



# Full wwPDB X-ray Structure Validation Report i

Feb 26, 2014 – 03:29 PM GMT

PDB ID : 3HOZ  
Title : Complete RNA polymerase II elongation complex IV with a T-U mismatch and a frayed RNA 3'-guanine  
Authors : Sydow, J.F.; Brueckner, F.; Cheung, A.C.M.; Damsma, G.E.; Dengl, S.; Lehmann, E.; Vassylyev, D.; Cramer, P.  
Deposited on : 2009-06-03  
Resolution : 3.65 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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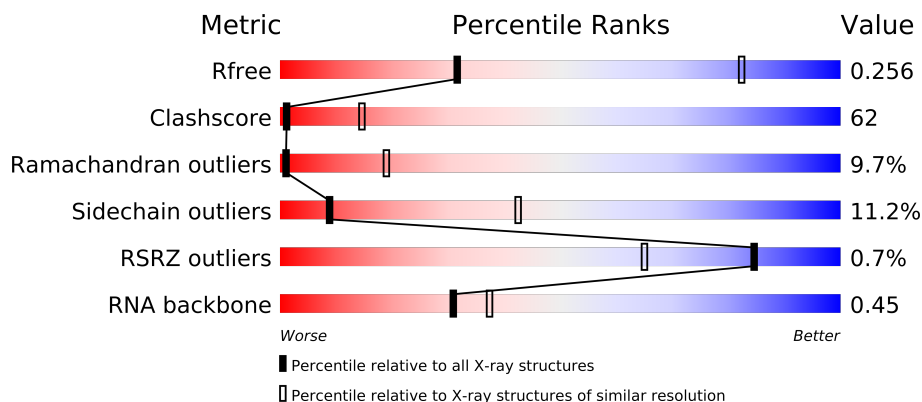
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.65 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.



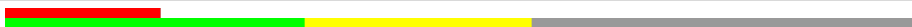


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1021 (3.94-3.38)
Clashscore	79885	1025 (3.90-3.42)
Ramachandran outliers	78287	1195 (3.92-3.40)
Sidechain outliers	78261	1193 (3.92-3.40)
RSRZ outliers	66119	1021 (3.94-3.38)
RNA backbone	1838	1008 (4.52-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1733	
2	B	1224	
3	C	347	
4	D	221	
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	

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Mol	Chain	Length	Quality of chain
13	N	12	
14	T	26	
15	P	18	

## 2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 31961 atoms, of which 0 are hydrogen and 0 are deuterium.

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	1418	Total	C	N	O	S	0	0	0
			11158	7030	1951	2115	62			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1109	Total	C	N	O	S	0	0	0
			8821	5584	1546	1636	55			

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

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

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-28	MET	-	EXPRESSION TAG	UNP P16370
C	-27	GLY	-	EXPRESSION TAG	UNP P16370
C	-26	SER	-	EXPRESSION TAG	UNP P16370
C	-25	HIS	-	EXPRESSION TAG	UNP P16370
C	-24	HIS	-	EXPRESSION TAG	UNP P16370
C	-23	HIS	-	EXPRESSION TAG	UNP P16370
C	-22	HIS	-	EXPRESSION TAG	UNP P16370
C	-21	HIS	-	EXPRESSION TAG	UNP P16370
C	-20	HIS	-	EXPRESSION TAG	UNP P16370
C	-19	SER	-	EXPRESSION TAG	UNP P16370
C	-18	ASN	-	EXPRESSION TAG	UNP P16370
C	-17	SER	-	EXPRESSION TAG	UNP P16370
C	-16	GLY	-	EXPRESSION TAG	UNP P16370
C	-15	LEU	-	EXPRESSION TAG	UNP P16370

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-14	ASN	-	EXPRESSION TAG	UNP P16370
C	-13	ASP	-	EXPRESSION TAG	UNP P16370
C	-12	ILE	-	EXPRESSION TAG	UNP P16370
C	-11	PHE	-	EXPRESSION TAG	UNP P16370
C	-10	GLU	-	EXPRESSION TAG	UNP P16370
C	-9	ALA	-	EXPRESSION TAG	UNP P16370
C	-8	GLN	-	EXPRESSION TAG	UNP P16370
C	-7	LYS	-	EXPRESSION TAG	UNP P16370
C	-6	ILE	-	EXPRESSION TAG	UNP P16370
C	-5	GLU	-	EXPRESSION TAG	UNP P16370
C	-4	TRP	-	EXPRESSION TAG	UNP P16370
C	-3	HIS	-	EXPRESSION TAG	UNP P16370
C	-2	GLU	-	EXPRESSION TAG	UNP P16370
C	-1	ASP	-	EXPRESSION TAG	UNP P16370
C	0	THR	-	EXPRESSION TAG	UNP P16370
C	1	GLY	-	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	179	Total	C	N	O	S	0	0	0
			1443	892	258	291	2			

- 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	87	Total	C	N	O	S	0	0	0
			705	451	119	132	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	136	Total	C	N	O	S	0	0	0
			1092	688	184	215	5			

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

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

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, 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	115	Total	C	N	O	S	0	0	0
			924	593	157	172	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	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

- Molecule 13 is a DNA chain called 5'-D(\*AP\*CP\*TP\*AP\*CP\*TP\*TP\*GP\*AP\*GP\*CP\*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	7	Total	C	N	O	P	0	0	0
			137	68	22	41	6			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
14	T	19	Total	Br	C	N	O	P	0	0	0
			387	1	185	69	114	18			

- Molecule 15 is a RNA chain called 5'-R(\*UP\*GP\*CP\*AP\*UP\*UP\*U\*CP\*AP\*AP\*CP\*CP

\*AP\*GP\*GP\*CP\*UP\*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	P	11	Total	C	N	O	P	0	0	0
			232	105	44	73	10			

- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	P	1	Total	Mg	0	0
			1	1		





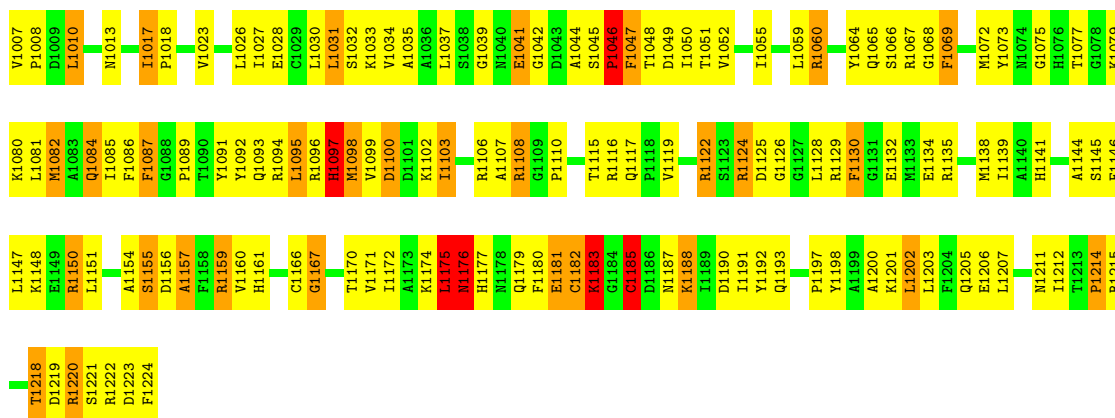
THR	SER	THR	SER	THR	GLY	GLN	GLU	F1389	T1325	E1263	M1202	E1139	T1077	Q1011	R940	Q872	R806
SER	PRO	GLY	PRO	N1390	E1264	N1203	GLN	N1390	R1326	E1265	N1203	H1140	Q1078	R1012	K941	M873	R809
THR	THR	ALA	THR	R1391	T1266	D1204	ILE	R1391	T1141	T1267	D1205	T1141	T1079	V1015	F942	A875	P810
THR	THR	THR	THR	N1393	T1268	D1206	GLU	N1393	K1144	T1269	D1207	S1145	ASN	L1081	R944	A876	Q811
PRO	PRO	THR	THR	T1394	E1269	T1208	THR	T1394	V1146	T1209	T1208	V1146	THR	F1018	V946	R877	F813
SER	SER	PHE	PRO	G1395	N1270	M1209	ILE	G1395	T1147	M1209	T1208	T1147	PHE	C1019	F947	I878	F814
THR	THR	GLY	GLY	A1396	I1271	G1210	GLY	A1396	I1148	G1210	G1210	I1148	HIS	C1020	A952	S882	F815
PRO	PRO	ALA	GLY	M1398	T1272	V1211	GLY	M1398	I1149	T1272	V1211	I1149	PHE	L1021	A952	L883	H816
THR	THR	THR	GLN	M1399	T1273	Q1212	THR	M1399	S1150	T1273	Q1212	S1150	ALA	L1022	N953	D884	A817
THR	THR	GLY	GLY	C1400	R1274	G1213	GLY	C1400	E1151	G1213	G1213	E1151	VAL	R1023	W954	T885	M818
SER	SER	GLY	GLY	S1401	G1275	E1214	GLY	S1401	I1152	G1275	E1214	I1152	GLY	S1024	G819	G819	G819
PRO	PRO	ALA	GLY	F1402	V1276	R1215	GLY	F1402	V1153	V1276	R1215	V1153	ALA	R1025	V958	G820	G820
THR	THR	VAL	VAL	E1403	E1277	I1216	VAL	E1403	T1154	E1277	I1216	T1154	SER	L1026	N959	G888	R821
THR	THR	THR	THR	E1404	M1278	I1217	THR	E1404	D1155	M1278	I1217	D1155	LYS	A1027	I960	E822	E822
PRO	PRO	PRO	PRO	T1405	I1279	Q1218	PRO	T1405	P1158	I1279	Q1218	P1158	K1093	R1028	R961	G823	G823
SER	SER	TYR	TYR	F1407	R1281	F1220	SER	F1407	R1159	R1281	F1220	R1159	V1094	R1029	R962	L824	L824
THR	THR	GLY	GLY	I1408	V1282	K1221	ASN	I1408	S1160	V1282	K1221	S1160	T1095	R1030	I963	I825	I825
PRO	PRO	PHE	PHE	L1409	G1283	M1222	ASN	L1409	T1161	G1283	M1222	T1161	S1096	V1031	I964	R826	R826
THR	THR	VAL	VAL	F1410	M1284	D1223	SER	F1410	V1162	M1284	D1223	V1162	V1098	Q1033	N966	T827	T827
SER	SER	GLY	GLY	E1411	M1285	L1224	GLY	E1411	I1163	M1285	L1224	I1163	P1099	E1034	A967	A828	A828
PRO	PRO	SER	SER	A1412	K1286	F1225	VAL	A1412	Q1171	K1286	F1225	Q1171	N1106	Y1035	Q968	X830	X830
ALA	PRO	VAL	VAL	G1413	V1287	V1226	VAL	G1413	H1172	V1287	V1226	H1172	L1101	R1036	L901	T831	T831
THR	THR	ASN	ASN	A1414	D1288	D1233	ASN	A1414	H1173	D1288	D1233	H1173	K1102	L1037	L902	A832	A832
SER	SER	PHE	PHE	E1417	K1290	I1227	ASP	E1417	F1174	K1290	I1227	F1174	E1103	L1038	N903	G833	G833
PRO	PRO	GLY	GLY	L1418	G1296	M1228	ASP	L1418	S1175	G1296	M1228	S1175	T1104	T1038	D974	Y836	Y836
THR	THR	PRO	PRO	F1419	E1297	S1229	GLY	F1419	LEU	E1297	S1229	LEU	K1112	K1039	H975	R898	R898
SER	SER	THR	THR	M1420	V1298	D1231	THR	M1420	ASP	V1298	D1231	ASP	T1113	Q1040	T976	H906	H906
PRO	PRO	SER	SER	A1421	G1299	N1232	PRO	A1421	GLU	G1299	N1232	GLU	P1114	Y1041	K977	H906	H906
SER	SER	PRO	PRO	C1421	K1300	M1232	LYS	C1421	GLU	K1300	M1232	GLU	S1115	F1042	P978	T907	T907
THR	THR	ALA	ALA	D1422	T1295	D1233	ASP	D1422	ALA	T1295	D1233	ALA	L1116	T1063	S979	L908	L908
PRO	PRO	VAL	VAL	G1423	G1296	I1236	VAL	G1423	GLN	G1296	I1236	GLN	Y1118	L1064	D980	D909	D909
PRO	PRO	THR	THR	L1432	E1297	M1238	THR	L1432	GLU	E1297	M1238	GLU	T1119	S1065	L981	S911	S911
THR	THR	GLY	GLY	I1436	V1300	I1238	GLY	I1436	LEU	V1300	I1238	LEU	K1112	K1048	H983	L912	L912
PRO	PRO	SER	SER	G1437	N1307	D1239	SER	G1437	ASP	N1307	D1239	ASP	T1114	I1049	K984	L913	L913
PRO	PRO	ASN	ASN	T1438	E1308	C1240	ASN	T1438	GLU	E1308	C1240	GLU	S1115	F1053	D985	E914	E914
THR	THR	ALA	ALA	A1440	M1312	M1241	ALA	A1440	THR	M1312	M1241	THR	L1122	L1065	L986	S915	S915
PRO	PRO	MET	MET	F1441	N1313	R1241	PRO	F1441	PHE	N1313	R1241	PHE	E1121	F1054	L988	I919	I919
THR	THR	ALA	ALA	D1442	G1314	V1242	THR	D1442	D1186	G1314	V1242	D1186	P1122	L1066	D992	G921	G921
SER	SER	GLY	GLY	V1443	E1315	GLU	GLY	V1443	Q1187	E1315	GLU	Q1187	G1123	G1061	D922	D922	D922
PRO	PRO	PHE	PHE	I1445	V1316	E1254	PHE	I1445	Q1188	V1316	E1254	Q1188	E995	E1062	K924	L923	L923
PRO	PRO	THR	THR	M1446	M1317	E1256	THR	M1446	S1189	M1317	E1256	S1189	N996	M1063	L925	L925	L925
SER	SER	THR	THR	L1381	T1318	D1257	THR	L1381	P1190	T1318	D1257	P1190	L998	V1064	Q926	Q926	Q926
PRO	PRO	ALA	ALA	V1384	V1319	M1258	ALA	V1384	L1192	V1319	M1258	L1192	V999	G1065	V927	S859	S859
PRO	PRO	SER	SER	V1451	P1320	G1259	SER	V1451	L1193	P1320	G1259	L1193	L1129	V1066	L1000	L928	L928
THR	THR	GLY	GLY	K1452	G1321	M1260	GLY	K1452	L1194	G1321	M1260	L1194	Q1070	K1002	G1002	Y933	Y933
SER	SER	THR	THR	Y1453	I1322	K1261	THR	Y1453	L1195	I1322	K1261	L1195	S1071	K1003	K954	F866	F866
PRO	PRO	ALA	ALA	M1454	D1323	L1261	ALA	M1454	L1197	D1323	L1261	L1197	I1134	E1005	N1004	Q935	Q935
PRO	PRO	ASN	ASN	P1455	P1324	K1262	ASN	P1455	D1198	P1324	K1262	D1198	G1073	I1006	I1006	L936	L936
									A1200			A1200	S1136	E1074	N1009	V937	V937
									A1201			A1201	A1137	P1075	K938	E870	E870
													I1138	A1076	A1010	D871	D871

