



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 05:58 am BST

PDB ID : 3I4M
Title : 8-oxoguanine containing RNA polymerase II elongation complex D
Authors : Damsma, G.E.; Cramer, P.
Deposited on : 2009-07-02
Resolution : 3.70 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

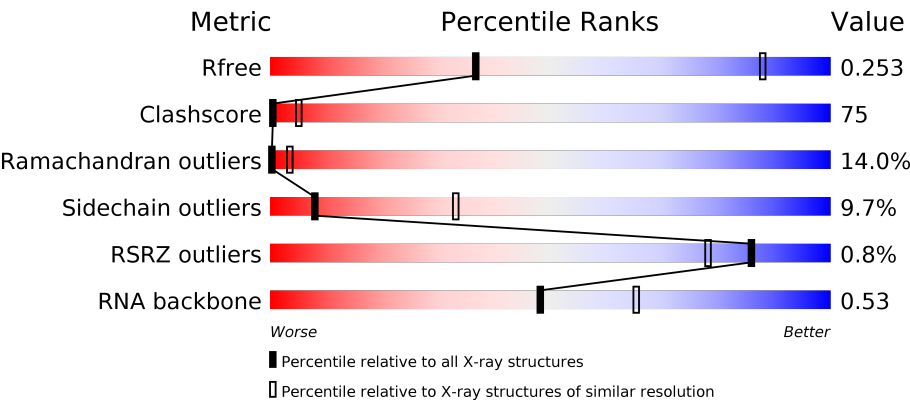
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	130704	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)
RNA backbone	3102	1027 (4.40-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	<div><div>16%</div><div>53%</div><div>13%</div><div>•</div><div>18%</div></div>
2	B	1224	<div><div>17%</div><div>58%</div><div>16%</div><div>•</div><div>8%</div></div>
3	C	324	<div><div>18%</div><div>50%</div><div>15%</div><div>•</div><div>17%</div></div>
4	D	221	<div><div>19%</div><div>51%</div><div>13%</div><div>•</div><div>15%</div></div>

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Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	T	26	
14	N	12	
15	P	16	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 32355 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 subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1429	Total	C	N	O	S	0	0	0
			11240	7079	1966	2133	62			

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1125	Total	C	N	O	S	0	0	0
			8942	5659	1571	1657	55			

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	270	Total	C	N	O	S	0	0	0
			2125	1336	353	422	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	HIS	-	EXPRESSION TAG	UNP P16370
C	-4	HIS	-	EXPRESSION TAG	UNP P16370
C	-3	HIS	-	EXPRESSION TAG	UNP P16370
C	-2	HIS	-	EXPRESSION TAG	UNP P16370
C	-1	HIS	-	EXPRESSION TAG	UNP P16370
C	0	HIS	-	EXPRESSION TAG	UNP P16370

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	187	Total	C	N	O	S	0	0	0
			1504	930	269	301	4			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

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 subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	88	Total	C	N	O	S	0	0	0
			712	455	120	134	3			

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

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 subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	137	Total	C	N	O	S	0	0	0
			1101	693	185	218	5			

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	116	Total	C	N	O	S	0	0	0
			944	581	172	181	10			

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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 subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	116	Total	C	N	O	S	0	0	0
			929	596	158	173	2			

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	47	Total	C	N	O	S	0	0	0
			370	228	73	65	4			

- Molecule 13 is a DNA chain called DNA (5'-D(*AP*G*CP*TP*CP*AP*AP*GP*TP*AP*CP*TP*TP*AP*(8OG)P*GP*CP*CP*(BRU)P*GP*GP*TP*CP*AP*TP*T)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
13	T	21	Total	Br	C	N	O	P	0	0	0
			426	1	203	75	127	20			

- Molecule 14 is a DNA chain called DNA (5'-D(*AP*GP*TP*AP*CP*TP*TP*GP*AP*GP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	11	Total	C	N	O	P	0	0	0
			224	108	42	64	10			

- Molecule 15 is a RNA chain called RNA (5'-R(*UP*GP*CP*AP*UP*C*UP*UP*CP*CP*AP*GP*GP*CP*CP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	P	10	Total	C	N	O	P	0	0	0
			205	93	33	70	9			

- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Mg	0	0
			1	1		

- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	J	1	Total	Zn	0	0
			1	1		
17	B	1	Total	Zn	0	0
			1	1		
17	I	2	Total	Zn	0	0
			2	2		
17	C	1	Total	Zn	0	0
			1	1		

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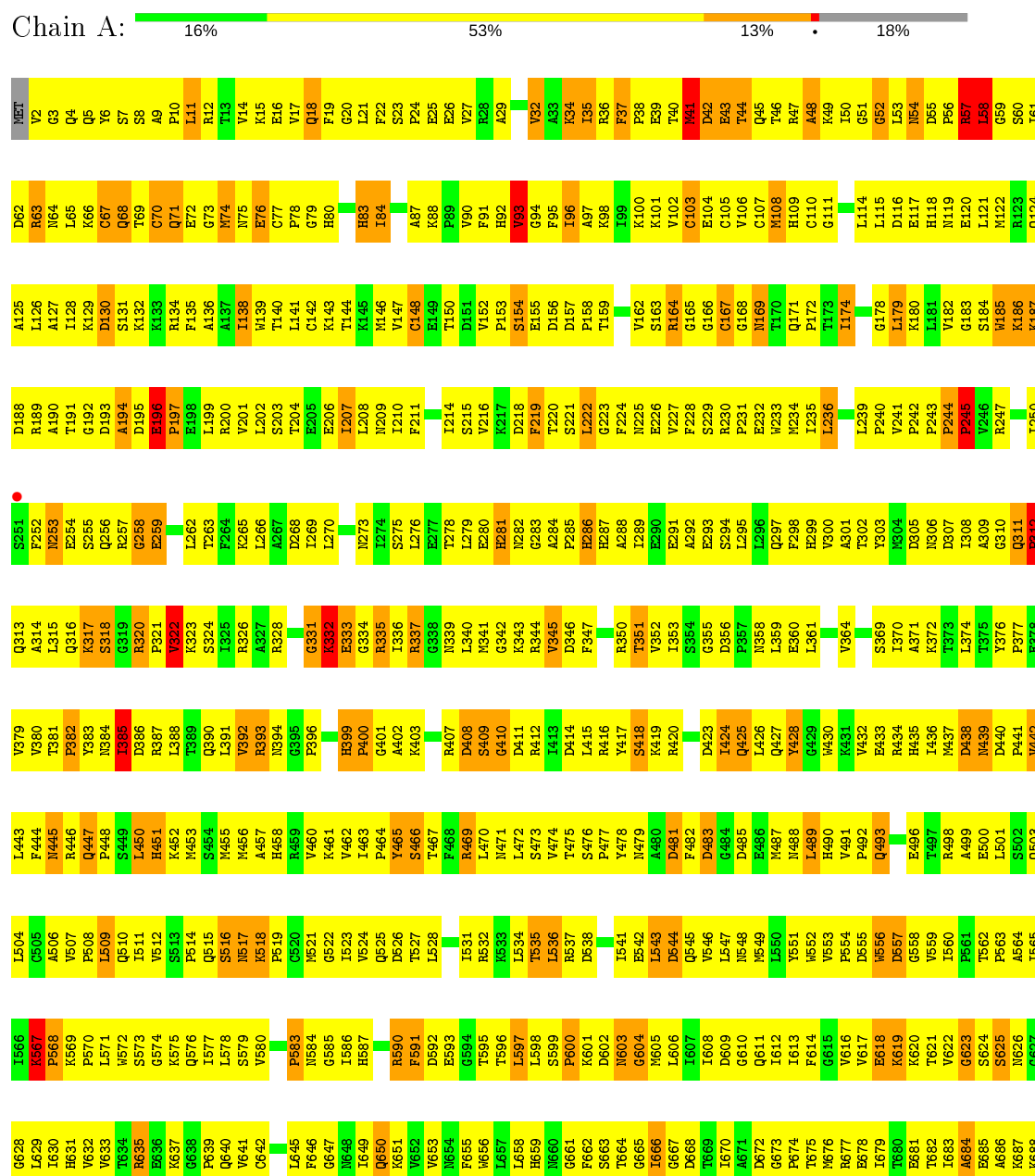
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	2	Total 2	Zn 2	0	0
17	L	1	Total 1	Zn 1	0	0

3 Residue-property plots

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

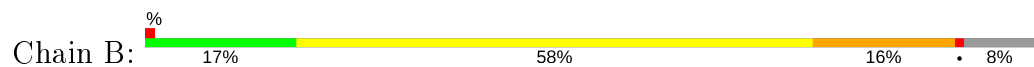
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1



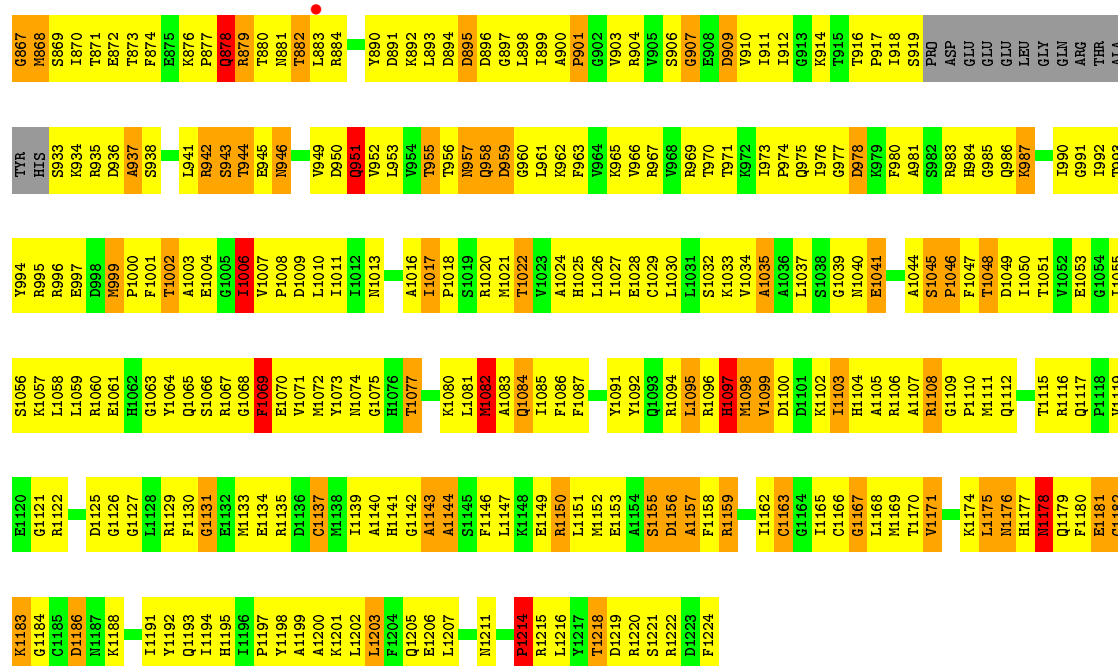
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PRO	THR	PHE	E1448	H1387	T1322	E1255	L1193	Q1130	Q1070	M1009	R944	Q881	M818	S764	V690
SER	SER	THR	S1449	G1388	T1322	E1256	R1194	A1131	S1071	A1010	E945	S882	G819	F755	L691
PRO	PRO	ALA	L1450	F1389	D1323	D1257	L1195	K1132	I1072	Q1011	R946	L883	G820	V756	D892
PRO	PRO	THR	L1451	M1390	P1324	M1258	E1196	L1133	E1074	R1012	F947	D884	R821	N757	V693
THR	THR	GLY	K1452	R1391	T1325	M1259	L1197	I1134	G1073	D1013	V948	T885	E822	T758	T694
SER	SER	ALA	Y1453	S1392	R1326	L1260	D1198	I1138	P1075	A1014	D949	I886	I825	A759	K695
SER	ASP	ALA	M1454	E1393	L1327	K1261	R1199	I1138	A1076	V1015	G950	G887	I826	A760	K696
PRO	PRO	ASP	P1455	T1394	Y1328	K1262	A1200	E1139	T1077	T1016	E951	G888	D826	M761	A697
THR	THR	TYR	G1455	T1395	T1329	L1263	A1201	H1140	Q1078	F1017	R952	S889	T827	S762	Q698
SER	SER	GLY	A1396	G1396	M1330	E1264	L1141	T1141	M1079	F1018	N953	D890	A828	A763	A699
PRO	PRO	GLU	L1397	L1397	S1331	T1265	T1142	T1142	T1080	C1019	N954	A891	V829	C764	N700
SER	PRO	ALA	M1398	M1398	F1332	T1266	L1143	L1143	L1081	C1020	P955	E894	K830	V765	L701
THR	THR	THR	A1399	A1399	I1333	M1267	K1144	K1144	ASN	L1021			T831	G766	L702
SER	SER	THR	C1400	C1400	D1334	L1268	S1145	S1145	THR	L1022			A832	Q768	A703
PRO	PRO	GLU	S1401	F1402	I1335	E1269	V1146	V1146	PHE				E833	Q767	T704
THR	THR	PHE	F1402	F1402	T1271	M1270	T1147	T1147	HIS	R1025			T834	S769	K705
SER	TYR	GLY	E1403	E1403	Q1211	L1271	L1148	L1148	PHE	L1026	R961	R898	G835	V770	H706
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SER	PRO	THR	T1405	T1405	G1213	L1273	S1150	S1150	GLY	T1028	1963	D900	I837		T709
THR	THR	GLY	ASP	ASP	E1214	L1274	E1151	E1151	VAL	R1029	1964	L901	Q838	R774	L710
GLY	GLY	GLY	GLN	GLN	G1215	G1275	T1152	T1152	ALA	R1030	Q965	N902	R839	I775	R711
GLY	GLY	GLY	GLY	GLY	A1342	V1276	L1153	L1153	SER	V1031	Q966	N903	R840	I776	E712
PRO	PRO	ALA	GLY	GLY	E1343	E1277	Y1154	Y1154	LVS	L1032	A967	D905	L841	F777	S713
SER	SER	THR	THR	THR	R1344	M1278	Q1218	D1155	K1093	G1033	Q968	D906	K843	G778	F714
PRO	PRO	SER	PRO	PRO	R1345	I1279	T1219	P1156	V1094	E1034	Q969	H906	K843	F779	E715
SER	PRO	THR	THR	THR	E1280	E1280	K1220	D1157	T1095	Y1035	T970	T907	L844	V780	
PRO	PRO	GLY	GLY	GLY	M1284	M1284	K1221	P1158	S1096	R1036	F971	L908	L845	R781	V718
THR	THR	ASN	ASN	ASN	E1351	E1351	D1222	R1159	G1097	L1037	H972	D909	R846	I783	V719
PRO	PRO	GLY	GLY	GLY	M1285	M1285	L1224	S1160	V1098	T1038	1973	P910	D847	R782	R720
THR	THR	VAL	VAL	VAL	E1352	E1352	F1225	T1161	P1099	K1039	D974	S911	I848	L784	F721
SER	SER	SER	SER	SER	Y1353	Y1353	F1226	V1162	R1100	Q1040	H975	L912	M849	P785	L722
PRO	PRO	LEU	LEU	LEU	M1354	M1354	V1226	I1163	L1101	A1041		L913		H723	R723
VAL	VAL	VAL	VAL	VAL	V1291	V1291	I1227	E1164	K1102	F1042	D980	D853	Y852	E724	E724
ASN	ASN	ASN	ASN	ASN	P1292	P1292	W1228	E1165	L1103	D1043	S915	S915	N854	A725	A725
ALA	ALA	ALA	ALA	ALA	S1293	S1293	S1229	D1166	I1104	W1044	G916	G916	R726	R726	R726
ASP	ASP	ASP	ASP	ASP	P1294	P1294	E1230	E1167	L1105	V1045	1981	S917	T855	D727	D727
LEU	LEU	LEU	LEU	LEU	T1295	T1295	D1231	E1168	M1106	L1046	T982	E918	T856	K728	K728
ASP	ASP	ASP	ASP	ASP	G1296	G1296	M1232	I1169	V1107	S1047	1983	I919	R857	P794	A729
VAL	VAL	VAL	VAL	VAL	E1297	E1297	D1233	I1170	A1108	M1048	D985	K924	N858	E795	G730
LVS	LVS	LVS	LVS	LVS	Y1298	Y1298	E1234	K1109	I1049	E1050	1986	K924	S859	S796	R731
THR	THR	THR	THR	THR	V1299	V1299	K1235	M1110	A1051	A1051	V987	L925	L860	K797	L732
GLY	GLY	GLY	GLY	GLY	K1300	K1300	L1236	F1173	M1111	Q1052	1988	L925	G861	A733	A733
LEU	LEU	LEU	LEU	LEU	E1303	E1303	I1237	S1175	K1112	F1053		V927		E734	E734
MET	MET	MET	MET	MET	W1304	W1304	I1238	L1176	T1113			L928	I864	V735	V735
THR	THR	THR	THR	THR	V1305	V1305	C1239	L1177	P1114	L1054	1993	L928	Q865	M736	M736
PRO	PRO	PRO	PRO	PRO	L1306	L1306	R1241	D1178	S1115	R1055	Q994	L929	F866	L737	L737
ALA	ALA	ALA	ALA	ALA	E1307	E1307	V1242	E1179	L1116	S1056	E995	D950	I867	S803	S803
VAL	VAL	VAL	VAL	VAL	T1308	T1308	V1243	GLU	T1117	V1057	N996	E951	Y868	Y804	D739
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THR	THR	THR	THR	THR	V1311	V1311	K1246	GLN	L1120	P1060	V999	K934	D871	M808	N742
THR	THR	THR	THR	THR	M1312	M1312	SER	SER	P1122	G1061	L1000	Q935	G872	T809	N743
PRO	PRO	PRO	PRO	PRO	L1313	L1313	LEU	PHE	E1122	E1062	R1001	L936	M873	K744	K744
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ASP	ASP	ASP	ASP	ASP	L1314	L1314	THR	Q1187	G1124	V1064	K1003	K938	A875	E812	E745
ALA	ALA	ALA	ALA	ALA	E1315	E1315	ALA	Q1188	A1126	G1065	N1004	D939	A876	F813	F747
MET	MET	MET	MET	MET	V1316	V1316	GLU	S1189	A1126	V1066	E1005	R940	B877	F814	F747
PRO	PRO	PRO	PRO	PRO	M1317	M1317	THR	P1190	D1127	L1067	I1006	K941	L878	F815	S751
THR	THR	THR	THR	THR	T1318	T1318	GLU	W1191	Q1128	A1068	I1007	F942	E879	H816	K752

PRO
SER
TYR
SER
LEU
PRO
THR
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PRO
ASN
TYR
TYR
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THR
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GLY
GLY
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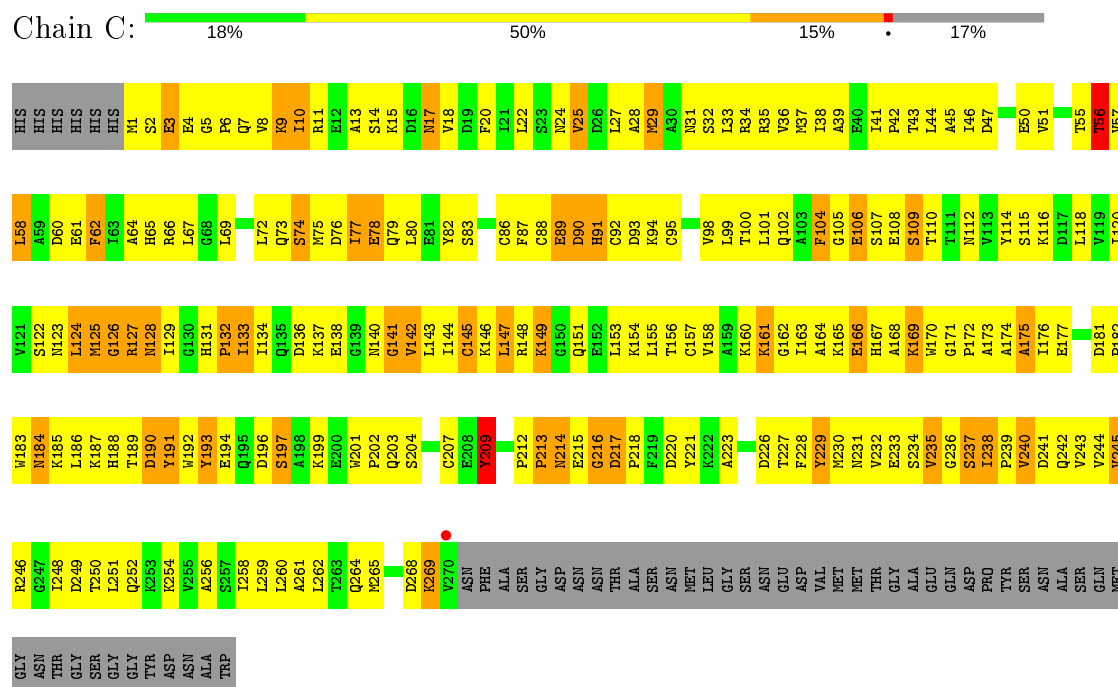
• Molecule 2: DNA-directed RNA polymerase II subunit RPB2



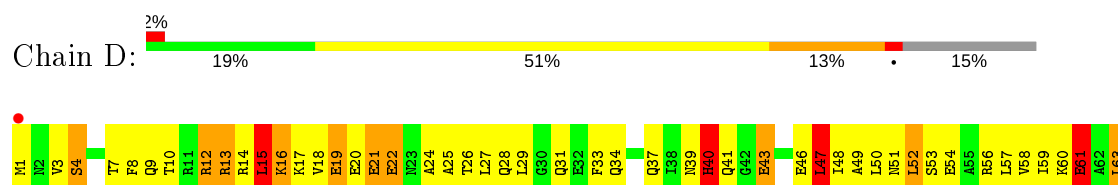
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ASP	I63	T123	I251	K315	K375	E437	T498	M663	A626	L748	A808
LEU	C64	Y124	L254	P316	F376	GLU	P501	L566	G627	G749	M809
ALA	E65	S125	L254	P316	F377	ALA	I502	L566	T628	L750	E810
ASN	D66	S126	L254	V318	L378	HIS	G503	E567	D629	V751	Y811
SER	S67	G127	L254	E319	G379	ASP	D505	E567	E630	A752	K812
GLU	T68	L128	L254	D320	Y380	PHE	D506	E567	G631	A753	L813
LYS	L69	F129	L189	D320	Y380	ASN	D506	E567	G632	T754	R814
TYR	L70	V130	K191	L192	G321	MET	K507	H508	G633	S755	R815
SER	D131	D131	K193	L192	G321	LYS	L508	O573	G634	I756	E816
ASP	GLU	V132	E262	E324	R384	L446	A509	S574	G635	P757	L817
GLU	GLN	K133	E262	E325	R385	A447	K510	S574	G636	P758	P818
ASP	LEU	K134	E262	E326	R386	T448	P511	D576	L637	P759	Q821
PRO	ALA	R135	E262	E327	L387	N449	R512	A577	G638	D760	N822
TYR	GLN	Y136	E262	E328	C388	A450	D513	T578	G639	H761	N823
GLY	HIS	T137	E262	E329	A389	K451	L514	R579	V640	L762	I824
PHE	THR	E138	E262	E330	L390	T452	H515	V580	E641	Q763	I824
GLU	THR	ALA	E262	E331	D391	T453	N516	F581	D642	S764	V825
D20	GLU	ILE	E262	E332	R392	T454	T517	F582	D643	P765	A826
E21	ASP	ASP	E262	E333	K393	S455	H518	V583	E644	R766	I827
S22	SER	VAL	E262	E334	D394	G456	N519	G584	G645	G767	A828
A23	ASN	PRO	E262	E335	Q395	L457	D520	V585	L646	T768	C829
E24	ILE	GLY	E262	E336	D396	K458	L521	V586	G647	Q769	R830
PRO	ARG	ARG	E262	E337	D397	T459	E522	H587	H648	Q770	Y831
T26	ARG	GLU	E262	E338	R398	A460	C523	G588	G649	S771	G832
E27	LYS	LEU	E262	E339	L461	L460	E526	V589	E650	A772	Y833
D28	TYR	LYS	E262	E340	H400	A462	T527	H590	L651	M773	N834
D29	GLU	TVR	E262	E341	F401	T463	T527	E591	K652	G774	Q835
S30	LEU	GLU	E262	E342	G402	G464	F528	N592	V653	K775	E836
K31	S91	LEU	E262	E343	R405	M465	E529	P493	G654	A776	S837
A32	F92	ILE	E262	E344	S550	M466	G530	A594	R655	T777	S838
V33	G93	ALA	E262	E345	K346	G467	Q531	R595	G656	U778	M839
I34	K94	GLU	E262	E346	K347	E468	E532	L596	H657	G779	I840
S35	S95	GLU	E262	E347	A409	Q469	V536	N597	A658	V780	M841
S36	F96	SER	E262	E348	G410	K470	T536	E598	A659	ASP	N842
F37	F97	GLU	E262	E349	P411	K471	K537	T599	G660	L782	U843
F38	R98	ASP	E262	E350	L412	A472	L538	L600	S844	T783	S844
R39	K99	ASP	E262	E351	L413	G662	N539	R601	M662	V784	S845
E40	F40	SER	E262	E352	A414	S475	T540	T602	A663	H785	I846
K41	M101	GLU	E262	E353	Q415	R476	S541	L603	T664	L786	D847
G42	V102	SER	E262	E354	L416	A477	H542	R604	E665	K787	R848
L43	H103	GLY	E262	E355	F417	G478	S543	R605	D668	R788	G849
V44	E104	A230	E262	E356	K418	V479	T544	G606	ILE	T729	L850
S45	S105	P231	E262	E357	T419	S480	I545	G607	GLU	D790	R851
Q46	D106	V166	E262	E358	L420	Q481	S546	D608	GLY	T791	R852
L48	G107	T222	E262	E359	F421	V482	V547	T609	GLY	M792	S853
L48	V108	G168	E262	E360	K422	L483	G548	N610	GLY	H793	L854
D49	D99	E299	E262	E361	R423	N484	T549	P611	PHE	T794	F855
S50	H10	L170	E262	E362	L424	R485	D550	E612	GLU	I795	R856
F51	F51	P171	E262	E363	T425	V486	P551	ASP	ASP	T736	R857
N52	N52	T172	E262	E364	K426	L487	N552	S614	VAL	T737	S858
Q53	Y113	M173	E262	E365	M427	Y488	P553	N615	GLU	F738	Y859
F54	P114	L174	E262	E366	I428	S489	T554	T616	E878	T739	M860
V55	Q115	S242	E262	E367	F429	S490	L555	R617	T680	D861	D861
D56	E116	E243	E262	E368	R430	T491	T556	H618	Q862	C741	Q862
T57	Y57	L244	E262	E369	M431	L492	F557	L619	E863	P802	E863
L58	R118	L244	E262	E370	Q309	Y432	F557	N620	S862	I743	K864
L59	L119	L311	E262	E371	K433	L495	S559	E621	G864	H744	K865
Q60	R120	E184	E262	E372	R434	P406	S560	T622	L864	T745	L864

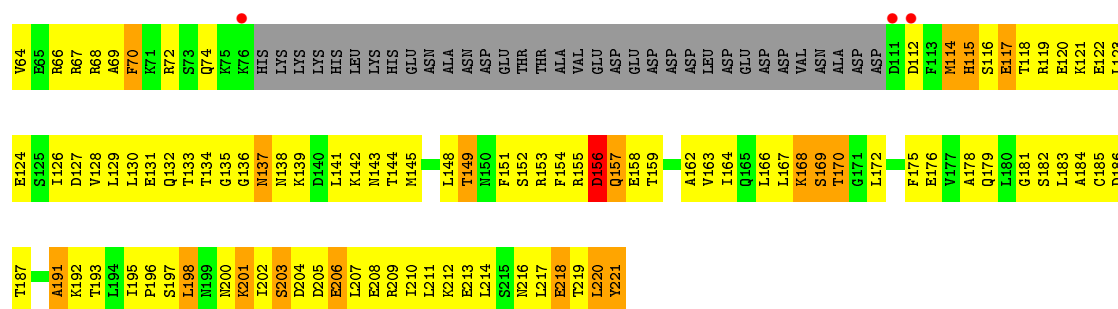


• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

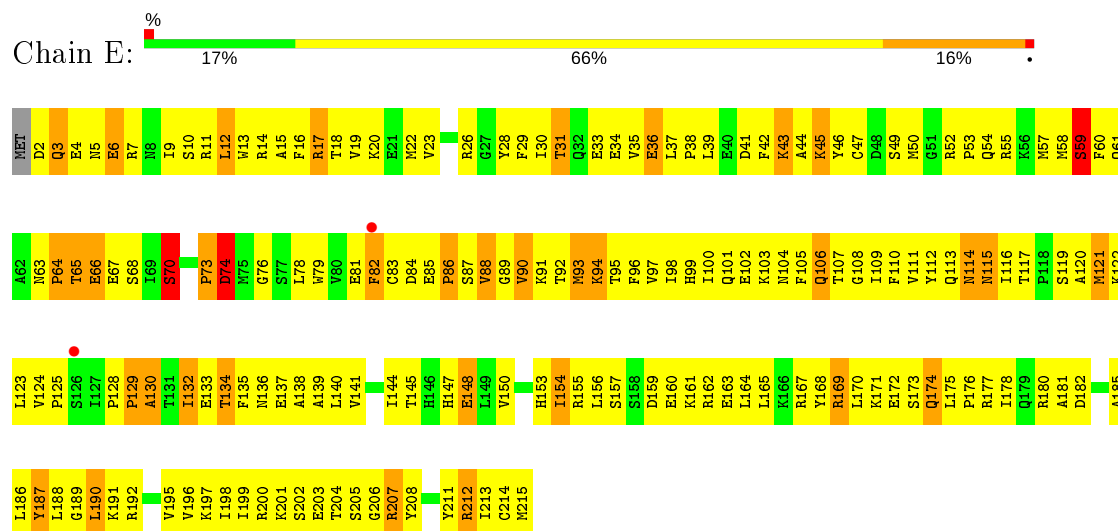


• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

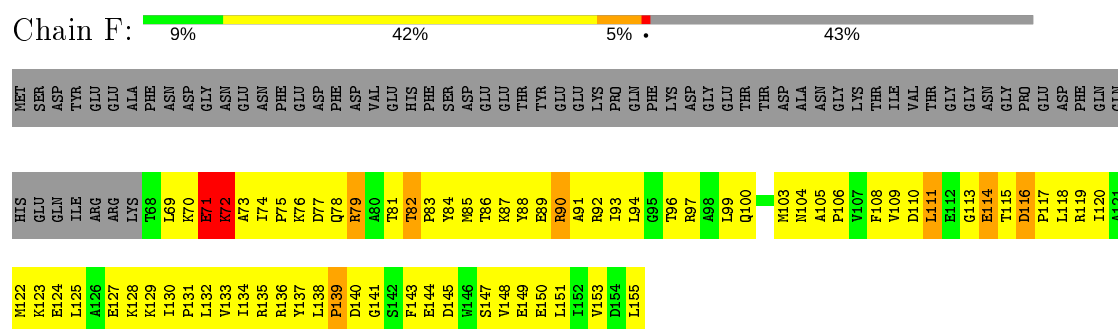




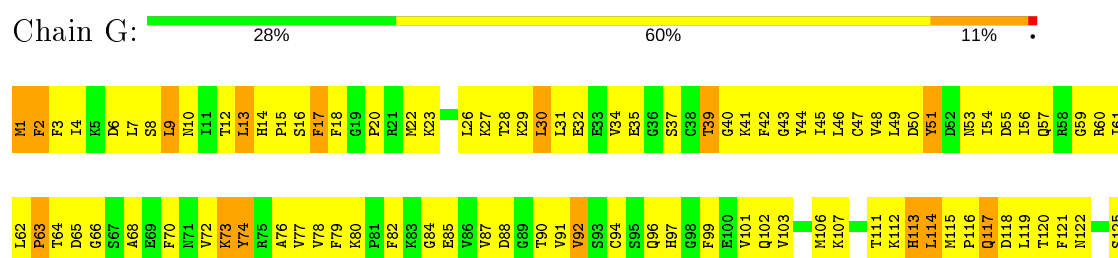
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

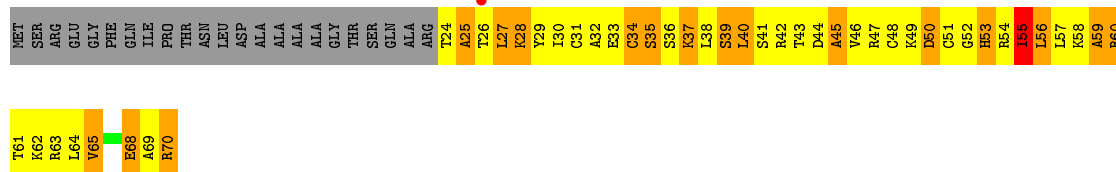


• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

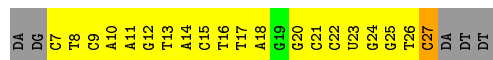
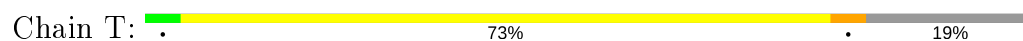


• Molecule 7: DNA-directed RNA polymerase II subunit RPB7





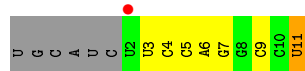
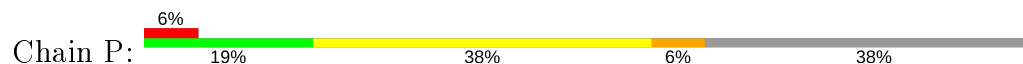
- Molecule 13: DNA (5'-D(*AP*G*CP*TP*CP*AP*AP*GP*TP*AP*CP*TP*TP*AP*(8OG)P*GP*CP*CP*(BRU)P*GP*GP*TP*CP*AP*TP*T)-3')



- Molecule 14: DNA (5'-D(*AP*GP*TP*AP*CP*TP*TP*GP*AP*GP*CP*T)-3')



- Molecule 15: RNA (5'-R(*UP*GP*CP*AP*UP*C*UP*UP*CP*CP*AP*GP*GP*CP*CP*U)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	220.65Å 392.00Å 281.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.70 49.00 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-3.70) 100.0 (49.00-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 3.67Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.225 , 0.258 0.227 , 0.253	Depositor DCC
R_{free} test set	2439 reflections (1.88%)	wwPDB-VP
Wilson B-factor (Å ²)	114.2	Xtriage
Anisotropy	0.492	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 97.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.029 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.034 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	32355	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.80% 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: MG, 8OG, ZN, BRU

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	0.44	0/11441	0.74	3/15473 (0.0%)
2	B	0.41	0/9116	0.70	0/12291
3	C	0.42	0/2163	0.69	0/2930
4	D	0.38	0/1516	0.63	0/2031
5	E	0.39	0/1788	0.64	0/2406
6	F	0.52	0/724	0.82	0/977
7	G	0.44	0/1368	0.72	0/1844
8	H	0.37	0/1119	0.68	0/1514
9	I	0.38	0/962	0.66	0/1295
10	J	0.44	0/541	0.74	0/727
11	K	0.46	0/947	0.68	0/1279
12	L	0.39	0/372	0.68	0/495
13	T	0.56	1/426 (0.2%)	0.87	0/650
14	N	0.41	0/251	0.81	0/386
15	P	0.42	0/227	0.80	0/351
All	All	0.43	1/32961 (0.0%)	0.71	3/44649 (0.0%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	T	27	DC	C1'-N1	5.98	1.57	1.49

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	567	LYS	C-N-CD	5.82	140.63	128.40
1	A	3	GLY	N-CA-C	-5.75	98.73	113.10
1	A	509	LEU	CA-CB-CG	-5.00	103.79	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1035	TYR	Sidechain
2	B	797	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11240	0	11311	1819	0
2	B	8942	0	8986	1481	0
3	C	2125	0	2090	340	0
4	D	1504	0	1518	205	0
5	E	1752	0	1776	286	0
6	F	712	0	738	138	0
7	G	1340	0	1357	217	0
8	H	1101	0	1075	206	0
9	I	944	0	901	162	0
10	J	532	0	542	129	0
11	K	929	0	939	135	0
12	L	370	0	394	90	0
13	T	426	0	236	37	0
14	N	224	0	126	11	0
15	P	205	0	109	8	0
16	A	1	0	0	0	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0
17	C	1	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	L	1	0	0	0	0
All	All	32355	0	32098	4821	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 75.

