET:CE	2:B:804:ARG:HH21	2.28	0.45
2:B:802:MET:HG2	2:B:843:PHE:CE1	2.51	0.45
2:B:1273:TRP:CD2	2:B:1297:LYS:HD3	2.50	0.45
2:B:1432:LYS:HD3	2:B:1433:PRO:HD2	1.98	0.45
2:B:1534:GLN:HB3	2:B:1538:TRP:HZ3	1.80	0.45
2:B:1601:THR:C	2:B:1605:ARG:HE	2.15	0.45
3:C:163:ARG:C	3:C:165:LEU:H	2.19	0.45
2:E:166:ARG:HB3	2:E:171:ASN:HA	1.97	0.45
2:E:446:ILE:HG12	2:E:626:ILE:HG12	1.98	0.45
2:E:531:PHE:CE2	2:E:571:VAL:HG22	2.50	0.45
2:E:1209:THR:O	2:E:1213:GLN:HB2	2.15	0.45
2:E:1357:ARG:NH1	2:E:1456:ALA:HB3	2.28	0.45
2:E:1566:TYR:HB3	2:E:1571:PHE:CE1	2.51	0.45
3:F:9:VAL:HG23	3:F:80:ILE:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:LEU:HB2	1:A:686:LEU:HD11	1.98	0.45
2:B:19:TYR:HE2	2:B:26:GLU:HB3	1.82	0.45
2:B:127:TRP:HD1	2:B:130:GLN:NE2	2.14	0.45
2:B:554:LEU:HA	2:B:562:LEU:HB2	1.97	0.45
2:B:792:ARG:NE	2:B:835:GLU:OE1	2.50	0.45
2:B:795:PHE:HZ	2:B:836:LEU:HD12	1.79	0.45
2:B:844:ILE:O	2:B:847:ILE:HB	2.16	0.45
2:B:899:HIS:HD2	2:B:943:MET:HG2	1.81	0.45
2:B:907:SER:OG	2:B:908:ASN:N	2.49	0.45
2:B:987:MET:O	2:B:991:ILE:HG12	2.15	0.45
2:B:1066:GLN:HA	2:B:1069:ARG:NH2	2.31	0.45
2:B:1337:GLY:HA2	2:B:1340:ASN:HD21	1.80	0.45
2:B:1382:ILE:HD11	2:B:1489:TYR:HB3	1.99	0.45
2:E:127:TRP:HD1	2:E:130:GLN:NE2	2.14	0.45
1:A:711:PRO:HD2	2:B:17:TYR:CE1	2.51	0.45
2:B:464:LYS:HE2	2:B:464:LYS:HA	1.99	0.45
2:B:1007:MET:HE3	2:B:1007:MET:H	1.81	0.45
2:B:1516:GLU:HA	2:B:1519:ILE:HD12	1.98	0.45
2:E:143:GLU:HA	2:E:146:LYS:HE2	1.97	0.45
2:E:823:ILE:HA	2:E:826:ASP:OD2	2.16	0.45
2:E:856:LYS:HZ1	2:E:857:LEU:HD21	1.81	0.45
2:E:934:ARG:HD2	2:E:985:PHE:CD1	2.52	0.45
2:E:1157:GLN:O	2:E:1160:GLU:HB3	2.17	0.45
2:E:1181:ARG:C	2:E:1183:HIS:H	2.19	0.45
2:E:1334:ASP:OD2	2:E:1337:GLY:HA3	2.17	0.45
2:E:1435:MET:HE3	2:E:1455:ARG:HG2	1.99	0.45
2:E:1566:TYR:HD1	2:E:1566:TYR:HA	1.62	0.45
2:B:529:PHE:HE2	2:B:552:VAL:HG12	1.81	0.45
2:B:654:LEU:HD13	2:B:692:LEU:HB2	1.99	0.45
2:B:1209:THR:O	2:B:1213:GLN:HB2	2.15	0.45
2:B:1249:ASP:O	2:B:1252:ARG:HD3	2.16	0.45
3:C:93:VAL:O	3:C:98:TYR:HB3	2.16	0.45
1:D:591:LEU:HD22	1:D:604:LEU:HD23	1.97	0.45
2:E:19:TYR:HE2	2:E:26:GLU:HB3	1.82	0.45
2:E:331:ASP:HB3	2:E:336:LYS:HB2	1.97	0.45
2:E:419:HIS:CD2	2:E:420:LEU:HG	2.51	0.45
2:E:643:TRP:HD1	2:E:675:ALA:HB1	1.82	0.45
2:E:787:PHE:O	2:E:791:ILE:HG12	2.17	0.45
2:E:806:LEU:HD22	2:E:851:GLN:HB3	1.99	0.45
2:E:853:VAL:O	2:E:857:LEU:HG	2.17	0.45
2:E:1384:ARG:HE	2:E:1495:PHE:HB3	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1516:GLU:HA	2:E:1519:ILE:HD12	1.98	0.45
1:A:551:GLN:HE22	1:A:555:ARG:HD3	1.81	0.45
2:B:68:GLU:HB3	2:B:76:GLN:HE22	1.82	0.45
2:B:89:GLN:O	2:B:92:THR:OG1	2.31	0.45
2:B:179:SER:H	2:B:183:LEU:CD1	2.28	0.45
2:B:285:SER:HB2	2:B:435:GLU:CD	2.37	0.45
2:B:446:ILE:HG12	2:B:626:ILE:HG12	1.98	0.45
2:B:1078:ASP:OD1	2:B:1080:ARG:HB2	2.16	0.45
2:B:1155:LEU:O	2:B:1159:VAL:HG23	2.17	0.45
2:B:1229:ASN:O	2:B:1233:GLU:HG3	2.16	0.45
2:B:1404:ASN:HB3	2:B:1423:LYS:HD2	1.98	0.45
3:C:39:ASN:HB3	3:C:56:TRP:HA	1.98	0.45
3:C:53:LEU:HD22	3:C:173:ILE:HD11	1.97	0.45
1:D:545:LEU:HB2	1:D:686:LEU:HD11	1.98	0.45
1:D:662:TYR:HA	1:D:665:TRP:HE3	1.82	0.45
1:D:722:PHE:CE1	2:E:1:MET:HB3	2.42	0.45
2:E:98:TRP:CE3	2:E:101:ILE:HG21	2.51	0.45
2:E:526:HIS:HE1	2:E:585:TYR:OH	1.99	0.45
2:E:658:MET:SD	2:E:699:PHE:HD2	2.40	0.45
2:E:844:ILE:O	2:E:847:ILE:HB	2.16	0.45
2:E:990:PHE:HB3	2:E:1045:ASN:OD1	2.16	0.45
2:E:1479:PHE:HA	2:E:1482:MET:HG2	1.99	0.45
3:F:39:ASN:HA	3:F:57:ASP:N	2.30	0.45
1:A:617:VAL:O	1:A:642:PHE:HA	2.15	0.45
2:B:3:ARG:O	2:B:3:ARG:HD3	2.16	0.45
2:B:163:LEU:HD22	2:B:187:HIS:HE1	1.80	0.45
2:B:419:HIS:CD2	2:B:420:LEU:HG	2.51	0.45
2:B:823:ILE:O	2:B:827:VAL:HG23	2.16	0.45
2:B:1168:TYR:CZ	2:B:1172:LEU:HD11	2.52	0.45
2:B:1258:THR:HG22	2:B:1262:TYR:HE2	1.81	0.45
2:B:1411:THR:HB	3:C:28:PHE:CE1	2.52	0.45
2:B:1479:PHE:HA	2:B:1482:MET:HG2	1.99	0.45
2:B:1551:LEU:HB3	2:B:1622:LEU:HD21	1.99	0.45
2:B:1579:HIS:O	2:B:1583:GLN:NE2	2.36	0.45
1:D:711:PRO:HG2	2:E:16:ILE:CD1	2.46	0.45
2:E:5:ILE:N	2:E:40:MET:H	2.01	0.45
2:E:68:GLU:HB3	2:E:76:GLN:HE22	1.82	0.45
2:E:302:ARG:HH22	2:E:375:GLU:HG2	1.82	0.45
2:E:456:ASP:HB3	2:E:573:LYS:NZ	2.32	0.45
2:E:816:ALA:O	2:E:820:LEU:CB	2.63	0.45
2:E:969:TYR:CD2	2:E:1023:GLN:HG3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1206:ASP:OD1	2:E:1207:TYR:N	2.49	0.45
1:A:617:VAL:HG13	1:A:645:LEU:HD11	1.98	0.45
2:B:485:HIS:HA	2:B:492:GLY:HA2	1.98	0.45
2:B:681:MET:HE1	2:B:729:ALA:HA	1.99	0.45
2:B:1466:ARG:O	2:B:1484:ILE:HA	2.17	0.45
3:C:9:VAL:HG23	3:C:80:ILE:HA	1.98	0.45
2:E:229:LYS:HE3	2:E:343:GLN:HG2	1.99	0.45
2:E:470:MET:CG	2:E:496:TYR:HB3	2.46	0.45
2:E:640:LEU:HD23	2:E:672:THR:HG23	1.98	0.45
2:E:1114:LEU:HA	2:E:1168:TYR:CZ	2.52	0.45
2:E:1120:LEU:HD12	2:E:1121:ARG:N	2.32	0.45
2:E:1268:ALA:HA	2:E:1271:LEU:HD13	1.99	0.45
2:E:1361:GLU:HB3	2:E:1430:THR:HG23	1.99	0.45
3:F:7:VAL:HB	3:F:78:PHE:CD1	2.52	0.45
3:F:39:ASN:HB3	3:F:56:TRP:HA	1.98	0.45
1:A:588:TYR:HE2	1:A:608:LEU:HB2	1.82	0.45
2:B:197:LYS:O	2:B:200:GLU:N	2.45	0.45
2:B:969:TYR:CD2	2:B:1023:GLN:HG3	2.52	0.45
2:B:1002:TYR:OH	2:B:1013:GLN:HB2	2.16	0.45
2:B:1170:VAL:O	2:B:1174:LYS:HG3	2.17	0.45
2:B:1365:VAL:N	2:B:1381:PHE:O	2.42	0.45
2:B:1601:THR:HG22	2:B:1605:ARG:CZ	2.46	0.45
2:B:1633:VAL:C	2:B:1639:VAL:HG22	2.37	0.45
1:D:711:PRO:CG	2:E:16:ILE:HG21	2.47	0.45
2:E:285:SER:HB2	2:E:435:GLU:CD	2.37	0.45
2:E:821:PRO:O	2:E:824:ILE:HG12	2.17	0.45
2:E:1062:GLU:OE2	2:E:1080:ARG:NH1	2.49	0.45
2:E:1065:SER:OG	2:E:1068:LYS:HE3	2.17	0.45
2:E:1111:GLU:HA	2:E:1114:LEU:HD12	1.98	0.45
2:E:1168:TYR:CZ	2:E:1172:LEU:HD11	2.52	0.45
3:F:93:VAL:O	3:F:98:TYR:HB3	2.16	0.45
1:A:544:ILE:HD11	1:A:689:LEU:HB2	1.98	0.45
1:A:662:TYR:HA	1:A:665:TRP:HE3	1.82	0.45
2:B:101:ILE:O	2:B:105:LEU:HG	2.17	0.45
2:B:103:ARG:HG3	2:B:104:LYS:N	2.32	0.45
2:B:470:MET:CG	2:B:496:TYR:HB3	2.46	0.45
2:B:957:MET:O	2:B:960:LEU:HB3	2.17	0.45
2:B:1283:LEU:HB3	2:B:1288:TYR:HE1	1.82	0.45
1:D:551:GLN:HE22	1:D:555:ARG:HD3	1.82	0.45
1:D:624:HIS:HB3	1:D:653:ASN:HB3	1.98	0.45
2:E:150:ALA:HB1	2:E:197:LYS:HZ1	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:856:LYS:NZ	2:E:885:GLN:HB2	2.31	0.45
2:E:862:LYS:O	2:E:865:GLU:HB3	2.17	0.45
2:E:871:GLN:HB2	2:E:918:VAL:O	2.16	0.45
2:E:1170:VAL:O	2:E:1174:LYS:HG3	2.17	0.45
2:E:1256:ASN:ND2	2:E:1500:LYS:HE2	2.32	0.45
2:B:1632:LYS:HA	2:B:1632:LYS:HD2	1.80	0.45
2:E:3:ARG:O	2:E:3:ARG:HD3	2.16	0.45
2:E:81:ILE:HD11	2:E:138:LYS:HE2	1.98	0.45
2:E:87:LEU:HB2	2:E:145:LYS:HE2	1.99	0.45
2:E:187:HIS:CD2	2:E:1008:VAL:HB	2.52	0.45
2:E:485:HIS:HA	2:E:492:GLY:HA2	1.98	0.45
2:E:1012:THR:O	2:E:1016:VAL:HG22	2.16	0.45
2:E:1078:ASP:OD1	2:E:1080:ARG:HB2	2.16	0.45
2:E:1369:GLY:HA3	2:E:1424:GLN:HA	1.99	0.45
2:E:1551:LEU:HB3	2:E:1622:LEU:HD21	1.99	0.45
3:F:60:GLY:HA2	3:F:97:TRP:CZ2	2.51	0.45
2:B:73:ASP:OD2	2:B:85:LEU:HB3	2.17	0.44
2:B:302:ARG:HH22	2:B:375:GLU:HG2	1.82	0.44
2:B:469:THR:HG22	2:B:495:GLU:HB3	1.99	0.44
2:B:640:LEU:HD23	2:B:672:THR:HG23	1.98	0.44
2:B:866:SER:C	2:B:868:LEU:H	2.19	0.44
2:B:1065:SER:OG	2:B:1068:LYS:HE3	2.17	0.44
2:B:1361:GLU:HB3	2:B:1430:THR:HG23	1.99	0.44
3:C:7:VAL:HB	3:C:78:PHE:CD1	2.52	0.44
1:D:577:CYS:SG	1:D:588:TYR:HB3	2.57	0.44
2:E:98:TRP:HE3	2:E:101:ILE:HG21	1.82	0.44
2:E:103:ARG:HG3	2:E:104:LYS:N	2.32	0.44
2:E:188:GLU:HG3	2:E:192:LYS:HZ3	1.82	0.44
2:E:349:GLN:NE2	2:E:350:GLN:O	2.32	0.44
2:E:422:ASP:OD1	2:E:422:ASP:N	2.50	0.44
2:E:792:ARG:NE	2:E:835:GLU:OE1	2.50	0.44
2:E:800:MET:O	2:E:804:ARG:HG3	2.17	0.44
2:E:929:MET:HG3	2:E:964:MET:HE1	1.99	0.44
2:E:987:MET:HE1	2:E:1042:LEU:HD13	1.99	0.44
2:E:1229:ASN:O	2:E:1233:GLU:HG3	2.16	0.44
2:E:1417:ASP:OD1	2:E:1418:ILE:HG12	2.17	0.44
2:E:1606:ILE:HG13	2:E:1607:HIS:N	2.31	0.44
1:A:696:LEU:HD12	1:A:697:ARG:HE	1.83	0.44
2:B:288:ASP:OD1	2:B:291:ARG:NH2	2.47	0.44
2:B:744:ALA:HB1	2:B:812:ILE:HD13	1.98	0.44
2:B:821:PRO:O	2:B:824:ILE:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:853:VAL:O	2:B:857:LEU:HG	2.17	0.44
2:B:862:LYS:O	2:B:865:GLU:HB3	2.17	0.44
2:B:922:ALA:HA	2:B:925:ILE:HD12	2.00	0.44
2:B:933:LEU:H	2:B:935:ARG:NH2	2.14	0.44
2:B:1042:LEU:HD12	2:B:1042:LEU:O	2.18	0.44
2:B:1114:LEU:HA	2:B:1168:TYR:CZ	2.52	0.44
2:B:1183:HIS:CG	2:B:1187:SER:HG	2.30	0.44
2:B:1597:MET:CE	2:B:1633:VAL:HG11	2.47	0.44
1:D:617:VAL:HG13	1:D:645:LEU:HD11	1.97	0.44
2:E:19:TYR:CD1	2:E:20:ASN:N	2.86	0.44
2:E:690:ASP:OD2	2:E:732:LYS:HB3	2.17	0.44
2:E:1199:SER:O	2:E:1202:GLU:HG2	2.18	0.44
2:E:1217:LYS:HD2	2:E:1220:ARG:HH22	1.82	0.44
2:E:1382:ILE:O	2:E:1502:PHE:N	2.42	0.44
2:E:1469:ARG:HB3	2:E:1473:LYS:HD2	1.98	0.44
1:A:616:VAL:HG23	1:A:643:SER:C	2.38	0.44
2:B:225:TYR:HD2	2:B:404:LYS:HB2	1.83	0.44
2:B:229:LYS:HE3	2:B:343:GLN:HG2	1.99	0.44
2:B:658:MET:SD	2:B:699:PHE:HD2	2.40	0.44
2:B:860:MET:SD	2:B:861:THR:N	2.91	0.44
2:B:1180:CYS:CB	2:B:1191:GLU:HG3	2.47	0.44
2:B:1369:GLY:HA3	2:B:1424:GLN:HA	1.99	0.44
2:B:1382:ILE:O	2:B:1502:PHE:N	2.42	0.44
2:B:1417:ASP:OD1	2:B:1418:ILE:HG12	2.17	0.44
2:B:1488:THR:O	2:B:1508:SER:N	2.39	0.44
3:C:11:ASP:OD1	3:C:11:ASP:N	2.49	0.44
2:E:930:GLU:HG2	2:E:972:TYR:CD1	2.53	0.44
2:E:1098:LYS:O	2:E:1102:ILE:N	2.50	0.44
2:E:1177:LEU:O	2:E:1181:ARG:HD2	2.18	0.44
2:E:1180:CYS:CB	2:E:1191:GLU:HG3	2.47	0.44
2:B:19:TYR:OH	2:B:44:TRP:HZ3	2.00	0.44
2:B:328:ASP:OD1	2:B:390:LYS:HE2	2.17	0.44
2:B:480:LEU:HD23	2:B:483:ALA:HB2	2.00	0.44
2:B:806:LEU:HD22	2:B:851:GLN:HB3	1.99	0.44
2:B:934:ARG:HD2	2:B:985:PHE:CD1	2.52	0.44
2:B:934:ARG:HH12	2:B:938:ARG:HB2	1.83	0.44
2:B:974:SER:HB2	2:B:1031:PHE:CE1	2.52	0.44
2:B:1002:TYR:CE1	2:B:1010:ASN:HA	2.52	0.44
2:B:1120:LEU:HD12	2:B:1121:ARG:N	2.32	0.44
2:B:1320:LEU:HA	2:B:1323:GLU:OE2	2.18	0.44
2:B:1334:ASP:OD2	2:B:1337:GLY:HA3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1398:LEU:HB3	2:B:1426:MET:SD	2.58	0.44
2:B:1441:TYR:HD2	2:B:1450:ILE:HG21	1.82	0.44
2:E:23:GLN:HG2	2:E:58:ILE:HB	2.00	0.44
2:E:104:LYS:HD3	2:E:107:VAL:HB	2.00	0.44
2:E:464:LYS:HE2	2:E:464:LYS:HA	1.99	0.44
2:E:468:VAL:HG21	2:E:620:PHE:CE1	2.53	0.44
2:E:889:GLN:NE2	2:E:898:ASP:OD2	2.50	0.44
2:E:994:LYS:HA	2:E:997:ILE:HG12	1.99	0.44
2:E:1393:ASP:O	2:E:1396:LEU:HB3	2.18	0.44
3:F:42:ALA:O	3:F:53:LEU:HG	2.17	0.44
2:B:816:ALA:O	2:B:820:LEU:CB	2.63	0.44
2:B:889:GLN:NE2	2:B:898:ASP:OD2	2.50	0.44
2:B:979:ARG:HA	2:B:982:ILE:HG22	2.00	0.44
2:B:1240:TYR:CE2	2:B:1244:LEU:HD11	2.53	0.44
2:E:19:TYR:CG	2:E:59:PHE:CE1	3.05	0.44
2:E:319:ARG:NH1	2:E:511:GLU:OE2	2.48	0.44
2:E:438:LEU:HB2	2:E:441:ASP:OD1	2.17	0.44
2:E:578:LYS:HD3	2:E:584:PHE:CZ	2.51	0.44
2:E:764:PHE:HD1	2:E:823:ILE:HB	1.83	0.44
2:E:802:MET:HE2	2:E:847:ILE:HD13	2.00	0.44
2:E:957:MET:O	2:E:960:LEU:HB3	2.17	0.44
2:E:1221:MET:SD	2:E:1250:LEU:HB3	2.58	0.44
2:E:1249:ASP:O	2:E:1252:ARG:NH1	2.51	0.44
2:E:1382:ILE:HD11	2:E:1489:TYR:HB3	1.99	0.44
2:E:1382:ILE:HD11	2:E:1504:VAL:HG23	1.99	0.44
2:E:1610:LYS:HD2	2:E:1610:LYS:HA	1.73	0.44
1:A:577:CYS:SG	1:A:588:TYR:HB3	2.57	0.44
2:B:166:ARG:CD	2:B:173:LEU:HB2	2.47	0.44
2:B:187:HIS:CD2	2:B:1008:VAL:HB	2.52	0.44
2:B:732:LYS:HA	2:B:732:LYS:HD3	1.84	0.44
2:B:819:TYR:O	2:B:822:SER:OG	2.23	0.44
2:B:868:LEU:O	2:B:918:VAL:HG13	2.18	0.44
2:B:958:ILE:HG21	2:B:1017:PHE:HE1	1.81	0.44
2:B:994:LYS:HA	2:B:997:ILE:HG12	2.00	0.44
2:B:1221:MET:SD	2:B:1250:LEU:HB3	2.58	0.44
2:B:1268:ALA:HB2	2:B:1300:LEU:HD13	1.99	0.44
2:B:1435:MET:HE3	2:B:1455:ARG:HG2	1.99	0.44
2:B:1560:MET:O	3:C:36:VAL:HG13	2.18	0.44
2:E:101:ILE:O	2:E:105:LEU:HG	2.17	0.44
2:E:974:SER:HB2	2:E:1031:PHE:CE1	2.52	0.44
2:E:1027:VAL:HG22	2:E:1032:PHE:HE1	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1320:LEU:HA	2:E:1323:GLU:OE2	2.17	0.44
2:E:1343:LYS:HE3	2:E:1343:LYS:HB3	1.85	0.44
2:E:1633:VAL:C	2:E:1639:VAL:HG22	2.37	0.44
1:A:551:GLN:HG3	2:B:106:TYR:CE2	2.53	0.44
2:B:166:ARG:HH21	2:B:169:ASN:ND2	2.14	0.44