- Molecule 2: DNA-directed RNA polymerase II subunit RPB2

Chain B:

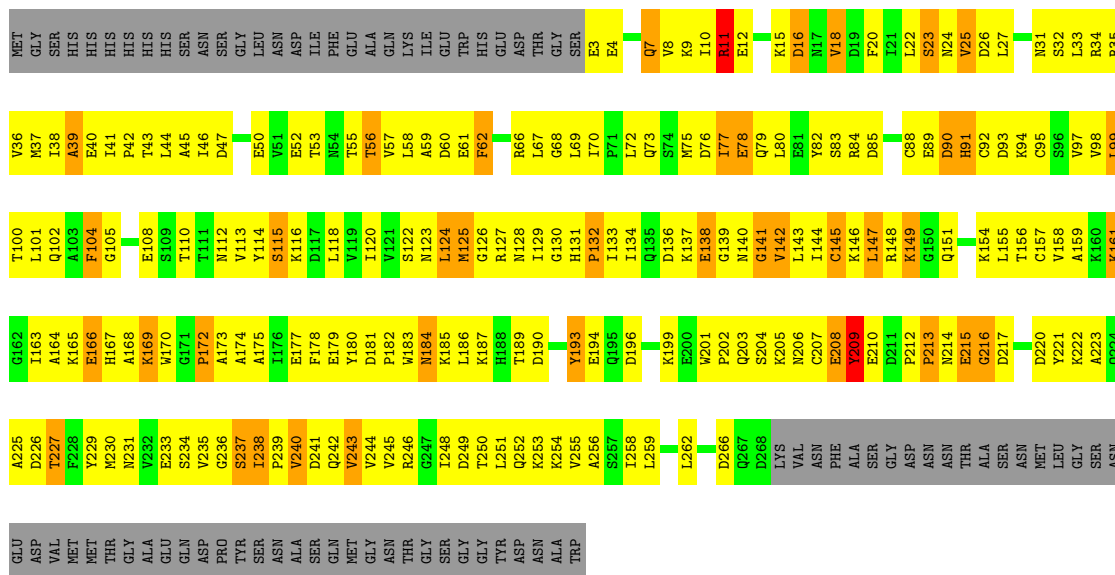


N946	G947	I948	V949	D950	Q951	V952	L953	T955	T956	N957	Q958	D959	G960	L961	G962	F963	P964	V965	K966	R967	R968	T969	V970	T971	K972	K973	P974	Q975	I976	G977	D978	F979	F980	R983	H984	Q985	Q986	K987	G988	T989	I990	G991	I992	T993	Y994	R995	R996	R997	E997	D998	M999	P1000	F1001	T1002	A1003	E1004	G1005	I1006				
T882	L883	R884	M885	K886	H887	G888	T889	Y890	S891	K892	L893	D896	G899	L900	P901	G902	S906	G907	D909	V910	I911	I912	G913	P914	T915	T916	P917	I918	S919	P920	ASP	GIJ	GIJ	H984	G985	LEU	GLY	G988	GLN	ARG	THR	ALA	THR	T993	S993	K994	R995	R996	R997	A997	D998	M999	P1000	F1001	T1002	A1003	E1004	G1005	I1006			
Q821	M822	A823	I824	V825	A826	H827	G830	F831	G832	G833	Y834	Q835	E836	A837	M838	P901	G902	S906	G907	D909	V910	I911	I912	G913	P914	T915	T916	P917	I918	S919	P920	ASP	GIJ	GIJ	H984	G985	LEU	GLY	G988	GLN	ARG	THR	ALA	THR	T993	S993	K994	R995	R996	R997	A997	D998	M999	P1000	F1001	T1002	A1003	E1004	G1005	I1006		
P757	F758	P759	D760	H761	H762	Q763	P764	F765	R766	H767	T768	Y769	Q770	A771	M772	P773	G774	K775	Q776	A777	M778	F779	F780	F781	Y785	M786	V787	R788	T789	D790	L791	M792	A793	M794	I795	L796	Y797	T798	Q799	Q800	K801	P802	L803	G804	T805	T806	R807	A808	M809	T810	E811	R815	E816	L817	P818	A819	G820					
Y692	I693	D694	A695	E696	E697	E698	E699	S700	I701	L702	I703	A704	M705	Q706	P707	E708	D709	L710	E711	P712	A715	ASN	GIJ	GIJ	ASN	ASN	P787	R788	T789	D790	L791	M792	A793	M794	I795	L796	Y797	T798	Q799	Q800	K801	P802	L803	G804	T805	T806	R807	A808	M809	T810	E811	R815	E816	L817	P818	A819	G820					
A630	G631	R632	V633	G634	R635	P636	L637	F638	I639	V640	E641	D642	D643	E644	G645	L646	G647	H648	K649	E650	L651	K652	V653	R654	K655	G656	L657	L658	L661	M662	A663	T664	E665	Y666	Q667	D668	I669	GLU	GLY	GLY	PHE	GLU	ASP	VAL	T805	T806	R807	A808	M809	T810	E811	R815	E816	L817	P818	A819	G820					
V570	P571	H572	GLY	LYS	L508	A509	K510	P511	R512	Q513	L514	H515	M516	L517	H518	G519	H520	H521	L522	V523	A525	E526	T527	P528	E529	G530	A532	V536	K537	M538	L539	M542	S546	G548	T549	D550	P553	I554	L555	T556	F557	L558	D559	E560	M561	G562	M563	E564	P565	L566	E567	Y569										
HIS	ASP	PHE	ASN	MET	LYS	L446	A447	L448	N449	A450	L453	T454	A455	K458	G459	H460	A461	A462	T463	G464	N465	K466	G467	Q468	K470	LYS	A473	K474	S475	R476	A477	G478	V479	S480	Q481	V482	L483	N484	A485	Y486	T487	S490	T491	K492	S493	G494	M495	L496	T497	A498	N499	L500	P501	L502								
G379	Y380	M381	I382	N383	R384	L385	L386	L387	C388	A389	L390	D391	R392	K393	D394	Q395	D396	D397	R398	R399	GLY	THR	ALA	ALA	GLY	ILE	LYS	K345	E346	K347	A352	K353	K354	L355	L356	Q357	K358	E359	F360	L361	F362	H363	K364	T365	Q366	L367	F370	Y371	M372	S373	K374	A375	F376	F377	L378							
Q255	V256	K257	L258	Y259	G260	R261	E262	S264	P196	M199	F203	L204	T268	L269	T272	L273	K277	D278	L280	P281	L282	V283	L284	L285	F286	R287	A288	L289	G290	I291	I292	P293	D294	G295	E296	I297	L298	E299	H300	Y303	D304	V305	N306	D307	W308	Q309	M310	S248	R249	L311	E312	M313	L314	K315	P316							
C317	V318	D320	V323	L324	Q326	R327	C328	L329	A330	L331	D332	D333	D334	Q335	L336	R337	R338	D339	ARG	GLY	THR	ALA	GLY	ILE	LYS	K345	E346	K347	A352	K353	K354	L355	L356	Q357	K358	E359	F360	L361	F362	H363	K364	T365	Q366	L367	F370	Y371	M372	S373	K374	A375	F376	F377	L378									
D188	L189	Y190	K191	L192	K193	E194	E195	P196	M199	F203	L204	T268	L269	T272	L273	K277	D278	L280	P281	L282	V283	L284	L285	F286	R287	A288	L289	G290	I291	I292	P293	D294	G295	E296	I297	L298	E299	H300	Y303	D304	V305	N306	D307	W308	Q309	M310	S248	R249	L311	E312	M313	L314	K315	P316								
S126	G127	L128	F129	D130	V131	Y132	K133	K134	ARG	THR	THR	TYR	GLU	ALA	ILE	VAL	PRO	GLY	ARG	ASP	GLU	ASN	ILE	LEU	LYS	TYR	ILE	ALA	GLU	GLU	ASP	ASP	GLU	GLY	K164	V165	F166	I167	G168	R169	I172	M173	S176	N178	C179	Y180	L181	S182	R183	L184	T185	E186	S187									
MET	SER	LEU	ALA	ASN	SER	GLU	LYS	TYR	ASP	GLU	ALA	GLN	HIS	THR	THR	GLY	PHE	GLY	D20	E21	ASN	ILE	S22	SER	A23	P24	GLY	LYS	TYR	T26	A27	E28	S29	F30	G31	A32	V33	I34	S35	A36	F37	F38	M101	V102	K41	G42	L43	V44	S45	Q46	Q47	S50	F51	F54	V55	D56	Y57	T58	L59	Q60	D61	I62