All (4821) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:LEU:HD13	2:B:429:PHE:CD1	1.39	1.55
2:B:69:LEU:HD13	2:B:429:PHE:CE1	1.66	1.30
2:B:577:ALA:HB1	2:B:589:VAL:HG11	1.24	1.17
2:B:806:THR:HG22	2:B:808:ALA:H	1.08	1.16
2:B:340:ALA:HB3	2:B:343:ILE:HG12	1.29	1.15
2:B:69:LEU:CD1	2:B:429:PHE:CD1	2.30	1.14
13:T:16:DT:H2''	13:T:17:DT:H5'	1.29	1.13
2:B:133:LYS:HE3	2:B:135:ARG:HH21	1.13	1.12
1:A:225:ASN:ND2	1:A:228:PHE:H	1.48	1.12
1:A:41:MET:HB2	1:A:49:LYS:HA	1.32	1.12
1:A:825:ILE:HD11	2:B:512:ARG:HB3	1.22	1.11
2:B:639:ILE:HD11	2:B:691:GLU:HG3	1.32	1.11
1:A:567:LYS:HG3	8:H:95:TYR:HA	1.11	1.10
2:B:637:LEU:HD12	2:B:693:ILE:HD12	1.32	1.10
2:B:622:LYS:HE2	9:I:59:VAL:HG22	1.28	1.10
3:C:43:THR:HG22	3:C:44:LEU:H	1.02	1.09
1:A:899:VAL:HB	1:A:929:LEU:HD11	1.14	1.09
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.27	1.09
7:G:138:THR:HG22	7:G:139:ILE:H	1.00	1.07
1:A:53:LEU:HD23	1:A:54:ASN:N	1.70	1.07
6:F:109:VAL:HG11	6:F:123:LYS:HD2	1.30	1.06
3:C:148:ARG:H	3:C:151:GLN:HG3	1.20	1.05
1:A:1244:ARG:HB3	1:A:1245:PRO:HA	1.28	1.05
2:B:244:LEU:HD11	2:B:366:GLN:HE22	1.20	1.05
2:B:506:GLY:HA2	2:B:512:ARG:HH21	1.21	1.05
1:A:666:ILE:H	2:B:1026:LEU:HD13	1.21	1.05
12:L:40:LEU:HD13	12:L:44:ASP:HB3	1.38	1.04
1:A:320:ARG:HB2	1:A:320:ARG:HH11	1.19	1.04
1:A:12:ARG:HB2	2:B:1218:THR:HG22	1.39	1.04
2:B:217:ARG:HE	2:B:405:ARG:HB2	1.20	1.04
8:H:12:VAL:HB	8:H:52:GLN:H	1.21	1.04
5:E:22:MET:HE3	5:E:26:ARG:HH11	1.23	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:273:LEU:HB2	2:B:276:ILE:HD12	1.40	1.02
8:H:81:PRO:HB2	8:H:82:PRO:CD	1.89	1.02
2:B:1097:HIS:H	2:B:1098:MET:HE2	1.23	1.02
8:H:64:ASN:HB2	8:H:88:SER:HB2	1.41	1.02
5:E:78:LEU:HA	5:E:107:THR:HB	1.38	1.01
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.41	1.01
1:A:903:ASN:HD22	1:A:904:THR:N	1.57	1.01
2:B:69:LEU:HB3	2:B:429:PHE:HE1	1.22	1.01
5:E:100:ILE:HG23	5:E:105:PHE:HB2	1.41	1.01
1:A:1445:ILE:HD12	1:A:1445:ILE:H	1.26	1.00
1:A:590:ARG:HH11	1:A:590:ARG:HB2	1.24	1.00
3:C:238:ILE:HG23	3:C:242:GLN:HB2	1.43	1.00
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.42	1.00
12:L:32:ALA:HB2	12:L:55:ILE:HG13	1.44	1.00
1:A:535:THR:HG21	1:A:616:VAL:HA	1.44	1.00
1:A:188:ASP:HB3	1:A:191:THR:HB	1.43	0.99
10:J:5:VAL:HG12	10:J:6:ARG:HG3	1.43	0.99
3:C:101:LEU:HD13	3:C:118:LEU:HD23	1.41	0.99
1:A:382:PRO:HD3	1:A:428:TYR:HD2	1.27	0.99
2:B:1065:GLN:HE21	2:B:1067:ARG:N	1.60	0.99
2:B:503:GLY:HA3	2:B:507:LYS:HE2	1.45	0.98
9:I:58:VAL:HG13	9:I:62:ILE:HD12	1.44	0.98
5:E:207:ARG:HH11	5:E:207:ARG:HB3	1.28	0.98
6:F:76:LYS:HA	6:F:79:ARG:HD3	1.45	0.98
2:B:69:LEU:CD1	2:B:429:PHE:CE1	2.45	0.98
3:C:148:ARG:N	3:C:151:GLN:HG3	1.78	0.98
1:A:567:LYS:HE2	8:H:47:PHE:HB2	1.44	0.97
2:B:583:ASN:HD21	2:B:628:THR:HG22	1.28	0.97
2:B:810:GLU:HA	2:B:815:ARG:HH22	1.29	0.97
6:F:111:LEU:HD12	6:F:111:LEU:H	1.27	0.97
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.45	0.97
8:H:40:LEU:HD22	8:H:123:MET:HE3	1.46	0.97
1:A:683:ILE:HD13	1:A:801:GLU:HG3	1.46	0.97
2:B:800:GLN:HB3	10:J:52:THR:CG2	1.92	0.96
5:E:124:VAL:HG13	5:E:132:ILE:HG13	1.46	0.96
1:A:1111:MET:HE2	1:A:1331:SER:HA	1.46	0.96
2:B:559:SER:HA	2:B:563:MET:HB3	1.47	0.96
7:G:138:THR:HG22	7:G:139:ILE:N	1.80	0.96
1:A:925:LEU:HD13	1:A:983:ILE:HD12	1.48	0.96
1:A:666:ILE:HD12	1:A:667:GLY:H	1.31	0.95
1:A:269:ILE:HG12	1:A:299:HIS:HB3	1.48	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1099:VAL:HG13	2:B:1100:ASP:H	1.32	0.95
2:B:800:GLN:HB3	10:J:52:THR:HG21	1.49	0.95
5:E:22:MET:CE	5:E:26:ARG:HH11	1.80	0.95
9:I:85:PHE:HD2	9:I:85:PHE:H	1.08	0.95
2:B:515:HIS:HD2	2:B:517:THR:H	1.01	0.95
6:F:73:ALA:HB1	6:F:143:PHE:H	1.31	0.94
2:B:866:TYR:HB2	2:B:870:ILE:HB	1.49	0.94
8:H:100:THR:HG23	8:H:138:GLU:HA	1.48	0.94
5:E:153:HIS:O	5:E:154:ILE:HG13	1.66	0.94
5:E:16:PHE:CZ	5:E:20:LYS:HE2	2.02	0.94
1:A:308:ILE:HG22	1:A:309:ALA:H	1.33	0.94
10:J:64:ASN:HB3	10:J:65:PRO:CD	1.97	0.94
8:H:128:ASN:H	8:H:130:ARG:NH1	1.65	0.94
1:A:754:SER:H	1:A:757:ASN:HD22	1.13	0.94
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.49	0.94
8:H:12:VAL:HB	8:H:52:GLN:N	1.83	0.94
1:A:320:ARG:HB2	1:A:320:ARG:NH1	1.83	0.94
8:H:81:PRO:HB2	8:H:82:PRO:HD3	1.48	0.93
3:C:114:TYR:CD2	3:C:140:ASN:HB3	2.02	0.93
1:A:567:LYS:CG	8:H:95:TYR:HA	1.97	0.93
12:L:27:LEU:H	12:L:27:LEU:HD23	1.34	0.93
2:B:1065:GLN:HE21	2:B:1067:ARG:H	0.96	0.93
1:A:541:ILE:HD13	1:A:549:MET:HE1	1.51	0.93
1:A:1144:LYS:HB2	1:A:1268:LEU:O	1.68	0.93
4:D:39:ASN:ND2	4:D:41:GLN:HB2	1.83	0.93
10:J:44:TYR:HA	10:J:47:ARG:HB2	1.51	0.93
11:K:21:ILE:HG23	11:K:33:ILE:HG12	1.51	0.93
1:A:466:SER:HB3	2:B:1103:ILE:HG12	1.52	0.92
7:G:127:PRO:HG2	7:G:138:THR:HG21	1.50	0.92
1:A:1424:VAL:HG13	1:A:1436:ILE:HD11	1.51	0.92
1:A:720:ARG:O	1:A:724:GLU:HB2	1.70	0.92
1:A:901:LEU:H	1:A:926:GLN:NE2	1.67	0.92
8:H:102:TYR:HD2	8:H:102:TYR:H	1.13	0.92
2:B:115:GLN:HG2	2:B:193:LYS:HB2	1.48	0.92
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.34	0.92
2:B:520:GLY:H	2:B:748:ILE:HG22	1.34	0.92
3:C:43:THR:HG22	3:C:44:LEU:N	1.85	0.92
8:H:33:GLN:HE21	8:H:35:GLN:HB2	1.31	0.92
7:G:122:ASN:HB2	7:G:131:GLN:HE21	1.34	0.91
2:B:911:ILE:HD11	2:B:941:LEU:HD13	1.52	0.91
1:A:897:TYR:HD2	1:A:936:LEU:HD13	1.34	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:LEU:HB3	2:B:429:PHE:CE1	2.05	0.91
1:A:1208:THR:HB	1:A:1211:GLN:HG3	1.52	0.91
1:A:1004:ASN:ND2	5:E:167:ARG:HD2	1.86	0.91
7:G:7:LEU:HB2	7:G:74:TYR:CE2	2.04	0.91
1:A:441:PRO:HG3	1:A:498:ARG:HB2	1.51	0.91
1:A:49:LYS:HZ1	1:A:61:ILE:HG13	1.34	0.91
3:C:203:GLN:HG2	3:C:207:CYS:SG	2.10	0.91
1:A:225:ASN:HD22	1:A:228:PHE:N	1.68	0.91
11:K:12:LEU:H	11:K:12:LEU:HD12	1.33	0.91
1:A:470:LEU:HD13	1:A:487:MET:HE1	1.52	0.90
3:C:258:ILE:HD11	11:K:42:LEU:HD11	1.52	0.90
1:A:335:ARG:HD3	2:B:1202:LEU:HD23	1.54	0.90
2:B:69:LEU:HD22	2:B:429:PHE:CE1	2.07	0.90
1:A:442:VAL:HG12	1:A:490:HIS:O	1.71	0.90
2:B:410:GLY:HA2	2:B:413:LEU:HD12	1.52	0.89
2:B:642:ASP:HA	2:B:649:LYS:HA	1.52	0.89
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.54	0.89
1:A:1409:LEU:HD13	2:B:1207:LEU:HD11	1.54	0.89
11:K:47:ARG:HB3	11:K:47:ARG:HH11	1.34	0.89
2:B:515:HIS:CD2	2:B:517:THR:H	1.90	0.89
4:D:3:VAL:HG21	7:G:10:ASN:HB2	1.52	0.89
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.14	0.89
1:A:1369:ALA:O	1:A:1372:VAL:HG12	1.72	0.89
2:B:384:ARG:HA	2:B:387:LEU:HD22	1.52	0.89
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.55	0.89
5:E:117:THR:HG22	5:E:119:SER:H	1.37	0.89
3:C:77:ILE:H	3:C:129:ILE:HD11	1.36	0.89
3:C:57:VAL:HG11	10:J:60:PHE:HB3	1.53	0.89
1:A:1308:THR:HG23	1:A:1309:ASP:N	1.84	0.89
3:C:43:THR:CG2	3:C:44:LEU:H	1.85	0.88
7:G:138:THR:CG2	7:G:139:ILE:H	1.82	0.88
1:A:1153:TYR:HB2	1:A:1192:LEU:HD23	1.55	0.88
1:A:18:GLN:HG2	1:A:1418:LEU:HD13	1.55	0.88
1:A:537:ARG:HD2	8:H:20:TYR:HE1	1.37	0.88
2:B:193:LYS:NZ	12:L:32:ALA:HB1	1.88	0.88
1:A:1227:ILE:HG22	1:A:1228:TRP:H	1.37	0.88
1:A:335:ARG:HD2	2:B:1206:GLU:OE1	1.73	0.88
1:A:568:PRO:HG2	8:H:46:LEU:HD22	1.55	0.88
5:E:17:ARG:NH1	5:E:17:ARG:HB2	1.88	0.88
1:A:946:VAL:HG13	5:E:201:LYS:HB3	1.55	0.88
2:B:880:THR:HB	2:B:934:LYS:CE	2.04	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1420:ASP:CB	1:A:1422:ARG:HG3	2.02	0.88
5:E:171:LYS:HG2	5:E:174:GLN:OE1	1.74	0.88
1:A:71:GLN:HG3	1:A:72:GLU:HG2	1.56	0.88
4:D:164:ILE:HG23	4:D:168:LYS:HD2	1.56	0.88
1:A:1030:ARG:HG3	1:A:1034:GLU:OE2	1.75	0.88
2:B:539:LEU:HD12	2:B:539:LEU:H	1.38	0.88
2:B:69:LEU:O	2:B:70:ILE:HG13	1.74	0.87
1:A:630:ILE:HD11	1:A:646:PHE:CZ	2.09	0.87
1:A:665:GLY:O	1:A:667:GLY:N	2.06	0.87
2:B:299:GLU:HB3	2:B:571:PRO:HG3	1.57	0.87
5:E:17:ARG:HB2	5:E:17:ARG:HH11	1.37	0.87
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.55	0.87
1:A:899:VAL:HB	1:A:929:LEU:CD1	2.04	0.87
2:B:1065:GLN:NE2	2:B:1067:ARG:H	1.73	0.87
1:A:901:LEU:H	1:A:926:GLN:HE21	1.19	0.87
12:L:61:THR:HG21	12:L:63:ARG:HE	1.38	0.87
3:C:175:ALA:HB2	10:J:10:CYS:HB2	1.57	0.87
1:A:899:VAL:HG13	1:A:908:LEU:HD21	1.55	0.87
1:A:182:VAL:HG22	1:A:201:VAL:HA	1.55	0.86
12:L:55:ILE:HD13	12:L:55:ILE:H	1.40	0.86
2:B:810:GLU:CA	2:B:815:ARG:HH22	1.88	0.86
1:A:1323:ASP:OD1	1:A:1325:THR:HG22	1.74	0.86
13:T:15:DC:H2"	13:T:16:DT:H72	1.55	0.86
1:A:1242:VAL:HG12	1:A:1243:VAL:H	1.39	0.86
1:A:40:THR:HG22	1:A:41:MET:HG3	1.54	0.86
2:B:278:GLN:HG2	2:B:279:ASP:H	1.38	0.86
9:I:82:GLU:HB3	9:I:104:LEU:HD12	1.58	0.86
1:A:567:LYS:HG3	8:H:95:TYR:CA	2.03	0.86
2:B:801:LYS:O	10:J:52:THR:HG23	1.75	0.86
12:L:34:CYS:HB3	12:L:51:CYS:SG	2.15	0.86
5:E:3:GLN:HG3	5:E:5:ASN:H	1.40	0.86
4:D:70:PHE:O	4:D:74:GLN:HG3	1.75	0.85
1:A:616:VAL:HG12	1:A:617:VAL:H	1.42	0.85
5:E:85:GLU:HB2	5:E:88:VAL:HG22	1.56	0.85
6:F:103:MET:CE	7:G:66:GLY:H	1.89	0.85
1:A:34:LYS:HZ1	1:A:57:ARG:NH2	1.74	0.85
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.56	0.85
9:I:65:ASP:HB3	9:I:68:LEU:HD12	1.56	0.85
13:T:15:DC:C2'	13:T:16:DT:H72	2.05	0.85
1:A:298:PHE:HZ	1:A:314:ALA:HB2	1.39	0.85
1:A:390:GLN:O	1:A:394:ASN:HB2	1.75	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:738:LYS:HB2	1:A:740:LEU:HG	1.58	0.85
6:F:72:LYS:HA	6:F:72:LYS:HE3	1.59	0.85
8:H:100:THR:OG1	8:H:138:GLU:HG3	1.76	0.85
1:A:1261:LYS:O	1:A:1264:GLU:HB3	1.76	0.85
3:C:244:VAL:O	3:C:248:ILE:HG13	1.75	0.85
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.58	0.85
1:A:134:ARG:HG2	1:A:138:ILE:HD11	1.56	0.85
7:G:45:ILE:HA	7:G:78:VAL:HG12	1.58	0.85
2:B:882:THR:HG22	2:B:884:ARG:HB2	1.56	0.85
11:K:49:GLU:OE2	11:K:97:LYS:HE3	1.76	0.85
5:E:156:LEU:HD12	5:E:195:VAL:HB	1.57	0.84
1:A:913:LEU:HD12	1:A:914:GLU:H	1.40	0.84
2:B:640:VAL:HG22	2:B:651:LEU:HD23	1.57	0.84
1:A:42:ASP:O	1:A:44:THR:N	2.11	0.84
2:B:1119:VAL:O	2:B:1126:GLY:HA3	1.78	0.84
2:B:289:LEU:HD13	2:B:375:ALA:HB2	1.58	0.84
2:B:880:THR:HB	2:B:934:LYS:HD3	1.58	0.84
2:B:69:LEU:HD13	2:B:429:PHE:HD1	1.11	0.84
11:K:65:HIS:CD2	11:K:67:PHE:H	1.96	0.84
2:B:604:ARG:HG3	2:B:611:PRO:HA	1.58	0.84
3:C:147:LEU:HB2	3:C:151:GLN:HB2	1.59	0.84
1:A:49:LYS:HZ1	1:A:61:ILE:N	1.75	0.84
3:C:32:SER:O	3:C:36:VAL:HG23	1.78	0.84
1:A:53:LEU:HD23	1:A:54:ASN:H	1.40	0.84
6:F:73:ALA:CB	6:F:143:PHE:H	1.90	0.84
1:A:414:ASP:OD1	1:A:416:ARG:HG2	1.78	0.84
1:A:1404:GLU:HB2	1:A:1408:ILE:HD12	1.58	0.83
12:L:55:ILE:O	12:L:56:LEU:HB2	1.77	0.83
5:E:19:VAL:O	5:E:23:VAL:HG23	1.77	0.83
1:A:1420:ASP:HB2	1:A:1422:ARG:HG3	1.59	0.83
1:A:563:PRO:HG3	1:A:572:TRP:CZ2	2.13	0.83
1:A:981:LEU:HD21	1:A:1039:LYS:HA	1.59	0.83
2:B:1180:PHE:HB3	2:B:1191:ILE:HD12	1.59	0.83
2:B:882:THR:CG2	2:B:884:ARG:HB2	2.08	0.83
3:C:47:ASP:HA	12:L:69:ALA:HB3	1.60	0.83
8:H:64:ASN:HD22	8:H:88:SER:CB	1.90	0.83
1:A:738:LYS:H	1:A:738:LYS:HD2	1.42	0.83
2:B:1084:GLN:NE2	2:B:1084:GLN:N	2.26	0.83
2:B:526:GLU:HG2	2:B:538:ASN:HD22	1.43	0.83
2:B:652:LYS:O	2:B:689:LEU:HD22	1.78	0.83
8:H:129:TYR:H	8:H:130:ARG:HH11	1.27	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:LYS:HG3	1:A:333:GLU:OE2	1.77	0.83
1:A:32:VAL:O	1:A:57:ARG:HD3	1.78	0.83
2:B:593:PRO:HG2	2:B:617:ARG:CZ	2.09	0.83
2:B:121:ASN:HA	2:B:207:GLY:HA2	1.58	0.83
1:A:1189:SER:O	1:A:1241:ARG:HD3	1.79	0.82
2:B:101:MET:HB2	2:B:169:ARG:HH22	1.44	0.82
7:G:1:MET:SD	7:G:2:PHE:N	2.52	0.82
12:L:32:ALA:CB	12:L:55:ILE:HG13	2.09	0.82
5:E:114:ASN:O	5:E:115:ASN:HB3	1.76	0.82
1:A:1095:THR:HG22	1:A:1100:ARG:HB2	1.61	0.82
2:B:770:GLN:CD	2:B:983:ARG:HA	1.98	0.82
2:B:309:GLN:OE1	9:I:52:ILE:HD11	1.79	0.82
1:A:196:GLU:HB2	1:A:197:PRO:HD2	1.61	0.82
1:A:590:ARG:HH11	1:A:590:ARG:CB	1.91	0.82
1:A:709:THR:HG22	1:A:711:ARG:H	1.45	0.82
2:B:1084:GLN:HE21	2:B:1084:GLN:H	1.24	0.82
1:A:351:THR:HB	2:B:1103:ILE:CD1	2.09	0.82
2:B:277:LYS:HG3	2:B:338:GLY:HA2	1.60	0.82
7:G:62:LEU:HB3	7:G:63:PRO:HD2	1.61	0.82
1:A:69:THR:O	1:A:71:GLN:N	2.13	0.82
1:A:770:VAL:HA	1:A:822:GLU:OE1	1.79	0.82
2:B:1095:LEU:HD12	2:B:1095:LEU:H	1.45	0.82
2:B:815:ARG:HD3	2:B:1041:GLU:OE2	1.79	0.82
2:B:1099:VAL:HG13	2:B:1100:ASP:N	1.95	0.82
2:B:850:LEU:HD12	2:B:851:PHE:N	1.94	0.82
7:G:49:LEU:HD21	7:G:77:VAL:HG23	1.61	0.82
1:A:1244:ARG:HB3	1:A:1245:PRO:CA	2.08	0.82
2:B:515:HIS:HD2	2:B:517:THR:N	1.77	0.82
2:B:65:GLU:HG3	2:B:66:ASP:H	1.45	0.82
2:B:830:TYR:CE2	2:B:1000:PRO:HD3	2.15	0.82
2:B:1084:GLN:HE21	2:B:1084:GLN:N	1.77	0.82
9:I:26:LEU:HD23	9:I:37:GLU:HA	1.59	0.82
3:C:142:VAL:H	10:J:16:ASP:HB3	1.45	0.82
1:A:855:THR:HG21	1:A:857:ARG:HE	1.44	0.81
1:A:1116:LEU:HB3	1:A:1308:THR:CG2	2.10	0.81
7:G:87:VAL:HB	7:G:103:VAL:HG11	1.61	0.81
1:A:225:ASN:HD22	1:A:228:PHE:H	0.83	0.81
3:C:133:ILE:HG21	3:C:236:GLY:HA3	1.62	0.81
1:A:49:LYS:NZ	1:A:61:ILE:HG13	1.94	0.81
1:A:1260:LEU:HD12	1:A:1260:LEU:O	1.81	0.81
2:B:69:LEU:CB	2:B:429:PHE:HE1	1.93	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:ARG:HB3	1:A:605:MET:H	1.46	0.81
2:B:69:LEU:HD22	2:B:429:PHE:CZ	2.16	0.81
5:E:128:PRO:HA	5:E:129:PRO:O	1.79	0.81
1:A:567:LYS:CE	8:H:47:PHE:HB2	2.11	0.81
2:B:622:LYS:CE	9:I:59:VAL:HG22	2.11	0.81
10:J:64:ASN:HB3	10:J:65:PRO:HD2	1.61	0.81
1:A:107:CYS:HA	1:A:171:GLN:OE1	1.79	0.81
1:A:1438:THR:HB	2:B:1144:ALA:HB3	1.63	0.81
2:B:289:LEU:HD13	2:B:375:ALA:CB	2.09	0.81
2:B:579:ARG:HB2	2:B:586:TRP:NE1	1.95	0.81
7:G:125:SER:OG	7:G:128:PRO:HA	1.80	0.81
1:A:1002:GLY:HA3	1:A:1007:ILE:HG21	1.60	0.81
2:B:1017:ILE:HB	2:B:1018:PRO:HD3	1.61	0.81
8:H:93:TYR:HB3	8:H:144:ILE:O	1.80	0.81
2:B:637:LEU:O	2:B:690:VAL:HG13	1.81	0.80
9:I:35:VAL:HG12	9:I:36:GLU:N	1.96	0.80
1:A:180:LYS:HZ2	1:A:294:SER:HB3	1.46	0.80
2:B:1182:CYS:SG	2:B:1182:CYS:O	2.38	0.80
2:B:882:THR:HG21	2:B:935:ARG:HA	1.63	0.80
1:A:321:PRO:O	1:A:322:VAL:HG12	1.81	0.80
2:B:1002:THR:HG23	2:B:1006:ILE:HG13	1.62	0.80
2:B:1150:ARG:HG3	2:B:1150:ARG:HH11	1.45	0.80
2:B:365:THR:OG1	2:B:367:LEU:HG	1.81	0.80
1:A:779:PHE:HE1	1:A:785:PRO:HD3	1.45	0.80
2:B:217:ARG:NE	2:B:405:ARG:HB2	1.97	0.80
6:F:77:ASP:O	6:F:78:GLN:HB2	1.79	0.80
8:H:101:ALA:HB2	8:H:116:TYR:CZ	2.15	0.80
1:A:600:PRO:HG2	1:A:601:LYS:H	1.44	0.80
2:B:336:ARG:HE	2:B:348:ARG:HH12	1.25	0.80
3:C:8:VAL:HG12	3:C:9:LYS:H	1.46	0.80
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.62	0.80
2:B:1084:GLN:HG2	3:C:201:TRP:CZ2	2.17	0.80
2:B:1159:ARG:HB3	2:B:1159:ARG:HH11	1.46	0.80
2:B:957:ASN:HD22	2:B:961:LEU:HB2	1.47	0.80
7:G:15:PRO:HA	7:G:18:PHE:CD1	2.17	0.80
1:A:1130:GLN:HE21	1:A:1134:ILE:HD11	1.47	0.80
1:A:23:SER:HA	1:A:233:TRP:NE1	1.96	0.80
3:C:98:VAL:C	3:C:99:LEU:HD23	2.02	0.80
5:E:52:ARG:HB3	5:E:53:PRO:HD2	1.64	0.80
1:A:1444:MET:HE1	6:F:135:ARG:HB2	1.64	0.80
2:B:422:LYS:O	2:B:426:LYS:HG2	1.80	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:47:LEU:HD13	4:D:48:ILE:H	1.46	0.79
13:T:15:DC:H2"	13:T:16:DT:C7	2.12	0.79
1:A:115:LEU:O	1:A:122:MET:HG2	1.83	0.79
3:C:45:ALA:HA	3:C:72:LEU:HD12	1.64	0.79
12:L:61:THR:HG22	12:L:63:ARG:H	1.47	0.79
2:B:824:ILE:HG22	2:B:1087:PHE:CE2	2.18	0.79
2:B:343:ILE:HG23	2:B:347:LYS:HE2	1.62	0.79
6:F:103:MET:HE2	7:G:66:GLY:H	1.47	0.79
10:J:9:SER:HB2	10:J:45:CYS:HB2	1.64	0.79
1:A:1206:ASP:HB3	1:A:1274:ARG:HH12	1.45	0.79
1:A:1254:ALA:O	1:A:1255:GLU:HB2	1.81	0.79
11:K:53:ASP:HB3	11:K:56:VAL:HG23	1.64	0.79
2:B:133:LYS:HE3	2:B:135:ARG:NH2	1.95	0.79
2:B:46:GLN:HB2	2:B:408:LEU:HD21	1.65	0.79
1:A:21:LEU:HD11	1:A:1414:ALA:HA	1.65	0.79
2:B:995:ARG:HH12	3:C:165:LYS:HG2	1.47	0.79
4:D:8:PHE:CD2	7:G:6:ASP:HB2	2.18	0.79
11:K:6:ARG:O	11:K:9:LEU:HG	1.81	0.79
7:G:7:LEU:HB2	7:G:74:TYR:HE2	1.43	0.79
11:K:12:LEU:N	11:K:12:LEU:HD12	1.97	0.79
1:A:148:CYS:O	1:A:168:GLY:HA2	1.82	0.78
2:B:35:SER:HA	2:B:811:TYR:HE2	1.48	0.78
3:C:238:ILE:HD11	3:C:246:ARG:HH11	1.47	0.78
3:C:39:ALA:CA	3:C:164:ALA:HB3	2.12	0.78
8:H:44:VAL:HG13	8:H:48:PRO:HA	1.63	0.78
12:L:30:ILE:O	12:L:56:LEU:HA	1.82	0.78
1:A:92:HIS:HB2	1:A:236:LEU:HD21	1.63	0.78
1:A:982:THR:H	1:A:985:ASP:HB2	1.47	0.78
3:C:73:GLN:HE21	3:C:74:SER:H	1.29	0.78
7:G:88:ASP:HB3	7:G:144:ARG:HA	1.66	0.78
1:A:372:LYS:HA	1:A:435:HIS:ND1	1.98	0.78
2:B:880:THR:CB	2:B:934:LYS:HD3	2.12	0.78
7:G:128:PRO:O	7:G:138:THR:HG23	1.83	0.78
3:C:235:VAL:HG12	10:J:13:VAL:HG23	1.64	0.78
2:B:1162:ILE:HD11	2:B:1194:ILE:HD13	1.64	0.78
5:E:207:ARG:NH1	5:E:207:ARG:HB3	1.98	0.78
8:H:27:GLU:HG2	8:H:39:THR:HA	1.66	0.78
12:L:28:LYS:HB2	12:L:39:SER:HB2	1.65	0.78
5:E:109:ILE:HG22	5:E:110:PHE:H	1.47	0.78
13:T:13:DT:H2"	13:T:14:DA:OP2	1.83	0.78
1:A:84:ILE:HD11	1:A:270:LEU:HD13	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:412:LEU:HB3	2:B:466:TRP:HE1	1.48	0.78
2:B:579:ARG:HB2	2:B:586:TRP:HE1	1.46	0.78
4:D:18:VAL:O	4:D:19:GLU:HB2	1.82	0.78
10:J:1:MET:N	10:J:57:ILE:H	1.82	0.78
1:A:567:LYS:HB3	1:A:568:PRO:HD3	1.65	0.78
2:B:613:VAL:HG13	2:B:627:PHE:O	1.84	0.78
2:B:549:THR:HB	2:B:628:THR:OG1	1.84	0.78
8:H:41:ASP:O	8:H:42:ILE:HG13	1.84	0.78
1:A:1004:ASN:HD21	5:E:167:ARG:HD2	1.46	0.78
2:B:294:ASP:O	2:B:296:GLU:N	2.17	0.78
11:K:30:ALA:HB2	11:K:76:GLN:HG3	1.64	0.78
1:A:1100:ARG:NH2	1:A:1351:GLU:HG2	1.99	0.78
1:A:320:ARG:CB	1:A:320:ARG:HH11	1.97	0.78
2:B:244:LEU:HD11	2:B:366:GLN:NE2	1.97	0.78
2:B:70:ILE:O	2:B:137:TYR:HB2	1.84	0.78
2:B:882:THR:HG22	2:B:884:ARG:H	1.49	0.78
2:B:880:THR:HB	2:B:934:LYS:CD	2.12	0.78
1:A:696:GLU:OE2	1:A:702:LEU:HD21	1.83	0.77
8:H:25:ARG:HA	8:H:41:ASP:HA	1.65	0.77
8:H:80:ARG:HH11	11:K:57:LEU:HD21	1.49	0.77
2:B:1095:LEU:HD12	2:B:1095:LEU:N	1.99	0.77
4:D:40:HIS:CB	7:G:73:LYS:HZ2	1.97	0.77
5:E:109:ILE:HG22	5:E:110:PHE:N	1.99	0.77
8:H:128:ASN:H	8:H:130:ARG:HH11	1.30	0.77
1:A:541:ILE:HD13	1:A:549:MET:CE	2.14	0.77
1:A:567:LYS:HD3	1:A:568:PRO:HD3	1.65	0.77
1:A:56:PRO:O	1:A:57:ARG:HG3	1.84	0.77
1:A:629:LEU:O	1:A:633:VAL:HG23	1.83	0.77
1:A:635:ARG:HH11	1:A:635:ARG:HA	1.50	0.77
2:B:611:PRO:HG2	2:B:685:LEU:HD21	1.67	0.77
4:D:139:LYS:HE2	4:D:143:ASN:HD21	1.47	0.77
11:K:55:LYS:HB3	11:K:81:TYR:CD1	2.20	0.77
2:B:277:LYS:O	2:B:278:GLN:HB2	1.83	0.77
3:C:38:ILE:HA	3:C:173:ALA:HB2	1.66	0.77
3:C:46:ILE:HG13	3:C:72:LEU:HD11	1.66	0.77
1:A:1175:SER:O	1:A:1176:LEU:HB2	1.84	0.77
2:B:723:VAL:HG12	2:B:724:ASP:H	1.49	0.77
8:H:130:ARG:N	8:H:130:ARG:HD2	1.98	0.77
9:I:7:CYS:HB3	9:I:14:LEU:HD21	1.66	0.77
1:A:284:ALA:C	1:A:286:HIS:H	1.88	0.77
1:A:1325:THR:O	5:E:148:GLU:HB2	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1444:MET:HG3	7:G:60:ARG:HA	1.66	0.77
1:A:189:ARG:HA	1:A:195:ASP:HA	1.65	0.77
1:A:477:PRO:HG2	1:A:521:MET:HG2	1.67	0.77
1:A:1343:ALA:HB2	5:E:150:VAL:HG22	1.64	0.77
1:A:49:LYS:NZ	1:A:61:ILE:H	1.82	0.77
11:K:107:THR:O	11:K:111:LEU:HG	1.85	0.77
11:K:31:VAL:HG12	11:K:32:VAL:H	1.50	0.77
11:K:55:LYS:HB3	11:K:81:TYR:HD1	1.49	0.77
1:A:899:VAL:HG22	1:A:1029:ARG:HG2	1.65	0.77
1:A:11:LEU:HD12	1:A:11:LEU:C	2.05	0.77
1:A:1115:SER:C	1:A:1308:THR:HG22	2.04	0.77
1:A:590:ARG:HH21	1:A:620:LYS:HB3	1.48	0.77
2:B:464:GLY:O	2:B:477:ALA:HA	1.85	0.77
15:P:3:U:H2'	15:P:4:C:C6	2.20	0.77
1:A:1160:SER:HA	1:A:1170:ILE:HD13	1.65	0.76
1:A:1308:THR:HG23	1:A:1310:GLY:H	1.50	0.76
2:B:506:GLY:HA2	2:B:512:ARG:NH2	1.99	0.76
2:B:906:SER:O	2:B:941:LEU:HD23	1.83	0.76
7:G:119:LEU:HD12	7:G:131:GLN:O	1.85	0.76
11:K:31:VAL:HG12	11:K:32:VAL:N	2.00	0.76
1:A:343:LYS:NZ	2:B:1151:LEU:HD12	2.00	0.76
2:B:1069:PHE:HD1	2:B:1069:PHE:H	1.31	0.76
2:B:800:GLN:HB3	10:J:52:THR:HG22	1.67	0.76
3:C:235:VAL:HG11	10:J:6:ARG:HH21	1.49	0.76
11:K:46:ILE:O	11:K:50:LEU:HB2	1.85	0.76
1:A:12:ARG:HD2	2:B:1218:THR:HB	1.67	0.76
1:A:837:ILE:HA	1:A:840:ARG:HD3	1.67	0.76
2:B:745:PRO:O	2:B:748:ILE:HG12	1.84	0.76
4:D:8:PHE:HD2	7:G:6:ASP:HB2	1.50	0.76
13:T:16:DT:C2'	13:T:17:DT:H5'	2.14	0.76
1:A:577:ILE:O	1:A:580:VAL:HG23	1.85	0.76
1:A:869:GLY:O	5:E:204:THR:HG21	1.86	0.76
2:B:803:LEU:HD12	2:B:1032:SER:HB3	1.67	0.76
2:B:326:ASP:OD2	2:B:328:GLU:HB3	1.85	0.76
1:A:115:LEU:HG	1:A:142:CYS:HB3	1.68	0.76
1:A:381:THR:C	1:A:383:TYR:H	1.88	0.76
1:A:754:SER:N	1:A:757:ASN:HD22	1.83	0.76
2:B:314:LEU:O	2:B:318:VAL:HG23	1.84	0.76
2:B:755:ILE:HG23	2:B:809:MET:HE3	1.65	0.76
1:A:852:TYR:CD2	1:A:1060:PRO:HB2	2.21	0.76
1:A:392:VAL:HG13	1:A:415:LEU:HD11	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:670:ILE:HG23	1:A:805:LEU:HD21	1.67	0.76
1:A:866:PHE:C	1:A:867:ILE:HD12	2.06	0.76
2:B:821:GLN:HE22	2:B:851:PHE:H	1.33	0.76
3:C:92:CYS:SG	3:C:94:LYS:HB2	2.26	0.76
2:B:1224:PHE:CE1	5:E:171:LYS:HG3	2.21	0.76
8:H:42:ILE:HG23	8:H:95:TYR:HE1	1.50	0.76
1:A:1101:LEU:HD12	1:A:1101:LEU:O	1.85	0.76
1:A:1315:GLU:C	1:A:1317:MET:H	1.88	0.75
2:B:758:PHE:CE1	2:B:1027:ILE:HG22	2.21	0.75
10:J:57:ILE:HA	10:J:60:PHE:HD2	1.51	0.75
1:A:34:LYS:NZ	1:A:57:ARG:HH21	1.84	0.75
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.22	0.75
2:B:757:PRO:HG3	2:B:1028:GLU:OE2	1.87	0.75
2:B:834:ASN:HA	2:B:838:SER:O	1.86	0.75
5:E:113:GLN:HA	5:E:137:GLU:HG3	1.68	0.75
1:A:504:LEU:HD11	6:F:91:ALA:CB	2.15	0.75
1:A:35:ILE:HG22	1:A:84:ILE:HD12	1.68	0.75
2:B:654:ARG:H	2:B:657:HIS:HD2	1.32	0.75
1:A:857:ARG:NH1	6:F:139:PRO:HB2	2.00	0.75
7:G:1:MET:SD	7:G:79:PHE:HD1	2.09	0.75
2:B:359:GLU:O	2:B:362:PRO:HD3	1.86	0.75
2:B:516:ASN:N	2:B:516:ASN:HD22	1.83	0.75
2:B:777:ALA:HA	2:B:1095:LEU:HA	1.66	0.75
5:E:212:ARG:HH11	5:E:212:ARG:HG3	1.50	0.75
1:A:34:LYS:NZ	1:A:57:ARG:NH2	2.35	0.75
2:B:806:THR:HG22	2:B:808:ALA:N	1.94	0.75
4:D:47:LEU:O	4:D:48:ILE:HD13	1.87	0.75
7:G:97:HIS:HA	7:G:112:LYS:HE2	1.68	0.75
1:A:43:GLU:HB2	1:A:46:THR:HB	1.67	0.75
1:A:583:PRO:HG2	1:A:586:ILE:HG13	1.69	0.75
4:D:40:HIS:HB3	7:G:73:LYS:HZ2	1.52	0.75
2:B:336:ARG:HE	2:B:348:ARG:NH1	1.84	0.75
2:B:855:PHE:HD1	2:B:856:PHE:N	1.84	0.75
2:B:97:VAL:HG22	2:B:128:LEU:HG	1.68	0.75
4:D:144:THR:HG21	7:G:46:LEU:HD13	1.69	0.75
3:C:89:GLU:O	3:C:90:ASP:HB3	1.86	0.75
8:H:99:GLY:HA3	8:H:118:PHE:HA	1.69	0.75
10:J:23:ASN:C	10:J:25:LEU:H	1.90	0.75
13:T:26:DT:H2"	13:T:27:DC:OP2	1.87	0.75
1:A:335:ARG:CD	2:B:1202:LEU:HD23	2.16	0.74
1:A:809:THR:H	1:A:812:GLU:HB2	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:28:THR:O	7:G:32:GLU:HG3	1.88	0.74
1:A:1394:THR:HG21	1:A:1398:MET:SD	2.26	0.74
1:A:463:ILE:HB	1:A:464:PRO:HD2	1.70	0.74
5:E:92:THR:O	5:E:95:THR:HB	1.87	0.74
1:A:1255:GLU:OE1	1:A:1258:HIS:HB2	1.88	0.74
2:B:69:LEU:CG	2:B:429:PHE:CE1	2.69	0.74
3:C:36:VAL:HG21	3:C:251:LEU:HB2	1.68	0.74
3:C:242:GLN:HA	3:C:245:VAL:HG23	1.68	0.74
5:E:23:VAL:HG13	5:E:78:LEU:HD13	1.70	0.74
10:J:44:TYR:HD2	10:J:44:TYR:H	1.31	0.74
1:A:298:PHE:CZ	1:A:314:ALA:HB2	2.22	0.74
1:A:940:ARG:HH11	1:A:940:ARG:HG2	1.51	0.74
2:B:850:LEU:HD12	2:B:851:PHE:H	1.52	0.74
2:B:957:ASN:O	2:B:959:ASP:N	2.20	0.74
3:C:93:ASP:OD1	3:C:122:SER:HB2	1.88	0.74
11:K:7:PHE:HB2	11:K:11:LEU:HD23	1.69	0.74
1:A:1280:GLU:O	1:A:1309:ASP:HB3	1.88	0.74
1:A:22:PHE:HB2	2:B:1211:ASN:OD1	1.88	0.74
1:A:132:LYS:HE2	1:A:1411:GLU:OE1	1.87	0.74
2:B:1180:PHE:HB3	2:B:1191:ILE:CD1	2.17	0.74
2:B:378:LEU:O	2:B:382:ILE:HG13	1.87	0.74
12:L:28:LYS:HD2	12:L:39:SER:OG	1.87	0.74
15:P:3:U:H2'	15:P:4:C:H6	1.53	0.74
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	2.23	0.74
1:A:1006:ILE:HD11	5:E:163:GLU:HG3	1.70	0.73
1:A:464:PRO:HG2	1:A:465:TYR:HD1	1.52	0.73
1:A:483:ASP:OD2	15:P:11:U:H5''	1.88	0.73
2:B:526:GLU:HG2	2:B:538:ASN:ND2	2.03	0.73
1:A:105:CYS:O	1:A:114:LEU:HG	1.88	0.73
1:A:889:SER:HB3	1:A:1297:GLU:HG3	1.70	0.73
1:A:7:SER:CB	2:B:1175:LEU:HD22	2.17	0.73
5:E:180:ARG:HH21	5:E:192:ARG:HB2	1.52	0.73
1:A:1391:ARG:HD2	1:A:1391:ARG:C	2.08	0.73
1:A:239:LEU:HD12	1:A:240:PRO:HD2	1.70	0.73
1:A:825:ILE:HD11	2:B:512:ARG:CB	2.13	0.73
2:B:1006:ILE:HG22	10:J:45:CYS:HB3	1.69	0.73
11:K:61:TYR:C	11:K:61:TYR:CD2	2.61	0.73
3:C:50:GLU:HG2	12:L:64:LEU:HD22	1.71	0.73
1:A:450:LEU:HD13	1:A:1074:GLU:HG2	1.69	0.73
2:B:23:ALA:HB1	2:B:24:PRO:HD2	1.69	0.73
3:C:128:ASN:O	3:C:129:ILE:HG13	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:109:LYS:HD2	8:H:111:LEU:HD11	1.71	0.73
12:L:60:ARG:HH21	12:L:65:VAL:HG21	1.52	0.73
1:A:288:ALA:HA	1:A:291:GLU:OE2	1.87	0.73
1:A:1219:THR:HG21	1:A:1271:ILE:HD11	1.71	0.73
1:A:14:VAL:N	1:A:1432:GLN:HE22	1.85	0.73
1:A:351:THR:HB	2:B:1103:ILE:HD12	1.69	0.73
1:A:591:PHE:HA	1:A:595:THR:HG21	1.70	0.73
3:C:112:ASN:HB3	3:C:114:TYR:CE1	2.24	0.73
9:I:111:THR:HG22	9:I:112:SER:H	1.54	0.73
1:A:10:PRO:HB3	4:D:3:VAL:HA	1.71	0.73
1:A:49:LYS:HZ1	1:A:61:ILE:H	1.32	0.73
3:C:22:LEU:HD13	3:C:230:MET:CE	2.19	0.73
6:F:79:ARG:NH2	6:F:150:GLU:OE1	2.22	0.73
1:A:438:ASP:OD2	1:A:461:LYS:HD2	1.89	0.72
1:A:464:PRO:HG2	1:A:465:TYR:CD1	2.23	0.72
1:A:506:ALA:HB1	1:A:508:PRO:HD2	1.71	0.72
1:A:682:THR:CG2	1:A:728:LYS:HE3	2.19	0.72
8:H:100:THR:HG22	8:H:101:ALA:N	2.03	0.72
1:A:1116:LEU:N	1:A:1308:THR:HG22	2.03	0.72
1:A:34:LYS:HB3	1:A:36:ARG:HH21	1.52	0.72
1:A:896:ARG:NH2	1:A:1030:ARG:HE	1.86	0.72
2:B:1097:HIS:N	2:B:1098:MET:HE2	2.02	0.72
2:B:708:GLU:HG3	2:B:709:ASP:H	1.53	0.72
11:K:65:HIS:HD2	11:K:67:PHE:H	1.36	0.72
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.29	0.72
1:A:335:ARG:HE	1:A:335:ARG:HA	1.54	0.72
1:A:511:ILE:HA	1:A:521:MET:HE3	1.69	0.72
1:A:535:THR:HG23	1:A:575:LYS:HG2	1.71	0.72
2:B:364:ILE:O	2:B:365:THR:HB	1.89	0.72
10:J:1:MET:N	10:J:56:LEU:N	2.36	0.72
2:B:193:LYS:HZ1	12:L:32:ALA:HB1	1.54	0.72
1:A:1420:ASP:O	1:A:1421:CYS:HB2	1.88	0.72
1:A:534:LEU:O	1:A:574:GLY:HA3	1.90	0.72
1:A:802:ASN:ND2	2:B:728:ARG:HB2	2.04	0.72
5:E:190:LEU:HD12	5:E:214:CYS:HB2	1.72	0.72
1:A:1101:LEU:HD11	1:A:1105:LEU:HD11	1.72	0.72
1:A:50:ILE:O	1:A:52:GLY:N	2.23	0.72
1:A:967:ALA:HA	1:A:1044:TRP:CZ3	2.24	0.72
4:D:119:ARG:HD3	4:D:221:TYR:CD2	2.25	0.72
5:E:61:GLN:HG3	5:E:78:LEU:O	1.89	0.72
8:H:129:TYR:H	8:H:130:ARG:NH1	1.87	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1193:LEU:HB2	1:A:1260:LEU:HD11	1.71	0.72
1:A:399:HIS:CB	1:A:400:PRO:HD3	2.20	0.72
2:B:1150:ARG:CG	2:B:1150:ARG:HH11	2.03	0.72
5:E:23:VAL:O	5:E:28:TYR:HB2	1.89	0.72
1:A:382:PRO:HB3	1:A:428:TYR:HE2	1.53	0.72
1:A:557:ASP:OD2	1:A:559:VAL:HB	1.88	0.72
1:A:890:ASP:H	1:A:1296:GLY:HA3	1.54	0.72
4:D:24:ALA:C	4:D:26:THR:H	1.92	0.72
6:F:79:ARG:HG3	6:F:144:GLU:HG2	1.72	0.72
1:A:470:LEU:HD23	1:A:470:LEU:H	1.51	0.72
3:C:44:LEU:HB2	3:C:77:ILE:HD11	1.71	0.72
1:A:1152:ILE:HD11	9:I:44:TYR:CD2	2.25	0.72
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.72	0.72
2:B:810:GLU:HA	2:B:815:ARG:NH2	2.02	0.72
2:B:906:SER:HA	2:B:946:ASN:HB2	1.70	0.72
12:L:30:ILE:O	12:L:56:LEU:HD23	1.90	0.72
1:A:763:ALA:O	1:A:803:SER:HB3	1.90	0.71
2:B:547:VAL:HG12	2:B:612:GLU:OE2	1.89	0.71
4:D:119:ARG:HG2	4:D:120:GLU:N	2.04	0.71
3:C:236:GLY:O	3:C:238:ILE:N	2.23	0.71
6:F:99:LEU:O	6:F:103:MET:HG2	1.90	0.71
9:I:105:SER:O	9:I:106:CYS:HB3	1.89	0.71
1:A:722:LEU:H	1:A:722:LEU:HD12	1.53	0.71
2:B:1106:ARG:NH1	2:B:1110:PRO:HG2	2.05	0.71
3:C:22:LEU:HD13	3:C:230:MET:HE3	1.73	0.71
5:E:195:VAL:HG12	5:E:196:VAL:H	1.54	0.71
1:A:356:ASP:HB2	1:A:469:ARG:NH1	2.05	0.71
1:A:903:ASN:HD22	1:A:904:THR:H	1.39	0.71
2:B:862:GLN:HG2	2:B:963:PHE:HD1	1.56	0.71
3:C:75:MET:HB3	3:C:128:ASN:HB3	1.72	0.71
9:I:74:GLU:HA	9:I:80:SER:O	1.90	0.71
13:T:9:DC:H2"	13:T:10:DA:C8	2.25	0.71
1:A:1116:LEU:HD13	1:A:1329:THR:HB	1.73	0.71
1:A:1436:ILE:HD13	2:B:1139:ILE:HG23	1.73	0.71
2:B:582:VAL:HB	2:B:587:HIS:HD2	1.54	0.71
8:H:64:ASN:OD1	8:H:90:ALA:N	2.20	0.71
12:L:61:THR:HG21	12:L:63:ARG:NE	2.05	0.71
1:A:32:VAL:HG23	1:A:57:ARG:HB2	1.71	0.71
1:A:567:LYS:HD2	8:H:95:TYR:CD2	2.26	0.71
2:B:412:LEU:HB3	2:B:466:TRP:NE1	2.06	0.71
2:B:60:GLN:O	2:B:63:ILE:HG22	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:147:LEU:HB2	3:C:151:GLN:CB	2.21	0.71
5:E:44:ALA:O	5:E:45:LYS:HB2	1.90	0.71
8:H:101:ALA:HB2	8:H:116:TYR:CE2	2.24	0.71
8:H:89:LEU:HB3	8:H:91:ASP:OD1	1.90	0.71
9:I:76:PRO:HD2	9:I:108:HIS:HD2	1.54	0.71
1:A:853:ASP:O	1:A:854:ASN:HB2	1.89	0.71
1:A:868:TYR:OH	1:A:1366:ARG:HD3	1.89	0.71
2:B:126:SER:OG	2:B:172:ILE:HD11	1.91	0.71
6:F:79:ARG:HB2	6:F:79:ARG:HH11	1.55	0.71
9:I:71:SER:OG	9:I:83:ASN:HB2	1.90	0.71
1:A:1032:LEU:O	1:A:1036:ARG:HD3	1.91	0.71
1:A:184:SER:HB3	1:A:199:LEU:HD23	1.73	0.71
1:A:524:VAL:HG12	1:A:525:GLN:N	2.04	0.71
1:A:816:HIS:CD2	2:B:764:SER:HB2	2.26	0.71
1:A:96:ILE:CG2	1:A:97:ALA:N	2.53	0.71
5:E:63:ASN:HB3	5:E:64:PRO:HD2	1.73	0.71
9:I:58:VAL:HG13	9:I:62:ILE:CD1	2.20	0.71
1:A:963:ILE:HD11	1:A:1048:ASN:CB	2.21	0.71
1:A:225:ASN:ND2	1:A:228:PHE:N	2.31	0.71
1:A:438:ASP:O	1:A:439:ASN:HB2	1.90	0.71
1:A:356:ASP:HB2	1:A:469:ARG:HH12	1.56	0.71
6:F:109:VAL:HG12	6:F:110:ASP:N	2.06	0.71
8:H:95:TYR:CE2	8:H:97:MET:HG3	2.26	0.71
12:L:61:THR:CG2	12:L:63:ARG:HE	2.03	0.71
14:N:3:DT:H1'	14:N:4:DA:C8	2.25	0.71
1:A:34:LYS:HZ1	1:A:57:ARG:HH21	1.34	0.71
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.71	0.71
2:B:713:ALA:HB1	2:B:714:GLU:OE1	1.91	0.71
3:C:73:GLN:NE2	3:C:74:SER:H	1.87	0.71
1:A:1006:ILE:CD1	5:E:163:GLU:HG3	2.21	0.70
1:A:1107:VAL:HG12	1:A:1107:VAL:O	1.91	0.70
1:A:117:GLU:H	1:A:117:GLU:CD	1.93	0.70
1:A:722:LEU:HD23	1:A:799:PHE:CD1	2.26	0.70
1:A:960:ILE:O	1:A:963:ILE:HG22	1.91	0.70
2:B:291:ILE:HD13	2:B:300:HIS:NE2	2.05	0.70
2:B:583:ASN:ND2	2:B:628:THR:HG22	2.05	0.70
7:G:23:LYS:HG3	7:G:56:ILE:HD11	1.73	0.70
1:A:515:GLN:HA	1:A:1367:HIS:HE2	1.57	0.70
1:A:381:THR:O	1:A:383:TYR:N	2.24	0.70
1:A:41:MET:HB2	1:A:49:LYS:CA	2.17	0.70
1:A:616:VAL:HG12	1:A:617:VAL:N	2.05	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:903:ASN:ND2	1:A:904:THR:N	2.37	0.70
2:B:294:ASP:C	2:B:296:GLU:H	1.95	0.70
2:B:977:GLY:HA3	2:B:1099:VAL:HB	1.73	0.70
4:D:9:GLN:NE2	4:D:31:GLN:HE21	1.89	0.70
8:H:64:ASN:HD22	8:H:88:SER:HB2	1.55	0.70
9:I:13:MET:CE	9:I:14:LEU:H	2.04	0.70
1:A:1027:ALA:O	1:A:1031:VAL:HG23	1.91	0.70
1:A:144:THR:O	1:A:146:MET:HG3	1.90	0.70
1:A:49:LYS:HZ1	1:A:61:ILE:CG1	2.04	0.70
1:A:567:LYS:CB	1:A:568:PRO:HD3	2.21	0.70
1:A:535:THR:CG2	1:A:616:VAL:HA	2.20	0.70
11:K:63:VAL:O	11:K:63:VAL:HG23	1.92	0.70
1:A:834:THR:HG21	1:A:1077:THR:HG23	1.72	0.70
1:A:466:SER:HB2	2:B:1099:VAL:CG2	2.21	0.70
4:D:119:ARG:HD3	4:D:221:TYR:CE2	2.26	0.70
1:A:896:ARG:NH2	1:A:1030:ARG:HH21	1.89	0.70
2:B:112:LEU:HD12	2:B:113:TYR:H	1.57	0.70
2:B:613:VAL:HG22	2:B:628:THR:HA	1.73	0.70
5:E:22:MET:HE3	5:E:26:ARG:NH1	2.04	0.70
6:F:132:LEU:HD21	7:G:61:ILE:HD11	1.72	0.70
8:H:129:TYR:N	8:H:130:ARG:HH11	1.89	0.70
1:A:37:PHE:HD1	1:A:37:PHE:N	1.89	0.70
1:A:382:PRO:HD3	1:A:428:TYR:CD2	2.19	0.70
1:A:885:THR:O	1:A:885:THR:HG22	1.91	0.70
2:B:229:ALA:HB1	2:B:231:PRO:HD2	1.72	0.70
2:B:603:LEU:HD13	2:B:608:ASP:HB3	1.74	0.70
9:I:35:VAL:HG12	9:I:36:GLU:H	1.56	0.70
9:I:85:PHE:HD2	9:I:85:PHE:N	1.87	0.70
10:J:24:LEU:HD12	10:J:39:LEU:HD11	1.73	0.70
12:L:38:LEU:O	12:L:39:SER:HB3	1.92	0.70
1:A:1057:VAL:HG12	1:A:1058:VAL:N	2.06	0.70
1:A:1066:VAL:O	1:A:1070:GLN:HG3	1.91	0.70
1:A:332:LYS:H	1:A:337:ARG:CB	2.05	0.70
2:B:244:LEU:HD21	2:B:366:GLN:HE21	1.56	0.70
2:B:69:LEU:CD2	2:B:429:PHE:CE1	2.74	0.70
3:C:107:SER:O	3:C:109:SER:N	2.23	0.70
3:C:5:GLY:O	3:C:7:GLN:HG3	1.92	0.70
9:I:111:THR:HG22	9:I:112:SER:N	2.06	0.70
2:B:918:ILE:HD12	2:B:935:ARG:CZ	2.22	0.70
1:A:1036:ARG:HH11	1:A:1036:ARG:HG2	1.56	0.70
1:A:1420:ASP:HB3	1:A:1422:ARG:HG3	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.74	0.70
1:A:230:ARG:H	1:A:233:TRP:HE3	1.38	0.70
1:A:252:PHE:O	1:A:256:GLN:HB2	1.92	0.70
1:A:774:ARG:NH1	1:A:797:LYS:HG3	2.07	0.70
3:C:73:GLN:HE21	3:C:75:MET:N	1.89	0.70
1:A:1149:ALA:HB2	9:I:47:GLU:HA	1.74	0.70
3:C:259:LEU:HD21	11:K:91:CYS:HB3	1.73	0.70
7:G:122:ASN:ND2	7:G:125:SER:HB3	2.07	0.70
8:H:118:PHE:O	8:H:120:GLY:N	2.25	0.70
8:H:125:LEU:HG	8:H:126:GLU:H	1.55	0.70
1:A:317:LYS:O	1:A:318:SER:HB3	1.92	0.69
1:A:596:THR:C	1:A:598:LEU:H	1.95	0.69
2:B:172:ILE:HD13	2:B:178:ASN:HD22	1.56	0.69
1:A:1116:LEU:HB3	1:A:1308:THR:HG21	1.73	0.69
1:A:332:LYS:H	1:A:337:ARG:HB2	1.57	0.69
1:A:35:ILE:HG22	1:A:35:ILE:O	1.92	0.69
1:A:567:LYS:HB2	8:H:96:VAL:H	1.56	0.69
1:A:885:THR:O	1:A:940:ARG:HD2	1.91	0.69
1:A:96:ILE:HG22	1:A:97:ALA:H	1.57	0.69
2:B:1095:LEU:CD1	2:B:1095:LEU:H	2.03	0.69
5:E:153:HIS:HB3	5:E:196:VAL:CG1	2.22	0.69
6:F:147:SER:OG	6:F:150:GLU:HG3	1.91	0.69
12:L:53:HIS:HB3	12:L:55:ILE:CD1	2.22	0.69
1:A:883:LEU:HD11	1:A:1017:LEU:HD11	1.75	0.69
1:A:12:ARG:HB2	2:B:1218:THR:CG2	2.20	0.69
1:A:202:LEU:HA	1:A:206:GLU:OE1	1.92	0.69
2:B:1007:VAL:CG2	2:B:1008:PRO:HD2	2.22	0.69
2:B:405:ARG:NE	2:B:632:ARG:HG2	2.07	0.69
2:B:637:LEU:HD21	2:B:742:GLU:OE2	1.92	0.69
5:E:117:THR:HG22	5:E:119:SER:N	2.07	0.69
8:H:104:PHE:CZ	8:H:136:LYS:HA	2.27	0.69
8:H:15:VAL:HG13	8:H:26:ILE:HG12	1.72	0.69
8:H:38:LEU:HD12	8:H:124:ARG:O	1.92	0.69
2:B:1215:ARG:O	2:B:1216:LEU:HD23	1.91	0.69
2:B:189:LEU:HD13	2:B:196:PRO:HA	1.74	0.69
8:H:106:GLU:HG2	8:H:112:ILE:HG12	1.71	0.69
1:A:1081:LEU:HD11	1:A:1097:GLY:HA3	1.73	0.69
1:A:829:VAL:C	1:A:831:THR:H	1.93	0.69
2:B:746:SER:HB2	2:B:1046:PRO:HG2	1.74	0.69
2:B:175:ARG:HH11	2:B:175:ARG:HG2	1.56	0.69
2:B:654:ARG:H	2:B:657:HIS:CD2	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1164:PRO:HG2	1:A:1165:GLU:H	1.55	0.69
2:B:911:ILE:HD11	2:B:941:LEU:CD1	2.23	0.69
2:B:999:MET:HB3	2:B:1007:VAL:HG21	1.73	0.69
4:D:155:ARG:HD3	4:D:221:TYR:CZ	2.27	0.69
5:E:173:SER:O	5:E:175:LEU:N	2.24	0.69
1:A:913:LEU:CD1	1:A:914:GLU:H	2.06	0.69
12:L:53:HIS:O	12:L:55:ILE:HD13	1.91	0.69
1:A:608:ILE:HB	1:A:613:ILE:HD11	1.73	0.69
7:G:30:LEU:HD13	7:G:72:VAL:HG11	1.73	0.69
12:L:26:THR:HG23	12:L:62:LYS:NZ	2.07	0.69
1:A:49:LYS:NZ	1:A:61:ILE:N	2.41	0.69
2:B:497:ARG:HH22	2:B:775:LYS:CE	2.04	0.69
3:C:212:PRO:HB3	3:C:213:PRO:HD2	1.74	0.69
2:B:430:ARG:O	2:B:434:ARG:HD2	1.93	0.69
10:J:48:ARG:HE	10:J:49:MET:HE2	1.57	0.69
1:A:567:LYS:CG	1:A:568:PRO:HD3	2.22	0.69
1:A:552:TRP:HE3	1:A:651:LYS:HB3	1.57	0.69
2:B:1000:PRO:O	2:B:1007:VAL:HG23	1.92	0.69
2:B:1142:GLY:HA3	6:F:88:TYR:HE2	1.58	0.69
2:B:213:ILE:HD11	2:B:497:ARG:HB3	1.74	0.69
3:C:137:LYS:HB2	3:C:138:GLU:OE1	1.92	0.69
1:A:852:TYR:CD1	6:F:136:ARG:HB3	2.28	0.69
7:G:127:PRO:HG3	7:G:139:ILE:CD1	2.23	0.69
7:G:139:ILE:HG22	7:G:140:LYS:HD3	1.75	0.69
1:A:709:THR:HB	1:A:712:GLU:H	1.58	0.68
1:A:870:GLU:O	5:E:205:SER:HB3	1.93	0.68
6:F:106:PRO:HG2	7:G:18:PHE:O	1.93	0.68
6:F:75:PRO:HG2	6:F:77:ASP:O	1.93	0.68
1:A:90:VAL:HG13	1:A:297:GLN:CD	2.13	0.68
1:A:630:ILE:HD11	1:A:646:PHE:HZ	1.55	0.68
2:B:1159:ARG:HB3	2:B:1159:ARG:NH1	2.08	0.68
2:B:483:LEU:HD11	2:B:491:THR:HG23	1.75	0.68
3:C:235:VAL:HG11	10:J:6:ARG:NH2	2.07	0.68
4:D:134:THR:HG22	4:D:136:GLY:H	1.58	0.68
2:B:100:PRO:HA	2:B:125:SER:O	1.93	0.68
2:B:273:LEU:HD12	2:B:276:ILE:HD12	1.75	0.68
2:B:751:VAL:HG13	2:B:812:LEU:HD22	1.75	0.68
3:C:100:THR:HG22	3:C:101:LEU:H	1.57	0.68
1:A:504:LEU:HD11	6:F:91:ALA:HB1	1.75	0.68
1:A:475:THR:HG23	1:A:476:SER:N	2.08	0.68
1:A:866:PHE:HE1	5:E:211:TYR:H	1.41	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:273:LEU:CB	2:B:276:ILE:HD12	2.21	0.68
2:B:364:ILE:HG12	2:B:585:VAL:HG13	1.76	0.68
2:B:879:ARG:NH1	2:B:883:LEU:HD22	2.07	0.68
2:B:955:THR:CG2	2:B:956:THR:N	2.56	0.68
3:C:184:ASN:ND2	3:C:187:LYS:HA	2.08	0.68
1:A:1100:ARG:HH21	1:A:1351:GLU:HG2	1.58	0.68
1:A:382:PRO:HB3	1:A:428:TYR:CE2	2.27	0.68
2:B:852:ARG:HH22	12:L:70:ARG:C	1.97	0.68
4:D:170:THR:C	4:D:172:LEU:H	1.97	0.68
14:N:2:DG:H4'	14:N:3:DT:OP1	1.94	0.68
1:A:2:VAL:HG11	2:B:1157:ALA:HB1	1.74	0.68
1:A:883:LEU:HD23	1:A:1021:LEU:HD13	1.76	0.68
2:B:497:ARG:HH22	2:B:775:LYS:HE2	1.58	0.68
2:B:863:GLU:OE2	2:B:873:THR:HA	1.94	0.68
8:H:84:ALA:HB2	8:H:87:ARG:HD2	1.75	0.68
1:A:857:ARG:HD3	1:A:861:GLY:O	1.94	0.68
2:B:638:PHE:HA	2:B:690:VAL:HG22	1.74	0.68
5:E:111:VAL:HG12	5:E:137:GLU:HG2	1.76	0.68
1:A:852:TYR:CE2	1:A:1060:PRO:HB2	2.27	0.68
1:A:285:PRO:HG2	1:A:288:ALA:HB3	1.75	0.68
1:A:427:GLN:HB2	1:A:430:TRP:CD1	2.28	0.68
1:A:658:LEU:HD23	1:A:659:HIS:CE1	2.29	0.68
2:B:1007:VAL:HG22	2:B:1008:PRO:HD2	1.76	0.68
2:B:423:LYS:HA	2:B:426:LYS:HE2	1.76	0.68
1:A:1339:LEU:HD13	5:E:147:HIS:CD2	2.29	0.68
6:F:109:VAL:HG11	6:F:123:LYS:CD	2.15	0.68
3:C:66:ARG:NH2	10:J:3:VAL:O	2.25	0.68
11:K:87:LEU:O	11:K:91:CYS:HB2	1.94	0.68
1:A:528:LEU:O	1:A:531:ILE:HG22	1.93	0.68
2:B:167:ILE:HD12	2:B:167:ILE:N	2.09	0.68
2:B:520:GLY:N	2:B:748:ILE:HG22	2.09	0.68
2:B:60:GLN:NE2	2:B:95:ILE:HG22	2.08	0.68
8:H:111:LEU:HA	8:H:127:GLY:O	1.93	0.68
1:A:11:LEU:HD12	1:A:11:LEU:O	1.94	0.68
2:B:114:PRO:HG3	2:B:181:LEU:HD11	1.76	0.68
2:B:582:VAL:HA	2:B:626:ILE:HB	1.74	0.68
7:G:102:GLN:HG3	7:G:106:MET:O	1.94	0.68
1:A:1308:THR:HG21	1:A:1310:GLY:O	1.94	0.67
1:A:910:PRO:HB3	1:A:916:GLY:HA3	1.75	0.67
3:C:80:LEU:HD11	3:C:95:CYS:C	2.14	0.67
1:A:1127:ASP:CG	1:A:1130:GLN:HB2	2.15	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1262:LYS:C	1:A:1264:GLU:H	1.97	0.67
1:A:402:ALA:CB	1:A:434:ARG:HA	2.25	0.67
1:A:825:ILE:CG2	1:A:826:ASP:N	2.58	0.67
1:A:84:ILE:HG23	1:A:84:ILE:O	1.93	0.67
1:A:903:ASN:HD22	1:A:903:ASN:C	1.97	0.67
1:A:981:LEU:CD2	1:A:1039:LYS:HA	2.23	0.67
2:B:519:TRP:HE1	2:B:635:ARG:NH2	1.92	0.67
2:B:855:PHE:HD1	2:B:855:PHE:C	1.97	0.67
3:C:193:TYR:HD2	3:C:197:SER:HB3	1.60	0.67
3:C:146:LYS:HB2	10:J:61:LEU:HD11	1.77	0.67
12:L:40:LEU:HD22	12:L:44:ASP:CG	2.15	0.67
1:A:447:GLN:NE2	13:T:20:DG:H4'	2.09	0.67
1:A:216:VAL:O	1:A:219:PHE:HB2	1.94	0.67
1:A:353:ILE:HD13	1:A:487:MET:HE2	1.75	0.67
2:B:408:LEU:HD22	2:B:545:ILE:HD12	1.77	0.67
3:C:123:ASN:HD21	3:C:125:MET:HA	1.60	0.67
8:H:4:THR:HG22	8:H:5:LEU:H	1.59	0.67
8:H:89:LEU:C	8:H:91:ASP:H	1.98	0.67
1:A:1224:LEU:HD11	1:A:1240:CYS:HB2	1.75	0.67
2:B:1181:GLU:O	2:B:1182:CYS:HB3	1.93	0.67
3:C:99:LEU:HD22	3:C:120:ILE:HG12	1.75	0.67
3:C:77:ILE:N	3:C:129:ILE:HD11	2.08	0.67
5:E:195:VAL:HG12	5:E:196:VAL:N	2.09	0.67
2:B:98:THR:O	2:B:126:SER:HB2	1.95	0.67
2:B:168:GLY:HA2	2:B:454:THR:OG1	1.94	0.67
3:C:77:ILE:HG22	3:C:78:GLU:N	2.09	0.67
4:D:69:ALA:HA	4:D:72:ARG:HD2	1.77	0.67
5:E:15:ALA:O	5:E:19:VAL:HG23	1.94	0.67
7:G:96:GLN:O	7:G:112:LYS:HD3	1.94	0.67
1:A:446:ARG:HB2	1:A:487:MET:SD	2.33	0.67
2:B:193:LYS:HZ2	12:L:32:ALA:HB1	1.57	0.67
2:B:288:ALA:HA	2:B:331:LEU:HD12	1.74	0.67
2:B:810:GLU:CB	2:B:815:ARG:HH22	2.06	0.67
2:B:999:MET:HA	2:B:999:MET:HE2	1.77	0.67
3:C:238:ILE:CG2	3:C:242:GLN:HB2	2.20	0.67
4:D:39:ASN:HD22	4:D:41:GLN:HB2	1.60	0.67
5:E:154:ILE:H	5:E:196:VAL:HG13	1.58	0.67
9:I:17:ARG:HG3	9:I:28:GLU:OE1	1.95	0.67
1:A:416:ARG:NH1	1:A:417:TYR:HE2	1.93	0.67
2:B:515:HIS:H	2:B:518:HIS:CD2	2.12	0.67
2:B:596:LEU:O	2:B:600:LEU:HG	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25:ILE:HG23	2:B:658:ILE:HD11	1.76	0.67
2:B:999:MET:HA	2:B:999:MET:CE	2.25	0.67
8:H:55:LEU:HB3	8:H:144:ILE:HG23	1.76	0.67
10:J:36:LEU:HB2	10:J:47:ARG:HH12	1.60	0.67
1:A:37:PHE:N	1:A:37:PHE:CD1	2.60	0.67
1:A:606:LEU:HG	1:A:613:ILE:HB	1.76	0.67
2:B:133:LYS:CE	2:B:135:ARG:HH21	2.01	0.67
3:C:56:THR:HG21	3:C:145:CYS:SG	2.34	0.67
1:A:1264:GLU:HG3	1:A:1265:ASN:N	2.10	0.67
1:A:552:TRP:CE3	1:A:651:LYS:HB3	2.29	0.67
1:A:855:THR:HG21	1:A:857:ARG:NE	2.08	0.67
2:B:383:ASN:C	2:B:387:LEU:HD13	2.15	0.67
2:B:546:SER:OG	2:B:631:GLY:N	2.27	0.67
2:B:616:ILE:HD12	2:B:616:ILE:N	2.10	0.67
2:B:744:HIS:HD2	2:B:746:SER:OG	1.78	0.67
2:B:1084:GLN:HG2	3:C:201:TRP:HZ2	1.59	0.67
7:G:48:VAL:HA	7:G:76:ALA:HB2	1.75	0.67
1:A:1148:ILE:HD11	1:A:1198:ASP:HA	1.76	0.67
1:A:1227:ILE:HG22	1:A:1228:TRP:N	2.07	0.67
1:A:802:ASN:HD21	2:B:729:ILE:H	1.41	0.67
2:B:1201:LYS:HE2	2:B:1205:GLN:OE1	1.94	0.67
2:B:29:ASP:CG	2:B:658:ILE:HD13	2.14	0.67
5:E:157:SER:OG	5:E:160:GLU:HG3	1.95	0.67
3:C:35:ARG:NH1	11:K:41:THR:OG1	2.27	0.67
1:A:1313:LEU:HD23	1:A:1338:VAL:HG21	1.75	0.66
1:A:451:HIS:O	2:B:1137:CYS:SG	2.52	0.66
2:B:822:ASN:HD21	10:J:52:THR:HG21	1.60	0.66
4:D:8:PHE:CZ	4:D:37:GLN:HB2	2.30	0.66
8:H:15:VAL:HA	8:H:26:ILE:HG23	1.76	0.66
9:I:73:ARG:HH12	9:I:112:SER:HB3	1.60	0.66
1:A:1151:GLU:OE2	9:I:45:ARG:HD2	1.96	0.66
3:C:3:GLU:HG3	11:K:104:ASN:OD1	1.95	0.66
11:K:67:PHE:C	11:K:68:PHE:HD2	1.98	0.66
11:K:45:LEU:HG	11:K:94:ILE:HD13	1.77	0.66
2:B:593:PRO:HA	2:B:596:LEU:HB3	1.76	0.66
2:B:1080:LYS:HD2	3:C:188:HIS:HB2	1.77	0.66
3:C:238:ILE:CD1	3:C:246:ARG:HH11	2.08	0.66
4:D:208:GLU:HG3	4:D:212:LYS:HE3	1.77	0.66
5:E:124:VAL:CG1	5:E:132:ILE:HG13	2.23	0.66
1:A:868:TYR:HD2	1:A:1058:VAL:HG21	1.60	0.66
1:A:929:LEU:HD23	1:A:983:ILE:CG2	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:136:ARG:O	6:F:143:PHE:HB2	1.95	0.66
1:A:1191:TRP:HB3	1:A:1260:LEU:HD23	1.77	0.66
1:A:1291:VAL:HG13	1:A:1292:PRO:HD2	1.77	0.66
1:A:524:VAL:HG12	1:A:525:GLN:H	1.59	0.66
1:A:833:GLU:HG2	1:A:1102:LYS:HD2	1.76	0.66
1:A:345:VAL:HG21	2:B:1150:ARG:HH22	1.61	0.66
2:B:273:LEU:O	2:B:276:ILE:HB	1.95	0.66
2:B:527:THR:OG1	2:B:528:PRO:HD2	1.95	0.66
2:B:755:ILE:HG23	2:B:809:MET:CE	2.26	0.66
3:C:36:VAL:HG21	3:C:251:LEU:HD13	1.77	0.66
3:C:73:GLN:HE21	3:C:75:MET:H	1.43	0.66
4:D:53:SER:HB3	4:D:152:SER:HB2	1.78	0.66
4:D:40:HIS:HB2	7:G:73:LYS:CE	2.26	0.66
8:H:102:TYR:N	8:H:102:TYR:HD2	1.91	0.66
1:A:698:GLN:HA	9:I:97:MET:O	1.96	0.66
1:A:1057:VAL:HG12	1:A:1058:VAL:H	1.61	0.66
2:B:230:ALA:N	2:B:231:PRO:HD2	2.11	0.66
2:B:511:PRO:O	2:B:513:GLN:N	2.28	0.66
1:A:1124:HIS:HB2	1:A:1130:GLN:HG2	1.78	0.66
1:A:116:ASP:OD2	1:A:164:ARG:HD2	1.95	0.66
2:B:487:THR:HG22	2:B:488:TYR:N	2.10	0.66
2:B:859:TYR:CZ	2:B:941:LEU:HD12	2.29	0.66
3:C:115:SER:O	3:C:118:LEU:HG	1.96	0.66
8:H:100:THR:HG23	8:H:138:GLU:CA	2.22	0.66
10:J:24:LEU:HA	10:J:28:ASP:HB2	1.77	0.66
1:A:106:VAL:HG12	1:A:107:CYS:H	1.58	0.66
1:A:456:MET:HE2	1:A:507:VAL:HA	1.76	0.66
1:A:903:ASN:ND2	1:A:905:ASP:H	1.93	0.66
2:B:102:VAL:HB	2:B:110:HIS:HB3	1.76	0.66
5:E:23:VAL:HG13	5:E:78:LEU:CD1	2.25	0.66
6:F:76:LYS:HA	6:F:79:ARG:CD	2.25	0.66
9:I:13:MET:HE2	9:I:14:LEU:H	1.59	0.66
10:J:1:MET:H1	10:J:57:ILE:H	1.40	0.66
1:A:14:VAL:H	1:A:1432:GLN:NE2	1.92	0.66
2:B:1072:MET:CE	2:B:1085:ILE:HB	2.25	0.66
2:B:276:ILE:HA	2:B:337:ARG:O	1.95	0.66
2:B:583:ASN:HD21	2:B:628:THR:CG2	2.08	0.66
1:A:1312:ASN:O	1:A:1316:VAL:HG23	1.95	0.66
1:A:79:GLY:HA3	1:A:243:PRO:CG	2.26	0.66
1:A:265:LYS:HD3	1:A:302:THR:HG23	1.76	0.66
1:A:372:LYS:HA	1:A:435:HIS:HD1	1.57	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LYS:CD	1:A:568:PRO:HD3	2.25	0.66
1:A:596:THR:O	1:A:598:LEU:N	2.28	0.66
1:A:899:VAL:CG1	1:A:908:LEU:HD21	2.25	0.66
1:A:979:SER:OG	1:A:980:ASP:N	2.28	0.66
2:B:648:HIS:CG	2:B:649:LYS:H	2.13	0.66
2:B:827:ILE:O	2:B:828:ALA:HB2	1.95	0.66
2:B:853:SER:O	2:B:854:LEU:HD23	1.96	0.66
2:B:860:MET:HG3	2:B:965:LYS:HG2	1.78	0.66
3:C:166:GLU:HG3	11:K:10:PHE:HZ	1.60	0.66
3:C:181:ASP:CG	3:C:186:LEU:HD13	2.15	0.66
2:B:996:ARG:NH1	3:C:38:ILE:HG23	2.11	0.66
5:E:144:ILE:HG13	5:E:145:THR:N	2.10	0.66
7:G:27:LYS:HE2	7:G:54:ILE:HB	1.78	0.66
7:G:49:LEU:HG	7:G:76:ALA:HA	1.78	0.66
13:T:21:DC:H2''	13:T:22:DC:H5'	1.76	0.66
1:A:129:LYS:O	1:A:130:ASP:HB2	1.95	0.66
1:A:442:VAL:O	1:A:457:ALA:HA	1.96	0.66
1:A:41:MET:CB	1:A:49:LYS:HA	2.18	0.66
2:B:1108:ARG:HG2	2:B:1109:GLY:N	2.11	0.66
2:B:1202:LEU:O	2:B:1206:GLU:HG3	1.96	0.66
2:B:220:GLY:O	2:B:222:ILE:HG13	1.96	0.66
2:B:613:VAL:HG13	2:B:628:THR:HA	1.78	0.66
2:B:975:GLN:O	2:B:990:ILE:HD12	1.95	0.66
3:C:238:ILE:HG22	3:C:243:VAL:HG23	1.77	0.66
4:D:148:LEU:O	4:D:152:SER:HB3	1.95	0.66
6:F:111:LEU:CD1	6:F:111:LEU:H	2.07	0.66
8:H:135:LEU:HD22	8:H:137:GLN:HE21	1.61	0.66
10:J:48:ARG:HD2	10:J:49:MET:N	2.10	0.66
1:A:96:ILE:HG22	1:A:97:ALA:N	2.11	0.65
3:C:239:PRO:HB2	3:C:241:ASP:OD1	1.96	0.65
9:I:31:THR:O	9:I:32:CYS:HB3	1.96	0.65
10:J:9:SER:CB	10:J:45:CYS:HB2	2.25	0.65
1:A:1198:ASP:HB3	1:A:1201:ALA:HB3	1.77	0.65
1:A:1438:THR:HB	2:B:1144:ALA:CB	2.25	0.65
1:A:38:PRO:HA	1:A:270:LEU:HD23	1.76	0.65
1:A:310:GLY:O	1:A:312:PRO:HD2	1.95	0.65
1:A:57:ARG:HG2	1:A:57:ARG:HH11	1.60	0.65
2:B:345:LYS:O	2:B:348:ARG:HG2	1.96	0.65
2:B:515:HIS:CD2	2:B:516:ASN:N	2.64	0.65
3:C:83:SER:HA	3:C:95:CYS:HB2	1.78	0.65
4:D:130:LEU:O	4:D:132:GLN:N	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:LEU:HD22	11:K:58:PHE:CE1	2.32	0.65
11:K:7:PHE:C	11:K:9:LEU:H	2.00	0.65
1:A:1028:THR:O	1:A:1032:LEU:HD12	1.96	0.65
1:A:1237:ILE:HG22	1:A:1238:ILE:N	2.11	0.65
1:A:253:ASN:HD22	1:A:256:GLN:NE2	1.94	0.65
1:A:7:SER:HB3	2:B:1175:LEU:HD22	1.78	0.65
2:B:314:LEU:O	2:B:317:CYS:HB3	1.97	0.65
2:B:464:GLY:C	2:B:465:ASN:HD22	1.99	0.65
3:C:161:LYS:HG3	3:C:162:GLY:N	2.12	0.65
3:C:18:VAL:HG23	3:C:240:VAL:CG1	2.26	0.65
5:E:96:PHE:O	5:E:99:HIS:HB3	1.96	0.65
11:K:50:LEU:HD11	11:K:75:ILE:HD13	1.77	0.65
1:A:1225:PHE:CZ	1:A:1227:ILE:HD11	2.32	0.65
1:A:836:TYR:CD2	1:A:840:ARG:HD2	2.31	0.65
2:B:102:VAL:O	2:B:102:VAL:HG12	1.96	0.65
2:B:282:ILE:HD11	2:B:317:CYS:SG	2.36	0.65
2:B:605:ARG:NH1	2:B:639:ILE:HG21	2.10	0.65
1:A:1392:SER:O	1:A:1394:THR:N	2.29	0.65
1:A:1447:GLU:OE2	7:G:23:LYS:HB2	1.97	0.65
1:A:55:ASP:C	1:A:57:ARG:H	2.00	0.65
2:B:978:ASP:OD2	2:B:1098:MET:HG2	1.96	0.65
2:B:773:MET:SD	2:B:987:LYS:HG2	2.37	0.65
5:E:28:TYR:C	5:E:65:THR:HG22	2.17	0.65
7:G:1:MET:HG2	7:G:85:GLU:OE2	1.96	0.65
11:K:53:ASP:HB3	11:K:56:VAL:CG2	2.27	0.65
12:L:55:ILE:HG12	12:L:56:LEU:N	2.11	0.65
1:A:276:LEU:HD13	1:A:293:GLU:HA	1.79	0.65
1:A:858:ASN:C	1:A:858:ASN:HD22	1.98	0.65
2:B:806:THR:HG23	2:B:1046:PRO:HD3	1.78	0.65
1:A:7:SER:HB2	2:B:1175:LEU:HD22	1.77	0.65
2:B:955:THR:HG22	2:B:956:THR:O	1.96	0.65
5:E:198:ILE:HD12	5:E:198:ILE:H	1.60	0.65
8:H:64:ASN:CB	8:H:88:SER:HB2	2.21	0.65
1:A:565:ILE:HG22	1:A:565:ILE:O	1.97	0.65
1:A:630:ILE:HG23	1:A:631:HIS:N	2.11	0.65
1:A:848:ILE:HA	1:A:857:ARG:O	1.95	0.65
1:A:466:SER:HB2	2:B:1099:VAL:HG21	1.79	0.65
2:B:508:LEU:O	2:B:509:ALA:HB2	1.97	0.65
5:E:124:VAL:N	5:E:125:PRO:HD2	2.12	0.65
5:E:7:ARG:HD2	5:E:7:ARG:C	2.17	0.65
8:H:40:LEU:HD13	8:H:123:MET:HB2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:8:ARG:HG3	9:I:34:TYR:CE1	2.32	0.65
11:K:18:LYS:NZ	11:K:38:GLU:HG2	2.11	0.65
1:A:739:ASP:OD2	8:H:19:ARG:HD2	1.97	0.65
1:A:855:THR:CG2	1:A:857:ARG:HE	2.10	0.65
1:A:91:PHE:HB3	1:A:96:ILE:HD12	1.79	0.65
2:B:1162:ILE:HD11	2:B:1194:ILE:CD1	2.26	0.65
2:B:589:VAL:HG12	2:B:590:HIS:N	2.12	0.65
2:B:843:GLN:N	2:B:994:TYR:O	2.19	0.65
5:E:197:LYS:HG2	5:E:199:ILE:HG13	1.78	0.65
8:H:135:LEU:HD22	8:H:137:GLN:NE2	2.12	0.65
9:I:7:CYS:N	9:I:14:LEU:HD21	2.12	0.65
11:K:12:LEU:HD23	11:K:16:GLU:O	1.96	0.65
13:T:7:DC:H2"	13:T:8:DT:C5	2.32	0.65
1:A:35:ILE:HB	1:A:83:HIS:O	1.97	0.65
1:A:767:GLN:HB2	1:A:799:PHE:HD1	1.60	0.65
1:A:785:PRO:HG2	1:A:786:HIS:CD2	2.32	0.65
1:A:898:ARG:HD2	1:A:899:VAL:N	2.12	0.65
2:B:165:VAL:HG11	2:B:448:ILE:CD1	2.27	0.65
2:B:449:ASN:O	2:B:451:LYS:N	2.30	0.65
4:D:123:LEU:O	4:D:127:ASP:HB2	1.97	0.65
7:G:13:LEU:HD23	7:G:14:HIS:H	1.60	0.65
1:A:1208:THR:HB	1:A:1211:GLN:CG	2.26	0.65
1:A:567:LYS:HZ3	8:H:95:TYR:CB	2.09	0.65
1:A:954:TRP:HB3	1:A:955:PRO:HD2	1.78	0.65
2:B:38:PHE:HD1	2:B:811:TYR:CD2	2.15	0.65
2:B:867:GLY:C	2:B:869:SER:H	1.99	0.65
3:C:167:HIS:ND1	3:C:169:LYS:HG2	2.11	0.65
5:E:198:ILE:HD12	5:E:198:ILE:N	2.12	0.65
6:F:70:LYS:O	6:F:72:LYS:HD2	1.96	0.65
1:A:35:ILE:CG2	1:A:84:ILE:HD12	2.27	0.64
1:A:565:ILE:O	1:A:570:PRO:HA	1.97	0.64
1:A:962:ARG:HA	1:A:965:GLN:HB2	1.77	0.64
2:B:100:PRO:HD2	2:B:180:TYR:CE1	2.32	0.64
2:B:26:THR:HA	2:B:708:GLU:OE1	1.96	0.64
2:B:766:ARG:HG3	2:B:1022:THR:HG23	1.78	0.64
3:C:261:ALA:O	3:C:265:MET:HB2	1.97	0.64
5:E:111:VAL:CG1	5:E:137:GLU:HG2	2.27	0.64
5:E:202:SER:OG	5:E:204:THR:HG22	1.97	0.64
7:G:59:GLY:HA3	7:G:70:PHE:CD2	2.31	0.64
8:H:100:THR:HG22	8:H:101:ALA:H	1.60	0.64
11:K:21:ILE:CG2	11:K:33:ILE:HG12	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:967:ALA:HA	1:A:1044:TRP:HZ3	1.62	0.64
1:A:172:PRO:HD3	1:A:185:TRP:NE1	2.12	0.64
1:A:34:LYS:CB	1:A:36:ARG:HH21	2.10	0.64
1:A:381:THR:HG23	1:A:382:PRO:HD2	1.78	0.64
1:A:469:ARG:HB3	1:A:469:ARG:HH11	1.60	0.64
11:K:102:LYS:O	11:K:106:GLU:HG3	1.97	0.64
1:A:1341:ILE:HG23	1:A:1342:GLU:N	2.11	0.64
1:A:474:VAL:HG22	1:A:474:VAL:O	1.96	0.64
1:A:828:ALA:HB2	2:B:530:GLY:HA2	1.79	0.64
2:B:1099:VAL:CG1	2:B:1100:ASP:H	2.08	0.64
6:F:79:ARG:HG3	6:F:144:GLU:CG	2.27	0.64
2:B:597:MET:HA	2:B:597:MET:CE	2.27	0.64
2:B:870:ILE:HG22	2:B:917:PRO:HG2	1.78	0.64
3:C:56:THR:HG22	3:C:57:VAL:H	1.61	0.64
4:D:22:GLU:H	4:D:22:GLU:CD	2.01	0.64
8:H:44:VAL:HG12	8:H:44:VAL:O	1.96	0.64
11:K:68:PHE:HB3	11:K:70:ARG:NH1	2.12	0.64
12:L:28:LYS:CB	12:L:39:SER:HB2	2.27	0.64
1:A:106:VAL:HG12	1:A:107:CYS:N	2.13	0.64
1:A:1242:VAL:HG12	1:A:1243:VAL:N	2.12	0.64
1:A:1438:THR:HG23	6:F:92:ARG:HB2	1.79	0.64
1:A:172:PRO:HB3	1:A:185:TRP:CD2	2.33	0.64
1:A:370:ILE:HG12	2:B:1105:ALA:HB2	1.79	0.64
1:A:590:ARG:HB3	1:A:605:MET:N	2.12	0.64
1:A:809:THR:HG23	1:A:812:GLU:OE1	1.97	0.64
2:B:90:ILE:HD12	2:B:432:MET:SD	2.38	0.64
1:A:315:LEU:HD13	2:B:471:LYS:HB3	1.78	0.64
11:K:50:LEU:HD11	11:K:75:ILE:CD1	2.28	0.64
1:A:506:ALA:HB3	1:A:509:LEU:HD12	1.79	0.64
2:B:1002:THR:HG21	2:B:1006:ILE:HD12	1.80	0.64
2:B:1186:ASP:O	4:D:17:LYS:HE2	1.97	0.64
2:B:243:ALA:CB	2:B:251:ILE:HG12	2.28	0.64
2:B:51:PHE:O	2:B:54:PHE:HB3	1.97	0.64
2:B:865:LYS:HG3	2:B:961:LEU:HD21	1.77	0.64
1:A:675:THR:OG1	1:A:736:ASN:ND2	2.29	0.64
2:B:288:ALA:HA	2:B:331:LEU:CD1	2.27	0.64
2:B:604:ARG:C	2:B:606:LYS:H	1.98	0.64
2:B:642:ASP:CA	2:B:649:LYS:HG3	2.28	0.64
2:B:918:ILE:CG2	2:B:919:SER:N	2.61	0.64
7:G:13:LEU:HD21	7:G:17:PHE:CD1	2.33	0.64
1:A:185:TRP:H	1:A:185:TRP:HE3	1.46	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:PHE:CD1	1:A:222:LEU:HD22	2.33	0.64
1:A:637:LYS:HB3	1:A:641:VAL:HG21	1.79	0.64
2:B:1174:LYS:O	2:B:1176:ASN:N	2.31	0.64
2:B:123:THR:OG1	2:B:458:LYS:HE2	1.98	0.64
2:B:502:ILE:HD12	2:B:502:ILE:H	1.62	0.64
2:B:891:ASP:C	2:B:893:LEU:H	2.00	0.64
2:B:863:GLU:O	2:B:961:LEU:HD22	1.98	0.64
5:E:54:GLN:O	5:E:57:MET:HB3	1.97	0.64
8:H:91:ASP:O	8:H:93:TYR:N	2.25	0.64
9:I:2:THR:HG22	9:I:3:THR:N	2.13	0.64
1:A:868:TYR:CD2	1:A:1058:VAL:HG21	2.33	0.64
1:A:90:VAL:HG13	1:A:297:GLN:OE1	1.97	0.64
1:A:39:GLU:OE1	1:A:50:ILE:HD12	1.98	0.64
1:A:666:ILE:HD12	1:A:667:GLY:N	2.08	0.64
1:A:900:ASP:HA	1:A:926:GLN:NE2	2.12	0.64
1:A:666:ILE:N	2:B:1026:LEU:HD13	2.03	0.64
2:B:1110:PRO:HG3	2:B:1125:ASP:HB3	1.78	0.64
2:B:1159:ARG:HE	2:B:1193:GLN:HE21	1.44	0.64
2:B:515:HIS:CD2	2:B:516:ASN:H	2.16	0.64
2:B:25:ILE:HD11	2:B:653:VAL:C	2.18	0.64
2:B:855:PHE:CD1	2:B:855:PHE:C	2.69	0.64
2:B:899:ILE:HD11	2:B:911:ILE:HA	1.78	0.64
2:B:822:ASN:ND2	10:J:52:THR:HG21	2.13	0.64
11:K:82:ASP:OD1	11:K:84:LYS:HG3	1.98	0.64
1:A:1130:GLN:O	1:A:1134:ILE:HG13	1.97	0.64
1:A:547:LEU:HD22	11:K:58:PHE:CD1	2.32	0.64
2:B:135:ARG:HB2	2:B:137:TYR:CE1	2.33	0.64
2:B:387:LEU:O	2:B:392:ARG:HB2	1.98	0.64
2:B:791:THR:HA	2:B:858:SER:HB2	1.79	0.64
2:B:953:LEU:HD23	2:B:965:LYS:O	1.98	0.64
3:C:8:VAL:O	3:C:9:LYS:HD2	1.98	0.64
4:D:60:LYS:CE	4:D:126:ILE:HD11	2.28	0.64
1:A:963:ILE:HD11	1:A:1048:ASN:HB2	1.78	0.63
1:A:1191:TRP:CE3	1:A:1191:TRP:HA	2.32	0.63
2:B:1034:VAL:HG12	2:B:1035:ALA:N	2.14	0.63
2:B:758:PHE:CZ	2:B:1044:ALA:HA	2.33	0.63
2:B:847:ASP:C	2:B:849:GLY:H	2.00	0.63
2:B:899:ILE:CD1	2:B:911:ILE:HA	2.28	0.63
4:D:9:GLN:HE21	4:D:31:GLN:NE2	1.95	0.63
11:K:47:ARG:HH11	11:K:47:ARG:CB	2.09	0.63
1:A:1308:THR:HG23	1:A:1309:ASP:H	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1364:ASN:HD22	1:A:1365:TYR:N	1.97	0.63
1:A:515:GLN:HA	1:A:1367:HIS:NE2	2.13	0.63
2:B:1002:THR:CG2	2:B:1006:ILE:HG13	2.27	0.63
3:C:242:GLN:HA	3:C:245:VAL:CG2	2.28	0.63
4:D:56:ARG:NH2	4:D:155:ARG:HA	2.12	0.63
4:D:9:GLN:HE21	4:D:31:GLN:HE21	1.43	0.63
8:H:139:ASN:O	8:H:140:ALA:HB2	1.97	0.63
12:L:32:ALA:HB3	12:L:33:GLU:OE2	1.99	0.63
1:A:1187:GLN:HG3	1:A:1188:GLN:HG3	1.79	0.63
1:A:1142:THR:HA	1:A:1273:LEU:HD13	1.78	0.63
3:C:148:ARG:H	3:C:151:GLN:CG	2.06	0.63
8:H:142:LEU:C	8:H:143:LEU:HD12	2.18	0.63
10:J:14:VAL:HG12	10:J:14:VAL:O	1.96	0.63
2:B:1096:ARG:O	2:B:1097:HIS:HB2	1.98	0.63
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.80	0.63
4:D:139:LYS:HE2	4:D:143:ASN:ND2	2.13	0.63
5:E:165:LEU:HD23	5:E:165:LEU:N	2.13	0.63
5:E:204:THR:HG23	5:E:205:SER:N	2.13	0.63
1:A:1100:ARG:HH22	1:A:1111:MET:CE	2.11	0.63
1:A:93:VAL:HG21	1:A:301:ALA:O	1.99	0.63
2:B:1096:ARG:O	2:B:1097:HIS:CB	2.47	0.63
2:B:114:PRO:HG2	2:B:115:GLN:H	1.63	0.63
2:B:217:ARG:C	2:B:217:ARG:HD2	2.19	0.63
2:B:343:ILE:HG23	2:B:347:LYS:CE	2.28	0.63
2:B:637:LEU:C	2:B:690:VAL:HG13	2.19	0.63
2:B:99:LYS:HA	2:B:178:ASN:HD21	1.63	0.63
4:D:60:LYS:HE3	4:D:126:ILE:HD11	1.79	0.63
12:L:26:THR:HG23	12:L:62:LYS:HZ3	1.64	0.63
1:A:1364:ASN:C	1:A:1364:ASN:HD22	1.98	0.63
1:A:55:ASP:CG	1:A:55:ASP:O	2.36	0.63
1:A:901:LEU:N	1:A:926:GLN:HE21	1.95	0.63
5:E:117:THR:HB	5:E:120:ALA:CB	2.29	0.63
5:E:180:ARG:NH2	5:E:192:ARG:HD2	2.14	0.63
5:E:116:ILE:HG22	5:E:117:THR:N	2.12	0.63
7:G:34:VAL:CG1	7:G:45:ILE:HG21	2.28	0.63
1:A:877:HIS:ND1	1:A:1056:SER:HA	2.14	0.63
1:A:535:THR:HG22	1:A:575:LYS:HE2	1.81	0.63
2:B:363:HIS:O	2:B:364:ILE:HB	1.98	0.63
2:B:244:LEU:HD21	2:B:366:GLN:NE2	2.14	0.63
5:E:204:THR:HG23	5:E:205:SER:H	1.64	0.63
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:LYS:C	1:A:334:GLY:H	2.02	0.63
2:B:276:ILE:HD13	2:B:280:ILE:HD11	1.80	0.63
2:B:383:ASN:O	2:B:387:LEU:HD13	1.98	0.63
2:B:686:ASN:C	2:B:688:GLY:H	2.02	0.63
2:B:857:ARG:HD2	2:B:945:GLU:OE1	1.97	0.63
3:C:13:ALA:O	11:K:114:LEU:HD13	1.99	0.63
5:E:159:ASP:HA	5:E:162:ARG:NH2	2.13	0.63
5:E:167:ARG:O	5:E:168:TYR:HD2	1.82	0.63