2:B:1006:TRP:CE3	2:B:1009:MET:HG3	2.49	0.44
2:B:1383:TYR:HA	2:B:1501:TRP:HA	1.98	0.44
2:B:1495:PHE:HE1	2:B:1502:PHE:CD2	2.31	0.44
2:B:1567:GLU:O	2:B:1572:THR:N	2.47	0.44
3:C:42:ALA:O	3:C:53:LEU:HG	2.17	0.44
2:E:73:ASP:OD2	2:E:85:LEU:HB3	2.17	0.44
2:E:95:LEU:HA	2:E:98:TRP:HB2	2.00	0.44
2:E:145:LYS:O	2:E:148:VAL:HG12	2.17	0.44
2:E:166:ARG:HH21	2:E:169:ASN:ND2	2.14	0.44
2:E:247:ASP:O	2:E:251:SER:N	2.42	0.44
2:E:654:LEU:HD13	2:E:692:LEU:HB2	1.98	0.44
2:E:795:PHE:CZ	2:E:836:LEU:HD12	2.53	0.44
2:E:795:PHE:CE2	2:E:839:LEU:HD13	2.52	0.44
2:E:860:MET:SD	2:E:861:THR:N	2.90	0.44
2:E:940:VAL:HA	2:E:943:MET:HE2	2.00	0.44
2:E:1218:GLU:HB2	2:E:1501:TRP:CZ2	2.52	0.44
2:E:1417:ASP:OD1	2:E:1417:ASP:N	2.51	0.44
3:F:72:TYR:HB2	3:F:73:PRO:HD3	2.00	0.44
1:A:532:PRO:O	1:A:536:LEU:HD13	2.18	0.44
1:A:544:ILE:HG23	1:A:545:LEU:H	1.83	0.44
2:B:19:TYR:CD1	2:B:20:ASN:N	2.86	0.44
2:B:643:TRP:HD1	2:B:675:ALA:HB1	1.82	0.44
2:B:795:PHE:CE2	2:B:839:LEU:HD13	2.52	0.44
2:B:1393:ASP:O	2:B:1396:LEU:HB3	2.18	0.44
2:B:1469:ARG:HB3	2:B:1473:LYS:HD2	1.98	0.44
3:C:21:ILE:HD11	3:C:35:THR:HG23	2.00	0.44
3:C:72:TYR:HB2	3:C:73:PRO:HD3	2.00	0.44
3:C:85:VAL:O	3:C:129:LEU:HD21	2.18	0.44
1:D:585:VAL:HB	1:D:606:ASP:O	2.18	0.44
2:E:19:TYR:CZ	2:E:60:PRO:HD3	2.53	0.44
2:E:204:ILE:HG23	2:E:211:ARG:CZ	2.48	0.44
2:E:1361:GLU:OE2	2:E:1388:TYR:HA	2.18	0.44
2:E:1567:GLU:O	2:E:1572:THR:N	2.47	0.44
2:E:1597:MET:CE	2:E:1633:VAL:HG11	2.47	0.44
2:B:285:SER:OG	2:B:288:ASP:OD2	2.33	0.44
2:B:663:GLY:O	2:B:667:LYS:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:690:ASP:OD2	2:B:732:LYS:HB3	2.17	0.44
2:B:787:PHE:O	2:B:791:ILE:HG12	2.17	0.44
2:B:820:LEU:HB3	2:B:821:PRO:HD3	2.00	0.44
2:B:931:ARG:C	2:B:932:LEU:HD12	2.38	0.44
2:B:1217:LYS:HD2	2:B:1220:ARG:HH22	1.82	0.44
2:B:1224:THR:HA	2:B:1227:VAL:HG12	1.99	0.44
2:B:1483:TRP:HA	2:B:1512:ILE:O	2.18	0.44
1:D:616:VAL:HG23	1:D:643:SER:C	2.38	0.44
2:E:19:TYR:OH	2:E:44:TRP:HZ3	2.00	0.44
2:E:162:ASP:OD2	2:E:1071:LYS:NZ	2.51	0.44
2:E:302:ARG:HG3	2:E:320:ARG:HB2	2.00	0.44
2:E:471:SER:N	2:E:528:ARG:O	2.35	0.44
2:E:663:GLY:O	2:E:667:LYS:HG3	2.17	0.44
2:E:911:GLU:O	2:E:915:ARG:HG2	2.18	0.44
2:E:958:ILE:HB	2:E:1016:VAL:CG2	2.48	0.44
2:E:1002:TYR:CE1	2:E:1010:ASN:HA	2.52	0.44
2:E:1268:ALA:HB2	2:E:1300:LEU:HD13	1.99	0.44
2:E:1337:GLY:HA2	2:E:1340:ASN:ND2	2.33	0.44
2:B:572:TYR:OH	2:B:589:PRO:HD2	2.17	0.43
2:B:800:MET:O	2:B:804:ARG:HG3	2.17	0.43
2:B:820:LEU:O	2:B:824:ILE:HG23	2.18	0.43
2:B:930:GLU:HG2	2:B:972:TYR:CD1	2.53	0.43
2:B:987:MET:HE1	2:B:1042:LEU:HD13	1.99	0.43
2:B:1056:HIS:HD1	2:B:1057:GLU:CD	2.17	0.43
2:B:1256:ASN:ND2	2:B:1500:LYS:HE2	2.32	0.43
2:B:1368:TYR:HB2	2:B:1408:MET:HE1	1.99	0.43
2:E:572:TYR:OH	2:E:589:PRO:HD2	2.17	0.43
2:E:1062:GLU:O	2:E:1069:ARG:HD3	2.18	0.43
2:E:1063:THR:HA	2:E:1069:ARG:HD2	2.00	0.43
2:E:1398:LEU:HB3	2:E:1426:MET:SD	2.58	0.43
2:E:1483:TRP:HA	2:E:1512:ILE:O	2.18	0.43
1:A:585:VAL:HB	1:A:606:ASP:O	2.18	0.43
1:A:711:PRO:HD2	2:B:17:TYR:CD1	2.53	0.43
2:B:87:LEU:HA	2:B:90:GLU:HG3	2.00	0.43
2:B:98:TRP:HE3	2:B:101:ILE:HG21	1.82	0.43
2:B:438:LEU:HB2	2:B:441:ASP:OD1	2.17	0.43
2:B:556:ASN:N	2:B:560:THR:O	2.41	0.43
2:B:853:VAL:HG23	2:B:854:ARG:N	2.33	0.43
2:B:908:ASN:O	2:B:912:VAL:HG22	2.18	0.43
2:B:1218:GLU:HB2	2:B:1501:TRP:CZ2	2.52	0.43
2:B:1263:THR:HA	2:B:1266:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1545:HIS:O	2:B:1549:MET:HG2	2.18	0.43
1:D:532:PRO:O	1:D:536:LEU:HD13	2.18	0.43
1:D:588:TYR:HE2	1:D:608:LEU:HB2	1.82	0.43
2:E:87:LEU:HA	2:E:90:GLU:HG3	2.00	0.43
2:E:730:TYR:CE1	2:E:771:ARG:HD3	2.53	0.43
2:E:853:VAL:HG23	2:E:854:ARG:N	2.33	0.43
2:E:1056:HIS:HD1	2:E:1057:GLU:CD	2.17	0.43
2:E:1240:TYR:CE2	2:E:1244:LEU:HD11	2.53	0.43
3:F:39:ASN:CA	3:F:57:ASP:H	2.27	0.43
2:B:5:ILE:N	2:B:40:MET:H	2.01	0.43
2:B:145:LYS:O	2:B:148:VAL:HG12	2.17	0.43
2:B:204:ILE:HG23	2:B:211:ARG:CZ	2.48	0.43
2:B:305:HIS:CD2	2:B:314:HIS:HB2	2.53	0.43
2:B:305:HIS:HA	2:B:315:THR:O	2.18	0.43
2:B:499:VAL:HB	2:B:509:TRP:HD1	1.84	0.43
2:B:821:PRO:HA	2:B:824:ILE:HG12	2.01	0.43
2:B:1157:GLN:O	2:B:1160:GLU:HB3	2.17	0.43
2:B:1268:ALA:HA	2:B:1271:LEU:HD13	1.99	0.43
2:E:225:TYR:HD2	2:E:404:LYS:HB2	1.83	0.43
2:E:1022:ASN:O	2:E:1026:GLU:OE1	2.36	0.43
2:E:1324:LEU:HD23	2:E:1341:LEU:HD13	2.01	0.43
2:E:1365:VAL:N	2:E:1381:PHE:O	2.42	0.43
2:E:1583:GLN:O	2:E:1586:VAL:HG12	2.18	0.43
1:A:579:LEU:HD12	1:A:580:SER:H	1.84	0.43
2:B:438:LEU:N	2:B:441:ASP:OD2	2.51	0.43
2:B:500:VAL:HG11	2:B:534:ARG:HB2	2.00	0.43
2:B:714:PRO:O	2:B:718:THR:OG1	2.26	0.43
2:B:730:TYR:CE1	2:B:771:ARG:HD3	2.53	0.43
2:B:1063:THR:HA	2:B:1069:ARG:HD2	2.00	0.43
2:B:1249:ASP:O	2:B:1252:ARG:NH1	2.51	0.43
2:B:1382:ILE:HD11	2:B:1504:VAL:HG23	2.00	0.43
2:B:1457:ASN:O	2:B:1459:VAL:HG13	2.16	0.43
1:D:544:ILE:HG23	1:D:545:LEU:H	1.83	0.43
2:E:302:ARG:HD3	2:E:322:PHE:CD1	2.47	0.43
2:E:305:HIS:HA	2:E:315:THR:O	2.18	0.43
2:E:340:GLU:HG2	2:E:420:LEU:HD11	2.00	0.43
2:E:795:PHE:HE1	2:E:840:PHE:CD1	2.36	0.43
2:E:821:PRO:HA	2:E:824:ILE:HG12	2.00	0.43
2:E:857:LEU:CB	2:E:905:LEU:HD21	2.47	0.43
2:E:908:ASN:O	2:E:912:VAL:HG22	2.18	0.43
2:E:922:ALA:HA	2:E:925:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:926:GLN:HG2	2:E:971:HIS:ND1	2.34	0.43
2:E:979:ARG:HA	2:E:982:ILE:HG22	2.00	0.43
2:E:1258:THR:HG22	2:E:1262:TYR:HE2	1.80	0.43
2:E:1500:LYS:HB2	2:E:1501:TRP:CE3	2.53	0.43
2:E:1522:MET:HE3	2:E:1589:LEU:HB3	2.01	0.43
3:F:45:MET:HA	3:F:50:PRO:HA	2.00	0.43
2:B:19:TYR:CZ	2:B:60:PRO:HD3	2.53	0.43
2:B:23:GLN:HG2	2:B:58:ILE:HB	2.00	0.43
2:B:87:LEU:HB2	2:B:145:LYS:HE2	1.99	0.43
2:B:95:LEU:HA	2:B:98:TRP:HB2	2.00	0.43
2:B:182:ALA:HA	2:B:185:LYS:HZ3	1.83	0.43
2:B:643:TRP:HE1	2:B:675:ALA:HA	1.83	0.43
2:B:895:ASN:O	2:B:898:ASP:N	2.51	0.43
2:B:911:GLU:O	2:B:915:ARG:HG2	2.18	0.43
2:B:1062:GLU:O	2:B:1069:ARG:HD3	2.18	0.43
2:B:1596:GLN:O	2:B:1599:LEU:HB3	2.18	0.43
2:E:156:ASN:HD22	2:E:161:LEU:HB2	1.84	0.43
2:E:469:THR:HG22	2:E:495:GLU:HB3	1.99	0.43
2:E:499:VAL:HB	2:E:509:TRP:HD1	1.84	0.43
2:E:528:ARG:HG3	2:E:551:PHE:HB3	2.01	0.43
2:E:831:PHE:CD2	2:E:836:LEU:HB2	2.54	0.43
2:E:1042:LEU:HD12	2:E:1042:LEU:O	2.18	0.43
2:B:8:LYS:HA	2:B:10:GLN:HE22	1.84	0.43
2:B:1290:VAL:HG13	2:B:1291:TYR:N	2.34	0.43
2:B:1417:ASP:CG	2:B:1418:ILE:HG12	2.39	0.43
2:E:248:PRO:HB3	2:E:387:ILE:CG2	2.49	0.43
2:E:328:ASP:OD1	2:E:390:LYS:HE2	2.17	0.43
2:E:673:LEU:HD13	2:E:719:TYR:CD2	2.53	0.43
2:E:735:LYS:HG2	2:E:739:PHE:CE2	2.54	0.43
2:E:836:LEU:HG	2:E:840:PHE:CE2	2.53	0.43
2:E:889:GLN:CA	2:E:895:ASN:HD21	2.31	0.43
2:E:976:PHE:HB2	2:E:982:ILE:HD12	2.01	0.43
2:E:1048:HIS:HE1	2:E:1105:MET:HA	1.84	0.43
2:E:1227:VAL:HG22	2:E:1231:TYR:CE2	2.54	0.43
2:E:1290:VAL:HG13	2:E:1291:TYR:N	2.34	0.43
2:E:1545:HIS:O	2:E:1549:MET:HG2	2.18	0.43
2:E:1556:ASP:O	2:E:1558:ALA:N	2.51	0.43
3:F:21:ILE:HD11	3:F:35:THR:HG23	2.00	0.43
3:F:85:VAL:O	3:F:129:LEU:HD21	2.18	0.43
3:F:154:TYR:OH	3:F:156:GLU:OE2	2.31	0.43
2:B:167:ASP:OD1	2:B:168:ASP:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:214:SER:O	2:B:217:SER:OG	2.37	0.43
2:B:302:ARG:HG3	2:B:320:ARG:HB2	2.00	0.43
2:B:958:ILE:HB	2:B:1016:VAL:CG2	2.48	0.43
2:B:995:ASP:OD1	2:B:999:LYS:HE3	2.18	0.43
2:B:1061:LEU:HA	2:B:1064:PHE:CZ	2.53	0.43
2:B:1243:TYR:HD2	2:B:1246:LYS:HG3	1.83	0.43
2:B:1337:GLY:HA2	2:B:1340:ASN:ND2	2.33	0.43
2:B:1500:LYS:HB2	2:B:1501:TRP:CE3	2.53	0.43
1:D:575:TRP:CZ3	1:D:588:TYR:HB2	2.54	0.43
1:D:693:GLU:OE1	1:D:696:LEU:HD11	2.19	0.43
2:E:53:LYS:HG3	2:E:53:LYS:O	2.19	0.43
2:E:123:SER:O	2:E:126:GLU:HG3	2.19	0.43
2:E:1061:LEU:HA	2:E:1064:PHE:CZ	2.53	0.43
2:E:1206:ASP:O	2:E:1210:ILE:HG12	2.19	0.43
2:E:1313:MET:SD	2:E:1453:TYR:OH	2.71	0.43
1:A:579:LEU:HA	1:A:586:LEU:HD13	2.01	0.43
2:B:528:ARG:HG3	2:B:551:PHE:HB3	2.00	0.43
2:B:764:PHE:HD1	2:B:823:ILE:HB	1.83	0.43
2:B:976:PHE:HB2	2:B:982:ILE:HD12	2.00	0.43
2:B:1059:LEU:HD21	2:B:1117:GLU:OE2	2.19	0.43
2:B:1177:LEU:O	2:B:1181:ARG:HD2	2.18	0.43
2:B:1239:ILE:HG23	2:B:1242:ARG:HH21	1.83	0.43
2:B:1275:ASP:OD2	2:B:1275:ASP:N	2.45	0.43
1:D:615:ALA:H	1:D:645:LEU:HB2	1.84	0.43
2:E:88:VAL:HB	2:E:128:ARG:HH22	1.84	0.43
2:E:91:LEU:HD12	2:E:91:LEU:HA	1.81	0.43
2:E:804:ARG:HD2	2:E:808:GLU:OE2	2.19	0.43
2:E:820:LEU:HB3	2:E:821:PRO:HD3	2.00	0.43
2:E:934:ARG:HH12	2:E:938:ARG:HB2	1.83	0.43
2:E:1155:LEU:O	2:E:1159:VAL:HG23	2.17	0.43
2:E:1283:LEU:HB3	2:E:1288:TYR:HE1	1.82	0.43
2:E:1495:PHE:HE1	2:E:1502:PHE:CD2	2.31	0.43
2:E:1617:PRO:HB2	2:E:1621:ARG:HH22	1.84	0.43
1:A:564:LYS:NZ	1:A:590:ASP:OD1	2.40	0.43
1:A:652:LEU:HD13	1:A:654:PHE:CZ	2.54	0.43
2:B:118:GLN:HB3	2:B:122:TYR:OH	2.19	0.43
2:B:380:THR:HG21	2:B:510:TYR:CD2	2.54	0.43
2:B:673:LEU:HD13	2:B:719:TYR:CD2	2.53	0.43
2:B:718:THR:HG23	2:B:722:LYS:NZ	2.34	0.43
2:B:795:PHE:HE1	2:B:840:PHE:CD1	2.36	0.43
2:B:1111:GLU:O	2:B:1114:LEU:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1199:SER:O	2:B:1202:GLU:HG2	2.18	0.43
1:D:543:GLU:OE1	1:D:543:GLU:N	2.49	0.43
1:D:640:LEU:O	1:D:655:ILE:HA	2.19	0.43
2:E:305:HIS:CD2	2:E:314:HIS:HB2	2.53	0.43
2:E:500:VAL:HG11	2:E:534:ARG:HB2	2.00	0.43
2:E:710:GLN:HA	2:E:713:ASN:OD1	2.19	0.43
2:E:1224:THR:HA	2:E:1227:VAL:HG12	1.99	0.43
2:E:1309:ASP:O	2:E:1312:LYS:HE2	2.19	0.43
2:E:1406:GLU:OE1	2:E:1423:LYS:NZ	2.52	0.43
2:E:1417:ASP:CG	2:E:1418:ILE:HG12	2.39	0.43
1:A:615:ALA:H	1:A:645:LEU:HB2	1.84	0.43
1:A:640:LEU:O	1:A:655:ILE:HA	2.19	0.43
2:B:162:ASP:OD2	2:B:1071:LYS:NZ	2.50	0.43
2:B:468:VAL:HG21	2:B:620:PHE:CE1	2.53	0.43
2:B:470:MET:HA	2:B:529:PHE:HA	2.01	0.43
2:B:582:ALA:HA	2:B:585:TYR:CE2	2.54	0.43
2:B:773:LEU:HA	2:B:776:ARG:CZ	2.49	0.43
2:B:795:PHE:CZ	2:B:836:LEU:HD12	2.53	0.43
2:B:804:ARG:HD2	2:B:808:GLU:OE2	2.18	0.43
2:B:1115:THR:O	2:B:1121:ARG:NH2	2.52	0.43
2:B:1324:LEU:HD23	2:B:1341:LEU:HD13	2.01	0.43
2:B:1361:GLU:OE2	2:B:1388:TYR:HA	2.18	0.43
2:B:1406:GLU:OE1	2:B:1423:LYS:NZ	2.52	0.43
2:B:1556:ASP:O	2:B:1558:ALA:N	2.51	0.43
3:C:45:MET:HA	3:C:50:PRO:HA	2.00	0.43
1:D:704:ILE:HD11	2:E:65:HIS:CD2	2.54	0.43
2:E:166:ARG:CD	2:E:173:LEU:HB2	2.47	0.43
2:E:287:MET:HA	2:E:290:ILE:HG12	2.01	0.43
2:E:326:VAL:H	2:E:386:VAL:HG11	1.84	0.43
2:E:480:LEU:HD23	2:E:483:ALA:HB2	1.99	0.43
2:E:519:ILE:HG23	2:E:631:LEU:HG	2.01	0.43
2:E:636:ASP:HB2	2:E:660:VAL:HG22	2.01	0.43
2:E:868:LEU:HD12	2:E:868:LEU:HA	1.78	0.43
2:E:868:LEU:O	2:E:918:VAL:HG13	2.18	0.43
2:E:1223:CYS:HA	2:E:1226:ASN:ND2	2.34	0.43
2:E:1568:LYS:O	2:E:1572:THR:OG1	2.37	0.43
3:F:9:VAL:HB	3:F:97:TRP:CE3	2.54	0.43
2:B:435:GLU:HA	2:B:708:LYS:HZ2	1.81	0.42
2:B:463:PRO:HD2	2:B:503:GLN:HB3	2.01	0.42
2:B:1386:LYS:HG3	2:B:1387:GLU:H	1.84	0.42
2:B:1617:PRO:HB2	2:B:1621:ARG:HH22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:633:GLN:HB3	1:D:637:VAL:HG21	2.01	0.42
1:D:652:LEU:HD13	1:D:654:PHE:CZ	2.54	0.42
2:E:468:VAL:HG22	2:E:531:PHE:CD1	2.54	0.42
2:E:473:HIS:HD2	2:E:528:ARG:HB3	1.84	0.42
2:E:773:LEU:HA	2:E:776:ARG:CZ	2.49	0.42
2:E:995:ASP:OD1	2:E:999:LYS:HE3	2.18	0.42
2:E:1248:ARG:HD2	2:E:1249:ASP:N	2.34	0.42
2:E:1318:ILE:O	2:E:1322:LYS:HG2	2.19	0.42
2:E:1367:TYR:CZ	2:E:1402:PHE:HE2	2.36	0.42
2:E:1596:GLN:O	2:E:1599:LEU:HB3	2.18	0.42
2:E:1631:GLU:O	2:E:1635:LYS:HG2	2.19	0.42
3:F:20:LEU:O	3:F:24:THR:HG23	2.19	0.42
3:F:82:PHE:HB3	3:F:93:VAL:HG21	2.01	0.42
2:B:11:LYS:NZ	2:B:36:HIS:HB2	2.34	0.42
2:B:53:LYS:HG3	2:B:53:LYS:O	2.19	0.42
2:B:153:ASP:HA	2:B:156:ASN:OD1	2.19	0.42
2:B:248:PRO:HB3	2:B:387:ILE:HG21	2.01	0.42
2:B:857:LEU:CB	2:B:905:LEU:HD21	2.47	0.42
2:B:889:GLN:CA	2:B:895:ASN:HD21	2.31	0.42
2:B:930:GLU:HG2	2:B:972:TYR:CG	2.54	0.42
2:B:1048:HIS:CE1	2:B:1108:PRO:HG2	2.54	0.42
2:B:1206:ASP:O	2:B:1210:ILE:HG12	2.19	0.42
2:B:1318:ILE:O	2:B:1322:LYS:HG2	2.19	0.42
2:B:1357:ARG:NE	2:B:1452:ASN:O	2.53	0.42
2:B:1367:TYR:CZ	2:B:1402:PHE:HE2	2.36	0.42