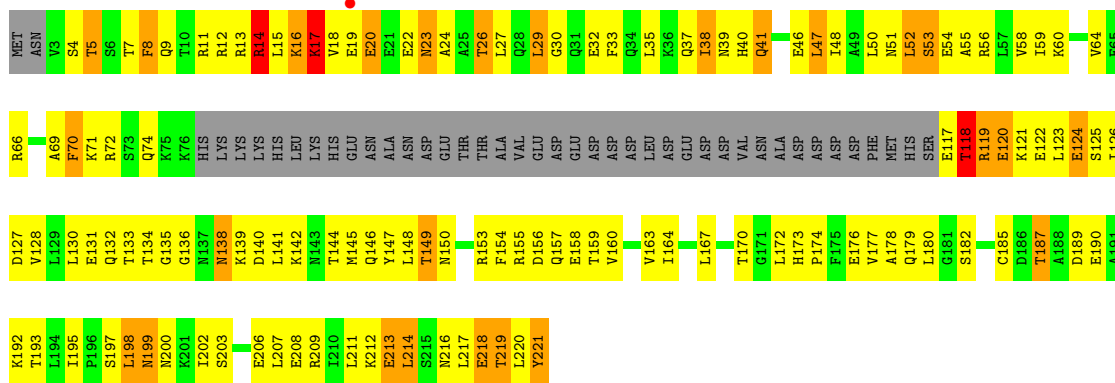
- Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C:



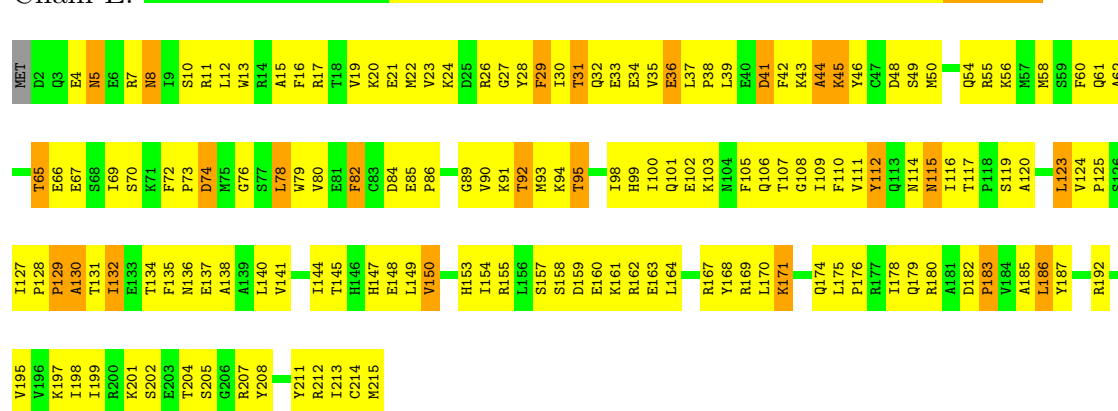
- Molecule 4: DNA-directed RNA polymerase II subunit RPB4

Chain D:



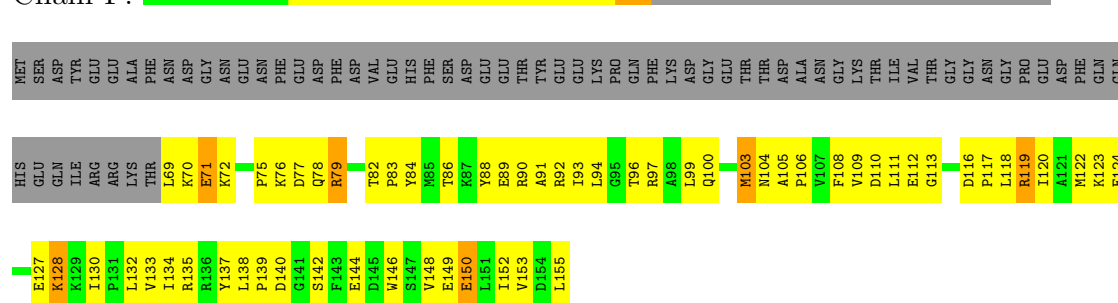
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

## Chain E:



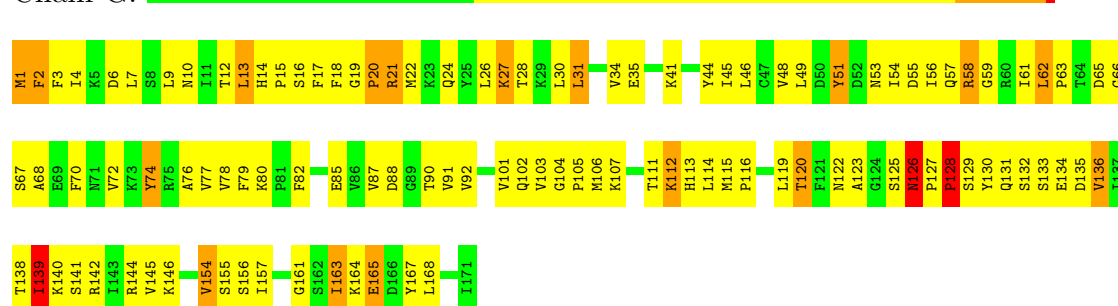
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:



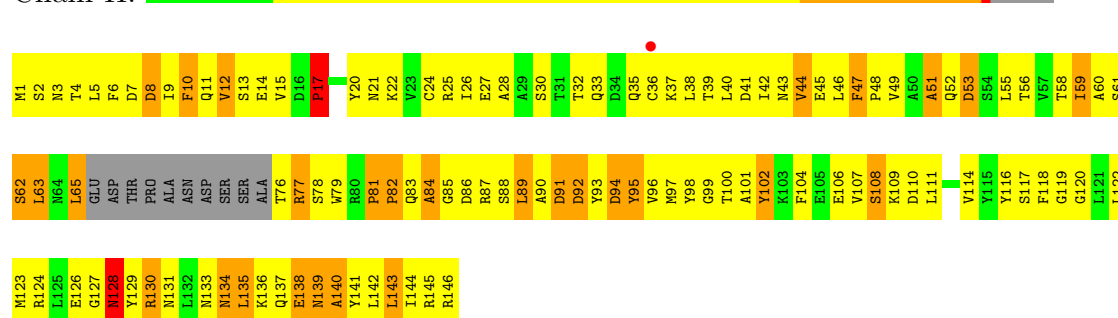
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7

## Chain G:



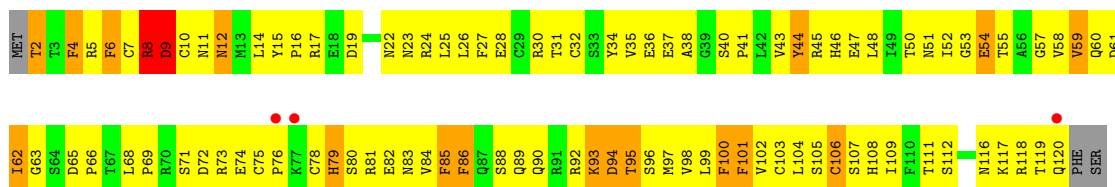
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

## Chain H:



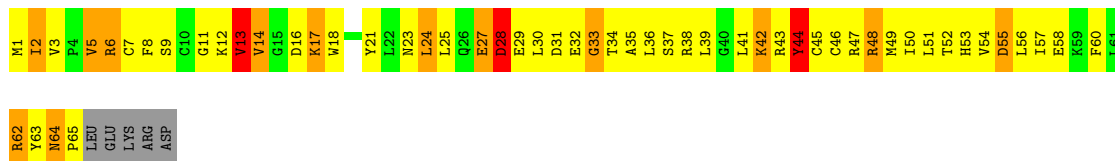
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I:



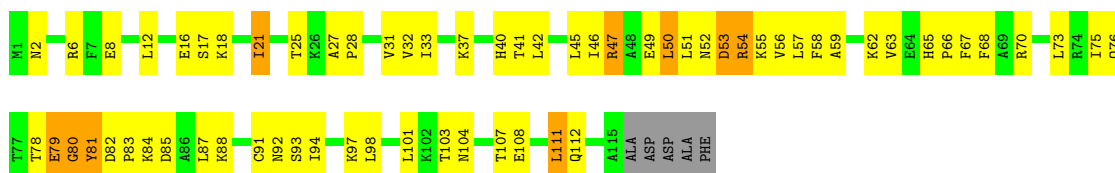
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



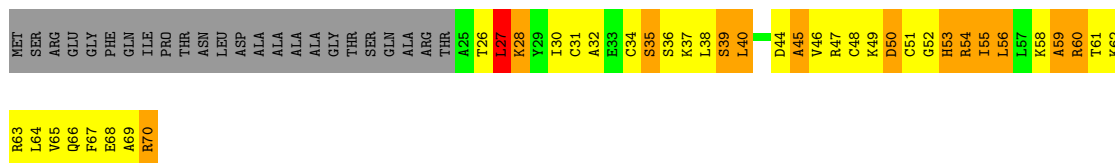
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11

Chain K:



- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:



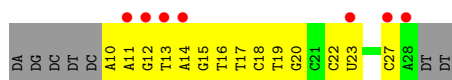
- Molecule 13: 5'-D(\*AP\*CP\*TP\*AP\*CP\*TP\*TP\*GP\*AP\*GP\*CP\*T)-3'

Chain N:



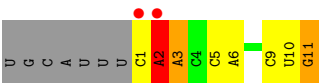
- Molecule 14: 5'-D(\*AP\*GP\*CP\*TP\*C\*AP\*AP\*GP\*TP\*AP\*GP\*TP\*TP\*CP\*TP\*GP\*CP\*C P\*(BRU)P\*GP\*GP\*TP\*CP\*AP\*TP\*T)-3'

Chain T:



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

Chain P: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	221.43Å 393.75Å 281.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.65 49.84 – 3.65	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-3.65) 100.0 (49.84-3.65)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.21 (at 3.67Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.210 , 0.253 0.212 , 0.256	Depositor DCC
$R_{free}$ test set	2674 reflections (2.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	88.8	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 75.8	EDS
Estimated twinning fraction	0.017 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.025 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 135971 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	31961	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.01% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.51	0/11358	0.79	4/15360 (0.0%)
2	B	0.49	0/8991	0.74	4/12121 (0.0%)
3	C	0.50	0/2133	0.74	1/2891 (0.0%)
4	D	0.48	0/1453	0.77	1/1947 (0.1%)
5	E	0.48	0/1788	0.71	2/2406 (0.1%)
6	F	0.57	0/717	0.83	1/967 (0.1%)
7	G	0.54	0/1368	0.81	1/1844 (0.1%)
8	H	0.45	0/1110	0.74	0/1502
9	I	0.44	0/989	0.72	0/1331
10	J	0.51	0/541	0.85	1/727 (0.1%)
11	K	0.49	0/942	0.68	0/1272
12	L	0.56	0/365	0.82	0/485
13	N	0.60	0/152	0.90	0/232
14	T	0.58	0/410	0.82	0/629
15	P	0.57	0/259	0.82	1/402 (0.2%)
All	All	0.50	0/32576	0.76	16/44116 (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
10	J	0	1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	26	THR	N-CA-C	-6.48	93.51	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	39	ALA	N-CA-C	6.32	128.07	111.00
1	A	331	GLY	N-CA-C	5.96	128.00	113.10
7	G	65	ASP	N-CA-C	-5.92	95.02	111.00
1	A	3	GLY	N-CA-C	-5.78	98.65	113.10
1	A	56	PRO	N-CA-C	-5.52	97.74	112.10
5	E	171	LYS	N-CA-C	-5.47	96.22	111.00
5	E	186	LEU	CA-CB-CG	-5.35	102.99	115.30
6	F	71	GLU	N-CA-C	-5.33	96.62	111.00
2	B	624	LEU	CA-CB-CG	-5.30	103.11	115.30
15	P	2	A	C2'-C3'-O3'	5.26	122.11	113.70
2	B	1130	PHE	N-CA-C	-5.25	96.82	111.00
1	A	311	GLN	N-CA-C	5.25	125.17	111.00
2	B	1185	CYS	N-CA-C	-5.16	97.06	111.00
10	J	5	VAL	N-CA-C	-5.14	97.13	111.00
2	B	363	HIS	N-CA-C	-5.02	97.45	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	J	44	TYR	Sidechain

## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11158	0	11228	1381	0
2	B	8821	0	8850	1234	0
3	C	2095	0	2051	306	0
4	D	1443	0	1466	213	0
5	E	1752	0	1776	214	0
6	F	705	0	731	92	0
7	G	1340	0	1357	168	0
8	H	1092	0	1069	179	0
9	I	971	0	929	137	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J	532	0	542	112	0
11	K	924	0	934	105	0
12	L	363	0	388	83	0
13	N	137	0	82	4	0
14	T	387	0	214	25	0
15	P	232	0	122	14	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	C	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
17	P	1	0	0	0	0
All	All	31961	0	31739	3920	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 62.