5:E:198:ILE:HD11	5:E:212:ARG:HB2	1.81	0.63
7:G:27:LYS:O	7:G:31:LEU:HG	1.98	0.63
1:A:1094:VAL:HG12	1:A:1113:THR:HG21	1.80	0.62
1:A:278:THR:HG23	1:A:282:ASN:HD22	1.63	0.62
1:A:343:LYS:HE2	2:B:1156:ASP:HB2	1.81	0.62
1:A:41:MET:SD	1:A:42:ASP:N	2.71	0.62
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.33	0.62
2:B:357:GLN:O	2:B:366:GLN:HA	1.98	0.62
2:B:90:ILE:HG23	2:B:133:LYS:O	1.99	0.62
3:C:209:TYR:H	3:C:209:TYR:HD1	1.47	0.62
6:F:118:LEU:O	6:F:122:MET:HG3	1.99	0.62
8:H:144:ILE:HG22	8:H:145:ARG:N	2.14	0.62
8:H:36:CYS:HA	8:H:126:GLU:O	1.98	0.62
2:B:578:THR:H	2:B:589:VAL:CG1	2.12	0.62
2:B:596:LEU:HD11	2:B:600:LEU:HD11	1.81	0.62
3:C:238:ILE:HD13	3:C:246:ARG:HD2	1.80	0.62
7:G:142:ARG:HB3	7:G:171:ILE:HD11	1.80	0.62
1:A:1436:ILE:O	1:A:1437:GLY:C	2.37	0.62
1:A:266:LEU:HD21	1:A:303:TYR:CE1	2.35	0.62
1:A:645:LEU:O	1:A:649:ILE:HG13	2.00	0.62
1:A:847:ASP:O	1:A:858:ASN:HA	2.00	0.62
2:B:351:TYR:O	2:B:355:ILE:HG13	2.00	0.62
5:E:93:MET:HE1	5:E:123:LEU:HB2	1.81	0.62
5:E:168:TYR:HB3	5:E:170:LEU:HG	1.81	0.62
8:H:105:GLU:O	8:H:112:ILE:HG23	1.99	0.62
1:A:79:GLY:HA3	1:A:243:PRO:HG3	1.80	0.62
1:A:335:ARG:O	1:A:339:ASN:HB2	1.97	0.62
2:B:1072:MET:HE3	2:B:1085:ILE:HB	1.81	0.62
2:B:614:SER:HB3	2:B:694:ASP:HB2	1.81	0.62
2:B:797:TYR:HE1	2:B:971:THR:HG23	1.64	0.62
2:B:862:GLN:HG2	2:B:963:PHE:CD1	2.34	0.62
3:C:31:ASN:O	3:C:35:ARG:HG3	2.00	0.62
9:I:86:PHE:CE1	9:I:100:PHE:HB2	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:GLN:HG3	1:A:430:TRP:CZ2	2.33	0.62
2:B:69:LEU:CB	2:B:429:PHE:CE1	2.74	0.62
2:B:449:ASN:O	2:B:450:ALA:C	2.38	0.62
3:C:65:HIS:CE1	3:C:69:LEU:HD11	2.35	0.62
5:E:145:THR:HG21	5:E:187:TYR:CE2	2.34	0.62
8:H:32:THR:HG22	8:H:33:GLN:H	1.65	0.62
8:H:4:THR:HG22	8:H:5:LEU:N	2.15	0.62
12:L:55:ILE:O	12:L:56:LEU:CB	2.48	0.62
1:A:472:LEU:O	1:A:475:THR:HB	1.99	0.62
1:A:475:THR:CG2	1:A:476:SER:N	2.62	0.62
1:A:646:PHE:O	1:A:650:GLN:HB2	1.99	0.62
1:A:466:SER:O	2:B:1103:ILE:HD11	1.98	0.62
2:B:232:SER:O	2:B:261:ARG:HD3	1.99	0.62
8:H:30:SER:HB2	8:H:36:CYS:HB3	1.81	0.62
1:A:1152:ILE:HD11	9:I:44:TYR:HD2	1.64	0.62
1:A:1424:VAL:HG11	2:B:1139:ILE:HD13	1.79	0.62
2:B:105:SER:O	2:B:106:ASP:HB2	1.99	0.62
2:B:221:ASN:N	2:B:241:ARG:O	2.31	0.62
2:B:284:ILE:HD13	2:B:333:PHE:CD2	2.35	0.62
2:B:510:LYS:CB	2:B:511:PRO:HD3	2.30	0.62
2:B:768:THR:O	2:B:771:SER:HB2	1.99	0.62
2:B:871:THR:O	2:B:917:PRO:HG3	1.98	0.62
2:B:898:LEU:HD13	2:B:952:VAL:HG11	1.80	0.62
7:G:23:LYS:HG3	7:G:56:ILE:CD1	2.30	0.62
9:I:80:SER:OG	9:I:105:SER:HB2	2.00	0.62
1:A:1109:LYS:O	1:A:1110:ASN:HB3	2.00	0.62
1:A:1161:THR:HG22	1:A:1163:ILE:N	2.11	0.62
1:A:247:ARG:NH1	1:A:263:THR:HG23	2.15	0.62
1:A:399:HIS:HB3	1:A:400:PRO:CD	2.25	0.62
2:B:1177:HIS:C	2:B:1178:ASN:HD22	2.03	0.62
7:G:145:VAL:HG12	7:G:146:LYS:N	2.15	0.62
1:A:899:VAL:CG2	1:A:1029:ARG:HG2	2.29	0.62
1:A:110:CYS:HB3	1:A:167:CYS:SG	2.40	0.62
1:A:1118:VAL:HG12	1:A:1327:ILE:HG13	1.81	0.62
1:A:268:ASP:HB3	1:A:299:HIS:CE1	2.35	0.62
2:B:99:LYS:HB3	2:B:100:PRO:HD2	1.81	0.62
2:B:196:PRO:HG2	2:B:197:PHE:H	1.65	0.62
2:B:258:LEU:HG	2:B:258:LEU:O	2.00	0.62
2:B:282:ILE:HD12	2:B:382:ILE:HD13	1.82	0.62
2:B:916:THR:HB	2:B:935:ARG:CG	2.30	0.62
6:F:72:LYS:CA	6:F:72:LYS:HE3	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:21:ILE:HG22	11:K:31:VAL:CG1	2.29	0.62
1:A:1329:THR:CG2	1:A:1335:ILE:HG13	2.30	0.62
1:A:1345:ARG:NH1	5:E:200:ARG:HH22	1.98	0.62
1:A:1371:LEU:O	1:A:1375:MET:HG3	2.00	0.62
1:A:188:ASP:CB	1:A:191:THR:HB	2.25	0.62
2:B:128:LEU:HB2	2:B:167:ILE:O	2.00	0.62
2:B:549:THR:HG22	2:B:550:ASP:H	1.64	0.62
2:B:801:LYS:O	10:J:52:THR:CG2	2.47	0.62
7:G:18:PHE:HA	7:G:22:MET:CE	2.30	0.62
8:H:40:LEU:HG	8:H:41:ASP:O	1.98	0.62
9:I:78:CYS:O	9:I:80:SER:N	2.32	0.62
8:H:82:PRO:HG3	11:K:54:ARG:HH11	1.65	0.62
1:A:847:ASP:HB3	1:A:1424:VAL:HG23	1.81	0.61
2:B:351:TYR:CZ	2:B:355:ILE:HD11	2.35	0.61
2:B:593:PRO:HG2	2:B:617:ARG:NH1	2.15	0.61
2:B:903:VAL:HG12	2:B:904:ARG:N	2.15	0.61
5:E:83:CYS:C	5:E:85:GLU:H	2.04	0.61
5:E:89:GLY:HA2	5:E:117:THR:OG1	1.99	0.61
8:H:4:THR:HA	8:H:60:ALA:HB2	1.80	0.61
11:K:41:THR:HG22	11:K:42:LEU:N	2.14	0.61
11:K:60:ALA:O	11:K:73:LEU:HD12	1.99	0.61
11:K:61:TYR:HD2	11:K:61:TYR:C	2.02	0.61
12:L:55:ILE:HG12	12:L:56:LEU:H	1.65	0.61
1:A:1100:ARG:HH21	1:A:1351:GLU:CG	2.12	0.61
1:A:523:ILE:HG23	1:A:527:THR:HB	1.82	0.61
1:A:929:LEU:HD23	1:A:983:ILE:HG23	1.82	0.61
2:B:243:ALA:HA	2:B:250:PHE:O	2.00	0.61
2:B:807:ARG:HG2	2:B:1045:SER:OG	1.99	0.61
5:E:100:ILE:CG2	5:E:105:PHE:HB2	2.25	0.61
6:F:86:THR:OG1	6:F:89:GLU:HG3	2.00	0.61
9:I:6:PHE:HB3	9:I:12:ASN:O	2.00	0.61
11:K:7:PHE:O	11:K:9:LEU:N	2.33	0.61
1:A:1018:PHE:O	1:A:1021:LEU:HB3	2.01	0.61
1:A:1276:VAL:HG12	1:A:1277:GLU:H	1.65	0.61
1:A:1315:GLU:O	1:A:1317:MET:N	2.33	0.61
1:A:541:ILE:HG22	1:A:546:VAL:HG23	1.83	0.61
1:A:986:ILE:HD12	1:A:1032:LEU:HD11	1.83	0.61
2:B:286:PHE:HA	2:B:289:LEU:HD12	1.83	0.61
2:B:378:LEU:HD12	2:B:378:LEU:O	2.00	0.61
2:B:393:LYS:HA	2:B:393:LYS:HE3	1.81	0.61
2:B:510:LYS:HG3	2:B:511:PRO:HD3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:40:HIS:CB	7:G:73:LYS:NZ	2.63	0.61
8:H:14:GLU:HG2	8:H:15:VAL:N	2.13	0.61
9:I:53:GLY:HA2	9:I:56:ALA:HB2	1.82	0.61
11:K:12:LEU:H	11:K:12:LEU:CD1	2.10	0.61
1:A:1155:ASP:OD2	1:A:1161:THR:HA	2.01	0.61
1:A:233:TRP:C	1:A:235:ILE:H	2.03	0.61
2:B:273:LEU:HB2	2:B:276:ILE:CD1	2.24	0.61
2:B:56:ASP:HB2	2:B:57:TYR:HD1	1.65	0.61
4:D:144:THR:O	4:D:148:LEU:HB2	2.00	0.61
4:D:63:LEU:HD13	4:D:133:THR:OG1	2.00	0.61
5:E:103:LYS:HB3	5:E:105:PHE:CE2	2.35	0.61
11:K:1:MET:HG3	11:K:2:ASN:N	2.15	0.61
13:T:15:DC:H2"	13:T:16:DT:OP2	2.01	0.61
1:A:115:LEU:O	1:A:122:MET:HE2	2.00	0.61
1:A:1199:ARG:NH2	1:A:1234:GLU:HA	2.16	0.61
1:A:830:LYS:HE2	1:A:1081:LEU:HB2	1.82	0.61
1:A:849:MET:HE1	1:A:1061:GLY:HA2	1.82	0.61
2:B:190:TYR:CE2	10:J:62:ARG:HB3	2.34	0.61
2:B:737:THR:CG2	9:I:66:PRO:HA	2.31	0.61
2:B:497:ARG:NH2	2:B:775:LYS:HE2	2.14	0.61
5:E:129:PRO:O	5:E:130:ALA:C	2.39	0.61
9:I:69:PRO:HG2	9:I:85:PHE:CD2	2.36	0.61
10:J:64:ASN:HD22	10:J:65:PRO:HD3	1.64	0.61
11:K:44:ASN:N	11:K:61:TYR:CE1	2.68	0.61
1:A:1035:TYR:HD1	1:A:1037:LEU:HD23	1.64	0.61
1:A:1214:GLU:OE1	1:A:1214:GLU:HA	2.01	0.61
1:A:1450:LEU:HG	1:A:1450:LEU:O	2.01	0.61
1:A:18:GLN:NE2	1:A:228:PHE:HE1	1.99	0.61
1:A:196:GLU:CB	1:A:197:PRO:HD2	2.29	0.61
1:A:98:LYS:HE2	1:A:224:PHE:CZ	2.35	0.61
1:A:901:LEU:N	1:A:926:GLN:NE2	2.44	0.61
2:B:1201:LYS:HE2	2:B:1205:GLN:NE2	2.15	0.61
2:B:559:SER:CA	2:B:563:MET:HB3	2.26	0.61
2:B:651:LEU:C	2:B:653:VAL:H	2.03	0.61
2:B:1080:LYS:HB2	3:C:188:HIS:HB3	1.80	0.61
7:G:112:LYS:O	7:G:115:MET:HG2	2.00	0.61
11:K:7:PHE:HA	11:K:10:PHE:CE2	2.35	0.61
1:A:1154:TYR:HD1	1:A:1191:TRP:CZ3	2.19	0.61
1:A:225:ASN:ND2	1:A:227:VAL:H	1.99	0.61
1:A:43:GLU:HG3	1:A:48:ALA:HB3	1.82	0.61
2:B:1065:GLN:HB3	2:B:1069:PHE:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:944:THR:HG21	2:B:1122:ARG:NH2	2.14	0.61
3:C:66:ARG:HH21	10:J:5:VAL:H	1.49	0.61
1:A:882:SER:H	1:A:1025:ARG:NH2	1.98	0.61
1:A:1039:LYS:HE3	1:A:1043:ASP:OD2	2.01	0.61
1:A:1149:ALA:CB	9:I:47:GLU:HA	2.31	0.61
1:A:152:VAL:CG1	1:A:153:PRO:HD2	2.31	0.61
1:A:590:ARG:NH1	1:A:590:ARG:HB2	2.08	0.61
2:B:999:MET:HB3	2:B:1007:VAL:CG2	2.30	0.61
2:B:261:ARG:HH11	2:B:262:GLU:H	1.48	0.61
2:B:259:TYR:HB2	2:B:268:THR:HG23	1.83	0.61
2:B:573:GLN:O	2:B:575:PRO:HD3	2.00	0.61
3:C:177:GLU:HG3	3:C:231:ASN:HB3	1.83	0.61
6:F:94:LEU:HD21	6:F:122:MET:HA	1.81	0.61
2:B:776:GLN:OE1	15:P:9:C:H4'	2.01	0.61
1:A:403:LYS:O	1:A:415:LEU:HB2	2.00	0.61
1:A:382:PRO:CD	1:A:428:TYR:HD2	2.09	0.61
4:D:56:ARG:HB2	4:D:148:LEU:HD22	1.82	0.61
1:A:573:SER:O	1:A:576:GLN:HB3	2.01	0.61
1:A:665:GLY:O	1:A:666:ILE:HD12	2.00	0.61
1:A:741:ASN:ND2	1:A:744:LYS:H	1.99	0.61
2:B:352:ALA:HA	2:B:355:ILE:HD12	1.83	0.61
4:D:53:SER:H	4:D:148:LEU:CD2	2.13	0.61
6:F:130:ILE:O	6:F:148:VAL:HG21	2.01	0.61
1:A:695:LYS:HG2	1:A:698:GLN:OE1	2.01	0.60
1:A:74:MET:CE	1:A:74:MET:H	2.13	0.60
2:B:680:THR:OG1	2:B:681:TRP:N	2.33	0.60
3:C:66:ARG:NH1	10:J:2:ILE:HG21	2.16	0.60
7:G:17:PHE:N	7:G:17:PHE:CD2	2.68	0.60
8:H:26:ILE:HG22	8:H:27:GLU:H	1.66	0.60
10:J:12:LYS:O	10:J:14:VAL:HG23	2.00	0.60
1:A:1427:ASN:H	1:A:1427:ASN:HD22	1.50	0.60
1:A:20:GLY:O	1:A:21:LEU:HD23	2.01	0.60
2:B:1072:MET:HG3	2:B:1085:ILE:HD13	1.81	0.60
2:B:1201:LYS:HE2	2:B:1205:GLN:CD	2.21	0.60
2:B:236:HIS:CE1	2:B:389:ALA:HA	2.35	0.60
2:B:582:VAL:HB	2:B:587:HIS:CD2	2.35	0.60
2:B:653:VAL:HA	2:B:657:HIS:CD2	2.35	0.60
4:D:119:ARG:HG2	4:D:120:GLU:H	1.64	0.60
8:H:32:THR:HG22	8:H:33:GLN:N	2.16	0.60
8:H:40:LEU:HD22	8:H:123:MET:CE	2.27	0.60
1:A:1173:HIS:CD2	1:A:1227:ILE:HG23	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:SER:HB3	1:A:162:VAL:HG23	1.82	0.60
1:A:679:ILE:HG12	1:A:732:LEU:HD12	1.83	0.60
1:A:930:ASP:O	1:A:934:LYS:HG2	2.01	0.60
2:B:327:ARG:O	2:B:331:LEU:HD13	2.02	0.60
5:E:182:ASP:HB3	5:E:185:ALA:HB2	1.83	0.60
5:E:154:ILE:O	5:E:196:VAL:HA	2.01	0.60
6:F:125:LEU:O	6:F:125:LEU:HG	2.01	0.60
7:G:56:ILE:O	7:G:57:GLN:HB2	2.01	0.60
9:I:35:VAL:CG1	9:I:36:GLU:N	2.65	0.60
2:B:900:ALA:HB3	12:L:61:THR:OG1	2.02	0.60
1:A:512:VAL:HA	1:A:519:PRO:HA	1.83	0.60
1:A:857:ARG:NH2	6:F:139:PRO:HG3	2.16	0.60
2:B:277:LYS:CG	2:B:338:GLY:HA2	2.31	0.60
3:C:98:VAL:O	3:C:99:LEU:HD23	2.00	0.60
8:H:91:ASP:C	8:H:93:TYR:H	2.03	0.60
1:A:1313:LEU:O	1:A:1315:GLU:N	2.34	0.60
1:A:544:ASP:CG	1:A:545:GLN:H	2.05	0.60
2:B:20:ASP:C	2:B:22:SER:H	2.04	0.60
2:B:314:LEU:HD21	2:B:386:LEU:HD11	1.83	0.60
2:B:446:LEU:O	2:B:447:ALA:HB3	2.02	0.60
2:B:579:ARG:CB	2:B:586:TRP:HE1	2.13	0.60
2:B:611:PRO:CG	2:B:685:LEU:HD11	2.31	0.60
5:E:46:TYR:O	5:E:54:GLN:HG2	2.02	0.60
5:E:4:GLU:C	5:E:6:GLU:N	2.55	0.60
7:G:14:HIS:ND1	7:G:15:PRO:HD2	2.17	0.60
8:H:30:SER:CB	8:H:36:CYS:HB3	2.31	0.60
8:H:24:CYS:HB2	8:H:44:VAL:HG21	1.83	0.60
9:I:14:LEU:HA	9:I:28:GLU:O	2.01	0.60
1:A:343:LYS:HZ2	2:B:1151:LEU:HD12	1.65	0.60
1:A:722:LEU:N	1:A:722:LEU:HD12	2.16	0.60
1:A:731:ARG:O	1:A:734:GLU:HB3	2.00	0.60
1:A:746:MET:CE	2:B:1018:PRO:HG2	2.32	0.60
1:A:832:ALA:HA	13:T:18:DA:N7	2.15	0.60
1:A:666:ILE:HD11	2:B:1067:ARG:O	2.00	0.60
2:B:639:ILE:HD11	2:B:691:GLU:CG	2.22	0.60
2:B:941:LEU:HD21	2:B:946:ASN:HA	1.82	0.60
3:C:101:LEU:CD1	3:C:118:LEU:HD23	2.26	0.60
5:E:46:TYR:CD2	5:E:58:MET:HG2	2.36	0.60
12:L:68:GLU:N	12:L:68:GLU:OE1	2.31	0.60
1:A:1319:VAL:O	1:A:1322:ILE:HG12	2.02	0.60
1:A:1453:TYR:O	1:A:1454:MET:HB3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:GLN:NE2	1:A:228:PHE:CE1	2.70	0.60
1:A:186:LYS:O	1:A:194:ALA:HB1	2.02	0.60
2:B:361:LEU:HD21	2:B:377:PHE:CD2	2.36	0.60
2:B:723:VAL:HG12	2:B:724:ASP:N	2.14	0.60
3:C:173:ALA:O	3:C:174:ALA:HB3	2.01	0.60
7:G:1:MET:SD	7:G:79:PHE:CD1	2.93	0.60
12:L:44:ASP:O	12:L:45:ALA:HB3	2.02	0.60
1:A:1152:ILE:HG23	1:A:1193:LEU:HD13	1.84	0.60
1:A:154:SER:HB3	1:A:162:VAL:CG2	2.31	0.60
1:A:150:THR:HG23	1:A:165:GLY:O	2.01	0.60
1:A:420:ARG:HG2	1:A:423:ASP:HB3	1.84	0.60
1:A:441:PRO:CG	1:A:498:ARG:HB2	2.30	0.60
1:A:91:PHE:HB3	1:A:96:ILE:CD1	2.31	0.60
2:B:616:ILE:HD13	2:B:625:LYS:HB2	1.83	0.60
4:D:195:ILE:HG22	4:D:198:LEU:HG	1.83	0.60
5:E:55:ARG:C	5:E:57:MET:H	2.02	0.60
8:H:40:LEU:CD1	8:H:123:MET:HB2	2.32	0.60
10:J:7:CYS:HA	10:J:49:MET:HE3	1.84	0.60
1:A:369:SER:CB	11:K:2:ASN:HD21	2.15	0.60
1:A:339:ASN:O	1:A:343:LYS:HG2	2.01	0.60
2:B:654:ARG:N	2:B:657:HIS:HD2	1.98	0.60
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.37	0.60
9:I:2:THR:HG22	9:I:3:THR:H	1.66	0.60
1:A:172:PRO:HG3	1:A:185:TRP:CZ2	2.37	0.60
1:A:946:VAL:HG22	5:E:201:LYS:HD2	1.82	0.60
2:B:127:GLY:C	2:B:128:LEU:HD12	2.22	0.60
2:B:135:ARG:HB2	2:B:137:TYR:HE1	1.67	0.60
2:B:642:ASP:N	2:B:649:LYS:HG3	2.16	0.60
3:C:261:ALA:HA	3:C:264:GLN:OE1	2.02	0.60
11:K:18:LYS:HZ2	11:K:38:GLU:HG2	1.66	0.60
11:K:21:ILE:HG22	11:K:31:VAL:HG11	1.84	0.60
1:A:1315:GLU:C	1:A:1317:MET:N	2.55	0.59
1:A:784:LEU:HB3	1:A:785:PRO:HD2	1.84	0.59
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	1.84	0.59
3:C:3:GLU:CB	11:K:104:ASN:HD21	2.15	0.59
4:D:56:ARG:HA	4:D:148:LEU:HD13	1.83	0.59
5:E:136:ASN:O	5:E:140:LEU:HG	2.01	0.59
5:E:79:TRP:HE1	5:E:81:GLU:HB2	1.67	0.59
7:G:132:SER:HB3	7:G:135:ASP:HB2	1.83	0.59
1:A:1157:ASP:C	1:A:1159:ARG:H	2.05	0.59
1:A:1187:GLN:O	1:A:1244:ARG:HG3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1193:LEU:HD12	1:A:1194:ARG:N	2.17	0.59
2:B:1047:PHE:O	2:B:1048:THR:HG23	2.01	0.59
2:B:944:THR:HG21	2:B:1122:ARG:CZ	2.32	0.59
2:B:35:SER:O	2:B:39:ARG:HG3	2.02	0.59
2:B:510:LYS:CG	2:B:511:PRO:HD3	2.31	0.59
2:B:604:ARG:C	2:B:606:LYS:N	2.55	0.59
2:B:758:PHE:CE2	2:B:1044:ALA:HA	2.37	0.59
4:D:63:LEU:HD12	4:D:129:LEU:HG	1.84	0.59
4:D:50:LEU:HD11	7:G:4:ILE:HD11	1.83	0.59
1:A:56:PRO:O	1:A:57:ARG:CG	2.49	0.59
2:B:65:GLU:HG3	2:B:66:ASP:OD1	2.03	0.59
2:B:67:SER:HB2	2:B:92:PHE:HD1	1.67	0.59
2:B:842:ASN:HD22	2:B:845:SER:CB	2.15	0.59
3:C:18:VAL:HG23	3:C:240:VAL:HG12	1.82	0.59
5:E:153:HIS:C	5:E:154:ILE:HG13	2.22	0.59
6:F:103:MET:O	6:F:104:ASN:HB2	2.02	0.59
8:H:42:ILE:O	8:H:44:VAL:HG23	2.02	0.59
1:A:567:LYS:HZ3	8:H:95:TYR:HB2	1.67	0.59
12:L:34:CYS:SG	12:L:34:CYS:O	2.60	0.59
1:A:115:LEU:CG	1:A:142:CYS:HB3	2.32	0.59
1:A:1277:GLU:O	1:A:1279:ILE:N	2.34	0.59
1:A:115:LEU:CD1	1:A:142:CYS:HB3	2.32	0.59
1:A:49:LYS:HE2	1:A:61:ILE:HD12	1.84	0.59
1:A:697:ALA:HB2	1:A:702:LEU:HD12	1.84	0.59
1:A:829:VAL:C	1:A:831:THR:N	2.56	0.59
1:A:986:ILE:HG22	1:A:987:VAL:N	2.16	0.59
2:B:258:LEU:HB2	2:B:385:LEU:HD21	1.85	0.59
4:D:114:MET:CE	4:D:114:MET:HA	2.32	0.59
4:D:134:THR:HG22	4:D:135:GLY:N	2.16	0.59
4:D:207:LEU:HA	4:D:210:ILE:HD12	1.85	0.59
5:E:190:LEU:HD13	5:E:191:LYS:H	1.68	0.59
7:G:143:ILE:HG22	7:G:144:ARG:N	2.17	0.59
2:B:992:ILE:CD1	11:K:66:PRO:HB2	2.32	0.59
1:A:1121:GLU:HG2	1:A:1122:PRO:HD2	1.84	0.59
1:A:337:ARG:HD3	1:A:839:ARG:NH2	2.18	0.59
1:A:511:ILE:HA	1:A:521:MET:CE	2.32	0.59
1:A:590:ARG:CG	1:A:590:ARG:HH11	2.15	0.59
1:A:756:ILE:O	1:A:759:ALA:HB3	2.01	0.59
2:B:798:TYR:HD2	2:B:798:TYR:N	2.01	0.59
4:D:47:LEU:HD11	7:G:3:PHE:CD2	2.38	0.59
7:G:13:LEU:CD2	7:G:17:PHE:HB2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:ALA:O	8:H:97:MET:HA	2.02	0.59
11:K:7:PHE:HB2	11:K:11:LEU:CD2	2.31	0.59
1:A:409:SER:O	1:A:411:ASP:N	2.36	0.59
1:A:456:MET:CE	1:A:507:VAL:HG13	2.32	0.59
1:A:537:ARG:HD2	8:H:20:TYR:CE1	2.28	0.59
1:A:666:ILE:CD1	1:A:667:GLY:H	2.10	0.59
1:A:845:LEU:O	1:A:846:GLU:C	2.41	0.59
2:B:31:TRP:CE3	2:B:31:TRP:HA	2.37	0.59
2:B:652:LYS:HD3	2:B:688:GLY:O	2.01	0.59
2:B:830:TYR:HE2	2:B:1000:PRO:HD3	1.66	0.59
3:C:147:LEU:HD23	3:C:147:LEU:N	2.17	0.59
7:G:30:LEU:HD13	7:G:72:VAL:CG1	2.32	0.59
11:K:11:LEU:N	11:K:11:LEU:HD22	2.17	0.59
2:B:992:ILE:HD11	11:K:66:PRO:HB2	1.84	0.59
1:A:1030:ARG:HG3	1:A:1034:GLU:CD	2.23	0.59
1:A:785:PRO:HG2	1:A:786:HIS:HD2	1.68	0.59
1:A:853:ASP:OD1	1:A:855:THR:HB	2.03	0.59
2:B:172:ILE:HD13	2:B:178:ASN:ND2	2.18	0.59
2:B:235:SER:C	2:B:236:HIS:HD2	2.06	0.59
2:B:331:LEU:CD2	2:B:353:LYS:HG2	2.33	0.59
2:B:483:LEU:HD11	2:B:491:THR:CG2	2.32	0.59
2:B:891:ASP:O	2:B:893:LEU:N	2.35	0.59
4:D:3:VAL:HG12	4:D:4:SER:N	2.17	0.59
8:H:128:ASN:N	8:H:130:ARG:NH1	2.45	0.59
12:L:27:LEU:N	12:L:27:LEU:HD23	2.13	0.59
1:A:323:LYS:H	1:A:323:LYS:HD2	1.68	0.59
1:A:523:ILE:HB	1:A:622:VAL:CG2	2.33	0.59
1:A:69:THR:C	1:A:71:GLN:N	2.55	0.59
1:A:700:ASN:ND2	9:I:115:LYS:HD2	2.17	0.59
1:A:898:ARG:HD3	1:A:933:TYR:CD1	2.37	0.59
2:B:123:THR:O	2:B:125:SER:N	2.35	0.59
2:B:333:PHE:CE1	2:B:337:ARG:NH2	2.70	0.59
2:B:516:ASN:ND2	2:B:516:ASN:N	2.49	0.59
2:B:498:THR:O	2:B:536:VAL:HA	2.03	0.59
6:F:82:THR:CG2	6:F:84:TYR:H	2.16	0.59
9:I:64:SER:O	9:I:66:PRO:HD3	2.01	0.59
12:L:49:LYS:O	12:L:50:ASP:HB2	2.03	0.59
1:A:1130:GLN:HG3	1:A:1134:ILE:HD11	1.84	0.59
1:A:401:GLY:C	1:A:435:HIS:HD2	2.05	0.59
1:A:475:THR:CG2	1:A:476:SER:H	2.15	0.59
2:B:557:PHE:HZ	2:B:603:LEU:HD21	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:563:MET:CE	2:B:580:VAL:HB	2.32	0.59
2:B:732:SER:HB2	2:B:734:HIS:CE1	2.38	0.59
3:C:124:LEU:HD21	3:C:129:ILE:O	2.03	0.59
6:F:138:LEU:HB3	6:F:139:PRO:HD2	1.84	0.59
10:J:35:ALA:O	10:J:38:ARG:HB3	2.02	0.59
1:A:208:LEU:HD23	1:A:208:LEU:C	2.24	0.59
1:A:353:ILE:HG21	1:A:487:MET:HE3	1.84	0.59
1:A:528:LEU:O	1:A:528:LEU:HD12	2.02	0.59
1:A:731:ARG:HG3	1:A:755:PHE:CE1	2.38	0.59
1:A:867:ILE:HG22	1:A:872:GLY:H	1.66	0.59
2:B:1215:ARG:CZ	4:D:15:LEU:HD21	2.33	0.59
2:B:180:TYR:HD1	2:B:180:TYR:H	1.51	0.59
2:B:308:TRP:HA	2:B:311:LEU:HD12	1.84	0.59
2:B:956:THR:HG22	2:B:957:ASN:H	1.68	0.59
3:C:112:ASN:CB	3:C:114:TYR:HE1	2.15	0.59
5:E:182:ASP:O	5:E:185:ALA:HB3	2.03	0.59
4:D:40:HIS:HB3	7:G:6:ASP:HB3	1.85	0.59
8:H:95:TYR:O	8:H:143:LEU:HA	2.03	0.59
1:A:567:LYS:HD2	8:H:95:TYR:CG	2.38	0.59
9:I:95:THR:HG22	9:I:96:SER:O	2.03	0.59
1:A:1445:ILE:HD12	7:G:59:GLY:O	2.03	0.58
1:A:340:LEU:HD21	2:B:1199:ALA:HB3	1.85	0.58
1:A:471:ASN:OD1	1:A:472:LEU:N	2.36	0.58
2:B:864:LYS:HB2	2:B:872:GLU:HG3	1.85	0.58
8:H:110:ASP:HB2	8:H:128:ASN:ND2	2.17	0.58
8:H:64:ASN:ND2	8:H:88:SER:HB2	2.18	0.58
1:A:1173:HIS:ND1	1:A:1173:HIS:O	2.36	0.58
1:A:1224:LEU:HG	1:A:1226:VAL:HG23	1.85	0.58
1:A:164:ARG:HG3	1:A:165:GLY:H	1.68	0.58
2:B:1006:ILE:HG23	10:J:43:ARG:HG3	1.85	0.58
2:B:553:PRO:O	2:B:557:PHE:HB2	2.03	0.58
2:B:797:TYR:HB3	2:B:798:TYR:CD2	2.39	0.58
3:C:82:TYR:CE1	3:C:161:LYS:HG2	2.37	0.58
3:C:232:VAL:HG21	3:C:244:VAL:HG22	1.84	0.58
4:D:59:ILE:O	4:D:63:LEU:HB2	2.03	0.58
5:E:67:GLU:O	5:E:70:SER:HB2	2.03	0.58
1:A:23:SER:HA	1:A:233:TRP:CD1	2.38	0.58
1:A:590:ARG:O	1:A:591:PHE:HB2	2.03	0.58
1:A:523:ILE:HB	1:A:622:VAL:HG22	1.85	0.58
2:B:827:ILE:O	2:B:1085:ILE:HG23	2.03	0.58
2:B:164:LYS:HD3	2:B:164:LYS:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:274:PRO:CG	2:B:359:GLU:HB3	2.32	0.58
2:B:25:ILE:HD11	2:B:653:VAL:O	2.03	0.58
4:D:127:ASP:OD2	4:D:142:LYS:HE3	2.02	0.58
5:E:85:GLU:O	5:E:88:VAL:HG23	2.03	0.58
7:G:106:MET:HG2	7:G:107:LYS:N	2.18	0.58
1:A:525:GLN:OE1	2:B:836:GLU:HG2	2.02	0.58
1:A:709:THR:HG22	1:A:710:LEU:N	2.18	0.58
2:B:1169:MET:HE3	2:B:1201:LYS:HG2	1.84	0.58
2:B:20:ASP:O	2:B:22:SER:N	2.35	0.58
2:B:357:GLN:HG2	2:B:366:GLN:O	2.04	0.58
2:B:515:HIS:H	2:B:518:HIS:HD2	1.49	0.58
2:B:56:ASP:HB2	2:B:57:TYR:CD1	2.38	0.58
4:D:116:SER:O	4:D:118:THR:HG23	2.03	0.58
5:E:22:MET:HG3	5:E:187:TYR:CD1	2.38	0.58
7:G:91:VAL:HG23	7:G:141:SER:O	2.03	0.58
8:H:5:LEU:O	8:H:133:ASN:HB3	2.03	0.58
1:A:1101:LEU:C	1:A:1101:LEU:HD12	2.23	0.58
1:A:164:ARG:HG3	1:A:165:GLY:N	2.18	0.58
1:A:295:LEU:O	1:A:298:PHE:HB3	2.03	0.58
1:A:853:ASP:OD1	1:A:855:THR:N	2.33	0.58
1:A:901:LEU:HD11	1:A:983:ILE:HD13	1.85	0.58
1:A:901:LEU:HG	1:A:926:GLN:HE21	1.67	0.58
6:F:117:PRO:C	6:F:119:ARG:H	2.06	0.58
1:A:1036:ARG:HG2	1:A:1036:ARG:NH1	2.19	0.58
1:A:278:THR:HG23	1:A:282:ASN:ND2	2.19	0.58
2:B:1115:THR:HG22	2:B:1117:GLN:HG3	1.85	0.58
2:B:1163:CYS:HB2	2:B:1182:CYS:SG	2.43	0.58
2:B:603:LEU:HB3	2:B:609:ILE:HD11	1.86	0.58
2:B:615:MET:HA	2:B:625:LYS:O	2.04	0.58
2:B:811:TYR:N	2:B:811:TYR:CD1	2.71	0.58
2:B:916:THR:HB	2:B:935:ARG:HG3	1.86	0.58
4:D:49:ALA:HB1	4:D:178:ALA:HB2	1.86	0.58
7:G:140:LYS:O	7:G:141:SER:C	2.42	0.58
9:I:50:THR:HB	9:I:92:ARG:NH1	2.18	0.58
12:L:30:ILE:C	12:L:56:LEU:HD23	2.24	0.58
1:A:427:GLN:HB2	1:A:430:TRP:CG	2.39	0.58
1:A:456:MET:HE1	1:A:507:VAL:HG13	1.86	0.58
1:A:583:PRO:O	1:A:610:GLY:HA3	2.03	0.58
1:A:774:ARG:O	1:A:775:ILE:C	2.41	0.58
1:A:814:PHE:CE1	2:B:519:TRP:HA	2.38	0.58
1:A:998:LEU:HD12	1:A:998:LEU:H	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:326:ASP:C	2:B:328:GLU:H	2.06	0.58
2:B:641:GLU:HB2	2:B:643:ASP:OD2	2.03	0.58
2:B:798:TYR:CD2	2:B:798:TYR:N	2.72	0.58
5:E:98:ILE:HG22	5:E:102:GLU:HG3	1.86	0.58
10:J:39:LEU:N	10:J:39:LEU:HD12	2.18	0.58
1:A:1143:LEU:HD23	1:A:1267:MET:HB3	1.85	0.58
1:A:860:LEU:HD11	1:A:1393:ASN:ND2	2.18	0.58
1:A:2:VAL:HG11	2:B:1157:ALA:CB	2.33	0.58
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.69	0.58
1:A:984:LYS:O	1:A:988:LEU:HB2	2.04	0.58
2:B:1177:HIS:CB	2:B:1179:GLN:HE21	2.17	0.58
1:A:860:LEU:O	2:B:1224:PHE:HE2	1.86	0.58
2:B:274:PRO:HG2	2:B:359:GLU:HB3	1.85	0.58
2:B:918:ILE:HG22	2:B:919:SER:N	2.19	0.58
5:E:99:HIS:CE1	5:E:103:LYS:HG3	2.39	0.58
7:G:88:ASP:CB	7:G:144:ARG:HA	2.33	0.58
1:A:17:VAL:HB	1:A:1419:ASP:HB3	1.84	0.58
1:A:180:LYS:NZ	1:A:294:SER:HB3	2.16	0.58
1:A:317:LYS:HA	2:B:471:LYS:HE2	1.86	0.58
2:B:345:LYS:C	2:B:348:ARG:HG2	2.24	0.58
1:A:568:PRO:CG	8:H:46:LEU:HD22	2.29	0.58
2:B:1006:ILE:HD13	10:J:44:TYR:CE2	2.39	0.58
1:A:1197:LEU:HD11	1:A:1238:ILE:HD11	1.86	0.58
1:A:7:SER:C	1:A:9:ALA:H	2.07	0.58
1:A:947:PHE:CE2	1:A:954:TRP:CE2	2.92	0.58
2:B:479:VAL:HG12	2:B:480:SER:H	1.69	0.58
2:B:708:GLU:O	2:B:710:LEU:N	2.36	0.58
2:B:770:GLN:OE1	2:B:983:ARG:HA	2.04	0.58
2:B:899:ILE:CG2	2:B:949:VAL:HG21	2.34	0.58
2:B:918:ILE:HD12	2:B:935:ARG:NH1	2.19	0.58
2:B:95:ILE:HB	2:B:130:VAL:HG22	1.85	0.58
7:G:85:GLU:HB3	7:G:147:ILE:HD12	1.86	0.58
13:T:7:DC:H2"	13:T:8:DT:C7	2.34	0.58
1:A:265:LYS:O	1:A:269:ILE:HG13	2.04	0.57
1:A:302:THR:HA	1:A:305:ASP:O	2.04	0.57
1:A:381:THR:C	1:A:383:TYR:N	2.56	0.57
1:A:353:ILE:HG21	1:A:487:MET:HG3	1.84	0.57
2:B:1181:GLU:H	2:B:1188:LYS:HG3	1.69	0.57
1:A:825:ILE:CD1	2:B:512:ARG:HB3	2.15	0.57
2:B:216:GLU:OE1	2:B:537:LYS:HE3	2.04	0.57
2:B:615:MET:O	2:B:697:GLU:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:112:ASN:CB	3:C:114:TYR:CE1	2.87	0.57
3:C:189:THR:HG22	3:C:190:ASP:N	2.19	0.57
3:C:34:ARG:O	3:C:38:ILE:HG13	2.04	0.57
4:D:25:ALA:C	4:D:27:LEU:H	2.08	0.57
6:F:85:MET:HB3	6:F:155:LEU:HD11	1.86	0.57
9:I:51:ASN:O	9:I:54:GLU:HG3	2.03	0.57
10:J:44:TYR:N	10:J:44:TYR:CD2	2.69	0.57
1:A:1035:TYR:O	1:A:1036:ARG:C	2.41	0.57
1:A:147:VAL:HG13	1:A:168:GLY:O	2.04	0.57
1:A:434:ARG:HH11	1:A:434:ARG:HG2	1.69	0.57
1:A:62:ASP:O	1:A:63:ARG:C	2.42	0.57
2:B:953:LEU:HB3	12:L:57:LEU:HD23	1.86	0.57
1:A:1053:PHE:O	1:A:1056:SER:N	2.37	0.57
1:A:1427:ASN:O	1:A:1430:LEU:N	2.37	0.57
1:A:469:ARG:HB3	1:A:469:ARG:NH1	2.19	0.57
1:A:523:ILE:CG2	1:A:527:THR:HB	2.34	0.57
3:C:167:HIS:CD2	12:L:70:ARG:HB3	2.39	0.57
2:B:1165:ILE:CD1	4:D:17:LYS:HD3	2.34	0.57
6:F:85:MET:HB3	6:F:155:LEU:CD1	2.34	0.57
3:C:66:ARG:NH1	10:J:2:ILE:CG2	2.67	0.57
1:A:826:ASP:HB2	1:A:830:LYS:HD3	1.86	0.57
1:A:864:ILE:HG21	1:A:1374:VAL:HG22	1.85	0.57
1:A:897:TYR:CD2	1:A:936:LEU:HD13	2.27	0.57
2:B:1178:ASN:O	2:B:1179:GLN:C	2.43	0.57
2:B:39:ARG:HG2	2:B:39:ARG:HH11	1.69	0.57
2:B:487:THR:CG2	2:B:488:TYR:N	2.66	0.57
3:C:100:THR:HG22	3:C:101:LEU:N	2.19	0.57
3:C:24:ASN:O	3:C:25:VAL:HG13	2.04	0.57
9:I:76:PRO:HD2	9:I:108:HIS:CD2	2.36	0.57
11:K:49:GLU:HG3	11:K:94:ILE:HG12	1.87	0.57
1:A:1017:LEU:HD23	5:E:204:THR:O	2.05	0.57
1:A:1100:ARG:O	1:A:1103:GLU:HB3	2.04	0.57
1:A:1142:THR:HB	1:A:1271:ILE:O	2.04	0.57
1:A:41:MET:O	1:A:42:ASP:O	2.23	0.57
1:A:618:GLU:O	1:A:620:LYS:N	2.38	0.57
1:A:67:CYS:C	1:A:68:GLN:HG3	2.23	0.57
1:A:701:LEU:O	1:A:702:LEU:HG	2.03	0.57
1:A:709:THR:HG21	9:I:93:LYS:O	2.04	0.57
1:A:804:TYR:HE1	2:B:1021:MET:HE3	1.69	0.57
1:A:775:ILE:HD12	1:A:818:MET:SD	2.44	0.57
1:A:896:ARG:HH21	1:A:1030:ARG:NE	2.01	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1167:GLY:HA3	2:B:1216:LEU:H	1.68	0.57
2:B:642:ASP:HB3	2:B:649:LYS:HG3	1.86	0.57
2:B:640:VAL:HG13	2:B:650:GLU:C	2.24	0.57
2:B:640:VAL:CG2	2:B:651:LEU:HD23	2.32	0.57
5:E:106:GLN:HA	5:E:130:ALA:CB	2.35	0.57
6:F:74:ILE:HD12	6:F:144:GLU:HG3	1.85	0.57
7:G:91:VAL:HB	7:G:139:ILE:O	2.05	0.57
10:J:23:ASN:C	10:J:25:LEU:N	2.58	0.57
1:A:1445:ILE:HD12	1:A:1445:ILE:N	2.09	0.57
1:A:189:ARG:O	1:A:190:ALA:HB3	2.05	0.57
2:B:204:ILE:C	2:B:205:ILE:HD12	2.24	0.57
2:B:265:SER:O	2:B:267:ARG:N	2.37	0.57
2:B:351:TYR:CE1	2:B:355:ILE:HD11	2.40	0.57
3:C:18:VAL:HG12	3:C:20:PHE:HD2	1.70	0.57
4:D:60:LYS:HZ3	4:D:115:HIS:CE1	2.22	0.57
5:E:10:SER:O	5:E:13:TRP:HB3	2.04	0.57
5:E:178:ILE:HB	5:E:212:ARG:HD2	1.86	0.57
5:E:85:GLU:C	5:E:87:SER:H	2.08	0.57
6:F:132:LEU:CD2	7:G:61:ILE:HD11	2.34	0.57
7:G:44:TYR:HE1	7:G:157:ILE:H	1.52	0.57
2:B:1121:GLY:HA2	13:T:22:DC:OP2	2.05	0.57
1:A:1322:ILE:O	1:A:1324:PRO:HD3	2.05	0.57
1:A:590:ARG:HG2	1:A:591:PHE:N	2.19	0.57
2:B:603:LEU:CD1	2:B:608:ASP:HB3	2.34	0.57
2:B:794:ASN:C	2:B:795:ILE:HD12	2.24	0.57
2:B:950:ASP:O	2:B:951:GLN:HB3	2.04	0.57
3:C:164:ALA:HA	3:C:167:HIS:O	2.04	0.57
4:D:31:GLN:O	4:D:34:GLN:HG3	2.03	0.57
7:G:146:LYS:HB2	7:G:168:LEU:HD11	1.84	0.57
7:G:51:TYR:O	7:G:54:ILE:HG13	2.04	0.57
13:T:25:DG:H2''	13:T:26:DT:H5'	1.86	0.57
1:A:873:MET:C	1:A:1058:VAL:HG23	2.24	0.57
1:A:11:LEU:HB2	2:B:1193:GLN:O	2.04	0.57
1:A:416:ARG:HG3	1:A:417:TYR:CE2	2.39	0.57
1:A:470:LEU:CD1	1:A:487:MET:HE1	2.31	0.57
3:C:82:TYR:CD1	3:C:161:LYS:HG2	2.40	0.57
4:D:130:LEU:C	4:D:132:GLN:H	2.08	0.57
6:F:109:VAL:HG12	6:F:110:ASP:H	1.67	0.57
8:H:26:ILE:HD13	8:H:49:VAL:HG11	1.87	0.57
8:H:11:GLN:O	8:H:28:ALA:HB1	2.05	0.57
10:J:1:MET:H1	10:J:56:LEU:HB2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:ASP:OD2	11:K:65:HIS:HE1	1.87	0.57
13:T:24:DG:H2'	13:T:25:DG:C8	2.40	0.57
1:A:860:LEU:HD11	1:A:1393:ASN:HD22	1.69	0.57
1:A:1453:TYR:CE2	6:F:129:LYS:HA	2.39	0.57
1:A:898:ARG:HD2	1:A:899:VAL:H	1.68	0.57
2:B:558:LEU:HD21	2:B:600:LEU:HD11	1.87	0.57
4:D:159:THR:O	4:D:163:VAL:HG23	2.05	0.57
7:G:115:MET:HB2	7:G:116:PRO:HD2	1.86	0.57
7:G:18:PHE:HA	7:G:22:MET:HE3	1.86	0.57
9:I:58:VAL:HG12	9:I:58:VAL:O	2.03	0.57
1:A:1106:ASN:O	1:A:1107:VAL:HB	2.04	0.57
1:A:236:LEU:HD23	1:A:236:LEU:N	2.20	0.57
1:A:331:GLY:O	1:A:332:LYS:HB3	2.05	0.57
1:A:336:ILE:HD13	1:A:340:LEU:HD12	1.86	0.57
1:A:682:THR:HG23	1:A:728:LYS:HE3	1.85	0.57
2:B:186:GLU:CG	10:J:62:ARG:HH22	2.18	0.57
2:B:648:HIS:CG	2:B:649:LYS:N	2.71	0.57
2:B:653:VAL:CG2	2:B:689:LEU:HB3	2.33	0.57
2:B:864:LYS:HG3	2:B:872:GLU:OE1	2.04	0.57
3:C:214:ASN:HB3	3:C:217:ASP:OD2	2.04	0.57
3:C:36:VAL:HG21	3:C:251:LEU:CD1	2.35	0.57
4:D:214:LEU:C	4:D:216:ASN:H	2.09	0.57
6:F:87:LYS:HA	6:F:155:LEU:HD22	1.87	0.57
7:G:127:PRO:HG3	7:G:139:ILE:HG13	1.86	0.57
7:G:15:PRO:HA	7:G:18:PHE:CE1	2.39	0.57
1:A:1293:SER:OG	1:A:1295:THR:HG23	2.05	0.56
1:A:567:LYS:NZ	8:H:47:PHE:HB2	2.20	0.56
1:A:768:GLN:CG	1:A:816:HIS:HA	2.17	0.56
2:B:1116:ARG:HG3	2:B:1198:TYR:CE2	2.40	0.56
2:B:1130:PHE:CE1	2:B:1134:GLU:HB3	2.40	0.56
2:B:165:VAL:HG12	2:B:166:PHE:N	2.20	0.56
2:B:126:SER:CB	2:B:172:ILE:HD11	2.34	0.56
3:C:132:PRO:O	3:C:134:ILE:HG13	2.05	0.56
3:C:229:TYR:CD1	3:C:229:TYR:N	2.72	0.56
5:E:180:ARG:HH21	5:E:192:ARG:HD2	1.70	0.56
5:E:22:MET:HE3	5:E:26:ARG:HD2	1.86	0.56
5:E:59:SER:HB3	5:E:81:GLU:HA	1.85	0.56
6:F:75:PRO:O	6:F:77:ASP:O	2.23	0.56
1:A:1161:THR:C	1:A:1163:ILE:H	2.07	0.56
1:A:167:CYS:HB2	1:A:169:ASN:ND2	2.20	0.56
1:A:542:GLU:O	1:A:546:VAL:HG23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:750:GLY:O	2:B:751:VAL:C	2.42	0.56
3:C:212:PRO:CB	3:C:213:PRO:HD2	2.35	0.56
9:I:4:PHE:CE1	9:I:6:PHE:HE2	2.23	0.56
1:A:388:LEU:O	1:A:392:VAL:HG23	2.05	0.56
1:A:37:PHE:HB2	1:A:52:GLY:HA3	1.86	0.56
1:A:584:ASN:C	1:A:586:ILE:H	2.07	0.56
1:A:639:PRO:HG2	1:A:640:GLN:N	2.20	0.56
2:B:839:MET:HG3	2:B:1010:LEU:HD11	1.87	0.56
2:B:1017:ILE:CB	2:B:1018:PRO:HD3	2.33	0.56
2:B:343:ILE:HD12	2:B:347:LYS:NZ	2.21	0.56
2:B:604:ARG:NH2	2:B:613:VAL:O	2.35	0.56
2:B:997:GLU:H	2:B:997:GLU:CD	2.06	0.56
3:C:61:GLU:HA	3:C:64:ALA:HB3	1.86	0.56
5:E:156:LEU:HD12	5:E:195:VAL:CB	2.31	0.56
7:G:127:PRO:HG3	7:G:139:ILE:HD11	1.85	0.56
7:G:35:GLU:HG2	7:G:48:VAL:HG23	1.88	0.56
8:H:118:PHE:C	8:H:120:GLY:H	2.07	0.56
8:H:127:GLY:O	8:H:128:ASN:HB2	2.05	0.56
10:J:36:LEU:HD12	10:J:47:ARG:NH1	2.20	0.56
13:T:21:DC:H2''	13:T:22:DC:C5'	2.35	0.56
1:A:1226:VAL:HG22	1:A:1240:CYS:HB3	1.87	0.56
1:A:134:ARG:HG2	1:A:138:ILE:CD1	2.31	0.56
1:A:865:GLN:HE21	1:A:1370:LEU:HA	1.71	0.56
1:A:503:GLN:HE21	6:F:90:ARG:HH21	1.54	0.56
1:A:794:PRO:HG2	1:A:795:GLU:OE2	2.06	0.56
1:A:798:GLY:HA2	1:A:815:PHE:HD1	1.69	0.56
1:A:828:ALA:CB	2:B:530:GLY:HA2	2.36	0.56
1:A:881:GLN:NE2	1:A:958:VAL:O	2.39	0.56
2:B:465:ASN:HB3	2:B:475:SER:OG	2.05	0.56
2:B:299:GLU:CB	2:B:571:PRO:HG3	2.32	0.56
5:E:9:ILE:HD11	5:E:53:PRO:HD3	1.88	0.56
4:D:3:VAL:CG2	7:G:10:ASN:HB2	2.32	0.56
7:G:34:VAL:HG12	7:G:45:ILE:HG21	1.85	0.56
9:I:106:CYS:O	9:I:107:SER:HB2	2.05	0.56
9:I:71:SER:HG	9:I:101:PHE:HD2	1.53	0.56
12:L:60:ARG:NH2	12:L:65:VAL:HG21	2.20	0.56
1:A:108:MET:N	1:A:108:MET:SD	2.78	0.56
1:A:140:THR:HA	1:A:143:LYS:HE2	1.87	0.56
1:A:35:ILE:HA	1:A:52:GLY:O	2.06	0.56
1:A:503:GLN:HE21	6:F:90:ARG:NH2	2.04	0.56
1:A:477:PRO:CG	1:A:521:MET:HG2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:711:ARG:O	1:A:714:PHE:HB3	2.05	0.56
1:A:69:THR:C	1:A:71:GLN:H	2.07	0.56
2:B:879:ARG:O	2:B:934:LYS:HE2	2.05	0.56
2:B:957:ASN:O	2:B:957:ASN:CG	2.42	0.56
4:D:155:ARG:HD3	4:D:221:TYR:CE1	2.40	0.56
5:E:17:ARG:CB	5:E:17:ARG:HH11	2.14	0.56
9:I:101:PHE:N	9:I:101:PHE:CD1	2.73	0.56
1:A:1313:LEU:HD11	1:A:1317:MET:HE2	1.87	0.56
2:B:616:ILE:HG12	2:B:697:GLU:HA	1.85	0.56
3:C:243:VAL:HG12	3:C:243:VAL:O	2.05	0.56
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.86	0.56
1:A:1050:GLU:O	1:A:1053:PHE:HB3	2.05	0.56
1:A:1322:ILE:O	1:A:1322:ILE:HG13	2.06	0.56
2:B:235:SER:HB3	2:B:258:LEU:HG	1.88	0.56
2:B:603:LEU:HB3	2:B:609:ILE:CD1	2.35	0.56
2:B:792:MET:HA	2:B:856:PHE:O	2.05	0.56
3:C:169:LYS:HE3	3:C:170:TRP:CH2	2.40	0.56
3:C:89:GLU:O	3:C:90:ASP:CB	2.54	0.56
4:D:217:LEU:O	4:D:219:THR:N	2.39	0.56
7:G:29:LYS:HD2	7:G:32:GLU:OE1	2.06	0.56
8:H:99:GLY:HA3	8:H:117:SER:O	2.06	0.56
10:J:34:THR:O	10:J:35:ALA:C	2.44	0.56
1:A:64:ASN:H	1:A:74:MET:CE	2.19	0.56
1:A:821:ARG:HB2	1:A:821:ARG:NH1	2.20	0.56
3:C:39:ALA:HA	3:C:164:ALA:CB	2.31	0.56
3:C:2:SER:O	3:C:3:GLU:HB2	2.05	0.56
9:I:50:THR:CG2	9:I:52:ILE:HG12	2.35	0.56
1:A:1029:ARG:HG3	1:A:1029:ARG:HH11	1.71	0.56
1:A:1141:THR:HA	1:A:1205:LYS:HZ3	1.71	0.56
1:A:1356:ILE:HD12	1:A:1368:MET:SD	2.46	0.56
1:A:332:LYS:HG3	1:A:333:GLU:CD	2.26	0.56
1:A:500:GLU:OE2	1:A:1438:THR:HG21	2.06	0.56
1:A:57:ARG:O	1:A:58:LEU:O	2.23	0.56
1:A:715:GLU:OE1	1:A:774:ARG:HD3	2.05	0.56
1:A:93:VAL:CG2	1:A:301:ALA:HA	2.34	0.56
2:B:613:VAL:HG13	2:B:627:PHE:C	2.26	0.56
2:B:785:TYR:CE1	2:B:795:ILE:HG12	2.41	0.56
2:B:824:ILE:HG22	2:B:1087:PHE:HE2	1.71	0.56
3:C:138:GLU:OE1	3:C:138:GLU:N	2.39	0.56
3:C:242:GLN:C	3:C:244:VAL:H	2.07	0.56
8:H:84:ALA:O	8:H:89:LEU:HD21	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:98:TYR:HE1	8:H:139:ASN:HA	1.69	0.56
1:A:1220:PHE:O	1:A:1221:LYS:HB2	2.06	0.56
1:A:269:ILE:CG1	1:A:299:HIS:HB3	2.31	0.56
2:B:707:PRO:HA	2:B:741:CYS:SG	2.46	0.56
2:B:973:ILE:CG2	2:B:974:PRO:HD2	2.36	0.56
5:E:117:THR:HB	5:E:120:ALA:HB2	1.86	0.56
6:F:86:THR:HG23	6:F:89:GLU:OE1	2.05	0.56
1:A:125:ALA:C	1:A:127:ALA:H	2.08	0.56
1:A:1289:ARG:HD2	1:A:1303:GLU:OE2	2.06	0.56
1:A:1437:GLY:O	1:A:1439:GLY:N	2.39	0.56
1:A:172:PRO:HB3	1:A:185:TRP:CE3	2.41	0.56
1:A:340:LEU:CD2	2:B:1199:ALA:HB3	2.36	0.56
1:A:899:VAL:HG13	1:A:908:LEU:CD2	2.32	0.56
2:B:1147:LEU:HD23	2:B:1147:LEU:C	2.26	0.56
2:B:1169:MET:HE1	2:B:1201:LYS:HA	1.88	0.56
2:B:562:GLY:HA3	2:B:590:HIS:ND1	2.21	0.56
2:B:834:ASN:CA	2:B:838:SER:O	2.54	0.56
3:C:18:VAL:HG12	3:C:18:VAL:O	2.05	0.56
10:J:24:LEU:O	10:J:30:LEU:HB2	2.06	0.56
10:J:1:MET:H1	10:J:56:LEU:N	2.02	0.56
11:K:68:PHE:HB3	11:K:70:ARG:HH11	1.70	0.56
1:A:567:LYS:HB3	1:A:568:PRO:CD	2.36	0.55
1:A:61:ILE:HG22	1:A:62:ASP:N	2.21	0.55
1:A:919:ILE:HG21	1:A:983:ILE:HD11	1.88	0.55
2:B:467:GLY:O	2:B:469:GLN:N	2.39	0.55
2:B:402:GLY:HA2	2:B:695:ALA:HB3	1.87	0.55
3:C:77:ILE:HG23	3:C:161:LYS:NZ	2.21	0.55
3:C:58:LEU:N	3:C:58:LEU:HD22	2.21	0.55
5:E:114:ASN:O	5:E:115:ASN:CB	2.47	0.55
5:E:128:PRO:HA	5:E:129:PRO:C	2.25	0.55
5:E:136:ASN:OD1	5:E:137:GLU:N	2.38	0.55
8:H:100:THR:CG2	8:H:101:ALA:N	2.70	0.55
1:A:1317:MET:O	1:A:1322:ILE:HD11	2.06	0.55
1:A:150:THR:O	1:A:150:THR:HG22	2.05	0.55
1:A:818:MET:HG2	2:B:514:LEU:HG	1.87	0.55
1:A:849:MET:HB2	1:A:1062:GLU:O	2.05	0.55
2:B:1109:GLY:O	2:B:1111:MET:HG2	2.06	0.55
2:B:662:MET:HA	2:B:665:GLU:HB2	1.88	0.55
2:B:855:PHE:CD1	2:B:856:PHE:N	2.73	0.55
4:D:137:ASN:HD22	4:D:137:ASN:N	2.03	0.55
8:H:129:TYR:HA	8:H:131:ASN:ND2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:104:PHE:CE2	8:H:136:LYS:HG2	2.41	0.55
11:K:44:ASN:N	11:K:61:TYR:HE1	2.03	0.55
11:K:65:HIS:CD2	11:K:67:PHE:HB2	2.41	0.55
12:L:27:LEU:HB3	12:L:37:LYS:HB3	1.88	0.55
1:A:107:CYS:SG	1:A:148:CYS:HB2	2.47	0.55
1:A:903:ASN:ND2	1:A:903:ASN:C	2.58	0.55
1:A:913:LEU:HD12	1:A:914:GLU:N	2.18	0.55
5:E:173:SER:C	5:E:175:LEU:H	2.09	0.55
7:G:51:TYR:C	7:G:51:TYR:CD2	2.80	0.55
10:J:64:ASN:CB	10:J:65:PRO:CD	2.80	0.55
1:A:1155:ASP:OD2	1:A:1161:THR:HG23	2.06	0.55
1:A:1262:LYS:C	1:A:1264:GLU:N	2.59	0.55
1:A:915:SER:O	1:A:919:ILE:HG13	2.07	0.55
2:B:344:LYS:O	2:B:345:LYS:C	2.44	0.55
2:B:594:ALA:HB2	9:I:61:ASP:OD1	2.06	0.55
3:C:176:ILE:HG22	3:C:177:GLU:N	2.22	0.55
4:D:53:SER:HA	4:D:56:ARG:HB3	1.88	0.55
5:E:154:ILE:HG22	5:E:155:ARG:O	2.05	0.55
5:E:4:GLU:C	5:E:6:GLU:H	2.08	0.55
8:H:108:SER:O	8:H:110:ASP:N	2.39	0.55
9:I:50:THR:HB	9:I:92:ARG:HH12	1.71	0.55
1:A:104:GLU:HG3	1:A:174:ILE:HD12	1.88	0.55
1:A:21:LEU:HD12	1:A:229:SER:HB2	1.89	0.55
1:A:639:PRO:HG2	1:A:640:GLN:H	1.72	0.55
1:A:886:ILE:HG23	1:A:887:GLY:N	2.21	0.55
3:C:252:GLN:HG3	11:K:95:ILE:HG23	1.87	0.55
5:E:109:ILE:CG2	5:E:110:PHE:H	2.16	0.55
4:D:40:HIS:HD2	7:G:73:LYS:CG	2.19	0.55
9:I:34:TYR:CD2	9:I:35:VAL:N	2.75	0.55
1:A:35:ILE:HG13	1:A:241:VAL:HG21	1.88	0.55
2:B:244:LEU:HD12	2:B:250:PHE:H	1.71	0.55
2:B:243:ALA:HB2	2:B:251:ILE:HG12	1.89	0.55
2:B:284:ILE:HG23	2:B:324:ILE:HD13	1.89	0.55
2:B:549:THR:HG22	2:B:550:ASP:N	2.22	0.55
3:C:196:ASP:HB3	3:C:199:LYS:HB2	1.87	0.55
5:E:55:ARG:C	5:E:57:MET:N	2.60	0.55
9:I:73:ARG:HH12	9:I:112:SER:CB	2.19	0.55
9:I:52:ILE:HG13	9:I:52:ILE:O	2.05	0.55
10:J:6:ARG:HB3	10:J:11:GLY:O	2.07	0.55
1:A:1284:MET:HA	1:A:1306:LEU:HD23	1.89	0.55
1:A:1373:ASP:O	1:A:1377:THR:HG23	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1423:GLY:HA3	1:A:1426:GLU:HG2	1.88	0.55
1:A:535:THR:HG21	1:A:616:VAL:CA	2.28	0.55
1:A:935:GLN:HE22	1:A:938:LYS:HD2	1.71	0.55
3:C:6:PRO:HB2	11:K:101:LEU:HD12	1.89	0.55
5:E:133:GLU:HG2	5:E:135:PHE:HE1	1.70	0.55
1:A:1342:GLU:CD	5:E:198:ILE:HG21	2.26	0.55
5:E:38:PRO:HG2	5:E:41:ASP:HB2	1.87	0.55
4:D:40:HIS:HB2	7:G:73:LYS:HD3	1.88	0.55
9:I:99:LEU:O	9:I:111:THR:HG23	2.07	0.55
1:A:98:LYS:O	1:A:102:VAL:HG23	2.06	0.55
1:A:224:PHE:CD2	1:A:231:PRO:HG3	2.42	0.55
2:B:1115:THR:O	2:B:1116:ARG:HB2	2.06	0.55
2:B:579:ARG:HD2	2:B:586:TRP:CZ2	2.42	0.55
2:B:526:GLU:OE1	2:B:752:ALA:HB3	2.07	0.55
4:D:163:VAL:O	4:D:166:LEU:HB3	2.06	0.55
5:E:90:VAL:CA	5:E:120:ALA:HB2	2.37	0.55
5:E:153:HIS:HB3	5:E:196:VAL:HG11	1.87	0.55
5:E:206:GLY:O	5:E:207:ARG:HG2	2.07	0.55
5:E:52:ARG:HB3	5:E:53:PRO:CD	2.35	0.55
6:F:116:ASP:O	6:F:120:ILE:HG13	2.06	0.55
8:H:10:PHE:N	8:H:10:PHE:CD1	2.75	0.55
1:A:1341:ILE:HG23	1:A:1342:GLU:H	1.70	0.55
1:A:849:MET:CE	1:A:1061:GLY:HA2	2.35	0.55
1:A:929:LEU:HD13	1:A:929:LEU:O	2.06	0.55
2:B:69:LEU:CD1	2:B:429:PHE:HD1	1.89	0.55
2:B:842:ASN:HD22	2:B:845:SER:HB3	1.71	0.55
2:B:873:THR:O	2:B:914:LYS:HA	2.07	0.55
4:D:8:PHE:CE1	4:D:37:GLN:HB2	2.41	0.55
1:A:1318:THR:HB	5:E:141:VAL:HG11	1.87	0.55
5:E:177:ARG:C	5:E:212:ARG:HD3	2.27	0.55
6:F:99:LEU:O	6:F:103:MET:CG	2.55	0.55
8:H:5:LEU:O	8:H:6:PHE:HB2	2.06	0.55
1:A:1141:THR:OG1	1:A:1205:LYS:HD3	2.07	0.55
1:A:154:SER:C	1:A:156:ASP:H	2.10	0.55
1:A:590:ARG:CD	1:A:604:GLY:HA2	2.37	0.55
2:B:278:GLN:CG	2:B:279:ASP:H	2.13	0.55
2:B:696:GLU:O	2:B:699:GLU:HB2	2.07	0.55
2:B:708:GLU:HG3	2:B:709:ASP:N	2.22	0.55
7:G:7:LEU:O	7:G:73:LYS:HE2	2.07	0.55
2:B:620:ARG:NH1	9:I:68:LEU:HD21	2.23	0.55
1:A:1074:GLU:HB3	1:A:1075:PRO:CD	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1152:ILE:HG22	1:A:1192:LEU:O	2.06	0.54
1:A:1330:ASN:O	1:A:1332:PHE:N	2.40	0.54
1:A:134:ARG:O	1:A:138:ILE:HG13	2.07	0.54
1:A:55:ASP:C	1:A:57:ARG:N	2.58	0.54
2:B:390:LEU:O	2:B:392:ARG:N	2.40	0.54
2:B:613:VAL:CG2	2:B:628:THR:HA	2.35	0.54
2:B:807:ARG:NH1	2:B:807:ARG:HB3	2.22	0.54
2:B:893:LEU:HD22	2:B:897:GLY:C	2.27	0.54
4:D:14:ARG:O	4:D:16:LYS:HG2	2.07	0.54
7:G:22:MET:O	7:G:23:LYS:C	2.46	0.54
9:I:35:VAL:CG1	9:I:36:GLU:H	2.18	0.54
11:K:31:VAL:CG1	11:K:32:VAL:H	2.18	0.54
1:A:1308:THR:CG2	1:A:1309:ASP:N	2.57	0.54
1:A:41:MET:CB	1:A:50:ILE:H	2.19	0.54
2:B:788:ARG:NH1	2:B:790:ASP:OD1	2.41	0.54
2:B:847:ASP:C	2:B:849:GLY:N	2.59	0.54
5:E:124:VAL:N	5:E:125:PRO:CD	2.70	0.54
5:E:39:LEU:O	5:E:42:PHE:HB3	2.07	0.54
9:I:55:THR:HG21	9:I:109:ILE:HD13	1.88	0.54
1:A:1001:ARG:O	1:A:1002:GLY:O	2.25	0.54
1:A:1081:LEU:HD12	1:A:1098:VAL:HG23	1.89	0.54
1:A:658:LEU:HD23	1:A:659:HIS:HE1	1.69	0.54
1:A:9:ALA:HB3	2:B:1193:GLN:HB2	1.88	0.54
2:B:205:ILE:N	2:B:205:ILE:HD12	2.23	0.54
2:B:305:VAL:HG12	2:B:305:VAL:O	2.07	0.54
3:C:148:ARG:HG2	3:C:149:LYS:N	2.23	0.54
4:D:203:SER:OG	4:D:206:GLU:HB2	2.08	0.54
5:E:185:ALA:O	5:E:190:LEU:HB2	2.08	0.54
9:I:59:VAL:HG12	9:I:60:GLN:H	1.72	0.54
1:A:967:ALA:CA	1:A:1044:TRP:HZ3	2.21	0.54
1:A:1114:PRO:O	1:A:1115:SER:O	2.24	0.54
1:A:1161:THR:C	1:A:1163:ILE:N	2.61	0.54
1:A:427:GLN:HB2	1:A:430:TRP:CE2	2.42	0.54
1:A:427:GLN:HG3	1:A:430:TRP:CE2	2.42	0.54
1:A:746:MET:HE3	2:B:1018:PRO:HG2	1.90	0.54
2:B:360:PHE:O	2:B:361:LEU:C	2.46	0.54
2:B:936:ASP:OD1	2:B:937:ALA:N	2.40	0.54
5:E:89:GLY:C	5:E:91:LYS:H	2.10	0.54
7:G:96:GLN:HA	7:G:121:PHE:CZ	2.41	0.54
3:C:7:GLN:HG2	11:K:104:ASN:ND2	2.23	0.54
1:A:1019:CYS:O	1:A:1022:LEU:HB3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1223:ASP:HA	1:A:1243:VAL:HG11	1.88	0.54
1:A:185:TRP:CZ3	1:A:200:ARG:HB3	2.43	0.54
1:A:316:GLN:O	1:A:317:LYS:C	2.45	0.54
1:A:728:LYS:CA	1:A:731:ARG:HH21	2.20	0.54
2:B:455:SER:O	2:B:456:GLY:C	2.46	0.54
2:B:707:PRO:HG2	2:B:708:GLU:H	1.72	0.54
2:B:68:THR:HG23	2:B:91:SER:HB3	1.88	0.54
5:E:153:HIS:O	5:E:154:ILE:CG1	2.48	0.54
8:H:76:THR:O	8:H:77:ARG:HB2	2.08	0.54
9:I:12:ASN:OD1	9:I:31:THR:HG21	2.08	0.54
9:I:7:CYS:HB3	9:I:14:LEU:CD2	2.38	0.54
10:J:60:PHE:O	10:J:63:TYR:HD1	1.90	0.54
12:L:55:ILE:CG1	12:L:56:LEU:H	2.21	0.54
1:A:254:GLU:HB2	2:B:935:ARG:NH2	2.23	0.54
1:A:343:LYS:HZ3	2:B:1151:LEU:HD12	1.69	0.54
1:A:688:LYS:HA	1:A:691:LEU:HB3	1.88	0.54
1:A:831:THR:HG23	1:A:832:ALA:N	2.23	0.54
3:C:91:HIS:ND1	3:C:158:VAL:HG11	2.22	0.54
3:C:184:ASN:HD21	3:C:187:LYS:HA	1.72	0.54
4:D:170:THR:C	4:D:172:LEU:N	2.61	0.54
5:E:85:GLU:HB2	5:E:88:VAL:CG2	2.35	0.54
5:E:93:MET:O	5:E:95:THR:N	2.41	0.54
7:G:34:VAL:HG11	7:G:74:TYR:HE1	1.72	0.54
8:H:62:SER:OG	8:H:63:LEU:N	2.41	0.54
1:A:111:GLY:O	1:A:214:ILE:HA	2.07	0.54
1:A:1254:ALA:O	1:A:1255:GLU:CB	2.54	0.54
1:A:578:LEU:HD23	1:A:612:ILE:CD1	2.38	0.54
1:A:602:ASP:HB3	1:A:616:VAL:HG23	1.88	0.54
1:A:852:TYR:CD2	1:A:1060:PRO:CB	2.89	0.54
1:A:898:ARG:HA	1:A:933:TYR:CD1	2.42	0.54
2:B:170:LEU:HD12	2:B:170:LEU:C	2.27	0.54
2:B:68:THR:HG22	2:B:69:LEU:H	1.71	0.54
2:B:616:ILE:CG2	2:B:700:SER:OG	2.56	0.54
2:B:711:GLU:HB2	2:B:712:PRO:CD	2.38	0.54
3:C:177:GLU:CG	3:C:231:ASN:HB3	2.37	0.54
4:D:66:ARG:HD2	4:D:133:THR:HB	1.90	0.54
4:D:207:LEU:HD23	4:D:207:LEU:C	2.28	0.54
8:H:19:ARG:O	8:H:20:TYR:HD2	1.91	0.54
8:H:38:LEU:HD12	8:H:39:THR:H	1.73	0.54
9:I:4:PHE:HD1	9:I:4:PHE:C	2.11	0.54
1:A:105:CYS:SG	1:A:139:TRP:HA	2.48	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:VAL:HG12	1:A:153:PRO:HD2	1.90	0.54
1:A:193:ASP:O	1:A:194:ALA:HB3	2.08	0.54
1:A:1418:LEU:HB3	2:B:1222:ARG:NH1	2.23	0.54
2:B:63:ILE:HA	2:B:421:PHE:CE2	2.43	0.54
2:B:658:ILE:HG22	2:B:662:MET:HE2	1.89	0.54
2:B:802:PRO:HG2	2:B:805:THR:HG22	1.89	0.54
8:H:145:ARG:O	8:H:146:ARG:HB2	2.08	0.54
3:C:14:SER:HA	11:K:114:LEU:HD22	1.89	0.54
1:A:968:GLN:HE22	1:A:1035:TYR:HB2	1.72	0.54
1:A:1156:PRO:HA	1:A:1190:PRO:CB	2.38	0.54
1:A:407:ARG:HG2	1:A:430:TRP:CH2	2.42	0.54
1:A:556:TRP:CE3	1:A:558:GLY:HA2	2.42	0.54
1:A:590:ARG:HH21	1:A:620:LYS:CB	2.19	0.54
1:A:729:ALA:HA	1:A:732:LEU:HD12	1.88	0.54
1:A:738:LYS:H	1:A:738:LYS:CD	2.15	0.54
1:A:874:ASP:N	1:A:1058:VAL:HG23	2.23	0.54
2:B:230:ALA:N	2:B:231:PRO:CD	2.70	0.54
2:B:326:ASP:O	2:B:328:GLU:N	2.41	0.54
2:B:38:PHE:CD1	2:B:811:TYR:CD2	2.96	0.54
3:C:213:PRO:O	3:C:214:ASN:CB	2.55	0.54
8:H:81:PRO:CB	8:H:82:PRO:CD	2.74	0.54
1:A:1153:TYR:CD2	1:A:1163:ILE:HD11	2.43	0.54
1:A:1386:ARG:HB2	1:A:1403:GLU:OE1	2.08	0.54
1:A:1063:MET:CG	1:A:1436:ILE:HG23	2.38	0.54
1:A:1446:ASP:O	1:A:1447:GLU:C	2.45	0.54
1:A:18:GLN:HG2	1:A:1418:LEU:CD1	2.34	0.54
1:A:974:ASP:OD2	1:A:976:THR:OG1	2.26	0.54
2:B:124:TYR:HH	2:B:179:CYS:HG	1.55	0.54
2:B:95:ILE:CG1	2:B:130:VAL:HG22	2.38	0.54
2:B:60:GLN:NE2	2:B:94:LYS:HA	2.23	0.54
2:B:850:LEU:CD2	2:B:1009:ASP:HB3	2.38	0.54
3:C:34:ARG:HA	3:C:37:MET:HE2	1.89	0.54
5:E:13:TRP:CZ3	5:E:39:LEU:HB2	2.43	0.54
10:J:27:GLU:O	10:J:29:GLU:HG3	2.07	0.54
11:K:31:VAL:CG1	11:K:32:VAL:N	2.69	0.54
1:A:551:TYR:CZ	11:K:62:LYS:HE2	2.43	0.54
1:A:262:LEU:HD12	1:A:328:ARG:NH2	2.23	0.53
1:A:269:ILE:HD13	1:A:300:VAL:HG22	1.89	0.53
1:A:444:PHE:HB3	1:A:458:HIS:HD2	1.73	0.53
1:A:567:LYS:CB	1:A:568:PRO:CD	2.86	0.53
1:A:583:PRO:HG2	1:A:586:ILE:CG1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:884:ASP:O	1:A:886:ILE:N	2.41	0.53
2:B:1098:MET:H	2:B:1098:MET:HE3	1.73	0.53
2:B:1171:VAL:HA	2:B:1182:CYS:HB2	1.90	0.53
2:B:97:VAL:CG2	2:B:128:LEU:HG	2.38	0.53
3:C:102:GLN:HG2	3:C:154:LYS:HG2	1.90	0.53
4:D:24:ALA:C	4:D:26:THR:N	2.60	0.53
6:F:119:ARG:HH11	6:F:119:ARG:HG3	1.72	0.53
7:G:51:TYR:HD2	7:G:51:TYR:C	2.12	0.53
11:K:23:PRO:HA	11:K:31:VAL:HG13	1.90	0.53
3:C:165:LYS:O	11:K:6:ARG:NH1	2.39	0.53
13:T:22:DC:H2'	13:T:23:BRU:H6	1.90	0.53
1:A:1120:LEU:HD22	1:A:1124:HIS:O	2.09	0.53
1:A:1230:GLU:C	1:A:1232:ASN:H	2.11	0.53
1:A:396:PRO:HB3	1:A:403:LYS:HA	1.90	0.53
1:A:371:ALA:HB2	1:A:462:VAL:HG13	1.90	0.53
1:A:64:ASN:O	1:A:65:LEU:C	2.46	0.53
2:B:57:TYR:CD1	2:B:57:TYR:N	2.76	0.53
3:C:235:VAL:HG12	10:J:13:VAL:CG2	2.37	0.53
4:D:126:ILE:HD13	4:D:145:MET:HE2	1.91	0.53
4:D:139:LYS:HG3	4:D:143:ASN:ND2	2.23	0.53
4:D:40:HIS:CD2	7:G:73:LYS:HZ3	2.26	0.53
7:G:99:PHE:HZ	7:G:163:ILE:HD13	1.73	0.53
8:H:42:ILE:HG12	8:H:97:MET:HE1	1.90	0.53
10:J:7:CYS:SG	10:J:49:MET:HE3	2.48	0.53
11:K:7:PHE:C	11:K:9:LEU:N	2.62	0.53
1:A:1103:GLU:O	1:A:1108:ALA:HB2	2.08	0.53
1:A:233:TRP:C	1:A:235:ILE:N	2.61	0.53
1:A:384:ASN:OD1	1:A:388:LEU:HD12	2.07	0.53
1:A:825:ILE:HG22	1:A:826:ASP:N	2.22	0.53
2:B:1073:TYR:CE2	2:B:1080:LYS:HG2	2.43	0.53
2:B:563:MET:HE3	2:B:580:VAL:HB	1.91	0.53
2:B:685:LEU:HG	2:B:686:ASN:N	2.24	0.53
2:B:899:ILE:HG23	2:B:903:VAL:HG21	1.89	0.53
3:C:74:SER:OG	3:C:237:SER:HB2	2.07	0.53
5:E:121:MET:O	5:E:124:VAL:HG23	2.09	0.53
1:A:1008:GLN:O	1:A:1011:GLN:HB3	2.09	0.53
1:A:340:LEU:HD21	2:B:1200:ALA:N	2.23	0.53
1:A:353:ILE:CD1	1:A:487:MET:HE2	2.36	0.53
1:A:463:ILE:HD11	1:A:469:ARG:HG3	1.89	0.53
1:A:525:GLN:O	1:A:528:LEU:N	2.42	0.53
1:A:591:PHE:HA	1:A:595:THR:CG2	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1106:ARG:HH12	2:B:1110:PRO:HG2	1.72	0.53
2:B:377:PHE:O	2:B:380:TYR:N	2.42	0.53
2:B:465:ASN:N	2:B:465:ASN:ND2	2.55	0.53
2:B:39:ARG:HH21	2:B:665:GLU:CD	2.11	0.53
2:B:616:ILE:HG23	2:B:700:SER:OG	2.08	0.53
2:B:753:ALA:HA	2:B:756:ILE:CD1	2.39	0.53
2:B:880:THR:HB	2:B:934:LYS:HE2	1.88	0.53
3:C:193:TYR:HD1	3:C:193:TYR:O	1.91	0.53
3:C:245:VAL:O	3:C:249:ASP:N	2.40	0.53
4:D:52:LEU:O	4:D:54:GLU:N	2.39	0.53
4:D:60:LYS:O	4:D:64:VAL:HG23	2.08	0.53
8:H:64:ASN:ND2	8:H:88:SER:C	2.61	0.53
2:B:900:ALA:CB	12:L:61:THR:OG1	2.56	0.53
1:A:1397:LEU:O	1:A:1400:CYS:HB3	2.09	0.53
1:A:676:MET:O	1:A:679:ILE:HB	2.08	0.53
1:A:70:CYS:O	1:A:72:GLU:HG2	2.08	0.53
1:A:913:LEU:HG	1:A:914:GLU:N	2.23	0.53
1:A:92:HIS:O	1:A:94:GLY:N	2.42	0.53
2:B:284:ILE:HG23	2:B:324:ILE:CD1	2.38	0.53
2:B:469:GLN:CG	2:B:470:LYS:H	2.22	0.53
2:B:659:ALA:HA	2:B:662:MET:HE2	1.91	0.53
2:B:637:LEU:CD1	2:B:693:ILE:HD12	2.22	0.53
2:B:899:ILE:O	2:B:952:VAL:HG21	2.09	0.53
2:B:984:HIS:NE2	2:B:1025:HIS:HA	2.23	0.53
5:E:178:ILE:HG13	5:E:182:ASP:OD2	2.08	0.53
12:L:24:THR:O	12:L:25:ALA:HB3	2.08	0.53
1:A:997:LEU:HD13	1:A:1018:PHE:CE2	2.43	0.53
1:A:896:ARG:NH2	1:A:1030:ARG:NH2	2.56	0.53
1:A:182:VAL:CG2	1:A:201:VAL:HA	2.32	0.53
1:A:311:GLN:O	1:A:312:PRO:C	2.46	0.53
1:A:473:SER:HG	1:A:646:PHE:HD2	1.56	0.53
1:A:613:ILE:O	1:A:614:PHE:HB3	2.08	0.53
1:A:682:THR:HG22	1:A:728:LYS:HE3	1.91	0.53
1:A:687:LYS:O	1:A:690:VAL:HB	2.08	0.53
1:A:963:ILE:HD11	1:A:1048:ASN:HB3	1.89	0.53
2:B:1058:LEU:N	2:B:1058:LEU:HD23	2.23	0.53
2:B:1178:ASN:O	2:B:1180:PHE:CD1	2.61	0.53
2:B:802:PRO:HG2	2:B:805:THR:CG2	2.39	0.53
2:B:955:THR:HG23	2:B:956:THR:H	1.74	0.53
3:C:209:TYR:N	3:C:209:TYR:CD1	2.76	0.53
5:E:212:ARG:HH11	5:E:212:ARG:CG	2.20	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:89:LEU:C	8:H:91:ASP:N	2.62	0.53
1:A:1163:ILE:HG22	1:A:1165:GLU:HG2	1.91	0.53
1:A:1187:GLN:HA	1:A:1244:ARG:HD2	1.91	0.53
1:A:178:GLY:C	1:A:179:LEU:HD23	2.28	0.53
1:A:408:ASP:O	1:A:410:GLY:N	2.42	0.53
1:A:740:LEU:HD12	1:A:741:ASN:N	2.24	0.53
1:A:940:ARG:NH1	1:A:940:ARG:HG2	2.20	0.53
1:A:947:PHE:CD1	1:A:947:PHE:N	2.76	0.53
2:B:222:ILE:O	2:B:240:ILE:HA	2.08	0.53
2:B:265:SER:O	2:B:266:ALA:C	2.47	0.53
4:D:126:ILE:HD13	4:D:145:MET:CE	2.39	0.53
4:D:66:ARG:HG3	7:G:51:TYR:CD1	2.43	0.53
5:E:110:PHE:HE2	5:E:112:TYR:HB3	1.72	0.53
7:G:13:LEU:HD22	7:G:17:PHE:HB2	1.90	0.53
9:I:44:TYR:CD1	9:I:45:ARG:N	2.77	0.53
10:J:31:ASP:O	10:J:32:GLU:C	2.47	0.53
1:A:1015:VAL:CG1	1:A:1019:CYS:SG	2.96	0.53
1:A:704:ALA:O	1:A:705:LYS:C	2.46	0.53
1:A:798:GLY:HA2	1:A:815:PHE:CD1	2.44	0.53
1:A:343:LYS:HD3	2:B:1155:SER:OG	2.09	0.53
2:B:294:ASP:HB2	9:I:12:ASN:HA	1.91	0.53
2:B:309:GLN:CD	9:I:52:ILE:HD11	2.29	0.53
2:B:506:GLY:CA	2:B:512:ARG:HH21	2.07	0.53
2:B:896:ASP:OD2	12:L:58:LYS:HE3	2.09	0.53
4:D:137:ASN:ND2	4:D:137:ASN:H	2.06	0.53
4:D:51:ASN:O	4:D:52:LEU:O	2.27	0.53
5:E:112:TYR:CZ	5:E:136:ASN:HB2	2.44	0.53
1:A:1100:ARG:O	1:A:1104:ILE:HG13	2.08	0.53
1:A:135:PHE:HD1	1:A:222:LEU:HD22	1.74	0.53
1:A:224:PHE:CG	1:A:231:PRO:HG3	2.43	0.53
1:A:278:THR:CG2	1:A:282:ASN:HD22	2.21	0.53
1:A:675:THR:O	1:A:679:ILE:HG13	2.09	0.53
1:A:734:GLU:C	1:A:736:ASN:H	2.10	0.53
1:A:858:ASN:ND2	1:A:858:ASN:C	2.62	0.53
2:B:215:GLN:HA	2:B:215:GLN:NE2	2.24	0.53
2:B:273:LEU:HD12	2:B:276:ILE:CD1	2.37	0.53
2:B:62:ILE:HG23	2:B:418:LYS:HG3	1.91	0.53
2:B:63:ILE:HD12	2:B:421:PHE:CE2	2.43	0.53
2:B:745:PRO:C	2:B:747:MET:H	2.13	0.53
2:B:882:THR:HG21	2:B:934:LYS:O	2.09	0.53
3:C:174:ALA:O	3:C:175:ALA:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:181:ASP:OD2	3:C:184:ASN:HA	2.08	0.53
4:D:7:THR:HB	7:G:42:PHE:CZ	2.43	0.53
5:E:14:ARG:HA	5:E:17:ARG:HG2	1.91	0.53
5:E:22:MET:O	5:E:26:ARG:HB2	2.09	0.53
5:E:9:ILE:CD1	5:E:53:PRO:HD3	2.38	0.53
1:A:1446:ASP:HB2	6:F:133:VAL:CG2	2.38	0.53
6:F:85:MET:O	6:F:155:LEU:HD21	2.08	0.53
7:G:17:PHE:N	7:G:17:PHE:HD2	2.07	0.53
4:D:50:LEU:HD11	7:G:4:ILE:CD1	2.38	0.53
10:J:16:ASP:OD1	10:J:17:LYS:HD2	2.09	0.53
1:A:1206:ASP:HB3	1:A:1274:ARG:NH1	2.19	0.53
1:A:1272:THR:C	1:A:1273:LEU:HD12	2.30	0.53
1:A:1276:VAL:HG12	1:A:1277:GLU:N	2.23	0.53
1:A:1351:GLU:O	1:A:1355:VAL:HG23	2.09	0.53
1:A:308:ILE:HG22	1:A:309:ALA:N	2.12	0.53
1:A:401:GLY:C	1:A:435:HIS:CD2	2.82	0.53
1:A:598:LEU:O	1:A:599:SER:C	2.47	0.53
1:A:75:ASN:O	1:A:76:GLU:CB	2.56	0.53
2:B:1159:ARG:HD2	2:B:1159:ARG:C	2.29	0.53
2:B:133:LYS:HG3	2:B:135:ARG:HE	1.73	0.53
2:B:221:ASN:OD1	2:B:242:SER:HA	2.09	0.53
2:B:272:THR:O	2:B:273:LEU:HD23	2.09	0.53
2:B:589:VAL:HG12	2:B:590:HIS:H	1.73	0.53
2:B:710:LEU:HA	2:B:733:HIS:HB3	1.90	0.53
2:B:879:ARG:CZ	2:B:883:LEU:HD22	2.38	0.53
3:C:123:ASN:CG	3:C:125:MET:H	2.11	0.53
3:C:148:ARG:HG2	3:C:149:LYS:H	1.74	0.53
4:D:60:LYS:NZ	4:D:115:HIS:CE1	2.76	0.53
5:E:86:PRO:HA	5:E:113:GLN:HB2	1.90	0.53
5:E:63:ASN:HB3	5:E:64:PRO:CD	2.38	0.53
8:H:100:THR:CG2	8:H:101:ALA:H	2.22	0.53
8:H:135:LEU:HD13	8:H:137:GLN:HE21	1.73	0.53
2:B:955:THR:OG1	12:L:55:ILE:HA	2.09	0.53
1:A:107:CYS:N	1:A:114:LEU:HD21	2.24	0.52
1:A:168:GLY:O	1:A:169:ASN:C	2.46	0.52
1:A:867:ILE:HG13	1:A:1000:LEU:HD21	1.91	0.52
2:B:1065:GLN:NE2	2:B:1066:SER:N	2.57	0.52
2:B:1085:ILE:HD12	2:B:1085:ILE:N	2.23	0.52
2:B:318:VAL:C	2:B:320:ASP:N	2.62	0.52
2:B:605:ARG:CZ	2:B:639:ILE:HD13	2.38	0.52
2:B:687:GLU:HB3	2:B:689:LEU:HG	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:22:LEU:HD13	3:C:230:MET:HE1	1.90	0.52
3:C:69:LEU:HD12	3:C:69:LEU:N	2.24	0.52
4:D:64:VAL:C	4:D:66:ARG:N	2.62	0.52
5:E:94:LYS:HG3	5:E:98:ILE:CD1	2.39	0.52
8:H:80:ARG:NH1	11:K:57:LEU:HD21	2.20	0.52
1:A:21:LEU:HG	1:A:1413:GLY:O	2.09	0.52
1:A:23:SER:HB3	1:A:233:TRP:CZ2	2.45	0.52
1:A:523:ILE:HD12	1:A:622:VAL:HG21	1.91	0.52
2:B:273:LEU:CD1	2:B:276:ILE:HD12	2.39	0.52
2:B:313:MET:CE	2:B:390:LEU:HD21	2.39	0.52
2:B:859:TYR:HD1	2:B:859:TYR:H	1.57	0.52
5:E:162:ARG:HB3	5:E:162:ARG:CZ	2.39	0.52
7:G:112:LYS:HA	7:G:115:MET:CE	2.40	0.52
14:N:3:DT:OP2	14:N:3:DT:H3'	2.09	0.52
1:A:322:VAL:CG1	1:A:322:VAL:O	2.58	0.52
1:A:334:GLY:O	1:A:335:ARG:C	2.48	0.52
1:A:452:LYS:HG3	2:B:1140:ALA:HB1	1.90	0.52
1:A:618:GLU:OE2	1:A:620:LYS:HB2	2.09	0.52
1:A:677:ARG:HD2	1:A:678:GLU:N	2.25	0.52
1:A:825:ILE:HG22	1:A:826:ASP:H	1.73	0.52
2:B:1167:GLY:O	2:B:1215:ARG:HA	2.10	0.52
2:B:192:LEU:O	2:B:193:LYS:HB2	2.09	0.52
2:B:460:ALA:HB1	2:B:466:TRP:CZ3	2.44	0.52
2:B:597:MET:HE2	2:B:597:MET:HA	1.90	0.52
2:B:955:THR:HG23	2:B:956:THR:N	2.24	0.52
3:C:189:THR:HG22	3:C:190:ASP:H	1.73	0.52
1:A:954:TRP:CZ3	5:E:203:GLU:HB2	2.43	0.52
9:I:7:CYS:SG	9:I:8:ARG:O	2.67	0.52
1:A:1074:GLU:HB3	1:A:1075:PRO:HD3	1.90	0.52
1:A:1394:THR:CG2	1:A:1398:MET:SD	2.97	0.52
1:A:507:VAL:N	1:A:508:PRO:CD	2.72	0.52
1:A:884:ASP:HB3	1:A:896:ARG:HH12	1.74	0.52
2:B:1030:LEU:HD11	2:B:1059:LEU:HD22	1.92	0.52
2:B:1053:GLU:HB3	2:B:1057:LYS:HE3	1.90	0.52
2:B:175:ARG:NH1	2:B:175:ARG:HG2	2.23	0.52
2:B:260:GLY:O	2:B:267:ARG:NH1	2.43	0.52
2:B:368:GLU:O	2:B:370:PHE:N	2.38	0.52
2:B:542:MET:HG2	2:B:747:MET:HB3	1.91	0.52
2:B:613:VAL:CG1	2:B:628:THR:HA	2.39	0.52
2:B:805:THR:HB	2:B:809:MET:SD	2.49	0.52
2:B:952:VAL:HG12	2:B:953:LEU:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:956:THR:HG22	2:B:960:GLY:HA2	1.91	0.52
4:D:34:GLN:O	4:D:47:LEU:HD23	2.09	0.52
5:E:134:THR:C	5:E:135:PHE:HD1	2.13	0.52
6:F:90:ARG:HH11	6:F:90:ARG:HB2	1.73	0.52
7:G:34:VAL:HG11	7:G:74:TYR:CE1	2.45	0.52
12:L:33:GLU:C	12:L:35:SER:H	2.13	0.52
1:A:1313:LEU:C	1:A:1315:GLU:H	2.13	0.52
1:A:1063:MET:HG3	1:A:1436:ILE:HG23	1.92	0.52
1:A:179:LEU:O	1:A:180:LYS:HG3	2.09	0.52
1:A:219:PHE:CE2	1:A:231:PRO:HD2	2.45	0.52
1:A:555:ASP:O	1:A:556:TRP:O	2.27	0.52
1:A:575:LYS:HB3	1:A:612:ILE:HG21	1.92	0.52
1:A:63:ARG:HG3	1:A:63:ARG:O	2.09	0.52
1:A:64:ASN:H	1:A:74:MET:HE1	1.74	0.52
1:A:853:ASP:OD1	1:A:855:THR:CB	2.58	0.52
1:A:913:LEU:CG	1:A:914:GLU:N	2.72	0.52
2:B:376:PHE:O	2:B:586:TRP:HZ3	1.93	0.52
2:B:648:HIS:CD2	2:B:649:LYS:H	2.28	0.52
2:B:745:PRO:O	2:B:747:MET:N	2.43	0.52
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.92	0.52
2:B:485:ARG:CZ	2:B:782:LEU:HD11	2.40	0.52
3:C:132:PRO:O	3:C:133:ILE:C	2.47	0.52
4:D:179:GLN:O	4:D:183:LEU:HB2	2.10	0.52
5:E:178:ILE:HG23	5:E:178:ILE:O	2.08	0.52
5:E:22:MET:HE1	5:E:26:ARG:HH11	1.71	0.52
5:E:91:LYS:C	5:E:93:MET:H	2.11	0.52
8:H:135:LEU:HD13	8:H:137:GLN:NE2	2.24	0.52
8:H:64:ASN:OD1	8:H:90:ALA:CB	2.58	0.52
1:A:1225:PHE:HZ	1:A:1227:ILE:HD11	1.73	0.52
1:A:1299:VAL:HG12	1:A:1300:LYS:N	2.23	0.52
1:A:333:GLU:N	1:A:333:GLU:OE2	2.43	0.52
1:A:808:LEU:HD23	1:A:813:PHE:HA	1.90	0.52
1:A:919:ILE:HG21	1:A:983:ILE:CD1	2.39	0.52
2:B:1150:ARG:NH1	2:B:1150:ARG:HB3	2.25	0.52
2:B:724:ASP:HB3	2:B:727:LYS:HG3	1.91	0.52
2:B:755:ILE:HG22	2:B:755:ILE:O	2.09	0.52
3:C:154:LYS:O	3:C:155:LEU:HD23	2.10	0.52
4:D:159:THR:O	4:D:162:ALA:HB3	2.09	0.52
6:F:103:MET:HE3	7:G:66:GLY:H	1.74	0.52
9:I:82:GLU:O	9:I:104:LEU:HG	2.09	0.52
9:I:85:PHE:N	9:I:85:PHE:CD2	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:95:THR:HG22	9:I:96:SER:N	2.25	0.52
1:A:1224:LEU:HD12	1:A:1225:PHE:N	2.25	0.52
1:A:1316:VAL:HG12	1:A:1316:VAL:O	2.10	0.52
1:A:1438:THR:O	1:A:1438:THR:HG22	2.10	0.52
1:A:606:LEU:HG	1:A:613:ILE:HD12	1.90	0.52
1:A:919:ILE:HG23	1:A:925:LEU:HD12	1.91	0.52
2:B:1106:ARG:HD3	2:B:1127:GLY:CA	2.40	0.52
2:B:120:ARG:HE	2:B:955:THR:HG21	1.73	0.52
3:C:136:ASP:CB	3:C:141:GLY:H	2.23	0.52
5:E:65:THR:O	5:E:68:SER:N	2.42	0.52
6:F:71:GLU:O	6:F:72:LYS:C	2.48	0.52
8:H:15:VAL:HG21	8:H:49:VAL:HG12	1.91	0.52
1:A:567:LYS:HG3	8:H:94:ASP:O	2.10	0.52
14:N:6:DT:H2"	14:N:7:DT:OP2	2.10	0.52
13:T:11:DA:H2"	13:T:12:DG:C8	2.45	0.52
1:A:1263:ILE:O	1:A:1263:ILE:HG22	2.09	0.52
1:A:1434:ALA:O	1:A:1436:ILE:N	2.42	0.52
1:A:157:ASP:C	1:A:159:THR:H	2.13	0.52
1:A:244:PRO:HB2	1:A:245:PRO:HD3	1.92	0.52
1:A:298:PHE:O	1:A:301:ALA:HB3	2.10	0.52
2:B:203:PHE:HB3	2:B:205:ILE:CD1	2.39	0.52
2:B:309:GLN:O	2:B:310:MET:C	2.47	0.52
2:B:496:ARG:HD2	2:B:751:VAL:CG2	2.40	0.52
2:B:995:ARG:NH1	3:C:165:LYS:HA	2.25	0.52
3:C:123:ASN:ND2	3:C:125:MET:HA	2.25	0.52
5:E:85:GLU:O	5:E:87:SER:N	2.43	0.52
7:G:1:MET:HE1	7:G:80:LYS:O	2.09	0.52
9:I:82:GLU:HB3	9:I:104:LEU:CD1	2.37	0.52