2:B:1372:PHE:N	2:B:1424:GLN:HG2	2.35	0.42
3:C:8:VAL:HG11	3:C:20:LEU:HD11	2.02	0.42
3:C:44:VAL:HG12	3:C:45:MET:O	2.18	0.42
1:D:696:LEU:HD12	1:D:697:ARG:HE	1.83	0.42
2:E:718:THR:HG23	2:E:722:LYS:NZ	2.34	0.42
2:E:931:ARG:C	2:E:932:LEU:HD12	2.38	0.42
2:E:1263:THR:HA	2:E:1266:LEU:HD12	2.00	0.42
2:E:1386:LYS:HG3	2:E:1387:GLU:H	1.84	0.42
1:A:693:GLU:OE1	1:A:696:LEU:HD11	2.19	0.42
1:A:714:PRO:HD3	2:B:62:THR:HG21	2.00	0.42
2:B:104:LYS:HD3	2:B:107:VAL:HB	2.00	0.42
2:B:156:ASN:HD22	2:B:161:LEU:HB2	1.84	0.42
2:B:166:ARG:HG2	2:B:173:LEU:HB2	2.01	0.42
2:B:166:ARG:NE	2:B:169:ASN:OD1	2.52	0.42
2:B:248:PRO:HB3	2:B:387:ILE:CG2	2.49	0.42
2:B:468:VAL:HG22	2:B:531:PHE:CD1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:792:ARG:HG2	2:B:839:LEU:HD11	2.01	0.42
3:C:82:PHE:HB3	3:C:93:VAL:HG21	2.01	0.42
1:D:693:GLU:OE2	1:D:697:ARG:HD2	2.19	0.42
2:E:153:ASP:HA	2:E:156:ASN:OD1	2.19	0.42
2:E:306:MET:HE1	2:E:465:ASN:HB3	2.01	0.42
2:E:438:LEU:N	2:E:441:ASP:OD2	2.52	0.42
2:E:455:PHE:CD2	2:E:466:VAL:HG21	2.54	0.42
2:E:820:LEU:O	2:E:824:ILE:HG23	2.18	0.42
2:E:1243:TYR:HD2	2:E:1246:LYS:HG3	1.83	0.42
2:E:1625:CYS:O	2:E:1628:GLU:HB3	2.19	0.42
1:A:693:GLU:OE2	1:A:697:ARG:HD2	2.19	0.42
2:B:123:SER:O	2:B:126:GLU:HG3	2.19	0.42
2:B:156:ASN:HA	2:B:161:LEU:HD12	2.01	0.42
2:B:273:LYS:O	2:B:277:LEU:N	2.53	0.42
2:B:1227:VAL:HG22	2:B:1231:TYR:CE2	2.53	0.42
2:B:1367:TYR:CE2	2:B:1402:PHE:CE2	3.06	0.42
2:B:1583:GLN:O	2:B:1586:VAL:HG12	2.18	0.42
3:C:14:VAL:HG13	3:C:116:LYS:HZ3	1.83	0.42
3:C:20:LEU:O	3:C:24:THR:HG23	2.19	0.42
2:E:632:THR:HA	2:E:664:GLU:OE1	2.20	0.42
2:E:882:LEU:HD13	2:E:882:LEU:HA	1.87	0.42
2:E:895:ASN:O	2:E:898:ASP:N	2.51	0.42
2:E:1239:ILE:HG23	2:E:1242:ARG:HH21	1.83	0.42
3:F:11:ASP:OD1	3:F:11:ASP:N	2.49	0.42
2:B:25:VAL:HG12	2:B:55:LYS:HE3	2.01	0.42
2:B:326:VAL:H	2:B:386:VAL:HG11	1.84	0.42
2:B:656:LYS:HG3	2:B:659:GLU:OE2	2.20	0.42
2:B:735:LYS:HG2	2:B:739:PHE:CE2	2.54	0.42
2:B:769:GLN:HA	2:B:772:VAL:HG12	2.02	0.42
2:B:831:PHE:CD2	2:B:836:LEU:HB2	2.54	0.42
2:B:1022:ASN:O	2:B:1026:GLU:OE1	2.37	0.42
2:B:1308:PHE:O	2:B:1312:LYS:N	2.53	0.42
2:B:1363:PHE:HE1	2:B:1430:THR:HG1	1.67	0.42
2:B:1417:ASP:OD1	2:B:1417:ASP:N	2.51	0.42
2:B:1568:LYS:O	2:B:1572:THR:OG1	2.37	0.42
3:C:9:VAL:HB	3:C:97:TRP:CE3	2.54	0.42
1:D:657:PRO:HB2	1:D:661:GLU:OE2	2.20	0.42
2:E:25:VAL:HG12	2:E:55:LYS:HE3	2.01	0.42
2:E:158:MET:C	2:E:159:LEU:HD22	2.39	0.42
2:E:166:ARG:NE	2:E:169:ASN:OD1	2.52	0.42
2:E:197:LYS:O	2:E:200:GLU:N	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:278:GLN:O	2:E:426:ALA:N	2.49	0.42
2:E:582:ALA:HA	2:E:585:TYR:CE2	2.54	0.42
2:E:643:TRP:HE1	2:E:675:ALA:HA	1.83	0.42
2:E:1116:PRO:HA	2:E:1121:ARG:NH2	2.35	0.42
2:B:15:ALA:HA	2:B:59:PHE:CZ	2.54	0.42
2:B:632:THR:HA	2:B:664:GLU:OE1	2.20	0.42
2:B:1027:VAL:HG22	2:B:1032:PHE:HE1	1.82	0.42
2:B:1245:TYR:O	2:B:1248:ARG:HG3	2.20	0.42
2:B:1318:ILE:HD13	2:B:1349:TYR:CE2	2.55	0.42
3:C:17:THR:O	3:C:21:ILE:HG22	2.19	0.42
2:E:1:MET:HG3	2:E:4:TRP:HE1	1.84	0.42
2:E:118:GLN:HB3	2:E:122:TYR:OH	2.19	0.42
2:E:930:GLU:HG2	2:E:972:TYR:CG	2.53	0.42
2:E:1059:LEU:HD21	2:E:1117:GLU:OE2	2.19	0.42
2:E:1367:TYR:CE2	2:E:1402:PHE:CE2	3.06	0.42
3:F:44:VAL:HG12	3:F:45:MET:O	2.18	0.42
1:A:588:TYR:CE2	1:A:608:LEU:HB2	2.54	0.42
2:B:4:TRP:CE3	2:B:39:GLU:HB2	2.55	0.42
2:B:287:MET:HA	2:B:290:ILE:HG12	2.01	0.42
2:B:455:PHE:CD2	2:B:466:VAL:HG21	2.55	0.42
2:B:464:LYS:HD3	2:B:533:HIS:CD2	2.55	0.42
2:B:570:VAL:HG22	2:B:592:LYS:HD2	2.02	0.42
2:B:632:THR:HG21	2:B:637:LEU:HD23	2.02	0.42
2:B:926:GLN:HG2	2:B:971:HIS:ND1	2.34	0.42
2:B:1098:LYS:O	2:B:1102:ILE:N	2.50	0.42
2:B:1110:LEU:HA	2:B:1128:PHE:HZ	1.85	0.42
2:B:1243:TYR:HA	2:B:1246:LYS:CG	2.50	0.42
2:E:166:ARG:HG2	2:E:173:LEU:HB2	2.01	0.42
2:E:246:TYR:CE1	2:E:383:LEU:HD21	2.55	0.42
2:E:380:THR:HG21	2:E:510:TYR:CD2	2.54	0.42
2:E:545:ARG:HH11	2:E:576:ASN:HD21	1.66	0.42
2:E:1357:ARG:NE	2:E:1452:ASN:O	2.52	0.42
2:E:1401:GLN:HG3	2:E:1402:PHE:CD2	2.55	0.42
2:E:1598:PRO:O	2:E:1602:GLU:OE1	2.38	0.42
1:A:564:LYS:NZ	1:A:590:ASP:HA	2.35	0.42
2:B:158:MET:C	2:B:159:LEU:HD22	2.39	0.42
2:B:219:ILE:HG13	2:B:222:TYR:OH	2.20	0.42
2:B:340:GLU:HG2	2:B:420:LEU:HD11	2.00	0.42
2:B:636:ASP:HB2	2:B:660:VAL:HG22	2.01	0.42
2:B:879:LEU:HG	2:B:879:LEU:O	2.20	0.42
2:B:940:VAL:HA	2:B:943:MET:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1059:LEU:HA	2:B:1059:LEU:HD23	1.77	0.42
2:B:1116:PRO:HA	2:B:1121:ARG:NH2	2.35	0.42
2:B:1155:LEU:HD21	2:B:1197:VAL:HG13	2.02	0.42
2:B:1248:ARG:HD2	2:B:1249:ASP:N	2.34	0.42
2:B:1309:ASP:O	2:B:1312:LYS:HE2	2.19	0.42
2:B:1313:MET:SD	2:B:1453:TYR:OH	2.71	0.42
2:B:1392:GLU:OE2	3:C:166:LYS:HE2	2.19	0.42
2:B:1409:THR:HA	3:C:28:PHE:CZ	2.52	0.42
3:C:39:ASN:CA	3:C:57:ASP:H	2.27	0.42
1:D:551:GLN:O	1:D:555:ARG:HG2	2.20	0.42
2:E:214:SER:O	2:E:217:SER:OG	2.37	0.42
2:E:570:VAL:HG22	2:E:592:LYS:HD2	2.02	0.42
2:E:769:GLN:HA	2:E:772:VAL:HG12	2.02	0.42
2:E:909:ILE:O	2:E:913:LEU:HD12	2.20	0.42
2:E:926:GLN:NE2	2:E:930:GLU:OE2	2.48	0.42
2:E:1242:ARG:O	2:E:1246:LYS:HG2	2.20	0.42
2:E:1256:ASN:O	2:E:1260:ALA:N	2.29	0.42
2:E:1338:LEU:O	2:E:1342:LEU:HD23	2.20	0.42
3:F:129:LEU:O	3:F:134:LEU:N	2.29	0.42
1:A:532:PRO:HG2	1:A:706:ILE:O	2.20	0.42
1:A:633:GLN:HB3	1:A:637:VAL:HG21	2.01	0.42
1:A:657:PRO:HB2	1:A:661:GLU:OE2	2.20	0.42
1:A:695:LYS:NZ	2:B:122:TYR:CE1	2.88	0.42
2:B:95:LEU:CA	2:B:98:TRP:HD1	2.31	0.42
2:B:1022:ASN:OD1	2:B:1086:ARG:NH1	2.53	0.42
2:B:1028:LEU:HA	2:B:1032:PHE:CD1	2.43	0.42
2:B:1090:MET:O	2:B:1094:LEU:HD23	2.20	0.42
2:B:1362:TYR:HE2	2:B:1459:VAL:HG21	1.85	0.42
2:B:1506:GLN:NE2	2:B:1508:SER:OG	2.48	0.42
1:D:564:LYS:HZ1	1:D:590:ASP:HA	1.84	0.42
1:D:701:LEU:HD21	2:E:15:ALA:C	2.40	0.42
2:E:15:ALA:HA	2:E:59:PHE:CZ	2.54	0.42
2:E:156:ASN:HA	2:E:161:LEU:HD12	2.01	0.42
2:E:464:LYS:HD3	2:E:533:HIS:CD2	2.55	0.42
2:E:839:LEU:HG	2:E:842:LYS:HZ1	1.83	0.42
2:E:1115:THR:O	2:E:1121:ARG:NH2	2.52	0.42
2:E:1372:PHE:N	2:E:1424:GLN:HG2	2.34	0.42
3:F:53:LEU:HD13	3:F:169:PHE:CZ	2.55	0.42
1:A:541:GLN:O	1:A:543:GLU:N	2.53	0.42
1:A:575:TRP:CZ3	1:A:588:TYR:HB2	2.54	0.42
1:A:585:VAL:HG12	1:A:607:LYS:NZ	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:246:TYR:CE1	2:B:383:LEU:HD21	2.54	0.42
2:B:344:HIS:N	2:B:401:VAL:O	2.53	0.42
2:B:519:ILE:HG23	2:B:631:LEU:HG	2.01	0.42
2:B:545:ARG:HH11	2:B:576:ASN:HD21	1.67	0.42
2:B:768:ILE:HG13	2:B:826:ASP:O	2.20	0.42
2:B:933:LEU:HA	2:B:936:ILE:HG22	2.02	0.42
2:B:1392:GLU:OE1	2:B:1392:GLU:N	2.51	0.42
2:B:1418:ILE:HD13	2:B:1421:SER:HB3	2.01	0.42
3:C:53:LEU:HD13	3:C:169:PHE:CZ	2.55	0.42
1:D:532:PRO:HG2	1:D:706:ILE:O	2.20	0.42
1:D:585:VAL:HG12	1:D:607:LYS:NZ	2.34	0.42
2:E:4:TRP:CE3	2:E:39:GLU:HB2	2.55	0.42
2:E:44:TRP:HE3	2:E:58:ILE:HG22	1.85	0.42
2:E:127:TRP:O	2:E:131:ILE:HG12	2.20	0.42
2:E:273:LYS:O	2:E:277:LEU:N	2.53	0.42
2:E:656:LYS:HG3	2:E:659:GLU:OE2	2.20	0.42
2:E:854:ARG:HH11	2:E:858:ASN:HD21	1.68	0.42
2:E:1048:HIS:CE1	2:E:1108:PRO:HG2	2.55	0.42
2:E:1111:GLU:O	2:E:1114:LEU:HB2	2.19	0.42
2:E:1129:PHE:CZ	2:E:1183:HIS:HB2	2.55	0.42
2:E:1183:HIS:CG	2:E:1184:LYS:N	2.87	0.42
2:E:1245:TYR:O	2:E:1248:ARG:HG3	2.20	0.42
2:E:1441:TYR:HD2	2:E:1450:ILE:HG21	1.82	0.42
2:E:1444:LYS:HD3	2:E:1446:VAL:HG12	2.02	0.42
3:F:17:THR:O	3:F:21:ILE:HG22	2.20	0.42
3:F:58:THR:HB	3:F:68:ARG:NH1	2.35	0.42
3:F:124:ASP:O	3:F:127:GLU:HG2	2.20	0.42
1:A:620:LYS:HE2	1:A:638:LEU:HD11	2.02	0.41
2:B:38:LEU:HD21	2:B:48:TYR:CD2	2.55	0.41
2:B:306:MET:HE1	2:B:465:ASN:HB3	2.01	0.41
2:B:473:HIS:HD2	2:B:528:ARG:HB3	1.84	0.41
2:B:778:TYR:O	2:B:780:GLN:N	2.53	0.41
2:B:1171:LEU:O	2:B:1175:LEU:HD23	2.20	0.41
2:B:1205:LEU:HD22	2:B:1208:ARG:NH2	2.35	0.41
2:B:1431:VAL:HG12	2:B:1464:TYR:HB2	2.02	0.41
1:D:588:TYR:CE2	1:D:608:LEU:HB2	2.54	0.41
2:E:38:LEU:HD21	2:E:48:TYR:CD2	2.55	0.41
2:E:105:LEU:HB3	2:E:114:PHE:HB2	2.02	0.41
2:E:1259:GLU:O	2:E:1263:THR:HG23	2.20	0.41
2:E:1308:PHE:O	2:E:1312:LYS:N	2.53	0.41
2:E:1360:PRO:HA	2:E:1387:GLU:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:666:THR:HG23	1:A:678:MET:SD	2.60	0.41
2:B:147:LYS:O	2:B:151:LYS:HD3	2.21	0.41
2:B:157:ARG:NH2	2:B:198:ILE:HG12	2.35	0.41
2:B:875:ARG:NH1	2:B:920:ALA:O	2.52	0.41
2:B:1091:TRP:CD1	2:B:1127:ILE:HG23	2.55	0.41
2:B:1155:LEU:HA	2:B:1158:GLU:OE2	2.20	0.41
2:B:1323:GLU:O	2:B:1327:THR:HG23	2.21	0.41
2:B:1367:TYR:C	2:B:1368:TYR:HD1	2.24	0.41
2:B:1380:ILE:HB	2:B:1504:VAL:HG12	2.03	0.41
2:B:1401:GLN:HG3	2:B:1402:PHE:CD2	2.55	0.41
1:D:579:LEU:HA	1:D:586:LEU:HD13	2.01	0.41
2:E:8:LYS:HA	2:E:10:GLN:HE22	1.84	0.41
2:E:441:ASP:O	2:E:629:THR:OG1	2.26	0.41
2:E:470:MET:HA	2:E:529:PHE:HA	2.01	0.41
2:E:768:ILE:HG13	2:E:826:ASP:O	2.20	0.41
2:E:792:ARG:HG2	2:E:839:LEU:HD11	2.01	0.41
2:E:818:LYS:O	2:E:821:PRO:HD2	2.20	0.41
2:E:993:PHE:O	2:E:997:ILE:HG12	2.20	0.41
2:E:1109:ILE:HG12	2:E:1128:PHE:CE1	2.56	0.41
2:E:1155:LEU:HD21	2:E:1197:VAL:HG13	2.01	0.41
2:E:1171:LEU:O	2:E:1175:LEU:HD23	2.20	0.41
2:E:1238:ASP:OD1	2:E:1239:ILE:HG12	2.20	0.41
2:E:1418:ILE:HD13	2:E:1421:SER:HB3	2.01	0.41
2:E:1463:ARG:NH2	2:E:1465:SER:HA	2.35	0.41
1:A:551:GLN:O	1:A:555:ARG:HG2	2.20	0.41
1:A:652:LEU:HD23	1:A:652:LEU:HA	1.74	0.41
1:A:658:ASP:OD1	1:A:661:GLU:HG2	2.21	0.41
2:B:80:VAL:HG23	2:B:81:ILE:HG22	2.03	0.41
2:B:874:CYS:O	2:B:878:LEU:HG	2.20	0.41
2:B:926:GLN:NE2	2:B:930:GLU:OE2	2.48	0.41
2:B:993:PHE:O	2:B:997:ILE:HG12	2.20	0.41
2:B:1322:LYS:HE3	2:B:1345:ARG:HD3	2.02	0.41
2:B:1598:PRO:O	2:B:1602:GLU:OE1	2.38	0.41
3:C:21:ILE:HA	3:C:24:THR:OG1	2.20	0.41
1:D:579:LEU:HD12	1:D:580:SER:H	1.84	0.41
2:E:435:GLU:HA	2:E:708:LYS:HZ2	1.83	0.41
2:E:768:ILE:HD11	2:E:827:VAL:HG22	2.02	0.41
2:E:853:VAL:HG23	2:E:854:ARG:H	1.85	0.41
2:E:1269:GLU:OE1	2:E:1270:LEU:HD22	2.21	0.41
2:E:1363:PHE:HE1	2:E:1430:THR:HG1	1.64	0.41
2:E:1506:GLN:NE2	2:E:1508:SER:OG	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:19:TYR:CG	2:B:59:PHE:CE1	3.05	0.41
2:B:44:TRP:HE3	2:B:58:ILE:HG22	1.85	0.41
2:B:228:PHE:CZ	2:B:231:PHE:HB2	2.55	0.41
2:B:818:LYS:O	2:B:821:PRO:HD2	2.20	0.41
2:B:959:ALA:HB1	2:B:963:GLN:NE2	2.35	0.41
2:B:1019:ARG:O	2:B:1023:GLN:HG2	2.21	0.41
2:B:1223:CYS:HA	2:B:1226:ASN:ND2	2.34	0.41
2:B:1238:ASP:OD1	2:B:1239:ILE:HG12	2.20	0.41
2:B:1290:VAL:HG13	2:B:1291:TYR:H	1.85	0.41
2:B:1318:ILE:HD13	2:B:1349:TYR:CZ	2.55	0.41
2:B:1333:PHE:CZ	2:E:1444:LYS:HD3	2.47	0.41
2:B:1338:LEU:O	2:B:1342:LEU:HD23	2.20	0.41
1:D:548:ILE:CG2	1:D:682:THR:HG23	2.50	0.41
1:D:564:LYS:NZ	1:D:590:ASP:HA	2.35	0.41
2:E:11:LYS:NZ	2:E:36:HIS:HB2	2.34	0.41
2:E:45:TYR:HB2	2:E:64:ILE:HG13	2.02	0.41
2:E:191:SER:O	2:E:194:ILE:HB	2.20	0.41
2:E:526:HIS:NE2	2:E:586:LEU:HD11	2.36	0.41
2:E:856:LYS:HZ3	2:E:885:GLN:HB2	1.85	0.41
2:E:874:CYS:O	2:E:878:LEU:HG	2.20	0.41
2:E:875:ARG:NH1	2:E:920:ALA:O	2.52	0.41
2:E:1228:LEU:HD23	2:E:1228:LEU:HA	1.90	0.41
2:E:1322:LYS:HE3	2:E:1345:ARG:HD3	2.02	0.41
2:E:1392:GLU:OE1	2:E:1392:GLU:N	2.51	0.41
3:F:8:VAL:HG11	3:F:20:LEU:HD11	2.02	0.41
1:A:646:TYR:CE1	1:A:652:LEU:HG	2.56	0.41
2:B:221:THR:HG23	2:B:283:ASP:HA	2.02	0.41
2:B:471:SER:N	2:B:528:ARG:O	2.35	0.41
2:B:710:GLN:HA	2:B:713:ASN:OD1	2.19	0.41
2:B:937:ASN:O	2:B:941:ILE:HG13	2.21	0.41
2:B:1369:GLY:CA	2:B:1418:ILE:HG22	2.51	0.41
2:B:1461:GLN:HA	2:B:1489:TYR:O	2.21	0.41
2:B:1625:CYS:O	2:B:1628:GLU:HB3	2.19	0.41
1:D:541:GLN:O	1:D:543:GLU:N	2.53	0.41
1:D:667:ASP:HB3	1:D:677:MET:SD	2.60	0.41
2:E:65:HIS:ND1	2:E:65:HIS:O	2.53	0.41
2:E:219:ILE:HG13	2:E:222:TYR:OH	2.20	0.41
2:E:463:PRO:HD2	2:E:503:GLN:HB3	2.02	0.41
2:E:910:LEU:HD22	2:E:963:GLN:OE1	2.20	0.41
2:E:959:ALA:HB1	2:E:963:GLN:NE2	2.35	0.41
2:E:1044:ASN:HA	2:E:1101:PHE:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1081:LYS:O	2:E:1085:PHE:HD1	2.04	0.41
2:E:1155:LEU:HA	2:E:1158:GLU:OE2	2.20	0.41
2:E:1531:ASN:O	2:E:1535:GLN:HG3	2.20	0.41