All (3920) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:508:LEU:HD13	2:B:510:LYS:HE2	1.26	1.16
1:A:53:LEU:HD23	1:A:54:ASN:N	1.61	1.16
2:B:744:HIS:HD2	2:B:745:PRO:HD2	1.07	1.14
1:A:1208:THR:HB	1:A:1211:GLN:HG3	1.24	1.13
2:B:559:SER:HA	2:B:563:MET:HB3	1.15	1.13
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	1.85	1.11
2:B:577:ALA:HB1	2:B:589:VAL:HG11	1.25	1.11
2:B:806:THR:HG22	2:B:808:ALA:H	1.12	1.10
1:A:53:LEU:HD23	1:A:54:ASN:H	0.96	1.09
3:C:112:ASN:HB3	3:C:114:TYR:HE1	1.10	1.09
8:H:4:THR:HA	8:H:60:ALA:HB2	1.32	1.08
2:B:583:ASN:HD21	2:B:628:THR:HG22	1.17	1.08
2:B:744:HIS:CD2	2:B:745:PRO:HD2	1.89	1.07
3:C:112:ASN:HB3	3:C:114:TYR:CE1	1.89	1.07
1:A:1242:VAL:HG12	1:A:1243:VAL:N	1.68	1.05
2:B:261:ARG:HH11	2:B:261:ARG:HB3	1.19	1.05
2:B:345:LYS:HG2	2:B:346:GLU:H	1.17	1.05
5:E:117:THR:HG22	5:E:119:SER:H	1.21	1.05
1:A:567:LYS:HE3	1:A:568:PRO:HD2	1.38	1.05
6:F:90:ARG:HD3	6:F:155:LEU:HD13	1.38	1.05
1:A:567:LYS:HB3	8:H:96:VAL:H	1.21	1.04
1:A:1206:ASP:HB3	1:A:1274:ARG:HH22	1.19	1.04

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:273:LEU:HB2	2:B:276:ILE:HD12	1.40	1.03
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.39	1.02
10:J:64:ASN:HB3	10:J:65:PRO:CD	1.90	1.01
1:A:1242:VAL:HG12	1:A:1243:VAL:H	0.85	1.01
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.08	1.01
1:A:265:LYS:HE3	1:A:265:LYS:N	1.74	1.01
2:B:710:LEU:HA	2:B:733:HIS:HB3	1.41	1.00
7:G:26:LEU:HD12	7:G:56:ILE:HD11	1.37	1.00
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.43	1.00
1:A:1244:ARG:HE	1:A:1245:PRO:HD2	1.21	1.00
5:E:56:LYS:HE2	5:E:84:ASP:HB2	1.40	1.00
1:A:1242:VAL:CG1	1:A:1243:VAL:H	1.71	1.00
2:B:510:LYS:CG	2:B:511:PRO:HD3	1.92	0.99
1:A:1445:ILE:HD12	1:A:1445:ILE:H	1.28	0.99
1:A:323:LYS:H	1:A:323:LYS:HD2	1.21	0.99
2:B:510:LYS:HG3	2:B:511:PRO:HD3	1.00	0.99
1:A:12:ARG:HB3	2:B:1218:THR:HG22	1.40	0.98
2:B:846:ILE:HG23	2:B:974:PRO:HG2	1.43	0.98
1:A:244:PRO:HB2	1:A:245:PRO:HD3	1.43	0.98
1:A:381:THR:HG22	1:A:383:TYR:H	1.23	0.98
1:A:567:LYS:HB2	1:A:568:PRO:CD	1.94	0.97
1:A:41:MET:HB3	1:A:49:LYS:HA	1.44	0.97
7:G:34:VAL:HG11	7:G:74:TYR:HE1	1.30	0.97
7:G:139:ILE:HG23	7:G:140:LYS:HG3	1.46	0.97
2:B:882:THR:HG23	2:B:884:ARG:H	1.22	0.97
1:A:783:THR:HG21	1:A:796:SER:O	1.65	0.97
2:B:770:GLN:OE1	2:B:983:ARG:HA	1.64	0.96
2:B:806:THR:N	2:B:809:MET:HE3	1.80	0.96
7:G:138:THR:HG22	7:G:139:ILE:N	1.80	0.96
1:A:1364:ASN:OD1	1:A:1366:ARG:HG2	1.65	0.96
2:B:622:LYS:HE2	9:I:59:VAL:HG22	1.47	0.96
2:B:289:LEU:HD13	2:B:375:ALA:HB2	1.46	0.95
10:J:53:HIS:HD2	10:J:54:VAL:N	1.63	0.95
2:B:243:ALA:HB2	2:B:251:ILE:HD13	1.45	0.95
2:B:1187:ASN:O	2:B:1188:LYS:HB2	1.64	0.95
9:I:65:ASP:HB3	9:I:68:LEU:HD12	1.49	0.95
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.48	0.94
4:D:220:LEU:CD2	4:D:221:TYR:H	1.80	0.94
1:A:672:ASP:HB3	1:A:736:ASN:OD1	1.68	0.94
1:A:344:ARG:HB3	1:A:344:ARG:HH11	1.30	0.94
1:A:351:THR:HG22	2:B:1103:ILE:HA	1.47	0.93
2:B:510:LYS:HG3	2:B:511:PRO:CD	1.96	0.93

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.48	0.93
1:A:41:MET:CB	1:A:49:LYS:HA	1.98	0.93
1:A:1187:GLN:HB2	1:A:1244:ARG:HG2	1.48	0.93
1:A:66:LYS:HZ3	1:A:68:GLN:H	1.01	0.93
1:A:1329:THR:HG22	1:A:1331:SER:H	1.30	0.93
3:C:177:GLU:HG3	3:C:231:ASN:HB3	1.51	0.93
1:A:629:LEU:O	1:A:633:VAL:HG23	1.69	0.93
1:A:98:LYS:O	1:A:102:VAL:HG23	1.69	0.93
7:G:15:PRO:HA	7:G:18:PHE:CD1	2.04	0.93
2:B:865:LYS:HB2	2:B:961:LEU:HD11	1.52	0.92
6:F:77:ASP:O	6:F:78:GLN:HB2	1.66	0.92
10:J:3:VAL:HG21	10:J:18:TRP:HB2	1.48	0.92
1:A:913:LEU:HD12	1:A:914:GLU:H	1.32	0.92
7:G:138:THR:HG22	7:G:139:ILE:H	1.31	0.92
1:A:66:LYS:NZ	1:A:68:GLN:H	1.68	0.92
2:B:1065:GLN:HE21	2:B:1067:ARG:H	1.02	0.92
2:B:737:THR:HG21	9:I:66:PRO:HA	1.52	0.92
4:D:60:LYS:HE3	4:D:126:ILE:HD11	1.52	0.92
4:D:14:ARG:HB3	4:D:14:ARG:HH11	1.34	0.92
1:A:549:MET:HE3	1:A:656:TRP:HD1	1.35	0.91
1:A:182:VAL:HG22	1:A:201:VAL:HA	1.52	0.91
1:A:1095:THR:HG21	1:A:1112:LYS:HB2	1.52	0.91
1:A:1094:VAL:HG22	1:A:1113:THR:HG21	1.51	0.91
5:E:22:MET:HE1	5:E:26:ARG:HH21	1.34	0.91
1:A:154:SER:HB3	1:A:162:VAL:HG21	1.50	0.91
1:A:1063:MET:SD	1:A:1436:ILE:HG12	2.10	0.91
2:B:800:GLN:HB3	10:J:52:THR:CG2	2.00	0.91
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.53	0.91
2:B:773:MET:SD	2:B:987:LYS:HD2	2.11	0.91
2:B:642:ASP:HB3	2:B:649:LYS:HD2	1.53	0.91
3:C:57:VAL:HG11	10:J:60:PHE:HB3	1.51	0.90
12:L:40:LEU:HD13	12:L:44:ASP:HB3	1.53	0.90
2:B:241:ARG:HA	2:B:253:THR:HG22	1.53	0.90
2:B:114:PRO:HG3	2:B:181:LEU:HD11	1.53	0.90
5:E:94:LYS:HE2	5:E:98:ILE:HD11	1.50	0.90
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.53	0.90
15:P:10:U:H5'	15:P:11:G:O3'	1.71	0.90
1:A:107:CYS:HA	1:A:171:GLN:NE2	1.85	0.90
1:A:381:THR:HG23	1:A:382:PRO:HD2	1.54	0.90
8:H:59:ILE:HG22	8:H:60:ALA:H	1.37	0.90
4:D:24:ALA:HB3	4:D:26:THR:HG23	1.53	0.90
8:H:84:ALA:HB2	8:H:87:ARG:HD2	1.54	0.89