12:L:29:TYR:HA	12:L:57:LEU:O	2.10	0.52
1:A:1001:ARG:HH11	1:A:1001:ARG:HG2	1.73	0.52
1:A:1038:THR:HG23	1:A:1041:ALA:HB2	1.92	0.52
1:A:1389:PHE:CD1	1:A:1390:ASN:N	2.78	0.52
1:A:1423:GLY:CA	1:A:1426:GLU:HG2	2.39	0.52
1:A:41:MET:HE1	1:A:42:ASP:HB2	1.90	0.52
2:B:31:TRP:CZ3	2:B:34:ILE:HD12	2.45	0.52
2:B:616:ILE:CG1	2:B:697:GLU:HA	2.40	0.52
3:C:136:ASP:HB2	3:C:141:GLY:H	1.74	0.52
3:C:11:ARG:NH2	3:C:229:TYR:HD2	2.08	0.52
3:C:66:ARG:NH2	10:J:5:VAL:HG23	2.24	0.52
3:C:73:GLN:HG3	3:C:74:SER:N	2.25	0.52
5:E:124:VAL:H	5:E:125:PRO:HD2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:140:ASP:OD1	6:F:141:GLY:N	2.43	0.52
6:F:70:LYS:C	6:F:72:LYS:H	2.13	0.52
9:I:40:SER:OG	9:I:41:PRO:HD2	2.10	0.52
10:J:48:ARG:C	10:J:48:ARG:HD2	2.30	0.52
1:A:369:SER:HB3	11:K:2:ASN:HD21	1.75	0.52
14:N:5:DC:H2"	14:N:6:DT:O5'	2.10	0.52
1:A:1100:ARG:HH22	1:A:1111:MET:HE1	1.74	0.52
1:A:1121:GLU:HB3	1:A:1124:HIS:NE2	2.24	0.52
1:A:865:GLN:NE2	1:A:1370:LEU:HA	2.24	0.52
1:A:1402:PHE:O	1:A:1403:GLU:HB2	2.09	0.52
1:A:593:GLU:C	1:A:595:THR:H	2.14	0.52
1:A:61:ILE:HG22	1:A:62:ASP:H	1.74	0.52
1:A:942:PHE:HZ	5:E:207:ARG:CG	2.23	0.52
2:B:990:ILE:HG22	2:B:991:GLY:N	2.25	0.52
7:G:125:SER:C	7:G:126:ASN:HD22	2.13	0.52
8:H:63:LEU:HD13	8:H:64:ASN:H	1.74	0.52
10:J:8:PHE:H	10:J:49:MET:CE	2.23	0.52
10:J:53:HIS:CD2	10:J:54:VAL:N	2.78	0.52
8:H:80:ARG:NH1	11:K:57:LEU:HD11	2.25	0.52
1:A:445:ASN:CB	1:A:455:MET:HG2	2.29	0.51
1:A:481:ASP:CG	1:A:485:ASP:OD2	2.49	0.51
1:A:698:GLN:O	9:I:98:VAL:HG13	2.10	0.51
1:A:947:PHE:N	1:A:947:PHE:HD1	2.08	0.51
2:B:331:LEU:HD23	2:B:353:LYS:HG2	1.91	0.51
2:B:68:THR:HG22	2:B:69:LEU:N	2.25	0.51
2:B:60:GLN:HE22	2:B:94:LYS:HA	1.75	0.51
3:C:242:GLN:C	3:C:244:VAL:N	2.63	0.51
4:D:206:GLU:O	4:D:210:ILE:HG13	2.11	0.51
5:E:65:THR:O	5:E:66:GLU:C	2.48	0.51
9:I:58:VAL:CG1	9:I:62:ILE:HD12	2.29	0.51
1:A:700:ASN:HB2	9:I:98:VAL:HG21	1.92	0.51
2:B:1039:GLY:HA2	10:J:51:LEU:HD21	1.92	0.51
1:A:343:LYS:HZ2	2:B:1151:LEU:CD1	2.23	0.51
1:A:40:THR:HB	1:A:41:MET:CE	2.40	0.51
1:A:630:ILE:CG2	1:A:631:HIS:N	2.72	0.51
1:A:722:LEU:CD1	1:A:722:LEU:H	2.22	0.51
1:A:743:VAL:O	1:A:747:VAL:HG23	2.10	0.51
1:A:767:GLN:HA	1:A:799:PHE:HA	1.92	0.51
2:B:1002:THR:HG21	2:B:1006:ILE:CD1	2.40	0.51
2:B:1102:LYS:O	2:B:1103:ILE:C	2.48	0.51
2:B:120:ARG:NH1	12:L:54:ARG:HH11	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:298:LEU:N	2:B:298:LEU:HD22	2.26	0.51
2:B:638:PHE:HB3	2:B:651:LEU:HD22	1.90	0.51
2:B:952:VAL:HG13	2:B:966:VAL:HG22	1.92	0.51
3:C:204:SER:H	3:C:207:CYS:HG	1.56	0.51
3:C:31:ASN:OD1	3:C:34:ARG:HD3	2.10	0.51
3:C:77:ILE:O	3:C:79:GLN:N	2.43	0.51
4:D:118:THR:OG1	4:D:121:LYS:HB2	2.10	0.51
4:D:56:ARG:HD3	4:D:149:THR:HA	1.92	0.51
8:H:110:ASP:HB2	8:H:128:ASN:HD22	1.76	0.51
8:H:14:GLU:O	8:H:26:ILE:HG23	2.10	0.51
9:I:4:PHE:CD1	9:I:4:PHE:C	2.82	0.51
11:K:109:TRP:C	11:K:111:LEU:H	2.13	0.51
1:A:1017:LEU:O	1:A:1017:LEU:HD12	2.10	0.51
1:A:1098:VAL:HB	1:A:1099:PRO:CD	2.40	0.51
1:A:544:ASP:CG	1:A:545:GLN:N	2.62	0.51
1:A:817:ALA:O	1:A:820:GLY:N	2.43	0.51
1:A:450:LEU:HB2	1:A:838:GLN:HE21	1.74	0.51
2:B:120:ARG:NH1	12:L:54:ARG:NH1	2.58	0.51
2:B:100:PRO:HD2	2:B:180:TYR:HE1	1.72	0.51
2:B:244:LEU:O	2:B:249:ARG:HG2	2.10	0.51
2:B:508:LEU:O	2:B:509:ALA:CB	2.57	0.51
2:B:942:ARG:O	2:B:943:SER:C	2.48	0.51
4:D:63:LEU:HD23	7:G:47:CYS:SG	2.50	0.51
6:F:103:MET:CE	7:G:66:GLY:N	2.68	0.51
9:I:82:GLU:HB3	9:I:104:LEU:HB2	1.91	0.51
10:J:27:GLU:O	10:J:29:GLU:N	2.43	0.51
10:J:36:LEU:HB2	10:J:47:ARG:NH1	2.24	0.51
3:C:3:GLU:HG3	11:K:104:ASN:CG	2.31	0.51
11:K:78:THR:O	11:K:81:TYR:HB3	2.10	0.51
1:A:896:ARG:HH21	1:A:1030:ARG:HE	1.53	0.51
1:A:1102:LYS:O	1:A:1106:ASN:ND2	2.43	0.51
1:A:1167:GLU:HA	1:A:1170:ILE:HD12	1.92	0.51
1:A:284:ALA:O	1:A:286:HIS:N	2.41	0.51
1:A:306:ASN:ND2	1:A:322:VAL:HG12	2.26	0.51
1:A:343:LYS:NZ	2:B:1151:LEU:CD1	2.70	0.51
1:A:463:ILE:HB	1:A:464:PRO:CD	2.40	0.51
1:A:466:SER:HB2	2:B:1099:VAL:HG22	1.91	0.51
1:A:567:LYS:CG	1:A:568:PRO:CD	2.87	0.51
1:A:877:HIS:CD2	1:A:877:HIS:N	2.78	0.51
2:B:562:GLY:O	2:B:590:HIS:ND1	2.43	0.51
2:B:746:SER:CB	2:B:1046:PRO:HG2	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:124:LEU:O	3:C:126:GLY:N	2.44	0.51
3:C:31:ASN:ND2	3:C:35:ARG:HD2	2.26	0.51
4:D:145:MET:O	4:D:149:THR:HB	2.11	0.51
5:E:5:ASN:O	5:E:9:ILE:HG13	2.10	0.51
9:I:62:ILE:HD13	9:I:102:VAL:HG11	1.93	0.51
13:T:12:DG:H2"	13:T:13:DT:O5'	2.09	0.51
1:A:104:GLU:CG	1:A:174:ILE:HD12	2.41	0.51
1:A:1102:LYS:HG2	1:A:1106:ASN:HD21	1.75	0.51
1:A:1118:VAL:CG2	1:A:1306:LEU:HB2	2.41	0.51
1:A:1120:LEU:H	1:A:1120:LEU:HD12	1.75	0.51
1:A:284:ALA:HB1	1:A:289:ILE:HD11	1.91	0.51
1:A:477:PRO:HG2	1:A:521:MET:CG	2.40	0.51
1:A:543:LEU:O	1:A:546:VAL:N	2.44	0.51
1:A:562:THR:HG21	8:H:98:TYR:CD2	2.46	0.51
1:A:591:PHE:HA	1:A:595:THR:CB	2.41	0.51
1:A:725:ALA:HA	1:A:728:LYS:HE2	1.93	0.51
1:A:74:MET:HE2	1:A:74:MET:H	1.75	0.51
1:A:767:GLN:NE2	1:A:797:LYS:O	2.42	0.51
1:A:901:LEU:HD13	1:A:919:ILE:CG2	2.41	0.51
2:B:730:ARG:NH2	2:B:1047:PHE:HB3	2.26	0.51
2:B:737:THR:HG21	9:I:66:PRO:HA	1.91	0.51
2:B:781:PHE:O	2:B:782:LEU:HG	2.10	0.51
2:B:866:TYR:O	2:B:868:MET:N	2.41	0.51
2:B:884:ARG:O	2:B:936:ASP:HB2	2.10	0.51
2:B:899:ILE:HG21	2:B:949:VAL:HG21	1.92	0.51
3:C:82:TYR:CZ	3:C:161:LYS:HG2	2.45	0.51
5:E:117:THR:HG22	5:E:120:ALA:H	1.74	0.51
7:G:119:LEU:HA	7:G:131:GLN:O	2.09	0.51
8:H:10:PHE:O	8:H:54:SER:HA	2.09	0.51
9:I:6:PHE:HA	9:I:14:LEU:HG	1.93	0.51
10:J:1:MET:H1	10:J:57:ILE:N	2.05	0.51
13:T:8:DT:H2"	13:T:9:DC:OP2	2.10	0.51
1:A:230:ARG:O	1:A:231:PRO:C	2.49	0.51
1:A:556:TRP:CZ3	1:A:558:GLY:HA2	2.45	0.51
1:A:598:LEU:O	1:A:598:LEU:HD23	2.11	0.51
1:A:765:VAL:HG23	1:A:802:ASN:O	2.11	0.51
1:A:830:LYS:HG3	1:A:1098:VAL:HG11	1.91	0.51
2:B:1044:ALA:O	2:B:1045:SER:O	2.29	0.51
2:B:391:ASP:HB2	9:I:92:ARG:HG3	1.91	0.51
2:B:510:LYS:HB2	2:B:511:PRO:HD3	1.92	0.51
2:B:582:VAL:HG22	2:B:626:ILE:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:797:TYR:HB3	2:B:798:TYR:HD2	1.76	0.51
2:B:882:THR:HG22	2:B:884:ARG:CB	2.35	0.51
3:C:168:ALA:O	3:C:171:GLY:N	2.43	0.51
1:A:1446:ASP:HB2	6:F:133:VAL:HG21	1.91	0.51
10:J:23:ASN:O	10:J:25:LEU:N	2.43	0.51
2:B:186:GLU:HG3	10:J:62:ARG:NH2	2.26	0.51
1:A:1001:ARG:HH11	1:A:1001:ARG:CG	2.24	0.51
1:A:1345:ARG:NH1	1:A:1373:ASP:OD1	2.44	0.51
1:A:387:ARG:O	1:A:390:GLN:HB3	2.10	0.51
1:A:432:VAL:O	1:A:433:GLU:C	2.47	0.51
1:A:498:ARG:HG3	1:A:499:ALA:N	2.26	0.51
1:A:574:GLY:O	1:A:575:LYS:C	2.49	0.51
1:A:535:THR:CG2	1:A:575:LYS:HE2	2.39	0.51
1:A:637:LYS:HB3	1:A:641:VAL:HG11	1.93	0.51
1:A:76:GLU:O	1:A:78:PRO:HD3	2.11	0.51
1:A:843:LYS:HD3	1:A:846:GLU:OE2	2.11	0.51
1:A:898:ARG:O	1:A:1029:ARG:NH1	2.44	0.51
2:B:515:HIS:O	2:B:518:HIS:HB2	2.11	0.51
2:B:69:LEU:CD1	2:B:429:PHE:HE1	2.19	0.51
2:B:798:TYR:CE1	10:J:4:PRO:HA	2.46	0.51
4:D:137:ASN:N	4:D:137:ASN:ND2	2.58	0.51
6:F:93:ILE:HD13	6:F:148:VAL:HG12	1.93	0.51
9:I:61:ASP:C	9:I:63:GLY:H	2.13	0.51
9:I:6:PHE:N	9:I:6:PHE:CD2	2.75	0.51
1:A:1048:ASN:O	1:A:1052:GLN:HB2	2.11	0.51
1:A:1425:SER:HA	1:A:1428:VAL:CG2	2.40	0.51
1:A:284:ALA:C	1:A:286:HIS:N	2.59	0.51
1:A:427:GLN:HB2	1:A:430:TRP:CD2	2.46	0.51
1:A:524:VAL:CG1	1:A:525:GLN:N	2.73	0.51
1:A:677:ARG:HD2	1:A:677:ARG:C	2.31	0.51
2:B:842:ASN:O	2:B:846:ILE:HG13	2.11	0.51
2:B:857:ARG:HH21	2:B:942:ARG:NH2	2.09	0.51
3:C:36:VAL:CG2	3:C:251:LEU:HD13	2.41	0.51
4:D:8:PHE:CD2	7:G:6:ASP:O	2.64	0.51
5:E:153:HIS:HB3	5:E:196:VAL:HG13	1.93	0.51
7:G:55:ASP:OD1	7:G:57:GLN:HG3	2.10	0.51
8:H:101:ALA:HB2	8:H:116:TYR:CE1	2.46	0.51
9:I:50:THR:HG22	9:I:51:ASN:N	2.26	0.51
9:I:69:PRO:HB2	9:I:85:PHE:CE2	2.46	0.51
9:I:74:GLU:O	9:I:74:GLU:HG3	2.10	0.51
10:J:25:LEU:O	10:J:29:GLU:HA	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:36:SER:O	12:L:37:LYS:C	2.48	0.51
3:C:51:VAL:HB	12:L:65:VAL:HG23	1.93	0.51
1:A:832:ALA:HA	13:T:18:DA:C8	2.45	0.51
1:A:1015:VAL:O	1:A:1017:LEU:N	2.44	0.51
1:A:1151:GLU:HG2	9:I:45:ARG:HB2	1.93	0.51
1:A:130:ASP:O	1:A:132:LYS:N	2.44	0.51
1:A:391:LEU:HD22	1:A:401:GLY:O	2.10	0.51
1:A:42:ASP:OD1	1:A:47:ARG:HA	2.10	0.51
1:A:900:ASP:HA	1:A:926:GLN:HE22	1.75	0.51
2:B:114:PRO:O	2:B:116:GLU:N	2.44	0.51
2:B:1166:CYS:O	2:B:1168:LEU:N	2.33	0.51
2:B:521:LEU:HD22	2:B:633:VAL:CG1	2.27	0.51
2:B:601:ARG:HH11	2:B:605:ARG:NH2	2.08	0.51
2:B:797:TYR:C	2:B:798:TYR:HD2	2.15	0.51
2:B:912:ILE:O	2:B:938:SER:HA	2.10	0.51
2:B:95:ILE:CB	2:B:130:VAL:HG22	2.40	0.51
5:E:124:VAL:HA	5:E:132:ILE:CD1	2.40	0.51
5:E:181:ALA:O	5:E:182:ASP:C	2.49	0.51
5:E:98:ILE:HA	5:E:101:GLN:HB3	1.93	0.51
6:F:114:GLU:HA	6:F:114:GLU:OE2	2.11	0.51
7:G:112:LYS:HA	7:G:115:MET:HE3	1.93	0.51
7:G:48:VAL:HA	7:G:76:ALA:CB	2.40	0.51
1:A:1272:THR:HG22	1:A:1273:LEU:N	2.26	0.51
1:A:1388:GLY:O	1:A:1391:ARG:HG3	2.11	0.51
1:A:19:PHE:O	1:A:1416:ALA:HA	2.11	0.51
1:A:172:PRO:HD3	1:A:185:TRP:CE2	2.45	0.51
2:B:95:ILE:HG13	2:B:129:PHE:O	2.11	0.51
2:B:190:TYR:HD2	10:J:62:ARG:O	1.92	0.51
2:B:276:ILE:O	2:B:278:GLN:N	2.37	0.51
2:B:293:PRO:O	2:B:297:ILE:HG13	2.11	0.51
2:B:969:ARG:HG2	2:B:970:THR:N	2.25	0.51
2:B:992:ILE:HG12	2:B:993:THR:N	2.26	0.51
5:E:16:PHE:HE2	5:E:37:LEU:HD23	1.76	0.51
1:A:1445:ILE:HD13	7:G:70:PHE:CZ	2.46	0.51
13:T:11:DA:H2"	13:T:12:DG:H8	1.76	0.51
1:A:896:ARG:HH22	1:A:1030:ARG:HH21	1.57	0.50
1:A:531:ILE:HD11	1:A:578:LEU:HD21	1.93	0.50
1:A:787:PHE:CE1	1:A:796:SER:HA	2.46	0.50
2:B:1158:PHE:CG	2:B:1159:ARG:N	2.79	0.50
2:B:1182:CYS:O	2:B:1183:LYS:O	2.29	0.50
2:B:229:ALA:CB	2:B:231:PRO:HD2	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:606:LYS:HD3	2:B:608:ASP:HB2	1.93	0.50
2:B:685:LEU:C	2:B:685:LEU:HD12	2.31	0.50
2:B:891:ASP:C	2:B:893:LEU:N	2.64	0.50
3:C:168:ALA:O	3:C:170:TRP:N	2.44	0.50
5:E:116:ILE:CG2	5:E:117:THR:N	2.74	0.50
7:G:127:PRO:HG3	7:G:139:ILE:CG1	2.40	0.50
7:G:143:ILE:CG2	7:G:144:ARG:N	2.74	0.50
7:G:142:ARG:CB	7:G:171:ILE:HD11	2.41	0.50
7:G:39:THR:O	7:G:43:GLY:HA2	2.11	0.50
12:L:38:LEU:O	12:L:39:SER:CB	2.60	0.50
12:L:68:GLU:CD	12:L:68:GLU:H	2.15	0.50
1:A:1187:GLN:CD	1:A:1188:GLN:HE21	2.15	0.50
1:A:37:PHE:CD2	1:A:50:ILE:HG21	2.46	0.50
2:B:778:MET:HE2	2:B:1094:ARG:HG2	1.93	0.50
2:B:1115:THR:HG22	2:B:1117:GLN:CG	2.41	0.50
2:B:189:LEU:O	2:B:192:LEU:N	2.45	0.50
2:B:258:LEU:O	2:B:258:LEU:CG	2.59	0.50
2:B:307:ASP:O	2:B:309:GLN:N	2.44	0.50
2:B:464:GLY:C	2:B:465:ASN:ND2	2.63	0.50
2:B:469:GLN:HG3	2:B:470:LYS:H	1.74	0.50
2:B:619:ILE:O	2:B:622:LYS:N	2.44	0.50
2:B:644:GLU:OE2	2:B:646:LEU:HB2	2.11	0.50
2:B:785:TYR:HD2	2:B:785:TYR:N	2.09	0.50
3:C:248:ILE:HD13	11:K:102:LYS:HA	1.94	0.50
8:H:84:ALA:HA	8:H:87:ARG:HG3	1.92	0.50
1:A:1191:TRP:CB	1:A:1260:LEU:HD23	2.40	0.50
1:A:125:ALA:O	1:A:127:ALA:N	2.45	0.50
1:A:286:HIS:C	1:A:288:ALA:H	2.15	0.50
1:A:699:ALA:HB3	1:A:701:LEU:HG	1.92	0.50
2:B:542:MET:SD	2:B:747:MET:HE2	2.52	0.50
2:B:811:TYR:H	2:B:811:TYR:HD1	1.58	0.50
2:B:864:LYS:O	2:B:871:THR:HG23	2.11	0.50
2:B:877:PRO:C	2:B:878:GLN:HG3	2.31	0.50
3:C:8:VAL:HG12	3:C:9:LYS:N	2.22	0.50
7:G:88:ASP:HB3	7:G:144:ARG:CA	2.40	0.50
1:A:25:GLU:OE1	1:A:25:GLU:N	2.20	0.50
1:A:282:ASN:O	1:A:284:ALA:N	2.44	0.50
1:A:506:ALA:CB	1:A:508:PRO:HD2	2.39	0.50
1:A:58:LEU:HA	1:A:80:HIS:HB2	1.93	0.50
1:A:590:ARG:CG	1:A:590:ARG:NH1	2.74	0.50
2:B:983:ARG:HD2	2:B:1091:TYR:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:593:PRO:O	2:B:596:LEU:N	2.44	0.50
2:B:654:ARG:O	2:B:656:GLY:N	2.45	0.50
2:B:706:GLN:NE2	2:B:730:ARG:HH11	2.09	0.50
2:B:847:ASP:O	2:B:849:GLY:N	2.44	0.50
2:B:969:ARG:HD3	3:C:61:GLU:OE2	2.11	0.50
3:C:169:LYS:HE3	3:C:170:TRP:CZ2	2.47	0.50
4:D:14:ARG:O	4:D:16:LYS:N	2.42	0.50
4:D:54:GLU:O	4:D:58:VAL:HG23	2.11	0.50
7:G:45:ILE:HD13	7:G:78:VAL:CG1	2.41	0.50
8:H:44:VAL:CG1	8:H:48:PRO:HA	2.38	0.50
9:I:111:THR:HG22	9:I:113:ASP:H	1.76	0.50
10:J:16:ASP:O	10:J:18:TRP:N	2.45	0.50
1:A:1396:ALA:HA	1:A:1399:ARG:NH2	2.27	0.50
1:A:402:ALA:HB2	1:A:434:ARG:HA	1.94	0.50
1:A:40:THR:HB	1:A:41:MET:HE2	1.93	0.50
1:A:461:LYS:O	1:A:463:ILE:HG23	2.12	0.50
1:A:767:GLN:OE1	1:A:799:PHE:HB2	2.12	0.50
1:A:909:ASP:O	1:A:911:SER:N	2.42	0.50
2:B:1050:ILE:N	2:B:1050:ILE:HD12	2.26	0.50
1:A:345:VAL:HG21	2:B:1150:ARG:NH2	2.24	0.50
2:B:278:GLN:HG2	2:B:279:ASP:N	2.18	0.50
2:B:331:LEU:HD12	2:B:331:LEU:N	2.26	0.50
2:B:57:TYR:N	2:B:57:TYR:HD1	2.10	0.50
2:B:54:PHE:O	2:B:58:THR:HB	2.11	0.50
2:B:660:LYS:HB3	2:B:679:TYR:CE2	2.46	0.50
2:B:785:TYR:CD2	2:B:785:TYR:N	2.80	0.50
2:B:860:MET:CG	2:B:965:LYS:HG2	2.41	0.50
3:C:174:ALA:O	10:J:10:CYS:O	2.29	0.50
3:C:88:CYS:SG	3:C:91:HIS:C	2.90	0.50
5:E:186:LEU:O	5:E:189:GLY:N	2.41	0.50
9:I:33:SER:O	9:I:35:VAL:HG23	2.11	0.50
11:K:7:PHE:O	11:K:11:LEU:HD23	2.11	0.50
1:A:1138:ILE:C	1:A:1275:GLY:HA2	2.32	0.50
1:A:125:ALA:HA	1:A:128:ILE:HG13	1.93	0.50
1:A:1453:TYR:O	1:A:1454:MET:CB	2.59	0.50
1:A:87:ALA:CB	1:A:276:LEU:HD23	2.42	0.50
1:A:418:SER:C	1:A:420:ARG:H	2.14	0.50
1:A:699:ALA:O	1:A:700:ASN:HB3	2.11	0.50
2:B:68:THR:CG2	2:B:91:SER:HB3	2.41	0.50
2:B:914:LYS:HD3	2:B:937:ALA:O	2.11	0.50
3:C:146:LYS:C	3:C:147:LEU:HD23	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:59:ILE:HG21	4:D:145:MET:SD	2.52	0.50
5:E:42:PHE:HZ	5:E:58:MET:HE1	1.77	0.50
10:J:5:VAL:HG12	10:J:6:ARG:CG	2.29	0.50
1:A:1218:GLN:O	1:A:1221:LYS:HE3	2.12	0.50
1:A:1259:MET:C	1:A:1261:LYS:H	2.15	0.50
1:A:1443:VAL:CG1	6:F:132:LEU:HD13	2.42	0.50
1:A:244:PRO:HG2	1:A:245:PRO:HD3	1.94	0.50
1:A:441:PRO:HD2	1:A:498:ARG:CZ	2.41	0.50
1:A:575:LYS:HB3	1:A:612:ILE:CG2	2.42	0.50
1:A:523:ILE:CD1	1:A:649:ILE:HG21	2.41	0.50
1:A:728:LYS:HB3	1:A:731:ARG:HH21	1.77	0.50
1:A:929:LEU:HD23	1:A:983:ILE:HG21	1.94	0.50
2:B:839:MET:HG3	2:B:1010:LEU:CD1	2.41	0.50
2:B:1069:PHE:HA	2:B:1085:ILE:O	2.11	0.50
2:B:170:LEU:O	2:B:172:ILE:HG13	2.11	0.50
2:B:193:LYS:HD3	2:B:787:VAL:HG11	1.93	0.50
2:B:313:MET:O	2:B:316:PRO:HD2	2.11	0.50
2:B:34:ILE:HG12	2:B:542:MET:HE1	1.94	0.50
2:B:637:LEU:HD22	2:B:741:CYS:O	2.12	0.50
3:C:101:LEU:O	3:C:102:GLN:HG3	2.11	0.50
3:C:166:GLU:O	3:C:167:HIS:HB2	2.12	0.50
3:C:268:ASP:O	3:C:269:LYS:HB2	2.11	0.50
3:C:82:TYR:O	3:C:83:SER:C	2.49	0.50
4:D:153:ARG:NH2	4:D:184:ALA:HA	2.27	0.50
7:G:153:GLN:O	7:G:154:VAL:C	2.50	0.50
8:H:26:ILE:O	8:H:27:GLU:HG3	2.12	0.50
2:B:800:GLN:CB	10:J:52:THR:HG22	2.39	0.50
14:N:4:DA:H2"	14:N:5:DC:C5	2.46	0.50
1:A:1141:THR:CG2	1:A:1205:LYS:HD3	2.42	0.50
1:A:219:PHE:CD2	1:A:231:PRO:HD2	2.47	0.50
1:A:265:LYS:HG2	1:A:303:TYR:HA	1.94	0.50
1:A:262:LEU:HD22	1:A:303:TYR:HE1	1.77	0.50
1:A:65:LEU:O	1:A:66:LYS:C	2.49	0.50
1:A:741:ASN:HD22	1:A:744:LYS:HB2	1.75	0.50
1:A:960:ILE:HA	1:A:963:ILE:HG22	1.91	0.50
2:B:826:ALA:HB2	2:B:1008:PRO:HB3	1.92	0.50
2:B:390:LEU:O	2:B:392:ARG:HG3	2.12	0.50
2:B:547:VAL:N	2:B:612:GLU:OE2	2.38	0.50
2:B:744:HIS:CG	2:B:745:PRO:HD2	2.47	0.50
2:B:810:GLU:CA	2:B:815:ARG:NH2	2.66	0.50
3:C:112:ASN:HB2	3:C:114:TYR:HE1	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:249:ASP:O	3:C:250:THR:C	2.48	0.50
4:D:3:VAL:HG12	4:D:4:SER:H	1.77	0.50
5:E:121:MET:C	5:E:123:LEU:H	2.15	0.50
6:F:70:LYS:O	6:F:72:LYS:NZ	2.42	0.50
8:H:101:ALA:HA	8:H:116:TYR:HA	1.94	0.50
8:H:89:LEU:O	8:H:91:ASP:N	2.45	0.50
1:A:220:THR:O	1:A:221:SER:C	2.50	0.50
1:A:491:VAL:HG12	1:A:492:PRO:O	2.12	0.50
1:A:347:PHE:CE2	1:A:493:GLN:OE1	2.65	0.50
1:A:548:ASN:HA	11:K:60:ALA:HB1	1.92	0.50
1:A:870:GLU:HB2	5:E:204:THR:HG21	1.94	0.50
2:B:1178:ASN:N	2:B:1178:ASN:ND2	2.59	0.50
2:B:244:LEU:HB2	2:B:249:ARG:HA	1.93	0.50
2:B:558:LEU:O	2:B:560:GLU:N	2.30	0.50
2:B:731:VAL:HG12	2:B:732:SER:N	2.27	0.50
2:B:785:TYR:CD1	2:B:795:ILE:HG12	2.47	0.50
4:D:153:ARG:HB3	4:D:154:PHE:CE1	2.47	0.50
4:D:153:ARG:HB3	4:D:154:PHE:CD1	2.46	0.50
4:D:155:ARG:HG3	4:D:155:ARG:HH11	1.77	0.50
4:D:57:LEU:O	4:D:61:GLU:HB2	2.11	0.50
5:E:197:LYS:HE2	5:E:199:ILE:HD11	1.94	0.50
9:I:5:ARG:HG3	9:I:14:LEU:HD12	1.92	0.50
12:L:61:THR:HG22	12:L:63:ARG:N	2.24	0.50
1:A:1111:MET:HB2	1:A:1113:THR:O	2.12	0.49
1:A:1114:PRO:HB2	1:A:1311:VAL:HG23	1.93	0.49
1:A:1341:ILE:O	1:A:1344:GLY:N	2.45	0.49
1:A:1402:PHE:CD1	1:A:1403:GLU:HG3	2.47	0.49
1:A:95:PHE:O	1:A:96:ILE:C	2.51	0.49
2:B:243:ALA:HB1	2:B:251:ILE:HG12	1.92	0.49
2:B:298:LEU:N	2:B:298:LEU:CD2	2.75	0.49
2:B:49:ASP:HA	2:B:52:ASN:HD22	1.77	0.49
2:B:661:LEU:HD11	2:B:684:LEU:HD11	1.93	0.49
1:A:786:HIS:NE2	2:B:742:GLU:OE1	2.45	0.49
2:B:863:GLU:OE1	2:B:962:LYS:HB2	2.11	0.49
3:C:105:GLY:HA3	3:C:149:LYS:O	2.12	0.49
3:C:114:TYR:HB2	3:C:116:LYS:HG2	1.94	0.49
3:C:76:ASP:OD2	3:C:127:ARG:HB2	2.11	0.49
4:D:138:ASN:HD21	7:G:35:GLU:HB3	1.76	0.49
4:D:47:LEU:CD1	4:D:48:ILE:H	2.20	0.49
4:D:40:HIS:HB2	7:G:73:LYS:NZ	2.27	0.49
10:J:27:GLU:C	10:J:29:GLU:H	2.15	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.94	0.49
1:A:452:LYS:HG3	2:B:1140:ALA:CB	2.42	0.49
2:B:118:ARG:HH22	2:B:194:GLU:CD	2.16	0.49
2:B:405:ARG:CZ	2:B:632:ARG:HG2	2.41	0.49
2:B:455:SER:O	2:B:458:LYS:N	2.44	0.49
2:B:49:ASP:HA	2:B:52:ASN:ND2	2.27	0.49
2:B:821:GLN:HE22	2:B:851:PHE:N	2.06	0.49
3:C:236:GLY:O	3:C:237:SER:C	2.51	0.49
5:E:26:ARG:HA	5:E:188:LEU:HD23	1.93	0.49
9:I:73:ARG:NH1	9:I:112:SER:HB3	2.27	0.49
9:I:28:GLU:HG3	9:I:29:CYS:N	2.27	0.49
1:A:1273:LEU:N	1:A:1273:LEU:HD12	2.27	0.49
1:A:1291:VAL:HG13	1:A:1292:PRO:CD	2.40	0.49
1:A:345:VAL:HG23	1:A:346:ASP:O	2.13	0.49
1:A:402:ALA:HB1	1:A:433:GLU:O	2.12	0.49
1:A:543:LEU:O	1:A:544:ASP:C	2.50	0.49
1:A:741:ASN:ND2	1:A:744:LYS:N	2.60	0.49
1:A:866:PHE:O	1:A:867:ILE:HD12	2.10	0.49
1:A:889:SER:HA	1:A:1297:GLU:N	2.27	0.49
2:B:1215:ARG:C	2:B:1216:LEU:HD23	2.31	0.49
2:B:235:SER:C	2:B:236:HIS:CD2	2.86	0.49
2:B:291:ILE:HG22	2:B:291:ILE:O	2.11	0.49
2:B:609:ILE:O	2:B:609:ILE:HG13	2.12	0.49
2:B:654:ARG:O	2:B:657:HIS:N	2.45	0.49
2:B:661:LEU:C	2:B:663:ALA:N	2.66	0.49
2:B:958:GLN:C	2:B:960:GLY:H	2.15	0.49
3:C:124:LEU:C	3:C:126:GLY:H	2.14	0.49
5:E:161:LYS:HG3	5:E:195:VAL:HG21	1.94	0.49
7:G:138:THR:HG22	7:G:139:ILE:HG13	1.95	0.49
8:H:82:PRO:HG3	11:K:54:ARG:NH1	2.26	0.49
8:H:84:ALA:CB	8:H:87:ARG:HD2	2.42	0.49
1:A:1313:LEU:HD11	1:A:1317:MET:CE	2.43	0.49
1:A:1120:LEU:O	1:A:1323:ASP:HB2	2.12	0.49
1:A:334:GLY:O	1:A:336:ILE:N	2.46	0.49
1:A:511:ILE:HD11	1:A:646:PHE:HE1	1.76	0.49
1:A:655:PHE:O	1:A:658:LEU:HB3	2.12	0.49
1:A:741:ASN:HD22	1:A:744:LYS:CB	2.26	0.49
1:A:761:MET:HA	1:A:804:TYR:HB2	1.94	0.49
1:A:884:ASP:C	1:A:886:ILE:H	2.16	0.49
2:B:102:VAL:N	2:B:110:HIS:O	2.45	0.49
2:B:1156:ASP:OD2	2:B:1199:ALA:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:205:ILE:O	2:B:207:GLY:N	2.44	0.49
2:B:542:MET:HB3	2:B:636:PRO:CD	2.42	0.49
2:B:579:ARG:N	2:B:589:VAL:HG13	2.27	0.49
2:B:65:GLU:HG3	2:B:66:ASP:N	2.19	0.49
3:C:124:LEU:O	3:C:127:ARG:HG2	2.12	0.49
5:E:190:LEU:CD1	5:E:214:CYS:HB2	2.42	0.49
8:H:62:SER:OG	8:H:63:LEU:HD12	2.13	0.49
9:I:10:CYS:SG	9:I:10:CYS:O	2.70	0.49
1:A:836:TYR:HB2	13:T:18:DA:H5'	1.93	0.49
1:A:1118:VAL:HG23	1:A:1306:LEU:HB2	1.95	0.49
1:A:11:LEU:CD1	1:A:11:LEU:C	2.75	0.49
1:A:416:ARG:NH1	1:A:417:TYR:CE2	2.76	0.49
1:A:492:PRO:HB3	1:A:501:LEU:CD1	2.42	0.49
1:A:608:ILE:C	1:A:610:GLY:N	2.66	0.49
1:A:731:ARG:HA	1:A:734:GLU:HB3	1.95	0.49
1:A:795:GLU:CD	1:A:795:GLU:H	2.15	0.49
2:B:1084:GLN:NE2	2:B:1084:GLN:H	1.91	0.49
1:A:344:ARG:HA	2:B:1129:ARG:HA	1.94	0.49
2:B:102:VAL:CG2	2:B:112:LEU:HB2	2.43	0.49
2:B:240:ILE:CG2	2:B:254:LEU:HB3	2.42	0.49
2:B:281:PRO:O	2:B:283:VAL:N	2.46	0.49
2:B:485:ARG:NH1	2:B:782:LEU:HD11	2.28	0.49
5:E:31:THR:HG23	5:E:34:GLU:HB2	1.94	0.49
5:E:61:GLN:NE2	5:E:105:PHE:CZ	2.79	0.49
8:H:144:ILE:HG22	8:H:145:ARG:H	1.77	0.49
8:H:17:PRO:HB3	8:H:24:CYS:SG	2.52	0.49
9:I:61:ASP:O	9:I:63:GLY:N	2.45	0.49
1:A:1054:LEU:O	1:A:1057:VAL:HG23	2.12	0.49
1:A:189:ARG:O	1:A:190:ALA:CB	2.61	0.49
1:A:681:GLU:C	1:A:683:ILE:N	2.65	0.49
1:A:780:VAL:O	1:A:780:VAL:HG12	2.12	0.49
2:B:1096:ARG:O	2:B:1097:HIS:CG	2.66	0.49
1:A:412:ARG:HH22	2:B:1108:ARG:NH2	2.10	0.49
2:B:244:LEU:HD13	2:B:247:GLY:O	2.13	0.49
2:B:343:ILE:HG23	2:B:347:LYS:CD	2.42	0.49
2:B:348:ARG:HG3	2:B:349:ILE:N	2.28	0.49
2:B:372:SER:O	2:B:376:PHE:HB2	2.13	0.49
2:B:37:PHE:CE1	2:B:41:LYS:HG3	2.47	0.49
2:B:614:SER:HB3	2:B:694:ASP:CB	2.42	0.49
5:E:109:ILE:CG2	5:E:110:PHE:N	2.69	0.49
9:I:61:ASP:O	9:I:64:SER:N	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.92	0.49
15:P:5:C:O2'	15:P:6:A:H5'	2.12	0.49
1:A:1148:ILE:HG12	1:A:1198:ASP:HB2	1.95	0.49
1:A:208:LEU:HD23	1:A:209:ASN:N	2.28	0.49
1:A:23:SER:O	1:A:24:PRO:C	2.49	0.49
1:A:270:LEU:O	1:A:273:ASN:HB3	2.13	0.49
1:A:639:PRO:CG	1:A:640:GLN:N	2.76	0.49
1:A:412:ARG:NH2	2:B:1108:ARG:NH2	2.60	0.49
2:B:1221:SER:HB3	4:D:12:ARG:HE	1.77	0.49
2:B:203:PHE:HB3	2:B:205:ILE:HD11	1.94	0.49
2:B:210:LYS:HG3	2:B:461:LEU:O	2.12	0.49
2:B:531:GLN:HG3	2:B:532:ALA:H	1.77	0.49
2:B:558:LEU:C	2:B:560:GLU:H	2.12	0.49
2:B:952:VAL:HG22	2:B:966:VAL:HG13	1.94	0.49
4:D:204:ASP:O	4:D:208:GLU:HB2	2.12	0.49
5:E:89:GLY:CA	5:E:117:THR:OG1	2.60	0.49
7:G:1:MET:HE1	7:G:3:PHE:HE1	1.77	0.49
11:K:45:LEU:HG	11:K:94:ILE:CD1	2.41	0.49
13:T:7:DC:H2"	13:T:8:DT:H71	1.94	0.49
1:A:1125:ALA:C	1:A:1127:ASP:H	2.14	0.49
1:A:374:LEU:O	1:A:436:ILE:HG12	2.13	0.49
1:A:381:THR:CG2	1:A:382:PRO:HD2	2.42	0.49
1:A:49:LYS:HD2	1:A:55:ASP:HB3	1.94	0.49
1:A:730:GLY:O	1:A:731:ARG:C	2.50	0.49
1:A:6:TYR:CD1	1:A:7:SER:N	2.81	0.49
2:B:1072:MET:HE3	2:B:1085:ILE:CB	2.42	0.49
2:B:22:SER:HA	2:B:654:ARG:CB	2.43	0.49
2:B:529:GLU:OE1	2:B:769:TYR:HE1	1.96	0.49
2:B:579:ARG:HH11	2:B:579:ARG:HG2	1.77	0.49
2:B:882:THR:HG22	2:B:884:ARG:N	2.23	0.49
2:B:95:ILE:HG13	2:B:130:VAL:HG22	1.95	0.49
4:D:52:LEU:O	4:D:53:SER:OG	2.28	0.49
5:E:100:ILE:O	5:E:100:ILE:HG22	2.13	0.49
5:E:156:LEU:HA	5:E:160:GLU:OE1	2.13	0.49
7:G:117:GLN:OE1	7:G:117:GLN:N	2.46	0.49
7:G:50:ASP:OD1	7:G:50:ASP:O	2.30	0.49
8:H:143:LEU:N	8:H:143:LEU:HD12	2.27	0.49
10:J:14:VAL:CG1	10:J:50:ILE:HD11	2.42	0.49
12:L:53:HIS:HB3	12:L:55:ILE:HD12	1.92	0.49
1:A:1053:PHE:O	1:A:1055:ARG:N	2.46	0.49
1:A:670:ILE:HA	1:A:805:LEU:HD22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:774:ARG:CZ	1:A:797:LYS:HG3	2.42	0.49
2:B:115:GLN:HG2	2:B:193:LYS:CB	2.33	0.49
2:B:190:TYR:CD2	10:J:62:ARG:HB3	2.48	0.49
2:B:259:TYR:HD1	2:B:259:TYR:H	1.61	0.49
2:B:592:ASN:HD21	2:B:595:ARG:NH1	2.11	0.49
2:B:601:ARG:NH1	2:B:605:ARG:NH2	2.61	0.49
2:B:880:THR:O	2:B:880:THR:HG22	2.13	0.49
3:C:101:LEU:C	3:C:102:GLN:HG3	2.33	0.49
3:C:124:LEU:C	3:C:126:GLY:N	2.66	0.49
6:F:120:ILE:O	6:F:124:GLU:HG3	2.13	0.49
6:F:138:LEU:CB	6:F:139:PRO:HD2	2.43	0.49
8:H:102:TYR:N	8:H:102:TYR:CD2	2.63	0.49
9:I:25:LEU:HB3	9:I:38:ALA:HB2	1.93	0.49
1:A:1348:LEU:HG	1:A:1372:VAL:HG23	1.95	0.49
1:A:391:LEU:O	1:A:394:ASN:HB3	2.13	0.49
1:A:528:LEU:HA	1:A:531:ILE:HG22	1.94	0.49
1:A:535:THR:HG22	1:A:536:LEU:N	2.28	0.49
2:B:276:ILE:HG22	2:B:278:GLN:O	2.13	0.49
2:B:361:LEU:N	2:B:362:PRO:CD	2.75	0.49
2:B:792:MET:O	2:B:793:ALA:HB2	2.13	0.49
3:C:38:ILE:HA	3:C:173:ALA:CB	2.40	0.49
3:C:83:SER:HA	3:C:95:CYS:CB	2.43	0.49
5:E:11:ARG:C	5:E:13:TRP:N	2.66	0.49
5:E:161:LYS:HD2	5:E:195:VAL:HG23	1.95	0.49
6:F:85:MET:C	6:F:155:LEU:HD11	2.32	0.49
7:G:138:THR:CG2	7:G:139:ILE:N	2.53	0.49
7:G:37:SER:OG	7:G:45:ILE:HG13	2.12	0.49
9:I:111:THR:CG2	9:I:112:SER:H	2.25	0.49
13:T:18:DA:H8	13:T:18:DA:O5'	1.95	0.49
1:A:1074:GLU:C	1:A:1076:ALA:H	2.16	0.48
1:A:1120:LEU:N	1:A:1120:LEU:HD12	2.27	0.48
1:A:1134:ILE:O	1:A:1138:ILE:HG12	2.13	0.48
1:A:1211:GLN:O	1:A:1212:VAL:C	2.52	0.48
1:A:1197:LEU:O	1:A:1236:LEU:HD12	2.12	0.48
1:A:1237:ILE:CG2	1:A:1238:ILE:N	2.75	0.48
1:A:1389:PHE:CG	1:A:1390:ASN:N	2.80	0.48
1:A:55:ASP:N	1:A:56:PRO:HD3	2.28	0.48
1:A:605:MET:HG2	1:A:621:THR:CG2	2.43	0.48
1:A:728:LYS:HG3	1:A:729:ALA:N	2.28	0.48
1:A:868:TYR:CZ	1:A:1064:VAL:HG11	2.48	0.48
2:B:1097:HIS:H	2:B:1098:MET:CE	2.09	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:225:VAL:HA	2:B:237:VAL:O	2.13	0.48
2:B:295:GLY:N	2:B:298:LEU:HD23	2.28	0.48
2:B:44:VAL:O	2:B:45:SER:C	2.51	0.48
2:B:46:GLN:HG3	2:B:47:GLN:H	1.78	0.48
2:B:865:LYS:HE3	2:B:961:LEU:HD21	1.94	0.48
2:B:956:THR:CG2	2:B:960:GLY:HA2	2.43	0.48
3:C:76:ASP:OD2	3:C:128:ASN:N	2.46	0.48
1:A:1450:LEU:HD11	6:F:108:PHE:CZ	2.48	0.48
6:F:130:ILE:O	6:F:148:VAL:CG2	2.61	0.48
7:G:1:MET:HA	7:G:1:MET:HE2	1.94	0.48
4:D:7:THR:HB	7:G:42:PHE:CE2	2.48	0.48
7:G:44:TYR:OH	7:G:156:SER:HA	2.12	0.48
10:J:9:SER:OG	10:J:48:ARG:NH2	2.46	0.48
11:K:48:ALA:O	11:K:51:LEU:N	2.45	0.48
1:A:114:LEU:N	1:A:114:LEU:HD23	2.28	0.48
1:A:187:LYS:O	1:A:194:ALA:HB3	2.13	0.48
1:A:543:LEU:O	1:A:545:GLN:N	2.46	0.48
1:A:560:ILE:HG13	8:H:79:TRP:H	1.78	0.48
2:B:1007:VAL:HG22	2:B:1008:PRO:CD	2.43	0.48
2:B:1077:THR:HG22	11:K:44:ASN:ND2	2.28	0.48
2:B:1082:MET:HA	3:C:189:THR:HA	1.95	0.48
2:B:120:ARG:NE	2:B:955:THR:HG21	2.28	0.48
2:B:326:ASP:C	2:B:328:GLU:N	2.66	0.48
2:B:343:ILE:CG2	2:B:347:LYS:HG3	2.43	0.48
2:B:451:LYS:O	2:B:455:SER:OG	2.30	0.48
2:B:751:VAL:O	2:B:752:ALA:C	2.52	0.48
2:B:802:PRO:HA	2:B:822:ASN:OD1	2.13	0.48
2:B:873:THR:CG2	2:B:874:PHE:N	2.76	0.48
3:C:238:ILE:HG22	3:C:243:VAL:CG2	2.40	0.48
2:B:1215:ARG:NH1	4:D:15:LEU:HD21	2.28	0.48
4:D:214:LEU:C	4:D:216:ASN:N	2.64	0.48
4:D:53:SER:H	4:D:148:LEU:HD22	1.78	0.48
5:E:33:GLU:OE1	5:E:33:GLU:N	2.41	0.48
6:F:71:GLU:N	6:F:71:GLU:OE1	2.46	0.48
8:H:58:THR:C	8:H:59:ILE:HG13	2.34	0.48
8:H:91:ASP:C	8:H:93:TYR:N	2.66	0.48
1:A:1191:TRP:HA	1:A:1191:TRP:HE3	1.76	0.48
1:A:1271:ILE:HG22	1:A:1271:ILE:O	2.13	0.48
1:A:384:ASN:O	1:A:385:ILE:C	2.52	0.48
1:A:380:VAL:HG21	1:A:430:TRP:HB2	1.94	0.48
1:A:556:TRP:C	1:A:558:GLY:H	2.15	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ASP:OD2	1:A:55:ASP:O	2.31	0.48
1:A:57:ARG:O	1:A:68:GLN:HG2	2.13	0.48
2:B:1055:ILE:O	2:B:1058:LEU:N	2.46	0.48
2:B:34:ILE:O	2:B:37:PHE:HB3	2.14	0.48
2:B:798:TYR:HD1	10:J:4:PRO:HB3	1.78	0.48
2:B:890:TYR:CE2	2:B:910:VAL:HG21	2.49	0.48
4:D:22:GLU:N	4:D:22:GLU:CD	2.65	0.48
5:E:168:TYR:CB	5:E:170:LEU:HG	2.42	0.48
5:E:173:SER:OG	5:E:174:GLN:N	2.46	0.48
9:I:90:GLN:HE21	9:I:92:ARG:HB2	1.77	0.48
1:A:1105:LEU:HD22	1:A:1384:VAL:HG21	1.96	0.48
1:A:1187:GLN:HA	1:A:1244:ARG:CD	2.44	0.48
1:A:121:LEU:O	1:A:124:GLN:HB2	2.14	0.48
1:A:1115:SER:O	1:A:1311:VAL:HG22	2.13	0.48
1:A:247:ARG:HH11	1:A:263:THR:HG23	1.77	0.48
1:A:310:GLY:C	1:A:312:PRO:HD2	2.34	0.48
1:A:639:PRO:CG	1:A:640:GLN:H	2.26	0.48
1:A:730:GLY:O	1:A:732:LEU:N	2.46	0.48
1:A:679:ILE:HG12	1:A:732:LEU:CD1	2.43	0.48
2:B:909:ASP:N	2:B:909:ASP:OD1	2.47	0.48
3:C:168:ALA:O	3:C:169:LYS:C	2.50	0.48
3:C:260:LEU:O	3:C:264:GLN:HG3	2.13	0.48
8:H:84:ALA:HA	8:H:87:ARG:CG	2.43	0.48
10:J:7:CYS:CA	10:J:49:MET:HE3	2.42	0.48
11:K:63:VAL:O	11:K:63:VAL:CG2	2.61	0.48
13:T:10:DA:H2"	13:T:11:DA:C8	2.47	0.48
1:A:244:PRO:CB	1:A:245:PRO:HD3	2.43	0.48
1:A:266:LEU:HD21	1:A:303:TYR:CZ	2.48	0.48
1:A:358:ASN:ND2	2:B:833:TYR:OH	2.46	0.48
1:A:41:MET:N	1:A:41:MET:HE3	2.28	0.48
1:A:481:ASP:N	1:A:481:ASP:OD2	2.45	0.48
1:A:666:ILE:CD1	1:A:667:GLY:N	2.75	0.48
1:A:710:LEU:HD12	1:A:710:LEU:N	2.28	0.48
1:A:88:LYS:HD2	1:A:293:GLU:OE2	2.13	0.48
2:B:1030:LEU:CD1	2:B:1059:LEU:HD22	2.44	0.48
1:A:843:LYS:HZ3	2:B:1135:ARG:HH12	1.61	0.48
2:B:1177:HIS:HB2	2:B:1179:GLN:HE21	1.77	0.48
2:B:319:GLU:HA	2:B:322:PHE:HB2	1.96	0.48
2:B:50:SER:OG	2:B:411:PRO:HD3	2.13	0.48
3:C:79:GLN:HG3	3:C:127:ARG:HD2	1.94	0.48
8:H:43:ASN:OD1	8:H:46:LEU:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:1:MET:H1	10:J:56:LEU:CA	2.27	0.48
2:B:797:TYR:O	10:J:1:MET:HG2	2.12	0.48
10:J:2:ILE:HG12	10:J:57:ILE:HD12	1.95	0.48
10:J:24:LEU:CD1	10:J:38:ARG:HG2	2.44	0.48
1:A:1057:VAL:CG1	1:A:1058:VAL:N	2.76	0.48
1:A:1329:THR:HG23	1:A:1335:ILE:HG13	1.95	0.48
1:A:79:GLY:CA	1:A:243:PRO:HG3	2.44	0.48
1:A:427:GLN:O	1:A:428:TYR:C	2.51	0.48
1:A:444:PHE:HB3	1:A:458:HIS:CD2	2.48	0.48
1:A:587:HIS:CE1	1:A:609:ASP:H	2.31	0.48
2:B:1072:MET:CG	2:B:1085:ILE:HD13	2.43	0.48
2:B:1166:CYS:O	2:B:1166:CYS:SG	2.71	0.48
2:B:450:ALA:O	2:B:451:LYS:C	2.51	0.48
2:B:653:VAL:O	2:B:654:ARG:HD3	2.14	0.48
2:B:39:ARG:NH2	2:B:665:GLU:HG2	2.27	0.48
1:A:785:PRO:O	2:B:702:LEU:HD12	2.14	0.48
2:B:731:VAL:HG12	2:B:732:SER:H	1.79	0.48
2:B:864:LYS:HD2	2:B:872:GLU:OE2	2.14	0.48
4:D:134:THR:CG2	4:D:135:GLY:N	2.75	0.48
7:G:144:ARG:HG2	7:G:168:LEU:HD23	1.96	0.48
10:J:36:LEU:HD11	10:J:51:LEU:HB2	1.95	0.48
14:N:4:DA:H2''	14:N:5:DC:C6	2.48	0.48
1:A:356:ASP:OD1	1:A:358:ASN:N	2.35	0.48
1:A:567:LYS:HZ1	8:H:47:PHE:HB2	1.78	0.48
1:A:586:ILE:HD11	1:A:633:VAL:HA	1.95	0.48
1:A:993:LEU:HD23	1:A:1022:LEU:HD11	1.94	0.48
1:A:29:ALA:HB1	2:B:1184:GLY:CA	2.43	0.48
2:B:35:SER:HA	2:B:811:TYR:CE2	2.38	0.48
2:B:595:ARG:HH11	2:B:595:ARG:HG3	1.78	0.48
2:B:687:GLU:CB	2:B:689:LEU:HG	2.43	0.48
2:B:707:PRO:O	2:B:708:GLU:O	2.32	0.48
3:C:62:PHE:HD2	3:C:62:PHE:C	2.17	0.48
5:E:198:ILE:H	5:E:198:ILE:CD1	2.27	0.48
8:H:139:ASN:O	8:H:140:ALA:CB	2.61	0.48
11:K:42:LEU:HD21	11:K:46:ILE:HD12	1.94	0.48
12:L:43:THR:C	12:L:45:ALA:H	2.16	0.48
12:L:61:THR:CG2	12:L:63:ARG:HB2	2.44	0.48
1:A:1067:LEU:O	1:A:1068:ALA:C	2.51	0.48
1:A:334:GLY:C	1:A:336:ILE:N	2.64	0.48
1:A:40:THR:CG2	1:A:41:MET:HE2	2.44	0.48
1:A:466:SER:CB	2:B:1103:ILE:HG12	2.35	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:502:ILE:HD12	2:B:502:ILE:N	2.26	0.48
2:B:373:ARG:HG2	2:B:566:LEU:HD23	1.96	0.48
2:B:597:MET:O	2:B:599:THR:N	2.46	0.48
2:B:705:MET:N	2:B:710:LEU:HD12	2.28	0.48
3:C:88:CYS:O	3:C:90:ASP:N	2.47	0.48
1:A:866:PHE:N	5:E:208:TYR:OH	2.43	0.48
5:E:4:GLU:OE1	5:E:4:GLU:HA	2.14	0.48
9:I:102:VAL:HA	9:I:108:HIS:O	2.14	0.48
1:A:1123:GLY:O	1:A:1125:ALA:N	2.47	0.48
1:A:1130:GLN:HE21	1:A:1134:ILE:CD1	2.21	0.48
1:A:1224:LEU:HD12	1:A:1241:ARG:O	2.13	0.48
1:A:514:PRO:C	1:A:516:SER:H	2.16	0.48
1:A:787:PHE:CZ	1:A:796:SER:HA	2.49	0.48
1:A:859:SER:HB2	1:A:1422:ARG:HB2	1.96	0.48
1:A:865:GLN:NE2	1:A:1370:LEU:HD13	2.29	0.48
2:B:1016:ALA:HA	2:B:1020:ARG:NH1	2.29	0.48
2:B:262:GLU:HA	2:B:267:ARG:NH2	2.29	0.48
2:B:345:LYS:O	2:B:346:GLU:C	2.51	0.48
2:B:123:THR:CB	2:B:458:LYS:HE2	2.44	0.48
2:B:895:ASP:C	2:B:897:GLY:H	2.16	0.48
3:C:15:LYS:HG2	3:C:15:LYS:O	2.14	0.48
3:C:6:PRO:CB	11:K:101:LEU:HD12	2.44	0.48
4:D:47:LEU:HD13	4:D:48:ILE:N	2.22	0.48
5:E:90:VAL:O	5:E:90:VAL:HG22	2.14	0.48
4:D:151:PHE:HZ	7:G:90:THR:HG1	1.60	0.48
3:C:66:ARG:HH21	10:J:5:VAL:HG23	1.77	0.48
1:A:1161:THR:HG22	1:A:1163:ILE:HG13	1.95	0.48
1:A:1193:LEU:HD12	1:A:1193:LEU:C	2.34	0.48
1:A:1230:GLU:C	1:A:1232:ASN:N	2.67	0.48
1:A:1290:LYS:O	1:A:1291:VAL:HG23	2.14	0.48
1:A:1376:THR:O	1:A:1377:THR:C	2.52	0.48
1:A:150:THR:OG1	1:A:166:GLY:HA2	2.13	0.48
1:A:441:PRO:HD2	1:A:498:ARG:NH2	2.29	0.48
1:A:509:LEU:O	1:A:511:ILE:N	2.47	0.48
1:A:509:LEU:C	1:A:511:ILE:H	2.17	0.48
1:A:668:ASP:CG	1:A:742:ASN:HD22	2.18	0.48
1:A:341:MET:CE	2:B:1135:ARG:NH1	2.77	0.48
2:B:1156:ASP:O	2:B:1157:ALA:O	2.32	0.48
2:B:1163:CYS:SG	2:B:1165:ILE:HB	2.54	0.48
2:B:358:LYS:HA	2:B:366:GLN:HB3	1.96	0.48
2:B:430:ARG:O	2:B:434:ARG:CD	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:539:LEU:H	2:B:539:LEU:CD1	2.17	0.48
2:B:542:MET:HG2	2:B:747:MET:HE3	1.95	0.48
2:B:745:PRO:C	2:B:747:MET:N	2.67	0.48
2:B:899:ILE:HD11	2:B:910:VAL:O	2.14	0.48
2:B:1084:GLN:OE1	3:C:189:THR:CG2	2.61	0.48
4:D:164:ILE:CG2	4:D:168:LYS:HD2	2.38	0.48
1:A:1450:LEU:HD13	6:F:131:PRO:HG3	1.95	0.48
1:A:107:CYS:HB2	1:A:171:GLN:NE2	2.29	0.47
1:A:1424:VAL:HG13	1:A:1436:ILE:CD1	2.35	0.47
1:A:331:GLY:O	1:A:332:LYS:O	2.31	0.47
1:A:392:VAL:HG21	1:A:426:LEU:HD11	1.96	0.47
1:A:549:MET:HE2	1:A:656:TRP:HD1	1.78	0.47
1:A:341:MET:HE1	2:B:1135:ARG:NH1	2.29	0.47
1:A:1422:ARG:HH12	2:B:1224:PHE:HD2	1.62	0.47
2:B:174:LEU:HD22	2:B:202:TYR:CE1	2.49	0.47
2:B:345:LYS:O	2:B:347:LYS:N	2.47	0.47
2:B:578:THR:C	2:B:589:VAL:HG13	2.34	0.47
2:B:603:LEU:HD12	2:B:609:ILE:HG12	1.96	0.47
2:B:405:ARG:HA	2:B:631:GLY:O	2.14	0.47
2:B:519:TRP:NE1	2:B:635:ARG:NH2	2.61	0.47
2:B:708:GLU:CG	2:B:709:ASP:H	2.19	0.47
2:B:976:ILE:O	2:B:990:ILE:HB	2.13	0.47
3:C:8:VAL:HG21	11:K:105:PHE:HA	1.96	0.47
3:C:91:HIS:C	3:C:91:HIS:CD2	2.86	0.47
4:D:10:THR:O	4:D:10:THR:HG23	2.13	0.47
4:D:198:LEU:HA	4:D:201:LYS:HD2	1.95	0.47
7:G:115:MET:SD	7:G:119:LEU:HD23	2.53	0.47
11:K:46:ILE:O	11:K:46:ILE:HG22	2.14	0.47
1:A:1038:THR:HG23	1:A:1041:ALA:CB	2.44	0.47
1:A:1198:ASP:HB3	1:A:1201:ALA:CB	2.43	0.47
1:A:1313:LEU:CD1	1:A:1327:ILE:HD13	2.44	0.47
1:A:592:ASP:N	1:A:595:THR:OG1	2.46	0.47
1:A:596:THR:C	1:A:598:LEU:N	2.62	0.47
2:B:1058:LEU:O	2:B:1061:GLU:HB2	2.14	0.47
2:B:128:LEU:N	2:B:128:LEU:HD12	2.29	0.47
2:B:324:ILE:HD11	2:B:329:THR:O	2.14	0.47
2:B:52:ASN:O	2:B:55:VAL:N	2.44	0.47
2:B:613:VAL:HG13	2:B:628:THR:CA	2.43	0.47
2:B:642:ASP:CB	2:B:649:LYS:HG3	2.43	0.47
5:E:33:GLU:O	5:E:36:GLU:N	2.47	0.47
7:G:62:LEU:CB	7:G:63:PRO:HD2	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:16:ASP:CG	10:J:17:LYS:HD2	2.34	0.47
2:B:186:GLU:HG3	10:J:62:ARG:NH1	2.29	0.47
12:L:43:THR:O	12:L:43:THR:HG22	2.13	0.47
1:A:1054:LEU:HD13	6:F:84:TYR:OH	2.13	0.47
1:A:1159:ARG:HD3	1:A:1174:PHE:CZ	2.49	0.47
1:A:1199:ARG:HH21	1:A:1234:GLU:HA	1.78	0.47
1:A:185:TRP:CE3	1:A:185:TRP:N	2.82	0.47
1:A:322:VAL:O	1:A:322:VAL:HG13	2.13	0.47
1:A:44:THR:O	1:A:45:GLN:HB2	2.15	0.47
1:A:600:PRO:CG	1:A:601:LYS:H	2.20	0.47
1:A:518:LYS:HE2	1:A:624:SER:O	2.14	0.47
1:A:853:ASP:C	1:A:853:ASP:OD1	2.52	0.47
1:A:90:VAL:CG1	1:A:297:GLN:HA	2.43	0.47
2:B:762:ASN:HD21	2:B:1024:ALA:HB3	1.79	0.47
2:B:1033:LYS:NZ	2:B:1068:GLY:O	2.47	0.47
2:B:1167:GLY:HA3	2:B:1215:ARG:HB3	1.95	0.47
2:B:239:GLU:HA	2:B:254:LEU:O	2.14	0.47
2:B:306:ASN:C	2:B:308:TRP:H	2.17	0.47
2:B:605:ARG:HB3	2:B:688:GLY:CA	2.45	0.47
3:C:76:ASP:O	3:C:78:GLU:N	2.44	0.47
5:E:117:THR:CG2	5:E:119:SER:HB2	2.43	0.47
5:E:173:SER:C	5:E:175:LEU:N	2.67	0.47
7:G:96:GLN:HA	7:G:121:PHE:CE2	2.49	0.47
7:G:8:SER:O	7:G:9:LEU:HB2	2.14	0.47
8:H:130:ARG:N	8:H:130:ARG:CD	2.73	0.47
8:H:36:CYS:HB2	8:H:130:ARG:HH22	1.79	0.47
1:A:958:VAL:CG2	1:A:1053:PHE:HA	2.44	0.47
1:A:1273:LEU:CD1	1:A:1273:LEU:N	2.76	0.47
1:A:1430:LEU:HB3	1:A:1432:GLN:HG3	1.95	0.47
1:A:506:ALA:O	1:A:509:LEU:HB2	2.14	0.47
1:A:628:GLY:O	1:A:632:VAL:HG23	2.14	0.47
1:A:645:LEU:HG	1:A:649:ILE:HD11	1.95	0.47
1:A:725:ALA:O	1:A:728:LYS:HG2	2.14	0.47
2:B:1081:LEU:O	2:B:1083:ALA:N	2.48	0.47
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.97	0.47
2:B:39:ARG:HG2	2:B:39:ARG:NH1	2.29	0.47
2:B:635:ARG:HB2	2:B:636:PRO:HD2	1.96	0.47
2:B:766:ARG:HG3	2:B:1022:THR:CG2	2.41	0.47
2:B:911:ILE:O	2:B:911:ILE:HG22	2.14	0.47
3:C:183:TRP:O	3:C:184:ASN:HB3	2.14	0.47
3:C:190:ASP:O	3:C:191:TYR:C	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:86:CYS:SG	3:C:87:PHE:N	2.87	0.47
4:D:47:LEU:HD11	7:G:3:PHE:HD2	1.78	0.47
4:D:68:ARG:O	4:D:72:ARG:HG3	2.14	0.47
5:E:138:ALA:HA	5:E:141:VAL:HG23	1.96	0.47
5:E:157:SER:C	5:E:159:ASP:N	2.67	0.47
6:F:109:VAL:CG1	6:F:110:ASP:N	2.76	0.47
9:I:25:LEU:CB	9:I:38:ALA:HB2	2.45	0.47
10:J:27:GLU:C	10:J:29:GLU:N	2.67	0.47
1:A:447:GLN:HE22	13:T:20:DG:H4'	1.79	0.47
1:A:1243:VAL:HG22	1:A:1244:ARG:H	1.80	0.47
1:A:1243:VAL:HG22	1:A:1244:ARG:N	2.28	0.47
1:A:1332:PHE:N	1:A:1332:PHE:CD2	2.83	0.47
1:A:381:THR:HG22	1:A:383:TYR:CD2	2.49	0.47
1:A:728:LYS:O	1:A:732:LEU:HG	2.14	0.47
2:B:261:ARG:NH1	2:B:262:GLU:H	2.13	0.47
2:B:288:ALA:N	2:B:330:ALA:HB1	2.29	0.47
2:B:370:PHE:HD2	2:B:373:ARG:HD2	1.79	0.47
2:B:412:LEU:HD13	2:B:479:VAL:HG11	1.96	0.47
2:B:604:ARG:O	2:B:606:LYS:N	2.47	0.47
2:B:686:ASN:C	2:B:688:GLY:N	2.68	0.47
2:B:867:GLY:C	2:B:869:SER:N	2.67	0.47
5:E:90:VAL:HB	5:E:120:ALA:HB2	1.96	0.47
5:E:30:ILE:HG23	5:E:34:GLU:OE1	2.15	0.47
1:A:1443:VAL:HG11	6:F:132:LEU:HD13	1.96	0.47
6:F:135:ARG:HG2	6:F:137:TYR:CE1	2.48	0.47
7:G:139:ILE:HG22	7:G:140:LYS:N	2.29	0.47
9:I:111:THR:CG2	9:I:112:SER:N	2.76	0.47
1:A:852:TYR:HD2	1:A:1060:PRO:CB	2.27	0.47
1:A:1129:GLU:O	1:A:1130:GLN:C	2.51	0.47
1:A:230:ARG:HG3	1:A:233:TRP:CZ3	2.49	0.47
1:A:280:GLU:C	1:A:282:ASN:H	2.16	0.47
1:A:399:HIS:CB	1:A:400:PRO:CD	2.84	0.47
1:A:605:MET:HG2	1:A:621:THR:HG23	1.97	0.47
1:A:777:PHE:C	1:A:779:PHE:H	2.17	0.47
2:B:1104:HIS:CG	2:B:1122:ARG:HB2	2.50	0.47
4:D:40:HIS:HB2	7:G:73:LYS:CD	2.44	0.47
5:E:164:LEU:C	5:E:165:LEU:HD23	2.34	0.47
5:E:45:LYS:HB3	5:E:46:TYR:CD1	2.49	0.47
5:E:73:PRO:HB2	5:E:74:ASP:OD1	2.15	0.47
8:H:26:ILE:HG22	8:H:27:GLU:N	2.28	0.47
1:A:1037:LEU:HD13	1:A:1041:ALA:CB	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ARG:C	1:A:136:ALA:N	2.68	0.47
1:A:1378:GLN:HA	1:A:1378:GLN:OE1	2.15	0.47
1:A:233:TRP:O	1:A:235:ILE:N	2.47	0.47
2:B:1053:GLU:O	2:B:1057:LYS:HG3	2.15	0.47
2:B:54:PHE:HE1	2:B:414:ALA:HA	1.79	0.47
2:B:515:HIS:CD2	2:B:517:THR:HG23	2.49	0.47
2:B:539:LEU:N	2:B:539:LEU:HD12	2.17	0.47
2:B:591:ARG:O	2:B:593:PRO:HD3	2.15	0.47
2:B:557:PHE:CZ	2:B:603:LEU:HD21	2.49	0.47
2:B:496:ARG:HD2	2:B:751:VAL:HG23	1.97	0.47
2:B:955:THR:HG22	2:B:956:THR:N	2.30	0.47
4:D:12:ARG:HG3	4:D:14:ARG:NH2	2.30	0.47
4:D:157:GLN:O	4:D:158:GLU:C	2.53	0.47
1:A:1389:PHE:O	1:A:1391:ARG:N	2.44	0.47
1:A:1448:GLU:O	1:A:1449:SER:C	2.51	0.47
1:A:572:TRP:HA	1:A:576:GLN:OE1	2.14	0.47
1:A:822:GLU:O	1:A:825:ILE:HG22	2.15	0.47
1:A:890:ASP:OD2	1:A:1296:GLY:HA2	2.14	0.47
2:B:114:PRO:O	2:B:115:GLN:C	2.53	0.47
2:B:336:ARG:NE	2:B:348:ARG:HH12	2.03	0.47
2:B:618:ASP:O	2:B:622:LYS:N	2.47	0.47
2:B:898:LEU:HD13	2:B:952:VAL:CG1	2.44	0.47
5:E:78:LEU:HD23	5:E:79:TRP:N	2.29	0.47
8:H:11:GLN:O	8:H:28:ALA:CB	2.63	0.47
1:A:1063:MET:SD	1:A:1436:ILE:HG12	2.55	0.47
1:A:1209:MET:SD	1:A:1236:LEU:HB3	2.55	0.47
1:A:1362:TYR:CD1	1:A:1363:VAL:N	2.83	0.47
1:A:1399:ARG:HB3	1:A:1408:ILE:CD1	2.44	0.47
1:A:1399:ARG:HB3	1:A:1408:ILE:HD13	1.97	0.47
1:A:38:PRO:HG2	1:A:39:GLU:N	2.30	0.47
1:A:635:ARG:HA	1:A:635:ARG:NH1	2.24	0.47
1:A:755:PHE:O	1:A:758:ILE:HG13	2.15	0.47
1:A:933:TYR:O	1:A:937:VAL:HG23	2.15	0.47
1:A:7:SER:O	1:A:9:ALA:N	2.48	0.47
2:B:130:VAL:HG23	2:B:167:ILE:HD13	1.95	0.47
2:B:203:PHE:N	2:B:203:PHE:CD1	2.83	0.47
3:C:107:SER:C	3:C:109:SER:N	2.65	0.47
3:C:238:ILE:CD1	3:C:246:ARG:HD2	2.44	0.47
5:E:138:ALA:HA	5:E:141:VAL:CG2	2.45	0.47
8:H:84:ALA:C	8:H:86:ASP:N	2.68	0.47
9:I:14:LEU:HD22	9:I:28:GLU:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1035:TYR:CD1	1:A:1037:LEU:HD23	2.47	0.47
1:A:1366:ARG:HG2	1:A:1366:ARG:HH11	1.79	0.47
1:A:352:VAL:O	1:A:467:THR:HG22	2.15	0.47
1:A:489:LEU:HD12	1:A:489:LEU:C	2.35	0.47
1:A:531:ILE:HD11	1:A:578:LEU:CD2	2.44	0.47
1:A:783:THR:HB	1:A:787:PHE:CD1	2.50	0.47
1:A:829:VAL:O	1:A:831:THR:N	2.48	0.47
1:A:9:ALA:CB	2:B:1193:GLN:HB2	2.44	0.47
2:B:294:ASP:C	2:B:296:GLU:N	2.62	0.47
2:B:318:VAL:C	2:B:320:ASP:H	2.18	0.47
2:B:373:ARG:HA	2:B:566:LEU:HD23	1.97	0.47
3:C:105:GLY:HA3	3:C:148:ARG:O	2.15	0.47
3:C:62:PHE:CD2	3:C:62:PHE:C	2.88	0.47
6:F:82:THR:HG23	6:F:84:TYR:H	1.79	0.47
9:I:101:PHE:N	9:I:101:PHE:HD1	2.13	0.47
1:A:1345:ARG:HD2	1:A:1373:ASP:OD1	2.14	0.47
1:A:146:MET:HB3	1:A:171:GLN:O	2.15	0.47
1:A:162:VAL:HG12	1:A:163:SER:N	2.29	0.47
1:A:191:THR:HG22	1:A:192:GLY:N	2.30	0.47
1:A:108:MET:HB3	1:A:210:ILE:CD1	2.45	0.47
1:A:929:LEU:CD1	1:A:929:LEU:O	2.63	0.47
1:A:953:ASN:C	1:A:954:TRP:CD1	2.89	0.47
2:B:705:MET:H	2:B:710:LEU:CD1	2.27	0.47
2:B:540:SER:HB3	2:B:747:MET:O	2.15	0.47
2:B:973:ILE:HG23	2:B:974:PRO:HD2	1.96	0.47
3:C:258:ILE:O	3:C:262:LEU:HG	2.14	0.47
3:C:29:MET:HA	11:K:45:LEU:HD13	1.96	0.47
5:E:108:GLY:HA3	5:E:132:ILE:HG22	1.96	0.47
5:E:47:CYS:HA	5:E:52:ARG:O	2.15	0.47
5:E:169:ARG:HB3	6:F:140:ASP:OD2	2.14	0.47
8:H:103:LYS:HG2	8:H:104:PHE:N	2.29	0.47
8:H:113:ALA:HB1	8:H:125:LEU:O	2.14	0.47
9:I:16:PRO:HB2	9:I:25:LEU:HD11	1.97	0.47
10:J:56:LEU:O	10:J:59:LYS:N	2.48	0.47
11:K:89:ASN:C	11:K:91:CYS:N	2.68	0.47
1:A:1030:ARG:O	1:A:1034:GLU:HB2	2.15	0.46
1:A:1140:HIS:HA	1:A:1275:GLY:HA3	1.97	0.46
1:A:1236:LEU:C	1:A:1237:ILE:HG13	2.36	0.46
1:A:1259:MET:O	1:A:1263:ILE:HD12	2.14	0.46
1:A:606:LEU:CG	1:A:613:ILE:HD12	2.44	0.46
1:A:896:ARG:HD3	1:A:897:TYR:HE1	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1055:ILE:O	2:B:1057:LYS:N	2.48	0.46
1:A:342:GLY:HA3	2:B:1131:GLY:HA2	1.97	0.46
2:B:185:THR:O	2:B:186:GLU:C	2.53	0.46
2:B:453:ILE:O	2:B:454:THR:C	2.53	0.46
2:B:563:MET:HE1	2:B:580:VAL:HB	1.97	0.46
2:B:810:GLU:CB	2:B:815:ARG:NH2	2.77	0.46
3:C:104:PHE:HB3	3:C:106:GLU:OE1	2.14	0.46
3:C:125:MET:HG3	3:C:127:ARG:NH2	2.30	0.46
5:E:4:GLU:HB3	5:E:7:ARG:HE	1.80	0.46
6:F:89:GLU:HB3	6:F:134:ILE:CD1	2.45	0.46
4:D:29:LEU:HD22	7:G:82:PHE:CE2	2.50	0.46
8:H:82:PRO:HG2	8:H:83:GLN:N	2.30	0.46
11:K:110:ASN:O	11:K:111:LEU:HD23	2.15	0.46
11:K:65:HIS:HD2	11:K:67:PHE:N	2.07	0.46
12:L:55:ILE:H	12:L:55:ILE:CD1	2.19	0.46
12:L:60:ARG:HG2	12:L:61:THR:H	1.80	0.46
1:A:1011:GLN:NE2	1:A:1015:VAL:HG21	2.31	0.46
1:A:1143:LEU:O	1:A:1146:VAL:HG23	2.15	0.46
1:A:1265:ASN:C	1:A:1267:MET:N	2.68	0.46
1:A:1451:VAL:C	1:A:1453:TYR:H	2.17	0.46
1:A:695:LYS:HA	1:A:698:GLN:HB2	1.97	0.46
1:A:84:ILE:CG2	1:A:84:ILE:O	2.63	0.46
1:A:993:LEU:CD2	1:A:1022:LEU:HD11	2.45	0.46
2:B:1065:GLN:NE2	2:B:1067:ARG:N	2.43	0.46
2:B:1068:GLY:O	2:B:1069:PHE:O	2.33	0.46
2:B:235:SER:HB2	2:B:267:ARG:HH12	1.80	0.46
2:B:309:GLN:HG3	9:I:52:ILE:CD1	2.44	0.46
2:B:311:LEU:O	2:B:312:GLU:C	2.53	0.46
2:B:483:LEU:CD1	2:B:491:THR:HG23	2.45	0.46
2:B:611:PRO:O	2:B:692:TYR:HB2	2.16	0.46
2:B:871:THR:HG22	2:B:872:GLU:O	2.15	0.46
3:C:115:SER:HB3	3:C:142:VAL:HB	1.96	0.46
5:E:178:ILE:HG22	5:E:213:ILE:O	2.15	0.46
7:G:13:LEU:HD21	7:G:17:PHE:HB2	1.97	0.46
7:G:88:ASP:HA	7:G:144:ARG:HA	1.97	0.46
9:I:100:PHE:CD1	9:I:100:PHE:N	2.83	0.46
1:A:1040:GLN:O	1:A:1041:ALA:C	2.54	0.46
1:A:289:ILE:O	1:A:292:ALA:N	2.32	0.46
1:A:332:LYS:C	1:A:334:GLY:N	2.69	0.46
1:A:575:LYS:HD2	8:H:120:GLY:HA2	1.95	0.46
1:A:623:GLY:C	1:A:625:SER:H	2.17	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:670:ILE:HG22	1:A:676:MET:HE2	1.98	0.46
2:B:1060:ARG:HA	2:B:1060:ARG:HD2	1.68	0.46
2:B:1125:ASP:O	2:B:1125:ASP:OD1	2.34	0.46
2:B:126:SER:HB3	2:B:172:ILE:HD11	1.98	0.46
2:B:397:ASP:OD1	2:B:399:ASP:N	2.38	0.46
2:B:458:LYS:O	2:B:459:TYR:C	2.53	0.46
2:B:498:THR:N	2:B:537:LYS:O	2.49	0.46
2:B:53:GLN:HG2	2:B:547:VAL:CG2	2.46	0.46
2:B:547:VAL:HG13	2:B:548:GLY:N	2.30	0.46
2:B:806:THR:HB	2:B:809:MET:HG3	1.98	0.46
2:B:934:LYS:HG2	2:B:934:LYS:O	2.14	0.46
3:C:228:PHE:N	3:C:228:PHE:CD1	2.83	0.46
4:D:46:GLU:HG2	4:D:47:LEU:N	2.31	0.46
1:A:1441:PHE:CE1	6:F:92:ARG:HG2	2.50	0.46
1:A:1445:ILE:HD11	7:G:68:ALA:HB1	1.96	0.46
11:K:77:THR:HG21	11:K:83:PRO:HA	1.97	0.46
1:A:874:ASP:CA	1:A:1058:VAL:HG23	2.46	0.46
1:A:1152:ILE:HD11	9:I:44:TYR:CE2	2.50	0.46
1:A:889:SER:CB	1:A:1297:GLU:HG3	2.44	0.46
1:A:144:THR:O	1:A:146:MET:CE	2.63	0.46
1:A:40:THR:C	1:A:41:MET:HG3	2.34	0.46
1:A:949:ASP:OD2	1:A:951:GLU:HB2	2.15	0.46
2:B:1001:PHE:CE2	3:C:34:ARG:CZ	2.99	0.46
2:B:261:ARG:O	2:B:263:GLY:N	2.48	0.46
2:B:287:ARG:HH11	2:B:324:ILE:HG22	1.81	0.46
2:B:435:THR:CG2	2:B:437:GLU:HB2	2.45	0.46
2:B:509:ALA:O	2:B:510:LYS:C	2.54	0.46
2:B:581:PHE:O	2:B:626:ILE:HB	2.16	0.46
2:B:1065:GLN:HB2	3:C:201:TRP:CZ3	2.50	0.46
4:D:119:ARG:HD3	4:D:221:TYR:HE2	1.80	0.46
4:D:4:SER:O	7:G:9:LEU:HD13	2.15	0.46
6:F:82:THR:HG22	6:F:84:TYR:H	1.80	0.46
1:A:1284:MET:O	1:A:1285:MET:HG2	2.15	0.46
1:A:1341:ILE:CG2	1:A:1342:GLU:N	2.76	0.46
1:A:159:THR:O	1:A:159:THR:HG22	2.16	0.46
1:A:203:SER:O	1:A:206:GLU:HB3	2.16	0.46
1:A:226:GLU:HG2	1:A:226:GLU:O	2.14	0.46
1:A:427:GLN:HB2	1:A:430:TRP:NE1	2.31	0.46
1:A:608:ILE:CB	1:A:613:ILE:HD11	2.42	0.46
2:B:307:ASP:C	2:B:309:GLN:N	2.69	0.46
2:B:326:ASP:CG	2:B:328:GLU:HB3	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:802:ASN:HD21	2:B:728:ARG:HB2	1.76	0.46
4:D:8:PHE:HZ	4:D:37:GLN:HB2	1.79	0.46
5:E:29:PHE:N	5:E:65:THR:HG22	2.31	0.46
6:F:111:LEU:HD12	6:F:111:LEU:N	2.10	0.46
6:F:117:PRO:C	6:F:119:ARG:N	2.69	0.46
1:A:857:ARG:CZ	6:F:139:PRO:CB	2.93	0.46
7:G:18:PHE:HZ	7:G:68:ALA:HB2	1.80	0.46
9:I:25:LEU:CG	9:I:38:ALA:HB2	2.46	0.46
9:I:61:ASP:C	9:I:63:GLY:N	2.68	0.46
1:A:369:SER:HB2	11:K:2:ASN:HD21	1.81	0.46
1:A:218:ASP:O	1:A:219:PHE:C	2.54	0.46
1:A:280:GLU:C	1:A:282:ASN:N	2.69	0.46
1:A:393:ARG:CB	1:A:393:ARG:HH11	2.27	0.46
1:A:642:CYS:O	1:A:645:LEU:HB3	2.16	0.46
1:A:751:SER:O	1:A:752:LYS:HG2	2.15	0.46
1:A:83:HIS:CD2	1:A:83:HIS:C	2.89	0.46
1:A:870:GLU:O	1:A:871:ASP:HB3	2.15	0.46
2:B:205:ILE:N	2:B:205:ILE:CD1	2.79	0.46
2:B:753:ALA:O	2:B:756:ILE:HG13	2.15	0.46
2:B:762:ASN:OD1	2:B:1022:THR:HA	2.14	0.46
2:B:529:GLU:OE2	2:B:769:TYR:CE1	2.68	0.46
3:C:13:ALA:O	11:K:114:LEU:HD22	2.14	0.46
3:C:82:TYR:CG	3:C:161:LYS:HG2	2.51	0.46
5:E:145:THR:HG21	5:E:187:TYR:CD2	2.50	0.46
5:E:17:ARG:HG3	5:E:18:THR:N	2.31	0.46
6:F:114:GLU:OE2	6:F:119:ARG:HG2	2.15	0.46
7:G:145:VAL:HG12	7:G:146:LYS:H	1.80	0.46
7:G:59:GLY:CA	7:G:70:PHE:CD2	2.97	0.46
9:I:25:LEU:HG	9:I:38:ALA:HB2	1.97	0.46
9:I:62:ILE:HG12	9:I:62:ILE:O	2.15	0.46
10:J:14:VAL:CG1	10:J:14:VAL:O	2.63	0.46
1:A:1067:LEU:HD13	1:A:1067:LEU:C	2.36	0.46
1:A:1140:HIS:HB2	1:A:1276:VAL:O	2.16	0.46
1:A:1340:GLY:O	1:A:1342:GLU:N	2.48	0.46
1:A:1438:THR:O	6:F:92:ARG:NH1	2.49	0.46
1:A:184:SER:HB3	1:A:199:LEU:CD2	2.44	0.46
1:A:372:LYS:HA	1:A:435:HIS:CE1	2.50	0.46
1:A:516:SER:O	1:A:518:LYS:HB3	2.16	0.46
1:A:672:ASP:OD2	1:A:674:PRO:HG2	2.16	0.46
1:A:720:ARG:HB3	1:A:720:ARG:CZ	2.46	0.46
1:A:79:GLY:H	2:B:1205:GLN:HE22	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:827:ILE:HD12	2:B:1086:PHE:CD2	2.51	0.46
2:B:641:GLU:C	2:B:643:ASP:H	2.18	0.46
2:B:844:SER:O	2:B:847:ASP:HB2	2.16	0.46
2:B:860:MET:HG2	2:B:861:ASP:H	1.80	0.46
2:B:895:ASP:C	2:B:897:GLY:N	2.69	0.46
3:C:58:LEU:N	3:C:58:LEU:CD2	2.79	0.46
3:C:99:LEU:HD23	3:C:99:LEU:N	2.30	0.46
5:E:186:LEU:O	5:E:187:TYR:C	2.53	0.46
5:E:35:VAL:C	5:E:37:LEU:H	2.19	0.46
1:A:852:TYR:CE1	6:F:136:ARG:HG2	2.51	0.46
1:A:1444:MET:HG3	7:G:59:GLY:O	2.16	0.46
11:K:61:TYR:HD2	11:K:61:TYR:O	1.98	0.46
1:A:1258:HIS:HB3	1:A:1259:MET:CE	2.46	0.46
1:A:1345:ARG:NH1	5:E:200:ARG:NH2	2.64	0.46
1:A:718:VAL:O	1:A:721:PHE:HB2	2.16	0.46
1:A:826:ASP:C	1:A:828:ALA:N	2.68	0.46
1:A:875:ALA:HA	1:A:878:ILE:CD1	2.45	0.46
1:A:897:TYR:CD1	1:A:897:TYR:N	2.83	0.46
1:A:932:GLU:O	1:A:936:LEU:HG	2.16	0.46
2:B:100:PRO:HD3	2:B:172:ILE:HD13	1.98	0.46
2:B:240:ILE:HG23	2:B:240:ILE:O	2.15	0.46
2:B:292:ILE:HG23	2:B:326:ASP:HA	1.98	0.46
2:B:333:PHE:O	2:B:333:PHE:CD2	2.69	0.46
2:B:834:ASN:O	2:B:838:SER:O	2.32	0.46
2:B:890:TYR:O	2:B:893:LEU:HB2	2.16	0.46
3:C:226:ASP:O	3:C:227:THR:HB	2.16	0.46
3:C:35:ARG:HH11	11:K:41:THR:CA	2.29	0.46
4:D:155:ARG:CZ	4:D:155:ARG:HB2	2.45	0.46
4:D:185:CYS:HB2	4:D:211:LEU:HD21	1.96	0.46
4:D:29:LEU:HD22	7:G:82:PHE:CD2	2.51	0.46
5:E:82:PHE:CD1	5:E:82:PHE:N	2.83	0.46
9:I:55:THR:O	9:I:55:THR:HG22	2.16	0.46
10:J:64:ASN:ND2	10:J:65:PRO:HD3	2.31	0.46
11:K:89:ASN:O	11:K:91:CYS:N	2.49	0.46
1:A:377:PRO:HG3	1:A:493:GLN:HG3	1.98	0.46
1:A:407:ARG:HA	1:A:430:TRP:CD2	2.51	0.46
1:A:896:ARG:HH21	1:A:1030:ARG:CZ	2.29	0.46
2:B:1020:ARG:HG3	2:B:1020:ARG:HH11	1.80	0.46
2:B:1106:ARG:HD3	2:B:1127:GLY:N	2.31	0.46
2:B:291:ILE:HD13	2:B:300:HIS:CD2	2.51	0.46
2:B:552:MET:N	2:B:553:PRO:HD2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:579:ARG:HA	2:B:589:VAL:HG22	1.98	0.46
2:B:654:ARG:C	2:B:656:GLY:N	2.68	0.46
3:C:245:VAL:HA	3:C:248:ILE:HD12	1.98	0.46
5:E:22:MET:CE	5:E:26:ARG:HD2	2.46	0.46
6:F:116:ASP:C	6:F:116:ASP:OD1	2.54	0.46
6:F:148:VAL:HA	6:F:151:LEU:HD12	1.96	0.46
8:H:25:ARG:HB2	8:H:41:ASP:OD1	2.15	0.46
3:C:10:ILE:HG13	11:K:108:GLU:HB3	1.98	0.46
11:K:82:ASP:OD1	11:K:84:LYS:N	2.46	0.46
12:L:39:SER:O	12:L:40:LEU:HG	2.15	0.46
1:A:1018:PHE:O	1:A:1021:LEU:N	2.49	0.46
1:A:1261:LYS:HE3	9:I:44:TYR:CE2	2.51	0.46
1:A:1118:VAL:O	1:A:1305:VAL:HG13	2.16	0.46
1:A:1111:MET:CE	1:A:1331:SER:HA	2.31	0.46
1:A:1372:VAL:O	1:A:1376:THR:HG23	2.16	0.46
1:A:1402:PHE:CG	1:A:1402:PHE:O	2.67	0.46
1:A:616:VAL:CG1	1:A:617:VAL:H	2.19	0.46
1:A:619:LYS:O	1:A:623:GLY:HA3	2.16	0.46
2:B:1065:GLN:HG3	2:B:1067:ARG:H	1.80	0.46
2:B:1081:LEU:C	2:B:1083:ALA:N	2.69	0.46
2:B:1221:SER:HB3	4:D:12:ARG:NE	2.30	0.46
1:A:1418:LEU:HB3	2:B:1222:ARG:HH11	1.79	0.46
2:B:334:ILE:C	2:B:336:ARG:H	2.20	0.46
2:B:591:ARG:O	2:B:592:ASN:C	2.55	0.46
2:B:756:ILE:O	2:B:759:PRO:HD3	2.16	0.46
3:C:215:GLU:O	3:C:216:GLY:C	2.54	0.46
3:C:46:ILE:HD12	3:C:67:LEU:O	2.16	0.46
4:D:119:ARG:HD3	4:D:221:TYR:HD2	1.76	0.46
5:E:167:ARG:HA	5:E:167:ARG:HD3	1.66	0.46
5:E:190:LEU:HD12	5:E:214:CYS:CB	2.45	0.46
5:E:195:VAL:CG1	5:E:196:VAL:N	2.78	0.46
7:G:127:PRO:HG2	7:G:138:THR:CG2	2.34	0.46
7:G:34:VAL:HG13	7:G:45:ILE:HG21	1.98	0.46
7:G:51:TYR:HD2	7:G:51:TYR:O	1.98	0.46
8:H:15:VAL:HG22	8:H:26:ILE:CG2	2.45	0.46
8:H:37:LYS:HD2	8:H:126:GLU:OE1	2.16	0.46
11:K:68:PHE:N	11:K:68:PHE:CD2	2.84	0.46
12:L:30:ILE:HG22	12:L:31:CYS:N	2.31	0.46
1:A:1239:ARG:HB3	1:A:1239:ARG:NH1	2.30	0.45
1:A:1427:ASN:ND2	1:A:1427:ASN:H	2.14	0.45
1:A:42:ASP:C	1:A:44:THR:N	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:GLN:NE2	6:F:90:ARG:HH21	2.12	0.45
1:A:584:ASN:C	1:A:586:ILE:N	2.69	0.45
1:A:590:ARG:HD3	1:A:592:ASP:OD2	2.16	0.45
1:A:699:ALA:O	1:A:700:ASN:CB	2.64	0.45
1:A:944:ARG:NE	1:A:1298:TYR:HE1	2.14	0.45
2:B:1007:VAL:HG23	2:B:1008:PRO:HD2	1.97	0.45
2:B:128:LEU:O	2:B:167:ILE:HD12	2.16	0.45
2:B:235:SER:OG	2:B:236:HIS:CD2	2.69	0.45
2:B:25:ILE:HG23	2:B:658:ILE:CD1	2.43	0.45
2:B:286:PHE:HE1	2:B:382:ILE:HD12	1.81	0.45
2:B:459:TYR:CD2	2:B:459:TYR:C	2.88	0.45
2:B:479:VAL:HG12	2:B:480:SER:N	2.31	0.45
2:B:601:ARG:O	2:B:605:ARG:HG3	2.16	0.45
2:B:601:ARG:NH1	2:B:605:ARG:HH22	2.14	0.45
2:B:680:THR:HG23	2:B:683:SER:H	1.81	0.45
2:B:693:ILE:HD13	2:B:701:ILE:HD13	1.97	0.45
4:D:51:ASN:O	4:D:52:LEU:C	2.54	0.45
5:E:164:LEU:HD11	5:E:211:TYR:CE1	2.51	0.45
6:F:103:MET:CE	7:G:65:ASP:HB2	2.45	0.45
6:F:77:ASP:O	6:F:78:GLN:CB	2.55	0.45
7:G:13:LEU:HD23	7:G:14:HIS:N	2.27	0.45
8:H:4:THR:HG22	8:H:6:PHE:H	1.81	0.45
1:A:560:ILE:CG1	8:H:79:TRP:H	2.29	0.45
11:K:100:ALA:O	11:K:103:THR:HB	2.17	0.45
3:C:35:ARG:NH1	11:K:41:THR:CA	2.79	0.45
12:L:34:CYS:O	12:L:35:SER:C	2.52	0.45
1:A:1051:ALA:O	1:A:1055:ARG:HG3	2.16	0.45
1:A:1110:ASN:CG	1:A:1110:ASN:O	2.55	0.45
1:A:1262:LYS:O	1:A:1264:GLU:N	2.49	0.45
1:A:150:THR:O	1:A:163:SER:HA	2.16	0.45
1:A:239:LEU:HA	1:A:240:PRO:HD2	1.81	0.45
1:A:728:LYS:HA	1:A:731:ARG:HH21	1.80	0.45
1:A:88:LYS:HG3	1:A:276:LEU:HD21	1.98	0.45
1:A:896:ARG:HH21	1:A:1030:ARG:NH2	2.14	0.45
2:B:102:VAL:HG23	2:B:110:HIS:O	2.16	0.45
2:B:1181:GLU:HG2	2:B:1188:LYS:HD2	1.98	0.45
2:B:59:LEU:HD12	2:B:417:PHE:CD2	2.51	0.45
2:B:656:GLY:O	2:B:657:HIS:C	2.53	0.45
3:C:133:ILE:HG13	3:C:237:SER:H	1.80	0.45
7:G:50:ASP:O	7:G:51:TYR:C	2.53	0.45
8:H:93:TYR:CD1	8:H:143:LEU:HD23	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:56:LEU:O	10:J:57:ILE:C	2.55	0.45
11:K:107:THR:HG22	11:K:108:GLU:N	2.30	0.45
11:K:110:ASN:C	11:K:111:LEU:HD23	2.36	0.45
1:A:1332:PHE:H	1:A:1332:PHE:HD2	1.61	0.45
1:A:332:LYS:H	1:A:337:ARG:HB3	1.81	0.45
1:A:509:LEU:C	1:A:511:ILE:N	2.70	0.45
1:A:54:ASN:HA	1:A:247:ARG:HH22	1.82	0.45
1:A:684:ALA:O	1:A:687:LYS:HB2	2.16	0.45
1:A:7:SER:C	1:A:9:ALA:N	2.70	0.45
2:B:834:ASN:ND2	2:B:1013:ASN:HA	2.31	0.45
2:B:128:LEU:HD11	2:B:170:LEU:HB3	1.98	0.45
2:B:469:GLN:O	2:B:470:LYS:HB2	2.16	0.45
2:B:570:VAL:HB	2:B:573:GLN:HB3	1.99	0.45
2:B:882:THR:C	2:B:884:ARG:H	2.20	0.45
3:C:56:THR:CG2	3:C:58:LEU:HD23	2.46	0.45
7:G:1:MET:CE	7:G:80:LYS:O	2.64	0.45
2:B:1039:GLY:HA2	10:J:51:LEU:CD2	2.47	0.45
1:A:1166:ASP:OD2	1:A:1239:ARG:NE	2.40	0.45
1:A:1191:TRP:HD1	1:A:1256:GLU:HB3	1.80	0.45
1:A:1402:PHE:O	1:A:1403:GLU:CB	2.64	0.45
1:A:524:VAL:CG1	1:A:525:GLN:H	2.28	0.45
1:A:821:ARG:HB2	1:A:821:ARG:HH11	1.81	0.45
1:A:964:ILE:O	1:A:967:ALA:N	2.48	0.45
2:B:1149:GLU:HA	2:B:1153:GLU:OE1	2.16	0.45
2:B:324:ILE:HG23	2:B:325:GLN:N	2.30	0.45
2:B:487:THR:H	2:B:490:SER:HB3	1.79	0.45
2:B:558:LEU:C	2:B:560:GLU:N	2.70	0.45
2:B:782:LEU:HB3	2:B:784:ASN:OD1	2.16	0.45
3:C:91:HIS:HA	3:C:95:CYS:SG	2.56	0.45
4:D:191:ALA:O	4:D:193:THR:N	2.49	0.45
4:D:208:GLU:O	4:D:212:LYS:HG3	2.16	0.45
5:E:11:ARG:O	5:E:13:TRP:N	2.49	0.45
5:E:50:MET:HB3	5:E:52:ARG:NH1	2.32	0.45
9:I:82:GLU:C	9:I:104:LEU:HG	2.37	0.45
9:I:15:TYR:CD1	9:I:15:TYR:N	2.83	0.45
11:K:40:HIS:O	11:K:41:THR:C	2.55	0.45
13:T:10:DA:H2"	13:T:11:DA:OP2	2.16	0.45
1:A:1012:ARG:O	1:A:1013:ASP:C	2.54	0.45
1:A:996:ASN:HB3	1:A:1050:GLU:OE2	2.17	0.45
1:A:1100:ARG:NH2	1:A:1351:GLU:CG	2.72	0.45
1:A:1131:ALA:O	1:A:1132:LYS:C	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1313:LEU:CD2	1:A:1338:VAL:HG21	2.43	0.45
1:A:108:MET:SD	1:A:210:ILE:HD13	2.56	0.45
1:A:424:ILE:C	1:A:425:GLN:OE1	2.55	0.45
1:A:600:PRO:C	1:A:602:ASP:H	2.20	0.45
1:A:663:SER:OG	1:A:664:THR:N	2.48	0.45
1:A:896:ARG:NH2	1:A:1030:ARG:NE	2.55	0.45
2:B:131:ASP:HA	2:B:164:LYS:N	2.32	0.45
2:B:180:TYR:N	2:B:180:TYR:CD1	2.78	0.45
2:B:383:ASN:ND2	2:B:387:LEU:HD11	2.32	0.45
2:B:498:THR:HG22	2:B:498:THR:O	2.15	0.45
2:B:502:ILE:HG22	2:B:507:LYS:CG	2.47	0.45
2:B:503:GLY:HA3	2:B:507:LYS:CE	2.32	0.45
2:B:766:ARG:NH1	2:B:766:ARG:HG2	2.30	0.45
2:B:529:GLU:CD	2:B:769:TYR:HE1	2.18	0.45
2:B:880:THR:HB	2:B:934:LYS:HE3	1.95	0.45
6:F:116:ASP:OD1	6:F:119:ARG:HB2	2.17	0.45
