



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:37 AM UTC

PDB ID : 1Y1V / pdb_00001y1v
Title : Refined RNA Polymerase II-TFIIS complex
Authors : Kettenberger, H.; Armache, K.-J.; Cramer, P.
Deposited on : 2004-11-19
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

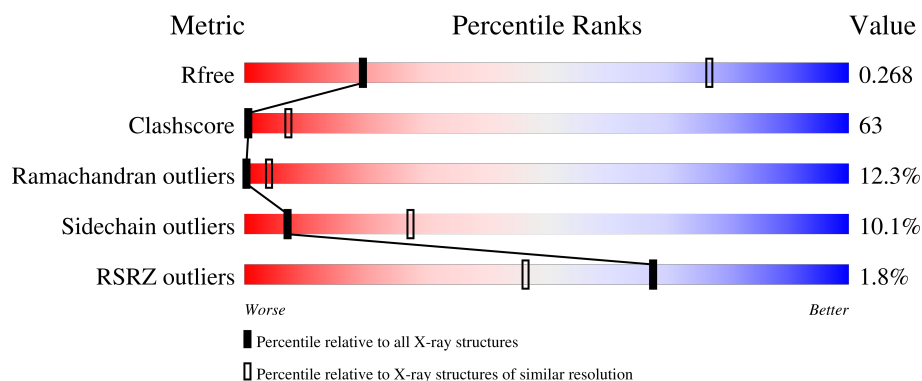
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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

Mol	Chain	Length	Quality of chain
1	A	1733	
2	B	1224	
3	C	318	
4	D	221	
5	E	215	

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Mol	Chain	Length	Quality of chain
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	S	179	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 31803 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase II largest subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1426	Total	C	N	O	S	0	0	0
			11214	7069	1959	2124	62			

- Molecule 2 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1112	Total	C	N	O	S	58	0	0
			8837	5594	1548	1640	55			

- Molecule 3 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 4 is a protein called DNA-directed RNA polymerase II 32 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	177	Total	C	N	O	S	0	0	0
			1356	840	241	273	2			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

- Molecule 7 is a protein called DNA-directed RNA polymerase II 19 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

- Molecule 10 is a protein called DNA-directed RNA polymerases I/II/III subunit 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 11 is a protein called DNA-directed RNA polymerase II 13.6 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			364	224	72	64	4			

- Molecule 13 is a protein called Transcription elongation factor S-II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	S	174	Total	C	N	O	S	0	0	104
			666	454	99	108	5			

- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	2	Total	Zn	0	0
			2	2		
14	B	1	Total	Zn	0	0
			1	1		
14	C	1	Total	Zn	0	0
			1	1		
14	I	2	Total	Zn	0	0
			2	2		
14	J	1	Total	Zn	0	0
			1	1		
14	L	1	Total	Zn	0	0
			1	1		
14	S	1	Total	Zn	0	0
			1	1		

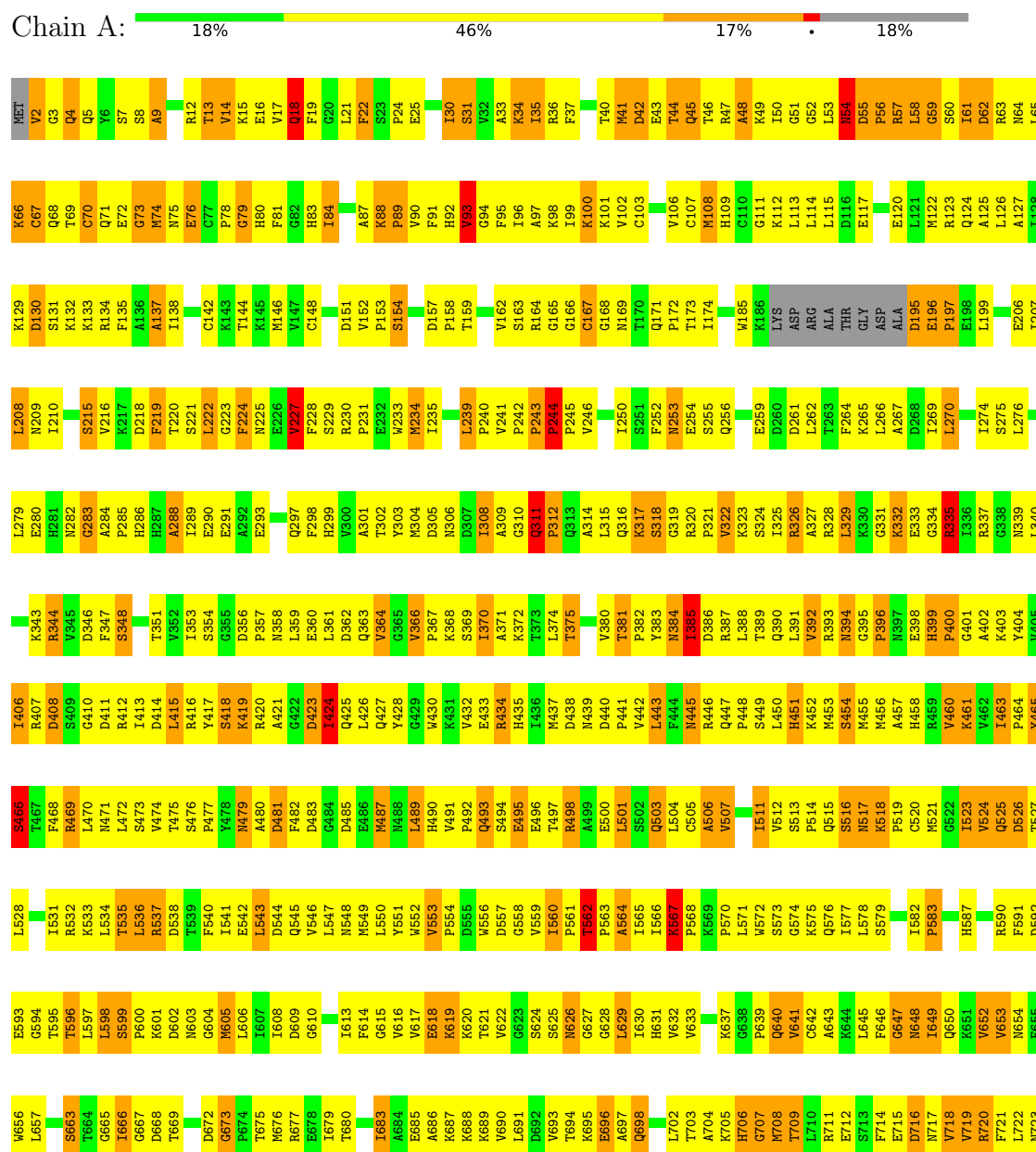
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	S	1	Total	Mg	0	0
			1	1		

3 Residue-property plots

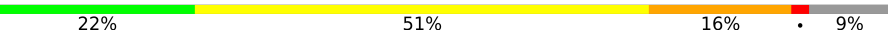
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: DNA-directed RNA polymerase II largest subunit

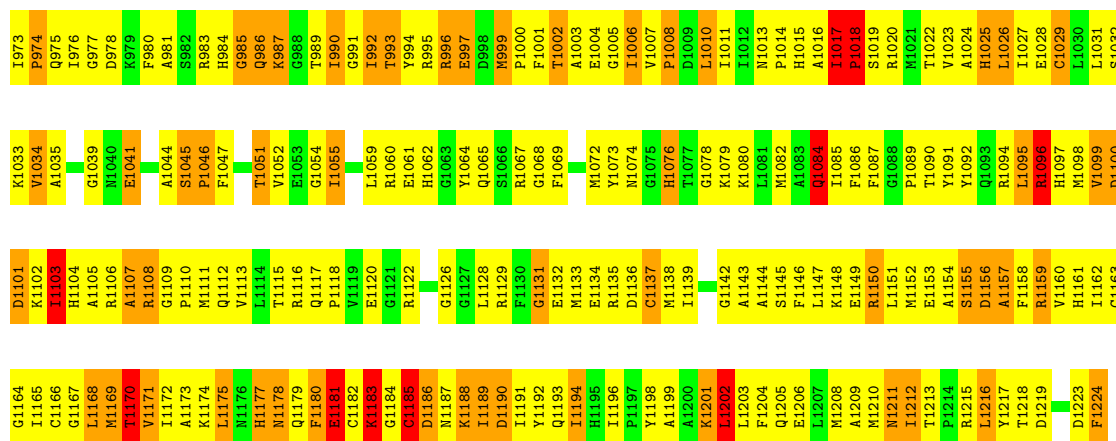




● Molecule 2: DNA-directed RNA polymerase II 140 kDa polypeptide

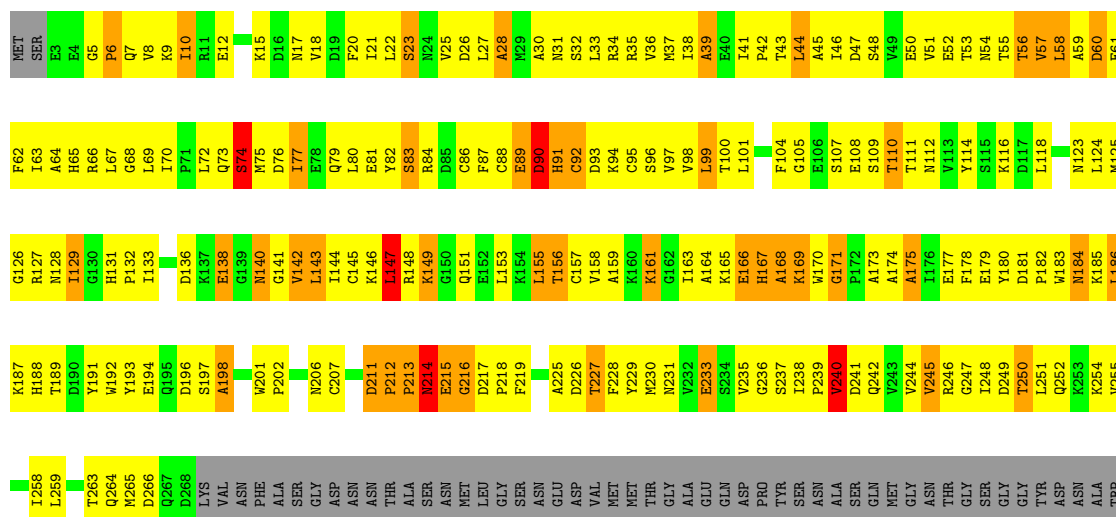
Chain B: 

MET	SER	LEU	LEU	ALA	ASN	SER	GLY	LEU	D20	E21	S22	A23	P24	I25	T26	A27	E28	D29	S30	S31	V31	I34	S35	A36	F37	F38	R39	E40	K41	G42	L43	V44	S45	Q46	Q47	L48	D49	S50	F51	N52	Q53	F54	V55	D56	Y57	T58	L59	Q60	D61																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
162	163	C64	E65	D66	S67	ASN	G68	T68	L69	I70	LEU	GLN	GLU	ALA	ASP	PRO	THR	THR	GLY	THR	GLU	SER	ASP	Y94	Y96	V97	T98	K99	P100	M101	V102	G103	V108	T109	L112	Y113	P114	Q115	E116	A117	R118	L119	R120	N121	L122	T123	Y124	S125	L126	G127																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
L128	F129	V130	K131	V132	K133	K134	ARG	THR	THR	TYR	GLU	ALA	ILE	ASP	VAL	PRO	GLY	ARG	GLU	GLU	LEU	LYS	ASP	ASP	GLU	GLY	V165	F166	I167	G168	R169	P231	A230	P233	L234	M173	L174	H236	V237	A238	E239	N240	C178	Y180	L181	N182	S187	L188	L189																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
Y190	K191	L192	K193	E194	G195	P196	F197	D198	M199	Q200	G201	Y202	F203	I204	I205	N206	G207	S208	E209	K210	V211	L212	L213	Q215	E216	R217	L218	A219	G220	N221	L222	Q223	Q224	V225	F226	K227	K228	A229	L230	P231	S232	P233	L234	S235	H236	V237	A238	E239	N240	C178	Y180	L181	N182	S187	L188	L189																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
L254	Q255	L256	K257	L258	Y259	G260	E261	S262	S263	T264	F265	I266	I267	I268	I269	K270	A271	L272	L273	P274	S275	I276	K277	Q278	D279	L280	P281	I282	V283	L284	I285	F286	R287	A288	L289	L290	L291	L292	L293	D294	G295	E296	L297	L298	E299	H300	Y303	W308	Q309	K310	L311	E312	M313	L314	M315	M316	M317	M318	M319	M320	M321	M322	M323	M324	M325	M326	M327	M328	M329	M330	M331	M332	M333	M334	M335	M336	M337	M338	M339	M340	M341	M342	M343	M344	M345	M346	M347	M348	M349	M350	M351	M352	M353	M354	M355	M356	M357	M358	M359	M360	M361	M362	M363	M364	M365	M366	M367	M368	M369	M370	M371	M372	M373	M374	M375	M376	M377	M378	M379	M380	M381	M382	M383	M384	M385	M386	M387	M388	M389	M390	M391	M392	M393	M394	M395	M396	M397	M398	M399	M400	M401	M402	M403	M404	M405	M406	M407	M408	M409	M410	M411	M412	M413	M414	M415	M416	M417	M418	M419	M420	M421	M422	M423	M424	M425	M426	M427	M428	M429	M430	M431	M432	M433	M434	M435	M436	M437	M438	M439	M440	M441	M442	M443	M444	M445	M446	M447	M448	M449	M450	M451	M452	M453	M454	M455	M456	M457	M458	M459	M460	M461	M462	M463	M464	M465	M466	M467	M468	M469	M470	M471	M472	M473	M474	M475	M476	M477	M478	M479	M480	M481	M482	M483	M484	M485	M486	M487	M488	M489	M490	M491	M492	M493	M494	M495	M496	M497	M498	M499	M500	M501	M502	M503	M504	M505	M506	M507	M508	M509	M510	M511	M512	M513	M514	M515	M516	M517	M518	M519	M520	M521	M522	M523	M524	M525	M526	M527	M528	M529	M530	M531	M532	M533	M534	M535	M536	M537	M538	M539	M540	M541	M542	M543	M544	M545	M546	M547	M548	M549	M550	M551	M552	M553	M554	M555	M556	M557	M558	M559	M560	M561	M562	M563	M564	M565	M566	M567	M568	M569	M570	M571	M572	M573	M574	M575	M576	M577	M578	M579	M580	M581	M582	M583	M584	M585	M586	M587	M588	M589	M590	M591	M592	M593	M594	M595	M596	M597	M598	M599	M600	M601	M602	M603	M604	M605	M606	M607	M608	M609	M610	M611	M612	M613	M614	M615	M616	M617	M618	M619	M620	M621	M622	M623	M624	M625	M626	M627	M628	M629	M630	M631	M632	M633	M634	M635	M636	M637	M638	M639	M640	M641	M642	M643	M644	M645	M646	M647	M648	M649	M650	M651	M652	M653	M654	M655	M656	M657	M658	M659	M660	M661	M662	M663	M664	M665	M666	M667	M668	M669	M670	M671	M672	M673	M674	M675	M676	M677	M678	M679	M680	M681	M682	M683	M684	M685	M686	M687	M688	M689	M690	M691	M692	M693	M694	M695	M696	M697	M698	M699	M700	M701	M702	M703	M704	M705	M706	M707	M708	M709	M710	M711	M712	M713	M714	M715	M716	M717	M718	M719	M720	M721	M722	M723	M724	M725	M726	M727	M728	M729	M730	M731	M732	M733	M734	M735	M736	M737	M738	M739	M740	M741	M742	M743	M744	M745	M746	M747	M748	M749	M750	M751	M752	M753	M754	M755	M756	M757	M758	M759	M760	M761	M762	M763	M764	M765	M766	M767	M768	M769	M770	M771	M772	M773	M774	M775	M776	M777	M778	M779	M780	M781	M782	M783	M784	M785	M786	M787	M788	M789	M790	M791	M792	M793	M794	M795	M796	M797	M798	M799	M800	M801	M802	M803	M804	M805	M806	M807	M808	M809	M810	M811	M812	M813	M814	M815	M816	M817	M818	M819	M820	M821	M822	M823	M824	M825	M826	M827	M828	M829	M830	M831	M832	M833	M834	M835	M836	M837	M838	M839	M840	M841	M842	M843	M844	M845	M846	M847	M848	M849	M850	M851	M852	M853	M854	M855	M856	M857	M858	M859	M860	M861	M862	M863	M864	M865	M866	M867	M868	M869	M870	M871	M872	M873	M874	M875	M876	M877	M878	M879	M880	M881	M882	M883	M884	M885	M886	M887	M888	M889	M890	M891	M892	M893	M894	M895	M896	M897	M898	M899	M900	M901	M902	M903	M904	M905	M906	M907	M908	M909	M910	M911	M912	M913	M914	M915	M916	M917	M918	M919	M920	M921	M922	M923	M924	M925	M926	M927	M928	M929	M930	M931	M932	M933	M934	M935	M936	M937	M938	M939	M940	M941	M942	M943	M944	M945	M946	M947	M948	M949	M950	M951	M952	M953	M954	M955	M956	M957	M958	M959	M960	M961	M962	M963	M964	M965	M966	M967	M968	M969	M970	M971	M972	M973	M974	M975	M976	M977	M978	M979	M980	M981	M982	M983	M984	M985	M986	M987	M988	M989	M990	M991	M992	M993	M994	M995	M996	M997	M998	M999	M1000	M1001	M1002	M1003	M1004	M1005	M1006	M1007	M1008	M1009	M1010	M1011	M1012	M1013	M1014	M1015	M1016	M1017	M1018	M1019	M1020	M1021	M1022	M1023	M1024	M1025	M1026	M1027	M1028	M1029	M1030	M1031	M1032	M1033	M1034	M1035	M1036	M1037	M1038	M1039	M1040	M1041	M1042	M1043	M1044	M1045	M1046	M1047	M1048	M1049	M1050	M1051	M1052	M1053	M1054	M1055	M1056	M1057	M1058	M1059	M1060	M1061	M1062	M1063	M1064	M1065	M1066	M1067	M1068	M1069	M1070	M1071	M1072	M1073	M1074	M1075	M1076	M1077	M1078	M1079	M1080	M1081	M1082	M1083	M1084	M1085	M1086	M1087	M1088	M1089	M1090	M1091	M1092	M1093	M1094	M1095	M1096	M1097	M1098	M1099	M1100	M1101	M1102	M1103	M1104	M1105	M1106	M1107	M1108	M1109	M1110	M1111	M1112	M1113	M1114	M1115	M1116	M1117	M1118	M1119	M1120	M1121	M1122	M1123	M1124	M1125	M1126	M1127	M1128	M1129	M1130	M1131	M1132	M1133	M1134	M1135	M1136	M1137	M1138	M1139	M1140	M1141	M1142	M1143	M1144	M1145	M1146	M1147	M1148	M1149	M1150	M1151	M1152	M1153	M1154	M1155	M1156	M1157	M1158	M1159	M1160	M1161	M1162	M1163	M1164	M1165	M1166	M1167	M1168	M1169	M1170	M1171	M1172	M1173	M1174	M1175	M1176	M1177	M1178	M1179	M1180	M1181	M1182	M1183	M1184	M1185	M1186	M1187	M1188	M1189	M1190	M1191	M1192	M1193	M1194	M1195	M1196	M1197	M1198	M1199	M1200	M1201	M1202	M1203	M1204	M1205	M1206	M1207	M1208	M1209	M1210	M1211	M1212	M1213	M1214	M1215	M1216	M1217	M1218	M1219	M1220	M1221	M1222	M1223	M1224	M1225	M1226	M1227	M1228	M1229	M1230	M1231	M1232	M1233	M1234	M1235	M1236	M1237	M1238	M1239	M1240	M1241	M1242	M1243	M1244	M1245	M1246	M1247	M1248	M1249	M1250	M1251	M1252	M1253	M1254	M1255	M1256	M1257	M1258	M1259	M1260	M1261	M1262	M1263	M1264	M1265	M1266	M1267	M1268	M1269	M1270	M1271	M1272	M1273	M1274	M1275	M1276	M1277	M1278	M1279	M1280	M1281	M1282	M1283	M1284	M1285	M1286	M1287	M1288	M1289	M1290	M1291	M1292	M1293	M1294	M1295	M1296	M1297	M1298	M1299	M1300	M1301	M1302	M1303	M1304	M1305	M1306	M1307	M1308	M1309	M1310	M1311	M1312	M1313	M1314	M1315	M1316	M1317	M1318	M1319	M1320	M1321	M1322	M1323	M1324	M1325	M1326	M1327	M1328	M1329	M1330	M1331	M1332	M1333	M1334	M1335	M1336	M1337	M1338	M1339	M1340	M1341	M1342	M1343	M1344	M1345	M1346	M1347	M1348	M1349	M1350	M1351	M1352	M1353	M1354	M1355	M1356	M1357	M1358	M1359	M1360	M1361	M1362	M1363	M1364	M1365	M1366	M1367	M1368	M1369	M1370	M1371	M1372	M1373	M1374	M1375	M1376	M1377	M1378	M1379	M1380	M1381	M1382	M1383	M1384	M1385	M1386	M1387	M1388	M1389	M1390	M1391	M1392	M1393	M1394	M1395	M1396	M1397	M1398	M1399	M1400	M1401	M1402	M1403	M1404	M1405	M1406	M1407	M1408	M1409	M1410	M1411	M1412	M1413	M1414	M1415	M1416	M1417	M1418	M1419	M1420	M1421	M1422	M1423	M1424	M1425	M1426	M1427	M1428	M1429	M1430	M1431	M1432	M1433	M1434	M1435	M1436	M1437	M1438	M1439	M1440	M1441	M1442	M1443	M1444	M1445	M1446	M1447	M1448	M1449	M1450	M1451	M1452	M1453	M1454	M1455	M1456	M1457	M1458	M1459	M1460	M1461	M1462	M1463	M1464	M1465	M1466	M1467	M1468	M1469	M1470	M1471	M1472	M1473	M1474	M1475	M1476	M1477	M1478	M1479	M1480	M1481	M1482	M1483	M1484	M1485	M1486	M1487	M1488	M1489	M1490	M1491	M1492	M1493	M1494	M1495	M1496	M1497	M1498	M1499	M1500	M1501	M1502	M1503	M1504	M1505	M1506	M1507	M1508	M1509



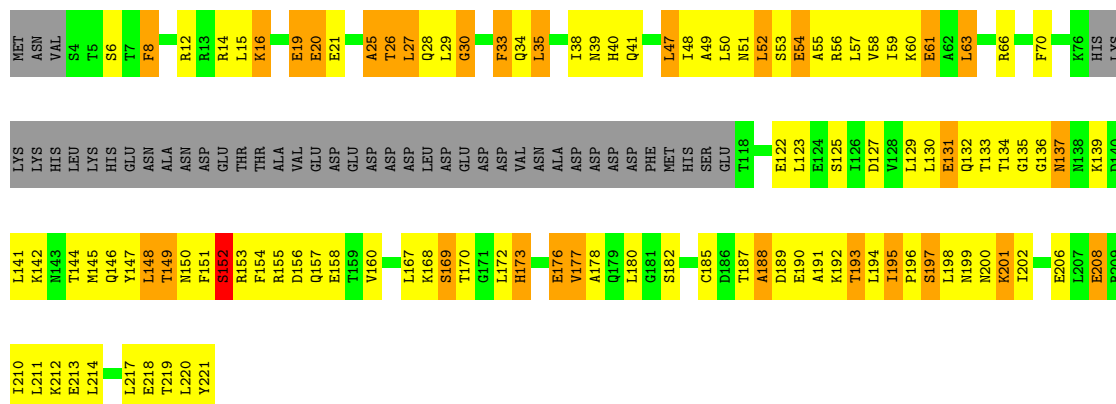
• Molecule 3: DNA-directed RNA polymerase II 45 kDa polypeptide

Chain C: 19% 49% 14% 16%

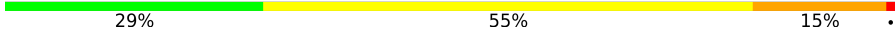


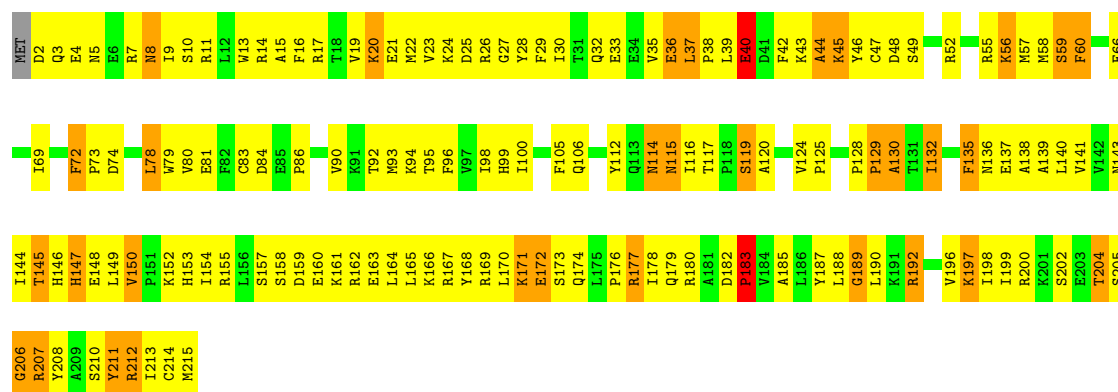
• Molecule 4: DNA-directed RNA polymerase II 32 kDa polypeptide

Chain D: 29% 37% 13% 20%



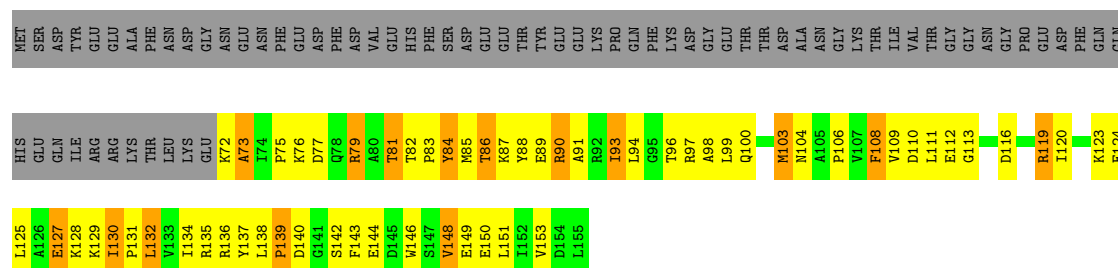
• Molecule 5: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide

Chain E: 



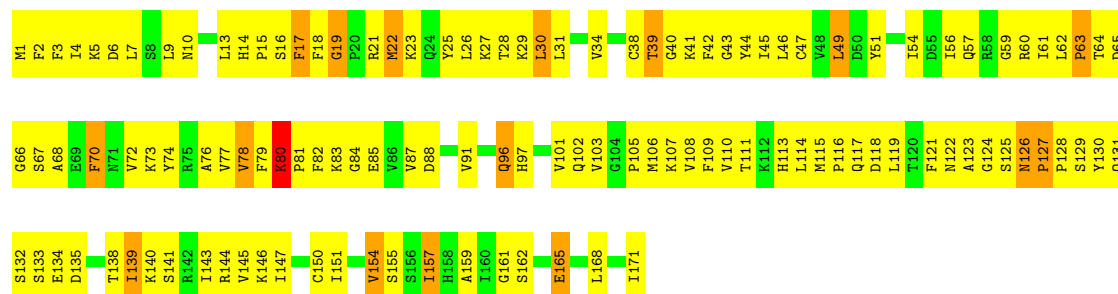
- Molecule 6: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide

Chain F: 



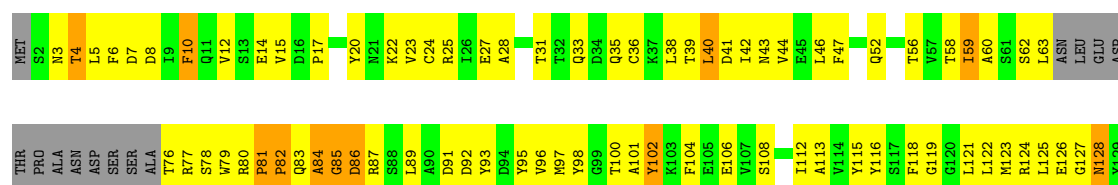
- Molecule 7: DNA-directed RNA polymerase II 19 kDa polypeptide

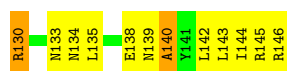
Chain G: 



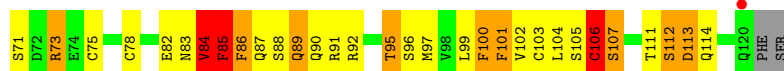
- Molecule 8: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide

Chain H: 

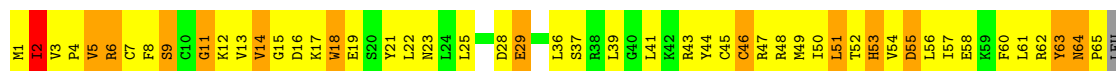




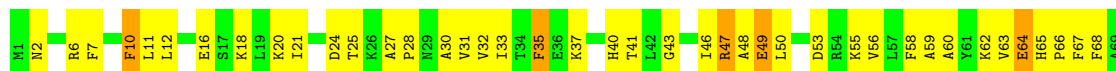
- Molecule 9: DNA-directed RNA polymerase II subunit 9



- Molecule 10: DNA-directed RNA polymerases I/II/III subunit 10



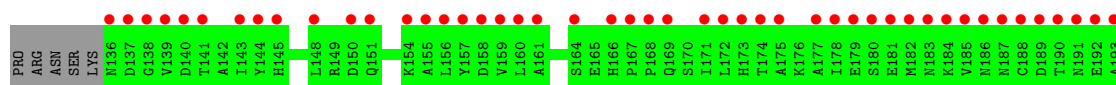
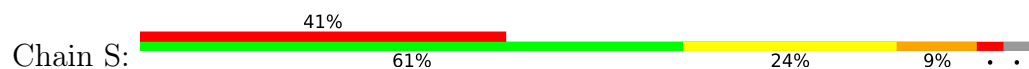
- Molecule 11: DNA-directed RNA polymerase II 13.6 kDa polypeptide

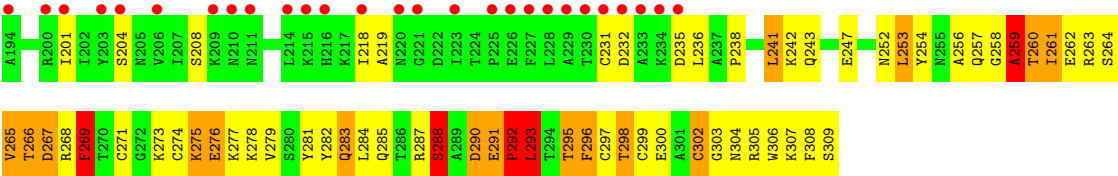


- Molecule 12: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide



- Molecule 13: Transcription elongation factor S-II





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	218.90Å 395.30Å 281.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.80 50.00 – 3.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.80) 86.8 (50.00-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.52 (at 3.77Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.282 , 0.294 0.259 , 0.268	Depositor DCC
R_{free} test set	2439 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å ²)	68.0	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 116.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.30$, $\langle L^2 \rangle = 0.13$	Xtriage
Estimated twinning fraction	0.199 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.206 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	31803	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.61	3/11417 (0.0%)	1.16	111/15442 (0.7%)
2	B	0.62	8/9009 (0.1%)	1.15	69/12146 (0.6%)
3	C	0.58	0/2133	1.10	17/2891 (0.6%)
4	D	0.48	0/1365	1.05	15/1837 (0.8%)
5	E	0.54	0/1788	1.03	13/2406 (0.5%)
6	F	0.62	0/691	1.17	5/933 (0.5%)
7	G	0.57	0/1368	1.12	11/1844 (0.6%)
8	H	0.43	0/1086	0.98	5/1470 (0.3%)
9	I	0.52	0/989	1.17	9/1331 (0.7%)
10	J	0.56	0/541	0.99	2/727 (0.3%)
11	K	0.53	0/937	0.96	1/1265 (0.1%)
12	L	0.66	0/366	0.99	1/485 (0.2%)
13	S	1.91	9/571 (1.6%)	2.23	15/765 (2.0%)
All	All	0.64	20/32261 (0.1%)	1.15	274/43542 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	3
13	S	0	2
All	All	0	5

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	S	269	PHE	C-N	-26.87	0.95	1.33
13	S	260	THR	CA-CB	21.08	1.80	1.53
2	B	467	GLY	C-O	-14.31	1.04	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	510	LYS	CA-C	8.03	1.62	1.52
13	S	260	THR	N-CA	6.34	1.54	1.46
2	B	510	LYS	N-CA	6.06	1.54	1.46
13	S	269	PHE	CA-C	6.04	1.59	1.52
13	S	259	ALA	CA-C	5.93	1.60	1.52
1	A	195	ASP	CA-C	5.86	1.65	1.52
1	A	195	ASP	N-CA	5.81	1.57	1.46
1	A	196	GLU	N-CA	5.71	1.54	1.46
13	S	266	THR	C-O	5.63	1.30	1.24
2	B	509	ALA	CA-CB	-5.50	1.44	1.53
2	B	467	GLY	CA-C	5.49	1.59	1.51
13	S	269	PHE	CA-CB	5.32	1.62	1.53
2	B	468	GLU	CB-CG	5.22	1.68	1.52
2	B	469	GLN	N-CA	5.17	1.52	1.46
13	S	268	ARG	CA-C	5.16	1.59	1.52
2	B	510	LYS	CB-CG	5.06	1.67	1.52
13	S	290	ASP	N-CA	5.05	1.52	1.46

All (274) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	S	269	PHE	O-C-N	-25.49	92.27	123.36
2	B	510	LYS	CA-C-N	24.64	145.30	119.19
2	B	510	LYS	C-N-CA	24.64	145.30	119.19
13	S	269	PHE	CA-C-N	23.92	163.51	122.37
13	S	269	PHE	C-N-CA	23.92	163.51	122.37
2	B	1185	CYS	N-CA-C	-12.62	97.88	113.02
2	B	296	GLU	N-CA-C	-11.27	96.79	112.45
4	D	26	THR	N-CA-C	-11.01	97.73	112.26
1	A	1262	LYS	N-CA-C	-10.04	100.34	111.28
1	A	243	PRO	CA-C-N	10.01	130.69	120.38
1	A	243	PRO	C-N-CA	10.01	130.69	120.38
1	A	344	ARG	N-CA-C	-9.86	95.93	110.52
2	B	512	ARG	N-CA-C	-9.81	100.41	112.38
9	I	28	GLU	N-CA-C	9.17	120.02	107.73
1	A	227	VAL	N-CA-C	9.10	119.27	111.90
7	G	19	GLY	CA-C-N	9.10	128.83	119.64
7	G	19	GLY	C-N-CA	9.10	128.83	119.64
1	A	195	ASP	N-CA-C	9.02	136.25	111.00
7	G	80	LYS	CA-C-N	8.74	129.28	119.92
7	G	80	LYS	C-N-CA	8.74	129.28	119.92
2	B	213	ILE	N-CA-C	8.70	121.10	108.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	466	SER	N-CA-C	8.67	123.18	113.21
1	A	1310	GLY	N-CA-C	-8.53	96.88	110.18
1	A	366	VAL	CA-C-N	-8.10	111.55	120.14
1	A	366	VAL	C-N-CA	-8.10	111.55	120.14
1	A	567	LYS	CA-C-N	-8.10	109.72	119.84
1	A	567	LYS	C-N-CA	-8.10	109.72	119.84
1	A	866	PHE	N-CA-C	-7.95	103.31	113.16
2	B	1052	VAL	N-CA-C	-7.74	102.90	110.72
2	B	468	GLU	N-CA-C	7.65	127.09	110.80
2	B	510	LYS	CB-CA-C	-7.63	95.14	110.17
2	B	681	TRP	N-CA-C	-7.56	101.16	112.04
2	B	1025	HIS	N-CA-C	-7.55	102.74	110.97
2	B	832	GLY	N-CA-C	-7.52	103.72	115.67
2	B	511	PRO	CB-CA-C	-7.48	101.19	112.11
4	D	188	ALA	N-CA-C	-7.48	103.06	111.14
2	B	208	SER	N-CA-C	7.45	121.03	110.23
2	B	508	LEU	CA-C-N	-7.39	107.43	121.54
2	B	508	LEU	C-N-CA	-7.39	107.43	121.54
1	A	1088	GLY	N-CA-C	-7.35	104.68	115.63
13	S	292	PRO	N-CA-C	7.34	127.59	112.47
9	I	65	ASP	CA-C-N	7.32	126.95	119.56
9	I	65	ASP	C-N-CA	7.32	126.95	119.56
13	S	266	THR	N-CA-C	7.27	121.53	109.46
2	B	805	THR	N-CA-C	7.23	120.39	109.41
1	A	173	THR	N-CA-C	-7.20	100.84	110.55
13	S	303	GLY	N-CA-C	7.11	125.85	115.32
2	B	1061	GLU	N-CA-C	-7.11	104.73	113.19
6	F	130	ILE	CA-C-N	7.09	128.70	119.84
6	F	130	ILE	C-N-CA	7.09	128.70	119.84
7	G	2	PHE	N-CA-C	-7.05	100.05	110.48
1	A	227	VAL	CB-CA-C	-7.05	104.53	111.30
2	B	475	SER	N-CA-C	7.02	119.59	110.53
8	H	80	ARG	CA-C-N	6.96	127.55	120.38
8	H	80	ARG	C-N-CA	6.96	127.55	120.38
1	A	769	SER	N-CA-C	6.94	119.06	108.52
1	A	927	VAL	N-CA-C	-6.91	104.26	111.58
10	J	5	VAL	N-CA-C	-6.89	99.79	108.89
9	I	85	PHE	N-CA-C	6.88	119.84	110.35
1	A	22	PHE	N-CA-C	6.87	119.04	109.15
2	B	112	LEU	N-CA-C	6.86	119.59	110.53
1	A	288	ALA	N-CA-C	-6.86	103.32	113.61
3	C	193	TYR	N-CA-C	6.86	117.53	108.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	452	LYS	N-CA-C	-6.82	103.84	111.28
4	D	38	ILE	N-CA-C	6.81	118.39	108.58
13	S	267	ASP	N-CA-C	6.80	122.75	113.37
1	A	398	GLU	N-CA-C	-6.78	100.44	110.48
1	A	827	THR	N-CA-C	-6.78	105.29	113.97
2	B	835	GLN	N-CA-C	6.78	119.05	110.24
1	A	865	GLN	N-CA-C	-6.74	96.45	110.80
1	A	244	PRO	N-CA-C	6.72	118.90	110.70
6	F	127	GLU	N-CA-C	-6.69	103.05	113.02
13	S	291	GLU	CA-C-N	6.66	128.16	119.84
13	S	291	GLU	C-N-CA	6.66	128.16	119.84
1	A	698	GLN	N-CA-C	-6.65	105.20	113.38
1	A	463	ILE	CA-C-N	6.65	126.59	120.21
1	A	463	ILE	C-N-CA	6.65	126.59	120.21
4	D	25	ALA	N-CA-C	-6.64	103.49	112.26
1	A	1413	GLY	N-CA-C	-6.64	107.36	114.67
7	G	140	LYS	N-CA-C	6.60	120.93	113.01
2	B	507	LYS	CA-C-N	-6.56	112.29	122.59
2	B	507	LYS	C-N-CA	-6.56	112.29	122.59
4	D	54	GLU	N-CA-C	-6.51	104.02	112.23
1	A	234	MET	N-CA-C	-6.51	105.34	113.28
7	G	129	SER	N-CA-C	6.50	117.16	108.38
6	F	132	LEU	N-CA-C	6.46	120.58	110.17
1	A	562	THR	CA-C-N	6.44	126.47	119.90
1	A	562	THR	C-N-CA	6.44	126.47	119.90
1	A	999	VAL	N-CA-C	-6.42	106.70	111.90
9	I	54	GLU	N-CA-C	6.42	119.63	109.81
5	E	20	LYS	N-CA-C	-6.41	103.92	111.03
5	E	5	ASN	N-CA-C	-6.39	106.44	114.56
3	C	226	ASP	N-CA-C	-6.38	100.76	110.14
1	A	311	GLN	N-CA-C	6.37	123.89	109.81
2	B	35	SER	N-CA-C	-6.36	103.26	111.02
2	B	829	CYS	N-CA-C	-6.36	98.91	109.46
2	B	473	MET	N-CA-C	-6.35	105.50	113.18
1	A	1339	LEU	N-CA-C	6.34	119.01	111.71
13	S	302	CYS	N-CA-C	6.31	120.72	112.89
1	A	977	LYS	CA-C-N	6.28	126.25	120.03
1	A	977	LYS	C-N-CA	6.28	126.25	120.03
2	B	1177	HIS	N-CA-C	-6.27	105.57	112.72
1	A	984	LYS	N-CA-C	-6.26	103.99	111.69
6	F	103	MET	N-CA-C	-6.25	105.52	113.02
2	B	825	VAL	N-CA-C	6.25	118.38	108.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	93	ASP	N-CA-C	-6.24	104.92	112.54
1	A	384	ASN	N-CA-C	6.21	121.37	113.55
1	A	432	VAL	CB-CA-C	-6.17	105.00	111.23
1	A	1404	GLU	N-CA-C	6.17	120.84	112.88
3	C	225	ALA	N-CA-C	6.17	120.09	107.69
2	B	511	PRO	CA-N-CD	-6.17	103.37	112.00
1	A	293	GLU	N-CA-C	-6.16	104.47	112.23
2	B	1113	VAL	N-CA-C	6.16	116.21	110.42
1	A	954	TRP	N-CA-C	6.14	118.14	108.55
1	A	1102	LYS	N-CA-C	-6.14	104.27	110.97
1	A	196	GLU	CA-C-N	6.14	127.52	119.84
1	A	196	GLU	C-N-CA	6.14	127.52	119.84
9	I	52	ILE	N-CA-C	6.14	116.71	107.75
1	A	222	LEU	N-CA-C	-6.11	102.31	110.55
2	B	918	ILE	N-CA-C	6.10	116.65	108.11
8	H	85	GLY	N-CA-C	-6.10	107.63	114.40
3	C	259	LEU	N-CA-C	-6.04	104.69	111.28
1	A	553	VAL	CA-C-N	6.04	127.39	119.84
1	A	553	VAL	C-N-CA	6.04	127.39	119.84
1	A	1405	THR	N-CA-C	6.03	123.63	110.80
1	A	137	ALA	N-CA-C	-6.02	103.89	112.13
5	E	150	VAL	CA-C-N	6.00	127.34	119.84
5	E	150	VAL	C-N-CA	6.00	127.34	119.84
13	S	261	ILE	N-CA-C	-6.00	100.07	108.12
3	C	23	SER	N-CA-C	6.00	118.59	109.95
1	A	229	SER	N-CA-C	5.99	117.20	107.32
1	A	729	ALA	N-CA-C	-5.99	104.83	111.71
2	B	510	LYS	N-CA-C	5.98	123.02	109.81
2	B	363	HIS	N-CA-C	-5.97	102.11	110.35
5	E	147	HIS	N-CA-C	5.97	118.92	109.96
1	A	440	ASP	N-CA-C	-5.97	102.53	109.93
1	A	1421	CYS	N-CA-C	-5.96	103.18	111.52
1	A	454	SER	N-CA-C	-5.92	105.89	114.12
2	B	1107	ALA	N-CA-C	-5.92	98.19	110.80
1	A	1085	HIS	N-CA-C	-5.88	106.11	113.28
3	C	39	ALA	N-CA-C	5.88	121.23	112.94
4	D	66	ARG	N-CA-C	-5.87	104.24	111.40
5	E	171	LYS	N-CA-C	-5.86	99.70	109.24
1	A	535	THR	N-CA-C	5.82	118.51	111.40
5	E	204	THR	N-CA-C	-5.81	104.95	112.68
4	D	157	GLN	N-CA-C	-5.81	106.04	113.01
1	A	506	ALA	N-CA-C	5.80	118.12	109.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	564	ALA	N-CA-C	-5.77	104.90	111.07
2	B	606	LYS	N-CA-C	-5.77	106.79	113.88
3	C	211	ASP	CA-C-N	5.74	126.29	120.38
3	C	211	ASP	C-N-CA	5.74	126.29	120.38
1	A	1444	MET	N-CA-C	5.73	117.79	109.07
9	I	25	LEU	N-CA-C	5.71	118.54	109.24
1	A	1071	SER	N-CA-C	5.71	119.34	112.38
4	D	173	HIS	CA-C-N	5.70	126.96	119.84
4	D	173	HIS	C-N-CA	5.70	126.96	119.84
1	A	239	LEU	N-CA-C	5.70	118.67	108.47
5	E	200	ARG	N-CA-C	5.69	118.15	109.95
3	C	155	LEU	N-CA-C	5.67	118.49	109.81
2	B	428	ILE	N-CA-C	-5.67	104.00	111.09
2	B	934	LYS	N-CA-C	5.67	117.16	109.11
1	A	18	GLN	N-CA-C	5.67	118.12	109.62
2	B	1173	ALA	N-CA-C	5.66	117.95	107.99
1	A	982	THR	N-CA-C	-5.66	101.26	110.20
12	L	30	ILE	N-CA-C	5.64	116.49	108.42
1	A	511	ILE	N-CA-C	5.64	118.95	111.17
1	A	88	LYS	CA-C-N	5.63	126.88	119.84
1	A	88	LYS	C-N-CA	5.63	126.88	119.84
1	A	1449	SER	N-CA-C	-5.63	106.41	113.28
1	A	424	ILE	N-CA-C	5.63	121.05	109.34
3	C	168	ALA	N-CA-C	5.63	118.14	111.33
4	D	195	ILE	CA-C-N	5.61	125.45	119.28
4	D	195	ILE	C-N-CA	5.61	125.45	119.28
1	A	439	ASN	N-CA-C	5.61	120.07	113.23
1	A	31	SER	N-CA-C	5.60	118.14	110.24
1	A	1072	ILE	N-CA-C	-5.60	107.00	111.81
2	B	427	ASP	N-CA-C	-5.58	107.11	114.31
2	B	510	LYS	CA-C-O	5.57	127.80	120.16
2	B	1194	ILE	N-CA-C	5.57	116.72	108.65
2	B	1008	PRO	N-CA-C	5.56	119.92	111.19
2	B	297	ILE	N-CA-C	-5.56	105.08	110.42
1	A	513	SER	N-CA-C	5.55	116.66	109.72
1	A	950	GLY	N-CA-C	-5.55	108.08	114.69
1	A	1092	LYS	N-CA-C	-5.54	104.05	111.87
1	A	663	SER	N-CA-C	5.54	115.59	108.34
4	D	33	PHE	N-CA-C	5.53	117.97	110.06
4	D	169	SER	N-CA-C	-5.52	104.79	112.30
5	E	152	LYS	N-CA-C	5.52	118.24	109.96
1	A	1419	ASP	N-CA-C	5.51	117.50	108.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1101	ASP	N-CA-C	-5.50	106.34	113.16
3	C	92	CYS	CA-CB-SG	-5.49	101.77	114.40
2	B	1180	PHE	N-CA-C	5.48	119.47	112.12
1	A	199	LEU	N-CA-C	5.47	117.15	108.67
1	A	1081	LEU	N-CA-C	5.47	118.31	109.40
8	H	40	LEU	N-CA-C	5.45	117.26	108.32
2	B	846	ILE	N-CA-C	-5.42	105.09	110.62
1	A	1325	THR	N-CA-C	-5.42	107.32	114.04
2	B	857	ARG	N-CA-C	-5.42	101.89	109.69
2	B	1168	LEU	N-CA-C	5.41	117.48	109.69
2	B	1131	GLY	N-CA-C	5.41	121.43	112.89
4	D	176	GLU	N-CA-C	-5.38	104.30	112.04
2	B	854	LEU	N-CA-C	-5.37	102.51	110.46
2	B	833	TYR	N-CA-C	-5.37	106.74	113.72
1	A	158	PRO	N-CA-C	-5.37	109.10	114.68
2	B	978	ASP	N-CA-C	5.36	117.80	110.24
2	B	580	VAL	N-CA-C	5.36	116.30	108.58
7	G	127	PRO	CA-C-N	5.36	125.30	119.78
7	G	127	PRO	C-N-CA	5.36	125.30	119.78
1	A	1155	ASP	CA-C-N	5.35	126.53	119.84
1	A	1155	ASP	C-N-CA	5.35	126.53	119.84
1	A	756	ILE	CB-CA-C	-5.34	105.04	111.88
1	A	1021	LEU	N-CA-C	-5.33	105.14	111.69
10	J	11	GLY	N-CA-C	5.33	120.03	113.79
2	B	277	LYS	N-CA-C	5.32	117.83	111.71
1	A	797	LYS	N-CA-C	-5.32	106.64	113.02
5	E	173	SER	N-CA-C	5.31	117.82	111.71
13	S	298	THR	CB-CA-C	-5.31	103.42	110.79
2	B	1016	ALA	N-CA-C	-5.30	106.67	112.72
1	A	1403	GLU	N-CA-C	5.30	122.09	110.80
1	A	1343	ALA	N-CA-C	-5.30	105.17	111.69
1	A	495	GLU	N-CA-C	-5.28	105.11	112.45
11	K	77	THR	N-CA-C	5.28	116.83	108.96
13	S	276	GLU	N-CA-C	5.28	118.01	109.40
9	I	8	ARG	N-CA-C	-5.28	101.42	109.65
2	B	492	LEU	N-CA-C	-5.27	104.59	111.02
2	B	1181	GLU	N-CA-C	5.27	122.02	110.80
5	E	119	SER	N-CA-C	-5.27	106.00	112.90
1	A	1360	GLY	N-CA-C	-5.27	104.93	114.46
1	A	120	GLU	N-CA-C	5.26	116.70	111.07
2	B	436	VAL	N-CA-C	-5.25	106.41	112.98
2	B	949	VAL	N-CA-C	-5.25	102.21	110.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	PHE	N-CA-C	5.25	116.26	108.86
3	C	12	GLU	N-CA-C	-5.25	103.56	110.43
13	S	253	LEU	N-CA-C	-5.23	105.50	111.14
2	B	66	ASP	N-CA-C	-5.22	106.77	112.72
1	A	1391	ARG	N-CA-C	-5.21	107.59	114.31
1	A	174	ILE	N-CA-C	5.21	116.22	108.46
1	A	706	HIS	N-CA-C	-5.21	105.57	112.34
1	A	537	ARG	N-CA-C	-5.20	105.79	111.82
1	A	1036	ARG	N-CA-C	5.20	121.87	110.80
1	A	230	ARG	N-CA-C	-5.19	103.40	110.36
3	C	147	LEU	N-CA-C	5.19	116.41	108.52
7	G	22	MET	N-CA-C	-5.19	105.07	111.40
1	A	479	ASN	N-CA-C	-5.19	104.84	110.91
1	A	1098	VAL	CB-CA-C	-5.18	108.85	114.35
2	B	1084	GLN	N-CA-C	-5.18	101.53	109.41
5	E	177	ARG	N-CA-C	5.16	118.14	110.14
2	B	872	GLU	N-CA-C	-5.15	103.81	110.19
2	B	1201	LYS	N-CA-C	-5.14	105.37	110.97
8	H	4	THR	N-CA-C	-5.14	101.55	109.52
5	E	197	LYS	N-CA-C	5.14	116.95	109.71
2	B	1045	SER	CA-C-N	5.13	126.25	119.84
2	B	1045	SER	C-N-CA	5.13	126.25	119.84
7	G	40	GLY	N-CA-C	-5.12	107.43	113.99
1	A	857	ARG	N-CA-C	5.12	117.32	109.95
1	A	166	GLY	N-CA-C	5.11	120.43	112.31
2	B	1120	GLU	N-CA-C	5.10	118.02	110.48
1	A	1032	LEU	N-CA-C	5.09	119.46	112.68
1	A	1368	MET	N-CA-C	-5.09	105.17	111.33
1	A	1311	VAL	N-CA-C	5.08	119.92	109.34
2	B	687	GLU	N-CA-C	-5.08	105.56	112.26
1	A	683	ILE	N-CA-C	-5.07	106.73	111.45
4	D	8	PHE	N-CA-C	5.07	121.60	110.80
2	B	510	LYS	C-N-CD	-5.06	104.24	125.00
2	B	772	ALA	N-CA-C	-5.06	105.89	113.89
3	C	38	ILE	N-CA-C	5.06	115.35	110.74
1	A	1283	VAL	N-CA-C	5.05	115.45	108.23
13	S	241	LEU	N-CA-C	-5.04	106.29	112.90
1	A	1316	VAL	N-CA-C	-5.04	106.45	113.00
3	C	90	ASP	N-CA-C	5.03	121.51	110.80
9	I	112	SER	N-CA-C	-5.03	105.53	113.02
1	A	1264	GLU	N-CA-C	-5.02	105.47	112.45
1	A	56	PRO	N-CA-C	-5.01	102.15	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	92	CYS	N-CA-C	-5.00	102.16	109.81

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	510	LYS	Mainchain
2	B	785	TYR	Sidechain
2	B	833	TYR	Sidechain
13	S	269	PHE	Sidechain,Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11214	0	11281	1626	0
2	B	8837	0	8871	1272	0
3	C	2095	0	2052	275	0
4	D	1356	0	1319	111	0
5	E	1752	0	1776	216	0
6	F	679	0	701	82	0
7	G	1340	0	1357	167	0
8	H	1068	0	1040	119	0
9	I	971	0	929	117	0
10	J	532	0	542	113	0
11	K	919	0	929	103	0
12	L	364	0	387	70	0
13	S	666	0	553	106	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
14	S	1	0	0	0	0
15	S	1	0	0	0	0
All	All	31803	0	31737	4021	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 63.