1:A:599:VAL:HA	1:A:600:PRO:HD3	1.86	0.41
1:A:614:LYS:H	1:A:614:LYS:HD2	1.85	0.41
1:A:640:LEU:HD13	1:A:656:ALA:O	2.21	0.41
2:B:570:VAL:HA	2:B:592:LYS:NZ	2.36	0.41
2:B:1048:HIS:HE1	2:B:1105:MET:HA	1.84	0.41
2:B:1063:THR:HA	2:B:1069:ARG:CD	2.51	0.41
2:B:1233:GLU:C	2:B:1234:LYS:HE2	2.41	0.41
2:B:1259:GLU:O	2:B:1263:THR:HG23	2.20	0.41
2:B:1436:SER:OG	2:B:1437:LEU:N	2.54	0.41
2:B:1449:GLN:OE1	2:B:1449:GLN:N	2.54	0.41
2:B:1463:ARG:NH2	2:B:1465:SER:HA	2.35	0.41
2:B:1489:TYR:HB3	2:B:1504:VAL:HG23	2.02	0.41
2:B:1522:MET:HE3	2:B:1589:LEU:HB3	2.02	0.41
2:E:764:PHE:HA	2:E:767:ILE:HB	2.03	0.41
2:E:933:LEU:HA	2:E:936:ILE:HG22	2.02	0.41
2:E:937:ASN:O	2:E:941:ILE:HG13	2.21	0.41
2:E:1034:ASP:OD1	2:E:1097:HIS:CD2	2.74	0.41
2:E:1090:MET:O	2:E:1094:LEU:HD23	2.20	0.41
2:E:1099:ILE:HD11	2:E:1134:CYS:O	2.21	0.41
2:E:1231:TYR:HB3	2:E:1240:TYR:HB2	2.03	0.41
2:E:1483:TRP:CE2	2:E:1513:SER:HA	2.55	0.41
2:E:1601:THR:HG1	2:E:1626:PHE:HZ	1.69	0.41
3:F:21:ILE:HA	3:F:24:THR:OG1	2.20	0.41
2:B:25:VAL:HB	2:B:56:LYS:O	2.20	0.41
2:B:836:LEU:HG	2:B:840:PHE:CE2	2.53	0.41
2:B:1129:PHE:CZ	2:B:1183:HIS:HB2	2.55	0.41
2:B:1154:LYS:O	2:B:1158:GLU:HG2	2.21	0.41
2:B:1279:VAL:HA	2:B:1280:PRO:HD3	1.93	0.41
2:B:1444:LYS:HD3	2:B:1446:VAL:HG12	2.02	0.41
2:B:1490:THR:N	2:B:1506:GLN:O	2.53	0.41
2:B:1631:GLU:O	2:B:1635:LYS:HG2	2.19	0.41
1:D:575:TRP:HE3	1:D:589:GLY:O	2.04	0.41
1:D:658:ASP:OD1	1:D:661:GLU:HG2	2.20	0.41
2:E:25:VAL:HB	2:E:56:LYS:O	2.20	0.41
2:E:38:LEU:H	2:E:47:GLY:HA3	1.86	0.41
2:E:166:ARG:HH12	2:E:168:ASP:H	1.67	0.41
2:E:1155:LEU:HA	2:E:1158:GLU:HG2	2.02	0.41
2:E:1205:LEU:HD22	2:E:1208:ARG:NH2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1323:GLU:O	2:E:1327:THR:HG23	2.21	0.41
2:E:1362:TYR:HE2	2:E:1459:VAL:HG21	1.85	0.41
2:E:1490:THR:N	2:E:1506:GLN:O	2.53	0.41
2:E:1575:TYR:CE1	2:E:1579:HIS:CE1	3.09	0.41
2:E:1612:THR:H	2:E:1615:LEU:HB2	1.86	0.41
1:A:693:GLU:O	1:A:696:LEU:HG	2.21	0.41
2:B:1:MET:HG3	2:B:4:TRP:HE1	1.84	0.41
2:B:45:TYR:HB2	2:B:64:ILE:HG13	2.02	0.41
2:B:65:HIS:ND1	2:B:65:HIS:O	2.53	0.41
2:B:191:SER:O	2:B:194:ILE:HB	2.21	0.41
2:B:737:LEU:HD12	2:B:737:LEU:HA	1.77	0.41
2:B:764:PHE:HA	2:B:767:ILE:HB	2.03	0.41
2:B:768:ILE:HD11	2:B:827:VAL:HG22	2.02	0.41
2:B:854:ARG:HH11	2:B:858:ASN:HD21	1.68	0.41
2:B:909:ILE:O	2:B:913:LEU:HD12	2.20	0.41
2:B:1109:ILE:HG12	2:B:1128:PHE:CE1	2.56	0.41
2:B:1175:LEU:O	2:B:1179:HIS:CD2	2.74	0.41
2:B:1180:CYS:HB2	2:B:1191:GLU:HG3	2.03	0.41
2:B:1408:MET:HB3	2:B:1410:SER:H	1.85	0.41
3:C:94:ARG:HH12	3:C:112:LEU:HD21	1.86	0.41
2:E:46:ARG:CB	2:E:58:ILE:HG13	2.46	0.41
2:E:89:GLN:O	2:E:92:THR:OG1	2.31	0.41
2:E:167:ASP:OD1	2:E:168:ASP:N	2.52	0.41
2:E:219:ILE:O	2:E:222:TYR:OH	2.21	0.41
2:E:332:ILE:HG12	2:E:337:VAL:HB	2.02	0.41
2:E:344:HIS:N	2:E:401:VAL:O	2.53	0.41
2:E:470:MET:HG2	2:E:496:TYR:HB3	2.03	0.41
2:E:473:HIS:HD1	2:E:478:LYS:C	2.24	0.41
2:E:972:TYR:HA	2:E:975:THR:HB	2.03	0.41
2:E:1091:TRP:CD1	2:E:1127:ILE:HG23	2.55	0.41
2:E:1109:ILE:O	2:E:1112:VAL:HG22	2.21	0.41
3:F:66:ARG:HD3	3:F:66:ARG:H	1.86	0.41
1:A:575:TRP:HE3	1:A:589:GLY:O	2.04	0.41
2:B:127:TRP:O	2:B:131:ILE:HG12	2.20	0.41
2:B:162:ASP:OD1	2:B:162:ASP:N	2.54	0.41
2:B:169:ASN:OD1	2:B:173:LEU:HD13	2.20	0.41
2:B:259:LEU:HD23	2:B:490:TYR:CG	2.56	0.41
2:B:406:LEU:HD12	2:B:413:VAL:HG13	2.03	0.41
2:B:436:ILE:HG23	2:B:711:HIS:NE2	2.36	0.41
2:B:483:ALA:O	2:B:515:VAL:HA	2.21	0.41
2:B:1018:LEU:O	2:B:1022:ASN:ND2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1034:ASP:OD1	2:B:1097:HIS:CD2	2.74	0.41
2:B:1081:LYS:O	2:B:1085:PHE:HD1	2.04	0.41
2:B:1201:LEU:HD23	2:B:1201:LEU:HA	1.92	0.41
2:B:1242:ARG:O	2:B:1246:LYS:HG2	2.20	0.41
2:B:1330:SER:O	2:B:1331:LYS:HD3	2.20	0.41
2:B:1483:TRP:CE2	2:B:1513:SER:HA	2.55	0.41
2:B:1532:CYS:HA	2:B:1535:GLN:HG3	2.03	0.41
3:C:28:PHE:CD2	3:C:29:PRO:HD2	2.56	0.41
3:C:58:THR:HB	3:C:68:ARG:NH1	2.35	0.41
3:C:82:PHE:HD1	3:C:112:LEU:HD11	1.86	0.41
3:C:120:ARG:NH2	3:C:139:TYR:H	2.19	0.41
3:C:124:ASP:O	3:C:127:GLU:HG2	2.20	0.41
1:D:580:SER:HB3	1:D:583:HIS:N	2.36	0.41
2:E:14:VAL:O	2:E:64:ILE:HA	2.21	0.41
2:E:189:VAL:HG13	2:E:193:ARG:CZ	2.50	0.41
2:E:221:THR:HG23	2:E:283:ASP:HA	2.02	0.41
2:E:228:PHE:CZ	2:E:231:PHE:HB2	2.55	0.41
2:E:234:ASN:O	2:E:322:PHE:HZ	2.04	0.41
2:E:248:PRO:HB3	2:E:387:ILE:HG21	2.01	0.41
2:E:259:LEU:HD23	2:E:490:TYR:CG	2.56	0.41
2:E:281:PHE:HE2	2:E:296:LEU:HD11	1.86	0.41
2:E:894:SER:O	2:E:897:PRO:HD2	2.21	0.41
2:E:928:ILE:CA	2:E:932:LEU:HD13	2.48	0.41
2:E:1002:TYR:HE1	2:E:1010:ASN:HA	1.85	0.41
2:E:1019:ARG:O	2:E:1023:GLN:HG2	2.21	0.41
2:E:1132:MET:HE1	2:E:1187:SER:HA	2.02	0.41
2:E:1318:ILE:HD13	2:E:1349:TYR:CE2	2.54	0.41
2:E:1318:ILE:HD13	2:E:1349:TYR:CZ	2.55	0.41
2:E:1330:SER:O	2:E:1331:LYS:HD3	2.21	0.41
2:E:1408:MET:HB3	2:E:1410:SER:H	1.85	0.41
2:E:1411:THR:HB	3:F:28:PHE:CE2	2.55	0.41
2:E:1461:GLN:HA	2:E:1489:TYR:O	2.21	0.41
2:E:1482:MET:C	2:E:1517:ASN:HD22	2.24	0.41
2:E:1566:TYR:CE1	2:E:1570:PHE:HE2	2.39	0.41
1:A:556:LEU:HD11	1:A:668:GLY:C	2.41	0.41
1:A:667:ASP:HB3	1:A:677:MET:SD	2.60	0.41
2:B:105:LEU:HB3	2:B:114:PHE:HB2	2.02	0.41
2:B:853:VAL:HG23	2:B:854:ARG:H	1.85	0.41
2:B:1531:ASN:O	2:B:1535:GLN:HG3	2.20	0.41
1:D:584:LYS:NZ	2:E:1405:ALA:HB2	2.34	0.41
1:D:646:TYR:CE1	1:D:652:LEU:HG	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:147:LYS:O	2:E:151:LYS:HD3	2.21	0.41
2:E:169:ASN:OD1	2:E:173:LEU:HD13	2.20	0.41
2:E:728:LEU:HD23	2:E:730:TYR:CE2	2.56	0.41
2:E:785:ASP:N	2:E:785:ASP:OD1	2.53	0.41
2:E:1072:ILE:HA	2:E:1076:TYR:HD2	1.86	0.41
2:E:1238:ASP:HA	2:E:1241:ILE:HD12	2.03	0.41
2:E:1361:GLU:OE1	2:E:1389:GLU:N	2.54	0.41
2:E:1380:ILE:HB	2:E:1504:VAL:HG12	2.03	0.41
2:E:1449:GLN:OE1	2:E:1449:GLN:N	2.54	0.41
1:A:580:SER:HB3	1:A:583:HIS:N	2.36	0.40
2:B:38:LEU:H	2:B:47:GLY:HA3	1.86	0.40
2:B:328:ASP:OD1	2:B:328:ASP:N	2.54	0.40
2:B:332:ILE:HG12	2:B:337:VAL:HB	2.02	0.40
2:B:730:TYR:CG	2:B:731:VAL:N	2.90	0.40
2:B:922:ALA:O	2:B:925:ILE:HB	2.21	0.40
2:B:1002:TYR:HE1	2:B:1010:ASN:HA	1.85	0.40
2:B:1109:ILE:O	2:B:1112:VAL:HG22	2.21	0.40
2:B:1168:TYR:HA	2:B:1171:LEU:HD12	2.03	0.40
2:B:1217:LYS:HB3	2:B:1221:MET:HE1	2.03	0.40
2:B:1231:TYR:HB3	2:B:1240:TYR:HB2	2.03	0.40
2:B:1283:LEU:HB3	2:B:1288:TYR:CE1	2.56	0.40
2:B:1369:GLY:HA2	2:B:1418:ILE:HG22	2.02	0.40
1:D:679:SER:HB2	1:D:682:THR:OG1	2.21	0.40
2:E:95:LEU:HD11	2:E:124:LEU:HD11	2.04	0.40
2:E:95:LEU:CA	2:E:98:TRP:HD1	2.31	0.40
2:E:157:ARG:NH2	2:E:198:ILE:HG12	2.36	0.40
2:E:406:LEU:HD12	2:E:413:VAL:HG13	2.03	0.40
2:E:964:MET:HG2	2:E:969:TYR:CZ	2.55	0.40
2:E:1110:LEU:HA	2:E:1128:PHE:HZ	1.85	0.40
2:E:1168:TYR:HA	2:E:1171:LEU:HD12	2.03	0.40
2:E:1374:SER:O	2:E:1377:ARG:HG2	2.21	0.40
2:E:1463:ARG:NH1	2:E:1465:SER:OG	2.54	0.40
2:E:1632:LYS:HD2	2:E:1632:LYS:HA	1.80	0.40
3:F:120:ARG:NH2	3:F:139:TYR:H	2.19	0.40
1:A:714:PRO:CG	2:B:60:PRO:HB3	2.51	0.40
2:B:14:VAL:O	2:B:64:ILE:HA	2.21	0.40
2:B:680:MET:O	2:B:684:SER:HB3	2.21	0.40
2:B:772:VAL:O	2:B:776:ARG:HG3	2.21	0.40
2:B:894:SER:O	2:B:897:PRO:HD2	2.21	0.40
2:B:932:LEU:N	2:B:935:ARG:HE	2.19	0.40
2:B:1579:HIS:O	2:B:1583:GLN:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:328:ASP:OD1	2:E:328:ASP:N	2.55	0.40
2:E:455:PHE:CE2	2:E:466:VAL:HG11	2.56	0.40
2:E:570:VAL:HA	2:E:592:LYS:NZ	2.36	0.40
2:E:632:THR:HG21	2:E:637:LEU:HD23	2.02	0.40
2:E:730:TYR:CG	2:E:731:VAL:N	2.90	0.40
2:E:772:VAL:O	2:E:776:ARG:HG3	2.21	0.40
2:E:922:ALA:O	2:E:925:ILE:HB	2.21	0.40
2:E:934:ARG:NH1	2:E:934:ARG:O	2.55	0.40
2:E:1175:LEU:O	2:E:1179:HIS:CD2	2.74	0.40
2:E:1233:GLU:C	2:E:1234:LYS:HE2	2.41	0.40
2:E:1283:LEU:HB3	2:E:1288:TYR:CE1	2.56	0.40
2:E:1290:VAL:HG13	2:E:1291:TYR:H	1.86	0.40
2:E:1369:GLY:CA	2:E:1418:ILE:HG22	2.51	0.40
2:E:1431:VAL:HG12	2:E:1464:TYR:HB2	2.02	0.40
2:E:1436:SER:OG	2:E:1437:LEU:N	2.54	0.40
3:F:86:SER:O	3:F:89:SER:OG	2.24	0.40
2:B:88:VAL:HB	2:B:128:ARG:HH22	1.84	0.40
2:B:222:TYR:HB3	2:B:405:LEU:HD11	2.04	0.40
2:B:455:PHE:CE2	2:B:466:VAL:HG11	2.56	0.40
2:B:470:MET:HG2	2:B:496:TYR:HB3	2.03	0.40
2:B:526:HIS:NE2	2:B:586:LEU:HD11	2.36	0.40
2:B:910:LEU:HD22	2:B:963:GLN:OE1	2.20	0.40
2:B:964:MET:HG2	2:B:969:TYR:CZ	2.55	0.40
2:B:969:TYR:HE2	2:B:1019:ARG:HH21	1.68	0.40
2:B:993:PHE:HB3	2:B:1049:LEU:HD11	2.03	0.40
2:B:1072:ILE:HA	2:B:1076:TYR:HD2	1.86	0.40
2:B:1080:ARG:HH21	2:B:1117:GLU:HG2	1.86	0.40
2:B:1155:LEU:HA	2:B:1158:GLU:HG2	2.02	0.40
2:B:1179:HIS:O	2:B:1182:LYS:HB2	2.22	0.40
2:B:1231:TYR:HB2	2:B:1240:TYR:HD1	1.86	0.40
2:B:1482:MET:C	2:B:1517:ASN:HD22	2.24	0.40
2:B:1575:TYR:CE1	2:B:1579:HIS:CE1	3.09	0.40
3:C:3:ALA:HA	3:C:52:ASN:HB2	2.03	0.40
1:D:539:LYS:NZ	1:D:540:ILE:HD11	2.37	0.40
1:D:580:SER:CB	1:D:585:VAL:H	2.34	0.40
1:D:666:THR:HG23	1:D:678:MET:SD	2.60	0.40
2:E:13:GLY:O	2:E:34:THR:HA	2.21	0.40
2:E:345:PHE:HB2	2:E:400:TRP:CZ3	2.56	0.40
2:E:408:GLY:HA3	2:E:412:GLN:HB2	2.04	0.40
2:E:802:MET:HE3	2:E:843:PHE:CE1	2.57	0.40
2:E:821:PRO:CG	2:E:863:ILE:HG13	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:874:CYS:O	2:E:877:VAL:HG12	2.22	0.40
2:E:899:HIS:HD2	2:E:943:MET:HG2	1.81	0.40
2:E:929:MET:HB2	2:E:964:MET:HE3	2.03	0.40
2:E:929:MET:HE1	2:E:972:TYR:HB3	2.03	0.40
2:E:1008:VAL:HG12	2:E:1009:MET:HE2	2.03	0.40
2:E:1011:MET:HA	2:E:1014:ASN:ND2	2.37	0.40
2:E:1022:ASN:OD1	2:E:1086:ARG:NH1	2.53	0.40
2:E:1059:LEU:HA	2:E:1059:LEU:HD23	1.77	0.40
2:E:1180:CYS:HB2	2:E:1191:GLU:HG3	2.03	0.40
2:E:1367:TYR:C	2:E:1368:TYR:HD1	2.24	0.40
3:F:3:ALA:HA	3:F:52:ASN:HB2	2.03	0.40
2:B:10:GLN:HB2	2:B:37:ILE:HD12	2.03	0.40
2:B:928:ILE:CA	2:B:932:LEU:HD13	2.48	0.40
2:B:950:ILE:O	2:B:954:VAL:HG23	2.21	0.40
2:B:997:ILE:HG13	2:B:998:GLY:N	2.36	0.40
2:B:1245:TYR:HA	2:B:1248:ARG:HG3	2.03	0.40
2:B:1360:PRO:HA	2:B:1387:GLU:HA	2.02	0.40
2:B:1612:THR:H	2:B:1615:LEU:HB2	1.86	0.40
3:C:43:ASN:OD1	3:C:50:PRO:HB2	2.21	0.40
2:E:186:ALA:O	2:E:189:VAL:HB	2.22	0.40
2:E:223:GLY:HA2	2:E:281:PHE:O	2.22	0.40
2:E:778:TYR:O	2:E:780:GLN:N	2.53	0.40
2:E:932:LEU:N	2:E:935:ARG:HE	2.19	0.40
2:E:950:ILE:O	2:E:954:VAL:HG23	2.21	0.40
2:E:997:ILE:HG13	2:E:998:GLY:N	2.36	0.40
2:E:1091:TRP:CZ2	2:E:1131:MET:HB3	2.56	0.40
2:E:1125:ILE:HG12	2:E:1172:LEU:HD23	2.04	0.40
2:E:1238:ASP:HB3	2:E:1281:HIS:HB3	2.04	0.40
2:E:1512:ILE:HG22	2:E:1517:ASN:HB2	2.03	0.40
3:F:43:ASN:OD1	3:F:50:PRO:HB2	2.21	0.40
3:F:82:PHE:HD1	3:F:112:LEU:HD11	1.86	0.40
2:B:103:ARG:NH1	2:B:104:LYS:HE3	2.30	0.40
2:B:345:PHE:HB2	2:B:400:TRP:CZ3	2.56	0.40
2:B:422:ASP:N	2:B:422:ASP:OD1	2.50	0.40
2:B:824:ILE:HD11	2:B:863:ILE:HA	2.04	0.40
2:B:1044:ASN:HA	2:B:1101:PHE:CZ	2.55	0.40
2:B:1238:ASP:HA	2:B:1241:ILE:HD12	2.03	0.40
1:D:530:SER:HB3	1:D:531:ARG:NH2	2.37	0.40
1:D:620:LYS:HE2	1:D:638:LEU:HD11	2.02	0.40
2:E:436:ILE:HG23	2:E:711:HIS:NE2	2.36	0.40
2:E:824:ILE:HD11	2:E:863:ILE:HA	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:828:LYS:HE2	2:E:870:ARG:NH2	2.37	0.40
2:E:886:LEU:HD13	2:E:932:LEU:CD2	2.51	0.40
2:E:993:PHE:HB3	2:E:1049:LEU:HD11	2.03	0.40
2:E:1095:GLY:HA3	2:E:1096:PRO:HD3	1.95	0.40
3:F:28:PHE:CD2	3:F:29:PRO:HD2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	196/733 (27%)	170 (87%)	26 (13%)	0	100	100
1	D	196/733 (27%)	170 (87%)	26 (13%)	0	100	100
2	B	1640/1648 (100%)	1476 (90%)	164 (10%)	0	100	100
2	E	1640/1648 (100%)	1476 (90%)	164 (10%)	0	100	100
3	C	175/184 (95%)	160 (91%)	15 (9%)	0	100	100
3	F	175/184 (95%)	160 (91%)	15 (9%)	0	100	100
All	All	4022/5130 (78%)	3612 (90%)	410 (10%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	183/664 (28%)	182 (100%)	1 (0%)	88	93
1	D	183/664 (28%)	182 (100%)	1 (0%)	88	93
2	B	1495/1497 (100%)	1485 (99%)	10 (1%)	84	90
2	E	1495/1497 (100%)	1484 (99%)	11 (1%)	84	90
3	C	153/157 (98%)	151 (99%)	2 (1%)	69	82
3	F	153/157 (98%)	151 (99%)	2 (1%)	69	82
All	All	3662/4636 (79%)	3635 (99%)	27 (1%)	84	90