7:G:94:CYS:HA	7:G:99:PHE:HA	1.98	0.45
8:H:58:THR:HG22	8:H:59:ILE:N	2.31	0.45
15:P:6:A:H2'	15:P:7:G:C8	2.51	0.45
15:P:6:A:H2'	15:P:7:G:H8	1.82	0.45
1:A:1176:LEU:O	1:A:1176:LEU:HD23	2.17	0.45
1:A:1441:PHE:HE1	6:F:92:ARG:HG2	1.81	0.45
1:A:254:GLU:O	1:A:255:SER:OG	2.32	0.45
1:A:402:ALA:HB1	1:A:434:ARG:HA	1.96	0.45
1:A:531:ILE:HG23	1:A:532:ARG:N	2.32	0.45
1:A:767:GLN:HE22	1:A:797:LYS:C	2.20	0.45
1:A:867:ILE:CG2	1:A:872:GLY:H	2.30	0.45
1:A:877:HIS:C	1:A:878:ILE:HG13	2.37	0.45
1:A:982:THR:C	1:A:984:LYS:N	2.66	0.45
2:B:186:GLU:HG3	10:J:62:ARG:HH22	1.80	0.45
2:B:20:ASP:C	2:B:22:SER:N	2.70	0.45
2:B:361:LEU:O	2:B:363:HIS:O	2.35	0.45
2:B:408:LEU:HA	2:B:408:LEU:HD12	1.74	0.45
2:B:975:GLN:HG2	2:B:976:ILE:H	1.82	0.45
3:C:6:PRO:HB3	3:C:25:VAL:HG12	1.98	0.45
3:C:77:ILE:C	3:C:79:GLN:H	2.20	0.45
4:D:136:GLY:C	4:D:138:ASN:H	2.20	0.45
4:D:210:ILE:HG13	4:D:210:ILE:H	1.42	0.45
5:E:22:MET:CE	5:E:26:ARG:NH1	2.64	0.45
6:F:93:ILE:CD1	6:F:148:VAL:HG12	2.47	0.45
7:G:92:VAL:CG2	7:G:102:GLN:HB2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:50:THR:HG22	9:I:52:ILE:H	1.81	0.45
9:I:90:GLN:NE2	9:I:92:ARG:HD2	2.31	0.45
1:A:11:LEU:HD22	2:B:1195:HIS:CD2	2.52	0.45
1:A:1140:HIS:N	1:A:1275:GLY:HA3	2.32	0.45
1:A:1427:ASN:O	1:A:1431:GLY:N	2.47	0.45
1:A:418:SER:O	1:A:420:ARG:N	2.45	0.45
1:A:700:ASN:HD22	9:I:115:LYS:HD2	1.81	0.45
2:B:1081:LEU:O	2:B:1083:ALA:O	2.34	0.45
2:B:199:MET:N	2:B:199:MET:SD	2.88	0.45
2:B:290:GLY:HA2	2:B:327:ARG:HD2	1.98	0.45
2:B:38:PHE:HD1	2:B:811:TYR:HD2	1.60	0.45
2:B:806:THR:HG21	2:B:808:ALA:HB3	1.99	0.45
2:B:806:THR:HG22	2:B:807:ARG:N	2.32	0.45
2:B:876:LYS:HD2	2:B:893:LEU:O	2.17	0.45
3:C:64:ALA:HA	3:C:67:LEU:HD12	1.97	0.45
1:A:7:SER:O	4:D:1:MET:HG3	2.17	0.45
4:D:8:PHE:HD2	7:G:6:ASP:O	1.99	0.45
5:E:45:LYS:HD3	5:E:46:TYR:HE1	1.81	0.45
6:F:116:ASP:OD1	6:F:119:ARG:N	2.50	0.45
7:G:111:THR:O	7:G:112:LYS:C	2.55	0.45
7:G:27:LYS:HG2	7:G:54:ILE:HD12	1.98	0.45
9:I:34:TYR:C	9:I:34:TYR:CD2	2.89	0.45
1:A:1194:ARG:HG3	1:A:1237:ILE:CG2	2.46	0.45
1:A:1350:LYS:O	1:A:1354:ASN:ND2	2.50	0.45
1:A:1436:ILE:O	1:A:1439:GLY:N	2.39	0.45
1:A:1444:MET:HG3	7:G:60:ARG:CA	2.41	0.45
1:A:350:ARG:O	1:A:351:THR:HG22	2.17	0.45
1:A:786:HIS:CE1	2:B:705:MET:SD	3.10	0.45
1:A:794:PRO:C	1:A:796:SER:H	2.20	0.45
1:A:345:VAL:CG2	2:B:1150:ARG:HH22	2.29	0.45
2:B:541:LEU:HB2	2:B:747:MET:HE3	1.99	0.45
2:B:638:PHE:HB2	2:B:741:CYS:HB3	1.99	0.45
2:B:906:SER:O	2:B:907:GLY:O	2.33	0.45
3:C:241:ASP:O	3:C:245:VAL:HG22	2.16	0.45
5:E:78:LEU:HD23	5:E:78:LEU:C	2.37	0.45
6:F:82:THR:HA	6:F:83:PRO:HD3	1.71	0.45
2:B:785:TYR:HE2	10:J:60:PHE:CE1	2.35	0.45
12:L:60:ARG:HG2	12:L:61:THR:N	2.32	0.45
1:A:134:ARG:C	1:A:136:ALA:H	2.20	0.45
1:A:323:LYS:N	1:A:323:LYS:HD2	2.30	0.45
1:A:369:SER:HB2	11:K:2:ASN:OD1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:MET:HB2	1:A:50:ILE:H	1.82	0.45
1:A:665:GLY:C	1:A:666:ILE:HD12	2.37	0.45
2:B:1159:ARG:HD3	2:B:1193:GLN:HG3	1.97	0.45
2:B:100:PRO:CG	2:B:180:TYR:HE1	2.30	0.45
2:B:383:ASN:O	2:B:385:LEU:N	2.49	0.45
2:B:529:GLU:CD	2:B:769:TYR:CE1	2.91	0.45
2:B:547:VAL:HG13	2:B:548:GLY:H	1.82	0.45
2:B:29:ASP:HB3	2:B:658:ILE:CD1	2.46	0.45
3:C:33:LEU:O	3:C:34:ARG:C	2.54	0.45
5:E:180:ARG:HB2	5:E:215:MET:OXT	2.16	0.45
5:E:74:ASP:N	5:E:74:ASP:OD1	2.49	0.45
7:G:14:HIS:ND1	7:G:15:PRO:CD	2.80	0.45
7:G:27:LYS:HD3	7:G:51:TYR:CE2	2.52	0.45
8:H:98:TYR:CE1	8:H:139:ASN:HA	2.51	0.45
11:K:10:PHE:CD2	11:K:10:PHE:N	2.84	0.45
11:K:49:GLU:HA	11:K:52:ASN:ND2	2.31	0.45
1:A:1167:GLU:O	1:A:1170:ILE:HG13	2.17	0.45
1:A:1175:SER:O	1:A:1176:LEU:CB	2.59	0.45
1:A:1161:THR:OG1	1:A:1239:ARG:NH2	2.50	0.45
1:A:1437:GLY:C	1:A:1439:GLY:H	2.21	0.45
1:A:21:LEU:CD1	1:A:229:SER:HB2	2.47	0.45
1:A:306:ASN:HB2	1:A:324:SER:HB3	1.98	0.45
1:A:608:ILE:HD12	1:A:613:ILE:CD1	2.47	0.45
1:A:645:LEU:CG	1:A:649:ILE:HD11	2.47	0.45
1:A:647:GLY:O	1:A:651:LYS:HG3	2.17	0.45
1:A:675:THR:O	1:A:675:THR:HG22	2.17	0.45
2:B:826:ALA:O	2:B:1011:ILE:HA	2.17	0.45
2:B:1034:VAL:O	2:B:1037:LEU:N	2.36	0.45
1:A:29:ALA:HB1	2:B:1184:GLY:HA3	1.98	0.45
2:B:266:ALA:C	2:B:268:THR:H	2.20	0.45
2:B:274:PRO:C	2:B:276:ILE:H	2.20	0.45
2:B:304:ASP:OD1	2:B:306:ASN:N	2.51	0.45
2:B:570:VAL:HA	2:B:571:PRO:HD2	1.85	0.45
2:B:593:PRO:CA	2:B:596:LEU:HB3	2.46	0.45
2:B:641:GLU:HB2	2:B:643:ASP:CG	2.37	0.45
3:C:80:LEU:O	3:C:80:LEU:HG	2.16	0.45
4:D:124:GLU:O	4:D:128:VAL:HG23	2.17	0.45
7:G:39:THR:HG22	7:G:40:GLY:H	1.82	0.45
9:I:68:LEU:HB3	9:I:84:VAL:HG23	1.99	0.45
11:K:49:GLU:HG3	11:K:94:ILE:CG1	2.47	0.45
12:L:26:THR:HG23	12:L:62:LYS:HZ1	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:44:ASP:O	12:L:45:ALA:CB	2.65	0.45
13:T:12:DG:N2	14:N:6:DT:C2	2.85	0.45
13:T:25:DG:H2"	13:T:26:DT:C5'	2.47	0.45
1:A:1341:ILE:CG2	1:A:1342:GLU:H	2.29	0.44
1:A:1447:GLU:O	1:A:1448:GLU:C	2.56	0.44
1:A:288:ALA:HA	1:A:291:GLU:CD	2.37	0.44
1:A:364:VAL:O	1:A:364:VAL:HG13	2.17	0.44
1:A:41:MET:CE	1:A:42:ASP:HB2	2.47	0.44
1:A:608:ILE:C	1:A:610:GLY:H	2.19	0.44
1:A:661:GLY:O	1:A:662:PHE:HB2	2.16	0.44
1:A:871:ASP:O	1:A:873:MET:N	2.50	0.44
2:B:451:LYS:O	2:B:452:THR:C	2.55	0.44
2:B:789:MET:HE2	2:B:953:LEU:HD21	1.98	0.44
2:B:814:PHE:C	2:B:816:GLU:N	2.68	0.44
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.99	0.44
3:C:220:ASP:OD1	3:C:223:ALA:N	2.50	0.44
3:C:239:PRO:O	3:C:241:ASP:N	2.50	0.44
4:D:185:CYS:CB	4:D:211:LEU:HD21	2.47	0.44
5:E:11:ARG:C	5:E:13:TRP:H	2.20	0.44
5:E:84:ASP:O	5:E:86:PRO:HD3	2.17	0.44
5:E:92:THR:HG22	5:E:92:THR:O	2.17	0.44
8:H:128:ASN:O	8:H:128:ASN:OD1	2.35	0.44
1:A:567:LYS:CB	8:H:96:VAL:H	2.26	0.44
1:A:1151:GLU:HG2	9:I:45:ARG:CB	2.47	0.44
3:C:114:TYR:OH	10:J:19:GLU:OE1	2.34	0.44
10:J:3:VAL:HG21	10:J:18:TRP:CB	2.47	0.44
12:L:40:LEU:HB3	12:L:41:SER:H	1.56	0.44
1:A:1383:SER:O	1:A:1388:GLY:HA3	2.17	0.44
1:A:186:LYS:O	1:A:187:LYS:HB3	2.16	0.44
1:A:618:GLU:O	1:A:621:THR:N	2.44	0.44
1:A:722:LEU:HB3	1:A:799:PHE:CE1	2.52	0.44
1:A:853:ASP:OD1	1:A:855:THR:HG22	2.17	0.44
1:A:968:GLN:O	1:A:970:THR:N	2.51	0.44
2:B:1201:LYS:HE2	2:B:1205:GLN:HE22	1.80	0.44
2:B:318:VAL:O	2:B:320:ASP:N	2.50	0.44
2:B:335:GLY:HA3	2:B:348:ARG:HB2	1.99	0.44
2:B:693:ILE:HD11	2:B:740:HIS:CD2	2.52	0.44
2:B:701:ILE:HB	2:B:739:THR:OG1	2.17	0.44
2:B:986:GLN:OE1	2:B:986:GLN:HA	2.18	0.44
2:B:980:PHE:HE1	2:B:990:ILE:HD11	1.82	0.44
3:C:173:ALA:O	3:C:174:ALA:CB	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:6:PRO:HB3	3:C:25:VAL:CG1	2.47	0.44
5:E:13:TRP:CH2	5:E:39:LEU:HB2	2.52	0.44
6:F:97:ARG:HG3	6:F:124:GLU:OE1	2.17	0.44
6:F:69:LEU:C	6:F:71:GLU:H	2.21	0.44
9:I:33:SER:O	9:I:34:TYR:C	2.55	0.44
10:J:2:ILE:HG23	10:J:3:VAL:O	2.18	0.44
11:K:29:ASN:O	11:K:76:GLN:HG3	2.16	0.44
1:A:1220:PHE:O	1:A:1221:LYS:CB	2.65	0.44
1:A:1404:GLU:HB2	1:A:1408:ILE:CD1	2.40	0.44
1:A:1409:LEU:O	1:A:1412:ALA:HB3	2.17	0.44
1:A:47:ARG:O	1:A:48:ALA:HB2	2.17	0.44
1:A:666:ILE:HD11	2:B:1086:PHE:HE1	1.83	0.44
1:A:683:ILE:O	1:A:686:ALA:N	2.44	0.44
1:A:700:ASN:HB2	9:I:98:VAL:CG2	2.48	0.44
1:A:770:VAL:O	1:A:771:GLU:HB2	2.16	0.44
1:A:858:ASN:ND2	1:A:860:LEU:H	2.15	0.44
2:B:172:ILE:HG22	2:B:173:MET:O	2.17	0.44
2:B:516:ASN:C	2:B:518:HIS:H	2.20	0.44
2:B:827:ILE:O	2:B:828:ALA:CB	2.61	0.44
3:C:181:ASP:OD2	3:C:185:LYS:N	2.50	0.44
3:C:258:ILE:N	3:C:258:ILE:HD12	2.32	0.44
4:D:22:GLU:OE1	4:D:22:GLU:N	2.38	0.44
5:E:212:ARG:NH1	5:E:212:ARG:CG	2.78	0.44
5:E:26:ARG:HG2	5:E:28:TYR:HE1	1.82	0.44
6:F:85:MET:CB	6:F:155:LEU:HD11	2.46	0.44
7:G:138:THR:O	7:G:139:ILE:C	2.56	0.44
7:G:163:ILE:HA	7:G:168:LEU:HD13	2.00	0.44
11:K:21:ILE:HG22	11:K:31:VAL:HG12	1.98	0.44
12:L:47:ARG:HG2	12:L:54:ARG:HG2	1.99	0.44
14:N:5:DC:H2'	14:N:6:DT:H72	1.98	0.44
1:A:1159:ARG:HD3	1:A:1174:PHE:HZ	1.81	0.44
1:A:116:ASP:C	1:A:118:HIS:N	2.68	0.44
1:A:119:ASN:O	1:A:122:MET:HB3	2.17	0.44
1:A:1392:SER:C	1:A:1394:THR:H	2.21	0.44
1:A:16:GLU:CD	2:B:1220:ARG:HA	2.37	0.44
1:A:6:TYR:CE1	4:D:1:MET:HG3	2.52	0.44
1:A:75:ASN:O	1:A:76:GLU:HB2	2.18	0.44
1:A:843:LYS:HA	1:A:843:LYS:HD3	1.82	0.44
1:A:879:GLU:OE2	1:A:959:ASN:ND2	2.48	0.44
2:B:1001:PHE:CD2	3:C:34:ARG:NH2	2.85	0.44
2:B:312:GLU:O	2:B:315:LYS:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:425:THR:O	2:B:428:ILE:HD12	2.17	0.44
1:A:315:LEU:HD13	2:B:471:LYS:O	2.18	0.44
2:B:953:LEU:HB3	12:L:57:LEU:CD2	2.47	0.44
3:C:143:LEU:HD21	3:C:146:LYS:HE3	1.99	0.44
4:D:167:LEU:O	4:D:169:SER:N	2.50	0.44
4:D:176:GLU:C	4:D:178:ALA:N	2.71	0.44
5:E:49:SER:C	5:E:50:MET:HE2	2.38	0.44
7:G:63:PRO:HG2	7:G:64:THR:H	1.82	0.44
9:I:22:ASN:O	9:I:23:ASN:HB2	2.15	0.44
12:L:40:LEU:CD1	12:L:44:ASP:HB3	2.28	0.44
1:A:1107:VAL:CG1	1:A:1107:VAL:O	2.63	0.44
1:A:1120:LEU:CD1	1:A:1120:LEU:H	2.29	0.44
1:A:1125:ALA:C	1:A:1127:ASP:N	2.70	0.44
1:A:130:ASP:C	1:A:132:LYS:H	2.21	0.44
1:A:134:ARG:CG	1:A:138:ILE:HD11	2.37	0.44
1:A:106:VAL:HG21	1:A:214:ILE:HD13	2.00	0.44
1:A:280:GLU:O	1:A:282:ASN:N	2.50	0.44
1:A:34:LYS:N	1:A:34:LYS:HD3	2.33	0.44
1:A:734:GLU:C	1:A:736:ASN:N	2.70	0.44
1:A:914:GLU:C	1:A:916:GLY:H	2.21	0.44
2:B:1107:ALA:O	2:B:1108:ARG:O	2.36	0.44
2:B:1200:ALA:HA	2:B:1203:LEU:HB3	1.99	0.44
2:B:401:PHE:HB2	2:B:517:THR:OG1	2.17	0.44
2:B:615:MET:O	2:B:615:MET:CE	2.66	0.44
2:B:784:ASN:O	2:B:788:ARG:HG3	2.17	0.44
2:B:827:ILE:HD12	2:B:1086:PHE:HD2	1.83	0.44
3:C:77:ILE:HG23	3:C:161:LYS:HZ2	1.81	0.44
3:C:268:ASP:O	3:C:269:LYS:CB	2.65	0.44
3:C:83:SER:OG	3:C:160:LYS:HD3	2.18	0.44
5:E:55:ARG:O	5:E:57:MET:N	2.51	0.44
7:G:91:VAL:HA	7:G:101:VAL:HA	2.00	0.44
7:G:26:LEU:HA	7:G:26:LEU:HD23	1.85	0.44
7:G:39:THR:HB	7:G:42:PHE:H	1.83	0.44
7:G:41:LYS:HD3	7:G:42:PHE:CE1	2.52	0.44
8:H:77:ARG:O	8:H:78:SER:O	2.34	0.44
9:I:100:PHE:N	9:I:100:PHE:HD1	2.15	0.44
9:I:83:ASN:OD1	9:I:103:CYS:HA	2.17	0.44
1:A:1217:LYS:O	1:A:1221:LYS:N	2.50	0.44
1:A:500:GLU:OE1	2:B:1143:ALA:C	2.56	0.44
1:A:608:ILE:CG1	1:A:613:ILE:HD11	2.47	0.44
1:A:7:SER:OG	2:B:1193:GLN:NE2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:811:GLN:O	1:A:812:GLU:C	2.55	0.44
2:B:1142:GLY:HA3	6:F:88:TYR:CE2	2.46	0.44
2:B:129:PHE:CE2	2:B:166:PHE:HD1	2.36	0.44
2:B:304:ASP:OD1	2:B:306:ASN:HB2	2.17	0.44
2:B:426:LYS:O	2:B:429:PHE:HB2	2.18	0.44
2:B:516:ASN:C	2:B:518:HIS:N	2.71	0.44
2:B:522:VAL:HG12	2:B:523:CYS:N	2.33	0.44
2:B:797:TYR:HE2	3:C:62:PHE:HA	1.82	0.44
1:A:472:LEU:HD11	2:B:835:GLN:NE2	2.33	0.44
2:B:797:TYR:CE1	2:B:971:THR:HG23	2.48	0.44
3:C:181:ASP:OD2	3:C:186:LEU:HD13	2.18	0.44
4:D:115:HIS:CD2	4:D:115:HIS:H	2.36	0.44
5:E:159:ASP:HA	5:E:162:ARG:HH22	1.80	0.44
5:E:202:SER:C	5:E:204:THR:H	2.19	0.44
5:E:83:CYS:C	5:E:85:GLU:N	2.70	0.44
10:J:20:SER:O	10:J:24:LEU:HG	2.18	0.44
10:J:24:LEU:HD12	10:J:39:LEU:CD1	2.44	0.44
10:J:24:LEU:CD1	10:J:39:LEU:HD11	2.45	0.44
2:B:798:TYR:HE1	10:J:4:PRO:HA	1.83	0.44
12:L:40:LEU:HD11	12:L:49:LYS:NZ	2.32	0.44
1:A:1100:ARG:HH12	1:A:1111:MET:CE	2.30	0.44
1:A:1141:THR:CB	1:A:1205:LYS:HZ3	2.31	0.44
1:A:1329:THR:HG22	1:A:1335:ILE:HG13	2.00	0.44
1:A:1381:LEU:HA	1:A:1381:LEU:HD23	1.71	0.44
1:A:108:MET:CE	1:A:210:ILE:HD13	2.48	0.44
1:A:447:GLN:H	1:A:447:GLN:HG3	1.55	0.44
1:A:492:PRO:HB3	1:A:501:LEU:HD11	1.99	0.44
1:A:49:LYS:HZ2	1:A:60:SER:HA	1.82	0.44
1:A:693:VAL:HG21	1:A:721:PHE:HE1	1.83	0.44
1:A:79:GLY:HA3	1:A:243:PRO:HG2	1.96	0.44
2:B:1080:LYS:HD2	3:C:188:HIS:CB	2.46	0.44
2:B:825:VAL:HG21	2:B:1092:TYR:CE1	2.53	0.44
2:B:1167:GLY:CA	2:B:1216:LEU:H	2.30	0.44
2:B:276:ILE:O	2:B:276:ILE:HG22	2.18	0.44
2:B:53:GLN:HG2	2:B:547:VAL:HG23	2.00	0.44
2:B:541:LEU:HB2	2:B:747:MET:CE	2.48	0.44
2:B:650:GLU:HG3	2:B:651:LEU:N	2.32	0.44
2:B:791:THR:O	2:B:792:MET:CB	2.66	0.44
2:B:871:THR:HG22	2:B:872:GLU:N	2.32	0.44
2:B:903:VAL:CG1	2:B:904:ARG:N	2.79	0.44
3:C:22:LEU:HD23	3:C:22:LEU:C	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:72:LEU:O	3:C:237:SER:HB3	2.17	0.44
4:D:130:LEU:C	4:D:132:GLN:N	2.71	0.44
4:D:40:HIS:HD2	7:G:73:LYS:HG3	1.81	0.44
4:D:56:ARG:HH21	4:D:155:ARG:HA	1.79	0.44
5:E:137:GLU:C	5:E:139:ALA:H	2.21	0.44
1:A:857:ARG:CZ	6:F:139:PRO:HB2	2.47	0.44
7:G:92:VAL:HG21	7:G:102:GLN:HB2	1.99	0.44
8:H:64:ASN:ND2	8:H:88:SER:O	2.50	0.44
8:H:82:PRO:HG2	8:H:83:GLN:H	1.82	0.44
1:A:1208:THR:HG22	1:A:1210:GLY:N	2.32	0.44
1:A:1220:PHE:CD1	1:A:1224:LEU:HD23	2.53	0.44
1:A:1244:ARG:CB	1:A:1245:PRO:CA	2.89	0.44
1:A:1293:SER:O	1:A:1294:PRO:C	2.54	0.44
1:A:203:SER:OG	1:A:206:GLU:HB2	2.18	0.44
1:A:258:GLY:O	1:A:259:GLU:O	2.36	0.44
1:A:446:ARG:HB3	1:A:478:TYR:HB3	1.99	0.44
1:A:532:ARG:HG2	1:A:532:ARG:NH1	2.33	0.44
1:A:910:PRO:HB3	1:A:917:SER:N	2.33	0.44
1:A:982:THR:HB	1:A:985:ASP:H	1.83	0.44
2:B:132:VAL:H	2:B:164:LYS:N	2.16	0.44
2:B:40:GLU:OE1	2:B:682:SER:HB2	2.17	0.44
2:B:620:ARG:HD2	9:I:68:LEU:HD11	1.99	0.44
2:B:758:PHE:HB3	2:B:761:HIS:HD2	1.82	0.44
2:B:846:ILE:HG23	2:B:974:PRO:HG2	2.00	0.44
4:D:166:LEU:HG	4:D:167:LEU:HD23	2.00	0.44
5:E:93:MET:C	5:E:95:THR:N	2.71	0.44
6:F:94:LEU:CD2	6:F:122:MET:HA	2.46	0.44
9:I:86:PHE:HE1	9:I:100:PHE:HB2	1.80	0.44
9:I:76:PRO:HG2	9:I:110:PHE:HB3	1.99	0.44
1:A:1265:ASN:O	1:A:1267:MET:N	2.51	0.44
1:A:320:ARG:HG2	1:A:322:VAL:H	1.83	0.44
1:A:332:LYS:HG3	1:A:333:GLU:HG2	2.00	0.44
1:A:496:GLU:O	1:A:499:ALA:HB3	2.18	0.44
1:A:994:GLN:HG2	1:A:1022:LEU:HD23	2.00	0.44
2:B:1064:TYR:O	2:B:1065:GLN:C	2.56	0.44
2:B:188:ASP:O	2:B:192:LEU:HD12	2.18	0.44
2:B:346:GLU:HG2	2:B:347:LYS:N	2.32	0.44
2:B:410:GLY:O	2:B:411:PRO:C	2.56	0.44
2:B:210:LYS:HE2	2:B:461:LEU:O	2.17	0.44
2:B:616:ILE:CD1	2:B:625:LYS:HB2	2.48	0.44
2:B:766:ARG:HH21	2:B:1020:ARG:HG2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:88:CYS:SG	3:C:91:HIS:CA	3.06	0.44
4:D:64:VAL:C	4:D:66:ARG:H	2.21	0.44
5:E:108:GLY:O	5:E:132:ILE:HG22	2.18	0.44
5:E:42:PHE:O	5:E:43:LYS:C	2.56	0.44
5:E:90:VAL:HA	5:E:93:MET:HB2	1.99	0.44
8:H:40:LEU:CD2	8:H:123:MET:HE3	2.31	0.44
1:A:1377:THR:OG1	1:A:1378:GLN:N	2.51	0.43
1:A:15:LYS:O	1:A:1420:ASP:O	2.35	0.43
1:A:262:LEU:CD2	1:A:303:TYR:CE1	3.01	0.43
1:A:543:LEU:CD1	1:A:547:LEU:HG	2.48	0.43
1:A:71:GLN:CG	1:A:72:GLU:N	2.80	0.43
2:B:257:LYS:N	2:B:270:LYS:O	2.51	0.43
2:B:224:GLN:HA	2:B:396:ASP:OD2	2.18	0.43
3:C:20:PHE:CE1	3:C:230:MET:HB2	2.52	0.43
1:A:1157:ASP:O	1:A:1159:ARG:N	2.51	0.43
1:A:1194:ARG:HG3	1:A:1237:ILE:HG23	2.00	0.43
1:A:276:LEU:HD11	1:A:293:GLU:HB2	2.00	0.43
1:A:377:PRO:HD3	1:A:493:GLN:OE1	2.18	0.43
1:A:384:ASN:HB3	1:A:387:ARG:HH21	1.82	0.43
1:A:595:THR:C	1:A:596:THR:HG23	2.38	0.43
1:A:71:GLN:HG3	1:A:72:GLU:N	2.32	0.43
1:A:784:LEU:HD11	1:A:815:PHE:CE2	2.53	0.43
1:A:883:LEU:CD2	1:A:1021:LEU:HB2	2.48	0.43
1:A:943:LEU:C	1:A:945:GLU:H	2.20	0.43
2:B:825:VAL:CG2	2:B:1010:LEU:HD23	2.48	0.43
2:B:1063:GLY:O	3:C:202:PRO:HG2	2.18	0.43
2:B:1098:MET:O	2:B:1099:VAL:C	2.55	0.43
2:B:1202:LEU:C	2:B:1206:GLU:HG3	2.37	0.43
2:B:205:ILE:HG12	2:B:461:LEU:HB3	2.00	0.43
2:B:258:LEU:O	2:B:259:TYR:O	2.36	0.43
2:B:446:LEU:O	2:B:447:ALA:CB	2.66	0.43
2:B:562:GLY:HA3	2:B:590:HIS:CE1	2.53	0.43
2:B:570:VAL:CG2	2:B:573:GLN:HB3	2.48	0.43
2:B:615:MET:HE2	2:B:697:GLU:CD	2.38	0.43
1:A:658:LEU:HD12	2:B:830:TYR:CD1	2.53	0.43
2:B:865:LYS:CG	2:B:961:LEU:HD21	2.46	0.43
5:E:204:THR:CG2	5:E:205:SER:N	2.79	0.43
7:G:112:LYS:HE3	7:G:113:HIS:CE1	2.53	0.43
8:H:129:TYR:C	8:H:130:ARG:HD2	2.38	0.43
8:H:56:THR:HB	8:H:145:ARG:HG2	2.00	0.43
1:A:1005:GLU:O	1:A:1009:ASN:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:VAL:C	1:A:114:LEU:HD21	2.38	0.43
1:A:353:ILE:HD13	1:A:487:MET:CE	2.45	0.43
1:A:481:ASP:OD1	1:A:485:ASP:OD2	2.37	0.43
2:B:1084:GLN:OE1	3:C:189:THR:HG22	2.18	0.43
2:B:1116:ARG:HD2	2:B:1198:TYR:CD1	2.53	0.43
2:B:46:GLN:CG	2:B:47:GLN:H	2.31	0.43
2:B:827:ILE:O	2:B:1085:ILE:CG2	2.66	0.43
2:B:843:GLN:NE2	2:B:847:ASP:OD1	2.43	0.43
2:B:865:LYS:HE3	2:B:961:LEU:CD2	2.49	0.43
3:C:77:ILE:C	3:C:79:GLN:N	2.72	0.43
4:D:9:GLN:HE22	4:D:31:GLN:HG2	1.83	0.43
6:F:119:ARG:HG3	6:F:119:ARG:NH1	2.33	0.43
8:H:144:ILE:CG2	8:H:145:ARG:N	2.81	0.43
8:H:24:CYS:HB2	8:H:44:VAL:CG2	2.46	0.43
9:I:7:CYS:HB2	9:I:34:TYR:CD2	2.53	0.43
11:K:22:ASP:O	11:K:31:VAL:HG13	2.18	0.43
1:A:1011:GLN:HE21	1:A:1015:VAL:HG21	1.82	0.43
1:A:1258:HIS:O	1:A:1262:LYS:HG3	2.18	0.43
1:A:1308:THR:CG2	1:A:1310:GLY:O	2.65	0.43
1:A:1450:LEU:CD1	6:F:108:PHE:CZ	3.01	0.43
1:A:17:VAL:HG23	1:A:1421:CYS:SG	2.58	0.43
1:A:877:HIS:O	1:A:878:ILE:HG12	2.17	0.43
1:A:877:HIS:O	1:A:878:ILE:CG1	2.66	0.43
2:B:1040:ASN:O	2:B:1041:GLU:C	2.57	0.43
2:B:1106:ARG:HD2	2:B:1125:ASP:O	2.17	0.43
2:B:1150:ARG:NH1	2:B:1150:ARG:CG	2.70	0.43
2:B:38:PHE:O	2:B:39:ARG:C	2.56	0.43
2:B:510:LYS:CB	2:B:511:PRO:CD	2.96	0.43
2:B:660:LYS:C	2:B:679:TYR:HD2	2.22	0.43
2:B:766:ARG:NH1	2:B:769:TYR:HE2	2.16	0.43
2:B:890:TYR:CZ	2:B:910:VAL:HG21	2.54	0.43
2:B:766:ARG:HD2	2:B:984:HIS:O	2.18	0.43
3:C:66:ARG:NH1	3:C:144:ILE:O	2.51	0.43
4:D:52:LEU:N	4:D:182:SER:HB3	2.34	0.43
5:E:93:MET:HG3	5:E:94:LYS:N	2.33	0.43
8:H:109:LYS:HD2	8:H:111:LEU:CD1	2.45	0.43
8:H:15:VAL:HG22	8:H:26:ILE:HG21	1.99	0.43
12:L:52:GLY:O	12:L:54:ARG:N	2.51	0.43
1:A:999:VAL:HG12	1:A:1000:LEU:HG	1.99	0.43
1:A:1105:LEU:CD2	1:A:1384:VAL:HG21	2.48	0.43
1:A:1124:HIS:ND1	1:A:1124:HIS:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1225:PHE:O	1:A:1240:CYS:CB	2.67	0.43
1:A:299:HIS:HA	1:A:302:THR:HG22	2.00	0.43
1:A:353:ILE:HG13	1:A:353:ILE:O	2.17	0.43
1:A:573:SER:O	1:A:574:GLY:C	2.57	0.43
1:A:715:GLU:OE2	1:A:774:ARG:NH1	2.51	0.43
1:A:777:PHE:C	1:A:779:PHE:N	2.71	0.43
1:A:779:PHE:CE1	1:A:785:PRO:HD3	2.37	0.43
1:A:783:THR:HB	1:A:787:PHE:HD1	1.84	0.43
1:A:885:THR:CG2	1:A:885:THR:O	2.60	0.43
1:A:923:LEU:O	1:A:927:VAL:HG23	2.18	0.43
2:B:1174:LYS:O	2:B:1175:LEU:C	2.56	0.43
2:B:23:ALA:O	2:B:654:ARG:HD2	2.19	0.43
2:B:595:ARG:NH1	2:B:595:ARG:HG3	2.33	0.43
2:B:658:ILE:HG22	2:B:659:ALA:N	2.33	0.43
2:B:705:MET:CE	2:B:705:MET:HA	2.49	0.43
2:B:526:GLU:CD	2:B:752:ALA:HB3	2.39	0.43
2:B:846:ILE:CG2	2:B:974:PRO:HG2	2.49	0.43
3:C:143:LEU:HD21	3:C:146:LYS:CE	2.48	0.43
4:D:202:ILE:HD11	4:D:206:GLU:OE1	2.19	0.43
7:G:122:ASN:HB3	7:G:129:SER:OG	2.18	0.43
4:D:138:ASN:ND2	7:G:35:GLU:HB3	2.33	0.43
7:G:51:TYR:O	7:G:51:TYR:CD2	2.71	0.43
9:I:7:CYS:CB	9:I:14:LEU:HD21	2.41	0.43
9:I:2:THR:CG2	9:I:3:THR:N	2.80	0.43
14:N:10:DG:H2"	14:N:11:DC:OP2	2.18	0.43
1:A:1154:TYR:CE2	1:A:1156:PRO:HD3	2.53	0.43
1:A:1223:ASP:HA	1:A:1243:VAL:CG1	2.47	0.43
1:A:125:ALA:C	1:A:127:ALA:N	2.72	0.43
1:A:115:LEU:CD1	1:A:141:LEU:HB3	2.49	0.43
1:A:172:PRO:HB2	1:A:183:GLY:HA3	2.00	0.43
1:A:49:LYS:CD	1:A:55:ASP:HB3	2.48	0.43
1:A:909:ASP:C	1:A:911:SER:H	2.21	0.43
1:A:961:ARG:HG3	1:A:961:ARG:NH1	2.34	0.43
2:B:1116:ARG:HG3	2:B:1198:TYR:CD2	2.54	0.43
2:B:192:LEU:C	2:B:194:GLU:H	2.22	0.43
2:B:785:TYR:HD2	2:B:785:TYR:H	1.66	0.43
2:B:800:GLN:HB2	2:B:821:GLN:HA	2.01	0.43
2:B:867:GLY:O	2:B:869:SER:N	2.46	0.43
3:C:186:LEU:O	3:C:187:LYS:HB2	2.19	0.43
3:C:41:ILE:CG2	3:C:172:PRO:HG3	2.49	0.43
3:C:55:THR:O	3:C:55:THR:HG22	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:73:PRO:HB2	5:E:74:ASP:H	1.66	0.43
7:G:111:THR:HG22	7:G:112:LYS:N	2.33	0.43
7:G:119:LEU:HD11	7:G:137:ILE:HD11	2.00	0.43
9:I:111:THR:HG22	9:I:113:ASP:N	2.32	0.43
12:L:48:CYS:O	12:L:50:ASP:N	2.44	0.43
1:A:1037:LEU:HD12	1:A:1042:PHE:CA	2.48	0.43
1:A:1425:SER:O	1:A:1426:GLU:C	2.57	0.43
1:A:289:ILE:C	1:A:291:GLU:N	2.71	0.43
1:A:342:GLY:O	2:B:1129:ARG:NH1	2.52	0.43
1:A:66:LYS:O	1:A:67:CYS:HB2	2.19	0.43
1:A:725:ALA:O	1:A:726:ARG:C	2.56	0.43
1:A:966:ASN:O	1:A:967:ALA:C	2.57	0.43
2:B:100:PRO:CD	2:B:180:TYR:HE1	2.31	0.43
2:B:23:ALA:O	2:B:654:ARG:HB3	2.18	0.43
2:B:261:ARG:HG3	2:B:261:ARG:NH1	2.33	0.43
2:B:29:ASP:OD1	2:B:658:ILE:HD13	2.17	0.43
2:B:328:GLU:C	2:B:330:ALA:N	2.71	0.43
2:B:37:PHE:CZ	2:B:41:LYS:HG3	2.54	0.43
2:B:784:ASN:ND2	2:B:788:ARG:HD2	2.33	0.43
2:B:996:ARG:HH21	3:C:175:ALA:HA	1.84	0.43
2:B:99:LYS:HA	2:B:178:ASN:ND2	2.32	0.43
3:C:146:LYS:HD2	10:J:57:ILE:HD13	2.00	0.43
3:C:148:ARG:CG	3:C:149:LYS:H	2.31	0.43
6:F:106:PRO:HG2	7:G:18:PHE:C	2.38	0.43
6:F:113:GLY:O	6:F:114:GLU:C	2.57	0.43
7:G:18:PHE:HA	7:G:22:MET:HE2	2.00	0.43
8:H:36:CYS:HB2	8:H:130:ARG:NH2	2.33	0.43
9:I:55:THR:HG1	9:I:100:PHE:HD2	1.62	0.43
10:J:35:ALA:O	10:J:39:LEU:CD1	2.67	0.43
12:L:39:SER:OG	12:L:40:LEU:N	2.51	0.43
1:A:1029:ARG:HG3	1:A:1029:ARG:NH1	2.34	0.43
1:A:1213:GLY:O	1:A:1216:ILE:N	2.51	0.43
1:A:1279:ILE:O	1:A:1280:GLU:HG3	2.19	0.43
1:A:101:LYS:HE2	1:A:139:TRP:CZ2	2.54	0.43
1:A:1418:LEU:HD23	2:B:1222:ARG:HD2	2.01	0.43
1:A:332:LYS:C	1:A:333:GLU:HG2	2.39	0.43
1:A:435:HIS:O	1:A:437:MET:HG3	2.19	0.43
1:A:458:HIS:CE1	1:A:507:VAL:HG21	2.53	0.43
1:A:541:ILE:HG21	1:A:549:MET:HE1	2.01	0.43
1:A:774:ARG:NH2	1:A:797:LYS:HB2	2.33	0.43
1:A:779:PHE:HD1	1:A:784:LEU:HA	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:855:THR:HG23	1:A:857:ARG:HG3	2.00	0.43
1:A:875:ALA:HA	1:A:878:ILE:HD12	2.01	0.43
1:A:997:LEU:HD13	1:A:1018:PHE:HE2	1.82	0.43
2:B:1122:ARG:HB3	13:T:22:DC:OP1	2.18	0.43
2:B:1167:GLY:HA3	2:B:1216:LEU:N	2.32	0.43
2:B:1178:ASN:HD22	2:B:1178:ASN:N	2.15	0.43
2:B:1197:PRO:C	2:B:1199:ALA:N	2.71	0.43
2:B:290:GLY:CA	2:B:327:ARG:HD2	2.48	0.43
2:B:277:LYS:HE3	2:B:338:GLY:O	2.18	0.43
2:B:340:ALA:C	2:B:342:GLY:H	2.21	0.43
2:B:361:LEU:HD21	2:B:364:ILE:HD12	1.99	0.43
2:B:492:LEU:O	2:B:495:LEU:N	2.51	0.43
2:B:642:ASP:C	2:B:644:GLU:H	2.22	0.43
2:B:872:GLU:HA	2:B:917:PRO:HD3	2.00	0.43
2:B:952:VAL:HG12	2:B:953:LEU:H	1.83	0.43
5:E:135:PHE:HD2	5:E:140:LEU:HD21	1.83	0.43
5:E:161:LYS:O	5:E:164:LEU:N	2.52	0.43
5:E:85:GLU:C	5:E:87:SER:N	2.71	0.43
8:H:4:THR:HA	8:H:60:ALA:CB	2.49	0.43
11:K:17:SER:O	11:K:18:LYS:C	2.56	0.43
1:A:1299:VAL:CG1	1:A:1300:LYS:N	2.82	0.43
1:A:1330:ASN:OD1	1:A:1331:SER:N	2.52	0.43
1:A:1343:ALA:HB2	5:E:150:VAL:CG2	2.41	0.43
1:A:279:LEU:O	1:A:289:ILE:HD11	2.19	0.43
1:A:409:SER:O	1:A:410:GLY:C	2.56	0.43
1:A:626:ASN:O	1:A:631:HIS:CD2	2.72	0.43
1:A:700:ASN:C	1:A:701:LEU:HD23	2.39	0.43
1:A:825:ILE:HA	1:A:825:ILE:HD12	1.70	0.43
2:B:1177:HIS:HB3	2:B:1179:GLN:HE21	1.83	0.43
2:B:186:GLU:HB3	2:B:187:SER:H	1.49	0.43
2:B:355:ILE:H	2:B:355:ILE:HG13	1.68	0.43
2:B:476:ARG:O	2:B:477:ALA:C	2.57	0.43
2:B:660:LYS:HB3	2:B:679:TYR:CD2	2.54	0.43
2:B:681:TRP:O	2:B:684:LEU:N	2.52	0.43
2:B:402:GLY:CA	2:B:695:ALA:HB3	2.49	0.43
4:D:64:VAL:HG22	4:D:129:LEU:CD2	2.49	0.43
5:E:137:GLU:C	5:E:139:ALA:N	2.72	0.43
5:E:15:ALA:HA	5:E:140:LEU:O	2.18	0.43
5:E:204:THR:CG2	5:E:205:SER:H	2.28	0.43
7:G:114:LEU:HA	7:G:114:LEU:HD12	1.89	0.43
8:H:40:LEU:HD13	8:H:123:MET:HE3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:CYS:C	1:A:144:THR:H	2.22	0.43
1:A:275:SER:O	1:A:279:LEU:HG	2.18	0.43
1:A:286:HIS:O	1:A:288:ALA:N	2.52	0.43
1:A:350:ARG:HB2	1:A:488:ASN:OD1	2.18	0.43
1:A:515:GLN:HB2	1:A:1071:SER:HB3	2.00	0.43
1:A:526:ASP:HB2	2:B:835:GLN:OE1	2.18	0.43
1:A:645:LEU:HG	1:A:649:ILE:CD1	2.48	0.43
1:A:826:ASP:O	1:A:830:LYS:N	2.37	0.43
1:A:899:VAL:O	1:A:929:LEU:HD12	2.19	0.43
2:B:1050:ILE:HG22	2:B:1051:THR:N	2.34	0.43
2:B:165:VAL:CG1	2:B:166:PHE:N	2.82	0.43
2:B:426:LYS:HG2	2:B:426:LYS:H	1.51	0.43
2:B:484:ASN:O	2:B:485:ARG:HD2	2.19	0.43
2:B:619:ILE:O	2:B:622:LYS:HG3	2.19	0.43
2:B:651:LEU:C	2:B:653:VAL:N	2.71	0.43
2:B:708:GLU:O	2:B:709:ASP:C	2.57	0.43
2:B:879:ARG:HA	2:B:879:ARG:HD3	1.46	0.43
3:C:136:ASP:OD1	3:C:137:LYS:N	2.52	0.43
3:C:17:ASN:H	3:C:240:VAL:HG21	1.84	0.43
3:C:35:ARG:HH11	11:K:41:THR:HA	1.83	0.43
3:C:3:GLU:HG3	11:K:104:ASN:ND2	2.34	0.43
4:D:13:ARG:O	4:D:13:ARG:CD	2.67	0.43
4:D:214:LEU:O	4:D:216:ASN:N	2.51	0.43
5:E:94:LYS:HE2	5:E:98:ILE:HD11	2.01	0.43
6:F:105:ALA:HB1	6:F:106:PRO:CD	2.49	0.43
7:G:44:TYR:HE1	7:G:157:ILE:N	2.16	0.43
9:I:13:MET:HE3	9:I:14:LEU:H	1.84	0.43
11:K:18:LYS:NZ	11:K:37:LYS:O	2.51	0.43
13:T:15:DC:C6	13:T:16:DT:H72	2.53	0.43
1:A:1451:VAL:O	1:A:1454:MET:HG2	2.19	0.42
1:A:460:VAL:HG12	1:A:461:LYS:N	2.34	0.42
1:A:536:LEU:O	1:A:537:ARG:C	2.58	0.42
1:A:555:ASP:O	1:A:556:TRP:C	2.56	0.42
1:A:596:THR:C	1:A:597:LEU:HD12	2.38	0.42
1:A:728:LYS:HA	1:A:731:ARG:HE	1.84	0.42
1:A:869:GLY:O	1:A:870:GLU:HB2	2.19	0.42
1:A:998:LEU:H	1:A:998:LEU:CD1	2.29	0.42
2:B:1020:ARG:HG3	2:B:1020:ARG:NH1	2.32	0.42
2:B:1146:PHE:CE1	2:B:1150:ARG:HD3	2.54	0.42
2:B:282:ILE:CD1	2:B:382:ILE:HD13	2.48	0.42
2:B:61:ASP:O	2:B:64:CYS:O	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:GLU:CG	2:B:66:ASP:H	2.25	0.42
2:B:637:LEU:CD1	2:B:703:ILE:HD13	2.48	0.42
2:B:860:MET:HG2	2:B:861:ASP:N	2.33	0.42
2:B:871:THR:CG2	2:B:872:GLU:N	2.81	0.42
2:B:773:MET:HE2	2:B:985:GLY:HA2	2.00	0.42
4:D:39:ASN:HB3	4:D:43:GLU:O	2.19	0.42
4:D:52:LEU:H	4:D:182:SER:HB3	1.84	0.42
6:F:85:MET:CE	6:F:93:ILE:HD12	2.49	0.42
7:G:116:PRO:HB2	7:G:118:ASP:OD1	2.19	0.42
7:G:84:GLY:N	7:G:147:ILE:O	2.47	0.42
10:J:2:ILE:HG12	10:J:57:ILE:CD1	2.48	0.42
12:L:36:SER:O	12:L:37:LYS:O	2.37	0.42
1:A:103:CYS:HB3	1:A:174:ILE:CD1	2.49	0.42
1:A:15:LYS:O	1:A:1421:CYS:HB2	2.19	0.42
1:A:185:TRP:CH2	1:A:200:ARG:HB3	2.54	0.42
1:A:384:ASN:O	1:A:386:ASP:N	2.52	0.42
1:A:387:ARG:HH11	1:A:437:MET:HE1	1.84	0.42
1:A:556:TRP:C	1:A:558:GLY:N	2.73	0.42
1:A:522:GLY:HA2	1:A:646:PHE:HE2	1.84	0.42
1:A:681:GLU:O	1:A:685:GLU:HG3	2.18	0.42
1:A:831:THR:CG2	1:A:832:ALA:N	2.82	0.42
1:A:882:SER:H	1:A:1025:ARG:HH21	1.67	0.42
1:A:910:PRO:HB3	1:A:917:SER:H	1.84	0.42
2:B:27:ALA:O	2:B:29:ASP:N	2.52	0.42
2:B:284:ILE:HD13	2:B:333:PHE:HD2	1.82	0.42
2:B:465:ASN:HD22	2:B:465:ASN:N	2.13	0.42
2:B:831:SER:CB	2:B:994:TYR:OH	2.67	0.42
5:E:31:THR:CG2	5:E:34:GLU:HB2	2.49	0.42
8:H:41:ASP:HB2	8:H:121:LEU:HB3	1.99	0.42
8:H:63:LEU:CD1	8:H:64:ASN:H	2.32	0.42
9:I:54:GLU:HB3	9:I:100:PHE:CE2	2.54	0.42
12:L:27:LEU:CB	12:L:37:LYS:HB3	2.48	0.42
1:A:108:MET:O	1:A:109:HIS:HB2	2.19	0.42
1:A:117:GLU:N	1:A:117:GLU:CD	2.69	0.42
1:A:1242:VAL:CG1	1:A:1243:VAL:H	2.13	0.42
1:A:1424:VAL:O	1:A:1428:VAL:HG23	2.18	0.42
1:A:1450:LEU:HD11	6:F:108:PHE:HZ	1.84	0.42
1:A:262:LEU:CD2	1:A:303:TYR:HE1	2.32	0.42
1:A:352:VAL:HG23	1:A:467:THR:HG22	1.99	0.42
1:A:600:PRO:HG2	1:A:601:LYS:HG3	2.00	0.42
1:A:69:THR:O	1:A:70:CYS:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:711:ARG:NH2	9:I:87:GLN:OE1	2.51	0.42
1:A:728:LYS:CB	1:A:731:ARG:HH21	2.32	0.42
1:A:733:ALA:O	1:A:736:ASN:HB3	2.19	0.42
1:A:894:GLU:O	1:A:896:ARG:N	2.52	0.42
2:B:1162:ILE:HG22	2:B:1163:CYS:O	2.19	0.42
2:B:170:LEU:HG	2:B:170:LEU:O	2.20	0.42
2:B:589:VAL:CG1	2:B:590:HIS:N	2.80	0.42
2:B:711:GLU:CB	2:B:712:PRO:CD	2.98	0.42
2:B:714:GLU:N	2:B:714:GLU:OE1	2.52	0.42
2:B:744:HIS:CD2	2:B:746:SER:OG	2.67	0.42
3:C:50:GLU:HB3	3:C:156:THR:HB	2.01	0.42
4:D:116:SER:O	4:D:117:GLU:C	2.57	0.42
4:D:186:ASP:O	4:D:211:LEU:HD13	2.18	0.42
6:F:108:PHE:HE1	6:F:131:PRO:HG3	1.85	0.42
6:F:75:PRO:C	6:F:77:ASP:N	2.70	0.42
6:F:103:MET:HE3	7:G:66:GLY:N	2.33	0.42
8:H:9:ILE:HG21	8:H:54:SER:HB2	2.01	0.42
8:H:79:TRP:O	8:H:80:ARG:C	2.57	0.42
9:I:61:ASP:HB3	9:I:64:SER:OG	2.19	0.42
2:B:186:GLU:HG3	10:J:62:ARG:HH12	1.84	0.42
12:L:27:LEU:H	12:L:27:LEU:CD2	2.14	0.42
1:A:1215:ARG:NH1	1:A:1272:THR:O	2.52	0.42
1:A:1423:GLY:O	1:A:1424:VAL:C	2.57	0.42
1:A:167:CYS:HB2	1:A:169:ASN:HD22	1.84	0.42
1:A:107:CYS:HB2	1:A:171:GLN:HE22	1.83	0.42
1:A:207:ILE:O	1:A:208:LEU:C	2.58	0.42
1:A:383:TYR:N	1:A:383:TYR:CD2	2.87	0.42
1:A:475:THR:HG23	1:A:476:SER:H	1.79	0.42
1:A:579:SER:HB3	1:A:611:GLN:HA	2.00	0.42
1:A:591:PHE:HD2	1:A:595:THR:HB	1.84	0.42
1:A:726:ARG:NH2	1:A:727:ASP:OD1	2.51	0.42
1:A:926:GLN:O	1:A:930:ASP:HB2	2.19	0.42
2:B:1029:CYS:HB3	2:B:1086:PHE:CE2	2.55	0.42
2:B:121:ASN:HA	2:B:207:GLY:CA	2.41	0.42
2:B:278:GLN:CG	2:B:279:ASP:N	2.80	0.42
2:B:327:ARG:HG2	2:B:327:ARG:O	2.19	0.42
2:B:348:ARG:O	2:B:351:TYR:HB3	2.19	0.42
2:B:388:CYS:C	2:B:390:LEU:N	2.72	0.42
2:B:436:VAL:O	2:B:436:VAL:HG12	2.18	0.42
2:B:572:HIS:O	2:B:573:GLN:C	2.58	0.42
2:B:69:LEU:O	2:B:70:ILE:CG1	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:822:ASN:HD21	10:J:52:THR:CG2	2.30	0.42
2:B:847:ASP:OD2	3:C:167:HIS:HA	2.20	0.42
3:C:91:HIS:HD2	3:C:91:HIS:O	2.02	0.42
4:D:63:LEU:CD1	4:D:133:THR:OG1	2.65	0.42
4:D:141:LEU:O	4:D:145:MET:HG2	2.19	0.42
4:D:196:PRO:O	4:D:197:SER:C	2.57	0.42
5:E:12:LEU:HD22	5:E:55:ARG:CZ	2.49	0.42
5:E:195:VAL:CG1	5:E:196:VAL:H	2.27	0.42
7:G:1:MET:O	7:G:2:PHE:C	2.58	0.42
7:G:62:LEU:HB3	7:G:63:PRO:CD	2.42	0.42
1:A:537:ARG:NH1	8:H:120:GLY:O	2.52	0.42
2:B:120:ARG:HH12	12:L:54:ARG:NH1	2.16	0.42
2:B:952:VAL:O	12:L:57:LEU:HD22	2.20	0.42
1:A:1001:ARG:NH1	1:A:1001:ARG:CG	2.82	0.42
1:A:1157:ASP:C	1:A:1159:ARG:N	2.70	0.42
1:A:1157:ASP:OD1	1:A:1159:ARG:HB2	2.19	0.42
1:A:276:LEU:HD13	1:A:293:GLU:CA	2.47	0.42
1:A:392:VAL:C	1:A:394:ASN:N	2.73	0.42
1:A:526:ASP:HB2	2:B:835:GLN:CD	2.40	0.42
1:A:568:PRO:CB	3:C:221:TYR:CZ	3.03	0.42
1:A:601:LYS:HB2	1:A:603:ASN:OD1	2.19	0.42
1:A:786:HIS:CE1	2:B:519:TRP:CZ2	3.08	0.42
2:B:1109:GLY:HA3	2:B:1110:PRO:HD2	1.75	0.42
2:B:1203:LEU:O	2:B:1207:LEU:HG	2.20	0.42
2:B:365:THR:O	2:B:374:LYS:HE3	2.19	0.42
1:A:317:LYS:HG3	2:B:471:LYS:NZ	2.34	0.42
2:B:557:PHE:CE1	2:B:603:LEU:HD11	2.53	0.42
2:B:615:MET:O	2:B:615:MET:HE2	2.19	0.42
2:B:825:VAL:HG21	2:B:1092:TYR:HE1	1.85	0.42
3:C:133:ILE:HG13	3:C:237:SER:N	2.34	0.42
3:C:187:LYS:C	3:C:189:THR:H	2.22	0.42
3:C:234:SER:OG	3:C:235:VAL:N	2.52	0.42
3:C:27:LEU:O	3:C:28:ALA:C	2.56	0.42
6:F:138:LEU:O	6:F:140:ASP:N	2.53	0.42
7:G:14:HIS:CE1	7:G:15:PRO:HD2	2.54	0.42
11:K:20:LYS:O	11:K:33:ILE:HA	2.20	0.42
1:A:1037:LEU:HD13	1:A:1041:ALA:HB3	2.01	0.42
1:A:102:VAL:O	1:A:105:CYS:HB2	2.19	0.42
1:A:1446:ASP:HB3	1:A:1449:SER:OG	2.20	0.42
1:A:90:VAL:HG11	1:A:297:GLN:HA	2.01	0.42
1:A:514:PRO:C	1:A:516:SER:N	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:TRP:CD2	1:A:558:GLY:HA2	2.55	0.42
2:B:104:GLU:OE1	12:L:54:ARG:CZ	2.67	0.42
2:B:1071:VAL:HG12	2:B:1072:MET:N	2.33	0.42
1:A:1431:GLY:HA3	2:B:1197:PRO:HD3	2.00	0.42
2:B:1192:TYR:CD2	2:B:1218:THR:HG21	2.55	0.42
2:B:190:TYR:CE1	2:B:196:PRO:HG3	2.54	0.42
2:B:32:ALA:O	2:B:35:SER:HB2	2.20	0.42
2:B:367:LEU:O	2:B:368:GLU:HB2	2.20	0.42
2:B:604:ARG:HA	2:B:609:ILE:HG13	2.01	0.42
2:B:801:LYS:HD2	2:B:815:ARG:HB3	2.01	0.42
2:B:60:GLN:HE22	2:B:95:ILE:HG22	1.80	0.42
2:B:98:THR:O	2:B:126:SER:CB	2.64	0.42
3:C:138:GLU:HB2	3:C:140:ASN:ND2	2.35	0.42
3:C:46:ILE:HD13	3:C:157:CYS:SG	2.60	0.42
3:C:166:GLU:HG3	11:K:10:PHE:CZ	2.46	0.42
2:B:996:ARG:NH2	3:C:175:ALA:HA	2.34	0.42
4:D:166:LEU:O	4:D:169:SER:OG	2.38	0.42
5:E:117:THR:HB	5:E:120:ALA:HB3	2.00	0.42
5:E:156:LEU:HD12	5:E:195:VAL:CG1	2.50	0.42
5:E:87:SER:O	5:E:88:VAL:C	2.58	0.42
6:F:74:ILE:HG13	6:F:74:ILE:H	1.64	0.42
8:H:109:LYS:HB3	8:H:110:ASP:OD1	2.20	0.42
9:I:49:ILE:HG22	9:I:49:ILE:O	2.20	0.42
10:J:1:MET:O	10:J:1:MET:HG3	2.19	0.42
11:K:65:HIS:HD2	11:K:67:PHE:HB2	1.84	0.42
1:A:1329:THR:O	1:A:1329:THR:HG23	2.19	0.42
1:A:1409:LEU:O	1:A:1410:PHE:C	2.58	0.42
1:A:47:ARG:NH1	1:A:254:GLU:OE1	2.51	0.42
1:A:355:GLY:HA3	1:A:482:PHE:CZ	2.55	0.42
1:A:524:VAL:HG12	1:A:525:GLN:CG	2.50	0.42
1:A:584:ASN:O	1:A:586:ILE:N	2.53	0.42
1:A:701:LEU:HD21	9:I:114:GLN:HB2	2.02	0.42
1:A:802:ASN:CG	2:B:728:ARG:HB2	2.39	0.42
2:B:1115:THR:HG22	2:B:1117:GLN:CB	2.50	0.42
2:B:126:SER:O	2:B:169:ARG:HA	2.20	0.42
2:B:205:ILE:C	2:B:207:GLY:N	2.73	0.42
2:B:428:ILE:HG13	2:B:428:ILE:H	1.72	0.42
2:B:806:THR:CG2	2:B:808:ALA:HB3	2.49	0.42
2:B:840:ILE:CG2	2:B:994:TYR:HD1	2.33	0.42
2:B:859:TYR:OH	2:B:941:LEU:HD12	2.18	0.42
2:B:857:ARG:NH2	2:B:942:ARG:CZ	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:860:MET:HG3	2:B:965:LYS:HE2	2.01	0.42
3:C:56:THR:CG2	3:C:145:CYS:SG	3.07	0.42
3:C:174:ALA:O	10:J:10:CYS:HB2	2.20	0.42
3:C:73:GLN:NE2	3:C:75:MET:H	2.14	0.42
7:G:88:ASP:OD2	7:G:88:ASP:N	2.47	0.42
8:H:32:THR:CG2	8:H:33:GLN:H	2.27	0.42
11:K:24:ASP:H	11:K:31:VAL:HA	1.85	0.42
1:A:1011:GLN:NE2	1:A:1015:VAL:CG2	2.82	0.42
1:A:1297:GLU:OE1	1:A:1297:GLU:N	2.52	0.42
1:A:332:LYS:O	1:A:333:GLU:HG2	2.19	0.42
1:A:556:TRP:O	1:A:558:GLY:N	2.53	0.42
1:A:57:ARG:HG2	1:A:57:ARG:NH1	2.32	0.42
1:A:637:LYS:HA	1:A:637:LYS:HD3	1.89	0.42
1:A:712:GLU:O	1:A:714:PHE:N	2.53	0.42
1:A:733:ALA:HA	1:A:736:ASN:HB3	2.01	0.42
1:A:781:ASP:O	1:A:790:ASP:N	2.52	0.42
1:A:839:ARG:CG	1:A:840:ARG:N	2.83	0.42
1:A:846:GLU:OE1	1:A:1425:SER:OG	2.34	0.42
1:A:919:ILE:HD13	1:A:983:ILE:CD1	2.49	0.42
2:B:1156:ASP:O	2:B:1157:ALA:C	2.58	0.42
2:B:1197:PRO:O	2:B:1199:ALA:N	2.53	0.42
1:A:1422:ARG:NH1	2:B:1224:PHE:HD2	2.18	0.42
2:B:247:GLY:O	2:B:248:SER:HB3	2.20	0.42
2:B:309:GLN:O	2:B:312:GLU:N	2.52	0.42
2:B:384:ARG:HD2	2:B:387:LEU:HD22	2.01	0.42
2:B:25:ILE:CD1	2:B:653:VAL:O	2.68	0.42
3:C:118:LEU:HD12	3:C:132:PRO:HG3	2.02	0.42
3:C:82:TYR:CE2	3:C:161:LYS:HG2	2.55	0.42
4:D:119:ARG:CG	4:D:221:TYR:HE2	2.33	0.42
4:D:175:PHE:CZ	7:G:85:GLU:HG3	2.55	0.42
5:E:164:LEU:HD11	5:E:211:TYR:CD1	2.54	0.42
8:H:100:THR:HG23	8:H:138:GLU:CB	2.49	0.42
8:H:145:ARG:O	8:H:146:ARG:CB	2.68	0.42
11:K:41:THR:CG2	11:K:42:LEU:N	2.83	0.42
1:A:1138:ILE:CA	1:A:1275:GLY:HA2	2.50	0.42
1:A:1150:SER:HA	1:A:1195:LEU:HA	2.01	0.42
1:A:120:GLU:O	1:A:121:LEU:C	2.58	0.42
1:A:1449:SER:C	1:A:1451:VAL:H	2.23	0.42
1:A:53:LEU:CD2	1:A:54:ASN:N	2.61	0.42
1:A:690:VAL:O	1:A:691:LEU:C	2.59	0.42
1:A:818:MET:HA	2:B:514:LEU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1002:THR:O	2:B:1004:GLU:N	2.52	0.42
2:B:505:ASP:O	2:B:506:GLY:C	2.57	0.42
2:B:661:LEU:HD23	2:B:679:TYR:O	2.20	0.42
2:B:529:GLU:OE1	2:B:769:TYR:CE1	2.72	0.42
2:B:843:GLN:O	2:B:844:SER:C	2.57	0.42
2:B:789:MET:CE	2:B:967:ARG:HB2	2.50	0.42
2:B:995:ARG:HH11	3:C:165:LYS:HA	1.84	0.42
3:C:88:CYS:SG	3:C:91:HIS:HA	2.60	0.42
4:D:26:THR:HG22	4:D:26:THR:O	2.20	0.42
4:D:47:LEU:CD1	7:G:3:PHE:HD2	2.31	0.42
4:D:64:VAL:CG2	4:D:129:LEU:HD21	2.50	0.42
6:F:70:LYS:O	6:F:72:LYS:N	2.43	0.42
1:A:1059:HIS:ND1	6:F:86:THR:HA	2.35	0.42
7:G:45:ILE:HD13	7:G:78:VAL:HG11	2.01	0.42
9:I:82:GLU:CB	9:I:104:LEU:HD12	2.40	0.42
1:A:1100:ARG:HH12	1:A:1111:MET:HE1	1.85	0.42
1:A:1277:GLU:HA	1:A:1277:GLU:OE1	2.19	0.42
1:A:179:LEU:HD23	1:A:179:LEU:N	2.35	0.42
1:A:452:LYS:HE3	2:B:1141:HIS:CE1	2.55	0.42
1:A:595:THR:O	1:A:596:THR:HG23	2.20	0.42
1:A:597:LEU:HD12	1:A:597:LEU:N	2.35	0.42
1:A:728:LYS:O	1:A:729:ALA:C	2.58	0.42
1:A:752:LYS:HD3	1:A:752:LYS:HA	1.87	0.42
1:A:826:ASP:O	1:A:827:THR:C	2.57	0.42
1:A:965:GLN:O	1:A:968:GLN:HB2	2.20	0.42
2:B:195:CYS:SG	2:B:196:PRO:HD2	2.60	0.42
2:B:36:ALA:O	2:B:39:ARG:HB2	2.20	0.42
2:B:566:LEU:O	2:B:567:GLU:C	2.58	0.42
3:C:100:THR:HG22	3:C:102:GLN:NE2	2.35	0.42
3:C:73:GLN:CG	3:C:74:SER:N	2.82	0.42
5:E:105:PHE:O	5:E:106:GLN:HB2	2.18	0.42
6:F:125:LEU:HB2	6:F:130:ILE:HD11	2.02	0.42
1:A:1192:LEU:HD13	1:A:1239:ARG:NH1	2.35	0.41
1:A:1230:GLU:O	1:A:1232:ASN:N	2.53	0.41
1:A:1425:SER:HA	1:A:1428:VAL:HG23	2.02	0.41
1:A:41:MET:HE3	1:A:41:MET:H	1.85	0.41
1:A:52:GLY:O	1:A:56:PRO:HG2	2.20	0.41
1:A:65:LEU:O	1:A:71:GLN:HA	2.20	0.41
1:A:790:ASP:OD2	9:I:87:GLN:HG3	2.20	0.41
1:A:877:HIS:C	1:A:878:ILE:CG1	2.89	0.41
2:B:210:LYS:HE2	2:B:462:ALA:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:287:ARG:NH1	2:B:324:ILE:O	2.52	0.41
2:B:654:ARG:C	2:B:656:GLY:H	2.23	0.41
2:B:810:GLU:HB3	2:B:811:TYR:CD1	2.54	0.41
2:B:818:PRO:HB2	2:B:1091:TYR:OH	2.20	0.41
2:B:830:TYR:HB3	2:B:831:SER:H	1.68	0.41
2:B:879:ARG:NH1	2:B:883:LEU:CD2	2.81	0.41
3:C:11:ARG:H	3:C:20:PHE:HA	1.85	0.41
4:D:168:LYS:O	4:D:169:SER:HB3	2.20	0.41
6:F:127:GLU:O	6:F:129:LYS:N	2.53	0.41
11:K:30:ALA:HB2	11:K:76:GLN:CG	2.41	0.41
1:A:1101:LEU:CD1	1:A:1105:LEU:HD11	2.46	0.41
1:A:841:LEU:HD22	1:A:1371:LEU:HD13	2.01	0.41
1:A:1400:CYS:O	1:A:1405:THR:HA	2.20	0.41
1:A:164:ARG:CG	1:A:165:GLY:N	2.82	0.41
1:A:562:THR:HA	1:A:563:PRO:HD3	1.87	0.41
1:A:602:ASP:C	1:A:603:ASN:O	2.57	0.41
1:A:685:GLU:OE2	1:A:686:ALA:HB2	2.20	0.41
1:A:705:LYS:O	1:A:706:HIS:C	2.58	0.41
1:A:733:ALA:O	1:A:737:LEU:HG	2.20	0.41
1:A:767:GLN:NE2	1:A:774:ARG:CB	2.83	0.41
2:B:236:HIS:N	2:B:236:HIS:CD2	2.87	0.41
2:B:435:THR:C	2:B:437:GLU:H	2.22	0.41
2:B:467:GLY:O	2:B:468:GLU:C	2.58	0.41
2:B:503:GLY:CA	2:B:507:LYS:HE2	2.31	0.41
2:B:601:ARG:HH11	2:B:605:ARG:HH22	1.66	0.41
2:B:831:SER:HB3	2:B:994:TYR:OH	2.20	0.41
3:C:47:ASP:HA	3:C:169:LYS:NZ	2.35	0.41
4:D:178:ALA:O	4:D:181:GLY:N	2.53	0.41
4:D:205:ASP:O	4:D:209:ARG:HG3	2.20	0.41
5:E:91:LYS:C	5:E:93:MET:N	2.72	0.41
8:H:55:LEU:HB3	8:H:144:ILE:CG2	2.48	0.41
10:J:18:TRP:CH2	10:J:22:LEU:HD11	2.55	0.41
1:A:1038:THR:OG1	1:A:1039:LYS:N	2.54	0.41
1:A:451:HIS:NE2	1:A:1074:GLU:HG3	2.35	0.41
1:A:108:MET:O	1:A:109:HIS:CB	2.69	0.41
1:A:1239:ARG:C	1:A:1240:CYS:SG	2.98	0.41
1:A:1305:VAL:HG12	1:A:1306:LEU:N	2.34	0.41
1:A:1425:SER:HA	1:A:1428:VAL:HG21	2.02	0.41
1:A:360:GLU:O	1:A:361:LEU:C	2.59	0.41
1:A:516:SER:O	1:A:517:ASN:C	2.58	0.41
1:A:54:ASN:HD21	1:A:61:ILE:HD11	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:958:VAL:HG13	1:A:1052:GLN:HB3	2.02	0.41
2:B:828:ALA:HB2	2:B:1085:ILE:HG23	2.02	0.41
2:B:1162:ILE:HG22	2:B:1163:CYS:N	2.35	0.41
2:B:1214:PRO:HG2	2:B:1214:PRO:O	2.19	0.41
2:B:261:ARG:HG3	2:B:261:ARG:HH11	1.85	0.41
2:B:373:ARG:HD2	2:B:567:GLU:OE2	2.19	0.41
2:B:416:LEU:O	2:B:420:LEU:HG	2.20	0.41
2:B:736:THR:O	2:B:736:THR:HG22	2.21	0.41
2:B:529:GLU:OE2	2:B:769:TYR:HE1	2.03	0.41
2:B:879:ARG:O	2:B:934:LYS:CE	2.69	0.41
1:A:469:ARG:NH2	2:B:991:GLY:O	2.46	0.41
3:C:176:ILE:HG22	3:C:177:GLU:O	2.20	0.41
3:C:254:LYS:O	3:C:256:ALA:N	2.53	0.41
5:E:89:GLY:C	5:E:91:LYS:N	2.72	0.41
6:F:135:ARG:NH2	6:F:145:ASP:OD2	2.52	0.41
7:G:137:ILE:HG21	7:G:143:ILE:HD11	2.03	0.41
8:H:64:ASN:ND2	8:H:88:SER:CB	2.68	0.41
9:I:50:THR:CG2	9:I:51:ASN:N	2.83	0.41
1:A:789:LYS:HE3	9:I:67:THR:OG1	2.21	0.41
13:T:7:DC:H2"	13:T:8:DT:C6	2.54	0.41
1:A:1002:GLY:HA3	1:A:1007:ILE:CG2	2.42	0.41
1:A:1390:ASN:OD1	1:A:1399:ARG:HA	2.20	0.41
1:A:23:SER:CA	1:A:233:TRP:NE1	2.76	0.41
1:A:24:PRO:O	1:A:27:VAL:HB	2.20	0.41
1:A:269:ILE:CD1	1:A:300:VAL:HA	2.49	0.41
1:A:50:ILE:C	1:A:52:GLY:N	2.73	0.41
1:A:567:LYS:HG2	1:A:568:PRO:CD	2.49	0.41
1:A:598:LEU:HA	8:H:122:LEU:HD13	2.03	0.41
2:B:311:LEU:O	2:B:314:LEU:N	2.53	0.41
2:B:312:GLU:O	2:B:315:LYS:N	2.45	0.41
2:B:424:LEU:HD23	2:B:453:ILE:HD11	2.03	0.41
2:B:555:ILE:HG22	2:B:556:THR:N	2.35	0.41
2:B:597:MET:O	2:B:598:GLU:C	2.58	0.41
2:B:593:PRO:CG	2:B:617:ARG:CZ	2.91	0.41
2:B:687:GLU:O	2:B:689:LEU:HD23	2.20	0.41
2:B:834:ASN:ND2	2:B:1013:ASN:CA	2.83	0.41
7:G:15:PRO:HG3	7:G:66:GLY:C	2.40	0.41
10:J:44:TYR:HD2	10:J:44:TYR:N	2.05	0.41
2:B:186:GLU:HG2	10:J:62:ARG:HH22	1.85	0.41
1:A:102:VAL:HG11	1:A:211:PHE:CE2	2.55	0.41
1:A:1146:VAL:HG11	1:A:1207:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1151:GLU:HB2	1:A:1153:TYR:HE1	1.86	0.41
1:A:1176:LEU:C	1:A:1176:LEU:HD23	2.41	0.41
1:A:1142:THR:CA	1:A:1273:LEU:HD13	2.48	0.41
1:A:1104:ILE:HD12	1:A:1355:VAL:HG21	2.02	0.41
1:A:1072:ILE:HD11	1:A:1368:MET:HA	2.01	0.41
1:A:1384:VAL:C	1:A:1385:THR:CG2	2.89	0.41
1:A:211:PHE:HA	1:A:214:ILE:HG13	2.01	0.41
1:A:309:ALA:O	1:A:311:GLN:N	2.49	0.41
1:A:563:PRO:HG2	8:H:79:TRP:CZ2	2.55	0.41
1:A:590:ARG:O	1:A:591:PHE:CB	2.69	0.41
1:A:860:LEU:O	2:B:1224:PHE:CE2	2.70	0.41
1:A:939:ASP:O	1:A:940:ARG:C	2.59	0.41
2:B:1001:PHE:CD1	2:B:1001:PHE:C	2.93	0.41
2:B:184:ALA:HB1	2:B:188:ASP:HB2	2.03	0.41
2:B:361:LEU:CD2	2:B:364:ILE:HD12	2.51	0.41
2:B:577:ALA:HB1	2:B:589:VAL:CG1	2.18	0.41
2:B:582:VAL:HG23	2:B:626:ILE:HD12	2.02	0.41
2:B:610:ASN:C	2:B:612:GLU:H	2.23	0.41
2:B:620:ARG:H	2:B:620:ARG:HG3	1.70	0.41
2:B:637:LEU:CD2	2:B:742:GLU:HA	2.51	0.41
2:B:825:VAL:HG22	2:B:1010:LEU:HB3	2.02	0.41
2:B:864:LYS:HD2	2:B:872:GLU:CD	2.40	0.41
2:B:969:ARG:CD	3:C:61:GLU:OE2	2.69	0.41
3:C:66:ARG:NH1	10:J:2:ILE:HG23	2.35	0.41
4:D:39:ASN:C	4:D:41:GLN:H	2.23	0.41
5:E:114:ASN:HD22	5:E:114:ASN:HA	1.58	0.41
5:E:45:LYS:HD3	5:E:46:TYR:CE1	2.55	0.41
5:E:52:ARG:CB	5:E:53:PRO:HD2	2.45	0.41
6:F:148:VAL:HG23	6:F:149:GLU:N	2.34	0.41
6:F:90:ARG:HG3	6:F:91:ALA:N	2.34	0.41
7:G:122:ASN:HB2	7:G:131:GLN:NE2	2.17	0.41
7:G:145:VAL:CG1	7:G:146:LYS:N	2.83	0.41
9:I:68:LEU:HB3	9:I:84:VAL:CG2	2.50	0.41
10:J:14:VAL:HG12	10:J:50:ILE:HD11	2.01	0.41
10:J:32:GLU:CD	10:J:32:GLU:H	2.24	0.41
1:A:1074:GLU:N	1:A:1075:PRO:HD2	2.35	0.41
1:A:1409:LEU:O	1:A:1412:ALA:N	2.51	0.41
1:A:1451:VAL:C	1:A:1453:TYR:N	2.73	0.41
1:A:1449:SER:O	1:A:1453:TYR:CD1	2.73	0.41
1:A:38:PRO:CG	1:A:39:GLU:N	2.83	0.41
1:A:440:ASP:O	1:A:460:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:ILE:HD13	1:A:653:VAL:HG21	2.01	0.41
1:A:841:LEU:HA	1:A:841:LEU:HD23	1.93	0.41
1:A:964:ILE:O	1:A:967:ALA:HB3	2.21	0.41
1:A:346:ASP:OD1	2:B:1108:ARG:HA	2.20	0.41
2:B:22:SER:HA	2:B:654:ARG:HB2	2.01	0.41
2:B:344:LYS:O	2:B:347:LYS:HG2	2.20	0.41
2:B:390:LEU:O	2:B:391:ASP:C	2.58	0.41
2:B:435:THR:C	2:B:437:GLU:N	2.73	0.41
2:B:43:LEU:HA	2:B:43:LEU:HD23	1.90	0.41
2:B:654:ARG:HH11	2:B:654:ARG:HG3	1.84	0.41
2:B:900:ALA:HA	2:B:901:PRO:HD3	1.90	0.41
3:C:77:ILE:CA	3:C:129:ILE:HD11	2.50	0.41
4:D:52:LEU:HA	4:D:148:LEU:HD21	2.03	0.41
5:E:13:TRP:O	5:E:16:PHE:HB3	2.21	0.41
5:E:64:PRO:O	5:E:65:THR:C	2.59	0.41
6:F:109:VAL:CG2	6:F:124:GLU:HA	2.51	0.41
6:F:70:LYS:HA	6:F:72:LYS:HZ1	1.85	0.41
6:F:72:LYS:HB3	6:F:73:ALA:H	1.64	0.41
7:G:121:PHE:HA	7:G:130:TYR:HA	2.02	0.41
8:H:83:GLN:C	8:H:85:GLY:H	2.23	0.41
2:B:799:PRO:HD3	10:J:1:MET:HG2	2.02	0.41
10:J:1:MET:H3	10:J:56:LEU:N	2.18	0.41
10:J:57:ILE:HG23	10:J:58:GLU:N	2.35	0.41
2:B:190:TYR:CE2	10:J:62:ARG:HD3	2.55	0.41
12:L:49:LYS:O	12:L:50:ASP:CB	2.69	0.41
1:A:101:LYS:HE2	1:A:139:TRP:CH2	2.55	0.41
1:A:456:MET:HE2	1:A:507:VAL:HG22	2.02	0.41
1:A:532:ARG:HG2	1:A:532:ARG:HH11	1.86	0.41
1:A:637:LYS:HB3	1:A:641:VAL:CG2	2.47	0.41
1:A:710:LEU:HD12	1:A:710:LEU:H	1.84	0.41
1:A:722:LEU:HD23	1:A:799:PHE:CG	2.55	0.41
1:A:779:PHE:HD2	1:A:779:PHE:HA	1.71	0.41
1:A:947:PHE:C	1:A:949:ASP:N	2.74	0.41
1:A:947:PHE:CE2	1:A:954:TRP:CD2	3.09	0.41
2:B:1055:ILE:C	2:B:1057:LYS:N	2.74	0.41
2:B:1106:ARG:HD3	2:B:1126:GLY:C	2.41	0.41
2:B:324:ILE:HG12	2:B:329:THR:HB	2.03	0.41
2:B:287:ARG:O	2:B:327:ARG:HA	2.21	0.41
2:B:865:LYS:CD	2:B:961:LEU:HD21	2.51	0.41
2:B:981:ALA:HB3	2:B:1095:LEU:HD11	2.03	0.41
3:C:183:TRP:CH2	3:C:203:GLN:NE2	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:42:PRO:HA	3:C:163:ILE:HG22	2.02	0.41
3:C:43:THR:CG2	3:C:44:LEU:N	2.57	0.41
2:B:798:TYR:CE2	3:C:62:PHE:CE2	3.07	0.41
4:D:153:ARG:CZ	4:D:184:ALA:HA	2.50	0.41
5:E:2:ASP:O	5:E:3:GLN:C	2.59	0.41
6:F:70:LYS:HA	6:F:72:LYS:NZ	2.35	0.41
6:F:96:THR:O	6:F:100:GLN:HG3	2.20	0.41
7:G:125:SER:HB2	7:G:127:PRO:O	2.21	0.41
7:G:8:SER:O	7:G:9:LEU:CB	2.68	0.41
8:H:64:ASN:CG	8:H:90:ALA:H	2.14	0.41
9:I:35:VAL:O	9:I:36:GLU:HB3	2.21	0.41
10:J:1:MET:H2	10:J:57:ILE:H	1.65	0.41
11:K:55:LYS:HB3	11:K:81:TYR:CE1	2.55	0.41
1:A:1141:THR:CA	1:A:1205:LYS:HZ3	2.32	0.41
1:A:1227:ILE:CG2	1:A:1228:TRP:H	2.20	0.41
1:A:37:PHE:H	1:A:37:PHE:HD1	1.63	0.41
1:A:630:ILE:CG2	1:A:631:HIS:H	2.34	0.41
1:A:683:ILE:HG22	1:A:684:ALA:N	2.35	0.41
2:B:487:THR:CG2	2:B:488:TYR:H	2.33	0.41
2:B:581:PHE:O	2:B:626:ILE:N	2.53	0.41
2:B:605:ARG:HB3	2:B:688:GLY:HA3	2.02	0.41
2:B:63:ILE:HD12	2:B:63:ILE:HA	1.89	0.41
2:B:693:ILE:HD13	2:B:701:ILE:CD1	2.50	0.41
2:B:859:TYR:CD1	2:B:859:TYR:N	2.88	0.41
3:C:104:PHE:HD2	3:C:105:GLY:H	1.68	0.41
3:C:131:HIS:O	3:C:133:ILE:N	2.53	0.41
2:B:996:ARG:HH12	3:C:38:ILE:HG23	1.86	0.41
3:C:77:ILE:HA	3:C:77:ILE:HD13	1.89	0.41
4:D:3:VAL:CG1	4:D:4:SER:N	2.83	0.41
5:E:93:MET:O	5:E:94:LYS:C	2.59	0.41
7:G:26:LEU:O	7:G:27:LYS:C	2.59	0.41
8:H:118:PHE:C	8:H:120:GLY:N	2.67	0.41
9:I:2:THR:O	9:I:3:THR:C	2.59	0.41
1:A:1037:LEU:HD12	1:A:1042:PHE:N	2.36	0.41
1:A:1239:ARG:HH11	1:A:1239:ARG:HB3	1.86	0.41
1:A:1144:LYS:HD2	1:A:1269:GLU:HG3	2.02	0.41
1:A:868:TYR:CZ	1:A:1366:ARG:HD3	2.56	0.41
1:A:244:PRO:HG2	1:A:245:PRO:CD	2.50	0.41
1:A:34:LYS:HZ3	1:A:34:LYS:HG2	1.77	0.41
1:A:376:TYR:HB3	1:A:434:ARG:NH1	2.36	0.41
1:A:38:PRO:HG2	1:A:39:GLU:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:746:MET:HE1	2:B:1018:PRO:HG2	2.03	0.41
2:B:1110:PRO:O	2:B:1119:VAL:HG22	2.21	0.41
2:B:112:LEU:HD12	2:B:113:TYR:N	2.32	0.41
2:B:368:GLU:O	2:B:371:GLU:OE1	2.38	0.41
2:B:457:LEU:O	2:B:458:LYS:C	2.58	0.41
3:C:102:GLN:HA	3:C:153:LEU:O	2.21	0.41
3:C:82:TYR:CD2	3:C:161:LYS:HG2	2.56	0.41
3:C:56:THR:HG22	3:C:58:LEU:HD23	2.02	0.41
3:C:77:ILE:CG2	3:C:78:GLU:N	2.76	0.41
4:D:60:LYS:HE2	4:D:126:ILE:HD11	2.03	0.41
4:D:155:ARG:O	4:D:156:ASP:HB2	2.20	0.41
4:D:175:PHE:O	4:D:179:GLN:HG2	2.21	0.41
1:A:1343:ALA:CB	5:E:150:VAL:HG22	2.43	0.41
8:H:100:THR:N	8:H:117:SER:O	2.45	0.41
8:H:82:PRO:O	8:H:84:ALA:N	2.41	0.41
9:I:55:THR:O	9:I:56:ALA:C	2.59	0.41
10:J:3:VAL:HA	10:J:4:PRO:HD3	1.87	0.41
2:B:186:GLU:HG3	10:J:62:ARG:CZ	2.51	0.41
11:K:14:GLU:O	11:K:15:GLY:O	2.39	0.41
1:A:1098:VAL:HB	1:A:1099:PRO:HD3	2.03	0.41
1:A:12:ARG:HD2	2:B:1218:THR:CB	2.43	0.41
1:A:16:GLU:HB3	1:A:1418:LEU:HD11	2.03	0.41
1:A:265:LYS:HG3	1:A:265:LYS:O	2.21	0.41
1:A:445:ASN:ND2	1:A:446:ARG:N	2.68	0.41
1:A:800:VAL:HG13	1:A:812:GLU:OE2	2.21	0.41
1:A:15:LYS:HB2	2:B:1219:ASP:O	2.21	0.41
2:B:265:SER:C	2:B:267:ARG:N	2.74	0.41
2:B:273:LEU:HD12	2:B:280:ILE:HD12	2.03	0.41
2:B:275:TYR:HB3	2:B:351:TYR:OH	2.21	0.41
2:B:227:LYS:HB2	2:B:395:GLN:OE1	2.21	0.41
3:C:183:TRP:O	3:C:184:ASN:CB	2.69	0.41
3:C:254:LYS:C	3:C:256:ALA:N	2.74	0.41
1:A:1143:LEU:CD2	1:A:1267:MET:HB3	2.48	0.41
1:A:1308:THR:HG23	1:A:1310:GLY:N	2.28	0.41
1:A:152:VAL:HG12	1:A:153:PRO:CD	2.51	0.41
1:A:390:GLN:O	1:A:394:ASN:N	2.54	0.41
1:A:49:LYS:NZ	1:A:61:ILE:CG1	2.72	0.41
1:A:553:VAL:HA	1:A:554:PRO:HD2	1.89	0.41
1:A:568:PRO:HB2	3:C:221:TYR:CZ	2.56	0.41
1:A:866:PHE:HB2	5:E:208:TYR:OH	2.21	0.41
1:A:966:ASN:C	1:A:968:GLN:N	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1017:ILE:CB	2:B:1018:PRO:CD	2.99	0.41
2:B:133:LYS:CG	2:B:135:ARG:HE	2.34	0.41
2:B:187:SER:O	2:B:191:LYS:HG3	2.21	0.41
2:B:343:ILE:CG2	2:B:347:LYS:HE2	2.42	0.41
2:B:413:LEU:O	2:B:416:LEU:HB2	2.21	0.41
2:B:488:TYR:CE2	2:B:813:LYS:HB2	2.55	0.41
2:B:601:ARG:HD3	2:B:605:ARG:HH21	1.85	0.41
3:C:192:TRP:CZ3	3:C:194:GLU:HG3	2.56	0.41
3:C:204:SER:N	3:C:207:CYS:HG	2.17	0.41
4:D:33:PHE:CE1	7:G:80:LYS:HD3	2.56	0.41
4:D:67:ARG:HH21	4:D:129:LEU:HD13	1.86	0.41
5:E:116:ILE:CG2	5:E:117:THR:H	2.34	0.41
5:E:145:THR:HG21	5:E:187:TYR:CZ	2.56	0.41
5:E:89:GLY:O	5:E:91:LYS:N	2.54	0.41
6:F:79:ARG:HH11	6:F:79:ARG:CB	2.29	0.41
7:G:164:LYS:O	7:G:164:LYS:HG2	2.21	0.41
8:H:31:THR:O	8:H:31:THR:HG22	2.20	0.41
12:L:52:GLY:O	12:L:53:HIS:C	2.59	0.41
1:A:106:VAL:CG1	1:A:107:CYS:N	2.82	0.40
1:A:1348:LEU:O	1:A:1352:VAL:HG23	2.20	0.40
1:A:1356:ILE:O	1:A:1356:ILE:HG22	2.21	0.40
1:A:569:LYS:O	1:A:571:LEU:HD13	2.20	0.40
1:A:595:THR:O	1:A:596:THR:CG2	2.68	0.40
1:A:714:PHE:O	1:A:715:GLU:C	2.60	0.40
1:A:731:ARG:O	1:A:732:LEU:C	2.59	0.40
1:A:767:GLN:HE21	1:A:774:ARG:HB3	1.87	0.40
1:A:814:PHE:O	1:A:814:PHE:CD2	2.74	0.40
2:B:980:PHE:CE2	2:B:1094:ARG:HB2	2.56	0.40
2:B:610:ASN:HA	2:B:611:PRO:HD3	1.89	0.40
1:A:472:LEU:CD1	2:B:835:GLN:NE2	2.84	0.40
3:C:116:LYS:HD3	3:C:140:ASN:HA	2.02	0.40
1:A:568:PRO:HB3	3:C:221:TYR:OH	2.21	0.40
4:D:60:LYS:NZ	4:D:122:GLU:OE2	2.53	0.40
4:D:51:ASN:C	4:D:52:LEU:O	2.57	0.40
5:E:124:VAL:HB	5:E:125:PRO:HD3	2.03	0.40
5:E:197:LYS:HG2	5:E:199:ILE:CG1	2.50	0.40
6:F:82:THR:HG22	6:F:84:TYR:N	2.35	0.40
6:F:90:ARG:CG	6:F:91:ALA:N	2.84	0.40
7:G:127:PRO:CG	7:G:139:ILE:HG13	2.50	0.40
7:G:53:ASN:HD22	7:G:53:ASN:N	2.18	0.40
8:H:4:THR:CG2	8:H:5:LEU:N	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:99:LEU:C	9:I:100:PHE:HD1	2.24	0.40
9:I:94:ASP:O	9:I:95:THR:O	2.40	0.40
10:J:47:ARG:HG2	10:J:47:ARG:NH1	2.35	0.40
3:C:252:GLN:CG	11:K:95:ILE:HG23	2.50	0.40
1:A:1026:LEU:HD23	1:A:1026:LEU:HA	1.89	0.40
1:A:100:LYS:O	1:A:104:GLU:HG3	2.20	0.40
1:A:1219:THR:HG21	1:A:1271:ILE:CD1	2.45	0.40
1:A:1342:GLU:OE2	5:E:212:ARG:NH1	2.53	0.40
1:A:1354:ASN:HA	1:A:1357:ALA:HB3	2.03	0.40
1:A:1425:SER:O	1:A:1428:VAL:HG23	2.22	0.40
1:A:253:ASN:ND2	1:A:256:GLN:NE2	2.67	0.40
1:A:26:GLU:O	1:A:27:VAL:C	2.58	0.40
1:A:49:LYS:HZ1	1:A:61:ILE:CB	2.34	0.40
1:A:606:LEU:HD11	1:A:608:ILE:HG13	2.03	0.40
1:A:779:PHE:CD1	1:A:784:LEU:HA	2.56	0.40
2:B:1033:LYS:NZ	2:B:1070:GLU:OE1	2.45	0.40
2:B:980:PHE:CD2	2:B:1094:ARG:HA	2.56	0.40
2:B:259:TYR:N	2:B:259:TYR:CD1	2.89	0.40
2:B:26:THR:O	2:B:29:ASP:HB2	2.22	0.40
2:B:287:ARG:NH1	2:B:325:GLN:HA	2.36	0.40
2:B:605:ARG:HB3	2:B:688:GLY:HA2	2.03	0.40
2:B:661:LEU:C	2:B:663:ALA:H	2.22	0.40
2:B:856:PHE:N	2:B:856:PHE:CD1	2.89	0.40
2:B:894:ASP:HB2	12:L:58:LYS:HZ1	1.85	0.40
3:C:191:TYR:HD2	3:C:201:TRP:CD1	2.39	0.40
3:C:249:ASP:O	3:C:252:GLN:HB3	2.21	0.40
4:D:138:ASN:OD1	4:D:141:LEU:HB2	2.21	0.40
5:E:28:TYR:CE2	5:E:78:LEU:HB2	2.56	0.40
7:G:1:MET:CE	7:G:3:PHE:CE1	3.05	0.40
7:G:88:ASP:HB3	7:G:144:ARG:CB	2.51	0.40
9:I:95:THR:CG2	9:I:96:SER:N	2.84	0.40
13:T:9:DC:H2"	13:T:10:DA:H8	1.78	0.40
1:A:1019:CYS:O	1:A:1020:CYS:C	2.59	0.40
1:A:1072:ILE:O	1:A:1075:PRO:HD2	2.21	0.40
1:A:1165:GLU:OE1	1:A:1194:ARG:NH2	2.54	0.40
1:A:241:VAL:O	1:A:242:PRO:C	2.58	0.40
1:A:265:LYS:HZ3	1:A:302:THR:HG21	1.86	0.40
1:A:359:LEU:HD23	1:A:359:LEU:HA	1.87	0.40
1:A:474:VAL:CG2	1:A:474:VAL:O	2.68	0.40
1:A:524:VAL:HG12	1:A:525:GLN:HG3	2.02	0.40
2:B:172:ILE:HG22	2:B:173:MET:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:222:ILE:N	2:B:240:ILE:HG13	2.36	0.40
2:B:324:ILE:HD13	2:B:330:ALA:HA	2.03	0.40
2:B:289:LEU:O	2:B:371:GLU:HB3	2.21	0.40
2:B:465:ASN:O	2:B:467:GLY:N	2.54	0.40
2:B:658:ILE:HG22	2:B:662:MET:CE	2.51	0.40
2:B:790:ASP:N	2:B:790:ASP:OD2	2.52	0.40
2:B:906:SER:HA	2:B:946:ASN:CB	2.44	0.40
2:B:878:GLN:O	2:B:934:LYS:HE2	2.21	0.40
3:C:259:LEU:O	3:C:262:LEU:N	2.53	0.40
4:D:205:ASP:O	4:D:208:GLU:HB3	2.21	0.40
4:D:218:GLU:O	4:D:219:THR:C	2.60	0.40
6:F:70:LYS:C	6:F:72:LYS:HZ2	2.22	0.40
7:G:144:ARG:O	7:G:168:LEU:HD22	2.22	0.40
7:G:26:LEU:O	7:G:29:LYS:N	2.54	0.40
1:A:600:PRO:HA	8:H:25:ARG:CZ	2.51	0.40
8:H:87:ARG:O	8:H:89:LEU:HG	2.21	0.40
11:K:11:LEU:N	11:K:11:LEU:CD2	2.82	0.40
11:K:83:PRO:O	11:K:84:LYS:C	2.60	0.40
1:A:975:HIS:HA	1:A:1036:ARG:HG3	2.02	0.40
1:A:1076:ALA:HA	1:A:1079:MET:CE	2.51	0.40
1:A:1126:ALA:O	1:A:1128:GLN:N	2.55	0.40
1:A:129:LYS:O	1:A:130:ASP:CB	2.66	0.40
1:A:1349:TYR:CD2	1:A:1349:TYR:C	2.94	0.40
1:A:1437:GLY:C	1:A:1439:GLY:N	2.75	0.40
1:A:215:SER:HB3	1:A:218:ASP:HB2	2.03	0.40
1:A:265:LYS:HE3	1:A:265:LYS:HA	2.03	0.40
1:A:447:GLN:HA	1:A:448:PRO:C	2.41	0.40
1:A:525:GLN:O	1:A:526:ASP:C	2.60	0.40
1:A:703:THR:C	1:A:705:LYS:H	2.24	0.40
2:B:102:VAL:HB	2:B:110:HIS:H	1.86	0.40
2:B:383:ASN:CG	2:B:387:LEU:HD11	2.42	0.40
2:B:530:GLY:C	2:B:531:GLN:HG2	2.41	0.40
2:B:814:PHE:C	2:B:816:GLU:H	2.24	0.40
2:B:901:PRO:HD2	12:L:59:ALA:O	2.22	0.40
4:D:139:LYS:HG3	4:D:143:ASN:HD22	1.87	0.40
4:D:175:PHE:HZ	7:G:85:GLU:HG3	1.87	0.40
4:D:39:ASN:HD21	4:D:41:GLN:HB2	1.79	0.40
5:E:117:THR:C	5:E:119:SER:N	2.75	0.40
5:E:117:THR:CG2	5:E:120:ALA:H	2.34	0.40
1:A:1006:ILE:HD12	5:E:163:GLU:HG3	2.00	0.40
5:E:164:LEU:HD21	5:E:211:TYR:CG	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:75:PRO:O	6:F:77:ASP:N	2.54	0.40
7:G:113:HIS:O	7:G:114:LEU:HB2	2.21	0.40
7:G:9:LEU:C	7:G:9:LEU:HD12	2.41	0.40
9:I:2:THR:CG2	9:I:3:THR:H	2.31	0.40
9:I:4:PHE:HD1	9:I:4:PHE:O	2.05	0.40
9:I:5:ARG:NE	9:I:36:GLU:OE2	2.55	0.40
2:B:737:THR:HG22	9:I:66:PRO:HA	2.02	0.40
2:B:391:ASP:CB	9:I:92:ARG:HG3	2.52	0.40
11:K:67:PHE:C	11:K:68:PHE:CD2	2.87	0.40
12:L:27:LEU:HD13	12:L:37:LYS:HG2	2.03	0.40
12:L:58:LYS:O	12:L:59:ALA:O	2.39	0.40
1:A:110:CYS:SG	1:A:111:GLY:N	2.94	0.40
1:A:1208:THR:HG22	1:A:1210:GLY:H	1.85	0.40
1:A:681:GLU:C	1:A:683:ILE:H	2.24	0.40
1:A:767:GLN:NE2	1:A:774:ARG:HB3	2.37	0.40
1:A:947:PHE:HE2	1:A:954:TRP:CD1	2.40	0.40
2:B:1045:SER:O	2:B:1046:PRO:O	2.39	0.40
2:B:1152:MET:C	2:B:1157:ALA:HB2	2.42	0.40
2:B:228:LYS:HD3	2:B:228:LYS:HA	1.94	0.40
2:B:293:PRO:CG	2:B:296:GLU:OE1	2.70	0.40
2:B:31:TRP:HE3	2:B:31:TRP:HA	1.85	0.40
2:B:351:TYR:CE2	2:B:355:ILE:HD11	2.55	0.40
2:B:469:GLN:CG	2:B:470:LYS:N	2.84	0.40
2:B:816:GLU:OE1	2:B:816:GLU:N	2.55	0.40
5:E:176:PRO:O	5:E:212:ARG:HA	2.21	0.40
6:F:89:GLU:HB3	6:F:134:ILE:HD11	2.03	0.40
6:F:138:LEU:HA	6:F:138:LEU:HD23	1.99	0.40
7:G:14:HIS:C	7:G:16:SER:N	2.75	0.40
7:G:12:THR:HA	7:G:68:ALA:O	2.22	0.40
8:H:128:ASN:N	8:H:130:ARG:HH11	2.10	0.40
11:K:42:LEU:HD23	11:K:42:LEU:C	2.42	0.40
2:B:766:ARG:HH21	15:P:11:U:H3	1.70	0.40
13:T:12:DG:N2	14:N:6:DT:O2	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1421/1733 (82%)	909 (64%)	310 (22%)	202 (14%)	0	3
2	B	1111/1224 (91%)	694 (62%)	257 (23%)	160 (14%)	0	3
3	C	268/324 (83%)	164 (61%)	66 (25%)	38 (14%)	0	3
4	D	183/221 (83%)	108 (59%)	49 (27%)	26 (14%)	0	3
5	E	212/215 (99%)	134 (63%)	49 (23%)	29 (14%)	0	3
6	F	86/155 (56%)	60 (70%)	20 (23%)	6 (7%)	1	15
7	G	169/171 (99%)	127 (75%)	32 (19%)	10 (6%)	1	18
8	H	133/146 (91%)	72 (54%)	37 (28%)	24 (18%)	0	1
9	I	114/122 (93%)	73 (64%)	26 (23%)	15 (13%)	0	4
10	J	63/70 (90%)	34 (54%)	13 (21%)	16 (25%)	0	0
11	K	114/120 (95%)	79 (69%)	26 (23%)	9 (8%)	1	12
12	L	45/70 (64%)	19 (42%)	11 (24%)	15 (33%)	0	0
All	All	3919/4571 (86%)	2473 (63%)	896 (23%)	550 (14%)	0	3