All (4021) 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)
13:S:260:THR:CA	13:S:260:THR:CB	1.80	1.53
13:S:269:PHE:CZ	13:S:297:CYS:SG	2.04	1.50
13:S:269:PHE:CE2	13:S:297:CYS:SG	2.14	1.39
1:A:1230:GLU:OE2	13:S:201:ILE:CA	1.75	1.32
1:A:1283:VAL:CG1	13:S:256:ALA:O	1.78	1.31
1:A:1172:LEU:CD1	13:S:204:SER:CA	2.12	1.27
1:A:1232:ASN:HD21	13:S:238:PRO:CA	1.48	1.25
13:S:235:ASP:CA	13:S:242:LYS:HE2	1.72	1.18
1:A:1283:VAL:HG13	13:S:256:ALA:O	1.41	1.15
7:G:138:THR:HG22	7:G:139:ILE:H	1.11	1.15
1:A:1017:LEU:HB2	5:E:206:GLY:H	1.11	1.14
1:A:353:ILE:HG21	1:A:487:MET:HG3	1.31	1.12
4:D:40:HIS:HB3	7:G:73:LYS:HZ3	1.09	1.12
1:A:794:PRO:HG2	1:A:795:GLU:OE2	1.49	1.11
1:A:225:ASN:ND2	1:A:228:PHE:H	1.47	1.11
10:J:57:ILE:HA	10:J:60:PHE:HD2	1.14	1.09
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	1.88	1.09
1:A:590:ARG:NH2	1:A:620:LYS:HB3	1.66	1.09
1:A:913:LEU:HD12	1:A:914:GLU:H	1.15	1.09
1:A:1329:THR:H	1:A:1335:ILE:HD11	1.02	1.09
1:A:899:VAL:HB	1:A:929:LEU:HD11	1.33	1.08
1:A:49:LYS:HZ1	1:A:61:ILE:HG13	0.96	1.08
1:A:855:THR:HG21	1:A:857:ARG:HE	1.10	1.08
2:B:1095:LEU:H	2:B:1095:LEU:HD12	1.11	1.08
7:G:14:HIS:HD2	7:G:16:SER:HB2	1.15	1.08
1:A:868:TYR:HE1	1:A:1064:VAL:HG11	1.15	1.07
3:C:45:ALA:HA	3:C:72:LEU:HD12	1.28	1.07
6:F:82:THR:HG22	6:F:84:TYR:H	1.15	1.07
1:A:1172:LEU:HD13	13:S:204:SER:CA	1.81	1.06
4:D:40:HIS:HB3	7:G:73:LYS:NZ	1.69	1.06
10:J:64:ASN:HB3	10:J:65:PRO:CD	1.86	1.05
2:B:112:LEU:HD12	2:B:113:TYR:H	1.19	1.05
1:A:779:PHE:HE1	1:A:785:PRO:HD3	1.20	1.05
1:A:47:ARG:HH12	1:A:254:GLU:HB3	1.21	1.05
13:S:235:ASP:CA	13:S:242:LYS:CE	2.34	1.05
2:B:579:ARG:HB2	2:B:586:TRP:HE1	1.19	1.04
2:B:839:MET:CG	2:B:1010:LEU:HD11	1.88	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:133:ILE:HD11	3:C:237:SER:HA	1.39	1.04
7:G:111:THR:HG22	7:G:113:HIS:H	1.19	1.04
1:A:834:THR:HG21	1:A:1077:THR:HG23	1.39	1.04
1:A:1135:ARG:NH1	13:S:256:ALA:HB2	1.72	1.03
1:A:901:LEU:H	1:A:926:GLN:NE2	1.54	1.03
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.39	1.02
2:B:1169:MET:HE1	2:B:1201:LYS:HA	1.41	1.02
13:S:291:GLU:N	13:S:292:PRO:HD2	1.72	1.02
2:B:508:LEU:CB	2:B:510:LYS:H	1.70	1.02
2:B:1065:GLN:HE21	2:B:1067:ARG:N	1.58	1.02
1:A:1172:LEU:HD11	13:S:204:SER:CA	1.85	1.02
2:B:705:MET:HA	2:B:705:MET:HE3	1.40	1.02
2:B:1159:ARG:HD3	2:B:1193:GLN:HG3	1.42	1.01
1:A:1199:ARG:HH22	13:S:241:LEU:HD13	1.21	1.01
2:B:589:VAL:HG12	2:B:590:HIS:H	1.24	1.00
1:A:164:ARG:HG3	1:A:165:GLY:H	1.26	1.00
2:B:273:LEU:HB2	2:B:276:ILE:HD12	1.43	1.00
2:B:918:ILE:HD12	2:B:935:ARG:HD2	1.43	1.00
2:B:23:ALA:HB1	2:B:24:PRO:HD2	1.44	1.00
1:A:53:LEU:HD23	1:A:54:ASN:N	1.76	1.00
1:A:886:ILE:HD11	1:A:943:LEU:HB3	1.44	0.99
1:A:896:ARG:HD3	1:A:897:TYR:HE1	1.26	0.99
1:A:1283:VAL:HG12	13:S:256:ALA:O	1.57	0.99
11:K:65:HIS:CD2	11:K:67:PHE:H	1.81	0.99
1:A:63:ARG:HA	1:A:74:MET:SD	2.01	0.99
2:B:510:LYS:O	2:B:510:LYS:HD2	1.60	0.99
1:A:853:ASP:OD1	1:A:855:THR:HB	1.62	0.99
1:A:1199:ARG:NH2	13:S:241:LEU:HD13	1.78	0.98
2:B:1162:ILE:HD11	2:B:1194:ILE:HD13	1.45	0.98
1:A:490:HIS:HB3	2:B:1150:ARG:NH1	1.79	0.98
2:B:65:GLU:HG3	2:B:66:ASP:H	1.27	0.98
2:B:295:GLY:H	2:B:298:LEU:HD23	1.27	0.98
3:C:56:THR:HG21	3:C:145:CYS:SG	2.03	0.98
2:B:839:MET:HG3	2:B:1010:LEU:HD11	1.01	0.97
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.45	0.97
3:C:33:LEU:HG	3:C:37:MET:HE2	1.43	0.97
1:A:225:ASN:HD22	1:A:228:PHE:H	1.03	0.97
2:B:863:GLU:OE2	2:B:873:THR:HA	1.64	0.97
1:A:913:LEU:HD12	1:A:914:GLU:N	1.81	0.96
1:A:1081:LEU:HD12	1:A:1082:ASN:OD1	1.66	0.96
1:A:1011:GLN:NE2	1:A:1015:VAL:HG21	1.78	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:882:THR:HG22	2:B:884:ARG:H	1.29	0.95
1:A:779:PHE:CE1	1:A:785:PRO:HD3	2.00	0.95
1:A:1172:LEU:CD2	13:S:204:SER:CA	2.44	0.95
2:B:211:VAL:O	2:B:480:SER:HA	1.65	0.95
2:B:824:ILE:HG12	10:J:48:ARG:HH12	1.31	0.95
1:A:1189:SER:O	1:A:1241:ARG:HD3	1.66	0.95
2:B:583:ASN:HD21	2:B:628:THR:HB	1.29	0.95
3:C:73:GLN:HE21	3:C:75:MET:H	1.03	0.95
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.45	0.94
1:A:103:CYS:SG	1:A:108:MET:HE1	2.07	0.94
1:A:1232:ASN:ND2	13:S:238:PRO:CA	2.29	0.94
2:B:1002:THR:HG21	2:B:1006:ILE:HD12	1.49	0.93
1:A:337:ARG:CZ	1:A:839:ARG:HH12	1.81	0.93
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.49	0.93
9:I:85:PHE:H	9:I:85:PHE:HD2	0.93	0.93
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	1.48	0.93
2:B:1065:GLN:NE2	2:B:1067:ARG:H	1.67	0.93
10:J:57:ILE:HA	10:J:60:PHE:CD2	2.04	0.93
1:A:70:CYS:O	1:A:72:GLU:HG2	1.68	0.93
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.48	0.92
2:B:987:LYS:HZ2	13:S:290:ASP:HB3	1.34	0.92
6:F:76:LYS:O	6:F:79:ARG:HD3	1.70	0.92
7:G:1:MET:HG3	7:G:85:GLU:CD	1.93	0.92
7:G:1:MET:HE1	7:G:80:LYS:H	1.33	0.92
13:S:279:VAL:HG22	13:S:299:CYS:HA	1.50	0.92
1:A:49:LYS:NZ	1:A:61:ILE:HG13	1.84	0.92
2:B:1183:LYS:N	2:B:1183:LYS:HE3	1.85	0.92
5:E:153:HIS:O	5:E:154:ILE:HG13	1.69	0.92
1:A:55:ASP:C	1:A:57:ARG:H	1.73	0.92
1:A:590:ARG:HH21	1:A:620:LYS:HB3	1.27	0.92
1:A:1341:ILE:HG23	1:A:1342:GLU:H	1.32	0.92
7:G:14:HIS:CD2	7:G:16:SER:HB2	2.04	0.92
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.05	0.91
1:A:708:MET:HE2	1:A:1089:VAL:HG13	1.52	0.91
3:C:167:HIS:HD2	3:C:169:LYS:H	1.17	0.91
2:B:168:GLY:H	2:B:450:ALA:HB1	1.34	0.91
3:C:63:ILE:HA	3:C:66:ARG:HG3	1.50	0.91
1:A:1362:TYR:HD1	1:A:1363:VAL:H	1.18	0.91
2:B:549:THR:HG22	2:B:550:ASP:H	1.35	0.91
1:A:1329:THR:HG22	1:A:1331:SER:H	1.36	0.91
1:A:864:ILE:O	1:A:865:GLN:HG3	1.72	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:846:ILE:HG23	2:B:974:PRO:HG2	1.51	0.90
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.36	0.90
1:A:490:HIS:HB3	2:B:1150:ARG:HH11	1.36	0.90
2:B:563:MET:HE3	2:B:580:VAL:HB	1.51	0.90
11:K:65:HIS:HD2	11:K:67:PHE:H	1.10	0.90
9:I:111:THR:HG22	9:I:112:SER:H	1.37	0.90
3:C:57:VAL:HG11	10:J:60:PHE:HB3	1.52	0.89
1:A:560:ILE:HG13	8:H:78:SER:HB2	1.51	0.89
1:A:1329:THR:N	1:A:1335:ILE:HD11	1.87	0.89
1:A:666:ILE:HD12	1:A:667:GLY:H	1.35	0.89
1:A:1118:VAL:O	1:A:1305:VAL:HG13	1.71	0.89
2:B:35:SER:HA	2:B:811:TYR:HE2	1.36	0.89
2:B:254:LEU:HD23	2:B:381:MET:HE1	1.55	0.89
1:A:1004:ASN:ND2	5:E:167:ARG:HD2	1.88	0.89
4:D:56:ARG:HB2	4:D:148:LEU:HD22	1.52	0.89
11:K:56:VAL:HA	11:K:77:THR:HG22	1.55	0.89
1:A:524:VAL:HG12	1:A:525:GLN:H	1.38	0.88
2:B:1095:LEU:HD12	2:B:1095:LEU:N	1.88	0.88
10:J:6:ARG:HG2	10:J:13:VAL:HA	1.55	0.88
2:B:800:GLN:HB3	10:J:52:THR:HG21	1.54	0.88
2:B:835:GLN:HA	2:B:1013:ASN:HD22	1.35	0.88
5:E:197:LYS:HE2	5:E:199:ILE:HD11	1.55	0.88
2:B:365:THR:HG23	2:B:367:LEU:HG	1.55	0.88
1:A:1029:ARG:HH11	1:A:1029:ARG:HG3	1.38	0.88
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.55	0.88
7:G:23:LYS:HG3	7:G:56:ILE:HD11	1.55	0.88
1:A:351:THR:HG22	2:B:1103:ILE:HA	1.55	0.88
1:A:567:LYS:HB3	8:H:96:VAL:H	1.39	0.88
1:A:1100:ARG:HH21	1:A:1351:GLU:HG2	1.39	0.88
5:E:117:THR:HG22	5:E:119:SER:H	1.39	0.88
7:G:13:LEU:HD21	7:G:17:PHE:HB2	1.56	0.88
8:H:40:LEU:HD13	8:H:123:MET:HB2	1.53	0.88
1:A:466:SER:O	2:B:1103:ILE:HD11	1.74	0.87
1:A:901:LEU:H	1:A:926:GLN:HE21	1.22	0.87
1:A:1121:GLU:HG2	1:A:1122:PRO:HD2	1.55	0.87
1:A:1313:LEU:HD23	1:A:1338:VAL:HG21	1.57	0.87
2:B:313:MET:HE2	2:B:390:LEU:HD21	1.57	0.87
2:B:579:ARG:HB2	2:B:586:TRP:NE1	1.90	0.87
2:B:830:TYR:CE2	2:B:1000:PRO:HD3	2.09	0.87
8:H:84:ALA:HB1	8:H:87:ARG:HB2	1.57	0.87
1:A:443:LEU:HG	2:B:1146:PHE:HE2	1.38	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:217:ARG:HE	2:B:405:ARG:HB2	1.40	0.87
2:B:582:VAL:HG23	2:B:626:ILE:HB	1.57	0.87
2:B:1007:VAL:HG22	2:B:1008:PRO:HD2	1.57	0.87
1:A:855:THR:HG21	1:A:857:ARG:NE	1.89	0.86
2:B:113:TYR:HB3	2:B:114:PRO:HD2	1.55	0.86
1:A:587:HIS:CD2	1:A:969:GLN:HG2	2.11	0.86
7:G:1:MET:HG3	7:G:85:GLU:OE2	1.75	0.86
2:B:466:TRP:O	2:B:468:GLU:N	2.08	0.86
3:C:213:PRO:O	3:C:214:ASN:HB2	1.74	0.86
2:B:467:GLY:O	2:B:468:GLU:HB2	1.73	0.86
9:I:29:CYS:SG	9:I:32:CYS:N	2.48	0.86
2:B:39:ARG:NH2	2:B:665:GLU:HG2	1.89	0.86
1:A:78:PRO:HA	2:B:1201:LYS:HZ1	1.41	0.86
1:A:1341:ILE:HG23	1:A:1342:GLU:N	1.89	0.85
13:S:265:VAL:CG1	13:S:278:LYS:HA	2.06	0.85
2:B:37:PHE:HE2	2:B:542:MET:HA	1.40	0.85
2:B:880:THR:HB	2:B:934:LYS:HD2	1.56	0.85
10:J:43:ARG:HG3	10:J:45:CYS:SG	2.16	0.85
2:B:493:SER:HA	2:B:751:VAL:HG21	1.57	0.85
2:B:562:GLY:HA3	2:B:590:HIS:CE1	2.12	0.85
1:A:665:GLY:HA2	2:B:1026:LEU:HD21	1.58	0.85
1:A:1362:TYR:CD1	1:A:1363:VAL:N	2.44	0.85
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.58	0.85
2:B:839:MET:HG3	2:B:1010:LEU:CD1	1.98	0.85
1:A:795:GLU:CD	1:A:795:GLU:H	1.83	0.85
1:A:1166:ASP:OD2	1:A:1239:ARG:HD2	1.76	0.85
2:B:955:THR:HG23	12:L:54:ARG:O	1.77	0.85
1:A:1116:LEU:N	1:A:1308:THR:HG22	1.92	0.85
1:A:963:ILE:HD13	1:A:1049:ILE:HG13	1.58	0.85
9:I:85:PHE:CD2	9:I:85:PHE:N	2.45	0.84
10:J:14:VAL:CG1	10:J:50:ILE:HD11	2.05	0.84
5:E:153:HIS:HB3	5:E:196:VAL:HG11	1.58	0.84
5:E:22:MET:HE3	5:E:26:ARG:HE	1.42	0.84
5:E:22:MET:HE3	5:E:26:ARG:NE	1.93	0.84
1:A:1116:LEU:H	1:A:1308:THR:HG22	1.41	0.84
2:B:510:LYS:HD2	2:B:510:LYS:C	1.98	0.84
2:B:781:PHE:O	2:B:782:LEU:HG	1.78	0.84
2:B:843:GLN:HB2	2:B:993:THR:HB	1.58	0.84
2:B:766:ARG:NH2	2:B:1020:ARG:HG2	1.92	0.84
7:G:138:THR:HG22	7:G:139:ILE:N	1.91	0.84
1:A:537:ARG:HD2	8:H:20:TYR:HE1	1.40	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:508:LEU:C	2:B:510:LYS:N	2.30	0.84
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.60	0.84
2:B:1065:GLN:HE21	2:B:1067:ARG:H	0.86	0.84
2:B:1107:ALA:O	2:B:1108:ARG:HG2	1.77	0.84
1:A:896:ARG:HD3	1:A:897:TYR:CE1	2.11	0.84
3:C:244:VAL:O	3:C:248:ILE:HG13	1.76	0.84
1:A:472:LEU:HD11	2:B:835:GLN:NE2	1.93	0.84
1:A:540:PHE:HB3	1:A:571:LEU:HD23	1.59	0.84
2:B:508:LEU:C	2:B:510:LYS:H	1.81	0.84
5:E:153:HIS:HB3	5:E:196:VAL:CG1	2.08	0.84
1:A:503:GLN:HE21	6:F:90:ARG:HH21	1.25	0.83
3:C:92:CYS:SG	3:C:95:CYS:SG	2.75	0.83
1:A:1079:MET:HE3	1:A:1098:VAL:HG22	1.61	0.83
10:J:3:VAL:HG21	10:J:18:TRP:HB2	1.59	0.83
1:A:1291:VAL:HG13	1:A:1292:PRO:HD2	1.59	0.83
8:H:100:THR:HG23	8:H:138:GLU:HA	1.58	0.83
1:A:353:ILE:HD12	1:A:470:LEU:HD21	1.61	0.83
1:A:1116:LEU:HD23	1:A:1311:VAL:HG22	1.60	0.83
10:J:9:SER:OG	10:J:45:CYS:HB2	1.79	0.83
1:A:743:VAL:O	1:A:747:VAL:HG23	1.79	0.83
3:C:98:VAL:C	3:C:99:LEU:HD23	2.04	0.82
2:B:510:LYS:O	2:B:510:LYS:CD	2.25	0.82
1:A:1283:VAL:HG13	13:S:256:ALA:C	2.04	0.82
2:B:510:LYS:HG2	2:B:512:ARG:H	1.43	0.82
13:S:291:GLU:H	13:S:292:PRO:HD2	1.42	0.82
10:J:16:ASP:OD1	10:J:17:LYS:HD2	1.80	0.82
13:S:288:SER:O	13:S:292:PRO:HD3	1.80	0.82
1:A:567:LYS:CG	1:A:568:PRO:HD2	2.09	0.82
2:B:502:ILE:HG22	2:B:502:ILE:O	1.79	0.82
2:B:1020:ARG:HG2	2:B:1020:ARG:HH11	1.44	0.82
9:I:111:THR:HG22	9:I:113:ASP:H	1.43	0.82
1:A:14:VAL:HG23	1:A:1432:GLN:NE2	1.95	0.82
1:A:1239:ARG:HH22	1:A:1241:ARG:HH22	1.25	0.82
2:B:295:GLY:N	2:B:298:LEU:HD23	1.94	0.81
6:F:103:MET:HE2	7:G:66:GLY:H	1.44	0.81
1:A:649:ILE:O	1:A:653:VAL:HG23	1.80	0.81
6:F:86:THR:OG1	6:F:89:GLU:HG3	1.80	0.81
1:A:1237:ILE:HG22	1:A:1238:ILE:N	1.96	0.81
2:B:102:VAL:HG23	2:B:112:LEU:HB2	1.63	0.81
7:G:111:THR:HG22	7:G:113:HIS:N	1.95	0.81
2:B:816:GLU:O	2:B:817:LEU:HD23	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:628:GLY:O	1:A:632:VAL:HG23	1.81	0.81
2:B:1007:VAL:CG2	2:B:1008:PRO:HD2	2.10	0.81
2:B:1159:ARG:HB3	2:B:1159:ARG:HH11	1.44	0.81
1:A:669:THR:O	1:A:762:SER:HB3	1.81	0.81
9:I:56:ALA:HB2	9:I:89:GLN:CG	2.10	0.81
1:A:1127:ASP:HB3	1:A:1130:GLN:HB3	1.63	0.81
1:A:1372:VAL:O	1:A:1376:THR:HG22	1.81	0.81
2:B:1169:MET:CE	2:B:1201:LYS:HA	2.11	0.81
13:S:235:ASP:CA	13:S:242:LYS:CG	2.58	0.81
1:A:1094:VAL:HG13	1:A:1113:THR:HG21	1.63	0.81
1:A:1317:MET:O	1:A:1322:ILE:HD11	1.80	0.81
9:I:6:PHE:HB3	9:I:12:ASN:O	1.80	0.81
1:A:666:ILE:HD12	1:A:667:GLY:N	1.95	0.80
7:G:18:PHE:HA	7:G:22:MET:HE3	1.63	0.80
1:A:78:PRO:HA	2:B:1201:LYS:NZ	1.96	0.80
1:A:471:ASN:O	1:A:474:VAL:HG12	1.81	0.80
2:B:862:GLN:HG2	2:B:963:PHE:HD1	1.45	0.80
1:A:399:HIS:O	1:A:401:GLY:N	2.14	0.80
2:B:1204:PHE:O	2:B:1208:MET:HG3	1.82	0.80
9:I:58:VAL:HG12	9:I:60:GLN:H	1.47	0.80
1:A:1017:LEU:HB2	5:E:206:GLY:N	1.93	0.80
2:B:1099:VAL:HG13	2:B:1100:ASP:H	1.44	0.80
6:F:82:THR:HG22	6:F:84:TYR:N	1.97	0.80
11:K:65:HIS:HD2	11:K:67:PHE:N	1.79	0.80
11:K:47:ARG:HB3	11:K:47:ARG:HH11	1.47	0.80
1:A:335:ARG:HE	1:A:339:ASN:ND2	1.79	0.79
1:A:49:LYS:HE2	1:A:61:ILE:HD12	1.62	0.79
1:A:56:PRO:O	1:A:57:ARG:HG3	1.82	0.79
1:A:1202:MET:HE1	1:A:1212:VAL:HG21	1.63	0.79
9:I:58:VAL:HG22	9:I:62:ILE:HD12	1.63	0.79
3:C:73:GLN:NE2	3:C:75:MET:H	1.79	0.79
1:A:825:ILE:HG21	2:B:510:LYS:HE3	1.64	0.79
9:I:55:THR:HG23	9:I:100:PHE:HD2	1.48	0.79
2:B:359:GLU:O	2:B:362:PRO:HD3	1.82	0.79
2:B:509:ALA:O	2:B:510:LYS:HD2	1.81	0.79
9:I:85:PHE:HD2	9:I:85:PHE:N	1.78	0.79
3:C:133:ILE:CD1	3:C:237:SER:HA	2.12	0.79
13:S:265:VAL:HG13	13:S:278:LYS:HA	1.65	0.79
1:A:299:HIS:HA	1:A:302:THR:HG22	1.65	0.79
1:A:494:SER:O	1:A:498:ARG:HG2	1.82	0.79
1:A:1435:PRO:HA	1:A:1439:GLY:O	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:1:MET:HE1	7:G:80:LYS:N	1.98	0.79
13:S:269:PHE:HZ	13:S:297:CYS:SG	1.97	0.79
2:B:364:ILE:HG12	2:B:585:VAL:HG13	1.65	0.79
2:B:806:THR:HG22	2:B:808:ALA:H	1.48	0.79
7:G:9:LEU:HD12	7:G:10:ASN:H	1.48	0.79
1:A:1444:MET:HG2	7:G:60:ARG:HA	1.65	0.78
2:B:613:VAL:HG13	2:B:627:PHE:O	1.84	0.78
1:A:608:ILE:HB	1:A:613:ILE:HD11	1.65	0.78
1:A:1135:ARG:NH1	13:S:256:ALA:CB	2.46	0.78
2:B:593:PRO:HG2	2:B:617:ARG:NH2	1.99	0.78
1:A:537:ARG:HD2	8:H:20:TYR:CE1	2.18	0.78
1:A:339:ASN:HB3	2:B:1117:GLN:HE22	1.48	0.78
3:C:167:HIS:CD2	3:C:169:LYS:H	2.02	0.78
3:C:212:PRO:HB3	3:C:213:PRO:HD2	1.64	0.78
5:E:124:VAL:HG13	5:E:132:ILE:HD12	1.64	0.78
5:E:154:ILE:H	5:E:196:VAL:HG13	1.49	0.78
13:S:271:CYS:SG	13:S:304:ASN:ND2	2.57	0.78
1:A:587:HIS:HD2	1:A:969:GLN:HG2	1.48	0.78
2:B:112:LEU:HD12	2:B:113:TYR:N	1.96	0.78
1:A:71:GLN:C	1:A:73:GLY:H	1.91	0.78
1:A:858:ASN:C	1:A:858:ASN:HD22	1.90	0.78
2:B:510:LYS:HG2	2:B:512:ARG:HG3	1.64	0.78
2:B:882:THR:HG22	2:B:884:ARG:N	1.99	0.78
2:B:987:LYS:NZ	13:S:290:ASP:HB3	1.98	0.78
4:D:40:HIS:CB	7:G:73:LYS:HZ3	1.94	0.78
4:D:48:ILE:HG21	7:G:4:ILE:HD12	1.66	0.77
1:A:765:VAL:HG23	1:A:802:ASN:O	1.84	0.77
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.18	0.77
1:A:866:PHE:O	1:A:867:ILE:HD12	1.85	0.77
1:A:1017:LEU:HB3	5:E:205:SER:HA	1.64	0.77
1:A:1127:ASP:HB3	1:A:1130:GLN:CB	2.14	0.77
1:A:164:ARG:HG3	1:A:165:GLY:N	1.98	0.77
1:A:1090:ALA:HA	1:A:1093:LYS:HE3	1.66	0.77
1:A:515:GLN:O	1:A:516:SER:HB3	1.85	0.77
2:B:508:LEU:HB3	2:B:510:LYS:H	1.48	0.77
2:B:1206:GLU:O	2:B:1209:ALA:HB3	1.83	0.77
2:B:615:MET:HB3	2:B:626:ILE:HG12	1.66	0.77
10:J:45:CYS:O	10:J:48:ARG:HG3	1.85	0.77
2:B:1106:ARG:HG3	2:B:1107:ALA:N	1.96	0.77
3:C:47:ASP:HA	12:L:69:ALA:CB	2.15	0.77
4:D:35:LEU:H	4:D:35:LEU:HD12	1.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:87:VAL:HB	7:G:103:VAL:HG11	1.67	0.77
12:L:30:ILE:HD11	12:L:59:ALA:HB2	1.64	0.77
1:A:908:LEU:HD12	1:A:983:ILE:HD11	1.67	0.77
3:C:73:GLN:HE21	3:C:75:MET:N	1.82	0.76
9:I:62:ILE:O	9:I:62:ILE:HG22	1.84	0.76
7:G:121:PHE:HB2	7:G:130:TYR:CE2	2.20	0.76
9:I:82:GLU:HB3	9:I:104:LEU:HD12	1.67	0.76
1:A:563:PRO:HG3	1:A:572:TRP:CZ2	2.20	0.76
1:A:590:ARG:HD3	1:A:604:GLY:HA2	1.67	0.76
1:A:767:GLN:OE1	1:A:799:PHE:HB2	1.83	0.76
1:A:830:LYS:HB2	1:A:1081:LEU:HD23	1.67	0.76
2:B:583:ASN:ND2	2:B:628:THR:HB	2.00	0.76
8:H:4:THR:HA	8:H:60:ALA:HB2	1.66	0.76
2:B:291:ILE:HD13	2:B:300:HIS:NE2	2.00	0.76
1:A:1224:LEU:HD12	1:A:1241:ARG:O	1.84	0.76
4:D:185:CYS:HA	4:D:190:GLU:OE1	1.85	0.76
5:E:124:VAL:HG13	5:E:132:ILE:HB	1.68	0.76
6:F:86:THR:HG23	6:F:89:GLU:CD	2.10	0.76
10:J:44:TYR:HA	10:J:47:ARG:HB2	1.68	0.76
1:A:963:ILE:HD11	1:A:1048:ASN:HB2	1.68	0.76
2:B:1165:ILE:HG22	2:B:1166:CYS:N	1.99	0.76
9:I:34:TYR:CD2	9:I:35:VAL:N	2.54	0.76
1:A:489:LEU:HD12	1:A:490:HIS:N	1.99	0.76
2:B:467:GLY:O	2:B:468:GLU:CB	2.29	0.76
10:J:1:MET:HE2	10:J:60:PHE:CE2	2.21	0.76
1:A:106:VAL:HG13	1:A:112:LYS:O	1.86	0.76
1:A:107:CYS:H	1:A:114:LEU:HD21	1.51	0.76
1:A:744:LYS:HG2	1:A:748:MET:HE2	1.68	0.76
1:A:1132:LYS:HE2	13:S:253:LEU:HD21	1.68	0.76
1:A:1444:MET:HE1	6:F:135:ARG:HB2	1.67	0.76
2:B:1084:GLN:N	2:B:1084:GLN:HE21	1.84	0.76
13:S:235:ASP:CA	13:S:242:LYS:HG2	2.16	0.76
2:B:589:VAL:HG12	2:B:590:HIS:N	1.95	0.76
2:B:794:ASN:C	2:B:795:ILE:HD12	2.11	0.76
2:B:1187:ASN:O	2:B:1188:LYS:HB2	1.84	0.76
5:E:7:ARG:HG3	5:E:8:ASN:N	2.00	0.76
11:K:113:THR:O	11:K:114:LEU:HB2	1.84	0.76
1:A:567:LYS:HB3	8:H:96:VAL:N	2.01	0.75
2:B:745:PRO:O	2:B:748:ILE:HG12	1.86	0.75
1:A:225:ASN:HD22	1:A:228:PHE:N	1.80	0.75
1:A:820:GLY:O	1:A:822:GLU:N	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1079:MET:HE1	1:A:1101:LEU:HD23	1.68	0.75
2:B:98:THR:O	2:B:126:SER:HB2	1.86	0.75
1:A:95:PHE:CD1	1:A:234:MET:HG2	2.20	0.75
1:A:826:ASP:O	1:A:830:LYS:HB3	1.85	0.75
1:A:1027:ALA:HB3	1:A:1030:ARG:HB2	1.68	0.75
1:A:1334:ASP:C	1:A:1336:MET:H	1.94	0.75
2:B:515:HIS:CD2	2:B:517:THR:H	2.02	0.75
2:B:918:ILE:HD12	2:B:935:ARG:CD	2.15	0.75
2:B:1224:PHE:HE2	5:E:171:LYS:HG3	1.52	0.75
1:A:754:SER:H	1:A:757:ASN:HD22	1.35	0.75
1:A:1204:ASP:HA	13:S:252:ASN:HB3	1.65	0.75
9:I:26:LEU:HD23	9:I:37:GLU:HA	1.67	0.75
2:B:39:ARG:HH21	2:B:665:GLU:HG2	1.46	0.75
3:C:90:ASP:O	3:C:91:HIS:CD2	2.39	0.75
2:B:777:ALA:HA	2:B:1095:LEU:HA	1.68	0.75
8:H:81:PRO:CB	8:H:82:PRO:HD2	2.17	0.75
1:A:95:PHE:O	1:A:99:ILE:HG13	1.87	0.75
1:A:285:PRO:HG2	1:A:288:ALA:HB3	1.67	0.75
2:B:510:LYS:HG2	2:B:512:ARG:CG	2.17	0.75
1:A:1107:VAL:HG12	1:A:1107:VAL:O	1.87	0.75
2:B:899:ILE:HD11	2:B:911:ILE:HA	1.68	0.75
1:A:346:ASP:HB3	2:B:1108:ARG:H	1.51	0.74
2:B:541:LEU:HB2	2:B:747:MET:HE3	1.66	0.74
4:D:145:MET:O	4:D:149:THR:HB	1.87	0.74
2:B:429:PHE:HA	2:B:432:MET:HE3	1.68	0.74
2:B:705:MET:HA	2:B:705:MET:CE	2.17	0.74
2:B:758:PHE:CE2	2:B:1044:ALA:HA	2.21	0.74
2:B:1160:VAL:HG12	2:B:1161:HIS:N	2.02	0.74
3:C:147:LEU:HB2	3:C:151:GLN:HB2	1.69	0.74
9:I:101:PHE:N	9:I:101:PHE:CD1	2.55	0.74
1:A:899:VAL:CB	1:A:929:LEU:HD11	2.16	0.74
1:A:1406:VAL:HG12	1:A:1410:PHE:CE1	2.21	0.74
2:B:1084:GLN:N	2:B:1084:GLN:NE2	2.35	0.74
1:A:1135:ARG:HH12	13:S:256:ALA:HB2	1.49	0.74
3:C:50:GLU:HG2	12:L:64:LEU:HD13	1.69	0.74
1:A:31:SER:HA	1:A:81:PHE:O	1.87	0.74
2:B:977:GLY:HA3	2:B:1099:VAL:HB	1.70	0.74
1:A:853:ASP:OD1	1:A:855:THR:N	2.21	0.74
1:A:1172:LEU:HD22	13:S:204:SER:CA	2.16	0.74
2:B:510:LYS:C	2:B:510:LYS:CD	2.61	0.74
7:G:122:ASN:ND2	7:G:125:SER:HB3	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:GLN:HE22	1:A:80:HIS:CD2	2.06	0.74
1:A:741:ASN:HD22	1:A:744:LYS:H	1.35	0.74
1:A:1239:ARG:HH22	1:A:1241:ARG:NH2	1.85	0.74
2:B:508:LEU:CB	2:B:510:LYS:N	2.50	0.74
2:B:508:LEU:HB2	2:B:510:LYS:H	1.52	0.74
9:I:111:THR:HG22	9:I:112:SER:N	2.03	0.74
10:J:7:CYS:SG	10:J:49:MET:HE3	2.27	0.74
1:A:337:ARG:CZ	1:A:839:ARG:NH1	2.50	0.74
1:A:897:TYR:N	1:A:897:TYR:HD1	1.85	0.74
2:B:515:HIS:HD2	2:B:517:THR:H	1.35	0.74
4:D:170:THR:CG2	4:D:172:LEU:HG	2.16	0.74
5:E:135:PHE:HD2	5:E:140:LEU:HD21	1.52	0.74
1:A:1170:ILE:HG23	1:A:1174:PHE:CE1	2.22	0.74
2:B:769:TYR:CE2	2:B:987:LYS:NZ	2.55	0.74
2:B:1142:GLY:HA3	6:F:88:TYR:HE2	1.52	0.74
1:A:1444:MET:CE	6:F:135:ARG:HB2	2.18	0.73
2:B:1180:PHE:HB3	2:B:1191:ILE:HD12	1.69	0.73
6:F:111:LEU:C	6:F:113:GLY:H	1.96	0.73
1:A:518:LYS:HB2	1:A:519:PRO:HD2	1.69	0.73
7:G:123:ALA:C	7:G:125:SER:H	1.96	0.73
1:A:364:VAL:HG12	1:A:458:HIS:HB3	1.71	0.73
1:A:1445:ILE:H	1:A:1445:ILE:HD12	1.53	0.73
2:B:827:ILE:HD12	2:B:1086:PHE:HD2	1.53	0.73
3:C:104:PHE:HD2	3:C:105:GLY:N	1.86	0.73
8:H:59:ILE:HG22	8:H:60:ALA:N	2.01	0.73
7:G:91:VAL:HG23	7:G:141:SER:O	1.88	0.73
9:I:101:PHE:HD1	9:I:101:PHE:H	1.34	0.73
8:H:36:CYS:HA	8:H:126:GLU:O	1.88	0.73
1:A:256:GLN:HE21	2:B:918:ILE:HD11	1.54	0.73
1:A:335:ARG:NH1	2:B:1206:GLU:OE2	2.22	0.73
1:A:265:LYS:HE2	1:A:322:VAL:CG1	2.19	0.73
1:A:903:ASN:HD22	1:A:904:THR:N	1.87	0.73
1:A:1283:VAL:CG1	13:S:256:ALA:C	2.62	0.73
3:C:6:PRO:HB3	3:C:25:VAL:HG12	1.69	0.73
4:D:144:THR:O	4:D:148:LEU:HB2	1.89	0.73
1:A:901:LEU:HG	1:A:926:GLN:HE21	1.53	0.73
4:D:130:LEU:C	4:D:132:GLN:H	1.97	0.73
2:B:1002:THR:CG2	2:B:1006:ILE:HD12	2.19	0.72
7:G:115:MET:HB2	7:G:116:PRO:HD2	1.70	0.72
1:A:1420:ASP:HB3	1:A:1422:ARG:HG3	1.71	0.72
1:A:1428:VAL:HG13	2:B:1151:LEU:HD21	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:145:VAL:HG12	7:G:146:LYS:N	2.03	0.72
1:A:648:ASN:O	1:A:652:VAL:HG23	1.88	0.72
1:A:979:SER:OG	1:A:980:ASP:N	2.22	0.72
1:A:1341:ILE:CG2	1:A:1342:GLU:H	2.03	0.72
2:B:801:LYS:O	10:J:52:THR:HG23	1.89	0.72
1:A:40:THR:HG21	1:A:259:GLU:OE2	1.89	0.72
1:A:55:ASP:C	1:A:57:ARG:N	2.46	0.72
1:A:288:ALA:HA	1:A:291:GLU:OE2	1.89	0.72
1:A:821:ARG:HB2	1:A:821:ARG:HH11	1.53	0.72
1:A:1057:VAL:HG12	1:A:1058:VAL:H	1.54	0.72
1:A:1402:PHE:CE1	1:A:1403:GLU:HG3	2.24	0.72
2:B:172:ILE:HD13	2:B:178:ASN:CB	2.19	0.72
2:B:873:THR:O	2:B:914:LYS:HA	1.88	0.72
5:E:213:ILE:HG12	5:E:214:CYS:H	1.54	0.72
6:F:111:LEU:HD12	6:F:111:LEU:H	1.54	0.72
7:G:80:LYS:O	7:G:80:LYS:HG2	1.87	0.72
9:I:59:VAL:O	9:I:60:GLN:HB2	1.88	0.72
1:A:289:ILE:C	1:A:291:GLU:H	1.95	0.72
1:A:310:GLY:O	1:A:312:PRO:HD2	1.89	0.72
3:C:45:ALA:CA	3:C:72:LEU:HD12	2.16	0.72
1:A:1385:THR:O	1:A:1388:GLY:N	2.21	0.72
2:B:773:MET:C	2:B:775:LYS:H	1.95	0.72
10:J:41:LEU:HD11	10:J:50:ILE:HG13	1.70	0.72
1:A:370:ILE:HG23	2:B:1105:ALA:HB2	1.72	0.72
1:A:668:ASP:HB3	1:A:743:VAL:HG23	1.71	0.72
1:A:1011:GLN:HE22	1:A:1015:VAL:HG21	1.52	0.72
1:A:55:ASP:CG	1:A:55:ASP:O	2.31	0.72
2:B:291:ILE:HD13	2:B:300:HIS:CD2	2.25	0.72
5:E:16:PHE:CZ	5:E:20:LYS:HE2	2.25	0.72
5:E:210:SER:C	5:E:211:TYR:CD1	2.68	0.72
9:I:34:TYR:CE2	9:I:36:GLU:HB3	2.25	0.72
1:A:1086:PHE:HE2	13:S:261:ILE:HD11	1.54	0.72
2:B:282:ILE:HD12	2:B:382:ILE:HD13	1.72	0.72
2:B:953:LEU:HD23	2:B:953:LEU:O	1.89	0.72
2:B:1031:LEU:HA	2:B:1055:ILE:HD13	1.72	0.71
7:G:43:GLY:HA3	7:G:80:LYS:HB3	1.70	0.71
8:H:44:VAL:O	8:H:44:VAL:HG12	1.89	0.71
1:A:215:SER:HB3	1:A:218:ASP:OD2	1.89	0.71
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.30	0.71
2:B:114:PRO:HG2	2:B:115:GLN:H	1.54	0.71
2:B:957:ASN:O	2:B:959:ASP:N	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:THR:HG23	1:A:382:PRO:HD2	1.70	0.71
1:A:666:ILE:HD11	2:B:1067:ARG:O	1.90	0.71
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.70	0.71
3:C:32:SER:O	3:C:36:VAL:HG23	1.89	0.71
9:I:71:SER:OG	9:I:83:ASN:HB2	1.90	0.71
13:S:271:CYS:SG	13:S:302:CYS:SG	2.89	0.71
1:A:375:THR:OG1	1:A:433:GLU:HB3	1.91	0.71
1:A:825:ILE:C	1:A:827:THR:H	1.96	0.71
1:A:1325:THR:O	5:E:148:GLU:HB2	1.90	0.71
2:B:123:THR:O	2:B:125:SER:N	2.22	0.71
2:B:313:MET:HE2	2:B:390:LEU:CD2	2.20	0.71
1:A:13:THR:O	2:B:1218:THR:HG22	1.90	0.71
1:A:49:LYS:HZ2	1:A:60:SER:HA	1.56	0.71
1:A:1172:LEU:HD21	13:S:204:SER:CA	2.21	0.71
2:B:363:HIS:O	2:B:364:ILE:HB	1.91	0.71
2:B:976:ILE:HD11	2:B:992:ILE:HA	1.71	0.71
2:B:1166:CYS:O	2:B:1168:LEU:N	2.22	0.71
4:D:54:GLU:O	4:D:58:VAL:HG23	1.89	0.71
9:I:56:ALA:HB2	9:I:89:GLN:HG3	1.72	0.71
1:A:225:ASN:ND2	1:A:228:PHE:N	2.32	0.71
1:A:463:ILE:HB	1:A:464:PRO:HD2	1.72	0.71
1:A:1436:ILE:HD13	2:B:1139:ILE:HG23	1.73	0.71
2:B:579:ARG:CB	2:B:586:TRP:HE1	2.00	0.71
2:B:986:GLN:NE2	2:B:1022:THR:HG21	2.05	0.71
1:A:59:GLY:HA2	1:A:67:CYS:SG	2.30	0.71
1:A:90:VAL:HG12	1:A:91:PHE:N	2.03	0.71
2:B:53:GLN:HG2	2:B:547:VAL:HG22	1.72	0.71
2:B:604:ARG:NH2	2:B:613:VAL:O	2.23	0.71
2:B:1102:LYS:O	2:B:1103:ILE:C	2.34	0.71
3:C:73:GLN:NE2	3:C:74:SER:H	1.89	0.71
12:L:32:ALA:HB3	12:L:55:ILE:CD1	2.21	0.71
1:A:441:PRO:HD2	1:A:498:ARG:NH2	2.06	0.70
1:A:605:MET:HE1	1:A:617:VAL:HA	1.73	0.70
2:B:261:ARG:O	2:B:267:ARG:HD3	1.90	0.70
2:B:1184:GLY:C	2:B:1186:ASP:H	1.96	0.70
1:A:135:PHE:C	1:A:137:ALA:H	1.97	0.70
1:A:315:LEU:HD23	1:A:321:PRO:HA	1.73	0.70
2:B:199:MET:HE2	2:B:492:LEU:HD23	1.72	0.70
2:B:510:LYS:HB2	2:B:511:PRO:CD	2.21	0.70
2:B:563:MET:CE	2:B:580:VAL:HB	2.21	0.70
3:C:263:THR:C	3:C:265:MET:H	1.99	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:THR:HB	2:B:1103:ILE:HD12	1.72	0.70
1:A:384:ASN:OD1	1:A:388:LEU:HD12	1.92	0.70
1:A:903:ASN:HD22	1:A:903:ASN:C	1.99	0.70
1:A:1147:THR:HG22	1:A:1149:ALA:H	1.56	0.70
1:A:95:PHE:HD1	1:A:234:MET:HG2	1.57	0.70
1:A:152:VAL:HG13	1:A:153:PRO:HD2	1.73	0.70
1:A:370:ILE:HG22	1:A:374:LEU:CD1	2.21	0.70
1:A:567:LYS:NZ	8:H:46:LEU:HB2	2.07	0.70
1:A:897:TYR:N	1:A:897:TYR:CD1	2.56	0.70
8:H:102:TYR:N	8:H:102:TYR:CD2	2.58	0.70
1:A:888:GLY:O	1:A:940:ARG:NH2	2.25	0.70
1:A:1435:PRO:O	1:A:1436:ILE:HG13	1.91	0.70
2:B:496:ARG:HB3	2:B:496:ARG:HH11	1.56	0.70
1:A:339:ASN:HB3	2:B:1117:GLN:NE2	2.05	0.70
1:A:414:ASP:OD1	1:A:416:ARG:HG3	1.91	0.70
1:A:1116:LEU:N	1:A:1308:THR:CG2	2.54	0.70
1:A:1279:ILE:HD11	1:A:1316:VAL:HG21	1.72	0.70
2:B:857:ARG:HG2	2:B:858:SER:H	1.55	0.70
5:E:135:PHE:CD2	5:E:140:LEU:HD21	2.26	0.70
1:A:608:ILE:HG23	1:A:969:GLN:OE1	1.91	0.70
1:A:698:GLN:HA	9:I:97:MET:O	1.90	0.70
1:A:870:GLU:HG2	5:E:208:TYR:CD2	2.27	0.70
1:A:1057:VAL:HG12	1:A:1058:VAL:N	2.06	0.70
4:D:137:ASN:C	4:D:137:ASN:HD22	2.00	0.70
5:E:202:SER:OG	5:E:204:THR:HG22	1.91	0.70
1:A:852:TYR:CD1	6:F:136:ARG:HB3	2.27	0.70
1:A:1280:GLU:O	1:A:1281:ARG:O	2.10	0.70
2:B:292:ILE:HD13	2:B:326:ASP:HA	1.73	0.70
10:J:2:ILE:HG12	10:J:57:ILE:HD12	1.74	0.70
1:A:1242:VAL:HG12	1:A:1243:VAL:H	1.56	0.70
2:B:857:ARG:HH21	2:B:942:ARG:CZ	2.04	0.70
1:A:239:LEU:HD12	1:A:240:PRO:HD2	1.74	0.70
3:C:191:TYR:HD2	3:C:201:TRP:CD1	2.09	0.70
11:K:67:PHE:C	11:K:68:PHE:HD2	1.98	0.70
1:A:567:LYS:HD2	1:A:568:PRO:HD2	1.73	0.69
2:B:510:LYS:HB2	2:B:511:PRO:HD2	1.74	0.69
2:B:637:LEU:O	2:B:690:VAL:HG13	1.90	0.69
2:B:831:SER:OG	2:B:840:ILE:HD11	1.92	0.69
3:C:105:GLY:HA3	3:C:149:LYS:O	1.92	0.69
2:B:483:LEU:HD11	2:B:491:THR:HG23	1.73	0.69
2:B:546:SER:OG	2:B:631:GLY:N	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:2:ASP:O	5:E:3:GLN:HG2	1.92	0.69
13:S:291:GLU:N	13:S:292:PRO:CD	2.53	0.69
1:A:855:THR:CG2	1:A:857:ARG:HE	1.99	0.69
3:C:147:LEU:HD12	3:C:151:GLN:O	1.91	0.69
1:A:347:PHE:H	2:B:1107:ALA:HA	1.57	0.69
1:A:1334:ASP:O	1:A:1336:MET:N	2.25	0.69
2:B:705:MET:HE1	2:B:742:GLU:OE1	1.92	0.69
2:B:1023:VAL:O	2:B:1027:ILE:HG13	1.93	0.69
3:C:238:ILE:CG2	3:C:242:GLN:HB2	2.22	0.69
5:E:124:VAL:HA	5:E:132:ILE:HD12	1.73	0.69
13:S:271:CYS:SG	13:S:274:CYS:SG	2.90	0.69
1:A:69:THR:O	1:A:71:GLN:N	2.25	0.69
1:A:265:LYS:N	1:A:265:LYS:HD2	2.06	0.69
1:A:367:PRO:HB3	1:A:465:TYR:O	1.91	0.69
2:B:862:GLN:HG2	2:B:963:PHE:CD1	2.28	0.69
1:A:92:HIS:O	1:A:94:GLY:N	2.25	0.69
1:A:407:ARG:HG2	1:A:430:TRP:CZ2	2.27	0.69
1:A:1283:VAL:HG12	1:A:1284:MET:H	1.58	0.69
9:I:56:ALA:HB2	9:I:89:GLN:HG2	1.72	0.69
11:K:12:LEU:H	11:K:12:LEU:HD12	1.58	0.69
1:A:1325:THR:HG22	1:A:1326:ARG:HG3	1.74	0.69
2:B:510:LYS:CB	2:B:511:PRO:HD2	2.21	0.69
2:B:606:LYS:HD2	2:B:608:ASP:OD2	1.92	0.69
1:A:606:LEU:HG	1:A:613:ILE:HD12	1.74	0.69
1:A:711:ARG:CG	9:I:97:MET:HE2	2.22	0.69
1:A:889:SER:HB3	1:A:1297:GLU:HG2	1.75	0.69
1:A:1261:LYS:HA	1:A:1264:GLU:HB3	1.73	0.69
1:A:1443:VAL:O	1:A:1444:MET:HG3	1.91	0.69
2:B:200:GLY:HA2	2:B:202:TYR:CE2	2.28	0.69
2:B:294:ASP:OD2	2:B:294:ASP:N	2.24	0.69
12:L:38:LEU:O	12:L:39:SER:HB3	1.91	0.69
1:A:84:ILE:HD11	1:A:270:LEU:HD13	1.74	0.69
1:A:367:PRO:HG2	1:A:370:ILE:HG13	1.74	0.69
2:B:824:ILE:HG12	10:J:48:ARG:NH1	2.08	0.69
2:B:871:THR:HG22	2:B:872:GLU:O	1.93	0.69
1:A:535:THR:HG21	1:A:616:VAL:HA	1.73	0.69
1:A:567:LYS:CD	1:A:568:PRO:HD2	2.23	0.69
1:A:1135:ARG:HH11	13:S:256:ALA:HB2	1.57	0.69
2:B:112:LEU:CD1	2:B:113:TYR:H	2.03	0.69
2:B:281:PRO:HG2	2:B:284:ILE:HG13	1.74	0.69
2:B:282:ILE:CD1	2:B:382:ILE:HD13	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:552:MET:HA	2:B:555:ILE:HB	1.75	0.69
2:B:983:ARG:NH1	2:B:1028:GLU:OE1	2.26	0.69
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.74	0.69
3:C:242:GLN:HA	3:C:245:VAL:HG23	1.73	0.69
2:B:839:MET:CE	2:B:1010:LEU:HD21	2.23	0.68
2:B:948:ILE:HG22	2:B:949:VAL:O	1.93	0.68
7:G:96:GLN:HA	7:G:121:PHE:CE2	2.28	0.68
1:A:996:ASN:C	1:A:998:LEU:HD12	2.18	0.68
1:A:1079:MET:CE	1:A:1101:LEU:HD23	2.23	0.68
7:G:106:MET:HG3	7:G:157:ILE:O	1.93	0.68
8:H:81:PRO:HB2	8:H:82:PRO:HD2	1.74	0.68
2:B:1165:ILE:HG22	2:B:1166:CYS:H	1.59	0.68
5:E:177:ARG:C	5:E:212:ARG:HD3	2.18	0.68
6:F:85:MET:HE1	6:F:148:VAL:HG12	1.74	0.68
7:G:1:MET:HE2	7:G:1:MET:O	1.92	0.68
1:A:390:GLN:HE21	1:A:394:ASN:ND2	1.91	0.68
3:C:6:PRO:HB3	3:C:25:VAL:CG1	2.24	0.68
6:F:119:ARG:HH11	6:F:119:ARG:HG3	1.57	0.68
1:A:858:ASN:ND2	1:A:860:LEU:H	1.92	0.68
2:B:294:ASP:C	2:B:296:GLU:H	2.01	0.68
2:B:986:GLN:OE1	2:B:986:GLN:HA	1.92	0.68
5:E:164:LEU:HD13	5:E:211:TYR:CE2	2.27	0.68
1:A:1237:ILE:HG22	1:A:1238:ILE:H	1.55	0.68
2:B:821:GLN:HE22	2:B:851:PHE:H	1.42	0.68
1:A:134:ARG:O	1:A:134:ARG:HG2	1.94	0.68
1:A:332:LYS:HG3	1:A:333:GLU:HG2	1.75	0.68
1:A:337:ARG:NH2	1:A:839:ARG:HH12	1.90	0.68
2:B:204:ILE:C	2:B:205:ILE:HD12	2.19	0.68
2:B:1146:PHE:CD1	2:B:1146:PHE:O	2.47	0.68
5:E:207:ARG:HB3	5:E:207:ARG:HH11	1.58	0.68
1:A:709:THR:HG22	1:A:712:GLU:H	1.59	0.68
1:A:901:LEU:HD22	1:A:919:ILE:CG2	2.24	0.68
2:B:597:MET:HA	2:B:597:MET:HE3	1.75	0.68
6:F:97:ARG:NH2	6:F:108:PHE:HE1	1.92	0.68
1:A:133:LYS:C	1:A:135:PHE:H	2.02	0.68
1:A:901:LEU:N	1:A:926:GLN:NE2	2.36	0.68
2:B:758:PHE:HE1	2:B:1027:ILE:HG22	1.56	0.68
1:A:837:ILE:HA	1:A:840:ARG:HD3	1.76	0.68
1:A:1081:LEU:HD21	1:A:1098:VAL:HG21	1.74	0.68
10:J:7:CYS:SG	10:J:46:CYS:HA	2.34	0.68
1:A:1364:ASN:OD1	1:A:1366:ARG:HD2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:642:ASP:HB3	2:B:649:LYS:CD	2.23	0.67
2:B:1115:THR:O	2:B:1116:ARG:HB2	1.92	0.67
5:E:143:ASN:HD22	5:E:146:HIS:CE1	2.12	0.67
13:S:279:VAL:HG13	13:S:298:THR:C	2.19	0.67
1:A:519:PRO:HG2	1:A:624:SER:O	1.94	0.67
1:A:1192:LEU:HG	1:A:1193:LEU:N	2.09	0.67
1:A:1227:ILE:HG22	1:A:1228:TRP:N	2.09	0.67
1:A:1410:PHE:HA	2:B:1212:ILE:HD11	1.75	0.67
2:B:378:LEU:HD12	2:B:378:LEU:O	1.94	0.67
7:G:127:PRO:HG2	7:G:138:THR:HG21	1.74	0.67
1:A:1121:GLU:CG	1:A:1122:PRO:HD2	2.24	0.67
1:A:1376:THR:OG1	1:A:1377:THR:N	2.23	0.67
2:B:594:ALA:HA	2:B:617:ARG:NH1	2.09	0.67
1:A:49:LYS:NZ	1:A:60:SER:HA	2.09	0.67
2:B:37:PHE:CE1	2:B:41:LYS:HG3	2.29	0.67
2:B:205:ILE:HD12	2:B:205:ILE:N	2.10	0.67
1:A:1100:ARG:HH21	1:A:1351:GLU:CG	2.07	0.67
2:B:273:LEU:CB	2:B:276:ILE:HD12	2.21	0.67
2:B:880:THR:O	2:B:881:ASN:HB2	1.94	0.67
2:B:1010:LEU:HD12	2:B:1011:ILE:H	1.60	0.67
6:F:103:MET:HE1	7:G:65:ASP:HB2	1.76	0.67
1:A:53:LEU:HD23	1:A:54:ASN:H	1.54	0.67
1:A:1342:GLU:CD	5:E:198:ILE:HG21	2.18	0.67
2:B:854:LEU:HB3	2:B:856:PHE:HE1	1.60	0.67
3:C:73:GLN:HB3	3:C:131:HIS:H	1.60	0.67
1:A:567:LYS:HD3	8:H:95:TYR:CG	2.30	0.67
1:A:1089:VAL:O	1:A:1089:VAL:HG12	1.95	0.67
7:G:13:LEU:HD23	7:G:14:HIS:N	2.10	0.67
1:A:709:THR:HB	1:A:712:GLU:HB2	1.76	0.67
1:A:1083:THR:HG21	1:A:1085:HIS:CE1	2.30	0.67
1:A:1447:GLU:OE2	7:G:23:LYS:HB2	1.94	0.67
7:G:91:VAL:HB	7:G:139:ILE:O	1.95	0.67
1:A:41:MET:O	1:A:50:ILE:HG13	1.94	0.67
1:A:337:ARG:HD3	2:B:1132:GLU:OE1	1.95	0.67
1:A:1118:VAL:HG12	1:A:1327:ILE:HG13	1.77	0.67
3:C:86:CYS:O	3:C:88:CYS:N	2.27	0.67
12:L:58:LYS:O	12:L:59:ALA:O	2.13	0.67
1:A:829:VAL:HG13	2:B:507:LYS:HG2	1.76	0.67
1:A:870:GLU:HB2	5:E:204:THR:HG21	1.76	0.67
1:A:886:ILE:CD1	1:A:943:LEU:HB3	2.22	0.67
1:A:982:THR:O	1:A:985:ASP:HB2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:VAL:HG12	2:B:178:ASN:ND2	2.09	0.67
2:B:654:ARG:H	2:B:657:HIS:HD2	1.41	0.67
2:B:1159:ARG:HB3	2:B:1159:ARG:NH1	2.09	0.67
2:B:1198:TYR:CE1	2:B:1201:LYS:HD2	2.30	0.67
9:I:34:TYR:HE2	9:I:36:GLU:HB3	1.60	0.67
1:A:1104:ILE:O	1:A:1107:VAL:N	2.23	0.66
1:A:1161:THR:OG1	1:A:1170:ILE:HD11	1.95	0.66
2:B:240:ILE:HG22	2:B:254:LEU:HB3	1.77	0.66
2:B:622:LYS:HE3	9:I:59:VAL:HG22	1.76	0.66
3:C:47:ASP:HA	12:L:69:ALA:HB3	1.77	0.66
5:E:198:ILE:HD11	5:E:212:ARG:HG3	1.76	0.66
13:S:265:VAL:HG11	13:S:278:LYS:HA	1.76	0.66
13:S:302:CYS:SG	13:S:304:ASN:ND2	2.68	0.66
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.75	0.66
7:G:73:LYS:HE2	7:G:74:TYR:O	1.95	0.66
1:A:265:LYS:HD2	1:A:265:LYS:H	1.60	0.66
1:A:1329:THR:H	1:A:1335:ILE:CD1	1.95	0.66
2:B:172:ILE:HD13	2:B:178:ASN:HB2	1.76	0.66
2:B:546:SER:OG	2:B:630:ALA:HA	1.95	0.66
2:B:750:GLY:O	2:B:751:VAL:C	2.39	0.66
2:B:898:LEU:HB2	12:L:58:LYS:NZ	2.10	0.66
12:L:31:CYS:HB3	12:L:34:CYS:C	2.21	0.66
1:A:90:VAL:HG13	1:A:297:GLN:OE1	1.96	0.66
1:A:254:GLU:HB2	2:B:935:ARG:HH22	1.60	0.66
1:A:997:LEU:HD13	1:A:1018:PHE:HE2	1.60	0.66
1:A:1331:SER:OG	1:A:1333:ILE:HG22	1.94	0.66
2:B:900:ALA:O	2:B:903:VAL:HG23	1.95	0.66
2:B:1099:VAL:HG13	2:B:1100:ASP:N	2.10	0.66
1:A:866:PHE:C	1:A:867:ILE:HD12	2.21	0.66
2:B:95:ILE:HG13	2:B:130:VAL:HG22	1.77	0.66
2:B:1065:GLN:HB2	3:C:201:TRP:CZ3	2.31	0.66
3:C:43:THR:HG22	3:C:44:LEU:N	2.10	0.66
8:H:84:ALA:CB	8:H:87:ARG:HB2	2.25	0.66
1:A:50:ILE:C	1:A:52:GLY:H	2.03	0.66
1:A:489:LEU:HD12	1:A:489:LEU:C	2.21	0.66
1:A:858:ASN:C	1:A:858:ASN:ND2	2.53	0.66
1:A:1283:VAL:HG12	1:A:1284:MET:N	2.11	0.66
5:E:157:SER:C	5:E:159:ASP:H	2.04	0.66
1:A:908:LEU:CD1	1:A:983:ILE:HD11	2.25	0.66
1:A:1283:VAL:O	1:A:1306:LEU:HA	1.96	0.66
1:A:1445:ILE:HD12	1:A:1445:ILE:N	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:705:MET:H	2:B:710:LEU:CD1	2.09	0.66
2:B:1065:GLN:HB3	2:B:1069:PHE:O	1.95	0.66
9:I:58:VAL:HG13	9:I:62:ILE:CG1	2.25	0.66
13:S:218:ILE:CA	13:S:219:ALA:CA	2.73	0.66
1:A:63:ARG:HG2	1:A:74:MET:SD	2.36	0.66
1:A:1313:LEU:HD23	1:A:1338:VAL:CG2	2.25	0.66
1:A:1437:GLY:HA3	6:F:88:TYR:CD2	2.30	0.66
2:B:770:GLN:HG2	2:B:983:ARG:O	1.96	0.66
2:B:910:VAL:HG12	2:B:911:ILE:N	2.11	0.66
12:L:28:LYS:HB2	12:L:39:SER:HB2	1.78	0.66
2:B:705:MET:H	2:B:710:LEU:HD12	1.61	0.66
2:B:991:GLY:O	2:B:992:ILE:HB	1.94	0.66
1:A:34:LYS:HB2	1:A:36:ARG:HH21	1.60	0.66
1:A:275:SER:O	1:A:279:LEU:HG	1.96	0.66
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.25	0.66
2:B:589:VAL:CG1	2:B:590:HIS:H	2.06	0.66
2:B:616:ILE:HD12	2:B:616:ILE:N	2.11	0.66
2:B:882:THR:CG2	2:B:884:ARG:HB2	2.25	0.66
2:B:899:ILE:CG2	2:B:903:VAL:HG21	2.25	0.66
2:B:1159:ARG:NE	2:B:1193:GLN:HE21	1.94	0.66
5:E:182:ASP:O	5:E:185:ALA:N	2.28	0.66
8:H:41:ASP:O	8:H:42:ILE:HG13	1.96	0.66
13:S:235:ASP:CA	13:S:242:LYS:HE3	2.26	0.66
1:A:264:PHE:O	1:A:267:ALA:HB3	1.96	0.65
1:A:886:ILE:HG22	1:A:887:GLY:N	2.11	0.65
2:B:802:PRO:HA	2:B:822:ASN:HD21	1.61	0.65
5:E:157:SER:OG	5:E:160:GLU:HG3	1.95	0.65
1:A:591:PHE:HA	1:A:595:THR:HG21	1.77	0.65
2:B:65:GLU:HG3	2:B:66:ASP:N	2.07	0.65
2:B:579:ARG:HD2	2:B:586:TRP:CZ2	2.30	0.65
2:B:322:PHE:HZ	9:I:30:ARG:HB3	1.61	0.65
2:B:953:LEU:CD2	2:B:965:LYS:HB2	2.26	0.65
3:C:63:ILE:CA	3:C:66:ARG:HG3	2.26	0.65
1:A:1291:VAL:HG13	1:A:1292:PRO:CD	2.25	0.65
2:B:23:ALA:HB1	2:B:24:PRO:CD	2.23	0.65
2:B:411:PRO:O	2:B:414:ALA:HB3	1.95	0.65
2:B:981:ALA:HB2	2:B:987:LYS:HA	1.79	0.65
3:C:241:ASP:O	3:C:245:VAL:HG23	1.96	0.65
5:E:78:LEU:HD23	5:E:79:TRP:N	2.11	0.65
12:L:61:THR:HG21	12:L:63:ARG:HG2	1.78	0.65
1:A:75:ASN:O	1:A:76:GLU:HB3	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:CYS:N	1:A:114:LEU:HD21	2.11	0.65
2:B:856:PHE:CD1	2:B:856:PHE:N	2.64	0.65
3:C:50:GLU:HG2	12:L:64:LEU:CD1	2.25	0.65
3:C:174:ALA:O	3:C:175:ALA:HB2	1.95	0.65
1:A:1161:THR:C	1:A:1163:ILE:H	2.04	0.65
1:A:1195:LEU:HD11	1:A:1267:MET:HE1	1.78	0.65
2:B:294:ASP:O	2:B:296:GLU:N	2.30	0.65
2:B:687:GLU:O	2:B:689:LEU:HG	1.96	0.65
5:E:55:ARG:C	5:E:57:MET:H	2.03	0.65
8:H:123:MET:HE1	8:H:142:LEU:CD1	2.26	0.65
1:A:55:ASP:N	1:A:56:PRO:HD3	2.11	0.65
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.29	0.65
1:A:1080:THR:HG21	13:S:284:LEU:HD13	1.77	0.65
2:B:594:ALA:HA	2:B:617:ARG:HH12	1.60	0.65
2:B:773:MET:C	2:B:775:LYS:N	2.48	0.65
2:B:794:ASN:O	2:B:795:ILE:HD12	1.96	0.65
3:C:5:GLY:O	3:C:7:GLN:HG3	1.96	0.65
3:C:92:CYS:SG	3:C:94:LYS:HB3	2.36	0.65
4:D:211:LEU:HD23	4:D:214:LEU:HD12	1.79	0.65
1:A:538:ASP:OD2	8:H:22:LYS:HB2	1.96	0.65
2:B:365:THR:HG23	2:B:367:LEU:H	1.61	0.65
1:A:689:LYS:HE2	1:A:721:PHE:CE2	2.32	0.65
2:B:322:PHE:CZ	9:I:30:ARG:HB3	2.32	0.65
3:C:107:SER:C	3:C:109:SER:H	2.04	0.65
12:L:60:ARG:HG2	12:L:61:THR:H	1.60	0.65
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.77	0.65
1:A:550:LEU:HD22	1:A:556:TRP:CE2	2.31	0.65
2:B:820:GLY:N	2:B:1091:TYR:OH	2.29	0.65
7:G:14:HIS:HD2	7:G:16:SER:CB	2.03	0.65
9:I:101:PHE:N	9:I:101:PHE:HD1	1.91	0.65
1:A:47:ARG:NH2	1:A:255:SER:H	1.95	0.64
1:A:593:GLU:O	1:A:595:THR:N	2.30	0.64
1:A:820:GLY:C	1:A:822:GLU:H	2.05	0.64
2:B:54:PHE:CE2	2:B:59:LEU:HD13	2.32	0.64
2:B:217:ARG:NE	2:B:405:ARG:HB2	2.10	0.64
2:B:825:VAL:HG22	2:B:1010:LEU:HB3	1.79	0.64
2:B:1223:ASP:O	2:B:1224:PHE:HB2	1.96	0.64
7:G:143:ILE:HG22	7:G:144:ARG:N	2.11	0.64
2:B:789:MET:HE2	2:B:965:LYS:O	1.98	0.64
1:A:14:VAL:N	1:A:1432:GLN:HE22	1.88	0.64
1:A:243:PRO:O	1:A:246:VAL:HG23	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.78	0.64
1:A:1334:ASP:C	1:A:1336:MET:N	2.55	0.64
1:A:1423:GLY:O	1:A:1424:VAL:C	2.40	0.64
2:B:37:PHE:HD2	2:B:542:MET:SD	2.21	0.64
2:B:39:ARG:HH21	2:B:665:GLU:CG	2.10	0.64
2:B:237:VAL:HG22	2:B:257:LYS:HA	1.78	0.64
2:B:361:LEU:HD21	2:B:377:PHE:CD2	2.32	0.64
2:B:797:TYR:C	2:B:798:TYR:HD2	2.04	0.64
2:B:835:GLN:HA	2:B:1013:ASN:ND2	2.10	0.64
4:D:47:LEU:HD13	4:D:48:ILE:H	1.63	0.64
8:H:91:ASP:C	8:H:93:TYR:H	2.04	0.64
1:A:370:ILE:HG22	1:A:374:LEU:HD11	1.80	0.64
1:A:550:LEU:HD22	1:A:556:TRP:NE1	2.11	0.64
1:A:1409:LEU:O	1:A:1412:ALA:HB3	1.98	0.64
2:B:227:LYS:HB2	2:B:395:GLN:OE1	1.97	0.64
2:B:827:ILE:HD12	2:B:1086:PHE:CD2	2.32	0.64
2:B:952:VAL:HG12	2:B:953:LEU:N	2.11	0.64
2:B:975:GLN:NE2	2:B:1100:ASP:OD2	2.30	0.64
7:G:138:THR:CG2	7:G:139:ILE:H	1.95	0.64
13:S:269:PHE:HE2	13:S:297:CYS:SG	2.14	0.64
1:A:115:LEU:O	1:A:122:MET:HE2	1.97	0.64
1:A:535:THR:HG21	1:A:617:VAL:H	1.63	0.64
1:A:1029:ARG:HH11	1:A:1029:ARG:CG	2.09	0.64
1:A:1199:ARG:HH22	13:S:241:LEU:CD1	2.02	0.64
1:A:1422:ARG:HH22	2:B:1224:PHE:C	2.06	0.64
1:A:1423:GLY:O	1:A:1426:GLU:N	2.31	0.64
2:B:54:PHE:HE1	2:B:414:ALA:HA	1.62	0.64
2:B:1060:ARG:HG2	2:B:1060:ARG:HH11	1.61	0.64
1:A:67:CYS:O	1:A:70:CYS:HB3	1.96	0.64
1:A:556:TRP:C	1:A:558:GLY:H	2.05	0.64
1:A:1074:GLU:HB3	1:A:1075:PRO:HD3	1.80	0.64
1:A:1148:ILE:O	1:A:1148:ILE:HG22	1.98	0.64
2:B:955:THR:HG22	2:B:956:THR:N	2.12	0.64
3:C:34:ARG:HA	3:C:37:MET:HE3	1.79	0.64
8:H:102:TYR:N	8:H:102:TYR:HD2	1.96	0.64
1:A:567:LYS:HG3	1:A:568:PRO:HD2	1.80	0.64
1:A:783:THR:HG21	1:A:815:PHE:CZ	2.33	0.64
1:A:1035:TYR:O	1:A:1037:LEU:N	2.25	0.64
2:B:315:LYS:N	2:B:316:PRO:HD2	2.11	0.64
3:C:179:GLU:HG2	3:C:180:TYR:N	2.12	0.64
6:F:86:THR:HG23	6:F:89:GLU:OE1	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:111:THR:CG2	7:G:113:HIS:H	2.04	0.64
1:A:1072:ILE:O	1:A:1075:PRO:HG2	1.98	0.64
2:B:261:ARG:NH1	2:B:261:ARG:HB3	2.11	0.64
2:B:1156:ASP:O	2:B:1157:ALA:O	2.15	0.64
2:B:1224:PHE:CE2	5:E:171:LYS:HG3	2.32	0.64
4:D:35:LEU:HD12	4:D:35:LEU:N	2.12	0.64
13:S:279:VAL:HG13	13:S:298:THR:O	1.98	0.64
13:S:282:TYR:CE2	13:S:296:PHE:HB2	2.33	0.64
1:A:768:GLN:CG	1:A:816:HIS:HA	2.22	0.64
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.13	0.64
1:A:1428:VAL:HG13	2:B:1151:LEU:CD2	2.28	0.64
2:B:63:ILE:HA	2:B:421:PHE:CE2	2.33	0.64
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.79	0.64
3:C:235:VAL:HG13	10:J:13:VAL:HG23	1.79	0.64
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.78	0.64
1:A:642:CYS:O	1:A:645:LEU:N	2.27	0.64
1:A:853:ASP:OD1	1:A:855:THR:CB	2.40	0.64
1:A:1120:LEU:O	1:A:1323:ASP:HB2	1.98	0.64
1:A:1206:ASP:O	1:A:1274:ARG:NH1	2.31	0.64
2:B:446:LEU:O	2:B:447:ALA:HB3	1.97	0.64
2:B:508:LEU:HB2	2:B:510:LYS:N	2.10	0.64
2:B:859:TYR:HD1	2:B:859:TYR:H	1.44	0.64
1:A:17:VAL:HG23	1:A:1421:CYS:SG	2.38	0.63
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	1.80	0.63
2:B:390:LEU:O	2:B:392:ARG:HG3	1.97	0.63
2:B:737:THR:HG21	9:I:66:PRO:HA	1.79	0.63
3:C:143:LEU:HD12	3:C:145:CYS:H	1.64	0.63
9:I:113:ASP:O	9:I:114:GLN:HG3	1.98	0.63
11:K:12:LEU:HD21	11:K:18:LYS:HG2	1.80	0.63
1:A:25:GLU:H	1:A:25:GLU:CD	2.06	0.63
1:A:845:LEU:HB3	1:A:848:ILE:HD12	1.80	0.63
1:A:849:MET:CE	1:A:1061:GLY:HA2	2.28	0.63
2:B:117:ALA:HA	2:B:122:LEU:HD12	1.78	0.63
12:L:28:LYS:HB2	12:L:39:SER:CB	2.28	0.63
1:A:1080:THR:O	1:A:1081:LEU:HD22	1.97	0.63
2:B:37:PHE:CE2	2:B:542:MET:HA	2.27	0.63
3:C:35:ARG:NH1	11:K:41:THR:N	2.47	0.63
7:G:14:HIS:ND1	7:G:15:PRO:HD2	2.12	0.63
8:H:81:PRO:CB	8:H:82:PRO:CD	2.77	0.63
1:A:637:LYS:HB3	1:A:641:VAL:HG21	1.81	0.63
1:A:706:HIS:CE1	13:S:257:GLN:OE1	2.51	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1051:THR:HB	2:B:1054:GLY:H	1.64	0.63
3:C:35:ARG:NH1	11:K:41:THR:H	1.96	0.63
8:H:93:TYR:HB3	8:H:144:ILE:O	1.98	0.63
1:A:265:LYS:O	1:A:266:LEU:C	2.41	0.63
7:G:6:ASP:O	7:G:7:LEU:HD23	1.98	0.63
7:G:14:HIS:CE1	7:G:15:PRO:HD2	2.34	0.63
1:A:704:ALA:O	1:A:705:LYS:HB2	1.97	0.63
2:B:508:LEU:HB2	2:B:510:LYS:CA	2.28	0.63
2:B:511:PRO:C	2:B:513:GLN:N	2.51	0.63
8:H:42:ILE:HG23	8:H:95:TYR:CE1	2.34	0.63
1:A:49:LYS:HZ1	1:A:61:ILE:CG1	1.90	0.63
1:A:367:PRO:HA	1:A:463:ILE:O	1.99	0.63
1:A:922:ASP:OD1	1:A:924:LYS:N	2.32	0.63
2:B:604:ARG:NH2	2:B:614:SER:HA	2.14	0.63
3:C:235:VAL:HG21	10:J:6:ARG:NH2	2.14	0.63
1:A:534:LEU:O	1:A:574:GLY:HA3	1.98	0.63
1:A:305:ASP:CG	1:A:326:ARG:HD2	2.24	0.63
2:B:519:TRP:C	2:B:519:TRP:CD1	2.77	0.63
2:B:604:ARG:HH22	2:B:614:SER:HA	1.62	0.63
2:B:1149:GLU:O	2:B:1151:LEU:N	2.32	0.63
9:I:2:THR:O	9:I:3:THR:C	2.41	0.63
1:A:61:ILE:O	1:A:63:ARG:N	2.32	0.62
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.80	0.62
1:A:1230:GLU:O	1:A:1232:ASN:N	2.32	0.62
2:B:292:ILE:HD11	2:B:327:ARG:H	1.64	0.62
4:D:144:THR:HG21	7:G:46:LEU:HD13	1.81	0.62
8:H:89:LEU:HB3	8:H:91:ASP:OD1	1.98	0.62
1:A:283:GLY:O	1:A:285:PRO:HD3	1.99	0.62
2:B:284:ILE:HD13	2:B:333:PHE:HD2	1.64	0.62
2:B:855:PHE:CD1	2:B:855:PHE:C	2.75	0.62
2:B:1020:ARG:HH11	2:B:1020:ARG:CG	2.09	0.62
2:B:1099:VAL:HG22	2:B:1103:ILE:HD13	1.80	0.62
2:B:1147:LEU:C	2:B:1147:LEU:HD23	2.24	0.62
3:C:147:LEU:HB2	3:C:151:GLN:CB	2.29	0.62
5:E:192:ARG:HH11	5:E:192:ARG:HG3	1.64	0.62
7:G:49:LEU:HD21	7:G:77:VAL:HG23	1.80	0.62
7:G:126:ASN:HD22	7:G:127:PRO:HA	1.63	0.62
2:B:526:GLU:OE2	2:B:752:ALA:HB2	1.98	0.62
5:E:86:PRO:O	5:E:114:ASN:HB2	1.99	0.62
7:G:34:VAL:HG12	7:G:45:ILE:HG21	1.80	0.62
11:K:47:ARG:HB3	11:K:47:ARG:NH1	2.12	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:GLY:O	1:A:169:ASN:C	2.43	0.62
1:A:265:LYS:HE2	1:A:322:VAL:HG13	1.81	0.62
1:A:549:MET:HE1	1:A:656:TRP:HD1	1.64	0.62
1:A:683:ILE:HG21	1:A:801:GLU:HG3	1.80	0.62
1:A:1402:PHE:O	1:A:1404:GLU:N	2.32	0.62
2:B:129:PHE:HA	2:B:165:VAL:O	1.99	0.62
7:G:117:GLN:C	7:G:119:LEU:H	2.07	0.62
8:H:40:LEU:CD1	8:H:123:MET:HB2	2.27	0.62
9:I:87:GLN:O	9:I:89:GLN:OE1	2.18	0.62
9:I:88:SER:C	9:I:90:GLN:H	2.07	0.62
13:S:274:CYS:O	13:S:276:GLU:N	2.32	0.62
1:A:1172:LEU:CG	13:S:204:SER:CA	2.77	0.62
1:A:1394:THR:HG23	1:A:1398:MET:HE3	1.82	0.62
2:B:604:ARG:NH1	2:B:691:GLU:OE2	2.33	0.62
2:B:952:VAL:HG12	2:B:953:LEU:H	1.64	0.62
2:B:999:MET:HA	2:B:999:MET:HE3	1.81	0.62
3:C:75:MET:HE2	3:C:239:PRO:HD3	1.81	0.62
6:F:97:ARG:NH2	6:F:108:PHE:CE1	2.68	0.62
10:J:5:VAL:HG12	10:J:6:ARG:HG3	1.80	0.62
1:A:708:MET:O	1:A:709:THR:O	2.17	0.62
1:A:1279:ILE:HD11	1:A:1316:VAL:CG2	2.29	0.62
2:B:780:VAL:HG12	2:B:782:LEU:O	1.99	0.62
3:C:67:LEU:HA	3:C:70:ILE:CD1	2.30	0.62
1:A:21:LEU:HG	1:A:1413:GLY:O	2.00	0.62
1:A:42:ASP:C	1:A:44:THR:H	2.07	0.62
1:A:44:THR:O	1:A:45:GLN:HB2	1.99	0.62
1:A:546:VAL:HG21	1:A:572:TRP:CE3	2.34	0.62
1:A:590:ARG:HG3	1:A:590:ARG:NH1	2.15	0.62
1:A:605:MET:SD	1:A:621:THR:HG21	2.40	0.62
1:A:998:LEU:HD12	1:A:998:LEU:H	1.65	0.62
1:A:1213:GLY:HA2	1:A:1216:ILE:HD12	1.81	0.62
1:A:1353:TYR:C	1:A:1353:TYR:CD2	2.77	0.62
2:B:31:TRP:CZ3	2:B:34:ILE:HD12	2.35	0.62
2:B:859:TYR:N	2:B:859:TYR:CD1	2.67	0.62
2:B:1145:SER:C	2:B:1147:LEU:N	2.55	0.62
5:E:168:TYR:HB3	5:E:170:LEU:HG	1.81	0.62
1:A:515:GLN:OE1	1:A:1071:SER:HA	1.99	0.62
1:A:818:MET:HG2	2:B:514:LEU:HG	1.81	0.62
1:A:823:GLY:C	1:A:825:ILE:H	2.08	0.62
1:A:1017:LEU:CB	5:E:205:SER:HA	2.29	0.62
1:A:1202:MET:HE1	1:A:1212:VAL:CG2	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:640:VAL:O	2:B:641:GLU:C	2.41	0.62
2:B:762:ASN:HD21	2:B:1024:ALA:HB3	1.64	0.62
2:B:763:GLN:NE2	13:S:293:LEU:HG	2.15	0.62
2:B:1084:GLN:HG2	3:C:201:TRP:CZ2	2.34	0.62
5:E:197:LYS:HG2	5:E:197:LYS:O	1.97	0.62