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	715	LYS
2	B	128	ARG
2	B	227	ASN
2	B	415	LYS
2	B	478	LYS
2	B	856	LYS
2	B	935	ARG
2	B	1252	ARG
2	B	1463	ARG
2	B	1540	ARG
2	B	1605	ARG
3	C	66	ARG
3	C	123	LYS
1	D	715	LYS
2	E	128	ARG
2	E	227	ASN
2	E	415	LYS
2	E	478	LYS
2	E	769	GLN
2	E	856	LYS
2	E	935	ARG
2	E	1252	ARG
2	E	1463	ARG
2	E	1540	ARG
2	E	1605	ARG
3	F	66	ARG
3	F	123	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	596	GLN
2	B	30	GLN
2	B	156	ASN
2	B	187	HIS
2	B	227	ASN
2	B	419	HIS
2	B	526	HIS
2	B	649	ASN
2	B	653	ASN
2	B	670	GLN
2	B	723	HIS
2	B	769	GLN
2	B	858	ASN
2	B	889	GLN
2	B	895	ASN
2	B	908	ASN
2	B	1014	ASN
2	B	1041	GLN
2	B	1044	ASN
2	B	1048	HIS
2	B	1256	ASN
2	B	1424	GLN
2	B	1517	ASN
2	B	1579	HIS
3	C	43	ASN
1	D	596	GLN
2	E	30	GLN
2	E	156	ASN
2	E	187	HIS
2	E	227	ASN
2	E	419	HIS
2	E	526	HIS
2	E	649	ASN
2	E	653	ASN
2	E	670	GLN
2	E	723	HIS
2	E	858	ASN
2	E	889	GLN
2	E	895	ASN
2	E	1014	ASN
2	E	1041	GLN
2	E	1044	ASN
2	E	1048	HIS