All (550) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	41	MET
1	A	43	GLU
1	A	48	ALA
1	A	58	LEU
1	A	63	ARG
1	A	67	CYS
1	A	70	CYS
1	A	74	MET
1	A	76	GLU
1	A	93	VAL
1	A	130	ASP

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Mol	Chain	Res	Type
1	A	154	SER
1	A	167	CYS
1	A	259	GLU
1	A	311	GLN
1	A	312	PRO
1	A	317	LYS
1	A	318	SER
1	A	399	HIS
1	A	409	SER
1	A	410	GLY
1	A	535	THR
1	A	536	LEU
1	A	543	LEU
1	A	544	ASP
1	A	556	TRP
1	A	567	LYS
1	A	583	PRO
1	A	619	LYS
1	A	666	ILE
1	A	705	LYS
1	A	846	GLU
1	A	871	ASP
1	A	885	THR
1	A	968	GLN
1	A	986	ILE
1	A	1002	GLY
1	A	1016	THR
1	A	1110	ASN
1	A	1114	PRO
1	A	1115	SER
1	A	1116	LEU
1	A	1122	PRO
1	A	1124	HIS
1	A	1177	LEU
1	A	1178	ASP
1	A	1206	ASP
1	A	1212	VAL
1	A	1244	ARG
1	A	1255	GLU
1	A	1314	SER
1	A	1341	ILE
1	A	1393	ASN