11:K:91:CYS:O	11:K:94:ILE:HB	1.99	0.62
1:A:90:VAL:CG1	1:A:91:PHE:N	2.63	0.62
1:A:886:ILE:HG13	1:A:943:LEU:CD1	2.30	0.62
2:B:37:PHE:CD1	2:B:41:LYS:HG3	2.35	0.62
2:B:839:MET:HE3	2:B:1010:LEU:HD21	1.81	0.62
2:B:1033:LYS:HD2	2:B:1087:PHE:O	2.00	0.62
6:F:97:ARG:HH22	6:F:108:PHE:HE1	1.45	0.62
7:G:114:LEU:HD23	7:G:161:GLY:O	2.00	0.62
8:H:84:ALA:C	8:H:86:ASP:H	2.06	0.62
1:A:289:ILE:O	1:A:291:GLU:N	2.33	0.62
1:A:897:TYR:HD2	1:A:936:LEU:HD13	1.65	0.62
2:B:69:LEU:HD22	2:B:429:PHE:CE1	2.35	0.62
2:B:236:HIS:CE1	2:B:389:ALA:HA	2.35	0.62
2:B:601:ARG:O	2:B:605:ARG:HG3	2.00	0.62
2:B:1001:PHE:CZ	2:B:1073:TYR:HB2	2.35	0.62
6:F:77:ASP:C	6:F:79:ARG:H	2.08	0.62
7:G:80:LYS:HE2	7:G:82:PHE:CZ	2.34	0.62
8:H:40:LEU:HD22	8:H:123:MET:HE3	1.82	0.62
1:A:90:VAL:HG13	1:A:297:GLN:CD	2.25	0.61
1:A:590:ARG:HH21	1:A:620:LYS:CB	2.08	0.61
1:A:1001:ARG:O	1:A:1002:GLY:O	2.18	0.61
1:A:1019:CYS:O	1:A:1022:LEU:HB3	1.99	0.61
2:B:557:PHE:C	2:B:557:PHE:CD2	2.77	0.61
2:B:1201:LYS:HE2	2:B:1205:GLN:OE1	2.00	0.61
5:E:35:VAL:C	5:E:37:LEU:H	2.08	0.61
7:G:1:MET:HE3	7:G:80:LYS:O	2.00	0.61
1:A:256:GLN:NE2	2:B:918:ILE:HD11	2.14	0.61
1:A:705:LYS:HA	13:S:254:TYR:OH	2.00	0.61
1:A:756:ILE:HG21	13:S:283:GLN:NE2	2.14	0.61
2:B:1182:CYS:C	2:B:1183:LYS:HE3	2.25	0.61
7:G:80:LYS:HE2	7:G:82:PHE:HZ	1.64	0.61
8:H:83:GLN:C	8:H:85:GLY:H	2.08	0.61
1:A:691:LEU:O	1:A:694:THR:HB	1.99	0.61
2:B:510:LYS:CG	2:B:512:ARG:H	2.11	0.61
2:B:773:MET:O	2:B:776:GLN:N	2.28	0.61
2:B:1106:ARG:HG3	2:B:1107:ALA:H	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:46:ILE:HD13	3:C:157:CYS:SG	2.41	0.61
1:A:289:ILE:C	1:A:291:GLU:N	2.58	0.61
1:A:442:VAL:O	1:A:457:ALA:HA	2.00	0.61
1:A:1203:ASN:O	1:A:1204:ASP:C	2.44	0.61
1:A:1206:ASP:O	1:A:1207:LEU:HG	2.00	0.61
1:A:1237:ILE:CG2	1:A:1238:ILE:N	2.63	0.61
2:B:292:ILE:CD1	2:B:326:ASP:HA	2.30	0.61
2:B:758:PHE:CE1	2:B:1027:ILE:HG22	2.35	0.61
3:C:58:LEU:H	3:C:58:LEU:CD2	2.14	0.61
5:E:78:LEU:HD21	5:E:80:VAL:HG23	1.81	0.61
6:F:79:ARG:HG3	6:F:144:GLU:OE1	2.00	0.61
1:A:412:ARG:NH2	2:B:1108:ARG:NH1	2.48	0.61
1:A:730:GLY:C	1:A:732:LEU:H	2.09	0.61
2:B:47:GLN:O	2:B:173:MET:HE1	2.01	0.61
2:B:542:MET:HE2	2:B:743:ILE:HG13	1.81	0.61
3:C:248:ILE:HD13	11:K:101:LEU:HD22	1.82	0.61
4:D:40:HIS:CE1	4:D:41:GLN:HG3	2.35	0.61
1:A:91:PHE:HD2	1:A:96:ILE:HG12	1.66	0.61
1:A:244:PRO:HG2	1:A:245:PRO:HD3	1.81	0.61
1:A:852:TYR:CE2	1:A:1060:PRO:HB2	2.36	0.61
1:A:1081:LEU:HD11	1:A:1098:VAL:HB	1.81	0.61
1:A:1227:ILE:HG22	1:A:1228:TRP:H	1.64	0.61
9:I:8:ARG:O	9:I:10:CYS:N	2.33	0.61
11:K:67:PHE:C	11:K:68:PHE:CD2	2.78	0.61
1:A:152:VAL:CG1	1:A:153:PRO:HD2	2.31	0.61
1:A:335:ARG:HE	1:A:339:ASN:HD22	1.45	0.61
1:A:629:LEU:O	1:A:633:VAL:HG23	2.01	0.61
1:A:857:ARG:HD3	1:A:861:GLY:O	2.00	0.61
1:A:1155:ASP:HB3	1:A:1241:ARG:HH21	1.66	0.61
2:B:562:GLY:HA3	2:B:590:HIS:HE1	1.65	0.61
2:B:899:ILE:CD1	2:B:911:ILE:HA	2.30	0.61
7:G:108:VAL:HG22	7:G:159:ALA:HB3	1.81	0.61
10:J:57:ILE:HG23	10:J:58:GLU:N	2.16	0.61
1:A:528:LEU:O	1:A:531:ILE:HG22	2.01	0.61
1:A:870:GLU:HG2	5:E:208:TYR:CG	2.36	0.61
1:A:1081:LEU:CD1	1:A:1098:VAL:HB	2.30	0.61
2:B:35:SER:HA	2:B:811:TYR:CE2	2.27	0.61
2:B:508:LEU:HB2	2:B:510:LYS:HB3	1.83	0.61
3:C:22:LEU:HD13	3:C:230:MET:HE1	1.81	0.61
3:C:143:LEU:HD12	3:C:143:LEU:C	2.25	0.61
1:A:694:THR:O	1:A:698:GLN:HG3	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:804:TYR:OH	2:B:763:GLN:HA	2.01	0.61
3:C:212:PRO:CB	3:C:213:PRO:HD2	2.31	0.61
8:H:23:VAL:HG13	8:H:42:ILE:O	2.00	0.61
9:I:106:CYS:O	9:I:107:SER:HB2	1.99	0.61
1:A:711:ARG:HA	9:I:97:MET:HE2	1.83	0.61
1:A:714:PHE:CD2	9:I:97:MET:HE1	2.36	0.61
1:A:849:MET:HE1	1:A:1061:GLY:HA2	1.83	0.61
1:A:869:GLY:O	5:E:204:THR:HG21	2.01	0.61
2:B:496:ARG:NH1	2:B:539:LEU:HB2	2.16	0.61
2:B:511:PRO:C	2:B:513:GLN:H	2.08	0.61
2:B:1177:HIS:C	2:B:1179:GLN:H	2.08	0.61
4:D:134:THR:HG22	4:D:135:GLY:N	2.16	0.61
13:S:241:LEU:O	13:S:242:LYS:C	2.43	0.61
1:A:902:LEU:O	1:A:903:ASN:HB2	2.01	0.60
2:B:533:CYS:O	2:B:535:LEU:N	2.34	0.60
5:E:198:ILE:CD1	5:E:212:ARG:HH11	2.14	0.60
1:A:446:ARG:CD	1:A:480:ALA:HB2	2.31	0.60
2:B:487:THR:HG22	2:B:488:TYR:N	2.15	0.60
4:D:51:ASN:O	4:D:54:GLU:HB3	2.01	0.60
9:I:55:THR:HG23	9:I:100:PHE:CD2	2.33	0.60
2:B:240:ILE:CG2	2:B:254:LEU:HB3	2.31	0.60
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.83	0.60
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.83	0.60
7:G:146:LYS:HB2	7:G:168:LEU:HD11	1.82	0.60
8:H:56:THR:O	8:H:144:ILE:HA	2.01	0.60
10:J:57:ILE:HG23	10:J:58:GLU:H	1.66	0.60
1:A:503:GLN:C	1:A:504:LEU:HD12	2.25	0.60
1:A:563:PRO:HG3	1:A:572:TRP:CE2	2.37	0.60
1:A:606:LEU:HB2	1:A:614:PHE:CE2	2.37	0.60
1:A:708:MET:HE2	1:A:1089:VAL:CG1	2.28	0.60
2:B:510:LYS:HG2	2:B:512:ARG:CB	2.30	0.60
2:B:545:ILE:HG22	2:B:546:SER:O	2.01	0.60
2:B:1096:ARG:O	2:B:1097:HIS:HB2	2.00	0.60
3:C:142:VAL:H	10:J:16:ASP:HB3	1.66	0.60
5:E:60:PHE:CE2	5:E:80:VAL:HB	2.36	0.60
13:S:291:GLU:H	13:S:292:PRO:CD	2.14	0.60
1:A:49:LYS:HE2	1:A:61:ILE:CD1	2.29	0.60
1:A:254:GLU:CB	2:B:935:ARG:HH22	2.14	0.60
1:A:786:HIS:N	1:A:786:HIS:CD2	2.69	0.60
1:A:1164:PRO:HG2	1:A:1165:GLU:H	1.66	0.60
2:B:605:ARG:CZ	2:B:639:ILE:HD13	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:113:ALA:HB2	8:H:126:GLU:HG3	1.84	0.60
13:S:298:THR:HG23	13:S:305:ARG:HG2	1.82	0.60
1:A:47:ARG:HH22	1:A:254:GLU:HA	1.65	0.60
1:A:69:THR:C	1:A:71:GLN:N	2.57	0.60
1:A:134:ARG:O	1:A:138:ILE:HG13	2.01	0.60
1:A:225:ASN:ND2	1:A:227:VAL:H	1.98	0.60
1:A:761:MET:HA	1:A:804:TYR:HB2	1.83	0.60
2:B:189:LEU:HA	2:B:192:LEU:HD12	1.82	0.60
2:B:642:ASP:HB3	2:B:649:LYS:HD2	1.84	0.60
2:B:705:MET:N	2:B:710:LEU:HD12	2.16	0.60
2:B:830:TYR:HE2	2:B:1000:PRO:HD3	1.66	0.60
4:D:35:LEU:H	4:D:35:LEU:CD1	2.14	0.60
6:F:72:LYS:O	6:F:73:ALA:HB3	2.02	0.60
7:G:23:LYS:HG3	7:G:56:ILE:CD1	2.28	0.60
1:A:853:ASP:CG	1:A:855:THR:HB	2.25	0.60
1:A:963:ILE:HD11	1:A:1048:ASN:CB	2.30	0.60
1:A:1116:LEU:HB3	1:A:1311:VAL:HG22	1.83	0.60
2:B:847:ASP:C	2:B:849:GLY:H	2.09	0.60
2:B:1159:ARG:HE	2:B:1193:GLN:HE21	1.50	0.60
3:C:31:ASN:O	3:C:32:SER:C	2.45	0.60
4:D:33:PHE:CE2	7:G:80:LYS:NZ	2.70	0.60
11:K:50:LEU:HD11	11:K:75:ILE:CD1	2.31	0.60
13:S:287:ARG:HD3	13:S:291:GLU:OE1	2.01	0.60
1:A:144:THR:O	1:A:146:MET:HG3	2.01	0.60
2:B:880:THR:HG21	2:B:934:LYS:HE3	1.82	0.60
10:J:3:VAL:HG21	10:J:18:TRP:CB	2.30	0.60
12:L:31:CYS:HB3	12:L:35:SER:HA	1.84	0.60
1:A:332:LYS:H	1:A:337:ARG:HB3	1.67	0.60
1:A:392:VAL:HG13	1:A:415:LEU:HD11	1.84	0.60
1:A:852:TYR:CE1	6:F:136:ARG:HG2	2.36	0.60
1:A:863:VAL:HG12	1:A:864:ILE:N	2.17	0.60
1:A:1134:ILE:O	1:A:1138:ILE:HG13	2.02	0.60
1:A:1164:PRO:HG2	1:A:1165:GLU:HG3	1.82	0.60
2:B:216:GLU:HA	2:B:406:LEU:HD23	1.84	0.60
2:B:578:THR:HG23	2:B:622:LYS:HA	1.84	0.60
4:D:210:ILE:O	4:D:214:LEU:HG	2.01	0.60
1:A:407:ARG:HG2	1:A:430:TRP:CH2	2.37	0.60
1:A:567:LYS:HD3	8:H:95:TYR:CD2	2.37	0.60
1:A:863:VAL:O	1:A:864:ILE:HG12	2.02	0.60
1:A:896:ARG:HB3	1:A:897:TYR:CD1	2.37	0.60
1:A:1261:LYS:O	1:A:1264:GLU:HB3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1180:PHE:HB3	2:B:1191:ILE:CD1	2.31	0.60
3:C:9:LYS:O	3:C:10:ILE:C	2.44	0.60
3:C:169:LYS:NZ	12:L:69:ALA:HB3	2.16	0.60
4:D:19:GLU:O	4:D:21:GLU:N	2.35	0.60
1:A:1372:VAL:CG1	1:A:1373:ASP:N	2.65	0.59
2:B:1159:ARG:HE	2:B:1193:GLN:NE2	2.00	0.59
5:E:23:VAL:HG13	5:E:78:LEU:HD13	1.84	0.59
1:A:399:HIS:CB	1:A:400:PRO:HD3	2.26	0.59
1:A:1104:ILE:O	1:A:1106:ASN:N	2.35	0.59
2:B:102:VAL:CG2	2:B:112:LEU:HB2	2.33	0.59
2:B:129:PHE:HE2	2:B:166:PHE:HD1	1.49	0.59
3:C:90:ASP:O	3:C:90:ASP:CG	2.43	0.59
1:A:469:ARG:HG2	1:A:469:ARG:HH11	1.67	0.59
1:A:541:ILE:HD13	1:A:549:MET:HE1	1.83	0.59
1:A:821:ARG:O	1:A:825:ILE:HG13	2.01	0.59
1:A:1237:ILE:CG2	1:A:1238:ILE:H	2.15	0.59
2:B:510:LYS:CB	2:B:511:PRO:CD	2.79	0.59
2:B:533:CYS:C	2:B:535:LEU:H	2.09	0.59
2:B:1183:LYS:N	2:B:1183:LYS:CE	2.62	0.59
4:D:176:GLU:OE2	4:D:198:LEU:HD23	2.02	0.59
5:E:46:TYR:CE2	5:E:58:MET:HA	2.37	0.59
8:H:56:THR:HB	8:H:145:ARG:HG2	1.84	0.59
8:H:59:ILE:HG22	8:H:60:ALA:H	1.64	0.59
12:L:61:THR:CG2	12:L:63:ARG:HG2	2.31	0.59
1:A:40:THR:HG23	1:A:54:ASN:HD21	1.67	0.59
1:A:343:LYS:HE2	2:B:1156:ASP:OD2	2.02	0.59
1:A:475:THR:HG23	1:A:476:SER:N	2.17	0.59
1:A:1265:ASN:C	1:A:1267:MET:N	2.60	0.59
2:B:310:MET:O	2:B:313:MET:HB2	2.02	0.59
2:B:653:VAL:CG2	2:B:689:LEU:HB3	2.30	0.59
2:B:778:MET:CE	2:B:1094:ARG:HD3	2.32	0.59
2:B:807:ARG:HB3	2:B:807:ARG:HH11	1.66	0.59
8:H:126:GLU:C	8:H:130:ARG:HH22	2.11	0.59
9:I:111:THR:CG2	9:I:112:SER:H	2.13	0.59
10:J:41:LEU:CD1	10:J:50:ILE:HG13	2.32	0.59
12:L:32:ALA:HB3	12:L:55:ILE:HD12	1.83	0.59
1:A:605:MET:HE2	1:A:615:GLY:O	2.02	0.59
1:A:730:GLY:C	1:A:732:LEU:N	2.59	0.59
1:A:855:THR:CG2	1:A:857:ARG:HG3	2.32	0.59
1:A:1017:LEU:HD23	5:E:204:THR:C	2.27	0.59
2:B:973:ILE:HG23	2:B:974:PRO:HD2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1166:CYS:HB2	2:B:1168:LEU:HD12	1.84	0.59
3:C:104:PHE:CD2	3:C:105:GLY:N	2.70	0.59
7:G:6:ASP:HB3	7:G:73:LYS:HZ1	1.66	0.59
7:G:145:VAL:CG1	7:G:146:LYS:N	2.64	0.59
9:I:58:VAL:HA	9:I:62:ILE:CD1	2.32	0.59
10:J:1:MET:HE2	10:J:60:PHE:CZ	2.38	0.59
2:B:46:GLN:HG3	2:B:47:GLN:H	1.68	0.59
3:C:58:LEU:CD2	3:C:58:LEU:N	2.65	0.59
5:E:48:ASP:CG	5:E:49:SER:H	2.11	0.59
5:E:94:LYS:HE2	5:E:98:ILE:HD11	1.84	0.59
7:G:1:MET:O	7:G:1:MET:SD	2.61	0.59
1:A:391:LEU:O	1:A:394:ASN:N	2.35	0.59
1:A:834:THR:HG23	1:A:1077:THR:HA	1.85	0.59
1:A:1424:VAL:HG11	2:B:1139:ILE:HD13	1.84	0.59
2:B:521:LEU:HB3	2:B:633:VAL:HG11	1.85	0.59
2:B:899:ILE:HG22	2:B:900:ALA:N	2.17	0.59
2:B:1169:MET:HE3	2:B:1201:LYS:HG2	1.85	0.59
1:A:41:MET:O	1:A:42:ASP:C	2.45	0.59
1:A:72:GLU:O	1:A:73:GLY:O	2.20	0.59
1:A:135:PHE:C	1:A:137:ALA:N	2.60	0.59
1:A:868:TYR:CE1	1:A:1064:VAL:CG1	2.77	0.59
1:A:905:ASP:C	1:A:906:HIS:HD1	2.10	0.59
2:B:240:ILE:HG23	2:B:240:ILE:O	2.02	0.59
2:B:546:SER:HG	2:B:630:ALA:HA	1.68	0.59
2:B:854:LEU:HB3	2:B:856:PHE:CE1	2.37	0.59
2:B:1095:LEU:H	2:B:1095:LEU:CD1	1.87	0.59
3:C:174:ALA:O	3:C:175:ALA:CB	2.51	0.59
4:D:170:THR:HG22	4:D:172:LEU:HG	1.82	0.59
1:A:567:LYS:HB3	8:H:95:TYR:HA	1.83	0.59
1:A:808:LEU:HD21	1:A:816:HIS:HD2	1.68	0.59
1:A:1397:LEU:HA	1:A:1400:CYS:CB	2.32	0.59
2:B:954:VAL:O	12:L:55:ILE:O	2.20	0.59
2:B:1160:VAL:CG1	2:B:1161:HIS:N	2.66	0.59
3:C:35:ARG:HH11	11:K:41:THR:N	2.01	0.59
5:E:164:LEU:HD22	5:E:211:TYR:CD2	2.37	0.59
10:J:23:ASN:C	10:J:25:LEU:H	2.09	0.59
1:A:782:ARG:NH2	2:B:699:GLU:O	2.34	0.59
1:A:1125:ALA:C	1:A:1127:ASP:H	2.10	0.59
1:A:1151:GLU:HB3	1:A:1153:TYR:HE1	1.68	0.59
1:A:1191:TRP:CD1	1:A:1256:GLU:HB2	2.37	0.59
1:A:1370:LEU:O	1:A:1374:VAL:HG23	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113:TYR:HB3	2:B:114:PRO:CD	2.29	0.59
2:B:798:TYR:CE1	10:J:4:PRO:HB3	2.38	0.59
2:B:841:MET:O	2:B:993:THR:HG22	2.02	0.59
8:H:40:LEU:HD12	8:H:122:LEU:O	2.03	0.59
9:I:101:PHE:O	9:I:102:VAL:HG23	2.03	0.59
1:A:68:GLN:C	1:A:70:CYS:H	2.09	0.58
1:A:69:THR:C	1:A:71:GLN:H	2.10	0.58
1:A:133:LYS:C	1:A:135:PHE:N	2.60	0.58
1:A:399:HIS:HB3	1:A:400:PRO:CD	2.26	0.58
1:A:687:LYS:O	1:A:690:VAL:HB	2.03	0.58
1:A:697:ALA:HB2	1:A:702:LEU:HD12	1.85	0.58
1:A:1116:LEU:HB3	1:A:1311:VAL:CG2	2.33	0.58
2:B:527:THR:OG1	2:B:528:PRO:HD2	2.03	0.58
2:B:541:LEU:HD12	2:B:747:MET:HE1	1.85	0.58
2:B:879:ARG:O	2:B:880:THR:HB	2.03	0.58
13:S:295:THR:O	13:S:295:THR:HG22	2.02	0.58
1:A:528:LEU:HD23	1:A:751:SER:HA	1.85	0.58
1:A:667:GLY:HA3	3:C:192:TRP:CH2	2.38	0.58
1:A:1030:ARG:HG3	1:A:1034:GLU:OE2	2.03	0.58
1:A:1095:THR:OG1	1:A:1112:LYS:HB2	2.03	0.58
2:B:549:THR:HG22	2:B:550:ASP:N	2.12	0.58
5:E:114:ASN:O	5:E:115:ASN:HB3	2.03	0.58
8:H:24:CYS:SG	8:H:44:VAL:HG21	2.43	0.58
1:A:22:PHE:HB2	2:B:1211:ASN:OD1	2.03	0.58
1:A:360:GLU:HB2	1:A:363:GLN:HG3	1.84	0.58
1:A:361:LEU:HG	1:A:507:VAL:HG11	1.85	0.58
1:A:1161:THR:C	1:A:1163:ILE:N	2.61	0.58
1:A:1342:GLU:CG	5:E:198:ILE:HD13	2.33	0.58
2:B:189:LEU:O	2:B:192:LEU:N	2.31	0.58
2:B:1034:VAL:HG12	2:B:1035:ALA:N	2.17	0.58
2:B:1065:GLN:HG3	2:B:1068:GLY:H	1.69	0.58
3:C:66:ARG:NH2	10:J:5:VAL:HG23	2.18	0.58
6:F:111:LEU:HD12	6:F:111:LEU:N	2.18	0.58
10:J:19:GLU:O	10:J:23:ASN:HB2	2.03	0.58
11:K:31:VAL:HG12	11:K:32:VAL:N	2.18	0.58
1:A:321:PRO:O	1:A:322:VAL:HG23	2.03	0.58
1:A:535:THR:CG2	1:A:616:VAL:HA	2.33	0.58
1:A:688:LYS:C	1:A:690:VAL:H	2.12	0.58
1:A:847:ASP:HB2	1:A:859:SER:H	1.68	0.58
1:A:1376:THR:O	1:A:1377:THR:C	2.46	0.58
2:B:763:GLN:HE22	13:S:293:LEU:HG	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:807:ARG:HB3	2:B:807:ARG:NH1	2.19	0.58
2:B:911:ILE:HD11	2:B:941:LEU:CD1	2.34	0.58
3:C:59:ALA:O	3:C:62:PHE:HB3	2.03	0.58
4:D:48:ILE:HG21	7:G:4:ILE:HB	1.85	0.58
5:E:198:ILE:CD1	5:E:212:ARG:HG3	2.34	0.58
8:H:42:ILE:HG23	8:H:95:TYR:HE1	1.67	0.58
1:A:848:ILE:HB	1:A:1065:GLY:HA3	1.85	0.58
1:A:1127:ASP:O	1:A:1130:GLN:HB3	2.03	0.58
1:A:1222:ASN:O	1:A:1223:ASP:HB3	2.04	0.58
1:A:1436:ILE:O	1:A:1437:GLY:C	2.46	0.58
2:B:570:VAL:HG23	2:B:573:GLN:HB3	1.85	0.58
2:B:815:ARG:HD3	2:B:1041:GLU:OE2	2.03	0.58
2:B:918:ILE:CD1	2:B:935:ARG:HD2	2.27	0.58
1:A:500:GLU:OE2	1:A:1438:THR:HG21	2.03	0.58
1:A:618:GLU:C	1:A:618:GLU:CD	2.71	0.58
1:A:785:PRO:HG2	1:A:786:HIS:HD2	1.68	0.58
1:A:820:GLY:C	1:A:822:GLU:N	2.60	0.58
1:A:1074:GLU:N	1:A:1075:PRO:HD2	2.19	0.58
2:B:235:SER:HB3	2:B:258:LEU:HG	1.86	0.58
2:B:404:LYS:HE2	2:B:404:LYS:HA	1.85	0.58
3:C:17:ASN:OD1	3:C:233:GLU:HG3	2.02	0.58
5:E:144:ILE:O	5:E:146:HIS:N	2.37	0.58
1:A:335:ARG:HH11	2:B:1206:GLU:CD	2.10	0.58
1:A:666:ILE:CD1	1:A:667:GLY:N	2.66	0.58
2:B:483:LEU:HD12	2:B:484:ASN:H	1.67	0.58
2:B:782:LEU:HD12	2:B:788:ARG:HH11	1.67	0.58
2:B:785:TYR:HE2	10:J:60:PHE:CE1	2.22	0.58
2:B:824:ILE:CG1	10:J:48:ARG:HH12	2.11	0.58
3:C:27:LEU:O	3:C:28:ALA:C	2.46	0.58
4:D:33:PHE:CE1	7:G:80:LYS:HE3	2.39	0.58
6:F:77:ASP:C	6:F:79:ARG:N	2.61	0.58
7:G:9:LEU:HD12	7:G:10:ASN:N	2.16	0.58
7:G:119:LEU:HD13	7:G:132:SER:HB2	1.86	0.58
13:S:300:GLU:HG3	13:S:300:GLU:O	2.04	0.58
1:A:567:LYS:CB	1:A:568:PRO:CD	2.81	0.58
1:A:827:THR:O	1:A:831:THR:HB	2.04	0.58
1:A:1265:ASN:C	1:A:1267:MET:H	2.09	0.58
1:A:1446:ASP:HB3	1:A:1449:SER:OG	2.04	0.58
3:C:124:LEU:O	3:C:127:ARG:HG2	2.04	0.58
5:E:13:TRP:O	5:E:16:PHE:HB3	2.03	0.58
7:G:117:GLN:O	7:G:119:LEU:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:ARG:HB2	1:A:487:MET:SD	2.43	0.58
1:A:903:ASN:ND2	1:A:905:ASP:H	2.02	0.58
2:B:461:LEU:HD12	2:B:461:LEU:H	1.68	0.58
2:B:762:ASN:HD21	2:B:1024:ALA:CB	2.17	0.58
2:B:1186:ASP:OD1	2:B:1186:ASP:O	2.22	0.58
9:I:58:VAL:HG13	9:I:62:ILE:HG13	1.84	0.58
11:K:53:ASP:HB3	11:K:56:VAL:HG23	1.86	0.58
1:A:598:LEU:HD22	8:H:25:ARG:NH1	2.18	0.58
1:A:1074:GLU:HB3	1:A:1075:PRO:CD	2.34	0.58
1:A:1316:VAL:O	1:A:1322:ILE:HD13	2.04	0.58
2:B:325:GLN:HG2	9:I:31:THR:CG2	2.34	0.58
2:B:708:GLU:O	2:B:710:LEU:N	2.37	0.58
2:B:1032:SER:C	2:B:1034:VAL:H	2.12	0.58
2:B:1132:GLU:O	2:B:1135:ARG:HB3	2.04	0.58
3:C:88:CYS:SG	3:C:91:HIS:C	2.87	0.58
4:D:47:LEU:HD11	7:G:3:PHE:CD2	2.39	0.58
5:E:162:ARG:HH11	5:E:162:ARG:HG2	1.68	0.58
8:H:84:ALA:C	8:H:86:ASP:N	2.60	0.58
9:I:61:ASP:C	9:I:63:GLY:H	2.12	0.58
1:A:115:LEU:HD12	1:A:142:CYS:SG	2.44	0.57
1:A:672:ASP:HB2	1:A:736:ASN:OD1	2.04	0.57
1:A:895:LYS:HG2	1:A:895:LYS:O	2.03	0.57
1:A:1086:PHE:O	1:A:1087:ALA:C	2.47	0.57
2:B:57:TYR:CD1	2:B:57:TYR:N	2.72	0.57
2:B:394:ASP:OD1	9:I:91:ARG:HB3	2.05	0.57
2:B:551:PRO:C	2:B:553:PRO:HD2	2.29	0.57
2:B:603:LEU:HB3	2:B:609:ILE:HD11	1.84	0.57
2:B:992:ILE:HD13	2:B:994:TYR:CE1	2.38	0.57
3:C:82:TYR:CE1	3:C:161:LYS:HD3	2.39	0.57
4:D:56:ARG:HA	4:D:148:LEU:HD13	1.86	0.57
5:E:157:SER:O	5:E:159:ASP:N	2.37	0.57
1:A:35:ILE:HD12	1:A:241:VAL:HG21	1.86	0.57
1:A:1161:THR:HG22	1:A:1163:ILE:N	2.14	0.57
1:A:1421:CYS:HA	1:A:1426:GLU:HB3	1.87	0.57
2:B:773:MET:O	2:B:775:LYS:N	2.37	0.57
7:G:123:ALA:C	7:G:125:SER:N	2.63	0.57
9:I:59:VAL:O	9:I:59:VAL:HG12	2.04	0.57
1:A:443:LEU:HG	2:B:1146:PHE:CE2	2.28	0.57
1:A:642:CYS:O	1:A:645:LEU:HB3	2.04	0.57
1:A:808:LEU:HD12	1:A:808:LEU:N	2.20	0.57
1:A:818:MET:HA	2:B:514:LEU:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:963:ILE:CD1	1:A:1049:ILE:HG13	2.30	0.57
3:C:69:LEU:H	3:C:69:LEU:HD12	1.69	0.57
3:C:167:HIS:CE1	12:L:70:ARG:HA	2.39	0.57
8:H:100:THR:HG22	8:H:101:ALA:N	2.19	0.57
10:J:8:PHE:HD1	10:J:49:MET:HE1	1.69	0.57
10:J:14:VAL:HG13	10:J:50:ILE:HD11	1.85	0.57
11:K:47:ARG:HD3	11:K:59:ALA:O	2.04	0.57
13:S:236:LEU:CA	13:S:242:LYS:HE3	2.34	0.57
1:A:57:ARG:O	1:A:58:LEU:O	2.21	0.57
1:A:115:LEU:HB2	1:A:122:MET:HE2	1.86	0.57
2:B:168:GLY:HA2	2:B:454:THR:OG1	2.05	0.57
5:E:161:LYS:C	5:E:163:GLU:N	2.61	0.57
9:I:4:PHE:CE1	9:I:13:MET:HE1	2.39	0.57
13:S:258:GLY:O	13:S:259:ALA:C	2.46	0.57
1:A:984:LYS:O	1:A:988:LEU:HB2	2.03	0.57
1:A:1164:PRO:O	1:A:1166:ASP:N	2.36	0.57
2:B:192:LEU:O	2:B:193:LYS:HB2	2.04	0.57
2:B:694:ASP:O	2:B:698:GLU:HB2	2.05	0.57
3:C:114:TYR:HB3	3:C:140:ASN:O	2.04	0.57
4:D:196:PRO:C	4:D:198:LEU:H	2.11	0.57
5:E:153:HIS:O	5:E:154:ILE:CG1	2.49	0.57
7:G:80:LYS:CE	7:G:82:PHE:HZ	2.17	0.57
1:A:1289:ARG:NH1	1:A:1326:ARG:NH1	2.52	0.57
2:B:860:MET:HB2	2:B:965:LYS:HG2	1.87	0.57
2:B:903:VAL:HG12	2:B:904:ARG:N	2.17	0.57
3:C:196:ASP:OD1	3:C:198:ALA:HB3	2.05	0.57
5:E:204:THR:CG2	5:E:205:SER:N	2.67	0.57
7:G:109:PHE:CD1	7:G:110:VAL:N	2.71	0.57
10:J:8:PHE:CD1	10:J:49:MET:SD	2.98	0.57
1:A:469:ARG:NH2	2:B:991:GLY:O	2.37	0.57
1:A:825:ILE:C	1:A:827:THR:N	2.61	0.57
1:A:1362:TYR:HD1	1:A:1363:VAL:N	1.85	0.57
2:B:296:GLU:O	2:B:299:GLU:HB2	2.04	0.57
2:B:644:GLU:C	2:B:646:LEU:H	2.13	0.57
2:B:953:LEU:HD21	2:B:965:LYS:HB2	1.87	0.57
3:C:239:PRO:O	3:C:240:VAL:C	2.46	0.57
3:C:263:THR:C	3:C:265:MET:N	2.63	0.57
5:E:78:LEU:HD23	5:E:78:LEU:C	2.30	0.57
1:A:92:HIS:O	1:A:95:PHE:N	2.37	0.57
1:A:403:LYS:O	1:A:404:TYR:CG	2.58	0.57
1:A:560:ILE:HD12	8:H:79:TRP:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1063:MET:CG	1:A:1436:ILE:HG23	2.35	0.57
1:A:1359:ASP:HB3	13:S:307:LYS:HE2	1.87	0.57
2:B:205:ILE:O	2:B:206:ASN:C	2.47	0.57
2:B:558:LEU:C	2:B:560:GLU:H	2.12	0.57
5:E:22:MET:HE3	5:E:26:ARG:CZ	2.35	0.57
5:E:84:ASP:O	5:E:86:PRO:HD3	2.05	0.57
9:I:6:PHE:HA	9:I:14:LEU:HG	1.85	0.57
9:I:58:VAL:HA	9:I:62:ILE:HD11	1.87	0.57
1:A:491:VAL:HG12	1:A:492:PRO:O	2.04	0.57
1:A:1335:ILE:HG22	1:A:1335:ILE:O	2.05	0.57
2:B:217:ARG:HE	2:B:405:ARG:CB	2.15	0.57
2:B:558:LEU:O	2:B:560:GLU:N	2.37	0.57
2:B:620:ARG:NH2	9:I:89:GLN:NE2	2.52	0.57
2:B:840:ILE:HB	2:B:1011:ILE:HB	1.85	0.57
2:B:1085:ILE:HG22	2:B:1086:PHE:N	2.19	0.57
1:A:316:GLN:O	1:A:317:LYS:C	2.47	0.57
1:A:492:PRO:O	1:A:493:GLN:NE2	2.38	0.57
1:A:711:ARG:HG3	9:I:97:MET:HE2	1.87	0.57
1:A:798:GLY:HA2	1:A:815:PHE:CD1	2.39	0.57
1:A:845:LEU:O	1:A:1065:GLY:HA3	2.05	0.57
2:B:247:GLY:H	2:B:418:LYS:HZ3	1.53	0.57
2:B:325:GLN:HG2	9:I:31:THR:HG23	1.86	0.57
2:B:360:PHE:O	2:B:361:LEU:C	2.47	0.57
2:B:1156:ASP:HB3	2:B:1198:TYR:H	1.70	0.57
3:C:181:ASP:OD1	3:C:186:LEU:HD13	2.05	0.57
6:F:75:PRO:O	6:F:77:ASP:O	2.23	0.57
12:L:43:THR:HG22	12:L:43:THR:O	2.04	0.57
1:A:18:GLN:HG3	1:A:228:PHE:CE1	2.40	0.56
1:A:382:PRO:HD3	1:A:428:TYR:CE2	2.40	0.56
1:A:495:GLU:O	1:A:498:ARG:HG3	2.04	0.56
1:A:666:ILE:H	2:B:1026:LEU:HD22	1.70	0.56
1:A:1080:THR:HG22	1:A:1081:LEU:N	2.20	0.56
1:A:1090:ALA:CA	1:A:1093:LYS:HE3	2.34	0.56
1:A:1443:VAL:C	1:A:1444:MET:HG3	2.30	0.56
2:B:172:ILE:HD13	2:B:178:ASN:HB3	1.86	0.56
2:B:1007:VAL:HG22	2:B:1008:PRO:CD	2.32	0.56
2:B:1172:ILE:HG22	2:B:1172:ILE:O	2.05	0.56
3:C:33:LEU:CG	3:C:37:MET:HE2	2.26	0.56
4:D:40:HIS:CB	7:G:73:LYS:NZ	2.58	0.56
1:A:688:LYS:C	1:A:690:VAL:N	2.61	0.56
1:A:730:GLY:O	1:A:732:LEU:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:603:LEU:HB3	2:B:609:ILE:CD1	2.35	0.56
3:C:82:TYR:O	3:C:84:ARG:N	2.38	0.56
3:C:167:HIS:HD2	3:C:169:LYS:N	1.97	0.56
3:C:236:GLY:C	3:C:238:ILE:H	2.13	0.56
1:A:34:LYS:CB	1:A:36:ARG:HH21	2.18	0.56
1:A:84:ILE:HG23	1:A:239:LEU:HB3	1.86	0.56
1:A:306:ASN:ND2	1:A:322:VAL:HB	2.21	0.56
1:A:685:GLU:HG3	1:A:686:ALA:N	2.20	0.56
1:A:695:LYS:C	1:A:697:ALA:H	2.11	0.56
1:A:775:ILE:HG13	1:A:798:GLY:HA3	1.86	0.56
1:A:899:VAL:CG2	1:A:908:LEU:HD21	2.35	0.56
1:A:996:ASN:O	1:A:998:LEU:HD12	2.04	0.56
1:A:1051:ALA:O	1:A:1053:PHE:N	2.39	0.56
1:A:1081:LEU:HD21	1:A:1098:VAL:CG2	2.35	0.56
1:A:1299:VAL:HG12	1:A:1300:LYS:N	2.19	0.56
2:B:278:GLN:HG2	2:B:279:ASP:H	1.68	0.56
2:B:1000:PRO:O	2:B:1007:VAL:HG23	2.05	0.56
2:B:1147:LEU:O	2:B:1148:LYS:C	2.45	0.56
2:B:1168:LEU:HD22	2:B:1208:MET:HE3	1.86	0.56
3:C:101:LEU:HD13	3:C:118:LEU:HD23	1.88	0.56
4:D:51:ASN:ND2	4:D:54:GLU:OE2	2.38	0.56
5:E:161:LYS:C	5:E:163:GLU:H	2.14	0.56
7:G:15:PRO:HA	7:G:18:PHE:CD1	2.41	0.56
8:H:89:LEU:C	8:H:91:ASP:H	2.12	0.56
11:K:65:HIS:CD2	11:K:67:PHE:N	2.60	0.56
12:L:62:LYS:H	12:L:62:LYS:HD2	1.70	0.56
1:A:130:ASP:O	1:A:132:LYS:N	2.39	0.56
1:A:532:ARG:HH22	1:A:745:GLN:HG2	1.69	0.56
1:A:1453:TYR:CZ	6:F:129:LYS:HA	2.40	0.56
2:B:29:ASP:HB3	2:B:658:ILE:CD1	2.34	0.56
2:B:528:PRO:HG2	2:B:533:CYS:HA	1.88	0.56
2:B:593:PRO:HG2	2:B:617:ARG:CZ	2.35	0.56
2:B:911:ILE:HD11	2:B:941:LEU:HD13	1.86	0.56
9:I:111:THR:HG22	9:I:113:ASP:N	2.19	0.56
1:A:78:PRO:CB	2:B:1201:LYS:HE3	2.36	0.56
1:A:1438:THR:HB	2:B:1144:ALA:CB	2.36	0.56
2:B:286:PHE:HE2	2:B:375:ALA:HB1	1.70	0.56
2:B:766:ARG:NH2	2:B:1020:ARG:CG	2.67	0.56
2:B:784:ASN:O	2:B:788:ARG:HG3	2.06	0.56
10:J:57:ILE:O	10:J:60:PHE:N	2.39	0.56
12:L:36:SER:O	12:L:37:LYS:C	2.48	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:928:LEU:O	1:A:930:ASP:N	2.39	0.56
2:B:522:VAL:HG12	2:B:523:CYS:N	2.19	0.56
2:B:857:ARG:HH21	2:B:942:ARG:NH1	2.04	0.56
2:B:1135:ARG:O	2:B:1139:ILE:HG13	2.06	0.56
3:C:18:VAL:HG12	3:C:20:PHE:HD2	1.70	0.56
3:C:123:ASN:ND2	3:C:125:MET:SD	2.79	0.56
5:E:19:VAL:O	5:E:23:VAL:HG23	2.06	0.56
5:E:55:ARG:C	5:E:57:MET:N	2.63	0.56
5:E:178:ILE:HG22	5:E:213:ILE:O	2.06	0.56
9:I:64:SER:O	9:I:66:PRO:HD3	2.05	0.56
10:J:13:VAL:HG12	10:J:14:VAL:N	2.21	0.56
1:A:4:GLN:O	1:A:5:GLN:HB2	2.05	0.56
1:A:98:LYS:O	1:A:102:VAL:HG23	2.05	0.56
1:A:547:LEU:HD22	11:K:58:PHE:CD1	2.40	0.56
1:A:1005:GLU:O	1:A:1006:ILE:C	2.49	0.56
1:A:1130:GLN:HA	1:A:1133:LEU:HD12	1.86	0.56
2:B:498:THR:O	2:B:536:VAL:HG13	2.05	0.56
2:B:642:ASP:O	2:B:644:GLU:N	2.30	0.56
2:B:1020:ARG:CG	2:B:1020:ARG:NH1	2.68	0.56
3:C:89:GLU:O	3:C:90:ASP:HB3	2.05	0.56
3:C:163:ILE:O	3:C:166:GLU:N	2.36	0.56
5:E:56:LYS:HE3	5:E:84:ASP:HB2	1.87	0.56
8:H:62:SER:O	8:H:63:LEU:C	2.48	0.56
8:H:123:MET:HE1	8:H:142:LEU:HD13	1.87	0.56
1:A:71:GLN:O	1:A:73:GLY:N	2.39	0.56
1:A:339:ASN:CB	2:B:1117:GLN:HE22	2.19	0.56
1:A:516:SER:O	1:A:517:ASN:C	2.47	0.56
1:A:663:SER:OG	2:B:1085:ILE:HG23	2.06	0.56
1:A:874:ASP:CA	1:A:1058:VAL:HG23	2.36	0.56
1:A:936:LEU:HD23	1:A:936:LEU:N	2.21	0.56
1:A:1134:ILE:O	1:A:1135:ARG:C	2.49	0.56
1:A:1140:HIS:HB2	1:A:1276:VAL:O	2.06	0.56
2:B:37:PHE:CD2	2:B:542:MET:SD	2.99	0.56
2:B:377:PHE:O	2:B:380:TYR:N	2.39	0.56
2:B:999:MET:HB3	2:B:1007:VAL:HG21	1.88	0.56
9:I:90:GLN:NE2	9:I:92:ARG:HD2	2.21	0.56
1:A:567:LYS:CB	8:H:95:TYR:HA	2.36	0.56
1:A:986:ILE:HD11	1:A:1032:LEU:HD11	1.87	0.56
2:B:44:VAL:O	2:B:45:SER:C	2.49	0.56
2:B:327:ARG:O	2:B:331:LEU:HD13	2.06	0.56
2:B:521:LEU:HB3	2:B:633:VAL:CG1	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:766:ARG:HH21	2:B:1020:ARG:HG2	1.71	0.56
2:B:798:TYR:HE1	10:J:4:PRO:HB3	1.71	0.56
2:B:996:ARG:NH2	3:C:175:ALA:HA	2.20	0.56
2:B:1098:MET:HE3	2:B:1101:ASP:OD2	2.05	0.56
3:C:82:TYR:CD1	3:C:161:LYS:HD3	2.41	0.56
3:C:242:GLN:O	3:C:246:ARG:N	2.37	0.56
5:E:176:PRO:O	5:E:212:ARG:HA	2.06	0.56
1:A:42:ASP:HB3	1:A:45:GLN:H	1.70	0.56
1:A:72:GLU:HB3	1:A:76:GLU:HG3	1.88	0.56
1:A:78:PRO:HB3	2:B:1201:LYS:HE3	1.88	0.56
1:A:306:ASN:HB2	1:A:324:SER:HB3	1.87	0.56
1:A:311:GLN:O	1:A:312:PRO:C	2.49	0.56
1:A:963:ILE:HD13	1:A:1049:ILE:CG1	2.32	0.56
1:A:1044:TRP:O	1:A:1047:SER:N	2.38	0.56
1:A:1323:ASP:C	1:A:1325:THR:H	2.14	0.56
2:B:575:PRO:C	2:B:577:ALA:H	2.13	0.56
2:B:744:HIS:CG	2:B:745:PRO:HD2	2.41	0.56
2:B:945:GLU:O	2:B:946:ASN:HB3	2.06	0.56
7:G:114:LEU:HG	7:G:162:SER:CB	2.36	0.56
11:K:21:ILE:HG23	11:K:31:VAL:HG11	1.88	0.56
1:A:92:HIS:O	1:A:93:VAL:C	2.48	0.55
1:A:470:LEU:CD2	1:A:487:MET:HE3	2.35	0.55
1:A:861:GLY:HA3	5:E:174:GLN:NE2	2.21	0.55
1:A:1349:TYR:C	1:A:1349:TYR:CD2	2.84	0.55
2:B:60:GLN:O	2:B:63:ILE:HG22	2.06	0.55
2:B:569:TYR:CE1	2:B:589:VAL:HG21	2.41	0.55
2:B:635:ARG:NH2	2:B:742:GLU:OE2	2.29	0.55
2:B:1065:GLN:HG2	2:B:1069:PHE:HB2	1.88	0.55
12:L:30:ILE:O	12:L:56:LEU:HA	2.06	0.55
1:A:391:LEU:O	1:A:392:VAL:C	2.49	0.55
1:A:1127:ASP:HB3	1:A:1130:GLN:HB2	1.89	0.55
2:B:209:GLU:CD	2:B:485:ARG:HE	2.14	0.55
2:B:1202:LEU:O	2:B:1203:LEU:C	2.49	0.55
3:C:133:ILE:CD1	3:C:237:SER:CA	2.82	0.55
7:G:1:MET:O	7:G:1:MET:CE	2.54	0.55
11:K:58:PHE:HE2	11:K:74:ARG:HE	1.53	0.55
1:A:384:ASN:O	1:A:385:ILE:C	2.49	0.55
1:A:414:ASP:OD1	1:A:416:ARG:CG	2.54	0.55
1:A:679:ILE:O	1:A:683:ILE:HG13	2.06	0.55
1:A:785:PRO:HG2	1:A:786:HIS:CD2	2.42	0.55
1:A:808:LEU:CD1	1:A:808:LEU:H	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1364:ASN:O	1:A:1365:TYR:C	2.49	0.55
2:B:31:TRP:CE3	2:B:34:ILE:HD12	2.41	0.55
2:B:582:VAL:HA	2:B:626:ILE:O	2.06	0.55
4:D:39:ASN:ND2	4:D:41:GLN:HB2	2.21	0.55
8:H:5:LEU:HB2	8:H:60:ALA:H	1.71	0.55
9:I:105:SER:O	9:I:106:CYS:HB3	2.06	0.55
1:A:265:LYS:HE2	1:A:322:VAL:HG11	1.89	0.55
1:A:705:LYS:C	1:A:707:GLY:N	2.62	0.55
1:A:774:ARG:O	1:A:775:ILE:C	2.49	0.55
1:A:1230:GLU:C	1:A:1232:ASN:H	2.14	0.55
1:A:1341:ILE:HD12	1:A:1379:GLY:O	2.05	0.55
1:A:1373:ASP:O	1:A:1376:THR:HG23	2.06	0.55
2:B:118:ARG:HH11	2:B:204:ILE:HD11	1.72	0.55
2:B:763:GLN:C	2:B:765:PRO:HD2	2.32	0.55
2:B:1189:ILE:HG22	2:B:1190:ASP:N	2.22	0.55
4:D:27:LEU:HD11	4:D:197:SER:HB2	1.89	0.55
4:D:52:LEU:C	4:D:54:GLU:H	2.14	0.55
5:E:47:CYS:HA	5:E:52:ARG:O	2.06	0.55
12:L:49:LYS:O	12:L:50:ASP:HB2	2.05	0.55
1:A:590:ARG:HG3	1:A:590:ARG:HH11	1.72	0.55
1:A:1208:THR:O	1:A:1209:MET:C	2.48	0.55
1:A:1420:ASP:O	1:A:1421:CYS:HB2	2.07	0.55
2:B:54:PHE:HA	2:B:58:THR:HB	1.88	0.55
2:B:242:SER:OG	2:B:252:SER:O	2.23	0.55
2:B:502:ILE:O	2:B:502:ILE:CG2	2.52	0.55
2:B:635:ARG:HB2	2:B:636:PRO:CD	2.36	0.55
4:D:51:ASN:O	4:D:52:LEU:C	2.48	0.55
1:A:18:GLN:HG3	1:A:228:PHE:HE1	1.72	0.55
1:A:78:PRO:O	1:A:79:GLY:O	2.25	0.55
1:A:648:ASN:O	1:A:649:ILE:C	2.47	0.55
1:A:896:ARG:HB3	1:A:897:TYR:HD1	1.70	0.55
1:A:896:ARG:O	1:A:1029:ARG:HB3	2.07	0.55
1:A:1313:LEU:O	1:A:1315:GLU:N	2.39	0.55
2:B:377:PHE:O	2:B:378:LEU:C	2.50	0.55
3:C:90:ASP:O	3:C:91:HIS:CG	2.60	0.55
5:E:211:TYR:CD1	5:E:211:TYR:N	2.74	0.55
6:F:84:TYR:N	6:F:84:TYR:CD1	2.73	0.55
6:F:100:GLN:O	6:F:103:MET:HB2	2.07	0.55
8:H:24:CYS:HB2	8:H:44:VAL:HG21	1.89	0.55
1:A:668:ASP:CB	1:A:743:VAL:HG23	2.36	0.55
1:A:965:GLN:O	1:A:968:GLN:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:997:LEU:HD13	1:A:1018:PHE:CE2	2.42	0.55
1:A:1038:THR:O	1:A:1039:LYS:C	2.49	0.55
2:B:681:TRP:C	2:B:683:SER:H	2.14	0.55
2:B:839:MET:HE2	2:B:1010:LEU:HD21	1.88	0.55
2:B:877:PRO:C	2:B:878:GLN:HG3	2.31	0.55
3:C:46:ILE:HG13	3:C:72:LEU:HD11	1.88	0.55
3:C:70:ILE:HD13	3:C:144:ILE:HD11	1.88	0.55
4:D:47:LEU:HD11	7:G:3:PHE:HD2	1.72	0.55
5:E:42:PHE:O	5:E:43:LYS:C	2.50	0.55
5:E:124:VAL:HG13	5:E:132:ILE:CD1	2.36	0.55
5:E:213:ILE:HG12	5:E:214:CYS:N	2.21	0.55
7:G:13:LEU:HD23	7:G:14:HIS:H	1.70	0.55
10:J:21:TYR:HA	10:J:39:LEU:HD11	1.87	0.55
1:A:390:GLN:HE21	1:A:394:ASN:HD21	1.53	0.55
1:A:453:MET:HE3	1:A:520:CYS:SG	2.47	0.55
1:A:472:LEU:CD1	2:B:835:GLN:CD	2.79	0.55
1:A:897:TYR:HB3	1:A:936:LEU:HD12	1.89	0.55
2:B:363:HIS:CD2	2:B:364:ILE:HG13	2.42	0.55
2:B:378:LEU:O	2:B:382:ILE:HG13	2.07	0.55
2:B:873:THR:HG22	2:B:874:PHE:N	2.22	0.55
2:B:1145:SER:C	2:B:1147:LEU:H	2.14	0.55
2:B:1149:GLU:O	2:B:1150:ARG:C	2.47	0.55
3:C:58:LEU:H	3:C:58:LEU:HD23	1.71	0.55
9:I:84:VAL:O	9:I:84:VAL:HG22	2.07	0.55
12:L:31:CYS:HB3	12:L:35:SER:N	2.21	0.55
1:A:848:ILE:HB	1:A:1065:GLY:CA	2.37	0.55
1:A:849:MET:HE3	1:A:1061:GLY:O	2.07	0.55
1:A:901:LEU:N	1:A:926:GLN:HE21	1.98	0.55
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.88	0.55
1:A:1344:GLY:O	1:A:1345:ARG:C	2.50	0.55
2:B:363:HIS:CD2	2:B:585:VAL:HG22	2.42	0.55
2:B:488:TYR:CE2	2:B:813:LYS:HB2	2.42	0.55
2:B:597:MET:SD	2:B:624:LEU:HD11	2.47	0.55
2:B:1020:ARG:HG2	2:B:1020:ARG:NH1	2.20	0.55
3:C:92:CYS:H	3:C:95:CYS:HG	1.55	0.55
8:H:7:ASP:O	8:H:8:ASP:HB2	2.06	0.55
9:I:25:LEU:HB3	9:I:38:ALA:HB2	1.89	0.55
10:J:1:MET:HE2	10:J:60:PHE:HE2	1.66	0.55
12:L:30:ILE:HG22	12:L:31:CYS:N	2.20	0.55
12:L:47:ARG:HH11	12:L:47:ARG:HG3	1.72	0.55
1:A:356:ASP:HB3	1:A:359:LEU:HG	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:715:GLU:O	1:A:717:ASN:N	2.39	0.55
1:A:1334:ASP:O	1:A:1337:GLU:N	2.40	0.55
2:B:25:ILE:HG23	2:B:29:ASP:HB3	1.89	0.55
2:B:265:SER:O	2:B:266:ALA:HB3	2.07	0.55
2:B:637:LEU:HD12	2:B:693:ILE:HD12	1.88	0.55
2:B:781:PHE:O	2:B:782:LEU:CG	2.54	0.55
2:B:800:GLN:CB	10:J:52:THR:HG21	2.33	0.55
2:B:1084:GLN:HE21	2:B:1084:GLN:H	1.55	0.55
3:C:27:LEU:HD12	3:C:228:PHE:HE2	1.70	0.55
8:H:127:GLY:HA3	8:H:130:ARG:NH2	2.22	0.55
10:J:21:TYR:C	10:J:23:ASN:H	2.15	0.55
1:A:15:LYS:HG3	2:B:1218:THR:O	2.06	0.54
1:A:786:HIS:HE1	2:B:519:TRP:CZ2	2.25	0.54
1:A:919:ILE:O	1:A:921:GLY:N	2.40	0.54
1:A:982:THR:HG22	1:A:984:LYS:H	1.73	0.54
1:A:1102:LYS:HG2	1:A:1106:ASN:ND2	2.22	0.54
1:A:1155:ASP:OD2	1:A:1161:THR:HG23	2.07	0.54
1:A:1410:PHE:C	1:A:1412:ALA:H	2.15	0.54
2:B:542:MET:HG2	2:B:747:MET:HB3	1.89	0.54
2:B:711:GLU:H	2:B:712:PRO:HD2	1.72	0.54
13:S:243:GLN:O	13:S:247:GLU:HG3	2.07	0.54
1:A:298:PHE:CZ	1:A:314:ALA:HB2	2.42	0.54
1:A:381:THR:HG23	1:A:382:PRO:CD	2.37	0.54
1:A:382:PRO:HD3	1:A:428:TYR:CD2	2.42	0.54
1:A:726:ARG:O	1:A:727:ASP:C	2.50	0.54
1:A:853:ASP:OD1	1:A:853:ASP:C	2.51	0.54
1:A:1329:THR:HG22	1:A:1331:SER:N	2.15	0.54
2:B:382:ILE:O	2:B:385:LEU:HB3	2.08	0.54
2:B:806:THR:O	2:B:807:ARG:C	2.50	0.54
3:C:67:LEU:HD23	3:C:70:ILE:HD11	1.89	0.54
5:E:124:VAL:CA	5:E:132:ILE:HD12	2.37	0.54
7:G:88:ASP:HA	7:G:144:ARG:HA	1.88	0.54
1:A:353:ILE:HG21	1:A:487:MET:CG	2.20	0.54
1:A:775:ILE:CG1	1:A:798:GLY:HA3	2.38	0.54
1:A:1397:LEU:O	1:A:1400:CYS:HB3	2.06	0.54
2:B:356:LEU:HA	2:B:360:PHE:HB2	1.90	0.54
2:B:1131:GLY:O	2:B:1132:GLU:C	2.50	0.54
3:C:63:ILE:O	3:C:64:ALA:C	2.50	0.54
3:C:183:TRP:O	3:C:185:LYS:HG3	2.06	0.54
6:F:93:ILE:O	6:F:94:LEU:C	2.49	0.54
8:H:139:ASN:O	8:H:140:ALA:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:46:ILE:O	11:K:50:LEU:HB2	2.07	0.54
1:A:597:LEU:HD12	1:A:597:LEU:N	2.21	0.54
1:A:604:GLY:O	1:A:605:MET:HB2	2.07	0.54
1:A:855:THR:HG23	1:A:856:THR:N	2.23	0.54
1:A:867:ILE:CG2	1:A:872:GLY:N	2.71	0.54
1:A:996:ASN:HA	1:A:998:LEU:CD1	2.38	0.54
1:A:1396:ALA:O	1:A:1398:MET:N	2.41	0.54
2:B:1165:ILE:CG2	2:B:1166:CYS:N	2.70	0.54
3:C:143:LEU:HD12	3:C:145:CYS:N	2.22	0.54
3:C:250:THR:O	3:C:254:LYS:HG3	2.07	0.54
5:E:90:VAL:O	5:E:90:VAL:HG22	2.07	0.54
7:G:18:PHE:HZ	7:G:68:ALA:HB2	1.71	0.54
9:I:34:TYR:HD2	9:I:35:VAL:N	2.05	0.54
13:S:293:LEU:N	13:S:293:LEU:HD23	2.23	0.54
1:A:470:LEU:CD2	1:A:487:MET:CE	2.86	0.54
1:A:1230:GLU:CD	13:S:201:ILE:CA	2.73	0.54
2:B:210:LYS:HA	2:B:481:GLN:O	2.07	0.54
2:B:459:TYR:C	2:B:459:TYR:CD2	2.85	0.54
2:B:693:ILE:HD11	2:B:740:HIS:CD2	2.43	0.54
2:B:861:ASP:OD1	2:B:862:GLN:N	2.41	0.54
2:B:1219:ASP:OD1	2:B:1219:ASP:O	2.25	0.54
5:E:39:LEU:O	5:E:42:PHE:HB3	2.08	0.54
8:H:143:LEU:C	8:H:144:ILE:HG13	2.33	0.54
1:A:71:GLN:C	1:A:73:GLY:N	2.60	0.54
1:A:308:ILE:HG22	1:A:309:ALA:H	1.73	0.54
1:A:476:SER:OG	1:A:477:PRO:HD3	2.08	0.54
1:A:626:ASN:O	1:A:631:HIS:HB2	2.07	0.54
1:A:877:HIS:CD2	1:A:1056:SER:HA	2.41	0.54
1:A:1017:LEU:HD12	1:A:1017:LEU:O	2.07	0.54
1:A:1021:LEU:O	1:A:1025:ARG:HG2	2.08	0.54
1:A:1127:ASP:O	1:A:1128:GLN:C	2.50	0.54
2:B:247:GLY:C	2:B:249:ARG:H	2.16	0.54
2:B:611:PRO:HB3	2:B:685:LEU:HD11	1.89	0.54
2:B:865:LYS:NZ	2:B:869:SER:HA	2.23	0.54
2:B:1099:VAL:O	2:B:1102:LYS:N	2.36	0.54
2:B:1106:ARG:CG	2:B:1107:ALA:N	2.69	0.54
3:C:39:ALA:CA	3:C:164:ALA:HB3	2.37	0.54
3:C:174:ALA:HB2	3:C:235:VAL:HG22	1.90	0.54
3:C:183:TRP:O	3:C:185:LYS:N	2.41	0.54
5:E:60:PHE:HE2	5:E:80:VAL:HB	1.73	0.54
5:E:90:VAL:HA	5:E:120:ALA:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:144:ILE:HG13	5:E:145:THR:H	1.72	0.54
7:G:81:PRO:HG3	7:G:106:MET:SD	2.47	0.54
8:H:58:THR:HG22	8:H:59:ILE:H	1.73	0.54
9:I:62:ILE:O	9:I:62:ILE:CG2	2.55	0.54
11:K:83:PRO:O	11:K:86:ALA:N	2.41	0.54
1:A:472:LEU:HD13	2:B:835:GLN:CD	2.33	0.54
1:A:703:THR:O	1:A:705:LYS:HG2	2.07	0.54
1:A:886:ILE:HG13	1:A:943:LEU:HD12	1.90	0.54
2:B:526:GLU:CD	2:B:752:ALA:HB2	2.32	0.54
3:C:44:LEU:HD23	3:C:72:LEU:HB2	1.90	0.54
6:F:84:TYR:N	6:F:84:TYR:HD1	2.06	0.54
8:H:14:GLU:HG2	8:H:15:VAL:N	2.22	0.54
8:H:95:TYR:HE2	8:H:97:MET:HG2	1.72	0.54
9:I:88:SER:O	9:I:90:GLN:N	2.41	0.54
1:A:75:ASN:O	1:A:76:GLU:CB	2.55	0.54
1:A:534:LEU:HD13	1:A:656:TRP:CG	2.43	0.54
1:A:1305:VAL:HG12	1:A:1306:LEU:N	2.23	0.54
1:A:1313:LEU:CD1	1:A:1327:ILE:HD13	2.38	0.54
2:B:431:TYR:CE2	2:B:447:ALA:HB2	2.42	0.54
2:B:498:THR:HB	2:B:537:LYS:O	2.08	0.54
2:B:555:ILE:HG22	2:B:556:THR:N	2.21	0.54
2:B:955:THR:CG2	2:B:956:THR:N	2.71	0.54
4:D:213:GLU:O	4:D:217:LEU:HG	2.07	0.54
9:I:7:CYS:SG	9:I:8:ARG:O	2.66	0.54
2:B:94:LYS:HG2	2:B:95:ILE:N	2.22	0.54
2:B:203:PHE:HB3	2:B:205:ILE:HD11	1.90	0.54
2:B:658:ILE:O	2:B:661:LEU:HB2	2.07	0.54
2:B:879:ARG:O	2:B:934:LYS:HD2	2.08	0.54
2:B:970:THR:HG22	2:B:971:THR:N	2.22	0.54
2:B:1163:CYS:SG	2:B:1165:ILE:HB	2.48	0.54
2:B:1165:ILE:CG2	2:B:1185:CYS:HB3	2.38	0.54
8:H:130:ARG:HA	8:H:133:ASN:HB2	1.90	0.54
11:K:65:HIS:CD2	11:K:66:PRO:CD	2.90	0.54
1:A:35:ILE:HA	1:A:52:GLY:O	2.07	0.54
1:A:711:ARG:HG2	9:I:97:MET:HE2	1.90	0.54
1:A:741:ASN:HD21	1:A:743:VAL:HB	1.72	0.54
1:A:877:HIS:C	1:A:878:ILE:HG13	2.33	0.54
1:A:1116:LEU:CD2	1:A:1311:VAL:HG22	2.36	0.54
2:B:94:LYS:HG2	2:B:95:ILE:H	1.73	0.54
2:B:230:ALA:N	2:B:231:PRO:HD2	2.23	0.54
2:B:1182:CYS:O	2:B:1182:CYS:SG	2.66	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:31:VAL:CG1	11:K:32:VAL:N	2.70	0.54
1:A:1123:GLY:O	1:A:1125:ALA:N	2.41	0.53
1:A:1441:PHE:HZ	6:F:89:GLU:HA	1.67	0.53
2:B:197:PHE:HZ	2:B:816:GLU:HG2	1.73	0.53
2:B:205:ILE:N	2:B:205:ILE:CD1	2.72	0.53
2:B:487:THR:HG22	2:B:488:TYR:H	1.73	0.53
3:C:168:ALA:C	3:C:170:TRP:H	2.17	0.53
8:H:33:GLN:C	8:H:35:GLN:H	2.16	0.53
9:I:55:THR:CG2	9:I:100:PHE:HD2	2.17	0.53
11:K:47:ARG:HH11	11:K:48:ALA:N	2.06	0.53
11:K:58:PHE:HB3	11:K:76:GLN:HE21	1.72	0.53
1:A:356:ASP:C	1:A:358:ASN:H	2.16	0.53
1:A:1063:MET:CE	1:A:1436:ILE:HG12	2.39	0.53
1:A:1173:HIS:CD2	1:A:1227:ILE:HG23	2.43	0.53
2:B:179:CYS:SG	2:B:181:LEU:HB2	2.48	0.53
2:B:203:PHE:HB3	2:B:205:ILE:CD1	2.37	0.53
2:B:224:GLN:O	2:B:238:ALA:HA	2.08	0.53
2:B:984:HIS:NE2	2:B:1025:HIS:HA	2.24	0.53
5:E:55:ARG:O	5:E:57:MET:N	2.41	0.53
8:H:116:TYR:HB2	8:H:123:MET:HB3	1.90	0.53
8:H:142:LEU:C	8:H:143:LEU:HD12	2.33	0.53
1:A:41:MET:HB3	1:A:48:ALA:O	2.08	0.53
1:A:423:ASP:OD1	1:A:424:ILE:N	2.42	0.53
1:A:468:PHE:CE2	1:A:489:LEU:HD23	2.43	0.53
1:A:1261:LYS:CA	1:A:1264:GLU:HB3	2.38	0.53
1:A:1305:VAL:CG1	1:A:1306:LEU:N	2.71	0.53
1:A:1329:THR:O	1:A:1330:ASN:C	2.50	0.53
1:A:1454:MET:O	1:A:1454:MET:HG3	2.08	0.53
2:B:817:LEU:O	2:B:818:PRO:O	2.26	0.53
2:B:827:ILE:CD1	2:B:1086:PHE:HD2	2.21	0.53
2:B:898:LEU:HB2	12:L:58:LYS:HZ2	1.73	0.53
2:B:1001:PHE:CE1	2:B:1073:TYR:HB2	2.43	0.53
6:F:116:ASP:O	6:F:120:ILE:HG13	2.09	0.53
1:A:129:LYS:O	1:A:130:ASP:HB2	2.08	0.53
1:A:381:THR:HG22	1:A:383:TYR:H	1.73	0.53
1:A:392:VAL:HG21	1:A:426:LEU:HD11	1.91	0.53
1:A:543:LEU:O	1:A:544:ASP:C	2.52	0.53
1:A:1204:ASP:HA	13:S:252:ASN:CB	2.36	0.53
1:A:1343:ALA:O	1:A:1346:ALA:HB3	2.09	0.53
3:C:97:VAL:HG12	3:C:98:VAL:N	2.23	0.53
4:D:123:LEU:HD23	4:D:149:THR:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:25:ASP:C	5:E:27:GLY:N	2.63	0.53
7:G:78:VAL:HG12	7:G:79:PHE:H	1.74	0.53
9:I:103:CYS:HB3	9:I:106:CYS:SG	2.48	0.53
1:A:63:ARG:CA	1:A:74:MET:SD	2.89	0.53
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.38	0.53
1:A:708:MET:SD	1:A:1091:SER:OG	2.66	0.53
1:A:720:ARG:O	1:A:724:GLU:HB2	2.09	0.53
1:A:1299:VAL:HG12	1:A:1300:LYS:H	1.74	0.53
2:B:1010:LEU:HD12	2:B:1011:ILE:N	2.23	0.53
2:B:1017:ILE:HG22	2:B:1018:PRO:N	2.21	0.53
2:B:1187:ASN:O	2:B:1188:LYS:CB	2.56	0.53
4:D:14:ARG:O	4:D:16:LYS:N	2.41	0.53
4:D:60:LYS:O	4:D:61:GLU:C	2.51	0.53
4:D:129:LEU:O	4:D:132:GLN:HB2	2.08	0.53
10:J:61:LEU:C	10:J:63:TYR:H	2.16	0.53
11:K:53:ASP:HB3	11:K:56:VAL:CG2	2.39	0.53
1:A:503:GLN:HE21	6:F:90:ARG:NH2	2.02	0.53
1:A:523:ILE:HG22	1:A:528:LEU:HB2	1.88	0.53
1:A:867:ILE:HG22	1:A:871:ASP:N	2.24	0.53
1:A:1396:ALA:O	1:A:1399:ARG:N	2.41	0.53
2:B:125:SER:HA	2:B:171:PRO:HA	1.89	0.53
2:B:214:ALA:HB3	2:B:498:THR:HA	1.90	0.53
3:C:112:ASN:HB3	3:C:114:TYR:CE1	2.44	0.53
3:C:144:ILE:O	3:C:145:CYS:HB2	2.08	0.53
3:C:166:GLU:O	3:C:167:HIS:HB2	2.07	0.53
1:A:151:ASP:OD1	1:A:163:SER:HB3	2.09	0.53
1:A:303:TYR:CE1	1:A:325:ILE:HD11	2.43	0.53
1:A:372:LYS:HA	1:A:435:HIS:ND1	2.24	0.53
1:A:817:ALA:O	1:A:818:MET:C	2.52	0.53
1:A:1072:ILE:C	1:A:1075:PRO:HD2	2.33	0.53
1:A:1385:THR:O	1:A:1387:HIS:N	2.42	0.53
2:B:31:TRP:O	2:B:34:ILE:N	2.42	0.53
2:B:39:ARG:HG2	2:B:39:ARG:HH11	1.73	0.53
2:B:293:PRO:C	2:B:294:ASP:O	2.47	0.53
2:B:681:TRP:C	2:B:683:SER:N	2.66	0.53
5:E:154:ILE:O	5:E:196:VAL:HA	2.09	0.53
5:E:163:GLU:O	5:E:164:LEU:C	2.51	0.53
7:G:128:PRO:O	7:G:138:THR:HG23	2.09	0.53
13:S:254:TYR:C	13:S:256:ALA:H	2.17	0.53
1:A:42:ASP:C	1:A:44:THR:N	2.64	0.53
1:A:122:MET:O	1:A:123:ARG:C	2.51	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:ILE:O	1:A:519:PRO:HA	2.08	0.53
1:A:587:HIS:HD2	1:A:969:GLN:CG	2.19	0.53
2:B:37:PHE:HE2	2:B:542:MET:CA	2.17	0.53
2:B:167:ILE:HG22	2:B:453:ILE:HD12	1.91	0.53
2:B:225:VAL:HA	2:B:237:VAL:O	2.08	0.53
2:B:1201:LYS:HE2	2:B:1205:GLN:CD	2.33	0.53
3:C:51:VAL:HG22	3:C:155:LEU:CD2	2.39	0.53
3:C:168:ALA:C	3:C:170:TRP:N	2.67	0.53
4:D:196:PRO:C	4:D:198:LEU:N	2.67	0.53
7:G:6:ASP:C	7:G:7:LEU:HD23	2.33	0.53
8:H:6:PHE:O	8:H:58:THR:HA	2.08	0.53
9:I:106:CYS:SG	9:I:107:SER:N	2.82	0.53
10:J:1:MET:H2	10:J:55:ASP:HA	1.73	0.53
10:J:57:ILE:O	10:J:60:PHE:HB2	2.09	0.53
13:S:231:CYS:CA	13:S:232:ASP:CA	2.86	0.53
1:A:47:ARG:NH1	1:A:254:GLU:HB3	2.06	0.53
1:A:84:ILE:HG22	1:A:239:LEU:O	2.08	0.53
1:A:317:LYS:O	1:A:318:SER:CB	2.57	0.53
1:A:437:MET:O	1:A:438:ASP:C	2.50	0.53
1:A:455:MET:HE3	2:B:1134:GLU:HG3	1.91	0.53
1:A:939:ASP:O	1:A:940:ARG:C	2.50	0.53
1:A:1036:ARG:HG2	1:A:1036:ARG:HH11	1.74	0.53
1:A:1097:GLY:O	1:A:1100:ARG:HB3	2.09	0.53
1:A:1148:ILE:O	1:A:1149:ALA:HB2	2.09	0.53
2:B:100:PRO:HD2	2:B:180:TYR:CE1	2.43	0.53
2:B:273:LEU:HD21	2:B:360:PHE:CE1	2.44	0.53
2:B:856:PHE:N	2:B:856:PHE:HD1	2.06	0.53
2:B:1169:MET:HE1	2:B:1201:LYS:CA	2.26	0.53
11:K:49:GLU:OE2	11:K:97:LYS:HE3	2.09	0.53
1:A:335:ARG:NH1	2:B:1206:GLU:CD	2.65	0.53
1:A:785:PRO:HG2	2:B:703:ILE:HD12	1.91	0.53
1:A:823:GLY:O	1:A:825:ILE:N	2.41	0.53
1:A:898:ARG:HD3	1:A:933:TYR:CD1	2.45	0.53
2:B:298:LEU:N	2:B:298:LEU:CD2	2.72	0.53
2:B:371:GLU:CD	2:B:371:GLU:H	2.17	0.53
2:B:458:LYS:O	2:B:459:TYR:C	2.50	0.53
2:B:906:SER:O	2:B:941:LEU:HD23	2.09	0.53
2:B:1149:GLU:C	2:B:1151:LEU:N	2.67	0.53
3:C:35:ARG:HH11	11:K:41:THR:CA	2.22	0.53
4:D:49:ALA:HB1	4:D:178:ALA:HB2	1.91	0.53
1:A:106:VAL:HA	1:A:114:LEU:HD21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:823:GLY:HA3	13:S:285:GLN:HB2	1.90	0.52
1:A:1313:LEU:O	1:A:1314:SER:C	2.52	0.52
2:B:294:ASP:C	2:B:296:GLU:N	2.68	0.52
2:B:562:GLY:HA3	2:B:590:HIS:ND1	2.24	0.52
2:B:619:ILE:C	2:B:621:GLU:H	2.17	0.52
2:B:806:THR:HG22	2:B:808:ALA:N	2.22	0.52
3:C:133:ILE:HD11	3:C:237:SER:CA	2.24	0.52
5:E:7:ARG:O	5:E:9:ILE:N	2.42	0.52
7:G:25:TYR:O	7:G:28:THR:HB	2.09	0.52
1:A:262:LEU:HD22	1:A:303:TYR:HE1	1.73	0.52
1:A:779:PHE:O	1:A:780:VAL:C	2.52	0.52
1:A:964:ILE:O	1:A:968:GLN:HG2	2.09	0.52
1:A:1011:GLN:O	1:A:1015:VAL:HG23	2.09	0.52
1:A:1272:THR:C	1:A:1273:LEU:HD12	2.34	0.52
1:A:1397:LEU:HA	1:A:1400:CYS:HB3	1.90	0.52
2:B:323:VAL:O	2:B:323:VAL:HG12	2.09	0.52
2:B:373:ARG:HA	2:B:566:LEU:HD23	1.91	0.52
2:B:1115:THR:HG22	2:B:1117:GLN:HG3	1.90	0.52
2:B:1166:CYS:O	2:B:1166:CYS:SG	2.68	0.52
5:E:124:VAL:HB	5:E:125:PRO:HD3	1.92	0.52
8:H:17:PRO:HB3	8:H:24:CYS:SG	2.49	0.52
1:A:583:PRO:O	1:A:610:GLY:HA3	2.10	0.52
1:A:751:SER:O	1:A:752:LYS:HG2	2.09	0.52
1:A:808:LEU:HD12	1:A:808:LEU:H	1.74	0.52
1:A:1114:PRO:O	1:A:1311:VAL:CG2	2.58	0.52
2:B:257:LYS:O	2:B:385:LEU:HD21	2.08	0.52
2:B:347:LYS:HG3	2:B:348:ARG:H	1.74	0.52
2:B:401:PHE:HB2	2:B:517:THR:OG1	2.10	0.52
2:B:901:PRO:O	2:B:903:VAL:N	2.41	0.52
3:C:9:LYS:O	3:C:10:ILE:O	2.26	0.52
3:C:61:GLU:HA	3:C:64:ALA:HB3	1.91	0.52
5:E:7:ARG:HG3	5:E:8:ASN:H	1.73	0.52
5:E:147:HIS:CD2	5:E:149:LEU:H	2.27	0.52
7:G:17:PHE:N	7:G:17:PHE:CD2	2.76	0.52
11:K:31:VAL:O	11:K:74:ARG:HA	2.10	0.52
1:A:14:VAL:HG23	1:A:1432:GLN:HE22	1.75	0.52
1:A:53:LEU:HD23	1:A:54:ASN:HB3	1.91	0.52
1:A:326:ARG:HG2	1:A:327:ALA:N	2.24	0.52
1:A:477:PRO:CG	1:A:521:MET:HG2	2.39	0.52
1:A:808:LEU:HD21	1:A:816:HIS:CD2	2.44	0.52
1:A:823:GLY:C	1:A:825:ILE:N	2.66	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:853:ASP:O	1:A:854:ASN:HB2	2.09	0.52
1:A:864:ILE:O	1:A:865:GLN:CG	2.50	0.52
1:A:1079:MET:HE1	1:A:1101:LEU:CD2	2.38	0.52
2:B:57:TYR:N	2:B:57:TYR:HD1	2.06	0.52
2:B:376:PHE:CE2	2:B:569:TYR:HD2	2.28	0.52
2:B:806:THR:N	2:B:809:MET:HE3	2.25	0.52
3:C:31:ASN:O	3:C:34:ARG:N	2.43	0.52
3:C:99:LEU:HD12	3:C:118:LEU:HD13	1.91	0.52
4:D:185:CYS:HB3	4:D:211:LEU:CD1	2.39	0.52
5:E:157:SER:C	5:E:159:ASP:N	2.68	0.52
7:G:18:PHE:CZ	7:G:68:ALA:HB2	2.44	0.52
7:G:109:PHE:CG	7:G:110:VAL:N	2.78	0.52
7:G:146:LYS:NZ	7:G:165:GLU:OE2	2.38	0.52
9:I:68:LEU:HB3	9:I:84:VAL:HG23	1.90	0.52
10:J:3:VAL:HG21	10:J:18:TRP:CG	2.43	0.52
1:A:514:PRO:O	1:A:875:ALA:HB1	2.08	0.52
1:A:744:LYS:HE2	1:A:748:MET:HE2	1.92	0.52
1:A:877:HIS:O	1:A:878:ILE:HG12	2.09	0.52
1:A:1104:ILE:O	1:A:1105:LEU:C	2.53	0.52
1:A:1310:GLY:O	1:A:1311:VAL:HG23	2.08	0.52
2:B:210:LYS:HD2	2:B:481:GLN:O	2.09	0.52
2:B:212:LEU:HD21	2:B:466:TRP:HH2	1.74	0.52
2:B:782:LEU:CD1	2:B:788:ARG:HH11	2.23	0.52
4:D:198:LEU:O	4:D:200:ASN:N	2.42	0.52
5:E:212:ARG:HG3	5:E:212:ARG:HH11	1.75	0.52
1:A:412:ARG:NH2	2:B:1108:ARG:HH12	2.07	0.52
1:A:866:PHE:CD2	5:E:168:TYR:CE1	2.98	0.52
1:A:1394:THR:O	1:A:1399:ARG:NE	2.38	0.52
1:A:1406:VAL:CG1	1:A:1410:PHE:CE1	2.90	0.52
2:B:225:VAL:HG22	2:B:396:ASP:OD2	2.10	0.52
2:B:413:LEU:O	2:B:414:ALA:C	2.52	0.52
2:B:522:VAL:CG1	2:B:523:CYS:N	2.71	0.52
3:C:99:LEU:HD23	3:C:99:LEU:N	2.23	0.52
3:C:215:GLU:O	3:C:217:ASP:N	2.43	0.52
8:H:128:ASN:CG	8:H:128:ASN:O	2.52	0.52
9:I:100:PHE:N	9:I:100:PHE:CD1	2.78	0.52
1:A:1073:GLY:HA2	1:A:1076:ALA:HB3	1.91	0.52
1:A:1157:ASP:C	1:A:1159:ARG:H	2.18	0.52
2:B:401:PHE:HD2	2:B:521:LEU:HD12	1.75	0.52
2:B:431:TYR:CZ	2:B:447:ALA:HB2	2.44	0.52
2:B:1184:GLY:C	2:B:1186:ASP:N	2.66	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:143:ILE:CG2	7:G:144:ARG:N	2.73	0.52
8:H:59:ILE:O	8:H:60:ALA:HB3	2.10	0.52
11:K:65:HIS:CD2	11:K:65:HIS:C	2.87	0.52
1:A:814:PHE:C	1:A:814:PHE:CD2	2.88	0.52
1:A:1088:GLY:O	1:A:1089:VAL:HG23	2.09	0.52
1:A:1102:LYS:C	1:A:1106:ASN:HD22	2.18	0.52
1:A:1213:GLY:O	1:A:1216:ILE:N	2.42	0.52
1:A:1280:GLU:O	1:A:1281:ARG:C	2.52	0.52
2:B:49:ASP:HA	2:B:52:ASN:HD22	1.75	0.52
2:B:314:LEU:O	2:B:315:LYS:C	2.53	0.52
2:B:457:LEU:O	2:B:461:LEU:HD12	2.10	0.52
2:B:857:ARG:NH2	2:B:942:ARG:NH1	2.57	0.52
3:C:58:LEU:N	3:C:58:LEU:HD22	2.25	0.52
3:C:227:THR:C	3:C:228:PHE:CD1	2.87	0.52
5:E:7:ARG:C	5:E:9:ILE:N	2.65	0.52
5:E:168:TYR:CB	5:E:170:LEU:HG	2.40	0.52
1:A:553:VAL:HG22	1:A:652:VAL:HG22	1.92	0.52
1:A:785:PRO:CG	2:B:703:ILE:HD12	2.40	0.52
1:A:1051:ALA:C	1:A:1053:PHE:N	2.67	0.52
1:A:1330:ASN:C	1:A:1330:ASN:OD1	2.52	0.52
1:A:1444:MET:O	6:F:132:LEU:HA	2.10	0.52
2:B:223:VAL:CG1	2:B:381:MET:HG2	2.40	0.52
2:B:865:LYS:HE2	2:B:871:THR:OG1	2.10	0.52
2:B:870:ILE:CG2	2:B:917:PRO:HG2	2.40	0.52
2:B:1045:SER:O	2:B:1046:PRO:O	2.27	0.52
3:C:31:ASN:OD1	3:C:34:ARG:HD3	2.10	0.52
10:J:55:ASP:OD2	10:J:58:GLU:HG2	2.10	0.52
12:L:28:LYS:HB2	12:L:39:SER:HA	1.91	0.52
1:A:18:GLN:HB3	2:B:1215:ARG:HG3	1.92	0.52
1:A:49:LYS:HZ2	1:A:60:SER:CA	2.20	0.52
1:A:55:ASP:N	1:A:56:PRO:CD	2.73	0.52
1:A:794:PRO:C	1:A:796:SER:H	2.18	0.52
1:A:898:ARG:HD3	1:A:933:TYR:CE1	2.45	0.52
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.91	0.52