Continued on next page...

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Mol	Chain	Res	Type
2	E	1256	ASN
2	E	1424	GLN
2	E	1517	ASN
2	E	1579	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

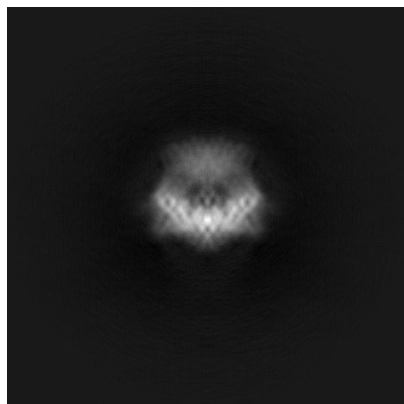
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60150. These allow visual inspection of the internal detail of the map and identification of artifacts.

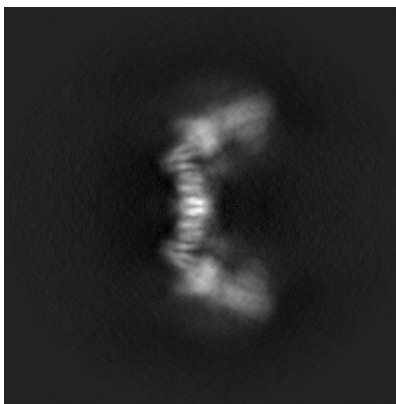
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

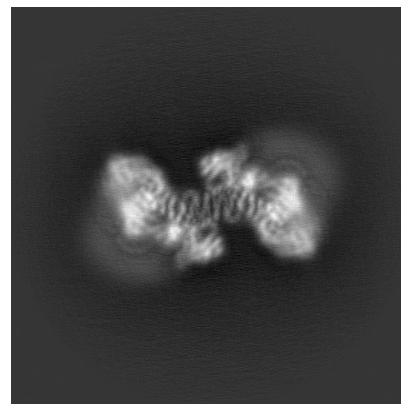
6.1.1 Primary map



X

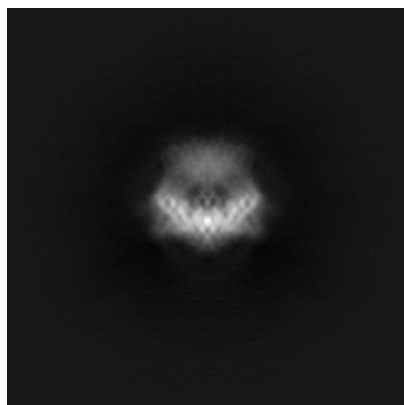


Y

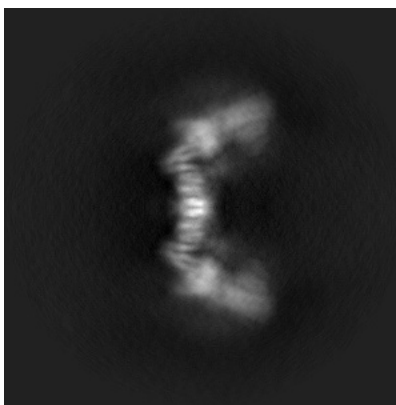


Z

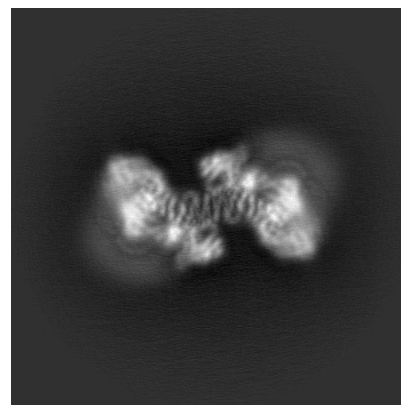
6.1.2 Raw map



X



Y

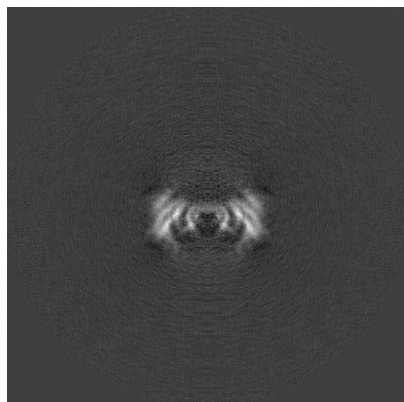


Z

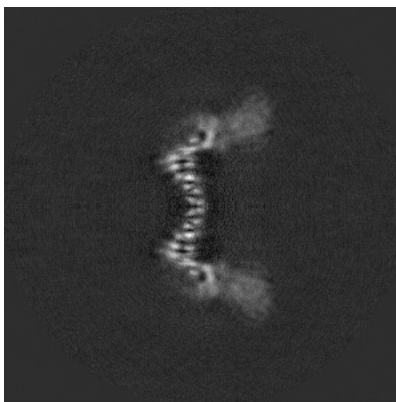
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