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Mol	Chain	Res	Type
1	A	1448	GLU
2	B	21	GLU
2	B	41	LYS
2	B	65	GLU
2	B	108	VAL
2	B	124	TYR
2	B	134	LYS
2	B	184	ALA
2	B	206	ASN
2	B	259	TYR
2	B	262	GLU
2	B	265	SER
2	B	266	ALA
2	B	278	GLN
2	B	282	ILE
2	B	295	GLY
2	B	343	ILE
2	B	344	LYS
2	B	345	LYS
2	B	346	GLU
2	B	365	THR
2	B	367	LEU
2	B	391	ASP
2	B	409	ALA
2	B	450	ALA
2	B	468	GLU
2	B	469	GLN
2	B	509	ALA
2	B	511	PRO
2	B	512	ARG
2	B	577	ALA
2	B	705	MET
2	B	708	GLU
2	B	709	ASP
2	B	751	VAL
2	B	878	GLN
2	B	879	ARG
2	B	892	LYS
2	B	958	GLN
2	B	987	LYS
2	B	1045	SER
2	B	1046	PRO

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Mol	Chain	Res	Type
2	B	1069	PHE
2	B	1097	HIS
2	B	1099	VAL
2	B	1143	ALA
2	B	1144	ALA
2	B	1157	ALA
2	B	1175	LEU
2	B	1183	LYS
3	C	4	GLU
3	C	56	THR
3	C	60	ASP
3	C	74	SER
3	C	90	ASP
3	C	141	GLY
3	C	149	LYS
3	C	161	LYS
3	C	213	PRO
3	C	214	ASN
3	C	237	SER
4	D	19	GLU
4	D	21	GLU
4	D	52	LEU
4	D	114	MET
4	D	131	GLU
4	D	169	SER
4	D	198	LEU
4	D	218	GLU
5	E	45	LYS
5	E	88	VAL
5	E	93	MET
5	E	97	VAL
5	E	106	GLN
5	E	115	ASN
5	E	129	PRO
5	E	174	GLN
6	F	72	LYS
6	F	81	THR
6	F	114	GLU
7	G	2	PHE
7	G	63	PRO
7	G	114	LEU
7	G	120	THR