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:112:ASN:CB	3:C:114:TYR:HE1	1.83	0.89
6:F:82:THR:HG22	6:F:84:TYR:H	1.34	0.89
2:B:615:MET:HB3	2:B:626:ILE:HG12	1.50	0.89
8:H:17:PRO:HB3	8:H:24:CYS:SG	2.12	0.89
3:C:102:GLN:HG2	3:C:154:LYS:HG3	1.52	0.89
5:E:180:ARG:HB2	5:E:215:MET:OXT	1.70	0.89
1:A:1170:ILE:HD12	1:A:1170:ILE:H	1.35	0.89
1:A:567:LYS:HE3	1:A:568:PRO:CD	2.01	0.89
1:A:779:PHE:HE1	1:A:785:PRO:HD3	1.38	0.89
1:A:107:CYS:HA	1:A:171:GLN:HE22	1.37	0.89
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.54	0.88
4:D:220:LEU:HD23	4:D:221:TYR:H	1.36	0.88
2:B:830:TYR:CE2	2:B:1000:PRO:HD3	2.08	0.88
2:B:364:ILE:HG13	2:B:585:VAL:HG22	1.54	0.88
8:H:95:TYR:HE2	8:H:97:MET:HG3	1.37	0.88
1:A:185:TRP:H	1:A:185:TRP:HE3	1.18	0.88
11:K:21:ILE:HG23	11:K:33:ILE:HG12	1.56	0.88
5:E:23:VAL:O	5:E:28:TYR:HB2	1.73	0.88
6:F:103:MET:CE	7:G:66:GLY:H	1.86	0.88
8:H:89:LEU:C	8:H:91:ASP:H	1.74	0.88
7:G:88:ASP:HB3	7:G:144:ARG:HA	1.54	0.88
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.56	0.87
9:I:26:LEU:HD23	9:I:37:GLU:HA	1.57	0.87
2:B:707:PRO:HG2	2:B:708:GLU:H	1.39	0.87
2:B:882:THR:HG23	2:B:884:ARG:N	1.90	0.87
12:L:55:ILE:HG12	12:L:56:LEU:H	1.40	0.87
1:A:225:ASN:HD22	1:A:228:PHE:H	1.16	0.87
4:D:138:ASN:HD21	7:G:35:GLU:HB3	1.37	0.87
5:E:78:LEU:HA	5:E:107:THR:HB	1.56	0.87
2:B:603:LEU:HD13	2:B:608:ASP:HB2	1.55	0.87
1:A:55:ASP:C	1:A:57:ARG:H	1.75	0.87
1:A:779:PHE:CE1	1:A:785:PRO:HD3	2.10	0.87
1:A:34:LYS:NZ	1:A:57:ARG:NH2	2.23	0.86
9:I:105:SER:O	9:I:106:CYS:HB3	1.75	0.86
1:A:671:ALA:HB3	1:A:676:MET:HG3	1.57	0.86
3:C:73:GLN:HE21	3:C:75:MET:H	1.21	0.86
2:B:168:GLY:H	2:B:450:ALA:HB1	1.38	0.86
1:A:868:TYR:HE1	1:A:1064:VAL:HG11	1.40	0.86
1:A:1308:THR:HG23	1:A:1309:ASP:N	1.90	0.86
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.58	0.86
5:E:16:PHE:CZ	5:E:20:LYS:HE2	2.11	0.85
1:A:1116:LEU:HB3	1:A:1308:THR:HG21	1.58	0.85

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:G:26:LEU:CD1	7:G:56:ILE:HD11	2.05	0.85
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.12	0.85
1:A:1107:VAL:HG12	1:A:1107:VAL:O	1.76	0.85
2:B:278:GLN:HG2	2:B:279:ASP:H	1.40	0.85
4:D:154:PHE:CD1	4:D:163:VAL:HG21	2.10	0.85
1:A:901:LEU:H	1:A:926:GLN:NE2	1.74	0.85
14:T:10:DA:H2"	14:T:11:DA:N7	1.90	0.85
2:B:597:MET:SD	2:B:624:LEU:HD11	2.16	0.85
6:F:69:LEU:HB3	6:F:71:GLU:CD	1.97	0.85
2:B:1007:VAL:HG22	2:B:1008:PRO:HD2	1.59	0.85
6:F:99:LEU:O	6:F:103:MET:HG2	1.77	0.85
1:A:668:ASP:HB3	1:A:741:ASN:HD21	1.41	0.85
1:A:1100:ARG:NH2	1:A:1351:GLU:HG2	1.92	0.85
5:E:120:ALA:O	5:E:123:LEU:HG	1.77	0.84
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.42	0.84
2:B:65:GLU:HG3	2:B:66:ASP:H	1.41	0.84
5:E:114:ASN:O	5:E:115:ASN:HB3	1.74	0.84
1:A:567:LYS:HB3	8:H:96:VAL:N	1.92	0.84
2:B:806:THR:HG22	2:B:808:ALA:N	1.92	0.84
2:B:664:THR:HA	2:B:667:GLN:HE21	1.41	0.84
2:B:345:LYS:HE2	2:B:349:ILE:HD11	1.60	0.83
2:B:579:ARG:HB2	2:B:586:TRP:NE1	1.93	0.83
2:B:911:ILE:HD11	2:B:941:LEU:HD13	1.59	0.83
2:B:841:MET:HG2	2:B:846:ILE:HD11	1.60	0.83
1:A:225:ASN:ND2	1:A:228:PHE:H	1.73	0.83
1:A:698:GLN:HA	9:I:97:MET:O	1.78	0.83
2:B:882:THR:HG23	2:B:884:ARG:HB2	1.59	0.83
8:H:130:ARG:NH1	8:H:130:ARG:HB2	1.93	0.83
1:A:1259:MET:HA	1:A:1262:LYS:HD2	1.60	0.83
4:D:23:ASN:H	4:D:23:ASN:HD22	1.24	0.83
1:A:503:GLN:HE21	6:F:90:ARG:NH2	1.76	0.83
1:A:1116:LEU:N	1:A:1308:THR:HG22	1.92	0.83
1:A:18:GLN:HG2	1:A:1418:LEU:HD13	1.58	0.83
2:B:805:THR:HG22	2:B:806:THR:H	1.43	0.83
7:G:138:THR:CG2	7:G:139:ILE:H	1.91	0.83
1:A:534:LEU:O	1:A:574:GLY:HA3	1.77	0.83
1:A:167:CYS:HB2	1:A:169:ASN:HD21	1.43	0.83
1:A:1224:LEU:HD11	1:A:1240:CYS:HB3	1.60	0.83
2:B:425:THR:HA	2:B:428:ILE:HD12	1.59	0.82
2:B:882:THR:HG21	2:B:935:ARG:HA	1.62	0.82
1:A:1293:SER:OG	1:A:1295:THR:HG23	1.79	0.82
7:G:122:ASN:ND2	7:G:125:SER:HB3	1.93	0.82