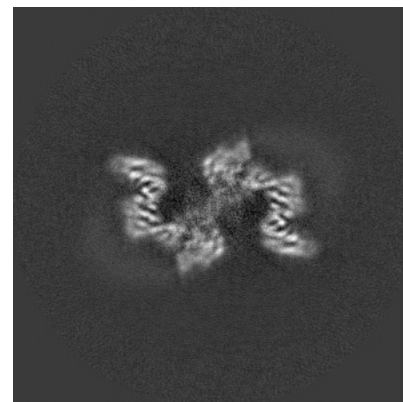
6.2.1 Primary map



X Index: 170

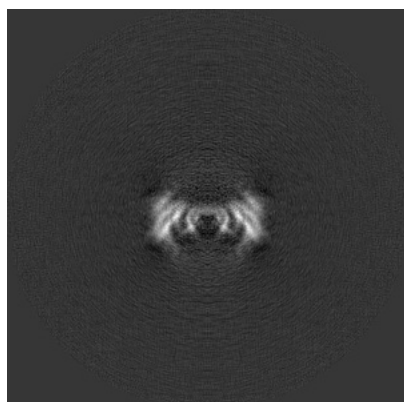


Y Index: 170

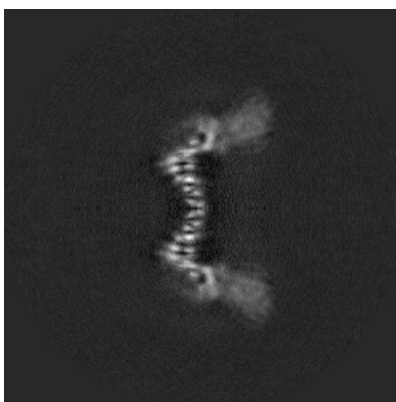


Z Index: 170

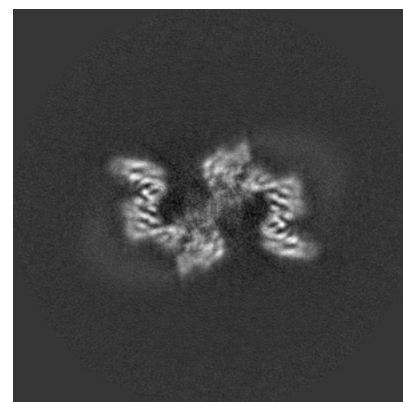
6.2.2 Raw map



X Index: 170



Y Index: 170

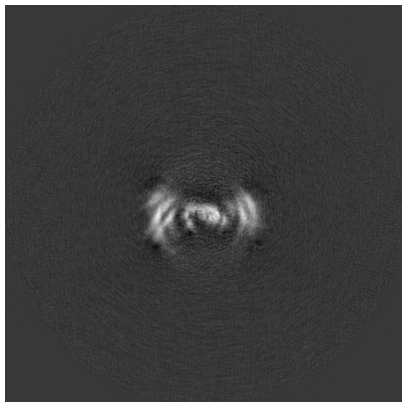


Z Index: 170

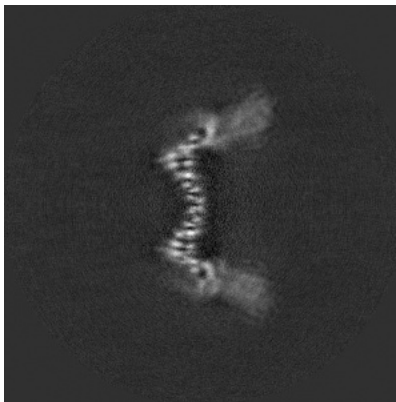
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

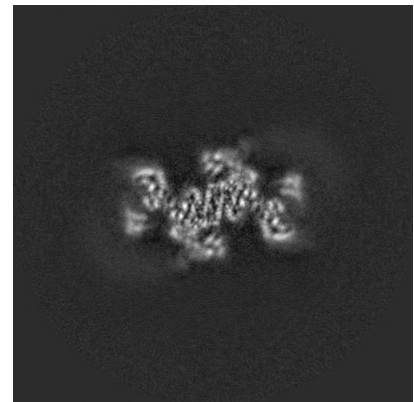
6.3.1 Primary map



X Index: 166

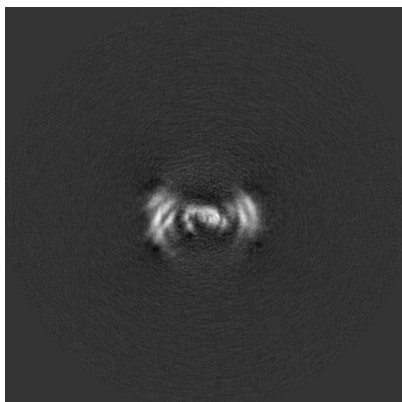


Y Index: 169

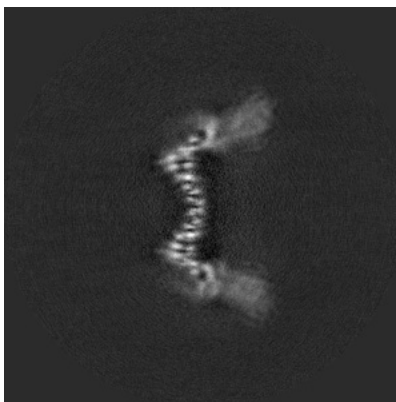


Z Index: 159

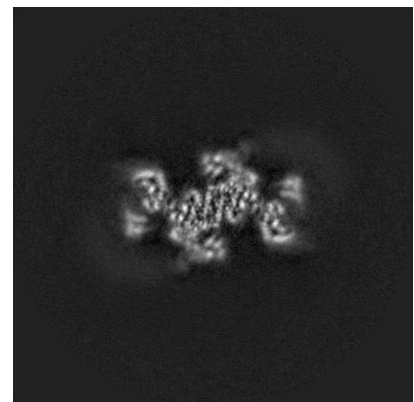
6.3.2 Raw map



X Index: 166



Y Index: 169

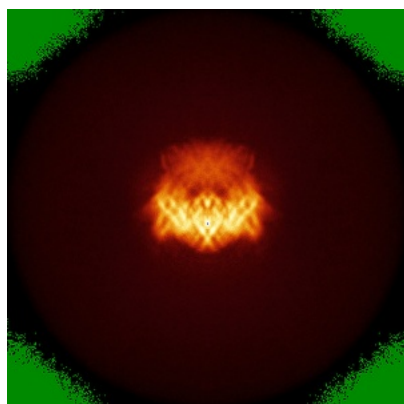


Z Index: 159

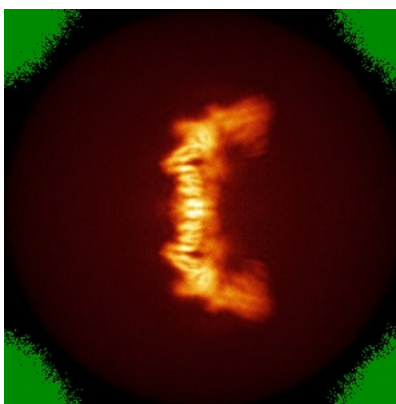
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

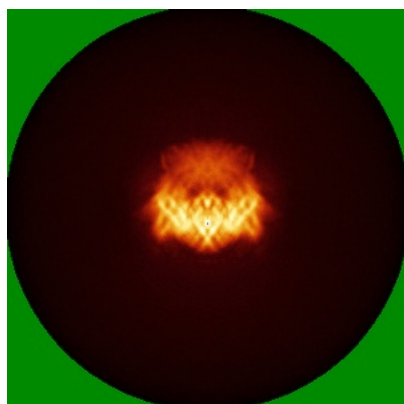


Y

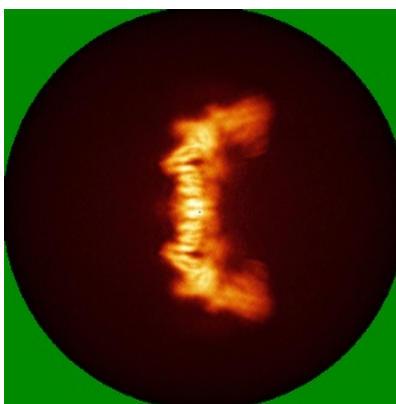


Z

6.4.2 Raw map



X



Y

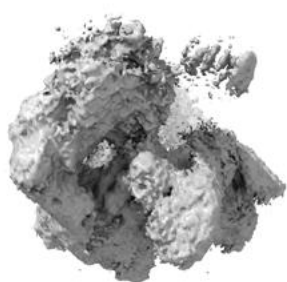


Z

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



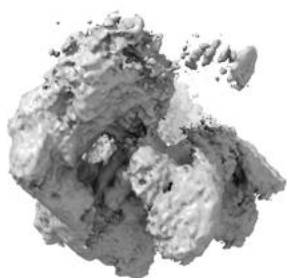
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. 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.

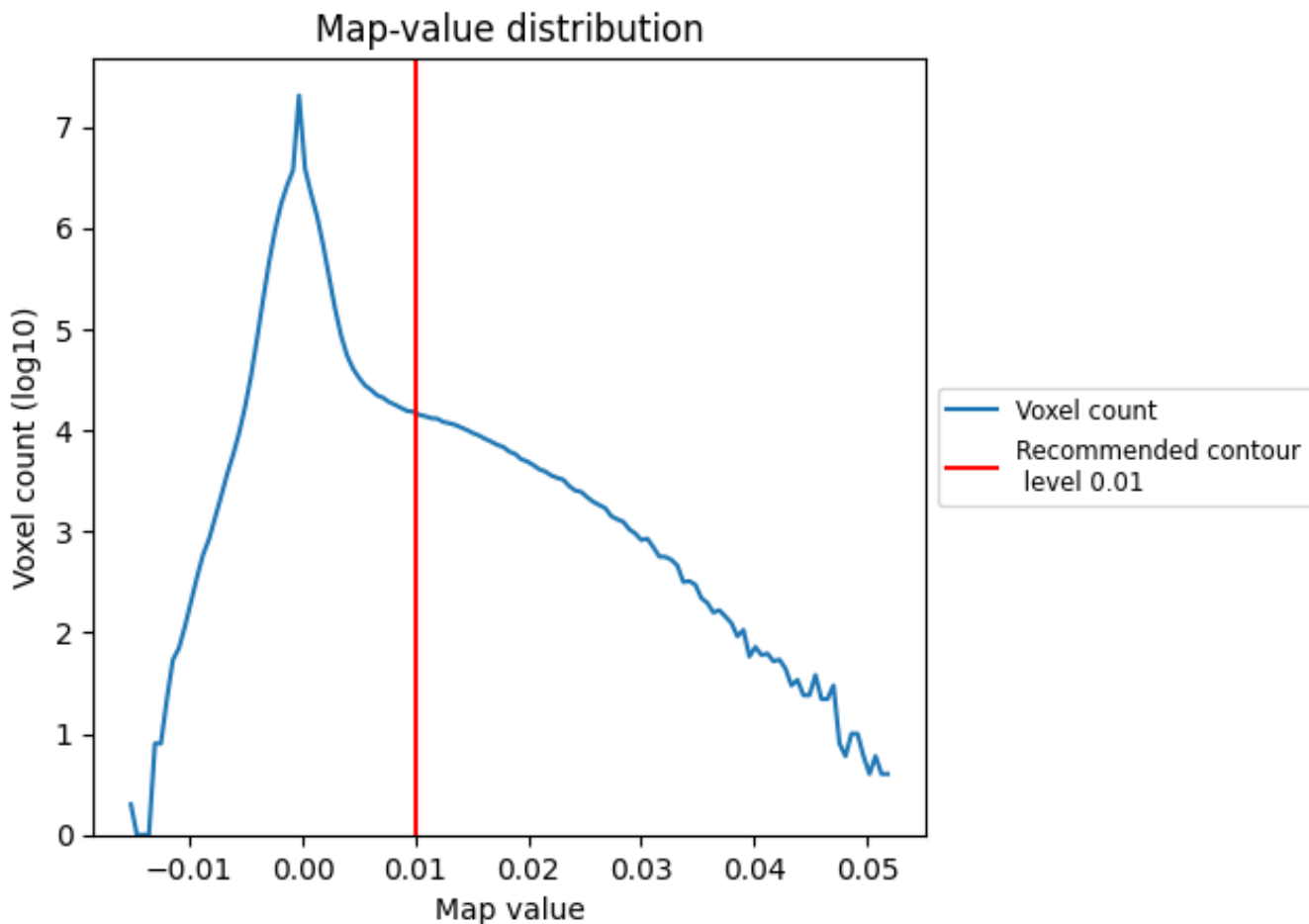
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

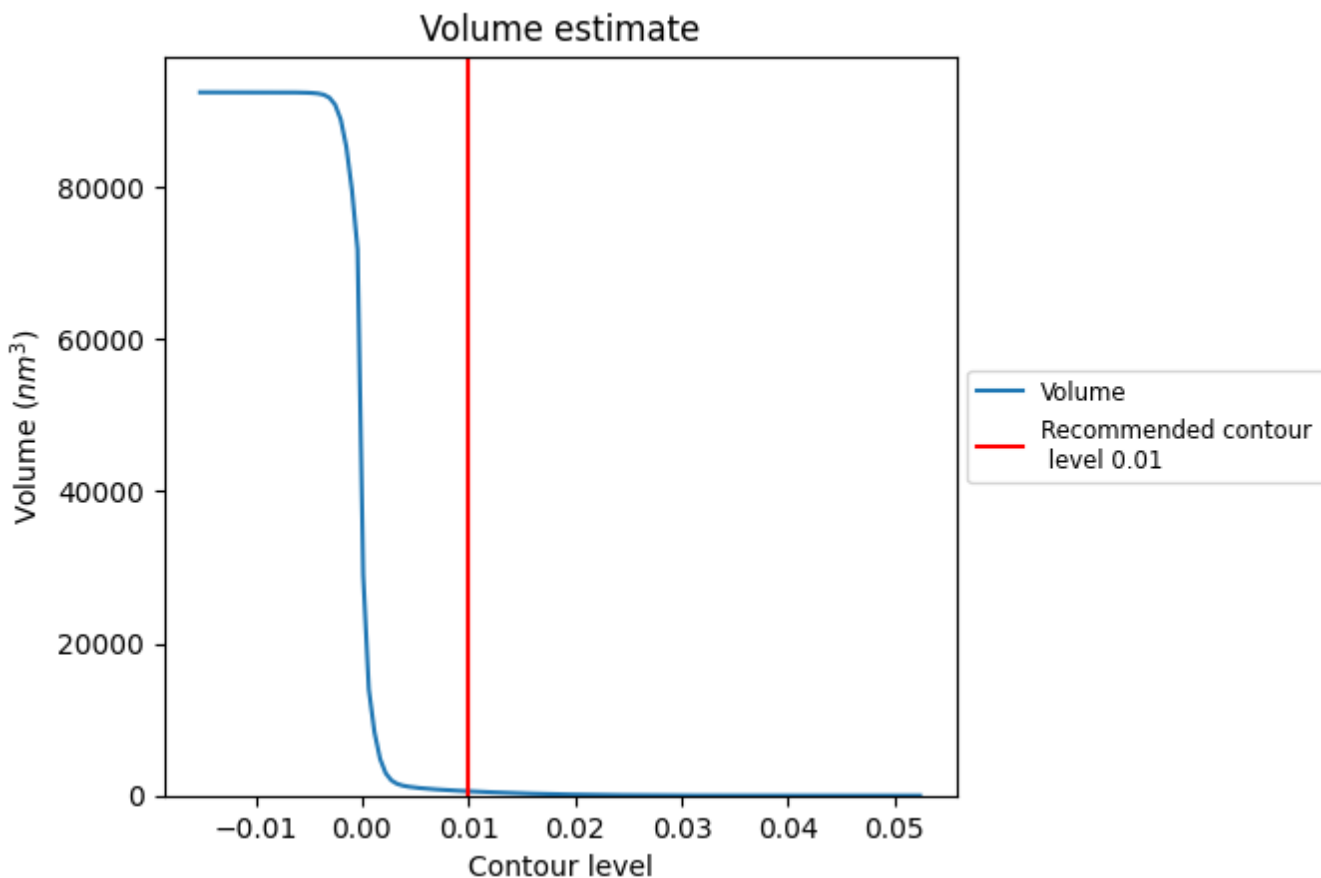
This section contains the results of statistical analysis of the map.

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.