1:A:1377:THR:O	1:A:1379:GLY:N	2.42	0.52
2:B:51:PHE:O	2:B:52:ASN:C	2.53	0.52
2:B:57:TYR:O	2:B:59:LEU:N	2.42	0.52
2:B:508:LEU:O	2:B:510:LYS:N	2.42	0.52
2:B:601:ARG:HG2	2:B:615:MET:HE1	1.92	0.52
2:B:640:VAL:HG23	2:B:740:HIS:HA	1.92	0.52
1:A:35:ILE:HG22	1:A:35:ILE:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:PRO:O	1:A:322:VAL:CB	2.57	0.51
1:A:351:THR:HG21	2:B:1103:ILE:HG13	1.91	0.51
1:A:841:LEU:O	1:A:845:LEU:HG	2.10	0.51
5:E:92:THR:O	5:E:95:THR:HB	2.10	0.51
13:S:235:ASP:CA	13:S:242:LYS:HG3	2.38	0.51
1:A:7:SER:O	1:A:8:SER:C	2.54	0.51
1:A:50:ILE:C	1:A:52:GLY:N	2.62	0.51
1:A:675:THR:O	1:A:679:ILE:HG13	2.11	0.51
1:A:725:ALA:O	1:A:729:ALA:N	2.42	0.51
1:A:856:THR:HB	1:A:865:GLN:HB2	1.93	0.51
1:A:1193:LEU:C	1:A:1193:LEU:HD12	2.35	0.51
2:B:54:PHE:CE1	2:B:414:ALA:HA	2.42	0.51
2:B:508:LEU:HB2	2:B:510:LYS:CB	2.40	0.51
2:B:758:PHE:CE2	2:B:1044:ALA:CA	2.92	0.51
2:B:781:PHE:CD1	2:B:781:PHE:C	2.88	0.51
2:B:1034:VAL:HG23	2:B:1059:LEU:CD1	2.40	0.51
2:B:1082:MET:O	3:C:189:THR:HG23	2.10	0.51
3:C:104:PHE:HD2	3:C:105:GLY:H	1.56	0.51
4:D:51:ASN:C	4:D:52:LEU:O	2.52	0.51
4:D:134:THR:HG22	4:D:136:GLY:H	1.75	0.51
9:I:54:GLU:O	9:I:100:PHE:CE2	2.63	0.51
12:L:38:LEU:HG	12:L:39:SER:N	2.26	0.51
1:A:348:SER:HB2	2:B:1128:LEU:HB2	1.90	0.51
1:A:894:GLU:C	1:A:896:ARG:H	2.18	0.51
1:A:1029:ARG:CG	1:A:1029:ARG:NH1	2.70	0.51
1:A:1148:ILE:O	1:A:1148:ILE:CG2	2.59	0.51
1:A:1325:THR:CG2	1:A:1326:ARG:HG3	2.40	0.51
1:A:1336:MET:HE2	1:A:1381:LEU:HG	1.92	0.51
2:B:62:ILE:HG23	2:B:418:LYS:HG2	1.92	0.51
2:B:380:TYR:OH	2:B:623:GLU:OE2	2.21	0.51
2:B:758:PHE:CE1	2:B:1027:ILE:CG2	2.94	0.51
2:B:879:ARG:O	2:B:880:THR:CB	2.58	0.51
2:B:1191:ILE:C	2:B:1192:TYR:CD1	2.88	0.51
3:C:31:ASN:O	3:C:34:ARG:HB3	2.10	0.51
9:I:100:PHE:N	9:I:100:PHE:HD1	2.08	0.51
11:K:65:HIS:CD2	11:K:66:PRO:HD2	2.46	0.51
11:K:67:PHE:O	11:K:68:PHE:HD2	1.93	0.51
11:K:78:THR:O	11:K:79:GLU:C	2.53	0.51
1:A:24:PRO:HG2	1:A:25:GLU:CD	2.35	0.51
1:A:602:ASP:OD2	1:A:616:VAL:HG23	2.11	0.51
1:A:898:ARG:HB2	1:A:933:TYR:HE1	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:928:LEU:O	1:A:929:LEU:C	2.53	0.51
1:A:1242:VAL:HG12	1:A:1243:VAL:N	2.25	0.51
2:B:38:PHE:CD1	2:B:811:TYR:CD2	2.98	0.51
2:B:46:GLN:CG	2:B:47:GLN:H	2.22	0.51
2:B:298:LEU:N	2:B:298:LEU:HD22	2.24	0.51
3:C:44:LEU:HB2	3:C:77:ILE:HD11	1.92	0.51
3:C:80:LEU:CD1	3:C:95:CYS:HA	2.40	0.51
3:C:107:SER:C	3:C:109:SER:N	2.69	0.51
9:I:95:THR:HG22	9:I:96:SER:N	2.25	0.51
10:J:48:ARG:HE	10:J:49:MET:HE2	1.75	0.51
11:K:87:LEU:HD12	11:K:87:LEU:O	2.09	0.51
1:A:56:PRO:O	1:A:57:ARG:CG	2.57	0.51
1:A:115:LEU:HB2	1:A:122:MET:CE	2.40	0.51
1:A:549:MET:O	1:A:550:LEU:C	2.53	0.51
1:A:1339:LEU:HD13	5:E:147:HIS:CD2	2.45	0.51
2:B:525:ALA:O	2:B:768:THR:HG23	2.11	0.51
2:B:843:GLN:O	2:B:846:ILE:HB	2.11	0.51
3:C:51:VAL:HG22	3:C:155:LEU:HD21	1.93	0.51
5:E:124:VAL:HG13	5:E:132:ILE:CB	2.39	0.51
7:G:123:ALA:O	7:G:125:SER:N	2.43	0.51
8:H:143:LEU:HD12	8:H:143:LEU:N	2.25	0.51
11:K:35:PHE:N	11:K:35:PHE:CD1	2.79	0.51
1:A:901:LEU:HD22	1:A:919:ILE:HG21	1.91	0.51
1:A:986:ILE:CD1	1:A:1032:LEU:HD11	2.40	0.51
1:A:1369:ALA:O	1:A:1372:VAL:HG12	2.11	0.51
2:B:59:LEU:HD12	2:B:417:PHE:CE2	2.46	0.51
2:B:97:VAL:HG12	2:B:178:ASN:HD21	1.74	0.51
2:B:118:ARG:HH22	2:B:194:GLU:CD	2.18	0.51
2:B:424:LEU:HD22	2:B:453:ILE:HD11	1.92	0.51
2:B:446:LEU:N	2:B:446:LEU:HD23	2.26	0.51
2:B:496:ARG:HH12	2:B:539:LEU:HB2	1.74	0.51
2:B:708:GLU:HG3	2:B:709:ASP:H	1.76	0.51
3:C:213:PRO:O	3:C:214:ASN:CB	2.55	0.51
5:E:7:ARG:C	5:E:9:ILE:H	2.19	0.51
5:E:144:ILE:HG13	5:E:145:THR:N	2.26	0.51
5:E:144:ILE:C	5:E:146:HIS:H	2.19	0.51
9:I:99:LEU:C	9:I:100:PHE:HD1	2.18	0.51
10:J:7:CYS:CA	10:J:49:MET:HE3	2.40	0.51
10:J:60:PHE:O	10:J:63:TYR:HD1	1.94	0.51
11:K:50:LEU:HD11	11:K:75:ILE:HD13	1.92	0.51
1:A:93:VAL:CG2	1:A:301:ALA:HA	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:LYS:O	1:A:101:LYS:C	2.54	0.51
1:A:647:GLY:O	1:A:648:ASN:C	2.54	0.51
1:A:770:VAL:O	1:A:771:GLU:HB2	2.11	0.51
1:A:877:HIS:CG	1:A:1056:SER:HA	2.46	0.51
2:B:102:VAL:HG22	2:B:112:LEU:HD22	1.92	0.51
2:B:378:LEU:HD12	2:B:378:LEU:C	2.35	0.51
2:B:726:ALA:HB1	2:B:1051:THR:HG21	1.91	0.51
2:B:1065:GLN:NE2	2:B:1067:ARG:HG2	2.25	0.51
5:E:79:TRP:HE1	5:E:81:GLU:HB2	1.76	0.51
9:I:43:VAL:O	9:I:43:VAL:HG12	2.09	0.51
1:A:34:LYS:HG2	1:A:36:ARG:NH2	2.26	0.51
1:A:472:LEU:CD1	2:B:835:GLN:NE2	2.69	0.51
1:A:556:TRP:C	1:A:558:GLY:N	2.65	0.51
1:A:645:LEU:O	1:A:646:PHE:C	2.54	0.51
1:A:795:GLU:CD	1:A:795:GLU:N	2.59	0.51
1:A:899:VAL:HG22	1:A:908:LEU:HD21	1.93	0.51
1:A:1169:ILE:O	1:A:1170:ILE:C	2.54	0.51
1:A:1191:TRP:HD1	1:A:1256:GLU:HB2	1.76	0.51
1:A:1372:VAL:HG12	1:A:1373:ASP:N	2.25	0.51
2:B:770:GLN:CD	2:B:983:ARG:HA	2.36	0.51
2:B:857:ARG:HG2	2:B:858:SER:N	2.24	0.51
2:B:865:LYS:HZ3	2:B:869:SER:HA	1.75	0.51
2:B:1032:SER:C	2:B:1034:VAL:N	2.64	0.51
2:B:1162:ILE:HG22	2:B:1163:CYS:N	2.25	0.51
3:C:60:ASP:OD2	12:L:60:ARG:NH2	2.44	0.51
5:E:16:PHE:O	5:E:17:ARG:C	2.54	0.51
7:G:1:MET:HE3	7:G:80:LYS:C	2.36	0.51
7:G:6:ASP:HB3	7:G:73:LYS:NZ	2.25	0.51
8:H:40:LEU:HG	8:H:41:ASP:O	2.11	0.51
10:J:5:VAL:O	10:J:6:ARG:O	2.28	0.51
1:A:14:VAL:H	1:A:1432:GLN:NE2	1.89	0.51
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.46	0.51
1:A:525:GLN:HB3	2:B:1015:HIS:HD2	1.74	0.51
1:A:556:TRP:O	1:A:558:GLY:N	2.44	0.51
1:A:738:LYS:HZ1	3:C:194:GLU:C	2.18	0.51
1:A:798:GLY:HA2	1:A:815:PHE:HD1	1.75	0.51
1:A:852:TYR:CD2	1:A:1060:PRO:HB2	2.45	0.51
1:A:903:ASN:C	1:A:903:ASN:ND2	2.65	0.51
1:A:1030:ARG:CG	1:A:1034:GLU:OE2	2.59	0.51
1:A:1090:ALA:O	1:A:1091:SER:OG	2.28	0.51
2:B:20:ASP:C	2:B:22:SER:H	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:LEU:HD22	2:B:429:PHE:HE1	1.74	0.51
2:B:334:ILE:HG22	2:B:334:ILE:O	2.09	0.51
5:E:100:ILE:CG2	5:E:105:PHE:HB2	2.40	0.51
7:G:114:LEU:HG	7:G:162:SER:HB3	1.93	0.51
12:L:49:LYS:O	12:L:50:ASP:CB	2.59	0.51
1:A:335:ARG:NE	1:A:339:ASN:HD22	2.09	0.51
1:A:399:HIS:O	1:A:400:PRO:C	2.54	0.51
1:A:474:VAL:HG22	1:A:474:VAL:O	2.10	0.51
1:A:496:GLU:OE1	7:G:64:THR:HA	2.11	0.51
1:A:1168:GLU:OE1	13:S:208:SER:CA	2.59	0.51
1:A:1277:GLU:O	1:A:1278:ASN:HB2	2.11	0.51
1:A:1290:LYS:O	1:A:1291:VAL:HG23	2.11	0.51
2:B:798:TYR:CD1	10:J:4:PRO:HG3	2.45	0.51
2:B:911:ILE:HG22	2:B:912:ILE:HG13	1.93	0.51
2:B:936:ASP:OD1	2:B:938:SER:N	2.42	0.51
3:C:35:ARG:HD3	11:K:41:THR:HA	1.93	0.51
8:H:25:ARG:HA	8:H:41:ASP:HA	1.93	0.51
10:J:46:CYS:O	10:J:49:MET:N	2.44	0.51
1:A:167:CYS:O	1:A:167:CYS:SG	2.69	0.50
1:A:456:MET:HE3	1:A:507:VAL:HG22	1.93	0.50
1:A:937:VAL:C	1:A:939:ASP:N	2.68	0.50
1:A:992:ASP:O	1:A:995:GLU:HB2	2.11	0.50
1:A:1167:GLU:O	1:A:1169:ILE:N	2.44	0.50
2:B:197:PHE:CZ	2:B:816:GLU:HG2	2.46	0.50
2:B:212:LEU:HD21	2:B:466:TRP:CH2	2.47	0.50
2:B:429:PHE:HA	2:B:432:MET:CE	2.40	0.50
2:B:1102:LYS:O	2:B:1103:ILE:O	2.29	0.50
3:C:163:ILE:O	3:C:164:ALA:C	2.54	0.50
3:C:168:ALA:O	3:C:170:TRP:N	2.44	0.50
4:D:47:LEU:HD13	4:D:48:ILE:N	2.25	0.50
5:E:10:SER:O	5:E:13:TRP:HB3	2.10	0.50
7:G:49:LEU:N	7:G:49:LEU:HD23	2.25	0.50
9:I:58:VAL:HG12	9:I:60:GLN:N	2.20	0.50
10:J:23:ASN:C	10:J:25:LEU:N	2.68	0.50
12:L:30:ILE:HG22	12:L:31:CYS:O	2.10	0.50
1:A:445:ASN:ND2	1:A:455:MET:HE3	2.26	0.50
1:A:646:PHE:O	1:A:647:GLY:C	2.55	0.50
1:A:996:ASN:HA	1:A:998:LEU:HD12	1.92	0.50
1:A:1385:THR:HG22	1:A:1386:ARG:N	2.26	0.50
2:B:242:SER:HB2	2:B:362:PRO:HG2	1.93	0.50
2:B:488:TYR:HE2	2:B:813:LYS:HB2	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:546:SER:HA	2:B:612:GLU:CD	2.35	0.50
2:B:546:SER:HA	2:B:612:GLU:OE2	2.11	0.50
2:B:994:TYR:HB2	2:B:999:MET:HE1	1.92	0.50
5:E:153:HIS:C	5:E:154:ILE:HG13	2.34	0.50
9:I:34:TYR:CD2	9:I:34:TYR:C	2.90	0.50
1:A:642:CYS:O	1:A:643:ALA:C	2.54	0.50
1:A:695:LYS:C	1:A:697:ALA:N	2.69	0.50
1:A:921:GLY:O	1:A:922:ASP:C	2.55	0.50
1:A:1067:LEU:O	1:A:1068:ALA:C	2.54	0.50
2:B:428:ILE:HG22	2:B:432:MET:HE2	1.94	0.50
2:B:510:LYS:O	2:B:513:GLN:HB2	2.11	0.50
7:G:70:PHE:N	7:G:70:PHE:CD1	2.79	0.50
10:J:52:THR:O	10:J:53:HIS:O	2.30	0.50
11:K:68:PHE:CD2	11:K:68:PHE:N	2.77	0.50
13:S:260:THR:CB	13:S:260:THR:C	2.80	0.50
1:A:335:ARG:HA	1:A:339:ASN:ND2	2.26	0.50
1:A:406:ILE:HG22	1:A:411:ASP:O	2.11	0.50
1:A:519:PRO:HG3	1:A:625:SER:O	2.12	0.50
1:A:811:GLN:O	1:A:812:GLU:C	2.55	0.50
1:A:858:ASN:HD21	1:A:860:LEU:HB2	1.75	0.50
1:A:871:ASP:CG	1:A:1366:ARG:HH22	2.19	0.50
1:A:1199:ARG:HG3	1:A:1236:LEU:HD11	1.93	0.50
1:A:1424:VAL:CG2	1:A:1436:ILE:HD11	2.32	0.50
2:B:269:ILE:HG22	2:B:282:ILE:HG23	1.94	0.50
2:B:303:TYR:CD2	2:B:303:TYR:N	2.80	0.50
2:B:996:ARG:HH22	3:C:175:ALA:HA	1.75	0.50
2:B:1111:MET:O	2:B:1112:GLN:C	2.54	0.50
2:B:1182:CYS:O	2:B:1183:LYS:C	2.53	0.50
3:C:53:THR:O	3:C:153:LEU:HA	2.10	0.50
3:C:239:PRO:HB2	3:C:241:ASP:OD1	2.12	0.50
6:F:119:ARG:HH11	6:F:119:ARG:CG	2.25	0.50
9:I:58:VAL:HG13	9:I:62:ILE:HD12	1.93	0.50
10:J:64:ASN:HB3	10:J:65:PRO:HD2	1.84	0.50
1:A:590:ARG:O	1:A:591:PHE:HB2	2.12	0.50
1:A:864:ILE:O	1:A:864:ILE:HG22	2.10	0.50
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.93	0.50
2:B:48:LEU:O	2:B:51:PHE:N	2.44	0.50
2:B:310:MET:HE1	2:B:383:ASN:OD1	2.11	0.50
2:B:570:VAL:HG21	2:B:573:GLN:CD	2.36	0.50
2:B:809:MET:O	2:B:812:LEU:N	2.37	0.50
2:B:839:MET:N	2:B:989:THR:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1029:CYS:SG	2:B:1086:PHE:CE2	3.05	0.50
2:B:1074:ASN:O	2:B:1078:GLY:N	2.44	0.50
3:C:43:THR:CG2	3:C:44:LEU:N	2.74	0.50
3:C:235:VAL:HG13	10:J:13:VAL:CG2	2.40	0.50
5:E:93:MET:C	5:E:95:THR:N	2.68	0.50
8:H:89:LEU:C	8:H:91:ASP:N	2.68	0.50
8:H:91:ASP:C	8:H:93:TYR:N	2.70	0.50
12:L:25:ALA:O	12:L:26:THR:HB	2.10	0.50
1:A:50:ILE:O	1:A:52:GLY:N	2.39	0.50
1:A:148:CYS:O	1:A:168:GLY:HA2	2.12	0.50
1:A:547:LEU:HD22	11:K:58:PHE:CE1	2.46	0.50
1:A:791:ASP:C	1:A:791:ASP:OD1	2.55	0.50
1:A:1213:GLY:O	1:A:1214:GLU:C	2.54	0.50
1:A:1308:THR:HG23	1:A:1309:ASP:N	2.26	0.50
1:A:1341:ILE:O	1:A:1344:GLY:N	2.45	0.50
1:A:1451:VAL:C	1:A:1453:TYR:H	2.19	0.50
2:B:758:PHE:HE2	2:B:1044:ALA:HA	1.73	0.50
4:D:26:THR:O	4:D:28:GLN:HG3	2.11	0.50
7:G:91:VAL:HA	7:G:101:VAL:HA	1.94	0.50
10:J:1:MET:HA	10:J:57:ILE:H	1.76	0.50
10:J:21:TYR:C	10:J:23:ASN:N	2.70	0.50
10:J:21:TYR:O	10:J:23:ASN:N	2.44	0.50
1:A:231:PRO:HA	1:A:234:MET:HE2	1.94	0.50
1:A:265:LYS:NZ	1:A:322:VAL:HG22	2.27	0.50
1:A:719:VAL:O	1:A:721:PHE:N	2.45	0.50
1:A:1114:PRO:O	1:A:1311:VAL:HG21	2.11	0.50
1:A:1398:MET:HB2	1:A:1426:GLU:OE2	2.11	0.50
2:B:509:ALA:C	2:B:510:LYS:HD2	2.36	0.50
2:B:851:PHE:CD2	2:B:1094:ARG:HB2	2.46	0.50
11:K:84:LYS:O	11:K:87:LEU:HB3	2.12	0.50
1:A:22:PHE:CE1	2:B:1213:THR:HG22	2.47	0.50
1:A:208:LEU:HG	1:A:235:ILE:HG21	1.93	0.50
1:A:709:THR:CG2	1:A:712:GLU:H	2.23	0.50
1:A:925:LEU:C	1:A:927:VAL:H	2.20	0.50
1:A:1053:PHE:O	1:A:1056:SER:N	2.44	0.50
2:B:196:PRO:HG2	2:B:197:PHE:H	1.77	0.50
2:B:376:PHE:HB3	2:B:586:TRP:CZ3	2.46	0.50
2:B:800:GLN:HB3	10:J:52:THR:CG2	2.35	0.50
2:B:980:PHE:CE2	2:B:1094:ARG:HG3	2.46	0.50
2:B:1022:THR:HG23	2:B:1022:THR:O	2.12	0.50
2:B:1060:ARG:HG2	2:B:1060:ARG:NH1	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:53:SER:HB3	4:D:152:SER:CB	2.42	0.50
4:D:130:LEU:C	4:D:132:GLN:N	2.61	0.50
5:E:25:ASP:C	5:E:27:GLY:H	2.17	0.50
6:F:127:GLU:O	6:F:129:LYS:HG3	2.12	0.50
6:F:143:PHE:C	6:F:143:PHE:CD1	2.90	0.50
12:L:52:GLY:O	12:L:53:HIS:C	2.54	0.50
1:A:12:ARG:CZ	2:B:1192:TYR:HE2	2.25	0.50
1:A:42:ASP:CG	1:A:45:GLN:HA	2.37	0.50
1:A:1122:PRO:O	1:A:1123:GLY:C	2.54	0.50
1:A:1125:ALA:O	1:A:1127:ASP:N	2.45	0.50
1:A:1213:GLY:HA2	1:A:1216:ILE:CD1	2.42	0.50
2:B:91:SER:OG	2:B:133:LYS:HB2	2.11	0.50
2:B:210:LYS:HE2	2:B:462:ALA:O	2.11	0.50
2:B:217:ARG:HD2	2:B:217:ARG:C	2.37	0.50
2:B:218:SER:O	2:B:219:ALA:O	2.29	0.50
2:B:578:THR:HA	2:B:622:LYS:HB3	1.94	0.50
2:B:843:GLN:O	2:B:846:ILE:N	2.44	0.50
2:B:901:PRO:O	2:B:902:GLY:C	2.53	0.50
5:E:3:GLN:HG3	5:E:4:GLU:N	2.27	0.50
5:E:171:LYS:O	5:E:172:GLU:C	2.55	0.50
6:F:103:MET:O	6:F:104:ASN:HB2	2.11	0.50
8:H:81:PRO:HB3	8:H:82:PRO:HD2	1.92	0.50
9:I:88:SER:C	9:I:90:GLN:N	2.70	0.50
12:L:28:LYS:HB2	12:L:39:SER:CA	2.42	0.50
12:L:60:ARG:HG2	12:L:61:THR:N	2.27	0.50
1:A:347:PHE:N	2:B:1107:ALA:HA	2.26	0.49
1:A:416:ARG:O	1:A:417:TYR:HD2	1.94	0.49
1:A:541:ILE:HD12	1:A:577:ILE:HD11	1.94	0.49
1:A:809:THR:OG1	1:A:812:GLU:HG3	2.12	0.49
1:A:863:VAL:HG12	1:A:865:GLN:H	1.76	0.49
2:B:117:ALA:HA	2:B:122:LEU:HB2	1.94	0.49
2:B:763:GLN:HG2	2:B:765:PRO:CD	2.38	0.49
2:B:984:HIS:CD2	2:B:1025:HIS:HB2	2.47	0.49
2:B:1178:ASN:O	2:B:1179:GLN:C	2.55	0.49
3:C:84:ARG:NH2	11:K:11:LEU:HD21	2.27	0.49
4:D:134:THR:CG2	4:D:135:GLY:N	2.75	0.49
6:F:103:MET:HE2	7:G:66:GLY:N	2.18	0.49
7:G:96:GLN:HG3	7:G:97:HIS:HD2	1.76	0.49
8:H:93:TYR:N	8:H:93:TYR:CD1	2.80	0.49
1:A:14:VAL:CG2	1:A:1430:LEU:HD13	2.42	0.49
1:A:254:GLU:HB2	2:B:935:ARG:NH2	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.93	0.49
1:A:755:PHE:HA	1:A:758:ILE:HG13	1.94	0.49
1:A:989:GLY:O	1:A:992:ASP:N	2.44	0.49
1:A:1019:CYS:O	1:A:1022:LEU:N	2.45	0.49
1:A:1161:THR:O	1:A:1163:ILE:N	2.45	0.49
1:A:1364:ASN:HD22	1:A:1365:TYR:N	2.10	0.49
2:B:25:ILE:HG23	2:B:29:ASP:CB	2.42	0.49
2:B:215:GLN:OE1	2:B:215:GLN:HA	2.12	0.49
2:B:314:LEU:O	2:B:317:CYS:HB3	2.12	0.49
2:B:526:GLU:HG2	2:B:538:ASN:HD22	1.77	0.49
2:B:850:LEU:HD12	2:B:851:PHE:H	1.77	0.49
3:C:86:CYS:SG	3:C:95:CYS:HB3	2.52	0.49
3:C:143:LEU:HD21	3:C:146:LYS:HE2	1.94	0.49
4:D:48:ILE:HG21	7:G:4:ILE:CD1	2.41	0.49
4:D:144:THR:OG1	7:G:105:PRO:HD3	2.12	0.49
6:F:72:LYS:HB2	6:F:142:SER:HB3	1.94	0.49
7:G:25:TYR:HE2	7:G:29:LYS:HD2	1.77	0.49
8:H:58:THR:HB	8:H:143:LEU:HD13	1.94	0.49
9:I:113:ASP:O	9:I:114:GLN:CG	2.61	0.49
13:S:269:PHE:HE2	13:S:306:TRP:CZ2	2.30	0.49
1:A:90:VAL:CG1	1:A:91:PHE:H	2.23	0.49
1:A:125:ALA:C	1:A:127:ALA:H	2.20	0.49
1:A:324:SER:O	1:A:325:ILE:C	2.52	0.49
1:A:838:GLN:O	1:A:842:VAL:HG23	2.13	0.49
1:A:898:ARG:HB2	1:A:933:TYR:CE1	2.47	0.49
1:A:1041:ALA:O	1:A:1044:TRP:HB3	2.12	0.49
1:A:1048:ASN:HD22	1:A:1048:ASN:N	2.10	0.49
2:B:261:ARG:HB3	2:B:261:ARG:HH11	1.76	0.49
2:B:882:THR:HB	2:B:934:LYS:O	2.11	0.49
3:C:69:LEU:HD12	3:C:69:LEU:N	2.27	0.49
3:C:186:LEU:N	3:C:186:LEU:CD1	2.75	0.49
5:E:23:VAL:O	5:E:28:TYR:HB2	2.12	0.49
5:E:164:LEU:CD2	5:E:211:TYR:CD2	2.95	0.49
1:A:24:PRO:HG2	1:A:25:GLU:OE2	2.11	0.49
1:A:564:ALA:HB2	1:A:576:GLN:OE1	2.12	0.49
1:A:717:ASN:O	1:A:721:PHE:CD1	2.66	0.49
1:A:874:ASP:N	1:A:1058:VAL:HG23	2.27	0.49
1:A:997:LEU:HB3	1:A:1053:PHE:CE2	2.47	0.49
1:A:1261:LYS:C	1:A:1264:GLU:H	2.20	0.49
1:A:1285:MET:HG3	1:A:1307:GLU:OE2	2.12	0.49
1:A:1360:GLY:HA3	13:S:306:TRP:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:563:MET:HA	2:B:589:VAL:O	2.13	0.49
2:B:583:ASN:HD21	2:B:628:THR:CB	2.13	0.49
2:B:843:GLN:O	2:B:844:SER:C	2.56	0.49
2:B:1165:ILE:HG22	2:B:1185:CYS:HB3	1.94	0.49
5:E:124:VAL:CG1	5:E:132:ILE:HD12	2.37	0.49
7:G:126:ASN:HA	7:G:127:PRO:C	2.36	0.49
13:S:273:LYS:C	13:S:275:LYS:H	2.18	0.49
1:A:470:LEU:HD11	1:A:482:PHE:CZ	2.46	0.49
1:A:821:ARG:HA	1:A:824:LEU:HD12	1.95	0.49
1:A:979:SER:HG	1:A:980:ASP:H	1.58	0.49
1:A:1097:GLY:C	1:A:1099:PRO:HD2	2.37	0.49
1:A:1444:MET:HG2	7:G:60:ARG:CA	2.40	0.49
2:B:175:ARG:HG2	2:B:175:ARG:HH11	1.77	0.49
2:B:497:ARG:NH2	2:B:775:LYS:NZ	2.60	0.49
2:B:642:ASP:HA	2:B:649:LYS:HA	1.95	0.49
2:B:1177:HIS:O	2:B:1179:GLN:N	2.44	0.49
4:D:147:TYR:CZ	7:G:103:VAL:HG13	2.47	0.49
5:E:72:PHE:N	5:E:72:PHE:CD1	2.80	0.49
7:G:1:MET:CE	7:G:80:LYS:C	2.85	0.49
1:A:37:PHE:N	1:A:37:PHE:CD1	2.81	0.49
1:A:601:LYS:HB2	1:A:603:ASN:ND2	2.27	0.49
1:A:869:GLY:O	1:A:870:GLU:HB2	2.11	0.49
1:A:871:ASP:O	1:A:873:MET:HE2	2.11	0.49
1:A:1226:VAL:C	1:A:1227:ILE:HG13	2.37	0.49
2:B:186:GLU:O	2:B:187:SER:C	2.55	0.49
2:B:351:TYR:CE1	2:B:355:ILE:HD11	2.47	0.49
2:B:615:MET:C	2:B:616:ILE:HD12	2.36	0.49
2:B:958:GLN:C	2:B:960:GLY:H	2.19	0.49
3:C:73:GLN:HE21	3:C:74:SER:H	1.60	0.49
4:D:137:ASN:C	4:D:137:ASN:ND2	2.70	0.49
7:G:30:LEU:O	7:G:34:VAL:HG23	2.12	0.49
1:A:88:LYS:HE3	1:A:280:GLU:OE2	2.12	0.49
1:A:321:PRO:O	1:A:322:VAL:HB	2.13	0.49
1:A:387:ARG:O	1:A:390:GLN:HB3	2.13	0.49
1:A:809:THR:H	1:A:812:GLU:HB2	1.78	0.49
1:A:1090:ALA:O	1:A:1091:SER:CB	2.60	0.49
2:B:54:PHE:O	2:B:59:LEU:HB2	2.12	0.49
2:B:693:ILE:HD11	2:B:740:HIS:NE2	2.27	0.49
2:B:899:ILE:HG22	2:B:900:ALA:H	1.75	0.49
2:B:1002:THR:O	2:B:1005:GLY:N	2.32	0.49
2:B:1106:ARG:HD3	2:B:1126:GLY:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:53:SER:O	4:D:57:LEU:HG	2.12	0.49
4:D:56:ARG:NH2	4:D:155:ARG:HA	2.28	0.49
4:D:127:ASP:O	4:D:131:GLU:HG3	2.13	0.49
8:H:27:GLU:HA	8:H:38:LEU:O	2.12	0.49
9:I:13:MET:HG3	9:I:14:LEU:N	2.27	0.49
1:A:3:GLY:O	1:A:4:GLN:O	2.31	0.49
1:A:433:GLU:OE2	2:B:1108:ARG:NH1	2.45	0.49
1:A:567:LYS:HZ1	8:H:46:LEU:HB2	1.74	0.49
1:A:626:ASN:O	1:A:628:GLY:N	2.42	0.49
1:A:1086:PHE:HE2	13:S:261:ILE:CD1	2.24	0.49
1:A:1209:MET:O	1:A:1210:GLY:C	2.55	0.49
1:A:1354:ASN:O	1:A:1355:VAL:C	2.54	0.49
1:A:1437:GLY:O	1:A:1438:THR:C	2.56	0.49
2:B:97:VAL:CG1	2:B:178:ASN:ND2	2.74	0.49
2:B:189:LEU:HD13	2:B:196:PRO:HA	1.94	0.49
2:B:247:GLY:H	2:B:418:LYS:NZ	2.10	0.49
2:B:361:LEU:N	2:B:362:PRO:CD	2.75	0.49
2:B:390:LEU:O	2:B:391:ASP:C	2.54	0.49
2:B:806:THR:C	2:B:808:ALA:N	2.68	0.49
2:B:910:VAL:CG1	2:B:911:ILE:N	2.76	0.49
2:B:1059:LEU:HD23	2:B:1065:GLN:O	2.12	0.49
4:D:170:THR:HG21	4:D:172:LEU:HG	1.94	0.49
4:D:173:HIS:O	4:D:177:VAL:HG23	2.13	0.49
12:L:31:CYS:HB3	12:L:35:SER:CA	2.42	0.49
1:A:154:SER:HB3	1:A:162:VAL:HG21	1.95	0.49
1:A:384:ASN:CG	1:A:388:LEU:HD12	2.37	0.49
1:A:907:THR:CG2	1:A:908:LEU:N	2.75	0.49
1:A:1161:THR:HG22	1:A:1163:ILE:HG13	1.94	0.49
1:A:1198:ASP:O	1:A:1202:MET:HG2	2.13	0.49
1:A:1342:GLU:HG3	5:E:198:ILE:HG21	1.95	0.49
2:B:234:ILE:HD12	2:B:234:ILE:N	2.27	0.49
2:B:371:GLU:CD	2:B:371:GLU:N	2.70	0.49
2:B:446:LEU:O	2:B:447:ALA:CB	2.61	0.49
2:B:510:LYS:HG2	2:B:512:ARG:N	2.19	0.49
2:B:642:ASP:C	2:B:644:GLU:H	2.19	0.49
2:B:992:ILE:CG2	2:B:994:TYR:HE1	2.26	0.49
2:B:999:MET:HA	2:B:999:MET:CE	2.42	0.49
2:B:1034:VAL:HG23	2:B:1059:LEU:HD12	1.95	0.49
5:E:32:GLN:HG3	5:E:36:GLU:OE2	2.12	0.49
5:E:136:ASN:OD1	5:E:137:GLU:N	2.46	0.49
10:J:37:SER:OG	10:J:47:ARG:NH2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:32:VAL:HG22	11:K:74:ARG:HG3	1.95	0.49
1:A:481:ASP:O	1:A:485:ASP:HB2	2.13	0.49
1:A:501:LEU:HD11	2:B:1146:PHE:CD2	2.48	0.49
2:B:67:SER:O	2:B:68:THR:C	2.56	0.49
2:B:360:PHE:C	2:B:360:PHE:CD2	2.91	0.49
2:B:594:ALA:CA	2:B:617:ARG:HH12	2.25	0.49
3:C:80:LEU:HD22	3:C:129:ILE:HD13	1.94	0.49
1:A:525:GLN:HB3	2:B:1015:HIS:CD2	2.48	0.48
1:A:877:HIS:C	1:A:878:ILE:CG1	2.86	0.48
2:B:760:ASP:O	2:B:761:HIS:CD2	2.66	0.48
6:F:72:LYS:O	6:F:73:ALA:CB	2.61	0.48
7:G:101:VAL:CG1	7:G:102:GLN:N	2.76	0.48
1:A:525:GLN:O	1:A:526:ASP:C	2.56	0.48
1:A:852:TYR:CE1	6:F:136:ARG:HB3	2.48	0.48
1:A:1210:GLY:O	1:A:1211:GLN:C	2.56	0.48
2:B:102:VAL:CG2	2:B:112:LEU:HD22	2.43	0.48
2:B:115:GLN:HG2	2:B:193:LYS:HB2	1.95	0.48
2:B:498:THR:HG22	2:B:537:LYS:H	1.78	0.48
2:B:558:LEU:C	2:B:560:GLU:N	2.70	0.48
2:B:811:TYR:CD1	2:B:811:TYR:N	2.80	0.48
2:B:845:SER:HB3	10:J:8:PHE:O	2.13	0.48
3:C:111:THR:O	3:C:147:LEU:HD23	2.12	0.48
3:C:136:ASP:OD1	3:C:138:GLU:N	2.45	0.48
5:E:17:ARG:O	5:E:20:LYS:HB2	2.13	0.48
5:E:117:THR:C	5:E:119:SER:H	2.21	0.48
7:G:15:PRO:O	7:G:18:PHE:HB2	2.12	0.48
12:L:30:ILE:CG2	12:L:31:CYS:N	2.75	0.48
1:A:64:ASN:O	1:A:65:LEU:C	2.56	0.48
1:A:348:SER:HB2	2:B:1128:LEU:HD12	1.93	0.48
1:A:472:LEU:HD13	2:B:835:GLN:OE1	2.13	0.48
1:A:503:GLN:O	1:A:504:LEU:HD12	2.13	0.48
1:A:668:ASP:CG	1:A:742:ASN:HD22	2.19	0.48
1:A:1263:ILE:O	1:A:1263:ILE:HG22	2.14	0.48
1:A:1308:THR:O	1:A:1309:ASP:HB2	2.12	0.48
2:B:38:PHE:HD1	2:B:811:TYR:CD2	2.31	0.48
2:B:899:ILE:HG23	2:B:903:VAL:HG21	1.95	0.48
2:B:1208:MET:HA	2:B:1212:ILE:O	2.13	0.48
8:H:10:PHE:N	8:H:10:PHE:CD1	2.81	0.48
10:J:36:LEU:HB2	10:J:47:ARG:NH1	2.28	0.48
11:K:88:LYS:O	11:K:89:ASN:C	2.56	0.48
1:A:98:LYS:O	1:A:99:ILE:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:780:VAL:O	1:A:780:VAL:HG12	2.14	0.48
1:A:877:HIS:O	1:A:878:ILE:CG1	2.61	0.48
1:A:929:LEU:HD23	1:A:983:ILE:HG21	1.95	0.48
2:B:166:PHE:C	2:B:167:ILE:HG13	2.39	0.48
2:B:579:ARG:HG2	2:B:579:ARG:HH11	1.79	0.48
2:B:616:ILE:N	2:B:625:LYS:O	2.37	0.48
2:B:622:LYS:CE	9:I:59:VAL:HG22	2.41	0.48
2:B:760:ASP:OD1	2:B:1046:PRO:HA	2.12	0.48
2:B:976:ILE:O	2:B:990:ILE:HB	2.12	0.48
3:C:164:ALA:O	3:C:167:HIS:N	2.43	0.48
6:F:99:LEU:O	6:F:103:MET:HG2	2.14	0.48
10:J:3:VAL:HG12	10:J:4:PRO:N	2.28	0.48
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.96	0.48
13:S:274:CYS:O	13:S:276:GLU:HG3	2.13	0.48
1:A:22:PHE:CD1	2:B:1213:THR:HG22	2.49	0.48
1:A:1329:THR:C	1:A:1331:SER:N	2.71	0.48
1:A:1335:ILE:HG23	1:A:1339:LEU:HD12	1.96	0.48
1:A:1372:VAL:HG12	1:A:1373:ASP:H	1.78	0.48
2:B:112:LEU:CD1	2:B:113:TYR:N	2.71	0.48
2:B:658:ILE:HG22	2:B:659:ALA:N	2.28	0.48
2:B:806:THR:CG2	2:B:808:ALA:HB3	2.44	0.48
2:B:1202:LEU:HD22	2:B:1206:GLU:CD	2.39	0.48
3:C:8:VAL:HG12	3:C:9:LYS:N	2.28	0.48
3:C:173:ALA:O	3:C:174:ALA:HB3	2.13	0.48
4:D:190:GLU:O	4:D:194:LEU:HG	2.14	0.48
4:D:208:GLU:O	4:D:212:LYS:HG3	2.13	0.48
5:E:16:PHE:CE2	5:E:20:LYS:HE2	2.48	0.48
7:G:145:VAL:CG1	7:G:146:LYS:H	2.27	0.48
9:I:27:PHE:O	9:I:28:GLU:HB3	2.11	0.48
11:K:47:ARG:HH11	11:K:47:ARG:CB	2.23	0.48
1:A:228:PHE:N	1:A:228:PHE:CD2	2.81	0.48
1:A:814:PHE:CD1	2:B:519:TRP:HE3	2.32	0.48
1:A:863:VAL:HG12	1:A:864:ILE:H	1.77	0.48
1:A:873:MET:HG2	1:A:957:PRO:HG3	1.96	0.48
1:A:896:ARG:CD	1:A:897:TYR:HE1	2.12	0.48
1:A:996:ASN:C	1:A:998:LEU:H	2.22	0.48
1:A:1029:ARG:HG3	1:A:1029:ARG:NH1	2.17	0.48
1:A:1051:ALA:O	1:A:1054:LEU:N	2.47	0.48
2:B:482:VAL:O	2:B:483:LEU:C	2.57	0.48
2:B:583:ASN:OD1	2:B:628:THR:N	2.47	0.48
2:B:976:ILE:CD1	2:B:992:ILE:HA	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:992:ILE:HD11	11:K:66:PRO:HB2	1.96	0.48
3:C:116:LYS:HD3	3:C:140:ASN:HB3	1.95	0.48
3:C:263:THR:O	3:C:265:MET:N	2.47	0.48
8:H:83:GLN:O	8:H:85:GLY:N	2.44	0.48
11:K:65:HIS:CD2	11:K:66:PRO:N	2.81	0.48
1:A:42:ASP:OD1	1:A:45:GLN:HA	2.13	0.48
1:A:821:ARG:HH11	1:A:821:ARG:CB	2.25	0.48
1:A:1057:VAL:CG1	1:A:1058:VAL:N	2.76	0.48
1:A:1116:LEU:C	1:A:1116:LEU:HD12	2.38	0.48
1:A:1438:THR:HB	2:B:1144:ALA:HB3	1.96	0.48
2:B:525:ALA:O	2:B:527:THR:HG22	2.13	0.48
2:B:764:SER:N	2:B:765:PRO:HD2	2.29	0.48
2:B:797:TYR:HB3	2:B:798:TYR:CD2	2.49	0.48
6:F:111:LEU:O	6:F:113:GLY:N	2.47	0.48
8:H:82:PRO:O	8:H:83:GLN:HB2	2.13	0.48
11:K:81:TYR:OH	11:K:86:ALA:HA	2.13	0.48
11:K:106:GLU:O	11:K:107:THR:C	2.56	0.48
13:S:236:LEU:CA	13:S:242:LYS:NZ	2.77	0.48
13:S:254:TYR:O	13:S:256:ALA:N	2.47	0.48
1:A:329:LEU:N	1:A:329:LEU:HD23	2.28	0.48
1:A:375:THR:HA	1:A:434:ARG:O	2.14	0.48
1:A:821:ARG:O	1:A:821:ARG:HG3	2.12	0.48
1:A:901:LEU:HB2	1:A:926:GLN:HG2	1.95	0.48
1:A:1059:HIS:O	1:A:1061:GLY:N	2.46	0.48
1:A:1121:GLU:O	1:A:1122:PRO:C	2.57	0.48
1:A:1193:LEU:HD12	1:A:1194:ARG:N	2.29	0.48
2:B:509:ALA:O	2:B:510:LYS:O	2.32	0.48
2:B:591:ARG:O	2:B:592:ASN:C	2.57	0.48
2:B:825:VAL:CG1	2:B:826:ALA:N	2.77	0.48
3:C:22:LEU:HD13	3:C:230:MET:CE	2.44	0.48
5:E:46:TYR:CD2	5:E:58:MET:HG2	2.48	0.48
10:J:7:CYS:HA	10:J:49:MET:HE3	1.95	0.48
1:A:14:VAL:HG21	1:A:1430:LEU:HD13	1.96	0.48
1:A:68:GLN:NE2	1:A:80:HIS:CD2	2.79	0.48
1:A:590:ARG:HD3	1:A:604:GLY:CA	2.41	0.48
1:A:744:LYS:HG2	1:A:748:MET:CE	2.41	0.48
1:A:1265:ASN:O	1:A:1267:MET:N	2.47	0.48
2:B:273:LEU:HD21	2:B:360:PHE:CD1	2.48	0.48
2:B:295:GLY:H	2:B:298:LEU:CD2	2.13	0.48
2:B:617:ARG:NE	2:B:619:ILE:HG12	2.29	0.48
2:B:644:GLU:C	2:B:646:LEU:N	2.71	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:681:TRP:O	2:B:683:SER:N	2.46	0.48
2:B:1135:ARG:NH2	2:B:1136:ASP:OD1	2.38	0.48
3:C:67:LEU:HD11	3:C:155:LEU:CD1	2.44	0.48
6:F:109:VAL:HG12	6:F:110:ASP:N	2.29	0.48
8:H:106:GLU:HG2	8:H:112:ILE:HG12	1.96	0.48
11:K:21:ILE:HG23	11:K:31:VAL:CG1	2.44	0.48
12:L:39:SER:O	12:L:40:LEU:HG	2.14	0.48
1:A:315:LEU:HD22	1:A:319:GLY:O	2.13	0.48
1:A:416:ARG:C	1:A:417:TYR:CD2	2.92	0.48
1:A:525:GLN:CD	2:B:836:GLU:HG2	2.39	0.48
1:A:1293:SER:OG	1:A:1295:THR:CG2	2.62	0.48
2:B:223:VAL:HG11	2:B:381:MET:HG2	1.96	0.48
2:B:465:ASN:HD22	2:B:465:ASN:N	2.12	0.48
2:B:910:VAL:HG12	2:B:911:ILE:H	1.79	0.48
2:B:1002:THR:HG22	2:B:1006:ILE:O	2.14	0.48
3:C:143:LEU:HD21	3:C:146:LYS:CE	2.43	0.48
4:D:185:CYS:HB3	4:D:211:LEU:HD13	1.95	0.48
6:F:111:LEU:C	6:F:113:GLY:N	2.62	0.48
7:G:88:ASP:HB3	7:G:144:ARG:HB2	1.95	0.48
13:S:253:LEU:O	13:S:256:ALA:HB3	2.14	0.48
1:A:157:ASP:C	1:A:159:THR:H	2.22	0.47
1:A:261:ASP:O	1:A:264:PHE:HB2	2.13	0.47
1:A:356:ASP:HB2	1:A:469:ARG:HG2	1.96	0.47
1:A:393:ARG:O	1:A:395:GLY:N	2.47	0.47
1:A:418:SER:O	1:A:421:ALA:N	2.46	0.47
1:A:859:SER:OG	1:A:1398:MET:HE1	2.13	0.47
1:A:1063:MET:HE2	1:A:1436:ILE:HG12	1.97	0.47
1:A:1064:VAL:O	1:A:1065:GLY:C	2.55	0.47
1:A:1293:SER:OG	1:A:1294:PRO:HD2	2.14	0.47
1:A:1394:THR:CG2	1:A:1398:MET:HE3	2.43	0.47
2:B:114:PRO:O	2:B:115:GLN:C	2.57	0.47
2:B:393:LYS:HA	2:B:393:LYS:HE3	1.96	0.47
2:B:508:LEU:O	2:B:509:ALA:C	2.51	0.47
2:B:540:SER:HA	2:B:749:LEU:O	2.14	0.47
2:B:806:THR:HG22	2:B:808:ALA:HB3	1.94	0.47
2:B:872:GLU:CD	2:B:914:LYS:HE2	2.39	0.47
3:C:42:PRO:HA	3:C:163:ILE:CG2	2.44	0.47
5:E:44:ALA:O	5:E:45:LYS:HB2	2.13	0.47
6:F:132:LEU:O	6:F:148:VAL:HG22	2.14	0.47
10:J:57:ILE:CA	10:J:60:PHE:CD2	2.90	0.47
1:A:768:GLN:HG2	1:A:816:HIS:CA	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:928:LEU:O	1:A:931:GLU:N	2.47	0.47
1:A:1051:ALA:O	1:A:1052:GLN:C	2.56	0.47
1:A:1116:LEU:HA	1:A:1329:THR:HA	1.96	0.47
1:A:1283:VAL:CG1	1:A:1284:MET:H	2.24	0.47
2:B:259:TYR:HB2	2:B:268:THR:HG23	1.95	0.47
2:B:457:LEU:O	2:B:461:LEU:CD1	2.61	0.47
2:B:486:TYR:CG	2:B:1096:ARG:NH2	2.82	0.47
2:B:689:LEU:O	2:B:690:VAL:HG23	2.14	0.47
2:B:810:GLU:HG3	2:B:815:ARG:HH22	1.79	0.47
2:B:942:ARG:O	2:B:944:THR:N	2.48	0.47
2:B:1017:ILE:HG22	2:B:1018:PRO:CD	2.44	0.47
2:B:1150:ARG:HA	2:B:1150:ARG:HE	1.79	0.47
2:B:1159:ARG:CD	2:B:1193:GLN:HE21	2.26	0.47
3:C:27:LEU:O	3:C:30:ALA:N	2.47	0.47
3:C:79:GLN:O	3:C:127:ARG:NH1	2.46	0.47
3:C:242:GLN:CA	3:C:245:VAL:HG23	2.43	0.47
8:H:84:ALA:HB2	8:H:87:ARG:HD2	1.96	0.47
9:I:2:THR:O	9:I:2:THR:HG22	2.14	0.47
13:S:281:TYR:CD1	13:S:281:TYR:C	2.93	0.47
1:A:81:PHE:CE2	1:A:242:PRO:HA	2.48	0.47
1:A:231:PRO:C	1:A:233:TRP:N	2.72	0.47
1:A:381:THR:HG21	1:A:383:TYR:CD1	2.50	0.47
1:A:419:LYS:HG3	1:A:420:ARG:N	2.28	0.47
1:A:715:GLU:C	1:A:717:ASN:N	2.71	0.47
1:A:919:ILE:O	1:A:920:LEU:C	2.57	0.47
1:A:993:LEU:HD11	1:A:997:LEU:HD21	1.96	0.47
1:A:1125:ALA:C	1:A:1127:ASP:N	2.72	0.47
2:B:168:GLY:N	2:B:450:ALA:HB1	2.14	0.47
2:B:510:LYS:O	2:B:510:LYS:HD3	2.13	0.47
2:B:702:LEU:C	2:B:703:ILE:HG13	2.39	0.47
2:B:846:ILE:HG23	2:B:974:PRO:CG	2.36	0.47
2:B:936:ASP:CG	2:B:938:SER:H	2.23	0.47
2:B:992:ILE:HG21	2:B:994:TYR:HE1	1.79	0.47
3:C:170:TRP:O	3:C:171:GLY:C	2.54	0.47
3:C:191:TYR:CD2	3:C:201:TRP:CD1	2.97	0.47
5:E:129:PRO:O	5:E:130:ALA:C	2.57	0.47
1:A:8:SER:O	1:A:9:ALA:C	2.57	0.47
1:A:789:LYS:HE3	9:I:67:THR:HB	1.97	0.47
1:A:852:TYR:CD2	1:A:1060:PRO:CB	2.97	0.47
1:A:944:ARG:NE	1:A:1298:TYR:HE1	2.12	0.47
1:A:1006:ILE:HD11	5:E:163:GLU:CG	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1090:ALA:CB	1:A:1093:LYS:HE3	2.43	0.47
1:A:1230:GLU:C	1:A:1232:ASN:N	2.71	0.47
1:A:1263:ILE:O	1:A:1267:MET:HG3	2.15	0.47
2:B:1106:ARG:HD3	2:B:1126:GLY:C	2.39	0.47
1:A:125:ALA:O	1:A:127:ALA:N	2.48	0.47
1:A:1118:VAL:HG23	1:A:1306:LEU:HB2	1.94	0.47
1:A:1282:VAL:C	1:A:1283:VAL:CG2	2.88	0.47
1:A:1335:ILE:O	1:A:1335:ILE:CG2	2.63	0.47
2:B:597:MET:C	2:B:599:THR:H	2.22	0.47
2:B:757:PRO:O	2:B:758:PHE:HB2	2.13	0.47
2:B:1033:LYS:HB2	2:B:1089:PRO:HD2	1.97	0.47
3:C:197:SER:O	3:C:198:ALA:C	2.58	0.47
4:D:51:ASN:O	4:D:52:LEU:O	2.33	0.47
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.96	0.47
10:J:48:ARG:HE	10:J:49:MET:CE	2.28	0.47
12:L:27:LEU:HD13	12:L:37:LYS:HE2	1.96	0.47
12:L:58:LYS:O	12:L:58:LYS:HG2	2.15	0.47
1:A:399:HIS:CB	1:A:400:PRO:CD	2.87	0.47
1:A:447:GLN:HB3	1:A:448:PRO:HA	1.97	0.47
1:A:535:THR:HG23	1:A:575:LYS:HG2	1.96	0.47
1:A:541:ILE:HD13	1:A:549:MET:CE	2.45	0.47
1:A:606:LEU:CB	1:A:614:PHE:CE2	2.97	0.47
1:A:711:ARG:HA	9:I:97:MET:CE	2.44	0.47
1:A:962:ARG:O	1:A:964:ILE:N	2.47	0.47
1:A:1057:VAL:CG1	1:A:1058:VAL:H	2.26	0.47
1:A:1216:ILE:O	1:A:1219:THR:HB	2.14	0.47
2:B:363:HIS:NE2	2:B:364:ILE:HG13	2.29	0.47
2:B:619:ILE:O	2:B:621:GLU:N	2.47	0.47
2:B:752:ALA:HB1	2:B:771:SER:HB3	1.96	0.47
2:B:798:TYR:CD2	2:B:798:TYR:N	2.83	0.47
2:B:847:ASP:C	2:B:849:GLY:N	2.72	0.47
2:B:903:VAL:CG1	2:B:904:ARG:N	2.76	0.47
2:B:1210:MET:O	2:B:1212:ILE:N	2.47	0.47
9:I:58:VAL:HG13	9:I:62:ILE:CD1	2.44	0.47
1:A:53:LEU:HD23	1:A:54:ASN:CB	2.45	0.47
1:A:253:ASN:OD1	2:B:884:ARG:HD2	2.14	0.47
1:A:302:THR:HA	1:A:305:ASP:O	2.14	0.47
1:A:370:ILE:O	1:A:371:ALA:C	2.57	0.47
1:A:451:HIS:O	2:B:1137:CYS:SG	2.73	0.47
1:A:556:TRP:NE1	1:A:559:VAL:H	2.13	0.47
1:A:608:ILE:O	1:A:609:ASP:C	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:650:GLN:O	1:A:654:ASN:HB2	2.14	0.47
1:A:714:PHE:CB	9:I:97:MET:HE1	2.45	0.47
1:A:814:PHE:O	1:A:817:ALA:HB3	2.15	0.47
1:A:897:TYR:HD2	1:A:936:LEU:CD1	2.28	0.47
1:A:928:LEU:C	1:A:930:ASP:N	2.70	0.47
1:A:1081:LEU:HD21	1:A:1098:VAL:CB	2.44	0.47
1:A:1311:VAL:HG21	1:A:1329:THR:HG23	1.96	0.47
1:A:1388:GLY:O	1:A:1391:ARG:HG2	2.15	0.47
2:B:221:ASN:OD1	2:B:242:SER:HA	2.14	0.47
2:B:298:LEU:CD2	2:B:298:LEU:H	2.27	0.47
2:B:371:GLU:N	2:B:371:GLU:OE1	2.48	0.47
2:B:544:CYS:O	2:B:545:ILE:HG13	2.15	0.47
2:B:545:ILE:C	2:B:634:TYR:HE2	2.22	0.47
2:B:847:ASP:OD2	11:K:6:ARG:NH2	2.48	0.47
3:C:47:ASP:O	3:C:48:SER:HB2	2.13	0.47
3:C:206:ASN:OD1	3:C:229:TYR:CD2	2.67	0.47
4:D:220:LEU:O	4:D:221:TYR:HD1	1.97	0.47
5:E:167:ARG:O	5:E:168:TYR:HD2	1.97	0.47
5:E:204:THR:HG23	5:E:205:SER:N	2.29	0.47
5:E:205:SER:O	5:E:206:GLY:C	2.56	0.47
6:F:124:GLU:HB3	6:F:130:ILE:HG12	1.95	0.47
6:F:124:GLU:O	6:F:130:ILE:HG13	2.14	0.47
7:G:62:LEU:HB3	7:G:63:PRO:HD2	1.95	0.47
8:H:39:THR:HB	8:H:124:ARG:HB3	1.97	0.47
8:H:102:TYR:HD2	8:H:102:TYR:H	1.51	0.47
9:I:5:ARG:O	9:I:14:LEU:HD12	2.13	0.47
11:K:105:PHE:O	11:K:106:GLU:C	2.57	0.47
11:K:113:THR:O	11:K:114:LEU:CB	2.58	0.47
1:A:95:PHE:HD1	1:A:234:MET:CG	2.25	0.47
1:A:254:GLU:H	2:B:935:ARG:HH12	1.63	0.47
1:A:873:MET:C	1:A:1058:VAL:HG23	2.40	0.47
1:A:1007:ILE:C	1:A:1009:ASN:N	2.71	0.47
1:A:1129:GLU:C	1:A:1131:ALA:N	2.67	0.47
2:B:283:VAL:O	2:B:284:ILE:C	2.57	0.47
2:B:831:SER:HB2	2:B:833:TYR:HD1	1.79	0.47
2:B:899:ILE:HG22	2:B:903:VAL:HG21	1.95	0.47
3:C:86:CYS:C	3:C:88:CYS:N	2.72	0.47
3:C:109:SER:O	3:C:110:THR:O	2.32	0.47
5:E:143:ASN:OD1	5:E:187:TYR:CE1	2.68	0.47
6:F:97:ARG:O	6:F:98:ALA:C	2.57	0.47
6:F:128:LYS:HD3	6:F:149:GLU:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:8:PHE:CE1	10:J:49:MET:SD	3.08	0.47
11:K:12:LEU:HD23	11:K:16:GLU:O	2.14	0.47
1:A:254:GLU:O	2:B:935:ARG:NH1	2.45	0.47
1:A:543:LEU:HD11	1:A:547:LEU:HD11	1.96	0.47
1:A:759:ALA:O	1:A:761:MET:N	2.47	0.47
1:A:1282:VAL:O	1:A:1283:VAL:HG22	2.14	0.47
2:B:758:PHE:C	2:B:760:ASP:N	2.72	0.47
2:B:850:LEU:HD12	2:B:851:PHE:N	2.30	0.47
3:C:236:GLY:C	3:C:238:ILE:N	2.73	0.47
3:C:245:VAL:C	3:C:247:GLY:N	2.73	0.47
4:D:146:GLN:O	4:D:147:TYR:C	2.58	0.47
5:E:124:VAL:CG1	5:E:132:ILE:HB	2.43	0.47
5:E:147:HIS:O	5:E:148:GLU:C	2.57	0.47
6:F:77:ASP:O	6:F:79:ARG:N	2.47	0.47
6:F:90:ARG:CG	6:F:91:ALA:N	2.78	0.47
6:F:94:LEU:HA	6:F:94:LEU:HD23	1.64	0.47
8:H:123:MET:HE1	8:H:142:LEU:HD11	1.96	0.47
1:A:117:GLU:H	1:A:117:GLU:CD	2.23	0.47
1:A:222:LEU:O	1:A:224:PHE:N	2.48	0.47
1:A:335:ARG:NE	1:A:339:ASN:ND2	2.57	0.47
1:A:551:TYR:CE2	11:K:62:LYS:HE2	2.50	0.47
1:A:566:ILE:O	1:A:567:LYS:C	2.57	0.47
1:A:893:PHE:C	1:A:893:PHE:CD2	2.92	0.47
1:A:946:VAL:HG12	1:A:947:PHE:N	2.29	0.47
1:A:1080:THR:C	1:A:1081:LEU:HD22	2.40	0.47
1:A:1104:ILE:C	1:A:1106:ASN:N	2.71	0.47
1:A:1162:VAL:O	1:A:1162:VAL:HG12	2.15	0.47
1:A:1227:ILE:O	1:A:1228:TRP:HB3	2.14	0.47
1:A:1398:MET:O	1:A:1401:SER:OG	2.22	0.47
1:A:1402:PHE:CD1	1:A:1403:GLU:HG3	2.50	0.47
2:B:95:ILE:HG13	2:B:130:VAL:CG2	2.44	0.47
2:B:97:VAL:CG1	2:B:178:ASN:HD21	2.28	0.47
2:B:834:ASN:HA	2:B:838:SER:O	2.15	0.47
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.48	0.47
3:C:112:ASN:CB	3:C:114:TYR:CE1	2.98	0.47
3:C:183:TRP:O	3:C:184:ASN:C	2.58	0.47
4:D:130:LEU:O	4:D:132:GLN:N	2.48	0.47
4:D:189:ASP:O	4:D:193:THR:HB	2.14	0.47
5:E:192:ARG:HG3	5:E:192:ARG:NH1	2.26	0.47
10:J:14:VAL:O	10:J:16:ASP:N	2.48	0.47
10:J:18:TRP:HA	10:J:18:TRP:CE3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:40:HIS:O	11:K:41:THR:C	2.58	0.47
1:A:500:GLU:O	1:A:504:LEU:HB2	2.15	0.46
1:A:548:ASN:HA	11:K:60:ALA:HB1	1.97	0.46
1:A:626:ASN:O	1:A:631:HIS:CB	2.63	0.46
1:A:809:THR:HG23	1:A:812:GLU:OE1	2.15	0.46
1:A:830:LYS:HB2	1:A:1081:LEU:CD2	2.43	0.46
1:A:936:LEU:HD23	1:A:936:LEU:H	1.78	0.46
1:A:1283:VAL:CG1	1:A:1284:MET:N	2.78	0.46
1:A:1342:GLU:CG	5:E:198:ILE:HG21	2.45	0.46
2:B:43:LEU:HD11	2:B:811:TYR:O	2.15	0.46
2:B:202:TYR:CE1	2:B:209:GLU:HG2	2.50	0.46
2:B:285:ILE:O	2:B:288:ALA:HB3	2.15	0.46
2:B:654:ARG:H	2:B:657:HIS:CD2	2.28	0.46
2:B:1090:THR:O	2:B:1091:TYR:C	2.57	0.46
2:B:1204:PHE:CE1	2:B:1216:LEU:HD11	2.50	0.46
5:E:7:ARG:CG	5:E:8:ASN:N	2.76	0.46
5:E:90:VAL:HG23	5:E:120:ALA:HA	1.97	0.46
6:F:135:ARG:HD3	6:F:143:PHE:CD2	2.51	0.46
13:S:269:PHE:CZ	13:S:308:PHE:CE1	3.03	0.46
1:A:70:CYS:O	1:A:71:GLN:C	2.58	0.46
1:A:80:HIS:O	1:A:243:PRO:HB3	2.16	0.46
1:A:370:ILE:HG23	2:B:1105:ALA:CB	2.41	0.46
1:A:535:THR:O	1:A:536:LEU:O	2.34	0.46
1:A:647:GLY:O	1:A:650:GLN:HB2	2.14	0.46
1:A:808:LEU:N	1:A:808:LEU:CD1	2.78	0.46
1:A:863:VAL:O	1:A:864:ILE:CG1	2.63	0.46
1:A:881:GLN:NE2	1:A:958:VAL:O	2.42	0.46
1:A:1131:ALA:O	1:A:1132:LYS:C	2.58	0.46
1:A:1327:ILE:HG22	5:E:147:HIS:CE1	2.51	0.46
2:B:58:THR:O	2:B:62:ILE:HG13	2.14	0.46
2:B:785:TYR:HA	2:B:788:ARG:HG3	1.97	0.46
3:C:247:GLY:C	3:C:249:ASP:N	2.72	0.46
9:I:83:ASN:HA	9:I:102:VAL:O	2.16	0.46
11:K:83:PRO:O	11:K:86:ALA:HB3	2.15	0.46
12:L:66:GLN:C	12:L:67:PHE:CD1	2.94	0.46
13:S:236:LEU:CA	13:S:242:LYS:CE	2.93	0.46
1:A:43:GLU:O	1:A:44:THR:HB	2.15	0.46
1:A:317:LYS:O	1:A:318:SER:HB3	2.14	0.46
1:A:344:ARG:HA	2:B:1129:ARG:HA	1.98	0.46
1:A:408:ASP:C	1:A:410:GLY:H	2.23	0.46
1:A:962:ARG:O	1:A:963:ILE:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1220:PHE:CE2	1:A:1263:ILE:HG23	2.50	0.46
1:A:1311:VAL:HG11	1:A:1329:THR:HG21	1.96	0.46
2:B:27:ALA:O	2:B:30:SER:OG	2.29	0.46
2:B:199:MET:HE2	2:B:492:LEU:CD2	2.42	0.46
2:B:593:PRO:O	2:B:594:ALA:C	2.59	0.46
2:B:753:ALA:O	2:B:756:ILE:N	2.46	0.46
2:B:834:ASN:O	2:B:838:SER:O	2.34	0.46
2:B:1098:MET:O	2:B:1099:VAL:C	2.59	0.46
3:C:95:CYS:O	3:C:96:SER:HB3	2.15	0.46
7:G:81:PRO:HA	7:G:85:GLU:OE1	2.15	0.46
9:I:73:ARG:HD2	9:I:101:PHE:CE2	2.50	0.46
10:J:36:LEU:HB2	10:J:47:ARG:HH12	1.81	0.46
10:J:52:THR:O	10:J:53:HIS:C	2.57	0.46
12:L:48:CYS:O	12:L:50:ASP:N	2.47	0.46
12:L:62:LYS:O	12:L:63:ARG:C	2.58	0.46
13:S:269:PHE:CE2	13:S:297:CYS:CB	2.96	0.46
1:A:209:ASN:O	1:A:210:ILE:C	2.58	0.46
1:A:414:ASP:O	1:A:416:ARG:N	2.48	0.46
1:A:618:GLU:O	1:A:621:THR:N	2.46	0.46
1:A:705:LYS:C	1:A:707:GLY:H	2.23	0.46
1:A:706:HIS:C	1:A:708:MET:H	2.22	0.46
1:A:1102:LYS:O	1:A:1106:ASN:ND2	2.46	0.46
2:B:45:SER:O	2:B:46:GLN:C	2.58	0.46
2:B:281:PRO:O	2:B:283:VAL:N	2.48	0.46
2:B:293:PRO:O	2:B:294:ASP:O	2.33	0.46
2:B:579:ARG:HA	2:B:589:VAL:HG13	1.96	0.46
2:B:788:ARG:HE	2:B:788:ARG:HB3	1.52	0.46
2:B:789:MET:CE	2:B:965:LYS:HB3	2.46	0.46
2:B:871:THR:HG22	2:B:872:GLU:N	2.31	0.46
2:B:956:THR:CG2	2:B:960:GLY:HA2	2.45	0.46
2:B:1079:LYS:HE3	3:C:188:HIS:CE1	2.51	0.46
3:C:88:CYS:SG	3:C:88:CYS:O	2.70	0.46
3:C:164:ALA:O	3:C:165:LYS:C	2.57	0.46
4:D:29:LEU:HD23	4:D:29:LEU:N	2.30	0.46
6:F:103:MET:CE	7:G:65:ASP:HB2	2.44	0.46
11:K:63:VAL:HG23	11:K:63:VAL:O	2.15	0.46
1:A:563:PRO:HB2	1:A:565:ILE:O	2.16	0.46
1:A:567:LYS:HE3	8:H:46:LEU:HD12	1.97	0.46
2:B:760:ASP:O	2:B:761:HIS:CG	2.69	0.46
2:B:1102:LYS:C	2:B:1103:ILE:O	2.58	0.46
3:C:228:PHE:CD1	3:C:228:PHE:N	2.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:154:PHE:HB2	4:D:160:VAL:HG22	1.97	0.46
5:E:24:LYS:HG3	5:E:25:ASP:N	2.30	0.46
5:E:197:LYS:O	5:E:199:ILE:HG13	2.16	0.46
6:F:87:LYS:HG3	6:F:88:TYR:CD1	2.51	0.46
8:H:76:THR:O	8:H:76:THR:HG22	2.14	0.46
9:I:99:LEU:HB2	9:I:101:PHE:CE1	2.50	0.46
10:J:61:LEU:O	10:J:63:TYR:N	2.48	0.46
11:K:55:LYS:HB3	11:K:81:TYR:HD1	1.80	0.46
12:L:30:ILE:O	12:L:56:LEU:HD23	2.15	0.46
1:A:541:ILE:HG22	1:A:546:VAL:HG23	1.97	0.46
1:A:696:GLU:O	1:A:696:GLU:HG2	2.15	0.46
1:A:715:GLU:O	1:A:718:VAL:N	2.48	0.46
1:A:784:LEU:C	1:A:786:HIS:H	2.23	0.46
1:A:867:ILE:CG2	1:A:872:GLY:H	2.29	0.46
1:A:889:SER:C	1:A:891:ALA:N	2.72	0.46
1:A:896:ARG:CD	1:A:897:TYR:CE1	2.93	0.46
1:A:897:TYR:HB3	1:A:936:LEU:CD1	2.45	0.46
2:B:34:ILE:O	2:B:35:SER:C	2.58	0.46
2:B:229:ALA:HB1	2:B:231:PRO:HD2	1.98	0.46
2:B:281:PRO:HG2	2:B:284:ILE:CG1	2.44	0.46
2:B:510:LYS:HD3	2:B:513:GLN:H	1.80	0.46
2:B:577:ALA:HB1	2:B:589:VAL:HG11	1.96	0.46
2:B:700:SER:C	2:B:701:ILE:CG2	2.89	0.46
2:B:863:GLU:O	2:B:961:LEU:HD22	2.15	0.46
2:B:995:ARG:O	2:B:996:ARG:C	2.59	0.46
2:B:999:MET:HB3	2:B:1007:VAL:CG2	2.45	0.46
2:B:1023:VAL:HG12	2:B:1027:ILE:HG13	1.97	0.46
3:C:251:LEU:O	3:C:254:LYS:N	2.49	0.46
5:E:117:THR:C	5:E:119:SER:N	2.73	0.46
8:H:31:THR:O	8:H:31:THR:HG22	2.15	0.46
12:L:54:ARG:HG3	12:L:54:ARG:NH1	2.29	0.46
1:A:231:PRO:C	1:A:233:TRP:H	2.23	0.46
1:A:266:LEU:O	1:A:267:ALA:C	2.58	0.46
1:A:351:THR:HB	2:B:1103:ILE:CD1	2.43	0.46
1:A:550:LEU:HD11	1:A:561:PRO:HD2	1.98	0.46
1:A:703:THR:O	1:A:704:ALA:C	2.59	0.46
1:A:907:THR:HG22	1:A:908:LEU:N	2.30	0.46
2:B:63:ILE:HD12	2:B:421:PHE:CE2	2.51	0.46
2:B:69:LEU:HD13	2:B:429:PHE:HD1	1.80	0.46
2:B:526:GLU:CD	2:B:752:ALA:CB	2.89	0.46
2:B:994:TYR:HB2	2:B:999:MET:CE	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:249:ASP:O	3:C:250:THR:C	2.58	0.46
4:D:53:SER:HB3	4:D:153:ARG:H	1.81	0.46
6:F:132:LEU:HD22	7:G:61:ILE:HD11	1.97	0.46
6:F:150:GLU:O	6:F:151:LEU:C	2.59	0.46
7:G:27:LYS:O	7:G:31:LEU:HG	2.16	0.46
8:H:143:LEU:O	8:H:144:ILE:HG13	2.16	0.46
9:I:11:ASN:O	9:I:12:ASN:ND2	2.48	0.46
9:I:69:PRO:O	9:I:84:VAL:HA	2.14	0.46
1:A:76:GLU:CG	1:A:76:GLU:O	2.63	0.46
1:A:100:LYS:O	1:A:103:CYS:N	2.49	0.46
1:A:285:PRO:CG	1:A:288:ALA:HB3	2.40	0.46
1:A:368:LYS:O	1:A:369:SER:C	2.58	0.46
1:A:443:LEU:HD23	1:A:443:LEU:HA	1.72	0.46
1:A:598:LEU:O	1:A:599:SER:C	2.58	0.46
1:A:707:GLY:O	1:A:708:MET:O	2.34	0.46
1:A:933:TYR:C	1:A:935:GLN:H	2.24	0.46
1:A:1063:MET:SD	1:A:1436:ILE:HG12	2.56	0.46
1:A:1083:THR:O	1:A:1084:PHE:O	2.34	0.46
1:A:1116:LEU:HB2	1:A:1329:THR:OG1	2.16	0.46
2:B:189:LEU:O	2:B:192:LEU:HB2	2.15	0.46
2:B:683:SER:O	2:B:687:GLU:HB2	2.16	0.46
2:B:882:THR:O	2:B:883:LEU:CB	2.63	0.46
2:B:992:ILE:HD13	2:B:994:TYR:HE1	1.81	0.46
2:B:1060:ARG:C	2:B:1062:HIS:H	2.22	0.46
3:C:114:TYR:N	3:C:114:TYR:CD1	2.83	0.46
3:C:147:LEU:HD23	3:C:147:LEU:N	2.31	0.46
4:D:33:PHE:CZ	7:G:80:LYS:NZ	2.84	0.46
5:E:33:GLU:C	5:E:35:VAL:N	2.72	0.46
5:E:90:VAL:HB	5:E:119:SER:HB2	1.98	0.46
5:E:165:LEU:O	5:E:166:LYS:C	2.58	0.46
6:F:138:LEU:O	6:F:139:PRO:C	2.59	0.46
1:A:63:ARG:HA	1:A:74:MET:CE	2.45	0.46
1:A:78:PRO:O	1:A:79:GLY:C	2.58	0.46
1:A:385:ILE:HG22	1:A:386:ASP:N	2.29	0.46
1:A:697:ALA:HB2	1:A:702:LEU:CD1	2.46	0.46
1:A:983:ILE:O	1:A:983:ILE:HG22	2.15	0.46
1:A:1100:ARG:NH2	1:A:1351:GLU:HG2	2.19	0.46
1:A:1385:THR:CG2	1:A:1386:ARG:N	2.79	0.46
2:B:385:LEU:HD12	2:B:385:LEU:O	2.15	0.46
2:B:510:LYS:HD3	2:B:513:GLN:N	2.31	0.46
2:B:604:ARG:C	2:B:606:LYS:H	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:613:VAL:HG22	2:B:628:THR:HA	1.98	0.46
3:C:15:LYS:O	3:C:240:VAL:HG22	2.16	0.46
3:C:215:GLU:O	3:C:216:GLY:C	2.59	0.46
4:D:59:ILE:O	4:D:60:LYS:C	2.58	0.46
4:D:167:LEU:C	4:D:169:SER:H	2.24	0.46
8:H:98:TYR:HE1	8:H:139:ASN:HA	1.80	0.46
11:K:71:PHE:CD1	11:K:71:PHE:C	2.94	0.46
1:A:243:PRO:CB	1:A:244:PRO:HD2	2.46	0.46
1:A:566:ILE:O	1:A:567:LYS:O	2.34	0.46
1:A:809:THR:HB	1:A:810:PRO:HD2	1.97	0.46
1:A:933:TYR:C	1:A:935:GLN:N	2.72	0.46
1:A:1018:PHE:O	1:A:1019:CYS:C	2.59	0.46
1:A:1119:TYR:CD2	1:A:1305:VAL:HG21	2.51	0.46
1:A:1129:GLU:HG3	1:A:1132:LYS:HE3	1.97	0.46
1:A:1167:GLU:O	1:A:1168:GLU:C	2.58	0.46
1:A:1227:ILE:CG2	1:A:1228:TRP:N	2.78	0.46
1:A:1377:THR:O	1:A:1378:GLN:C	2.57	0.46
2:B:401:PHE:C	2:B:403:LYS:H	2.24	0.46
2:B:543:SER:C	2:B:544:CYS:SG	2.99	0.46
3:C:80:LEU:O	3:C:80:LEU:HG	2.16	0.46
6:F:123:LYS:C	6:F:125:LEU:N	2.73	0.46
7:G:80:LYS:HA	7:G:81:PRO:HD2	1.74	0.46
9:I:15:TYR:O	9:I:28:GLU:HG2	2.16	0.46
11:K:10:PHE:N	11:K:10:PHE:CD2	2.84	0.46
1:A:18:GLN:CB	2:B:1215:ARG:HB2	2.45	0.45
1:A:73:GLY:O	1:A:74:MET:C	2.59	0.45
1:A:130:ASP:C	1:A:132:LYS:H	2.24	0.45
1:A:512:VAL:HG11	1:A:876:ALA:O	2.16	0.45
1:A:544:ASP:CG	1:A:545:GLN:N	2.74	0.45
1:A:989:GLY:C	1:A:991:LYS:N	2.69	0.45
1:A:1081:LEU:CD1	1:A:1099:PRO:HD3	2.46	0.45
1:A:1170:ILE:HG23	1:A:1174:PHE:HE1	1.77	0.45
1:A:1191:TRP:HB3	1:A:1260:LEU:HD23	1.97	0.45
1:A:1330:ASN:OD1	1:A:1331:SER:N	2.49	0.45
1:A:1437:GLY:CA	6:F:88:TYR:CD2	2.97	0.45
2:B:38:PHE:O	2:B:39:ARG:C	2.59	0.45
2:B:1020:ARG:HH12	13:S:291:GLU:HA	1.81	0.45
3:C:94:LYS:HB2	3:C:94:LYS:HE3	1.67	0.45
4:D:48:ILE:CG2	7:G:4:ILE:HB	2.46	0.45
5:E:177:ARG:O	5:E:212:ARG:HD3	2.15	0.45
11:K:21:ILE:HG12	11:K:33:ILE:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:70:ARG:O	11:K:70:ARG:HG3	2.16	0.45
1:A:18:GLN:C	1:A:18:GLN:OE1	2.59	0.45
1:A:33:ALA:O	1:A:83:HIS:HD2	1.99	0.45
1:A:321:PRO:O	1:A:322:VAL:CG2	2.63	0.45
1:A:353:ILE:HG13	1:A:482:PHE:CD2	2.51	0.45
1:A:915:SER:O	1:A:919:ILE:HG13	2.16	0.45
1:A:1435:PRO:C	1:A:1436:ILE:HG13	2.40	0.45
2:B:172:ILE:CG2	2:B:173:MET:N	2.79	0.45
2:B:386:LEU:O	2:B:388:CYS:N	2.50	0.45
2:B:661:LEU:C	2:B:663:ALA:N	2.75	0.45
2:B:838:SER:HA	2:B:989:THR:O	2.17	0.45
2:B:880:THR:HB	2:B:934:LYS:CD	2.36	0.45
2:B:906:SER:O	2:B:907:GLY:O	2.34	0.45
2:B:1064:TYR:O	2:B:1065:GLN:C	2.59	0.45
3:C:26:ASP:O	3:C:27:LEU:C	2.58	0.45
3:C:43:THR:HG22	3:C:44:LEU:H	1.81	0.45
3:C:46:ILE:HD13	3:C:157:CYS:CB	2.46	0.45
5:E:202:SER:HB3	5:E:205:SER:O	2.15	0.45
8:H:97:MET:HE3	8:H:118:PHE:CD1	2.52	0.45
1:A:44:THR:O	1:A:44:THR:HG22	2.16	0.45
1:A:393:ARG:C	1:A:395:GLY:N	2.75	0.45
1:A:515:GLN:O	1:A:516:SER:CB	2.58	0.45
1:A:556:TRP:CE2	1:A:558:GLY:HA2	2.51	0.45
1:A:590:ARG:HH11	1:A:590:ARG:CG	2.29	0.45
1:A:922:ASP:OD1	1:A:922:ASP:C	2.60	0.45
1:A:937:VAL:O	1:A:938:LYS:C	2.58	0.45
2:B:520:GLY:H	2:B:748:ILE:HG22	1.81	0.45
2:B:551:PRO:HG2	2:B:552:MET:H	1.81	0.45
2:B:806:THR:HG22	2:B:808:ALA:CB	2.46	0.45
3:C:22:LEU:CD2	3:C:25:VAL:HG21	2.47	0.45
3:C:35:ARG:NH1	11:K:41:THR:OG1	2.50	0.45
5:E:93:MET:O	5:E:94:LYS:C	2.59	0.45
10:J:48:ARG:HD2	10:J:48:ARG:C	2.41	0.45
11:K:88:LYS:O	11:K:91:CYS:N	2.49	0.45
12:L:59:ALA:O	12:L:60:ARG:O	2.34	0.45
1:A:269:ILE:HG12	1:A:299:HIS:HB3	1.99	0.45
1:A:362:ASP:OD2	1:A:362:ASP:N	2.48	0.45
1:A:920:LEU:C	1:A:920:LEU:CD2	2.89	0.45
1:A:1210:GLY:O	1:A:1214:GLU:HB2	2.16	0.45
1:A:1329:THR:O	1:A:1331:SER:N	2.49	0.45
1:A:1359:ASP:HB2	1:A:1361:SER:OG	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:170:LEU:O	2:B:170:LEU:HG	2.14	0.45
2:B:202:TYR:CD2	2:B:202:TYR:N	2.84	0.45
2:B:284:ILE:HG12	2:B:324:ILE:HD12	1.98	0.45
2:B:386:LEU:C	2:B:388:CYS:N	2.73	0.45
2:B:878:GLN:O	2:B:879:ARG:C	2.58	0.45
2:B:995:ARG:HB3	2:B:997:GLU:OE2	2.16	0.45
2:B:1026:LEU:HD23	2:B:1086:PHE:CE2	2.52	0.45
2:B:1115:THR:HG22	2:B:1117:GLN:CG	2.46	0.45
2:B:1164:GLY:HA3	2:B:1190:ASP:OD2	2.16	0.45
2:B:1169:MET:CE	2:B:1201:LYS:CA	2.89	0.45
3:C:118:LEU:HB2	3:C:132:PRO:HG2	1.97	0.45
7:G:22:MET:O	7:G:23:LYS:C	2.59	0.45
11:K:33:ILE:HB	11:K:35:PHE:HE1	1.81	0.45
1:A:19:PHE:O	1:A:1416:ALA:HA	2.17	0.45
1:A:130:ASP:C	1:A:132:LYS:N	2.75	0.45
1:A:298:PHE:HZ	1:A:314:ALA:HB2	1.80	0.45
1:A:343:LYS:NZ	2:B:1151:LEU:O	2.43	0.45
1:A:560:ILE:CG1	8:H:78:SER:HB2	2.36	0.45
1:A:707:GLY:C	1:A:708:MET:HG3	2.41	0.45
1:A:777:PHE:CE2	1:A:782:ARG:HA	2.51	0.45
1:A:937:VAL:HG12	1:A:938:LYS:N	2.30	0.45
1:A:942:PHE:C	1:A:942:PHE:CD2	2.94	0.45
1:A:1115:SER:OG	1:A:1116:LEU:N	2.49	0.45
1:A:1242:VAL:O	1:A:1243:VAL:HB	2.17	0.45
2:B:255:GLN:O	2:B:271:ALA:HB1	2.17	0.45
2:B:293:PRO:HG2	2:B:296:GLU:OE1	2.16	0.45
2:B:564:GLU:O	2:B:565:PRO:C	2.58	0.45
2:B:615:MET:HA	2:B:625:LYS:O	2.16	0.45
2:B:687:GLU:O	2:B:688:GLY:C	2.59	0.45