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Mol	Chain	Res	Type
7	G	139	ILE
7	G	141	SER
7	G	154	VAL
8	H	78	SER
8	H	81	PRO
8	H	82	PRO
8	H	87	ARG
8	H	109	LYS
8	H	128	ASN
8	H	131	ASN
8	H	140	ALA
9	I	32	CYS
9	I	79	HIS
9	I	95	THR
9	I	106	CYS
10	J	2	ILE
10	J	64	ASN
11	K	8	GLU
12	L	40	LEU
12	L	42	ARG
12	L	50	ASP
12	L	55	ILE
12	L	59	ALA
12	L	60	ARG
1	A	5	GLN
1	A	8	SER
1	A	42	ASP
1	A	57	ARG
1	A	84	ILE
1	A	96	ILE
1	A	126	LEU
1	A	131	SER
1	A	148	CYS
1	A	283	GLY
1	A	287	HIS
1	A	392	VAL
1	A	439	ASN
1	A	516	SER
1	A	517	ASN
1	A	591	PHE
1	A	604	GLY
1	A	625	SER

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Mol	Chain	Res	Type
1	A	706	HIS
1	A	726	ARG
1	A	775	ILE
1	A	852	TYR
1	A	872	GLY
1	A	958	VAL
1	A	969	GLN
1	A	1036	ARG
1	A	1054	LEU
1	A	1095	THR
1	A	1097	GLY
1	A	1123	GLY
1	A	1127	ASP
1	A	1133	LEU
1	A	1140	HIS
1	A	1167	GLU
1	A	1176	LEU
1	A	1221	LYS
1	A	1229	SER
1	A	1233	ASP
1	A	1278	ASN
1	A	1316	VAL
1	A	1331	SER
1	A	1365	TYR
1	A	1390	ASN
1	A	1405	THR
1	A	1438	THR
1	A	1450	LEU
1	A	1454	MET
2	B	46	GLN
2	B	115	GLN
2	B	168	GLY
2	B	229	ALA
2	B	257	LYS
2	B	258	LEU
2	B	260	GLY
2	B	277	LYS
2	B	294	ASP
2	B	308	TRP
2	B	312	GLU
2	B	327	ARG
2	B	368	GLU

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Mol	Chain	Res	Type
2	B	466	TRP
2	B	480	SER
2	B	483	LEU
2	B	506	GLY
2	B	575	PRO
2	B	598	GLU
2	B	629	ASP
2	B	655	LYS
2	B	711	GLU
2	B	712	PRO
2	B	728	ARG
2	B	735	ALA
2	B	752	ALA
2	B	882	THR
2	B	907	GLY
2	B	943	SER
2	B	951	GLN
2	B	1003	ALA
2	B	1006	ILE
2	B	1041	GLU
2	B	1075	GLY
2	B	1103	ILE
2	B	1108	ARG
2	B	1112	GLN
2	B	1155	SER
2	B	1167	GLY
2	B	1171	VAL
2	B	1176	ASN
2	B	1181	GLU
2	B	1186	ASP
3	C	17	ASN
3	C	78	GLU
3	C	89	GLU
3	C	110	THR
3	C	132	PRO
3	C	175	ALA
4	D	12	ARG
4	D	16	LYS
4	D	20	GLU
4	D	112	ASP
4	D	117	GLU
4	D	168	LYS

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Mol	Chain	Res	Type
4	D	201	LYS
4	D	220	LEU
5	E	3	GLN
5	E	43	LYS
5	E	66	GLU
5	E	70	SER
5	E	73	PRO
5	E	76	GLY
5	E	94	LYS
5	E	130	ALA
6	F	128	LYS
7	G	9	LEU
8	H	2	SER
8	H	6	PHE
8	H	84	ALA
8	H	92	ASP
8	H	110	ASP
8	H	119	GLY
8	H	137	GLN
9	I	3	THR
9	I	56	ALA
10	J	6	ARG
10	J	17	LYS
10	J	24	LEU
10	J	42	LYS
11	K	15	GLY
12	L	37	LYS
12	L	45	ALA
12	L	53	HIS
12	L	56	LEU
1	A	54	ASN
1	A	187	LYS
1	A	194	ALA
1	A	219	PHE
1	A	222	LEU
1	A	257	ARG
1	A	286	HIS
1	A	331	GLY
1	A	332	LYS
1	A	382	PRO
1	A	419	LYS
1	A	465	TYR

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Mol	Chain	Res	Type
1	A	483	ASP
1	A	510	GLN
1	A	538	ASP
1	A	557	ASP
1	A	568	PRO
1	A	597	LEU
1	A	600	PRO
1	A	731	ARG
1	A	734	GLU
1	A	789	LYS
1	A	875	ALA
1	A	895	LYS
1	A	910	PRO
1	A	979	SER
1	A	1098	VAL
1	A	1168	GLU
1	A	1211	GLN
1	A	1223	ASP
1	A	1270	ASN
1	A	1388	GLY
1	A	1416	ALA
1	A	1435	PRO
2	B	28	GLU
2	B	48	LEU
2	B	100	PRO
2	B	135	ARG
2	B	186	GLU
2	B	197	PHE
2	B	267	ARG
2	B	305	VAL
2	B	384	ARG
2	B	385	LEU
2	B	394	ASP
2	B	510	LYS
2	B	543	SER
2	B	591	ARG
2	B	707	PRO
2	B	746	SER
2	B	793	ALA
2	B	797	TYR
2	B	848	ARG
2	B	942	ARG

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Mol	Chain	Res	Type
2	B	957	ASN
2	B	1017	ILE
2	B	1056	SER
2	B	1074	ASN
2	B	1082	MET
3	C	9	LYS
3	C	10	ILE
3	C	25	VAL
3	C	109	SER
3	C	127	ARG
3	C	128	ASN
3	C	191	TYR
3	C	209	TYR
3	C	218	PRO
3	C	240	VAL
3	C	269	LYS
4	D	4	SER
4	D	47	LEU
4	D	61	GLU
4	D	156	ASP
4	D	192	LYS
5	E	36	GLU
5	E	64	PRO
5	E	74	ASP
5	E	86	PRO
5	E	148	GLU
6	F	71	GLU
8	H	14	GLU
8	H	32	THR
8	H	63	LEU
8	H	90	ALA
9	I	8	ARG
9	I	57	GLY
9	I	62	ILE
10	J	14	VAL
10	J	28	ASP
10	J	57	ILE
11	K	29	ASN
12	L	28	LYS
1	A	35	ILE
1	A	51	GLY
1	A	71	GLN

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Mol	Chain	Res	Type
1	A	169	ASN
1	A	186	LYS
1	A	232	GLU
1	A	253	ASN
1	A	281	HIS
1	A	418	SER
1	A	424	ILE
1	A	684	ALA
1	A	692	ASP
1	A	830	LYS
1	A	847	ASP
1	A	891	ALA
1	A	972	HIS
1	A	973	ILE
1	A	1067	LEU
1	A	1111	MET
1	A	1165	GLU
1	A	1242	VAL
1	A	1403	GLU
2	B	24	PRO
2	B	45	SER
2	B	114	PRO
2	B	309	GLN
2	B	341	LEU
2	B	369	GLY
2	B	456	GLY
2	B	559	SER
2	B	761	HIS
2	B	828	ALA
2	B	867	GLY
2	B	868	MET
2	B	881	ASN
2	B	901	PRO
2	B	937	ALA
2	B	1035	ALA
2	B	1203	LEU
3	C	125	MET
3	C	133	ILE
3	C	169	LYS
3	C	184	ASN
3	C	216	GLY
4	D	15	LEU

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Mol	Chain	Res	Type
4	D	157	GLN
4	D	203	SER
5	E	6	GLU
5	E	90	VAL
5	E	122	LYS
5	E	187	TYR
8	H	17	PRO
8	H	52	GLN
8	H	108	SER
9	I	9	ASP
9	I	34	TYR
9	I	58	VAL
10	J	9	SER
10	J	29	GLU
10	J	55	ASP
11	K	14	GLU
12	L	35	SER
12	L	39	SER
1	A	44	THR
1	A	155	GLU
1	A	164	ARG
1	A	196	GLU
1	A	234	MET
1	A	322	VAL
1	A	700	ASN
1	A	713	SER
1	A	718	VAL
1	A	1014	ALA
1	A	1108	ALA
1	A	1378	GLN
2	B	30	SER
2	B	37	PHE
2	B	325	GLN
2	B	334	ILE
2	B	353	LYS
2	B	467	GLY
2	B	566	LEU
2	B	613	VAL
2	B	687	GLU
2	B	792	MET
2	B	946	ASN
2	B	1178	ASN

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Mol	Chain	Res	Type
2	B	1214	PRO
3	C	3	GLU
3	C	108	GLU
3	C	142	VAL
4	D	40	HIS
5	E	12	LEU
5	E	59	SER
5	E	121	MET
6	F	139	PRO
8	H	105	GLU
9	I	65	ASP
9	I	107	SER
11	K	53	ASP
11	K	90	ALA
12	L	25	ALA
1	A	52	GLY
1	A	73	GLY
1	A	197	PRO
1	A	313	GLN
1	A	400	PRO
1	A	603	ASN
1	A	650	GLN
1	A	673	GLY
1	A	780	VAL
1	A	987	VAL
1	A	1164	PRO
2	B	187	SER
2	B	435	THR
2	B	540	SER
2	B	620	ARG
2	B	780	VAL
2	B	1131	GLY
4	D	191	ALA
9	I	11	ASN
10	J	13	VAL
10	J	32	GLU
11	K	79	GLU
12	L	46	VAL
1	A	59	GLY
1	A	138	ILE
1	A	250	ILE
1	A	623	GLY

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Mol	Chain	Res	Type
1	A	1437	GLY
3	C	126	GLY
7	G	20	PRO
11	K	43	GLY
1	A	77	CYS
1	A	223	GLY
1	A	245	PRO
1	A	258	GLY
1	A	719	VAL
1	A	765	VAL
1	A	1263	ILE
2	B	283	VAL
2	B	501	PRO
8	H	120	GLY
10	J	33	GLY
1	A	158	PRO
1	A	207	ILE
1	A	244	PRO
1	A	585	GLY
1	A	693	VAL
1	A	888	GLY
1	A	1428	VAL
2	B	284	ILE
2	B	355	ILE
2	B	562	GLY
2	B	729	ILE
3	C	182	PRO
10	J	4	PRO
11	K	66	PRO
1	A	385	ILE
2	B	592	ASN
7	G	92	VAL
1	A	948	VAL
5	E	154	ILE

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	1249/1520 (82%)	1135 (91%)	114 (9%)	9	36
2	B	974/1061 (92%)	879 (90%)	95 (10%)	8	33
3	C	238/280 (85%)	215 (90%)	23 (10%)	8	33
4	D	167/200 (84%)	145 (87%)	22 (13%)	4	22
5	E	196/197 (100%)	179 (91%)	17 (9%)	10	38
6	F	78/137 (57%)	69 (88%)	9 (12%)	5	27
7	G	152/152 (100%)	138 (91%)	14 (9%)	9	36
8	H	121/128 (94%)	112 (93%)	9 (7%)	13	44
9	I	110/116 (95%)	98 (89%)	12 (11%)	6	29
10	J	60/65 (92%)	55 (92%)	5 (8%)	11	40
11	K	99/102 (97%)	87 (88%)	12 (12%)	5	24
12	L	41/57 (72%)	35 (85%)	6 (15%)	3	18
All	All	3485/4015 (87%)	3147 (90%)	338 (10%)	8	33

All (338) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	18	GLN
1	A	32	VAL
1	A	34	LYS
1	A	37	PHE
1	A	41	MET
1	A	57	ARG
1	A	58	LEU
1	A	68	GLN
1	A	83	HIS
1	A	93	VAL
1	A	103	CYS
1	A	108	MET
1	A	174	ILE
1	A	179	LEU
1	A	185	TRP
1	A	196	GLU
1	A	204	THR
1	A	236	LEU
1	A	245	PRO
1	A	281	HIS
1	A	307	ASP

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Mol	Chain	Res	Type
1	A	312	PRO
1	A	320	ARG
1	A	322	VAL
1	A	326	ARG
1	A	332	LYS
1	A	333	GLU
1	A	335	ARG
1	A	337	ARG
1	A	345	VAL
1	A	351	THR
1	A	379	VAL
1	A	385	ILE
1	A	393	ARG
1	A	408	ASP
1	A	425	GLN
1	A	428	TYR
1	A	438	ASP
1	A	442	VAL
1	A	443	LEU
1	A	445	ASN
1	A	447	GLN
1	A	450	LEU
1	A	451	HIS
1	A	453	MET
1	A	466	SER
1	A	469	ARG
1	A	479	ASN
1	A	481	ASP
1	A	489	LEU
1	A	493	GLN
1	A	518	LYS
1	A	590	ARG
1	A	618	GLU
1	A	635	ARG
1	A	701	LEU
1	A	711	ARG
1	A	758	ILE
1	A	774	ARG
1	A	779	PHE
1	A	821	ARG
1	A	833	GLU
1	A	839	ARG

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Mol	Chain	Res	Type
1	A	858	ASN
1	A	903	ASN
1	A	906	HIS
1	A	923	LEU
1	A	929	LEU
1	A	930	ASP
1	A	942	PHE
1	A	961	ARG
1	A	969	GLN
1	A	998	LEU
1	A	1001	ARG
1	A	1009	ASN
1	A	1029	ARG
1	A	1035	TYR
1	A	1037	LEU
1	A	1038	THR
1	A	1058	VAL
1	A	1101	LEU
1	A	1120	LEU
1	A	1122	PRO
1	A	1124	HIS
1	A	1146	VAL
1	A	1152	ILE
1	A	1174	PHE
1	A	1178	ASP
1	A	1191	TRP
1	A	1193	LEU
1	A	1195	LEU
1	A	1214	GLU
1	A	1223	ASP
1	A	1240	CYS
1	A	1245	PRO
1	A	1255	GLU
1	A	1259	MET
1	A	1260	LEU
1	A	1264	GLU
1	A	1271	ILE
1	A	1295	THR
1	A	1297	GLU
1	A	1308	THR
1	A	1333	ILE
1	A	1364	ASN

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Mol	Chain	Res	Type
1	A	1371	LEU
1	A	1372	VAL
1	A	1393	ASN
1	A	1400	CYS
1	A	1408	ILE
1	A	1444	MET
1	A	1445	ILE
1	A	1449	SER
2	B	20	ASP
2	B	30	SER
2	B	44	VAL
2	B	46	GLN
2	B	57	TYR
2	B	61	ASP
2	B	100	PRO
2	B	164	LYS
2	B	167	ILE
2	B	170	LEU
2	B	175	ARG
2	B	194	GLU
2	B	203	PHE
2	B	213	ILE
2	B	217	ARG
2	B	272	THR
2	B	332	ASP
2	B	365	THR
2	B	371	GLU
2	B	376	PHE
2	B	378	LEU
2	B	393	LYS
2	B	396	ASP
2	B	426	LYS
2	B	429	PHE
2	B	455	SER
2	B	465	ASN
2	B	466	TRP
2	B	468	GLU
2	B	482	VAL
2	B	485	ARG
2	B	502	ILE
2	B	510	LYS
2	B	516	ASN

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Mol	Chain	Res	Type
2	B	557	PHE
2	B	563	MET
2	B	570	VAL
2	B	582	VAL
2	B	591	ARG
2	B	597	MET
2	B	601	ARG
2	B	602	THR
2	B	603	LEU
2	B	615	MET
2	B	616	ILE
2	B	635	ARG
2	B	636	PRO
2	B	680	THR
2	B	685	LEU
2	B	714	GLU
2	B	737	THR
2	B	748	ILE
2	B	766	ARG
2	B	785	TYR
2	B	798	TYR
2	B	811	TYR
2	B	815	ARG
2	B	830	TYR
2	B	839	MET
2	B	844	SER
2	B	855	PHE
2	B	859	TYR
2	B	878	GLN
2	B	895	ASP
2	B	909	ASP
2	B	933	SER
2	B	944	THR
2	B	951	GLN
2	B	955	THR
2	B	959	ASP
2	B	978	ASP
2	B	999	MET
2	B	1002	THR
2	B	1006	ILE
2	B	1022	THR
2	B	1048	THR

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Mol	Chain	Res	Type
2	B	1049	ASP
2	B	1069	PHE
2	B	1077	THR
2	B	1082	MET
2	B	1084	GLN
2	B	1095	LEU
2	B	1097	HIS
2	B	1098	MET
2	B	1133	MET
2	B	1137	CYS
2	B	1150	ARG
2	B	1156	ASP
2	B	1159	ARG
2	B	1163	CYS
2	B	1170	THR
2	B	1178	ASN
2	B	1182	CYS
2	B	1214	PRO
2	B	1218	THR
3	C	1	MET
3	C	29	MET
3	C	56	THR
3	C	58	LEU
3	C	62	PHE
3	C	77	ILE
3	C	91	HIS
3	C	104	PHE
3	C	106	GLU
3	C	124	LEU
3	C	145	CYS
3	C	147	LEU
3	C	166	GLU
3	C	190	ASP
3	C	193	TYR
3	C	197	SER
3	C	209	TYR
3	C	217	ASP
3	C	229	TYR
3	C	233	GLU
3	C	235	VAL
3	C	238	ILE
3	C	245	VAL

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Mol	Chain	Res	Type
4	D	13	ARG
4	D	15	LEU
4	D	21	GLU
4	D	22	GLU
4	D	28	GLN
4	D	40	HIS
4	D	43	GLU
4	D	47	LEU
4	D	61	GLU
4	D	63	LEU
4	D	70	PHE
4	D	115	HIS
4	D	137	ASN
4	D	149	THR
4	D	156	ASP
4	D	170	THR
4	D	187	THR
4	D	200	ASN
4	D	206	GLU
4	D	213	GLU
4	D	220	LEU
4	D	221	TYR
5	E	17	ARG
5	E	31	THR
5	E	59	SER
5	E	60	PHE
5	E	65	THR
5	E	70	SER
5	E	74	ASP
5	E	82	PHE
5	E	104	ASN
5	E	114	ASN
5	E	132	ILE
5	E	134	THR
5	E	169	ARG
5	E	172	GLU
5	E	190	LEU
5	E	207	ARG
5	E	212	ARG
6	F	71	GLU
6	F	72	LYS
6	F	79	ARG

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Mol	Chain	Res	Type
6	F	82	THR
6	F	90	ARG
6	F	111	LEU
6	F	115	THR
6	F	116	ASP
6	F	153	VAL
7	G	1	MET
7	G	13	LEU
7	G	17	PHE
7	G	30	LEU
7	G	39	THR
7	G	51	TYR
7	G	73	LYS
7	G	74	TYR
7	G	113	HIS
7	G	117	GLN
7	G	137	ILE
7	G	141	SER
7	G	165	GLU
7	G	171	ILE
8	H	8	ASP
8	H	10	PHE
8	H	17	PRO
8	H	63	LEU
8	H	64	ASN
8	H	86	ASP
8	H	91	ASP
8	H	95	TYR
8	H	102	TYR
9	I	4	PHE
9	I	6	PHE
9	I	7	CYS
9	I	8	ARG
9	I	15	TYR
9	I	37	GLU
9	I	44	TYR
9	I	85	PHE
9	I	86	PHE
9	I	94	ASP
9	I	100	PHE
9	I	101	PHE
10	J	2	ILE

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Mol	Chain	Res	Type
10	J	38	ARG
10	J	43	ARG
10	J	44	TYR
10	J	48	ARG
11	K	5	ASP
11	K	6	ARG
11	K	10	PHE
11	K	21	ILE
11	K	25	THR
11	K	41	THR
11	K	47	ARG
11	K	50	LEU
11	K	61	TYR
11	K	81	TYR
11	K	91	CYS
11	K	114	LEU
12	L	27	LEU
12	L	34	CYS
12	L	55	ILE
12	L	65	VAL
12	L	68	GLU
12	L	70	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (130) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	68	GLN
1	A	75	ASN
1	A	83	HIS
1	A	92	HIS
1	A	109	HIS
1	A	118	HIS
1	A	169	ASN
1	A	171	GLN
1	A	213	HIS
1	A	225	ASN
1	A	256	GLN
1	A	282	ASN
1	A	299	HIS
1	A	306	ASN
1	A	339	ASN

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Mol	Chain	Res	Type
1	A	358	ASN
1	A	390	GLN
1	A	394	ASN
1	A	435	HIS
1	A	439	ASN
1	A	445	ASN
1	A	447	GLN
1	A	493	GLN
1	A	517	ASN
1	A	611	GLN
1	A	654	ASN
1	A	659	HIS
1	A	700	ASN
1	A	736	ASN
1	A	741	ASN
1	A	757	ASN
1	A	767	GLN
1	A	786	HIS
1	A	802	ASN
1	A	858	ASN
1	A	877	HIS
1	A	903	ASN
1	A	926	GLN
1	A	935	GLN
1	A	968	GLN
1	A	975	HIS
1	A	1106	ASN
1	A	1130	GLN
1	A	1140	HIS
1	A	1188	GLN
1	A	1203	ASN
1	A	1278	ASN
1	A	1354	ASN
1	A	1364	ASN
1	A	1393	ASN
1	A	1427	ASN
1	A	1432	GLN
2	B	52	ASN
2	B	60	GLN
2	B	178	ASN
2	B	215	GLN
2	B	236	HIS

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Mol	Chain	Res	Type
2	B	357	GLN
2	B	366	GLN
2	B	383	ASN
2	B	465	ASN
2	B	484	ASN
2	B	513	GLN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	538	ASN
2	B	573	GLN
2	B	587	HIS
2	B	744	HIS
2	B	763	GLN
2	B	821	GLN
2	B	834	ASN
2	B	835	GLN
2	B	842	ASN
2	B	951	GLN
2	B	957	ASN
2	B	975	GLN
2	B	1065	GLN
2	B	1076	HIS
2	B	1084	GLN
2	B	1117	GLN
2	B	1141	HIS
2	B	1161	HIS
2	B	1178	ASN
2	B	1179	GLN
2	B	1193	GLN
2	B	1195	HIS
3	C	24	ASN
3	C	65	HIS
3	C	73	GLN
3	C	79	GLN
3	C	102	GLN
3	C	112	ASN
3	C	123	ASN
3	C	135	GLN
3	C	203	GLN
4	D	9	GLN
4	D	39	ASN

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Mol	Chain	Res	Type
4	D	40	HIS
4	D	115	HIS
4	D	137	ASN
4	D	138	ASN
4	D	143	ASN
4	D	179	GLN
5	E	54	GLN
5	E	101	GLN
5	E	104	ASN
5	E	114	ASN
5	E	147	HIS
7	G	53	ASN
7	G	126	ASN
7	G	131	GLN
7	G	158	HIS
8	H	33	GLN
8	H	35	GLN
8	H	131	ASN
8	H	137	GLN
8	H	139	ASN
9	I	89	GLN
9	I	90	GLN
9	I	108	HIS
9	I	114	GLN
10	J	53	HIS
10	J	64	ASN
11	K	44	ASN
11	K	52	ASN
11	K	65	HIS
11	K	76	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	9/16 (56%)	1 (11%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	P	11	U

There are no RNA pucker outliers to report.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
13	8OG	T	19	13,15	18,25,26	1.35	2 (11%)	21,37,40	2.64	6 (28%)
13	BRU	T	23	13,15	15,21,22	4.01	4 (26%)	17,30,33	4.23	5 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	8OG	T	19	13,15	-	0/3/21/22	0/3/3/3
13	BRU	T	23	13,15	-	0/4/21/22	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	T	23	BRU	BR-C5	-14.12	1.49	1.90
13	T	23	BRU	C4-C5	5.44	1.45	1.38
13	T	19	8OG	C6-N1	3.85	1.39	1.33
13	T	19	8OG	C8-N7	-2.73	1.31	1.34
13	T	23	BRU	C4-N3	2.61	1.37	1.33
13	T	23	BRU	C6-C5	-2.07	1.34	1.39

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	T	23	BRU	C4-N3-C2	15.07	127.86	115.14
13	T	19	8OG	C5-C6-N1	-8.63	111.62	123.43
13	T	23	BRU	C5-C4-N3	-7.10	115.14	123.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	T	19	8OG	C6-N1-C2	5.63	124.88	115.93
13	T	19	8OG	C2'-C1'-N9	2.98	119.27	116.01
13	T	23	BRU	C5-C6-N1	2.81	123.61	119.97
13	T	19	8OG	C2-N3-C4	-2.67	112.31	115.36
13	T	23	BRU	BR-C5-C6	2.48	122.95	117.31
13	T	19	8OG	N3-C2-N1	-2.43	123.98	127.22
13	T	19	8OG	C6-C5-C4	-2.26	118.64	120.80
13	T	23	BRU	O3'-C3'-C2'	-2.20	103.03	110.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	T	23	BRU	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	1429/1733 (82%)	-0.31	1 (0%) 95 94	15, 73, 135, 195	0
2	B	1125/1224 (91%)	-0.15	14 (1%) 79 69	11, 88, 154, 194	0
3	C	270/324 (83%)	-0.29	1 (0%) 92 88	34, 73, 131, 174	0
4	D	187/221 (84%)	-0.15	4 (2%) 63 52	58, 98, 152, 197	0
5	E	214/215 (99%)	-0.26	2 (0%) 84 76	42, 112, 155, 161	0
6	F	88/155 (56%)	-0.47	0 100 100	24, 48, 91, 122	0
7	G	171/171 (100%)	-0.23	0 100 100	48, 74, 117, 128	0
8	H	137/146 (93%)	0.16	3 (2%) 62 50	91, 125, 152, 157	0
9	I	116/122 (95%)	-0.13	3 (2%) 56 43	65, 121, 152, 153	0
10	J	65/70 (92%)	-0.42	0 100 100	48, 67, 106, 121	0
11	K	116/120 (96%)	-0.32	2 (1%) 70 59	32, 79, 108, 160	0
12	L	47/70 (67%)	-0.05	1 (2%) 63 52	73, 124, 147, 159	0
13	T	19/26 (73%)	0.44	0 100 100	128, 194, 200, 200	0
14	N	11/12 (91%)	0.88	1 (9%) 9 7	186, 198, 200, 200	0
15	P	10/16 (62%)	0.33	1 (10%) 7 5	177, 193, 199, 200	0
All	All	4005/4625 (86%)	-0.22	33 (0%) 86 78	11, 83, 152, 200	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	471	LYS	6.2
2	B	883	LEU	3.8
11	K	116	ALA	3.4
2	B	504	ARG	3.3
2	B	722	ASP	3.2
11	K	115	ALA	3.1
5	E	126	SER	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	507	LYS	2.7
2	B	339	THR	2.7
8	H	146	ARG	2.6
2	B	472	ALA	2.5
4	D	111	ASP	2.5
15	P	2	U	2.5
4	D	76	LYS	2.3
2	B	723	VAL	2.3
2	B	713	ALA	2.3
12	L	26	THR	2.3
9	I	102	VAL	2.3
4	D	112	ASP	2.3
8	H	142	LEU	2.3
8	H	83	GLN	2.2
2	B	468	GLU	2.2
14	N	8	DG	2.1
2	B	470	LYS	2.1
2	B	341	LEU	2.1
1	A	251	SER	2.1
3	C	270	VAL	2.1
2	B	714	GLU	2.1
5	E	82	PHE	2.1
2	B	248	SER	2.0
9	I	117	LYS	2.0
4	D	1	MET	2.0
9	I	84	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
13	BRU	T	23	20/21	0.68	0.27	153,162,167,170	0
13	8OG	T	19	23/24	0.89	0.17	131,141,154,155	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands

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(\AA^2)	Q<0.9
17	ZN	I	1122	1/1	0.92	0.04	134,134,134,134	0
16	MG	A	2458	1/1	0.95	0.09	69,69,69,69	0
17	ZN	A	2456	1/1	0.96	0.07	96,96,96,96	0
17	ZN	L	1071	1/1	0.97	0.06	111,111,111,111	0
17	ZN	I	1121	1/1	0.99	0.12	70,70,70,70	0
17	ZN	J	1066	1/1	0.99	0.23	47,47,47,47	0
17	ZN	B	2225	1/1	0.99	0.21	43,43,43,43	0
17	ZN	A	2457	1/1	1.00	0.14	38,38,38,38	0
17	ZN	C	1269	1/1	1.00	0.12	39,39,39,39	0

6.5 Other polymers

There are no such residues in this entry.