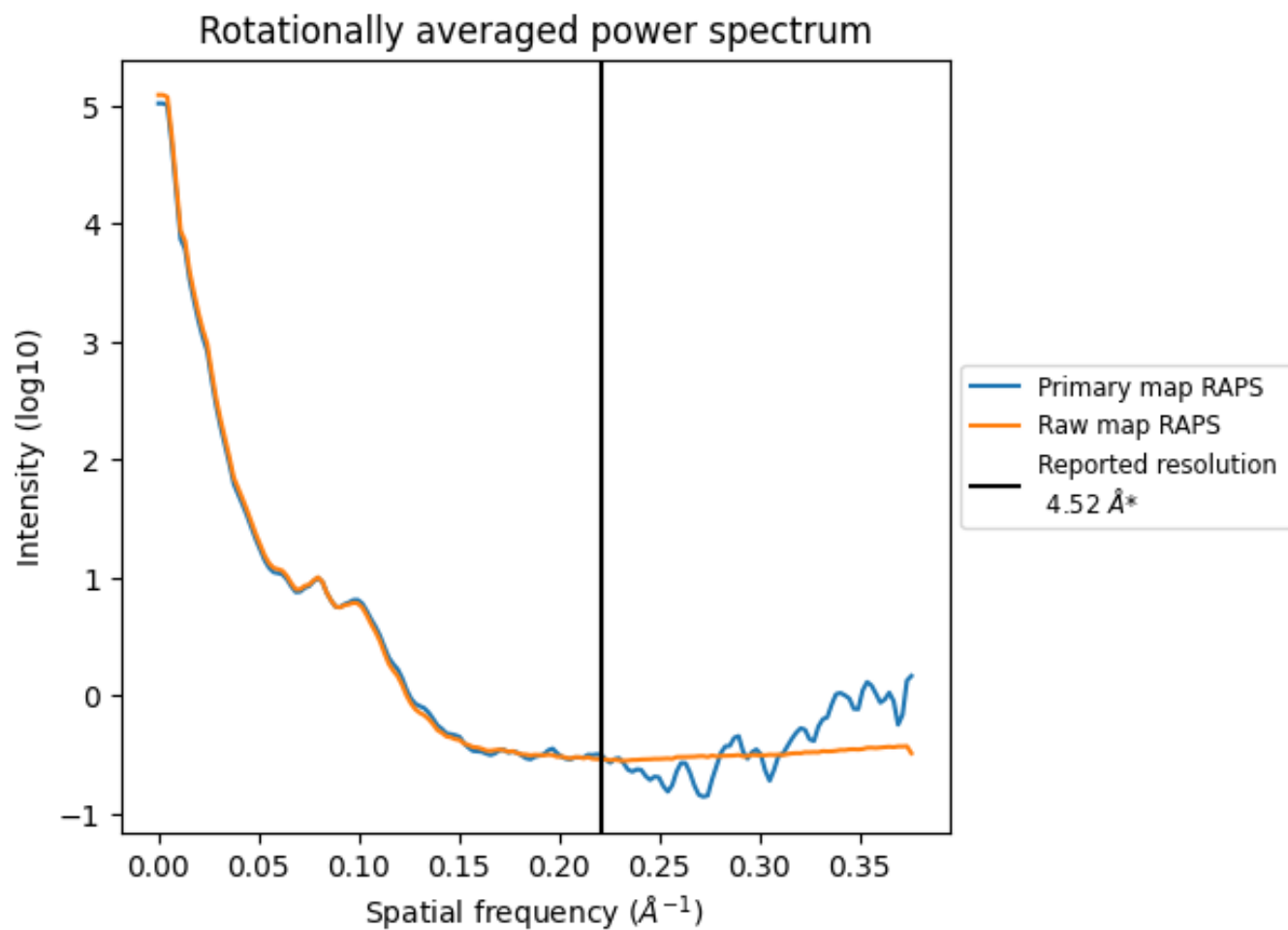
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 568 nm^3 ; this corresponds to an approximate mass of 513 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 i

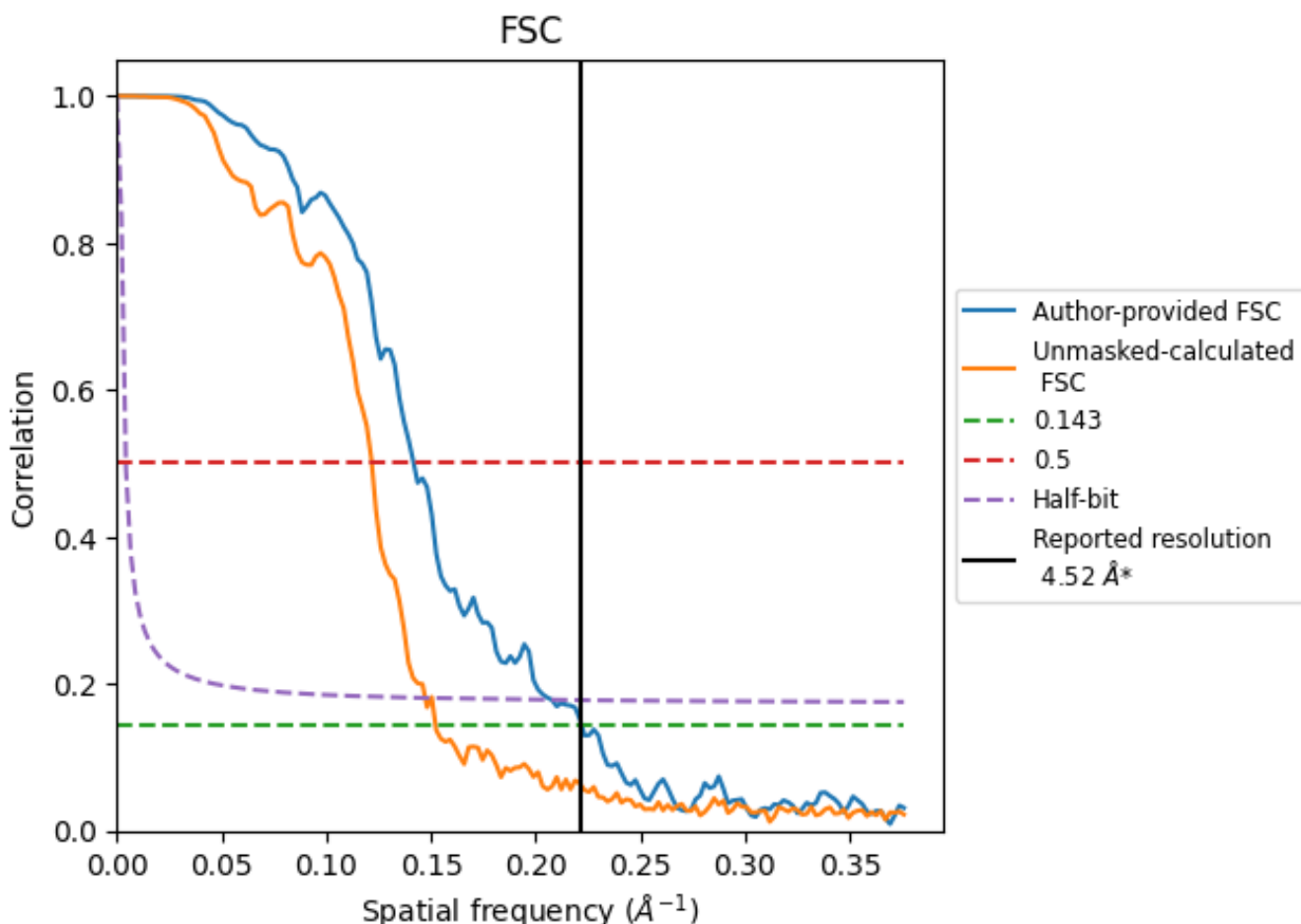


*Reported resolution corresponds to spatial frequency of 0.221 Å⁻¹

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 0.221 \AA^{-1}

8.2 Resolution estimates [i](#)

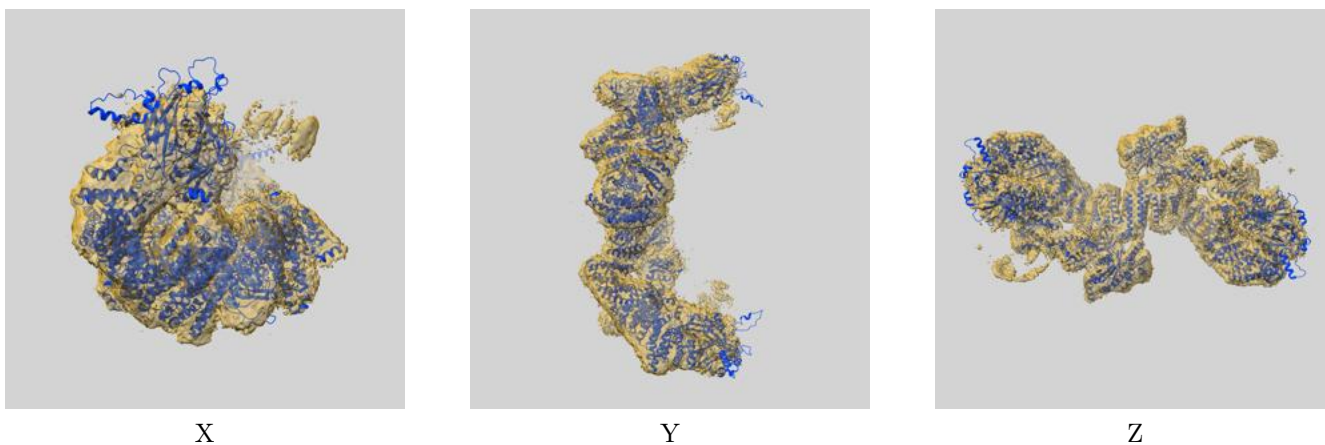
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.52	-	-
Author-provided FSC curve	4.50	7.05	4.81
Unmasked-calculated*	6.57	8.21	6.79

*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 6.57 differs from the reported value 4.52 by more than 10 %

9 Map-model fit [i](#)

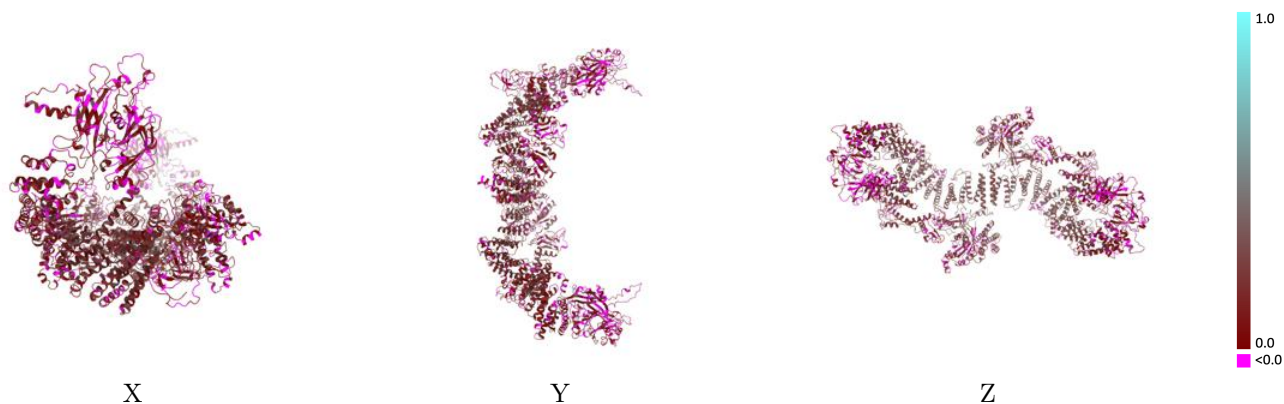
This section contains information regarding the fit between EMDB map EMD-60150 and PDB model 8ZJM. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



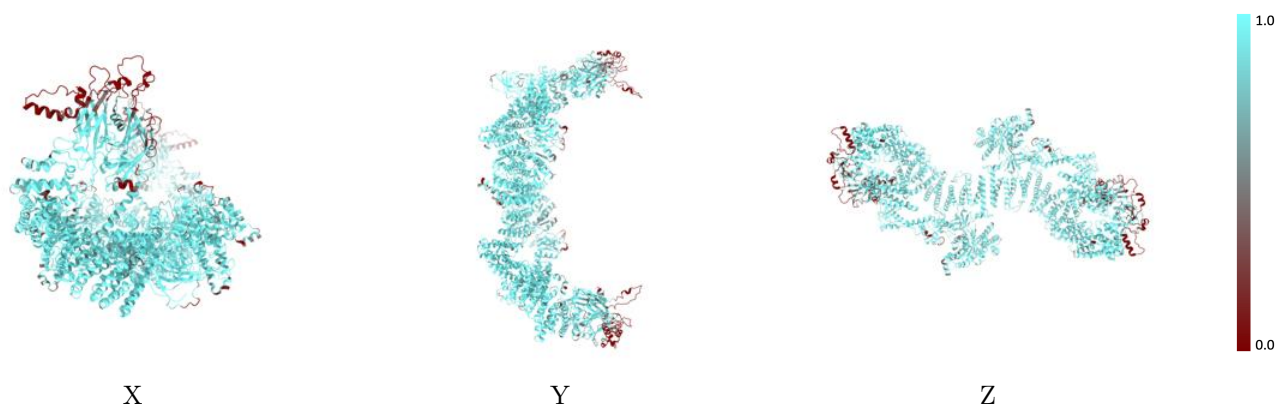
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



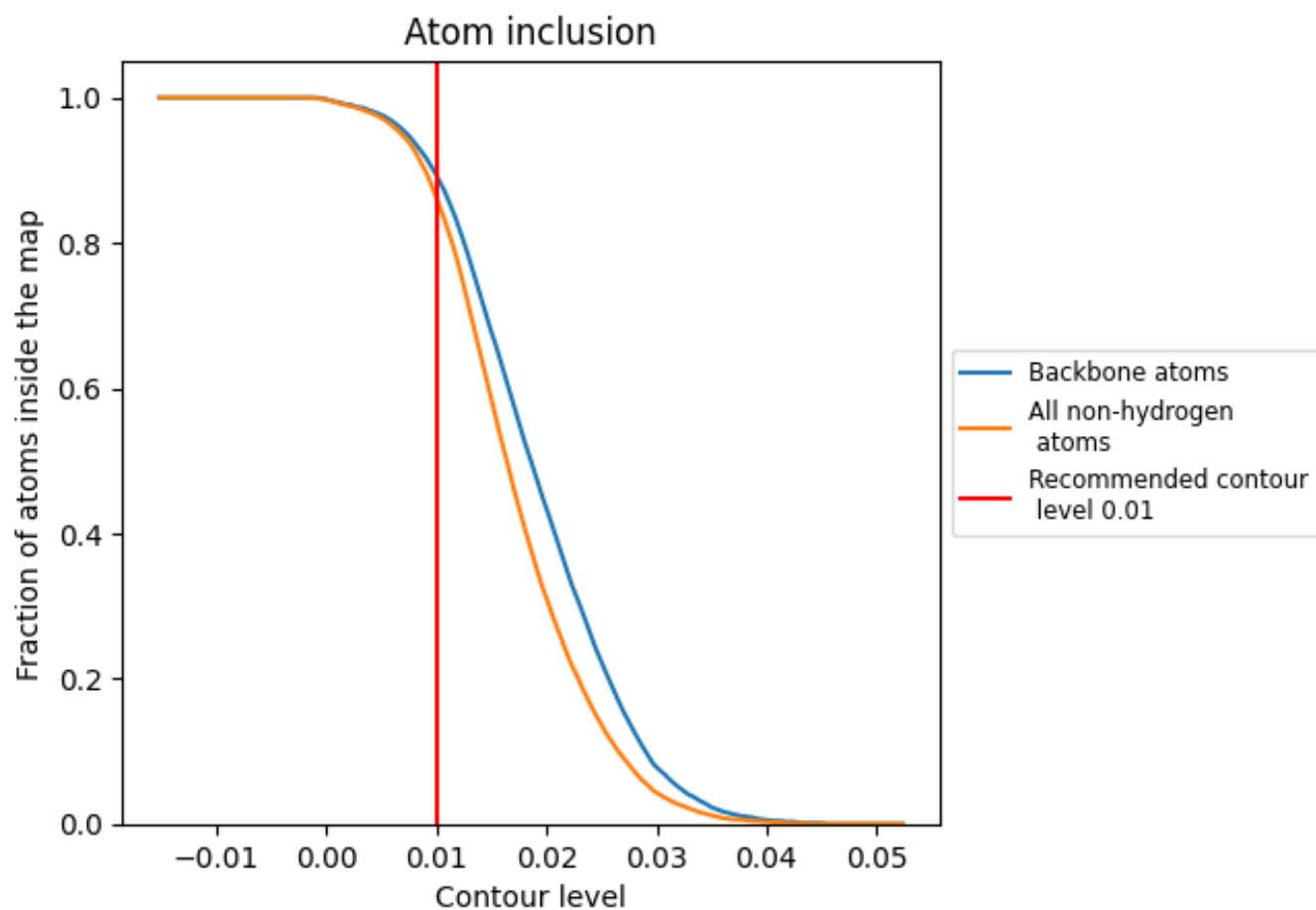
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).















9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 86% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8620	 0.1420
A	 0.8650	 0.1090
B	 0.8590	 0.1490
C	 0.8680	 0.1320
D	 0.8770	 0.1070
E	 0.8600	 0.1450
F	 0.8720	 0.1300