2:B:816:GLU:O	2:B:817:LEU:CD2	2.59	0.45
2:B:898:LEU:HB2	12:L:58:LYS:HZ3	1.80	0.45
2:B:1198:TYR:O	2:B:1199:ALA:C	2.59	0.45
3:C:158:VAL:HG12	3:C:158:VAL:O	2.17	0.45
5:E:135:PHE:HB3	5:E:140:LEU:HD11	1.98	0.45
7:G:39:THR:C	7:G:41:LYS:N	2.70	0.45
12:L:28:LYS:HG3	12:L:39:SER:OG	2.15	0.45
1:A:95:PHE:CD1	1:A:234:MET:CG	2.96	0.45
1:A:688:LYS:O	1:A:690:VAL:N	2.50	0.45
1:A:834:THR:CG2	1:A:1077:THR:HA	2.46	0.45
1:A:935:GLN:C	1:A:937:VAL:N	2.71	0.45
1:A:1016:THR:O	1:A:1018:PHE:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1151:GLU:HB3	1:A:1153:TYR:CE1	2.50	0.45
1:A:1173:HIS:CG	1:A:1227:ILE:HG23	2.51	0.45
2:B:984:HIS:CD2	2:B:1025:HIS:HA	2.51	0.45
2:B:1181:GLU:OE1	2:B:1183:LYS:HG3	2.17	0.45
3:C:46:ILE:HD13	3:C:157:CYS:HB3	1.99	0.45
4:D:122:GLU:HA	4:D:125:SER:OG	2.17	0.45
5:E:135:PHE:CB	5:E:140:LEU:HD11	2.47	0.45
7:G:132:SER:HB3	7:G:135:ASP:HB2	1.97	0.45
11:K:101:LEU:O	11:K:102:LYS:C	2.58	0.45
1:A:70:CYS:HA	2:B:1174:LYS:HG2	1.98	0.45
1:A:618:GLU:O	1:A:619:LYS:C	2.59	0.45
1:A:760:GLN:O	1:A:804:TYR:CD1	2.70	0.45
1:A:849:MET:O	1:A:851:HIS:HD2	1.99	0.45
1:A:1115:SER:O	1:A:1329:THR:HG23	2.17	0.45
1:A:1121:GLU:O	1:A:1122:PRO:O	2.35	0.45
1:A:1129:GLU:O	1:A:1130:GLN:C	2.60	0.45
1:A:1271:ILE:O	1:A:1271:ILE:CG2	2.65	0.45
1:A:1293:SER:OG	1:A:1295:THR:HG23	2.17	0.45
2:B:280:ILE:HG23	2:B:281:PRO:HD2	1.99	0.45
2:B:377:PHE:C	2:B:379:GLY:N	2.71	0.45
2:B:385:LEU:HD12	2:B:385:LEU:C	2.42	0.45
2:B:466:TRP:O	2:B:467:GLY:C	2.58	0.45
2:B:578:THR:HG23	2:B:622:LYS:CA	2.47	0.45
2:B:638:PHE:HD2	2:B:690:VAL:HG22	1.82	0.45
2:B:975:GLN:HG2	2:B:976:ILE:H	1.82	0.45
3:C:66:ARG:HH21	10:J:5:VAL:HG23	1.80	0.45
4:D:176:GLU:O	4:D:180:LEU:HB2	2.17	0.45
5:E:117:THR:O	5:E:120:ALA:N	2.45	0.45
7:G:82:PHE:O	7:G:84:GLY:N	2.50	0.45
8:H:83:GLN:C	8:H:85:GLY:N	2.74	0.45
11:K:90:ALA:O	11:K:94:ILE:HG13	2.17	0.45
1:A:30:ILE:HD11	2:B:1168:LEU:HD13	1.99	0.45
1:A:52:GLY:O	1:A:56:PRO:HG2	2.17	0.45
1:A:353:ILE:HG23	1:A:485:ASP:O	2.16	0.45
1:A:668:ASP:HA	1:A:741:ASN:OD1	2.17	0.45
1:A:783:THR:O	1:A:784:LEU:HD23	2.16	0.45
1:A:920:LEU:C	1:A:920:LEU:HD23	2.42	0.45
1:A:1011:GLN:NE2	1:A:1015:VAL:CG2	2.65	0.45
1:A:1143:LEU:HD12	1:A:1146:VAL:HG23	1.99	0.45
1:A:1313:LEU:HD11	1:A:1327:ILE:HD13	1.99	0.45
1:A:1347:ALA:O	1:A:1348:LEU:C	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:550:ASP:OD1	2:B:551:PRO:HD2	2.17	0.45
3:C:44:LEU:HG	3:C:159:ALA:HB1	1.99	0.45
3:C:75:MET:HE2	3:C:239:PRO:CD	2.46	0.45
3:C:88:CYS:SG	3:C:91:HIS:N	2.90	0.45
3:C:187:LYS:C	3:C:189:THR:H	2.23	0.45
3:C:214:ASN:HB3	3:C:217:ASP:OD2	2.16	0.45
5:E:117:THR:HG22	5:E:119:SER:N	2.20	0.45
5:E:198:ILE:CD1	5:E:212:ARG:NH1	2.78	0.45
8:H:95:TYR:HE2	8:H:97:MET:CG	2.29	0.45
11:K:7:PHE:HA	11:K:10:PHE:CE2	2.51	0.45
11:K:35:PHE:N	11:K:35:PHE:HD1	2.15	0.45
1:A:244:PRO:CG	1:A:245:PRO:HD3	2.47	0.45
1:A:849:MET:HE3	1:A:1061:GLY:HA2	1.99	0.45
1:A:1007:ILE:C	1:A:1009:ASN:H	2.24	0.45
2:B:710:LEU:O	2:B:711:GLU:HG2	2.17	0.45
2:B:851:PHE:O	2:B:974:PRO:HD3	2.17	0.45
2:B:855:PHE:CD1	2:B:856:PHE:N	2.85	0.45
2:B:964:VAL:HG12	2:B:965:LYS:N	2.32	0.45
2:B:1006:ILE:H	2:B:1006:ILE:HG13	1.19	0.45
4:D:156:ASP:C	4:D:158:GLU:N	2.74	0.45
5:E:210:SER:C	5:E:211:TYR:HD1	2.24	0.45
6:F:135:ARG:HG2	6:F:137:TYR:CE1	2.52	0.45
7:G:56:ILE:O	7:G:57:GLN:HB2	2.15	0.45
8:H:23:VAL:HG22	8:H:43:ASN:HA	1.99	0.45
8:H:100:THR:HG22	8:H:101:ALA:H	1.79	0.45
9:I:55:THR:HG22	9:I:56:ALA:N	2.32	0.45
10:J:1:MET:H2	10:J:56:LEU:N	2.14	0.45
10:J:46:CYS:O	10:J:47:ARG:C	2.60	0.45
10:J:56:LEU:O	10:J:57:ILE:C	2.59	0.45
11:K:53:ASP:OD1	11:K:55:LYS:HB2	2.17	0.45
13:S:260:THR:CA	13:S:260:THR:HB	2.20	0.45
1:A:492:PRO:C	1:A:493:GLN:HE21	2.25	0.45
1:A:563:PRO:HB3	1:A:571:LEU:O	2.17	0.45
1:A:706:HIS:ND1	13:S:257:GLN:HB2	2.32	0.45
1:A:789:LYS:HD2	9:I:67:THR:OG1	2.17	0.45
1:A:809:THR:O	1:A:810:PRO:C	2.58	0.45
1:A:840:ARG:O	1:A:841:LEU:C	2.60	0.45
1:A:866:PHE:HD2	5:E:168:TYR:CE1	2.33	0.45
1:A:1081:LEU:CD2	1:A:1098:VAL:HG21	2.45	0.45
1:A:1115:SER:HA	1:A:1308:THR:HG23	1.99	0.45
2:B:598:GLU:O	2:B:598:GLU:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:745:PRO:O	2:B:748:ILE:CG1	2.61	0.45
2:B:758:PHE:O	2:B:760:ASP:N	2.49	0.45
2:B:789:MET:HE2	2:B:965:LYS:HB3	1.99	0.45
2:B:800:GLN:HB2	2:B:821:GLN:HA	1.99	0.45
2:B:824:ILE:CD1	10:J:48:ARG:NH1	2.80	0.45
2:B:975:GLN:HG2	2:B:976:ILE:N	2.32	0.45
2:B:990:ILE:HG22	2:B:992:ILE:H	1.81	0.45
2:B:1183:LYS:CE	2:B:1183:LYS:H	2.27	0.45
4:D:51:ASN:OD1	4:D:52:LEU:O	2.34	0.45
8:H:95:TYR:CE2	8:H:97:MET:CG	3.00	0.45
9:I:15:TYR:N	9:I:15:TYR:CD1	2.85	0.45
10:J:2:ILE:HG12	10:J:57:ILE:CD1	2.46	0.45
11:K:55:LYS:HB3	11:K:81:TYR:CD1	2.52	0.45
1:A:51:GLY:HA2	1:A:56:PRO:HA	1.99	0.44
1:A:384:ASN:O	1:A:386:ASP:N	2.50	0.44
1:A:388:LEU:O	1:A:389:THR:C	2.61	0.44
1:A:465:TYR:N	11:K:2:ASN:HB3	2.32	0.44
1:A:673:GLY:O	1:A:676:MET:HB2	2.16	0.44
1:A:1101:LEU:O	1:A:1101:LEU:HD12	2.17	0.44
2:B:753:ALA:HA	2:B:756:ILE:HG13	1.99	0.44
2:B:785:TYR:CE2	10:J:60:PHE:CE1	3.04	0.44
2:B:828:ALA:HB2	2:B:1085:ILE:HG21	2.00	0.44
2:B:977:GLY:CA	2:B:1099:VAL:HB	2.44	0.44
2:B:1160:VAL:CG1	2:B:1161:HIS:H	2.30	0.44
3:C:52:GLU:HA	12:L:64:LEU:HD22	1.99	0.44
3:C:77:ILE:HG23	3:C:161:LYS:HE3	2.00	0.44
4:D:40:HIS:CE1	4:D:41:GLN:HE21	2.34	0.44
4:D:141:LEU:O	4:D:144:THR:HB	2.16	0.44
6:F:88:TYR:CD1	6:F:88:TYR:N	2.85	0.44
11:K:87:LEU:HD12	11:K:87:LEU:C	2.42	0.44
1:A:78:PRO:O	1:A:78:PRO:HG2	2.17	0.44
1:A:108:MET:O	1:A:109:HIS:HB2	2.16	0.44
1:A:299:HIS:C	1:A:301:ALA:N	2.73	0.44
1:A:576:GLN:O	1:A:579:SER:HB2	2.18	0.44
1:A:814:PHE:CD1	2:B:519:TRP:CE3	3.05	0.44
1:A:815:PHE:O	1:A:816:HIS:C	2.61	0.44
1:A:1132:LYS:CE	13:S:253:LEU:HD21	2.43	0.44
1:A:1170:ILE:O	1:A:1174:PHE:HD1	2.00	0.44
2:B:642:ASP:HB3	2:B:649:LYS:CG	2.47	0.44
2:B:806:THR:H	2:B:809:MET:HE3	1.81	0.44
2:B:981:ALA:CB	2:B:987:LYS:HA	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:73:GLN:NE2	3:C:75:MET:N	2.54	0.44
3:C:127:ARG:O	3:C:128:ASN:C	2.60	0.44
8:H:89:LEU:O	8:H:91:ASP:N	2.39	0.44
10:J:61:LEU:C	10:J:63:TYR:N	2.75	0.44
1:A:2:VAL:HG21	2:B:1157:ALA:C	2.42	0.44
1:A:381:THR:O	1:A:384:ASN:N	2.45	0.44
1:A:470:LEU:HD11	1:A:482:PHE:CE2	2.52	0.44
1:A:506:ALA:O	1:A:507:VAL:C	2.60	0.44
1:A:573:SER:CB	8:H:119:GLY:O	2.65	0.44
1:A:1161:THR:HG1	1:A:1170:ILE:HD11	1.82	0.44
1:A:1348:LEU:O	1:A:1349:TYR:C	2.60	0.44
1:A:1436:ILE:HD13	2:B:1139:ILE:CG2	2.45	0.44
2:B:373:ARG:HG3	2:B:566:LEU:HD23	2.00	0.44
2:B:408:LEU:HD12	2:B:408:LEU:HA	1.76	0.44
2:B:542:MET:CG	2:B:747:MET:HB3	2.48	0.44
2:B:555:ILE:HD11	2:B:587:HIS:NE2	2.32	0.44
2:B:1073:TYR:CE2	2:B:1080:LYS:HG2	2.53	0.44
3:C:62:PHE:C	3:C:62:PHE:CD2	2.95	0.44
3:C:67:LEU:O	3:C:68:GLY:C	2.61	0.44
4:D:147:TYR:CE1	7:G:103:VAL:HG13	2.53	0.44
7:G:14:HIS:CG	7:G:15:PRO:HD2	2.53	0.44
10:J:3:VAL:CG2	10:J:18:TRP:CG	2.99	0.44
13:S:283:GLN:HG2	13:S:295:THR:OG1	2.17	0.44
1:A:79:GLY:C	1:A:243:PRO:HG3	2.42	0.44
1:A:458:HIS:CE1	1:A:507:VAL:HG21	2.53	0.44
1:A:666:ILE:N	2:B:1026:LEU:HD22	2.32	0.44
1:A:1081:LEU:O	1:A:1082:ASN:C	2.61	0.44
1:A:1236:LEU:C	1:A:1237:ILE:HG13	2.43	0.44
2:B:274:PRO:O	2:B:275:TYR:HB2	2.16	0.44
2:B:287:ARG:NH1	2:B:324:ILE:O	2.50	0.44
2:B:372:SER:O	2:B:376:PHE:HD1	2.00	0.44
2:B:604:ARG:O	2:B:606:LYS:N	2.50	0.44
2:B:1150:ARG:HA	2:B:1150:ARG:NE	2.33	0.44
2:B:1155:SER:OG	2:B:1156:ASP:N	2.47	0.44
3:C:91:HIS:HB2	3:C:96:SER:OG	2.18	0.44
3:C:178:PHE:O	3:C:179:GLU:HB2	2.16	0.44
4:D:26:THR:C	4:D:28:GLN:N	2.75	0.44
5:E:39:LEU:O	5:E:40:GLU:C	2.59	0.44
5:E:42:PHE:CZ	5:E:58:MET:HE3	2.53	0.44
5:E:144:ILE:C	5:E:146:HIS:N	2.72	0.44
8:H:24:CYS:CB	8:H:44:VAL:HG21	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:1:MET:N	10:J:56:LEU:N	2.65	0.44
1:A:12:ARG:NE	2:B:1192:TYR:HE2	2.15	0.44
1:A:65:LEU:O	1:A:66:LYS:C	2.60	0.44
1:A:460:VAL:CG1	1:A:461:LYS:N	2.79	0.44
1:A:470:LEU:HD23	1:A:487:MET:HE3	1.98	0.44
1:A:483:ASP:HB2	2:B:987:LYS:HG3	1.99	0.44
1:A:596:THR:O	1:A:597:LEU:C	2.61	0.44
1:A:786:HIS:CE1	2:B:519:TRP:CZ2	3.05	0.44
1:A:843:LYS:HD2	1:A:843:LYS:HA	1.89	0.44
1:A:967:ALA:N	1:A:1044:TRP:HZ3	2.16	0.44
1:A:1205:LYS:O	1:A:1206:ASP:C	2.61	0.44
1:A:1434:ALA:HA	1:A:1435:PRO:HD3	1.91	0.44
2:B:95:ILE:CG1	2:B:130:VAL:HG22	2.44	0.44
2:B:233:PRO:HG2	2:B:234:ILE:CD1	2.47	0.44
2:B:394:ASP:OD2	9:I:91:ARG:HD2	2.17	0.44
2:B:806:THR:O	2:B:808:ALA:N	2.51	0.44
2:B:821:GLN:HE22	2:B:851:PHE:N	2.09	0.44
2:B:1017:ILE:O	2:B:1018:PRO:C	2.58	0.44
2:B:1107:ALA:O	2:B:1108:ARG:O	2.36	0.44
3:C:80:LEU:HD11	3:C:95:CYS:CA	2.47	0.44
5:E:22:MET:HE3	5:E:26:ARG:NH2	2.33	0.44
7:G:96:GLN:HA	7:G:121:PHE:CD2	2.52	0.44
7:G:101:VAL:HG12	7:G:102:GLN:N	2.32	0.44
13:S:269:PHE:HZ	13:S:308:PHE:CE1	2.35	0.44
1:A:76:GLU:HG3	1:A:76:GLU:O	2.18	0.44
1:A:834:THR:CG2	1:A:1077:THR:HG23	2.29	0.44
1:A:847:ASP:OD1	1:A:847:ASP:N	2.48	0.44
1:A:896:ARG:NH2	1:A:1030:ARG:NH2	2.66	0.44
1:A:1001:ARG:O	1:A:1002:GLY:C	2.59	0.44
1:A:1040:GLN:O	1:A:1041:ALA:C	2.60	0.44
1:A:1099:PRO:O	1:A:1102:LYS:HB3	2.17	0.44
1:A:1392:SER:C	1:A:1394:THR:H	2.25	0.44
2:B:27:ALA:O	2:B:28:GLU:C	2.61	0.44
2:B:324:ILE:CG2	2:B:325:GLN:N	2.81	0.44
2:B:489:SER:OG	2:B:490:SER:N	2.49	0.44
2:B:798:TYR:HD2	2:B:798:TYR:N	2.16	0.44
2:B:874:PHE:HA	2:B:913:GLY:O	2.17	0.44
2:B:882:THR:O	2:B:883:LEU:HB2	2.17	0.44
2:B:1002:THR:O	2:B:1003:ALA:C	2.59	0.44
2:B:1069:PHE:HA	2:B:1085:ILE:O	2.17	0.44
2:B:1182:CYS:O	2:B:1183:LYS:O	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:21:ILE:O	3:C:21:ILE:HG22	2.17	0.44
3:C:50:GLU:HB3	3:C:156:THR:HB	1.98	0.44
4:D:47:LEU:CD1	4:D:48:ILE:N	2.81	0.44
5:E:137:GLU:C	5:E:139:ALA:N	2.75	0.44
1:A:25:GLU:CD	1:A:25:GLU:N	2.75	0.44
1:A:164:ARG:CG	1:A:165:GLY:H	2.01	0.44
1:A:475:THR:CG2	1:A:476:SER:N	2.81	0.44
1:A:544:ASP:CG	1:A:545:GLN:H	2.26	0.44
1:A:910:PRO:C	1:A:912:LEU:H	2.26	0.44
1:A:1342:GLU:HG2	5:E:198:ILE:HD13	1.99	0.44
1:A:1343:ALA:HB2	5:E:150:VAL:HG22	1.98	0.44
2:B:129:PHE:CD2	2:B:166:PHE:HA	2.53	0.44
2:B:230:ALA:N	2:B:231:PRO:CD	2.81	0.44
2:B:281:PRO:O	2:B:282:ILE:C	2.60	0.44
2:B:293:PRO:O	2:B:296:GLU:HB3	2.18	0.44
2:B:374:LYS:O	2:B:375:ALA:C	2.60	0.44
3:C:44:LEU:HD23	3:C:72:LEU:CB	2.48	0.44
3:C:181:ASP:CG	3:C:186:LEU:HD13	2.42	0.44
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.52	0.44
4:D:52:LEU:C	4:D:54:GLU:N	2.75	0.44
5:E:177:ARG:HD3	5:E:215:MET:HG3	1.99	0.44
7:G:14:HIS:CD2	7:G:16:SER:H	2.34	0.44
8:H:38:LEU:HD12	8:H:39:THR:H	1.82	0.44
1:A:718:VAL:O	1:A:721:PHE:HB2	2.18	0.44
1:A:803:SER:C	1:A:805:LEU:N	2.75	0.44
1:A:890:ASP:H	1:A:1296:GLY:HA3	1.83	0.44
1:A:1206:ASP:HB2	1:A:1274:ARG:HH22	1.83	0.44
1:A:1312:ASN:O	1:A:1316:VAL:HG23	2.18	0.44
1:A:1313:LEU:HD12	1:A:1327:ILE:HD13	1.99	0.44
2:B:350:GLN:O	2:B:351:TYR:C	2.61	0.44
3:C:175:ALA:HB3	10:J:43:ARG:NH2	2.33	0.44
7:G:1:MET:CE	7:G:80:LYS:O	2.66	0.44
7:G:26:LEU:O	7:G:27:LYS:C	2.61	0.44
7:G:51:TYR:C	7:G:51:TYR:CD2	2.94	0.44
10:J:28:ASP:O	10:J:29:GLU:C	2.61	0.44
10:J:45:CYS:SG	10:J:46:CYS:N	2.91	0.44
12:L:47:ARG:NH2	12:L:54:ARG:HE	2.16	0.44
1:A:264:PHE:O	1:A:265:LYS:C	2.60	0.44
2:B:763:GLN:O	2:B:764:SER:C	2.59	0.44
2:B:952:VAL:CG1	2:B:953:LEU:N	2.79	0.44
3:C:80:LEU:HD11	3:C:96:SER:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:211:ASP:HA	3:C:212:PRO:HD3	1.84	0.44
4:D:146:GLN:O	4:D:150:ASN:N	2.51	0.44
5:E:207:ARG:HB3	5:E:207:ARG:NH1	2.28	0.44
7:G:66:GLY:O	7:G:67:SER:C	2.60	0.44
11:K:7:PHE:O	11:K:11:LEU:HB2	2.18	0.44
12:L:40:LEU:HD22	12:L:44:ASP:CB	2.47	0.44
1:A:135:PHE:CE1	1:A:222:LEU:HD22	2.53	0.43
1:A:185:TRP:O	1:A:197:PRO:HA	2.18	0.43
1:A:353:ILE:CD1	1:A:487:MET:HE2	2.48	0.43
1:A:449:SER:O	2:B:1133:MET:HB3	2.18	0.43
1:A:814:PHE:CE1	2:B:519:TRP:HA	2.52	0.43
1:A:1152:ILE:HG13	9:I:44:TYR:HD2	1.83	0.43
1:A:1343:ALA:O	1:A:1344:GLY:C	2.60	0.43
2:B:781:PHE:HD1	2:B:782:LEU:HG	1.83	0.43
2:B:1084:GLN:OE1	3:C:191:TYR:HA	2.17	0.43
2:B:1085:ILE:CG2	2:B:1086:PHE:N	2.80	0.43
3:C:98:VAL:O	3:C:99:LEU:HD23	2.18	0.43
5:E:138:ALA:HA	5:E:141:VAL:CG2	2.47	0.43
8:H:38:LEU:HD12	8:H:124:ARG:O	2.18	0.43
9:I:71:SER:O	9:I:83:ASN:ND2	2.51	0.43
10:J:1:MET:HE3	10:J:56:LEU:HD12	1.99	0.43
11:K:91:CYS:O	11:K:92:ASN:C	2.60	0.43
12:L:30:ILE:CD1	12:L:59:ALA:HB2	2.42	0.43
1:A:393:ARG:C	1:A:395:GLY:H	2.25	0.43
1:A:396:PRO:HB3	1:A:402:ALA:O	2.18	0.43
1:A:773:LYS:O	1:A:774:ARG:C	2.60	0.43
1:A:1189:SER:OG	1:A:1190:PRO:HD2	2.18	0.43
1:A:1406:VAL:HG12	1:A:1410:PHE:CD1	2.52	0.43
2:B:39:ARG:HG2	2:B:39:ARG:NH1	2.34	0.43
2:B:189:LEU:O	2:B:190:TYR:C	2.61	0.43
2:B:546:SER:HG	2:B:631:GLY:H	1.56	0.43
2:B:999:MET:HE3	2:B:999:MET:CA	2.48	0.43
3:C:62:PHE:O	3:C:65:HIS:HB3	2.17	0.43
5:E:21:GLU:O	5:E:24:LYS:HG2	2.19	0.43
7:G:1:MET:CE	7:G:80:LYS:H	2.18	0.43
7:G:47:CYS:O	7:G:76:ALA:HB1	2.19	0.43
1:A:43:GLU:HB2	1:A:46:THR:HB	2.00	0.43
1:A:693:VAL:O	1:A:693:VAL:HG12	2.18	0.43
1:A:720:ARG:HD2	13:S:262:GLU:HB3	1.99	0.43
1:A:814:PHE:HE1	2:B:519:TRP:HA	1.83	0.43
1:A:833:GLU:O	1:A:834:THR:C	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:971:PHE:CE2	1:A:1040:GLN:HG2	2.53	0.43
1:A:1239:ARG:NH1	1:A:1239:ARG:HB3	2.33	0.43
2:B:395:GLN:HG2	2:B:396:ASP:H	1.83	0.43
2:B:465:ASN:N	2:B:465:ASN:ND2	2.65	0.43
2:B:901:PRO:HB2	12:L:60:ARG:HA	2.00	0.43
2:B:911:ILE:HG23	2:B:966:VAL:HG11	2.00	0.43
2:B:987:LYS:O	2:B:987:LYS:HG2	2.18	0.43
2:B:1135:ARG:O	2:B:1136:ASP:C	2.61	0.43
2:B:1182:CYS:C	2:B:1183:LYS:O	2.60	0.43
3:C:169:LYS:NZ	12:L:69:ALA:CB	2.81	0.43
5:E:29:PHE:O	5:E:30:ILE:HG13	2.18	0.43
5:E:159:ASP:C	5:E:161:LYS:N	2.76	0.43
7:G:119:LEU:HD12	7:G:131:GLN:O	2.18	0.43
11:K:30:ALA:HA	11:K:75:ILE:O	2.18	0.43
11:K:32:VAL:HA	11:K:73:LEU:O	2.18	0.43
12:L:38:LEU:O	12:L:39:SER:CB	2.58	0.43
13:S:254:TYR:C	13:S:256:ALA:N	2.73	0.43
13:S:293:LEU:N	13:S:293:LEU:CD2	2.81	0.43
1:A:43:GLU:O	1:A:44:THR:CB	2.66	0.43
1:A:353:ILE:HD13	1:A:487:MET:HG3	2.00	0.43
1:A:477:PRO:HG2	1:A:521:MET:HG2	1.99	0.43
1:A:567:LYS:HD3	8:H:95:TYR:HA	1.99	0.43
1:A:962:ARG:O	1:A:965:GLN:N	2.51	0.43
2:B:48:LEU:O	2:B:49:ASP:C	2.60	0.43
2:B:59:LEU:CD1	2:B:417:PHE:CE2	3.01	0.43
2:B:214:ALA:HA	2:B:408:LEU:HD12	2.00	0.43
2:B:215:GLN:OE1	2:B:499:ASN:HB3	2.18	0.43
2:B:789:MET:CE	2:B:965:LYS:O	2.65	0.43
3:C:144:ILE:O	3:C:145:CYS:CB	2.66	0.43
8:H:12:VAL:HA	8:H:28:ALA:HB2	1.99	0.43
8:H:38:LEU:HD13	8:H:125:LEU:HD13	2.00	0.43
10:J:7:CYS:SG	10:J:49:MET:CE	3.01	0.43
10:J:25:LEU:O	10:J:29:GLU:HA	2.18	0.43
13:S:296:PHE:N	13:S:296:PHE:CD1	2.86	0.43
1:A:42:ASP:HB3	1:A:45:GLN:N	2.33	0.43
1:A:58:LEU:O	1:A:59:GLY:O	2.36	0.43
1:A:88:LYS:HA	1:A:89:PRO:HD2	1.72	0.43
1:A:108:MET:SD	1:A:210:ILE:HD13	2.59	0.43
1:A:476:SER:O	1:A:477:PRO:C	2.60	0.43
1:A:540:PHE:CB	1:A:571:LEU:HD23	2.39	0.43
1:A:735:VAL:O	1:A:735:VAL:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:845:LEU:HD22	1:A:1374:VAL:HG21	2.00	0.43
1:A:1001:ARG:HG2	1:A:1001:ARG:HH11	1.83	0.43
1:A:1261:LYS:C	1:A:1264:GLU:HB3	2.44	0.43
2:B:258:LEU:HG	2:B:258:LEU:O	2.18	0.43
2:B:540:SER:HB3	2:B:747:MET:O	2.18	0.43
2:B:547:VAL:H	2:B:612:GLU:CD	2.27	0.43
2:B:634:TYR:CE1	2:B:692:TYR:CD1	3.06	0.43
2:B:695:ALA:O	2:B:698:GLU:HB3	2.18	0.43
2:B:787:VAL:O	2:B:787:VAL:HG12	2.19	0.43
2:B:976:ILE:HG22	2:B:977:GLY:N	2.34	0.43
2:B:1145:SER:O	2:B:1147:LEU:N	2.51	0.43
3:C:237:SER:O	3:C:238:ILE:HG13	2.18	0.43
3:C:242:GLN:HA	3:C:245:VAL:CG2	2.45	0.43
4:D:56:ARG:CB	4:D:148:LEU:HD22	2.37	0.43
4:D:156:ASP:C	4:D:158:GLU:H	2.25	0.43
5:E:33:GLU:C	5:E:35:VAL:H	2.25	0.43
5:E:188:LEU:O	5:E:189:GLY:C	2.62	0.43
7:G:1:MET:SD	7:G:79:PHE:CD1	3.12	0.43
1:A:862:ASN:HA	5:E:174:GLN:O	2.19	0.43
1:A:1006:ILE:HD11	5:E:163:GLU:HG3	2.00	0.43
1:A:1080:THR:HG22	1:A:1081:LEU:H	1.81	0.43
1:A:1101:LEU:HD11	1:A:1105:LEU:HD11	2.00	0.43
1:A:1192:LEU:CG	1:A:1193:LEU:N	2.81	0.43
1:A:1396:ALA:O	1:A:1397:LEU:C	2.61	0.43
2:B:287:ARG:NH2	2:B:325:GLN:HE22	2.16	0.43
2:B:390:LEU:O	2:B:392:ARG:N	2.51	0.43
2:B:460:ALA:HB1	2:B:466:TRP:CE3	2.52	0.43
2:B:777:ALA:HA	2:B:1095:LEU:CA	2.45	0.43
2:B:780:VAL:HG21	10:J:56:LEU:HD11	1.99	0.43
2:B:866:TYR:O	2:B:867:GLY:C	2.61	0.43
2:B:952:VAL:CG1	2:B:953:LEU:H	2.31	0.43
3:C:242:GLN:HB3	3:C:246:ARG:HG3	1.99	0.43
5:E:11:ARG:C	5:E:13:TRP:N	2.74	0.43
5:E:198:ILE:HD11	5:E:212:ARG:HH11	1.84	0.43
7:G:117:GLN:C	7:G:119:LEU:N	2.71	0.43
12:L:63:ARG:O	12:L:63:ARG:HG3	2.19	0.43
1:A:2:VAL:HG21	2:B:1158:PHE:N	2.34	0.43
1:A:55:ASP:O	1:A:57:ARG:N	2.51	0.43
1:A:224:PHE:CD2	1:A:231:PRO:HG3	2.54	0.43
1:A:353:ILE:HG13	1:A:482:PHE:HD2	1.83	0.43
1:A:464:PRO:HG2	1:A:465:TYR:HD1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:703:THR:HB	1:A:705:LYS:HE2	2.01	0.43
1:A:715:GLU:C	1:A:717:ASN:H	2.27	0.43
1:A:1315:GLU:C	1:A:1317:MET:N	2.74	0.43
2:B:597:MET:O	2:B:599:THR:N	2.52	0.43
2:B:778:MET:HE1	2:B:853:SER:HB3	2.00	0.43
2:B:1099:VAL:CG1	2:B:1100:ASP:H	2.24	0.43
6:F:86:THR:O	6:F:89:GLU:HB2	2.18	0.43
8:H:145:ARG:O	8:H:146:ARG:HB2	2.18	0.43
11:K:62:LYS:HG3	11:K:62:LYS:O	2.19	0.43
1:A:49:LYS:NZ	1:A:60:SER:CA	2.81	0.43
1:A:79:GLY:HA3	1:A:243:PRO:CG	2.49	0.43
1:A:426:LEU:O	1:A:427:GLN:HG2	2.19	0.43
1:A:722:LEU:O	1:A:725:ALA:HB3	2.19	0.43
1:A:803:SER:C	1:A:805:LEU:H	2.26	0.43
1:A:1208:THR:O	1:A:1211:GLN:N	2.52	0.43
1:A:1304:TRP:C	1:A:1305:VAL:HG23	2.44	0.43
1:A:1319:VAL:O	1:A:1322:ILE:HG12	2.19	0.43
2:B:20:ASP:O	2:B:22:SER:N	2.48	0.43
2:B:376:PHE:HE2	2:B:569:TYR:HD2	1.65	0.43
2:B:486:TYR:CD1	2:B:1096:ARG:NH2	2.86	0.43
2:B:624:LEU:HD12	2:B:624:LEU:HA	1.79	0.43
2:B:1076:HIS:CD2	11:K:40:HIS:NE2	2.86	0.43
2:B:1177:HIS:C	2:B:1179:GLN:N	2.73	0.43
3:C:82:TYR:O	3:C:83:SER:C	2.62	0.43
3:C:97:VAL:HG12	3:C:98:VAL:H	1.84	0.43
5:E:128:PRO:HA	5:E:129:PRO:C	2.42	0.43
6:F:134:ILE:N	6:F:146:TRP:O	2.50	0.43
11:K:24:ASP:CG	11:K:74:ARG:NH1	2.77	0.43
11:K:55:LYS:HB2	11:K:81:TYR:HE1	1.84	0.43
1:A:253:ASN:HB2	2:B:935:ARG:NH1	2.34	0.43
1:A:496:GLU:OE1	7:G:63:PRO:O	2.37	0.43
1:A:582:ILE:O	1:A:583:PRO:O	2.36	0.43
1:A:858:ASN:O	1:A:860:LEU:N	2.52	0.43
1:A:955:PRO:O	1:A:955:PRO:HG2	2.18	0.43
1:A:1373:ASP:HA	1:A:1376:THR:CG2	2.49	0.43
1:A:1450:LEU:HD11	6:F:108:PHE:CZ	2.54	0.43
1:A:1451:VAL:C	1:A:1453:TYR:N	2.76	0.43
2:B:236:HIS:O	2:B:237:VAL:HG23	2.18	0.43
2:B:405:ARG:HD2	2:B:631:GLY:C	2.43	0.43
2:B:485:ARG:HH11	2:B:485:ARG:HG3	1.83	0.43
2:B:526:GLU:HG2	2:B:538:ASN:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:758:PHE:HB2	2:B:1024:ALA:HB1	2.00	0.43
2:B:798:TYR:HE2	3:C:62:PHE:CE2	2.37	0.43
2:B:995:ARG:O	2:B:997:GLU:N	2.52	0.43
8:H:118:PHE:O	8:H:119:GLY:C	2.60	0.43
10:J:54:VAL:HG12	10:J:56:LEU:HD23	2.00	0.43
1:A:536:LEU:H	1:A:536:LEU:HG	1.51	0.43
1:A:751:SER:OG	2:B:1015:HIS:CE1	2.72	0.43
1:A:841:LEU:HD13	1:A:1072:ILE:HB	2.00	0.43
1:A:1021:LEU:O	1:A:1024:SER:HB3	2.19	0.43
1:A:1074:GLU:N	1:A:1075:PRO:CD	2.82	0.43
1:A:1098:VAL:N	1:A:1099:PRO:CD	2.81	0.43
1:A:1348:LEU:HG	1:A:1372:VAL:HG23	2.01	0.43
2:B:63:ILE:O	2:B:67:SER:HB3	2.19	0.43
2:B:381:MET:O	2:B:382:ILE:C	2.61	0.43
3:C:41:ILE:HD11	3:C:247:GLY:CA	2.49	0.43
3:C:59:ALA:O	3:C:62:PHE:CB	2.67	0.43
3:C:76:ASP:HB2	3:C:128:ASN:O	2.18	0.43
4:D:26:THR:O	4:D:28:GLN:N	2.52	0.43
5:E:80:VAL:HG12	5:E:81:GLU:N	2.33	0.43
7:G:16:SER:C	7:G:18:PHE:H	2.26	0.43
8:H:97:MET:SD	8:H:121:LEU:HD12	2.59	0.43
8:H:115:TYR:CE2	8:H:124:ARG:HG3	2.54	0.43
12:L:32:ALA:CB	12:L:55:ILE:HG13	2.49	0.43
12:L:50:ASP:O	12:L:52:GLY:N	2.52	0.43
1:A:261:ASP:O	1:A:264:PHE:N	2.51	0.42
1:A:343:LYS:HE2	2:B:1156:ASP:HB2	2.01	0.42
1:A:366:VAL:O	1:A:463:ILE:HG12	2.19	0.42
1:A:719:VAL:C	1:A:721:PHE:N	2.76	0.42
1:A:727:ASP:O	1:A:731:ARG:HG3	2.18	0.42
1:A:784:LEU:HD11	1:A:815:PHE:CE2	2.54	0.42
1:A:925:LEU:C	1:A:927:VAL:N	2.76	0.42
1:A:1013:ASP:C	1:A:1015:VAL:H	2.26	0.42
1:A:1111:MET:HE1	1:A:1331:SER:HA	2.01	0.42
1:A:1169:ILE:HD11	1:A:1229:SER:HB3	2.01	0.42
1:A:1384:VAL:O	1:A:1384:VAL:HG12	2.19	0.42
1:A:1444:MET:HG2	7:G:59:GLY:O	2.19	0.42
2:B:281:PRO:C	2:B:283:VAL:N	2.75	0.42
2:B:324:ILE:HG22	2:B:325:GLN:N	2.34	0.42
2:B:518:HIS:O	2:B:519:TRP:C	2.60	0.42
2:B:1017:ILE:HG22	2:B:1018:PRO:HD3	2.01	0.42
2:B:1159:ARG:CD	2:B:1193:GLN:HG3	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:241:ASP:O	3:C:244:VAL:HB	2.19	0.42
5:E:154:ILE:HG22	5:E:155:ARG:O	2.19	0.42
8:H:27:GLU:HG2	8:H:39:THR:HG23	2.00	0.42
10:J:64:ASN:CB	10:J:65:PRO:CD	2.74	0.42
11:K:35:PHE:HD1	11:K:35:PHE:H	1.67	0.42
11:K:47:ARG:C	11:K:47:ARG:HD2	2.44	0.42
12:L:40:LEU:HD22	12:L:44:ASP:CG	2.44	0.42
1:A:304:MET:O	1:A:326:ARG:HB3	2.19	0.42
1:A:453:MET:HE3	1:A:520:CYS:CB	2.50	0.42
1:A:533:LYS:HE3	1:A:745:GLN:NE2	2.34	0.42
1:A:545:GLN:O	1:A:546:VAL:C	2.61	0.42
1:A:600:PRO:HA	8:H:25:ARG:NH2	2.34	0.42
1:A:679:ILE:O	1:A:680:THR:C	2.62	0.42
1:A:794:PRO:C	1:A:796:SER:N	2.77	0.42
1:A:1129:GLU:O	1:A:1131:ALA:N	2.52	0.42
1:A:1284:MET:HE3	1:A:1304:TRP:CZ3	2.54	0.42
2:B:176:SER:O	2:B:182:SER:HB3	2.19	0.42
2:B:292:ILE:N	2:B:293:PRO:HD2	2.34	0.42
2:B:401:PHE:C	2:B:403:LYS:N	2.76	0.42
2:B:984:HIS:O	2:B:985:GLY:C	2.62	0.42
2:B:1060:ARG:C	2:B:1062:HIS:N	2.76	0.42
2:B:1073:TYR:N	2:B:1073:TYR:CD1	2.87	0.42
2:B:1076:HIS:ND1	2:B:1076:HIS:N	2.66	0.42
2:B:1085:ILE:N	2:B:1085:ILE:HD12	2.34	0.42
3:C:63:ILE:O	3:C:67:LEU:HG	2.19	0.42
5:E:92:THR:O	5:E:92:THR:HG22	2.18	0.42
5:E:182:ASP:O	5:E:185:ALA:HB3	2.19	0.42
6:F:100:GLN:HG2	7:G:66:GLY:HA3	2.01	0.42
9:I:61:ASP:C	9:I:63:GLY:N	2.77	0.42
9:I:111:THR:HG21	9:I:113:ASP:HB2	2.00	0.42
1:A:47:ARG:CZ	1:A:255:SER:H	2.31	0.42
1:A:107:CYS:HB2	1:A:171:GLN:HG2	2.01	0.42
1:A:472:LEU:O	1:A:475:THR:HG22	2.19	0.42
1:A:483:ASP:HB2	2:B:987:LYS:CG	2.48	0.42
1:A:515:GLN:HB3	1:A:1071:SER:OG	2.20	0.42
1:A:526:ASP:HB3	1:A:657:LEU:HD23	2.01	0.42
1:A:527:THR:O	1:A:653:VAL:HG11	2.19	0.42
1:A:570:PRO:C	1:A:571:LEU:HD12	2.43	0.42
1:A:783:THR:HG21	1:A:815:PHE:CE2	2.53	0.42
1:A:1044:TRP:O	1:A:1045:VAL:C	2.62	0.42
1:A:1142:THR:O	1:A:1143:LEU:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1272:THR:HG22	1:A:1273:LEU:N	2.34	0.42
2:B:222:ILE:O	2:B:240:ILE:HA	2.19	0.42
2:B:431:TYR:CD2	2:B:447:ALA:HB2	2.54	0.42
2:B:549:THR:CG2	2:B:550:ASP:H	2.17	0.42
2:B:758:PHE:C	2:B:760:ASP:H	2.26	0.42
2:B:912:ILE:HD11	2:B:966:VAL:HG23	1.99	0.42
2:B:1003:ALA:HA	3:C:178:PHE:O	2.19	0.42
8:H:58:THR:HG22	8:H:59:ILE:N	2.35	0.42
11:K:95:ILE:O	11:K:96:ASN:C	2.63	0.42
1:A:738:LYS:NZ	3:C:194:GLU:C	2.78	0.42
1:A:1013:ASP:C	1:A:1015:VAL:N	2.76	0.42
1:A:1067:LEU:O	1:A:1067:LEU:HD12	2.20	0.42
1:A:1362:TYR:C	1:A:1363:VAL:HG23	2.44	0.42
2:B:295:GLY:HA2	2:B:298:LEU:HB2	2.01	0.42
2:B:546:SER:HG	2:B:630:ALA:CA	2.33	0.42
2:B:597:MET:C	2:B:599:THR:N	2.77	0.42
2:B:949:VAL:HG12	2:B:950:ASP:N	2.34	0.42
4:D:63:LEU:HD13	4:D:133:THR:OG1	2.19	0.42
5:E:25:ASP:O	5:E:27:GLY:N	2.52	0.42
5:E:147:HIS:HD2	5:E:149:LEU:H	1.67	0.42
12:L:32:ALA:CB	12:L:55:ILE:HD12	2.48	0.42
1:A:40:THR:CG2	1:A:259:GLU:OE2	2.65	0.42
1:A:52:GLY:N	1:A:56:PRO:HG3	2.35	0.42
1:A:626:ASN:C	1:A:631:HIS:HD2	2.27	0.42
1:A:672:ASP:O	1:A:673:GLY:C	2.62	0.42
1:A:1213:GLY:O	1:A:1215:ARG:N	2.53	0.42
1:A:1453:TYR:CE2	6:F:129:LYS:HA	2.54	0.42
2:B:235:SER:OG	2:B:236:HIS:CD2	2.72	0.42
2:B:259:TYR:N	2:B:259:TYR:CD1	2.88	0.42
2:B:386:LEU:O	2:B:387:LEU:C	2.62	0.42
2:B:603:LEU:HD13	2:B:608:ASP:HB2	2.00	0.42
2:B:615:MET:HA	2:B:626:ILE:HA	2.01	0.42
2:B:744:HIS:HD2	2:B:746:SER:CB	2.32	0.42
3:C:258:ILE:HD12	3:C:258:ILE:N	2.35	0.42
9:I:73:ARG:HH12	9:I:112:SER:HB2	1.83	0.42
10:J:6:ARG:HB3	10:J:11:GLY:O	2.20	0.42
1:A:231:PRO:O	1:A:233:TRP:N	2.52	0.42
1:A:252:PHE:HB2	1:A:256:GLN:HB3	2.01	0.42
1:A:489:LEU:C	1:A:489:LEU:CD1	2.91	0.42
1:A:695:LYS:O	1:A:697:ALA:N	2.53	0.42
1:A:784:LEU:C	1:A:786:HIS:N	2.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:929:LEU:O	1:A:929:LEU:HD13	2.19	0.42
1:A:1016:THR:O	1:A:1017:LEU:C	2.62	0.42
1:A:1081:LEU:HA	1:A:1081:LEU:HD13	1.84	0.42
1:A:1164:PRO:O	1:A:1167:GLU:HG3	2.19	0.42
1:A:1170:ILE:O	1:A:1171:GLN:C	2.61	0.42
1:A:1220:PHE:O	1:A:1221:LYS:HB2	2.18	0.42
2:B:843:GLN:HA	2:B:846:ILE:HG13	2.02	0.42
2:B:1162:ILE:HG22	2:B:1163:CYS:O	2.19	0.42
4:D:188:ALA:O	4:D:189:ASP:C	2.62	0.42
5:E:14:ARG:O	5:E:15:ALA:C	2.63	0.42
7:G:30:LEU:HD13	7:G:72:VAL:HG11	2.01	0.42
9:I:26:LEU:CD2	9:I:37:GLU:HA	2.41	0.42
10:J:11:GLY:O	10:J:12:LYS:C	2.60	0.42
1:A:282:ASN:O	1:A:284:ALA:N	2.53	0.42
1:A:325:ILE:O	1:A:328:ARG:HB2	2.20	0.42
1:A:380:VAL:HG11	1:A:427:GLN:C	2.45	0.42
1:A:417:TYR:O	1:A:418:SER:C	2.62	0.42
1:A:526:ASP:OD2	2:B:829:CYS:HB3	2.20	0.42
1:A:532:ARG:HD3	1:A:749:ALA:HB2	2.00	0.42
1:A:900:ASP:HA	1:A:926:GLN:HE22	1.84	0.42
1:A:1017:LEU:HD23	5:E:204:THR:O	2.18	0.42
1:A:1134:ILE:O	1:A:1137:ALA:N	2.48	0.42
2:B:227:LYS:H	2:B:395:GLN:CD	2.27	0.42
2:B:582:VAL:HG23	2:B:626:ILE:CB	2.39	0.42
2:B:634:TYR:HE1	2:B:692:TYR:CD1	2.38	0.42
2:B:680:THR:HB	2:B:681:TRP:H	1.58	0.42
2:B:814:PHE:C	2:B:816:GLU:N	2.76	0.42
2:B:1031:LEU:HD13	2:B:1055:ILE:HD11	2.00	0.42
2:B:1065:GLN:HG3	2:B:1067:ARG:H	1.83	0.42
3:C:62:PHE:C	3:C:62:PHE:HD2	2.27	0.42
3:C:86:CYS:C	3:C:88:CYS:H	2.27	0.42
5:E:135:PHE:CD1	5:E:135:PHE:N	2.88	0.42
5:E:162:ARG:HH11	5:E:162:ARG:CG	2.32	0.42
5:E:185:ALA:O	5:E:190:LEU:HG	2.18	0.42
7:G:106:MET:HG2	7:G:107:LYS:N	2.34	0.42
7:G:145:VAL:HG12	7:G:146:LYS:H	1.82	0.42
11:K:65:HIS:CD2	11:K:67:PHE:HB2	2.54	0.42
1:A:16:GLU:HB3	1:A:1418:LEU:HD11	2.02	0.42
1:A:523:ILE:HD12	1:A:622:VAL:CG2	2.49	0.42
1:A:853:ASP:OD2	1:A:857:ARG:NH2	2.52	0.42
2:B:315:LYS:HE2	9:I:4:PHE:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:515:HIS:HD2	2:B:517:THR:OG1	2.03	0.42
2:B:730:ARG:O	2:B:731:VAL:O	2.38	0.42
3:C:91:HIS:CD2	3:C:91:HIS:O	2.73	0.42
5:E:98:ILE:O	5:E:99:HIS:C	2.61	0.42
6:F:138:LEU:O	6:F:140:ASP:N	2.52	0.42
7:G:21:ARG:HD3	7:G:21:ARG:HA	1.92	0.42
9:I:13:MET:HA	9:I:13:MET:HE3	2.01	0.42
1:A:78:PRO:C	1:A:79:GLY:O	2.62	0.42
1:A:92:HIS:HB3	1:A:95:PHE:HB2	2.02	0.42
1:A:542:GLU:H	1:A:542:GLU:HG2	1.66	0.42
1:A:577:ILE:O	1:A:578:LEU:C	2.61	0.42
1:A:598:LEU:CD2	8:H:25:ARG:NH1	2.83	0.42
1:A:870:GLU:HG2	5:E:208:TYR:CE2	2.55	0.42
1:A:886:ILE:HG13	1:A:943:LEU:HD13	2.00	0.42
1:A:900:ASP:HA	1:A:926:GLN:NE2	2.35	0.42
1:A:1116:LEU:O	1:A:1308:THR:HG22	2.19	0.42
1:A:1348:LEU:HG	1:A:1372:VAL:CG2	2.50	0.42
2:B:23:ALA:CB	2:B:24:PRO:CD	2.95	0.42
2:B:254:LEU:HD23	2:B:381:MET:CE	2.36	0.42
2:B:515:HIS:CD2	2:B:517:THR:HG23	2.54	0.42
2:B:628:THR:O	2:B:629:ASP:O	2.38	0.42
2:B:642:ASP:HB3	2:B:649:LYS:CE	2.49	0.42
2:B:644:GLU:O	2:B:646:LEU:N	2.53	0.42
2:B:1147:LEU:C	2:B:1149:GLU:N	2.76	0.42
3:C:181:ASP:N	3:C:182:PRO:CD	2.83	0.42
3:C:251:LEU:O	3:C:252:GLN:C	2.62	0.42
7:G:44:TYR:HE1	7:G:157:ILE:HB	1.83	0.42
8:H:95:TYR:HB3	8:H:144:ILE:HB	2.00	0.42
11:K:58:PHE:CB	11:K:76:GLN:HE21	2.32	0.42
12:L:54:ARG:HG3	12:L:54:ARG:HH11	1.85	0.42
1:A:216:VAL:O	1:A:219:PHE:HB2	2.20	0.42
1:A:254:GLU:N	2:B:935:ARG:HH22	2.17	0.42
1:A:419:LYS:HG3	1:A:420:ARG:H	1.84	0.42
1:A:472:LEU:C	1:A:474:VAL:H	2.28	0.42
1:A:483:ASP:OD2	1:A:485:ASP:OD1	2.38	0.42
1:A:518:LYS:HE2	1:A:624:SER:O	2.20	0.42
1:A:552:TRP:O	1:A:554:PRO:HD3	2.20	0.42
1:A:716:ASP:OD1	1:A:716:ASP:O	2.37	0.42
1:A:825:ILE:O	1:A:827:THR:N	2.52	0.42
1:A:1215:ARG:HD2	1:A:1215:ARG:HA	1.87	0.42
2:B:409:ALA:O	2:B:410:GLY:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:410:GLY:O	2:B:411:PRO:C	2.63	0.42
2:B:591:ARG:O	2:B:593:PRO:HD3	2.19	0.42
2:B:805:THR:HA	2:B:809:MET:HE1	2.01	0.42
2:B:835:GLN:HE21	2:B:835:GLN:HB2	1.57	0.42
2:B:900:ALA:O	2:B:901:PRO:C	2.62	0.42
2:B:939:THR:HA	2:B:940:PRO:HD2	1.92	0.42
2:B:1073:TYR:HE2	3:C:180:TYR:CE2	2.37	0.42
2:B:1115:THR:CG2	2:B:1117:GLN:HB2	2.50	0.42
4:D:33:PHE:CE1	7:G:80:LYS:CE	3.02	0.42
5:E:197:LYS:O	5:E:197:LYS:CG	2.64	0.42
7:G:27:LYS:HE2	7:G:54:ILE:HB	2.02	0.42
12:L:53:HIS:O	12:L:55:ILE:HG12	2.20	0.42
1:A:96:ILE:O	1:A:97:ALA:C	2.63	0.41
1:A:114:LEU:O	1:A:115:LEU:HG	2.20	0.41
1:A:125:ALA:C	1:A:127:ALA:N	2.78	0.41
1:A:299:HIS:C	1:A:301:ALA:H	2.28	0.41
1:A:322:VAL:CG1	1:A:323:LYS:N	2.82	0.41
1:A:324:SER:O	1:A:327:ALA:HB3	2.19	0.41
1:A:675:THR:O	1:A:675:THR:HG22	2.19	0.41
1:A:726:ARG:O	1:A:729:ALA:N	2.53	0.41
1:A:845:LEU:O	1:A:846:GLU:C	2.61	0.41
1:A:874:ASP:HA	1:A:1058:VAL:HG23	2.01	0.41
1:A:1143:LEU:HD23	1:A:1267:MET:O	2.19	0.41
1:A:1282:VAL:HG22	1:A:1308:THR:HA	2.01	0.41
2:B:31:TRP:CE3	2:B:31:TRP:HA	2.55	0.41
2:B:57:TYR:HD1	2:B:57:TYR:H	1.67	0.41
2:B:172:ILE:HG22	2:B:173:MET:N	2.35	0.41
2:B:373:ARG:CG	2:B:566:LEU:HD23	2.50	0.41
2:B:419:THR:HG21	2:B:468:GLU:OE2	2.20	0.41
2:B:487:THR:CG2	2:B:488:TYR:N	2.82	0.41
2:B:492:LEU:O	2:B:495:LEU:N	2.42	0.41
2:B:616:ILE:N	2:B:616:ILE:CD1	2.81	0.41
2:B:637:LEU:HD21	2:B:742:GLU:OE2	2.20	0.41
2:B:785:TYR:HE2	10:J:60:PHE:CZ	2.38	0.41
2:B:981:ALA:C	2:B:1092:TYR:CD2	2.98	0.41
3:C:75:MET:O	3:C:246:ARG:NH2	2.31	0.41
3:C:249:ASP:O	3:C:252:GLN:N	2.53	0.41
6:F:86:THR:O	6:F:89:GLU:N	2.51	0.41
1:A:320:ARG:HH21	1:A:323:LYS:NZ	2.17	0.41
1:A:546:VAL:HG21	1:A:572:TRP:CD2	2.55	0.41
1:A:567:LYS:CE	8:H:46:LEU:HB2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:901:LEU:CG	1:A:926:GLN:HE21	2.28	0.41
1:A:1092:LYS:HD2	1:A:1092:LYS:HA	1.82	0.41
1:A:1157:ASP:C	1:A:1159:ARG:N	2.78	0.41
1:A:1450:LEU:HD21	7:G:19:GLY:O	2.20	0.41
2:B:247:GLY:C	2:B:249:ARG:N	2.78	0.41
2:B:510:LYS:HE2	2:B:513:GLN:OE1	2.21	0.41
2:B:544:CYS:O	2:B:545:ILE:CG1	2.68	0.41
2:B:866:TYR:O	2:B:868:MET:N	2.53	0.41
2:B:1098:MET:O	2:B:1101:ASP:HB2	2.20	0.41
3:C:18:VAL:O	3:C:20:PHE:CD2	2.73	0.41
4:D:19:GLU:O	4:D:20:GLU:C	2.61	0.41
5:E:42:PHE:CE1	5:E:58:MET:HE3	2.55	0.41
7:G:150:CYS:C	7:G:151:ILE:HG13	2.45	0.41
9:I:16:PRO:HA	9:I:26:LEU:O	2.21	0.41
9:I:55:THR:HG22	9:I:56:ALA:H	1.84	0.41
11:K:81:TYR:C	11:K:81:TYR:CD2	2.97	0.41
11:K:83:PRO:O	11:K:84:LYS:C	2.63	0.41
1:A:7:SER:HB2	2:B:1175:LEU:CD2	2.49	0.41
1:A:606:LEU:HB3	1:A:614:PHE:CD2	2.55	0.41
1:A:788:SER:O	1:A:789:LYS:C	2.63	0.41
1:A:962:ARG:C	1:A:964:ILE:N	2.76	0.41
1:A:1397:LEU:HA	1:A:1400:CYS:HB2	1.99	0.41
2:B:170:LEU:HA	2:B:171:PRO:HD2	1.87	0.41
2:B:174:LEU:HD11	2:B:204:ILE:CD1	2.49	0.41
2:B:233:PRO:HG2	2:B:234:ILE:HD12	2.02	0.41
2:B:303:TYR:N	2:B:303:TYR:HD2	2.18	0.41
2:B:708:GLU:O	2:B:709:ASP:C	2.62	0.41
2:B:745:PRO:O	2:B:746:SER:C	2.62	0.41
2:B:849:GLY:O	2:B:852:ARG:HG3	2.20	0.41
2:B:1032:SER:O	2:B:1034:VAL:N	2.53	0.41
2:B:1201:LYS:HE2	2:B:1205:GLN:NE2	2.35	0.41
3:C:8:VAL:CG1	3:C:9:LYS:N	2.83	0.41
4:D:149:THR:O	4:D:149:THR:HG23	2.20	0.41
4:D:151:PHE:O	4:D:152:SER:O	2.38	0.41
4:D:195:ILE:O	4:D:198:LEU:HG	2.21	0.41
4:D:217:LEU:O	4:D:219:THR:N	2.54	0.41
5:E:182:ASP:O	5:E:183:PRO:C	2.63	0.41
7:G:132:SER:C	7:G:134:GLU:N	2.77	0.41
11:K:12:LEU:HD11	11:K:18:LYS:HE2	2.02	0.41
1:A:254:GLU:H	2:B:935:ARG:NH1	2.18	0.41
1:A:550:LEU:HD22	1:A:556:TRP:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:630:ILE:HG23	1:A:642:CYS:SG	2.60	0.41
1:A:714:PHE:HD2	9:I:97:MET:HE1	1.81	0.41
1:A:763:ALA:C	1:A:803:SER:HB3	2.45	0.41
1:A:1164:PRO:C	1:A:1166:ASP:H	2.28	0.41
1:A:1260:LEU:HG	1:A:1260:LEU:O	2.20	0.41
1:A:1427:ASN:C	1:A:1429:ILE:N	2.77	0.41
2:B:121:ASN:HA	2:B:207:GLY:HA2	2.02	0.41
2:B:515:HIS:CG	2:B:516:ASN:N	2.88	0.41
2:B:542:MET:HE3	2:B:636:PRO:CG	2.50	0.41
2:B:770:GLN:OE1	2:B:983:ARG:HA	2.20	0.41
2:B:785:TYR:C	2:B:787:VAL:H	2.28	0.41
2:B:809:MET:O	2:B:811:TYR:N	2.54	0.41
3:C:44:LEU:HG	3:C:45:ALA:N	2.34	0.41
3:C:80:LEU:HD12	3:C:95:CYS:HA	2.01	0.41
3:C:187:LYS:HG3	3:C:219:PHE:CE1	2.55	0.41
3:C:255:VAL:HG21	11:K:94:ILE:HG21	2.03	0.41
4:D:40:HIS:CG	4:D:41:GLN:N	2.89	0.41
5:E:112:TYR:CE1	5:E:136:ASN:HB2	2.56	0.41
5:E:124:VAL:HG13	5:E:132:ILE:CG1	2.50	0.41
5:E:143:ASN:ND2	5:E:146:HIS:ND1	2.68	0.41
7:G:7:LEU:O	7:G:73:LYS:HD2	2.20	0.41
9:I:101:PHE:O	9:I:102:VAL:CG2	2.67	0.41
10:J:43:ARG:HG2	10:J:46:CYS:SG	2.61	0.41
11:K:85:ASP:O	11:K:89:ASN:ND2	2.54	0.41
13:S:269:PHE:CE2	13:S:306:TRP:CZ2	3.08	0.41
1:A:44:THR:O	1:A:45:GLN:CB	2.65	0.41
1:A:324:SER:O	1:A:327:ALA:N	2.53	0.41
1:A:334:GLY:O	1:A:335:ARG:C	2.63	0.41
1:A:894:GLU:C	1:A:896:ARG:N	2.78	0.41
2:B:62:ILE:HG23	2:B:418:LYS:CG	2.49	0.41
2:B:282:ILE:HD13	2:B:382:ILE:HD13	2.01	0.41
2:B:365:THR:CG2	2:B:367:LEU:HG	2.38	0.41
2:B:575:PRO:HG2	2:B:576:ASP:H	1.84	0.41
2:B:635:ARG:HG3	2:B:635:ARG:NH1	2.35	0.41
2:B:702:LEU:HD12	2:B:702:LEU:HA	1.85	0.41
2:B:952:VAL:O	2:B:953:LEU:HB3	2.20	0.41
2:B:956:THR:HG22	2:B:960:GLY:HA2	2.02	0.41
3:C:69:LEU:O	3:C:70:ILE:C	2.63	0.41
3:C:167:HIS:CD2	3:C:167:HIS:C	2.97	0.41
4:D:55:ALA:O	4:D:56:ARG:C	2.64	0.41
5:E:116:ILE:HG22	5:E:117:THR:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:75:PRO:C	6:F:77:ASP:N	2.74	0.41
1:A:69:THR:O	1:A:70:CYS:C	2.63	0.41
1:A:151:ASP:OD1	1:A:163:SER:CB	2.68	0.41
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.86	0.41
1:A:361:LEU:HG	1:A:507:VAL:CG1	2.51	0.41
1:A:475:THR:O	1:A:479:ASN:N	2.53	0.41
1:A:605:MET:HB2	1:A:605:MET:HE3	1.74	0.41
1:A:960:ILE:O	1:A:960:ILE:HG22	2.20	0.41
1:A:1260:LEU:O	1:A:1260:LEU:CG	2.68	0.41
1:A:1279:ILE:CD1	1:A:1316:VAL:HG21	2.48	0.41
1:A:1362:TYR:CE1	1:A:1364:ASN:HA	2.56	0.41
1:A:1369:ALA:O	1:A:1370:LEU:C	2.64	0.41
1:A:1397:LEU:H	1:A:1397:LEU:HG	1.64	0.41
2:B:129:PHE:HE2	2:B:166:PHE:CD1	2.35	0.41
2:B:274:PRO:CG	2:B:359:GLU:HB3	2.51	0.41
2:B:700:SER:O	2:B:701:ILE:HG22	2.20	0.41
2:B:830:TYR:HD1	2:B:830:TYR:HA	1.68	0.41
2:B:1072:MET:CE	2:B:1085:ILE:HB	2.51	0.41
3:C:241:ASP:HB3	11:K:109:TRP:CH2	2.55	0.41
5:E:48:ASP:CG	5:E:49:SER:N	2.79	0.41
5:E:114:ASN:O	5:E:115:ASN:CB	2.68	0.41
5:E:179:GLN:O	5:E:180:ARG:C	2.60	0.41
7:G:1:MET:SD	7:G:79:PHE:CE1	3.14	0.41
9:I:40:SER:HB2	9:I:41:PRO:HD2	2.03	0.41
11:K:55:LYS:O	11:K:77:THR:HG22	2.20	0.41
12:L:31:CYS:SG	12:L:34:CYS:N	2.93	0.41
1:A:443:LEU:HB2	1:A:501:LEU:HD21	2.03	0.41
1:A:541:ILE:CD1	1:A:577:ILE:HD11	2.51	0.41
1:A:825:ILE:O	1:A:828:ALA:N	2.49	0.41
1:A:839:ARG:O	1:A:842:VAL:HB	2.21	0.41
1:A:1116:LEU:H	1:A:1308:THR:CG2	2.18	0.41
1:A:1120:LEU:HD12	1:A:1120:LEU:N	2.36	0.41
1:A:1187:GLN:HG3	1:A:1188:GLN:H	1.85	0.41
1:A:1419:ASP:OD1	1:A:1426:GLU:OE1	2.39	0.41
1:A:1427:ASN:O	1:A:1430:LEU:N	2.43	0.41
2:B:293:PRO:CG	2:B:296:GLU:OE1	2.68	0.41
2:B:311:LEU:O	2:B:312:GLU:C	2.64	0.41
2:B:599:THR:O	2:B:603:LEU:HB2	2.20	0.41
2:B:642:ASP:C	2:B:644:GLU:N	2.79	0.41
3:C:8:VAL:HG12	3:C:10:ILE:H	1.86	0.41
3:C:229:TYR:CD1	3:C:229:TYR:N	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:50:LEU:HD11	7:G:4:ILE:CG1	2.51	0.41
5:E:66:GLU:HA	5:E:69:ILE:HD12	2.02	0.41
5:E:211:TYR:N	5:E:211:TYR:HD1	2.19	0.41
7:G:5:LYS:HG3	7:G:7:LEU:HD21	2.02	0.41
9:I:86:PHE:HB2	9:I:87:GLN:H	1.67	0.41
10:J:57:ILE:CG2	10:J:58:GLU:N	2.84	0.41
1:A:7:SER:HB2	2:B:1175:LEU:HD22	2.02	0.41
1:A:24:PRO:HG2	1:A:25:GLU:OE1	2.20	0.41
1:A:208:LEU:O	1:A:209:ASN:C	2.64	0.41
1:A:582:ILE:HA	1:A:583:PRO:HD2	1.84	0.41
1:A:653:VAL:O	1:A:654:ASN:C	2.63	0.41
1:A:883:LEU:HA	1:A:883:LEU:HD23	1.87	0.41
2:B:114:PRO:CG	2:B:115:GLN:H	2.25	0.41
2:B:360:PHE:CE2	2:B:361:LEU:HB2	2.55	0.41
2:B:824:ILE:HG22	2:B:1087:PHE:CE2	2.55	0.41
4:D:173:HIS:NE2	4:D:201:LYS:NZ	2.68	0.41
5:E:14:ARG:C	5:E:16:PHE:N	2.77	0.41
7:G:97:HIS:CD2	7:G:97:HIS:N	2.89	0.41
8:H:3:ASN:HB3	8:H:4:THR:H	1.61	0.41
8:H:96:VAL:HA	8:H:142:LEU:O	2.21	0.41
8:H:104:PHE:HZ	8:H:135:LEU:O	2.04	0.41
9:I:45:ARG:HE	9:I:47:GLU:HG3	1.85	0.41
13:S:308:PHE:O	13:S:309:SER:CB	2.69	0.41
1:A:35:ILE:HD12	1:A:241:VAL:CG2	2.50	0.41
1:A:206:GLU:O	1:A:207:ILE:C	2.64	0.41
1:A:218:ASP:HA	1:A:221:SER:OG	2.21	0.41
1:A:274:ILE:C	1:A:276:LEU:N	2.77	0.41
1:A:310:GLY:C	1:A:312:PRO:HD2	2.45	0.41
1:A:420:ARG:O	1:A:424:ILE:HG13	2.21	0.41
1:A:519:PRO:HG2	1:A:624:SER:C	2.46	0.41
1:A:556:TRP:CD2	1:A:558:GLY:HA2	2.55	0.41
1:A:562:THR:HA	1:A:563:PRO:HD3	1.84	0.41
1:A:971:PHE:N	1:A:971:PHE:CD1	2.88	0.41
1:A:996:ASN:CA	1:A:998:LEU:HD12	2.51	0.41
1:A:1027:ALA:O	1:A:1030:ARG:N	2.54	0.41
1:A:1114:PRO:O	1:A:1115:SER:O	2.38	0.41
1:A:1123:GLY:O	1:A:1124:HIS:C	2.63	0.41
1:A:1308:THR:OG1	1:A:1309:ASP:N	2.53	0.41
1:A:1451:VAL:O	1:A:1453:TYR:N	2.54	0.41
2:B:23:ALA:CB	2:B:24:PRO:HD2	2.31	0.41
2:B:37:PHE:CD1	2:B:37:PHE:C	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:90:ILE:HD11	2:B:432:MET:SD	2.60	0.41
2:B:102:VAL:O	2:B:109:THR:HG23	2.21	0.41
2:B:408:LEU:O	2:B:412:LEU:HG	2.21	0.41
2:B:455:SER:O	2:B:456:GLY:C	2.64	0.41
2:B:535:LEU:HA	2:B:535:LEU:HD23	1.87	0.41
2:B:570:VAL:HA	2:B:571:PRO:HD2	1.78	0.41
2:B:635:ARG:HH11	2:B:635:ARG:CG	2.33	0.41
2:B:792:MET:O	2:B:793:ALA:HB2	2.20	0.41
2:B:857:ARG:O	2:B:858:SER:HB3	2.21	0.41
2:B:1004:GLU:CB	2:B:1006:ILE:HD11	2.51	0.41
2:B:1142:GLY:O	2:B:1144:ALA:N	2.54	0.41
2:B:1145:SER:O	2:B:1146:PHE:C	2.63	0.41
2:B:1152:MET:O	2:B:1154:ALA:N	2.54	0.41
2:B:1170:THR:O	2:B:1171:VAL:C	2.64	0.41
3:C:69:LEU:H	3:C:69:LEU:CD1	2.32	0.41
3:C:143:LEU:C	3:C:143:LEU:CD1	2.94	0.41
4:D:34:GLN:O	4:D:47:LEU:HD23	2.21	0.41
4:D:47:LEU:CD1	7:G:3:PHE:HD2	2.33	0.41
5:E:24:LYS:CG	5:E:25:ASP:N	2.84	0.41
5:E:112:TYR:HE1	5:E:136:ASN:HD22	1.69	0.41
6:F:106:PRO:HG2	7:G:18:PHE:C	2.46	0.41
7:G:39:THR:HB	7:G:42:PHE:H	1.86	0.41
7:G:62:LEU:HB3	7:G:63:PRO:CD	2.50	0.41
10:J:13:VAL:C	10:J:14:VAL:HG23	2.45	0.41
10:J:18:TRP:HA	10:J:18:TRP:HE3	1.85	0.41
10:J:21:TYR:HB2	10:J:39:LEU:CD1	2.51	0.41
11:K:27:ALA:HB1	11:K:28:PRO:HD2	2.03	0.41
12:L:60:ARG:CG	12:L:61:THR:H	2.29	0.41
1:A:7:SER:CB	2:B:1175:LEU:HD22	2.51	0.41
1:A:53:LEU:HD23	1:A:53:LEU:C	2.42	0.41
1:A:90:VAL:HG12	1:A:91:PHE:O	2.20	0.41
1:A:113:LEU:HD23	1:A:113:LEU:HA	1.96	0.41
1:A:704:ALA:O	1:A:705:LYS:CB	2.66	0.41
1:A:967:ALA:HA	1:A:1044:TRP:CZ3	2.56	0.41
1:A:982:THR:C	1:A:984:LYS:N	2.77	0.41
1:A:1072:ILE:O	1:A:1075:PRO:CG	2.66	0.41
1:A:1142:THR:O	1:A:1145:SER:OG	2.27	0.41
1:A:1191:TRP:CE3	1:A:1191:TRP:HA	2.56	0.41
1:A:1217:LYS:C	1:A:1219:THR:H	2.28	0.41
1:A:1318:THR:HB	5:E:141:VAL:HG11	2.03	0.41
2:B:212:LEU:HD23	2:B:212:LEU:HA	1.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:351:TYR:O	2:B:355:ILE:HG13	2.20	0.41
2:B:483:LEU:HD12	2:B:484:ASN:N	2.35	0.41
2:B:1168:LEU:HB2	2:B:1170:THR:OG1	2.21	0.41
3:C:27:LEU:HA	3:C:228:PHE:CE2	2.56	0.41
5:E:59:SER:O	5:E:60:PHE:HB3	2.21	0.41
11:K:65:HIS:NE2	11:K:67:PHE:CG	2.88	0.41
13:S:258:GLY:O	13:S:259:ALA:O	2.38	0.41
1:A:470:LEU:C	1:A:470:LEU:HD12	2.46	0.40
1:A:599:SER:HA	1:A:600:PRO:HD2	1.86	0.40
1:A:677:ARG:C	1:A:679:ILE:N	2.78	0.40
1:A:706:HIS:CD2	1:A:706:HIS:H	2.38	0.40
1:A:723:ASN:O	1:A:724:GLU:C	2.64	0.40
1:A:848:ILE:O	1:A:1065:GLY:N	2.39	0.40
1:A:1037:LEU:N	1:A:1037:LEU:HD23	2.36	0.40
1:A:1061:GLY:O	1:A:1062:GLU:C	2.64	0.40
1:A:1147:THR:HG22	1:A:1148:ILE:N	2.36	0.40
1:A:1161:THR:CG2	1:A:1163:ILE:HG13	2.51	0.40
1:A:1165:GLU:H	1:A:1165:GLU:HG3	1.58	0.40
2:B:57:TYR:O	2:B:58:THR:C	2.63	0.40
2:B:121:ASN:HA	2:B:207:GLY:CA	2.51	0.40
2:B:222:ILE:O	2:B:240:ILE:HG13	2.21	0.40
2:B:329:THR:O	2:B:332:ASP:HB3	2.21	0.40
2:B:1023:VAL:O	2:B:1027:ILE:N	2.50	0.40
5:E:124:VAL:HA	5:E:132:ILE:CD1	2.47	0.40
5:E:124:VAL:HB	5:E:125:PRO:CD	2.50	0.40
5:E:137:GLU:C	5:E:139:ALA:H	2.29	0.40
7:G:1:MET:SD	7:G:1:MET:C	3.04	0.40
1:A:423:ASP:CG	1:A:424:ILE:H	2.29	0.40
1:A:445:ASN:HB2	1:A:455:MET:HG2	2.03	0.40
1:A:455:MET:HE1	2:B:1134:GLU:HB3	2.02	0.40
1:A:477:PRO:HG3	1:A:521:MET:HG2	2.03	0.40
1:A:626:ASN:HB3	1:A:627:GLY:H	1.71	0.40
1:A:639:PRO:HG2	1:A:640:GLN:H	1.85	0.40
1:A:901:LEU:HD22	1:A:919:ILE:HG22	1.99	0.40
1:A:989:GLY:C	1:A:991:LYS:H	2.29	0.40
1:A:1004:ASN:HD22	5:E:167:ARG:HD2	1.78	0.40
1:A:1067:LEU:HD12	1:A:1067:LEU:C	2.46	0.40
1:A:1164:PRO:C	1:A:1166:ASP:N	2.79	0.40
1:A:1211:GLN:O	1:A:1214:GLU:HB2	2.21	0.40
1:A:1327:ILE:HG22	5:E:147:HIS:HE1	1.85	0.40
2:B:38:PHE:CE2	2:B:43:LEU:HD23	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:114:PRO:HG3	2:B:194:GLU:HG3	2.03	0.40
2:B:382:ILE:O	2:B:383:ASN:C	2.63	0.40
2:B:508:LEU:HB3	2:B:510:LYS:N	2.25	0.40
2:B:796:LEU:HD12	2:B:796:LEU:HA	1.82	0.40
2:B:842:ASN:O	2:B:846:ILE:HG13	2.21	0.40
2:B:847:ASP:O	2:B:849:GLY:N	2.55	0.40
2:B:873:THR:CG2	2:B:874:PHE:N	2.84	0.40
2:B:903:VAL:O	2:B:948:ILE:HG23	2.21	0.40
2:B:1109:GLY:O	2:B:1110:PRO:C	2.64	0.40
2:B:1187:ASN:HD21	2:B:1190:ASP:HB3	1.86	0.40
3:C:80:LEU:CD1	3:C:95:CYS:CA	2.99	0.40
4:D:25:ALA:C	4:D:27:LEU:H	2.29	0.40
5:E:144:ILE:H	5:E:144:ILE:HG12	1.68	0.40
5:E:153:HIS:HB3	5:E:196:VAL:HG13	1.99	0.40
6:F:88:TYR:H	6:F:88:TYR:HD1	1.67	0.40
7:G:132:SER:O	7:G:134:GLU:N	2.54	0.40
8:H:47:PHE:CD2	8:H:95:TYR:HD1	2.39	0.40
9:I:34:TYR:HE2	9:I:36:GLU:CB	2.32	0.40
10:J:57:ILE:O	10:J:58:GLU:C	2.63	0.40
13:S:282:TYR:O	13:S:282:TYR:CG	2.73	0.40
1:A:34:LYS:HD3	1:A:34:LYS:H	1.86	0.40
1:A:135:PHE:O	1:A:137:ALA:N	2.54	0.40
1:A:515:GLN:HB2	1:A:1071:SER:HB3	2.02	0.40
1:A:532:ARG:NH2	1:A:745:GLN:HG2	2.36	0.40
1:A:1019:CYS:O	1:A:1022:LEU:CB	2.68	0.40
1:A:1212:VAL:O	1:A:1213:GLY:C	2.63	0.40
1:A:1438:THR:CG2	2:B:1144:ALA:HB3	2.51	0.40
2:B:213:ILE:HD13	2:B:213:ILE:HA	1.81	0.40
2:B:496:ARG:HB3	2:B:496:ARG:NH1	2.30	0.40
2:B:515:HIS:HD2	2:B:517:THR:N	2.12	0.40
2:B:996:ARG:HH22	3:C:175:ALA:CA	2.34	0.40
2:B:1034:VAL:CG1	2:B:1035:ALA:N	2.78	0.40
2:B:1039:GLY:HA2	10:J:51:LEU:CD2	2.50	0.40
2:B:1072:MET:HE2	2:B:1085:ILE:HB	2.02	0.40
2:B:1194:ILE:HD12	2:B:1196:ILE:CG2	2.52	0.40
2:B:1216:LEU:C	2:B:1217:TYR:HD1	2.28	0.40
3:C:41:ILE:HA	3:C:42:PRO:HD3	1.84	0.40
3:C:43:THR:CG2	3:C:44:LEU:H	2.34	0.40
4:D:29:LEU:O	4:D:30:GLY:O	2.39	0.40
4:D:188:ALA:O	4:D:191:ALA:N	2.55	0.40
5:E:60:PHE:HE2	5:E:80:VAL:CB	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:82:THR:HA	6:F:83:PRO:HD3	1.82	0.40
7:G:5:LYS:CG	7:G:7:LEU:HD21	2.51	0.40
7:G:154:VAL:HB	7:G:155:SER:H	1.71	0.40
10:J:13:VAL:HG12	10:J:14:VAL:H	1.86	0.40
10:J:47:ARG:HH11	10:J:47:ARG:HG2	1.85	0.40
12:L:32:ALA:HB3	12:L:55:ILE:CG1	2.52	0.40
1:A:254:GLU:H	2:B:935:ARG:HH22	1.70	0.40
1:A:493:GLN:HE21	1:A:493:GLN:CA	2.33	0.40
1:A:757:ASN:O	1:A:761:MET:HG3	2.20	0.40
1:A:899:VAL:HB	1:A:929:LEU:CD1	2.25	0.40
1:A:932:GLU:HG3	1:A:936:LEU:HD21	2.02	0.40
1:A:1336:MET:CE	1:A:1381:LEU:HG	2.52	0.40
2:B:187:SER:O	2:B:188:ASP:C	2.64	0.40
2:B:216:GLU:HB2	2:B:406:LEU:CD2	2.51	0.40
2:B:236:HIS:HE1	2:B:389:ALA:HA	1.83	0.40
2:B:349:ILE:O	2:B:349:ILE:HG22	2.20	0.40
2:B:530:GLY:O	2:B:532:ALA:N	2.54	0.40
2:B:763:GLN:OE1	13:S:292:PRO:HB3	2.21	0.40
2:B:936:ASP:OD2	2:B:938:SER:OG	2.38	0.40
2:B:1013:ASN:OD1	2:B:1014:PRO:HD2	2.21	0.40
2:B:1183:LYS:HA	2:B:1186:ASP:HA	2.04	0.40
3:C:75:MET:HE3	3:C:75:MET:HB2	1.82	0.40
4:D:50:LEU:HD11	7:G:4:ILE:HG13	2.03	0.40
4:D:52:LEU:O	4:D:54:GLU:N	2.46	0.40
5:E:37:LEU:HA	5:E:38:PRO:HD2	1.94	0.40
6:F:97:ARG:O	6:F:100:GLN:N	2.54	0.40
6:F:99:LEU:HD21	7:G:66:GLY:N	2.37	0.40
7:G:13:LEU:HD12	7:G:26:LEU:HD21	2.03	0.40
9:I:55:THR:HG1	9:I:100:PHE:HD2	1.55	0.40
10:J:21:TYR:HB2	10:J:39:LEU:HD13	2.02	0.40
1:A:356:ASP:C	1:A:358:ASN:N	2.80	0.40
1:A:461:LYS:O	1:A:463:ILE:HG23	2.22	0.40
1:A:501:LEU:HD11	2:B:1146:PHE:CE2	2.56	0.40
1:A:599:SER:HB2	1:A:603:ASN:H	1.87	0.40
1:A:867:ILE:HG22	1:A:871:ASP:H	1.85	0.40
1:A:1116:LEU:O	1:A:1116:LEU:HG	2.22	0.40
1:A:1138:ILE:CG2	1:A:1316:VAL:HG13	2.52	0.40
2:B:179:CYS:O	2:B:180:TYR:C	2.65	0.40
2:B:240:ILE:CG2	2:B:240:ILE:O	2.68	0.40
2:B:418:LYS:O	2:B:419:THR:C	2.64	0.40
2:B:516:ASN:HD22	2:B:516:ASN:H	1.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:533:CYS:SG	2:B:534:GLY:N	2.95	0.40
2:B:628:THR:O	2:B:629:ASP:C	2.65	0.40
2:B:800:GLN:CB	10:J:52:THR:CG2	2.98	0.40
2:B:1192:TYR:CD1	2:B:1192:TYR:N	2.89	0.40
5:E:93:MET:O	5:E:96:PHE:N	2.55	0.40
11:K:20:LYS:HB2	11:K:20:LYS:HE3	1.89	0.40
12:L:61:THR:HG22	12:L:63:ARG:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1418/1733 (82%)	914 (64%)	316 (22%)	188 (13%)	0	3
2	B	1096/1224 (90%)	726 (66%)	223 (20%)	147 (13%)	0	3
3	C	264/318 (83%)	169 (64%)	62 (24%)	33 (12%)	0	4
4	D	173/221 (78%)	129 (75%)	27 (16%)	17 (10%)	0	7
5	E	212/215 (99%)	141 (66%)	50 (24%)	21 (10%)	0	7
6	F	82/155 (53%)	60 (73%)	15 (18%)	7 (8%)	0	9
7	G	169/171 (99%)	123 (73%)	34 (20%)	12 (7%)	1	12
8	H	129/146 (88%)	93 (72%)	26 (20%)	10 (8%)	1	11
9	I	117/122 (96%)	80 (68%)	22 (19%)	15 (13%)	0	3
10	J	63/70 (90%)	36 (57%)	14 (22%)	13 (21%)	0	1
11	K	112/120 (93%)	82 (73%)	25 (22%)	5 (4%)	2	18
12	L	44/70 (63%)	18 (41%)	14 (32%)	12 (27%)	0	0
13	S	68/179 (38%)	51 (75%)	10 (15%)	7 (10%)	0	6
All	All	3947/4744 (83%)	2622 (66%)	838 (21%)	487 (12%)	0	4

All (487) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	48	ALA
1	A	55	ASP
1	A	58	LEU
1	A	62	ASP
1	A	70	CYS
1	A	73	GLY
1	A	76	GLU
1	A	93	VAL
1	A	130	ASP
1	A	286	HIS
1	A	311	GLN
1	A	322	VAL
1	A	385	ILE
1	A	399	HIS
1	A	423	ASP
1	A	516	SER
1	A	525	GLN
1	A	536	LEU
1	A	567	LYS
1	A	583	PRO
1	A	626	ASN
1	A	709	THR
1	A	780	VAL
1	A	821	ARG
1	A	920	LEU
1	A	1002	GLY
1	A	1036	ARG
1	A	1115	SER
1	A	1122	PRO
1	A	1124	HIS
1	A	1165	GLU
1	A	1167	GLU
1	A	1212	VAL
1	A	1223	ASP
1	A	1231	ASP
1	A	1242	VAL
1	A	1281	ARG
1	A	1308	THR
1	A	1309	ASP
1	A	1335	ILE
1	A	1341	ILE

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Mol	Chain	Res	Type
1	A	1366	ARG
1	A	1377	THR
1	A	1378	GLN
1	A	1386	ARG
1	A	1392	SER
1	A	1396	ALA
1	A	1397	LEU
1	A	1403	GLU
1	A	1405	THR
1	A	1424	VAL
2	B	43	LEU
2	B	45	SER
2	B	58	THR
2	B	67	SER
2	B	108	VAL
2	B	124	TYR
2	B	186	GLU
2	B	219	ALA
2	B	261	ARG
2	B	367	LEU
2	B	391	ASP
2	B	466	TRP
2	B	467	GLY
2	B	468	GLU
2	B	474	SER
2	B	510	LYS
2	B	530	GLY
2	B	531	GLN
2	B	571	PRO
2	B	591	ARG
2	B	620	ARG
2	B	629	ASP
2	B	636	PRO
2	B	643	ASP
2	B	648	HIS
2	B	709	ASP
2	B	727	LYS
2	B	731	VAL
2	B	751	VAL
2	B	752	ALA
2	B	818	PRO
2	B	901	PRO

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Mol	Chain	Res	Type
2	B	943	SER
2	B	958	GLN
2	B	992	ILE
2	B	1046	PRO
2	B	1108	ARG
2	B	1157	ALA
2	B	1167	GLY
2	B	1171	VAL
2	B	1175	LEU
2	B	1181	GLU
2	B	1188	LYS
2	B	1211	ASN
3	C	10	ILE
3	C	60	ASP
3	C	81	GLU
3	C	83	SER
3	C	87	PHE
3	C	110	THR
3	C	149	LYS
3	C	167	HIS
3	C	175	ALA
3	C	184	ASN
3	C	213	PRO
3	C	214	ASN
3	C	215	GLU
3	C	216	GLY
4	D	12	ARG
4	D	15	LEU
4	D	20	GLU
4	D	152	SER
5	E	130	ALA
5	E	158	SER
6	F	81	THR
7	G	118	ASP
8	H	81	PRO
8	H	84	ALA
8	H	140	ALA
9	I	9	ASP
9	I	11	ASN
9	I	84	VAL
10	J	6	ARG
10	J	15	GLY

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Mol	Chain	Res	Type
10	J	53	HIS
10	J	64	ASN
12	L	50	ASP
12	L	53	HIS
12	L	59	ALA
12	L	60	ARG
13	S	275	LYS
13	S	292	PRO
1	A	42	ASP
1	A	44	THR
1	A	45	GLN
1	A	54	ASN
1	A	57	ARG
1	A	61	ILE
1	A	74	MET
1	A	79	GLY
1	A	111	GLY
1	A	126	LEU
1	A	131	SER
1	A	154	SER
1	A	219	PHE
1	A	223	GLY
1	A	244	PRO
1	A	290	GLU
1	A	317	LYS
1	A	318	SER
1	A	331	GLY
1	A	332	LYS
1	A	335	ARG
1	A	400	PRO
1	A	415	LEU
1	A	418	SER
1	A	419	LYS
1	A	424	ILE
1	A	473	SER
1	A	557	ASP
1	A	594	GLY
1	A	598	LEU
1	A	619	LYS
1	A	708	MET
1	A	716	ASP
1	A	720	ARG

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Mol	Chain	Res	Type
1	A	738	LYS
1	A	760	GLN
1	A	765	VAL
1	A	775	ILE
1	A	824	LEU
1	A	846	GLU
1	A	847	ASP
1	A	859	SER
1	A	864	ILE
1	A	875	ALA
1	A	929	LEU
1	A	968	GLN
1	A	979	SER
1	A	1006	ILE
1	A	1016	THR
1	A	1052	GLN
1	A	1084	PHE
1	A	1089	VAL
1	A	1104	ILE
1	A	1105	LEU
1	A	1126	ALA
1	A	1128	GLN
1	A	1164	PRO
1	A	1168	GLU
1	A	1169	ILE
1	A	1170	ILE
1	A	1224	LEU
1	A	1314	SER
1	A	1365	TYR
1	A	1376	THR
2	B	21	GLU
2	B	46	GLN
2	B	65	GLU
2	B	68	THR
2	B	114	PRO
2	B	229	ALA
2	B	258	LEU
2	B	260	GLY
2	B	266	ALA
2	B	294	ASP
2	B	322	PHE
2	B	504	ARG

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Mol	Chain	Res	Type
2	B	509	ALA
2	B	526	GLU
2	B	534	GLY
2	B	559	SER
2	B	605	ARG
2	B	613	VAL
2	B	641	GLU
2	B	810	GLU
2	B	867	GLY
2	B	869	SER
2	B	880	THR
2	B	881	ASN
2	B	891	ASP
2	B	902	GLY
2	B	903	VAL
2	B	907	GLY
2	B	1018	PRO
2	B	1041	GLU
2	B	1096	ARG
2	B	1099	VAL
2	B	1150	ARG
2	B	1156	ASP
2	B	1170	THR
2	B	1183	LYS
2	B	1186	ASP
2	B	1190	ASP
3	C	74	SER
3	C	141	GLY
3	C	161	LYS
4	D	6	SER
4	D	8	PHE
4	D	16	LYS
4	D	19	GLU
4	D	30	GLY
4	D	199	ASN
4	D	218	GLU
5	E	36	GLU
5	E	45	LYS
5	E	59	SER
5	E	106	GLN
5	E	145	THR
5	E	189	GLY

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Mol	Chain	Res	Type
5	E	206	GLY
6	F	131	PRO
7	G	83	LYS
7	G	154	VAL
8	H	59	ILE
8	H	77	ARG
8	H	82	PRO
8	H	108	SER
8	H	128	ASN
9	I	3	THR
9	I	34	TYR
9	I	62	ILE
9	I	89	GLN
9	I	106	CYS
9	I	107	SER
10	J	2	ILE
10	J	62	ARG
11	K	37	LYS
11	K	103	THR
12	L	43	THR
12	L	51	CYS
12	L	56	LEU
13	S	259	ALA
1	A	59	GLY
1	A	66	LYS
1	A	89	PRO
1	A	124	GLN
1	A	167	CYS
1	A	283	GLY
1	A	394	ASN
1	A	396	PRO
1	A	517	ASN
1	A	543	LEU
1	A	592	ASP
1	A	640	GLN
1	A	647	GLY
1	A	707	GLY
1	A	731	ARG
1	A	774	ARG
1	A	903	ASN
1	A	1017	LEU
1	A	1060	PRO

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Mol	Chain	Res	Type
1	A	1062	GLU
1	A	1131	ALA
1	A	1221	LYS
1	A	1229	SER
1	A	1452	LYS
2	B	115	GLN
2	B	131	ASP
2	B	176	SER
2	B	206	ASN
2	B	295	GLY
2	B	308	TRP
2	B	334	ILE
2	B	365	THR
2	B	369	GLY
2	B	469	GLN
2	B	480	SER
2	B	551	PRO
2	B	598	GLU
2	B	645	SER
2	B	682	SER
2	B	688	GLY
2	B	711	GLU
2	B	712	PRO
2	B	738	PHE
2	B	761	HIS
2	B	792	MET
2	B	822	ASN
2	B	996	ARG
2	B	1017	ILE
2	B	1153	GLU
2	B	1155	SER
2	B	1189	ILE
3	C	6	PRO
3	C	28	ALA
3	C	91	HIS
3	C	169	LYS
3	C	202	PRO
3	C	212	PRO
3	C	218	PRO
3	C	264	GLN
4	D	52	LEU
5	E	8	ASN

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Mol	Chain	Res	Type
5	E	44	ALA
5	E	56	LYS
5	E	74	ASP
5	E	192	ARG
7	G	17	PHE
7	G	139	ILE
7	G	147	ILE
9	I	7	CYS
9	I	113	ASP
10	J	22	LEU
12	L	35	SER
12	L	49	LYS
13	S	295	THR
1	A	35	ILE
1	A	67	CYS
1	A	100	LYS
1	A	196	GLU
1	A	253	ASN
1	A	312	PRO
1	A	465	TYR
1	A	526	ASP
1	A	605	MET
1	A	986	ILE
1	A	1040	GLN
1	A	1139	GLU
1	A	1206	ASP
1	A	1266	THR
1	A	1280	GLU
1	A	1302	PRO
2	B	387	LEU
2	B	409	ALA
2	B	430	ARG
2	B	754	SER
2	B	848	ARG
2	B	884	ARG
2	B	946	ASN
2	B	1029	CYS
2	B	1143	ALA
2	B	1178	ASN
2	B	1202	LEU
3	C	90	ASP
3	C	198	ALA

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Mol	Chain	Res	Type
3	C	227	THR
3	C	240	VAL
4	D	131	GLU
4	D	168	LYS
5	E	73	PRO
5	E	115	ASN
6	F	73	ALA
6	F	112	GLU
7	G	133	SER
8	H	92	ASP
9	I	32	CYS
9	I	73	ARG
9	I	86	PHE
9	I	95	THR
10	J	9	SER
10	J	29	GLU
10	J	51	LEU
10	J	63	TYR
11	K	64	GLU
12	L	42	ARG
13	S	288	SER
1	A	84	ILE
1	A	197	PRO
1	A	696	GLU
1	A	759	ALA
1	A	789	LYS
1	A	795	GLU
1	A	808	LEU
1	A	817	ALA
1	A	958	VAL
1	A	1160	SER
1	A	1188	GLN
1	A	1435	PRO
2	B	22	SER
2	B	56	ASP
2	B	368	GLU
2	B	483	LEU
2	B	490	SER
2	B	565	PRO
2	B	878	GLN
2	B	879	ARG
2	B	883	LEU

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Mol	Chain	Res	Type
2	B	1019	SER
2	B	1100	ASP
3	C	148	ARG
4	D	27	LEU
4	D	142	LYS
5	E	40	GLU
5	E	172	GLU
5	E	183	PRO
6	F	108	PHE
7	G	30	LEU
7	G	124	GLY
7	G	165	GLU
8	H	52	GLN
11	K	70	ARG
13	S	277	LYS
13	S	293	LEU
1	A	599	SER
1	A	641	VAL
1	A	719	VAL
1	A	1162	VAL
1	A	1338	VAL
2	B	171	PRO
2	B	282	ILE
2	B	450	ALA
2	B	543	SER
2	B	694	ASP
2	B	758	PHE
2	B	906	SER
2	B	1103	ILE
2	B	1118	PRO
3	C	126	GLY
3	C	171	GLY
4	D	201	LYS
6	F	139	PRO
10	J	18	TRP
12	L	26	THR
12	L	46	VAL
1	A	507	VAL
1	A	1057	VAL
2	B	635	ARG
3	C	142	VAL
6	F	93	ILE

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Mol	Chain	Res	Type
1	A	9	ALA
1	A	653	VAL
1	A	886	ILE
1	A	963	ILE
1	A	1158	PRO
2	B	985	GLY
5	E	37	LEU
7	G	63	PRO
1	A	392	VAL
1	A	673	GLY
1	A	1379	GLY
2	B	410	GLY
2	B	502	ILE
2	B	552	MET
2	B	974	PRO
1	A	250	ILE
1	A	649	ILE
1	A	1031	VAL
10	J	14	VAL
11	K	43	GLY
1	A	357	PRO
1	A	1061	GLY
2	B	575	PRO
7	G	157	ILE
5	E	129	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1246/1520 (82%)	1116 (90%)	130 (10%)	7	26
2	B	964/1061 (91%)	866 (90%)	98 (10%)	7	27
3	C	234/274 (85%)	207 (88%)	27 (12%)	5	23
4	D	140/200 (70%)	121 (86%)	19 (14%)	3	18
5	E	196/197 (100%)	183 (93%)	13 (7%)	15	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	74/137 (54%)	65 (88%)	9 (12%)	5	21
7	G	152/152 (100%)	143 (94%)	9 (6%)	18	43
8	H	117/128 (91%)	112 (96%)	5 (4%)	26	50
9	I	113/116 (97%)	99 (88%)	14 (12%)	4	21
10	J	60/65 (92%)	57 (95%)	3 (5%)	22	47
11	K	99/102 (97%)	90 (91%)	9 (9%)	9	32
12	L	40/57 (70%)	34 (85%)	6 (15%)	3	16
13	S	62/156 (40%)	52 (84%)	10 (16%)	2	14
All	All	3497/4165 (84%)	3145 (90%)	352 (10%)	7	27

All (352) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	13	THR
1	A	14	VAL
1	A	18	GLN
1	A	30	ILE
1	A	34	LYS
1	A	41	MET
1	A	54	ASN
1	A	62	ASP
1	A	93	VAL
1	A	108	MET
1	A	195	ASP
1	A	208	LEU
1	A	215	SER
1	A	220	THR
1	A	227	VAL
1	A	270	LEU
1	A	308	ILE
1	A	326	ARG
1	A	329	LEU
1	A	335	ARG
1	A	348	SER
1	A	354	SER
1	A	364	VAL
1	A	370	ILE
1	A	375	THR

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Mol	Chain	Res	Type
1	A	381	THR
1	A	385	ILE
1	A	406	ILE
1	A	408	ASP
1	A	425	GLN
1	A	434	ARG
1	A	443	LEU
1	A	445	ASN
1	A	450	LEU
1	A	451	HIS
1	A	454	SER
1	A	460	VAL
1	A	461	LYS
1	A	466	SER
1	A	469	ARG
1	A	481	ASP
1	A	487	MET
1	A	489	LEU
1	A	493	GLN
1	A	497	THR
1	A	498	ARG
1	A	501	LEU
1	A	503	GLN
1	A	505	CYS
1	A	518	LYS
1	A	523	ILE
1	A	524	VAL
1	A	560	ILE
1	A	562	THR
1	A	596	THR
1	A	618	GLU
1	A	629	LEU
1	A	648	ASN
1	A	652	VAL
1	A	666	ILE
1	A	718	VAL
1	A	734	GLU
1	A	739	ASP
1	A	740	LEU
1	A	754	SER
1	A	762	SER
1	A	786	HIS

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Mol	Chain	Res	Type
1	A	791	ASP
1	A	795	GLU
1	A	821	ARG
1	A	829	VAL
1	A	830	LYS
1	A	831	THR
1	A	833	GLU
1	A	845	LEU
1	A	852	TYR
1	A	854	ASN
1	A	858	ASN
1	A	867	ILE
1	A	879	GLU
1	A	886	ILE
1	A	890	ASP
1	A	897	TYR
1	A	920	LEU
1	A	929	LEU
1	A	936	LEU
1	A	949	ASP
1	A	969	GLN
1	A	1029	ARG
1	A	1035	TYR
1	A	1037	LEU
1	A	1048	ASN
1	A	1050	GLU
1	A	1052	GLN
1	A	1058	VAL
1	A	1081	LEU
1	A	1082	ASN
1	A	1110	ASN
1	A	1111	MET
1	A	1114	PRO
1	A	1116	LEU
1	A	1117	THR
1	A	1122	PRO
1	A	1127	ASP
1	A	1136	SER
1	A	1142	THR
1	A	1155	ASP
1	A	1166	ASP
1	A	1236	LEU

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Mol	Chain	Res	Type
1	A	1242	VAL
1	A	1264	GLU
1	A	1271	ILE
1	A	1274	ARG
1	A	1276	VAL
1	A	1291	VAL
1	A	1295	THR
1	A	1297	GLU
1	A	1300	LYS
1	A	1317	MET
1	A	1325	THR
1	A	1333	ILE
1	A	1353	TYR
1	A	1358	SER
1	A	1370	LEU
1	A	1372	VAL
1	A	1376	THR
1	A	1398	MET
1	A	1445	ILE
1	A	1447	GLU
2	B	44	VAL
2	B	57	TYR
2	B	63	ILE
2	B	128	LEU
2	B	175	ARG
2	B	194	GLU
2	B	213	ILE
2	B	223	VAL
2	B	261	ARG
2	B	268	THR
2	B	286	PHE
2	B	294	ASP
2	B	298	LEU
2	B	365	THR
2	B	371	GLU
2	B	378	LEU
2	B	393	LYS
2	B	401	PHE
2	B	408	LEU
2	B	419	THR
2	B	427	ASP
2	B	429	PHE

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Mol	Chain	Res	Type
2	B	463	THR
2	B	466	TRP
2	B	476	ARG
2	B	482	VAL
2	B	485	ARG
2	B	496	ARG
2	B	498	THR
2	B	510	LYS
2	B	511	PRO
2	B	555	ILE
2	B	582	VAL
2	B	599	THR
2	B	603	LEU
2	B	615	MET
2	B	616	ILE
2	B	628	THR
2	B	629	ASP
2	B	635	ARG
2	B	636	PRO
2	B	644	GLU
2	B	658	ILE
2	B	682	SER
2	B	724	ASP
2	B	737	THR
2	B	742	GLU
2	B	743	ILE
2	B	748	ILE
2	B	751	VAL
2	B	766	ARG
2	B	807	ARG
2	B	815	ARG
2	B	830	TYR
2	B	835	GLN
2	B	839	MET
2	B	855	PHE
2	B	856	PHE
2	B	859	TYR
2	B	878	GLN
2	B	901	PRO
2	B	909	ASP
2	B	918	ILE
2	B	939	THR

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Mol	Chain	Res	Type
2	B	953	LEU
2	B	986	GLN
2	B	987	LYS
2	B	990	ILE
2	B	993	THR
2	B	997	GLU
2	B	999	MET
2	B	1002	THR
2	B	1006	ILE
2	B	1010	LEU
2	B	1017	ILE
2	B	1018	PRO
2	B	1026	LEU
2	B	1034	VAL
2	B	1047	PHE
2	B	1051	THR
2	B	1055	ILE
2	B	1076	HIS
2	B	1084	GLN
2	B	1095	LEU
2	B	1096	ARG
2	B	1103	ILE
2	B	1104	HIS
2	B	1137	CYS
2	B	1138	MET
2	B	1159	ARG
2	B	1169	MET
2	B	1170	THR
2	B	1183	LYS
2	B	1185	CYS
2	B	1202	LEU
2	B	1212	ILE
2	B	1216	LEU
2	B	1224	PHE
3	C	23	SER
3	C	44	LEU
3	C	54	ASN
3	C	55	THR
3	C	56	THR
3	C	57	VAL
3	C	58	LEU
3	C	74	SER

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Mol	Chain	Res	Type
3	C	77	ILE
3	C	89	GLU
3	C	99	LEU
3	C	100	THR
3	C	108	GLU
3	C	129	ILE
3	C	138	GLU
3	C	140	ASN
3	C	143	LEU
3	C	147	LEU
3	C	156	THR
3	C	166	GLU
3	C	186	LEU
3	C	214	ASN
3	C	233	GLU
3	C	240	VAL
3	C	245	VAL
3	C	250	THR
3	C	266	ASP
4	D	35	LEU
4	D	47	LEU
4	D	61	GLU
4	D	63	LEU
4	D	70	PHE
4	D	137	ASN
4	D	139	LYS
4	D	148	LEU
4	D	149	THR
4	D	152	SER
4	D	177	VAL
4	D	182	SER
4	D	187	THR
4	D	192	LYS
4	D	193	THR
4	D	197	SER
4	D	202	ILE
4	D	206	GLU
4	D	208	GLU
5	E	40	GLU
5	E	60	PHE
5	E	72	PHE
5	E	78	LEU

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Mol	Chain	Res	Type
5	E	83	CYS
5	E	114	ASN
5	E	132	ILE
5	E	135	PHE
5	E	169	ARG
5	E	183	PRO
5	E	207	ARG
5	E	211	TYR
5	E	212	ARG
6	F	79	ARG
6	F	81	THR
6	F	84	TYR
6	F	86	THR
6	F	90	ARG
6	F	96	THR
6	F	119	ARG
6	F	148	VAL
6	F	153	VAL
7	G	38	CYS
7	G	39	THR
7	G	49	LEU
7	G	70	PHE
7	G	78	VAL
7	G	80	LYS
7	G	96	GLN
7	G	126	ASN
7	G	171	ILE
8	H	10	PHE
8	H	86	ASP
8	H	102	TYR
8	H	130	ARG
8	H	134	ASN
9	I	6	PHE
9	I	8	ARG
9	I	9	ASP
9	I	10	CYS
9	I	13	MET
9	I	32	CYS
9	I	46	HIS
9	I	75	CYS
9	I	78	CYS
9	I	84	VAL

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Mol	Chain	Res	Type
9	I	85	PHE
9	I	100	PHE
9	I	101	PHE
9	I	106	CYS
10	J	2	ILE
10	J	46	CYS
10	J	55	ASP
11	K	10	PHE
11	K	25	THR
11	K	35	PHE
11	K	47	ARG
11	K	49	GLU
11	K	64	GLU
11	K	70	ARG
11	K	78	THR
11	K	114	LEU
12	L	33	GLU
12	L	51	CYS
12	L	55	ILE
12	L	63	ARG
12	L	65	VAL
12	L	68	GLU
13	S	263	ARG
13	S	264	SER
13	S	265	VAL
13	S	266	THR
13	S	267	ASP
13	S	283	GLN
13	S	288	SER
13	S	292	PRO
13	S	293	LEU
13	S	296	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (105) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	80	HIS
1	A	83	HIS
1	A	119	ASN
1	A	213	HIS
1	A	225	ASN

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Mol	Chain	Res	Type
1	A	256	GLN
1	A	299	HIS
1	A	316	GLN
1	A	339	ASN
1	A	390	GLN
1	A	394	ASN
1	A	435	HIS
1	A	493	GLN
1	A	503	GLN
1	A	587	HIS
1	A	611	GLN
1	A	631	HIS
1	A	659	HIS
1	A	741	ASN
1	A	742	ASN
1	A	757	ASN
1	A	760	GLN
1	A	768	GLN
1	A	786	HIS
1	A	851	HIS
1	A	858	ASN
1	A	877	HIS
1	A	903	ASN
1	A	926	GLN
1	A	1048	ASN
1	A	1070	GLN
1	A	1085	HIS
1	A	1106	ASN
1	A	1140	HIS
1	A	1173	HIS
1	A	1232	ASN
1	A	1265	ASN
1	A	1378	GLN
1	A	1432	GLN
2	B	52	ASN
2	B	60	GLN
2	B	121	ASN
2	B	178	ASN
2	B	236	HIS
2	B	325	GLN
2	B	366	GLN
2	B	465	ASN

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Mol	Chain	Res	Type
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	538	ASN
2	B	657	HIS
2	B	744	HIS
2	B	821	GLN
2	B	835	GLN
2	B	984	HIS
2	B	1015	HIS
2	B	1065	GLN
2	B	1076	HIS
2	B	1084	GLN
2	B	1117	GLN
2	B	1179	GLN
2	B	1193	GLN
3	C	65	HIS
3	C	73	GLN
3	C	79	GLN
3	C	91	HIS
3	C	112	ASN
3	C	123	ASN
3	C	167	HIS
3	C	252	GLN
4	D	39	ASN
4	D	40	HIS
4	D	41	GLN
4	D	51	ASN
4	D	137	ASN
4	D	216	ASN
5	E	101	GLN
5	E	104	ASN
5	E	114	ASN
5	E	143	ASN
5	E	147	HIS
7	G	10	ASN
7	G	14	HIS
7	G	53	ASN
7	G	57	GLN
7	G	97	HIS
7	G	102	GLN
7	G	122	ASN

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Mol	Chain	Res	Type
7	G	126	ASN
7	G	153	GLN
7	G	158	HIS
8	H	131	ASN
9	I	12	ASN
9	I	23	ASN
9	I	79	HIS
9	I	83	ASN
10	J	64	ASN
11	K	65	HIS
11	K	76	GLN
11	K	89	ASN
11	K	92	ASN
13	S	243	GLN
13	S	285	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	S	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S	269:PHE	C	270:THR	N	0.95

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	1426/1733 (82%)	-1.35	0 100 100	1, 54, 131, 183	0
2	B	1104/1224 (90%)	-1.29	0 100 100	4, 67, 147, 180	0
3	C	266/318 (83%)	-1.33	0 100 100	17, 61, 118, 143	0
4	D	177/221 (80%)	-1.30	0 100 100	23, 78, 141, 157	0
5	E	214/215 (99%)	-1.25	0 100 100	10, 93, 155, 173	0
6	F	84/155 (54%)	-1.46	0 100 100	1, 40, 79, 101	0
7	G	171/171 (100%)	-1.41	0 100 100	25, 56, 96, 113	0
8	H	133/146 (91%)	-1.12	0 100 100	60, 115, 156, 175	0
9	I	119/122 (97%)	-1.13	1 (0%) 82 62	45, 109, 153, 196	0
10	J	65/70 (92%)	-1.39	0 100 100	30, 56, 107, 124	0
11	K	114/120 (95%)	-1.32	0 100 100	21, 67, 121, 129	0
12	L	46/70 (65%)	-1.10	0 100 100	51, 117, 149, 169	0
13	S	174/179 (97%)	1.10	74 (42%) 0 1	50, 50, 110, 125	0
All	All	4093/4744 (86%)	-1.21	75 (1%) 67 46	1, 64, 141, 196	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	S	141	THR	6.9
13	S	145	HIS	5.9
13	S	218	ILE	5.5
13	S	154	LYS	5.0
13	S	230	THR	4.7
13	S	161	ALA	4.7
13	S	235	ASP	4.6
13	S	188	CYS	4.5
13	S	151	GLN	4.4

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Mol	Chain	Res	Type	RSRZ
13	S	167	PRO	4.4
13	S	158	ASP	4.2
13	S	192	GLU	4.2
13	S	143	ILE	4.0
13	S	148	LEU	3.9
13	S	233	ALA	3.9
13	S	137	ASP	3.8
13	S	164	SER	3.7
13	S	179	GLU	3.7
13	S	189	ASP	3.6
13	S	157	TYR	3.6
13	S	231	CYS	3.6
13	S	194	ALA	3.6
13	S	225	PRO	3.5
13	S	226	GLU	3.5
13	S	227	PHE	3.5
13	S	184	LYS	3.4
13	S	221	GLY	3.4
13	S	150	ASP	3.3
13	S	193	ALA	3.3
13	S	185	VAL	3.3
13	S	229	ALA	3.3
13	S	187	ASN	3.3
13	S	200	ARG	3.2
13	S	190	THR	3.2
13	S	191	ASN	3.2
13	S	228	LEU	3.2
13	S	183	ASN	3.1
13	S	155	ALA	3.0
13	S	172	LEU	3.0
13	S	203	TYR	2.9
13	S	215	LYS	2.9
9	I	120	GLN	2.8
13	S	175	ALA	2.8
13	S	136	ASN	2.8
13	S	181	GLU	2.8
13	S	186	ASN	2.8
13	S	173	HIS	2.8
13	S	138	GLY	2.8
13	S	168	PRO	2.7
13	S	171	ILE	2.7
13	S	232	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
13	S	144	TYR	2.7
13	S	178	ILE	2.6
13	S	216	HIS	2.6
13	S	182	MET	2.6
13	S	206	VAL	2.6
13	S	169	GLN	2.6
13	S	214	LEU	2.5
13	S	156	LEU	2.4
13	S	139	VAL	2.4
13	S	174	THR	2.4
13	S	159	VAL	2.4
13	S	220	ASN	2.4
13	S	201	ILE	2.4
13	S	209	LYS	2.4
13	S	234	LYS	2.4
13	S	210	ASN	2.3
13	S	211	ASN	2.3
13	S	140	ASP	2.3
13	S	204	SER	2.3
13	S	160	LEU	2.2
13	S	166	HIS	2.1
13	S	180	SER	2.1
13	S	223	ILE	2.1
13	S	177	ALA	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	MG	S	1	1/1	0.98	0.09	91,91,91,91	0
14	ZN	A	1735	1/1	1.00	0.01	15,15,15,15	0
14	ZN	B	1307	1/1	1.00	0.01	15,15,15,15	0
14	ZN	C	319	1/1	1.00	0.01	20,20,20,20	0
14	ZN	I	203	1/1	1.00	0.01	63,63,63,63	0
14	ZN	I	204	1/1	1.00	0.01	97,97,97,97	0
14	ZN	J	101	1/1	1.00	0.01	16,16,16,16	0
14	ZN	L	105	1/1	1.00	0.01	68,68,68,68	0
14	ZN	S	310	1/1	1.00	0.02	94,94,94,94	0
14	ZN	A	1734	1/1	1.00	0.01	58,58,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.