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:110:HIS:CB	12:L:54:ARG:HH22	1.92	0.82
2:B:559:SER:HA	2:B:563:MET:CB	2.07	0.82
1:A:40:THR:HG22	1:A:41:MET:HG3	1.62	0.82
1:A:14:VAL:H	1:A:1432:GLN:NE2	1.77	0.82
1:A:1348:LEU:O	1:A:1352:VAL:HG23	1.78	0.82
2:B:351:TYR:CE1	2:B:355:ILE:HD11	2.13	0.82
5:E:56:LYS:NZ	5:E:85:GLU:HG3	1.94	0.82
2:B:1065:GLN:HE21	2:B:1067:ARG:N	1.76	0.82
1:A:230:ARG:HG3	1:A:233:TRP:CZ3	2.13	0.82
1:A:591:PHE:HA	1:A:595:THR:HG21	1.59	0.82
11:K:47:ARG:HB3	11:K:47:ARG:HH11	1.44	0.82
3:C:120:ILE:HD13	3:C:124:LEU:HD11	1.61	0.82
3:C:128:ASN:O	3:C:129:ILE:HG13	1.77	0.82
1:A:1312:ASN:HD21	1:A:1315:GLU:HG3	1.45	0.82
8:H:65:LEU:HD23	8:H:65:LEU:N	1.95	0.82
2:B:583:ASN:ND2	2:B:628:THR:HG22	1.95	0.82
10:J:5:VAL:HG12	10:J:6:ARG:HG3	1.60	0.82
7:G:15:PRO:HA	7:G:18:PHE:CE1	2.15	0.82
2:B:1095:LEU:HD12	2:B:1095:LEU:H	1.45	0.81
2:B:798:TYR:HE2	3:C:62:PHE:CE2	1.97	0.81
1:A:831:THR:HG23	1:A:832:ALA:H	1.44	0.81
1:A:1420:ASP:HB2	1:A:1422:ARG:HG3	1.61	0.81
2:B:815:ARG:HD3	2:B:1041:GLU:OE2	1.79	0.81
1:A:646:PHE:O	1:A:650:GLN:HG3	1.80	0.81
2:B:1159:ARG:HB3	2:B:1159:ARG:HH11	1.46	0.81
8:H:101:ALA:HB2	8:H:116:TYR:CE2	2.15	0.81
1:A:390:GLN:HE21	1:A:394:ASN:HD22	1.27	0.81
1:A:1100:ARG:HH21	1:A:1351:GLU:HG2	1.44	0.81
1:A:332:LYS:HA	1:A:337:ARG:HB3	1.62	0.81
1:A:42:ASP:O	1:A:44:THR:N	2.13	0.81
10:J:53:HIS:CD2	10:J:54:VAL:N	2.47	0.81
8:H:40:LEU:HD13	8:H:123:MET:HE3	1.60	0.81
1:A:56:PRO:O	1:A:57:ARG:HG3	1.81	0.81
5:E:207:ARG:HH11	5:E:207:ARG:HB3	1.45	0.81
2:B:642:ASP:HA	2:B:649:LYS:HA	1.62	0.81
1:A:903:ASN:HD22	1:A:904:THR:N	1.78	0.81
5:E:124:VAL:HG13	5:E:132:ILE:HG13	1.62	0.81
7:G:119:LEU:HD11	7:G:130:TYR:HB3	1.63	0.81
1:A:11:LEU:O	1:A:11:LEU:HD23	1.81	0.81
1:A:666:ILE:HD12	1:A:667:GLY:H	1.45	0.81
4:D:195:ILE:HG22	4:D:198:LEU:HG	1.62	0.81
1:A:1387:HIS:HA	1:A:1391:ARG:HH11	1.45	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:H:130:ARG:HH11	8:H:130:ARG:HB2	1.45	0.81
2:B:577:ALA:CB	2:B:589:VAL:HG11	2.10	0.80
1:A:666:ILE:H	2:B:1026:LEU:HD13	1.44	0.80
1:A:49:LYS:NZ	1:A:61:ILE:HG13	1.96	0.80
2:B:842:ASN:HD22	2:B:845:SER:H	1.27	0.80
2:B:975:GLN:HG2	2:B:976:ILE:H	1.45	0.80
9:I:93:LYS:H	9:I:93:LYS:HD3	1.46	0.80
2:B:579:ARG:HB2	2:B:586:TRP:HE1	1.45	0.80
1:A:754:SER:H	1:A:757:ASN:HD22	1.29	0.80
3:C:177:GLU:HG3	3:C:231:ASN:HD22	1.45	0.80
1:A:332:LYS:C	1:A:334:GLY:H	1.85	0.80
1:A:896:ARG:HD3	1:A:897:TYR:CE1	2.16	0.80
1:A:889:SER:HB3	1:A:1297:GLU:HG3	1.64	0.80
1:A:683:ILE:HD13	1:A:801:GLU:HG3	1.63	0.80
2:B:613:VAL:HG13	2:B:627:PHE:O	1.82	0.80
1:A:1186:ASP:O	1:A:1187:GLN:HB3	1.81	0.80
2:B:1065:GLN:NE2	2:B:1067:ARG:H	1.78	0.80
14:T:15:DG:H2'	14:T:16:DT:H71	1.63	0.80
14:T:16:DT:H2''	14:T:17:DT:H5'	1.62	0.80
9:I:6:PHE:HB3	9:I:12:ASN:O	1.82	0.80
2:B:278:GLN:CG	2:B:279:ASP:H	1.93	0.80
1:A:901:LEU:HD22	1:A:919:ILE:HG23	1.64	0.80
3:C:66:ARG:NH1	10:J:2:ILE:HG21	1.97	0.80
1:A:14:VAL:N	1:A:1432:GLN:HE22	1.79	0.80
1:A:831:THR:HG23	1:A:832:ALA:N	1.96	0.80
2:B:1182:CYS:SG	2:B:1182:CYS:O	2.39	0.80
2:B:803:LEU:HD12	2:B:1032:SER:HB3	1.61	0.80
2:B:866:TYR:HB2	2:B:870:ILE:HB	1.63	0.79
7:G:30:LEU:HD22	7:G:72:VAL:HG11	1.63	0.79
5:E:22:MET:CE	5:E:26:ARG:HH21	1.94	0.79
2:B:172:ILE:HD13	2:B:178:ASN:HD22	1.46	0.79
5:E:44:ALA:O	5:E:45:LYS:HB2	1.81	0.79
1:A:697:ALA:HB2	1:A:702:LEU:HD12	1.64	0.79
1:A:571:LEU:HD22	8:H:46:LEU:HD11	1.65	0.79
2:B:165:VAL:HG11	2:B:448:ILE:HD13	1.64	0.79
6:F:119:ARG:HH11	6:F:119:ARG:HG3	1.46	0.79
1:A:427:GLN:HG3	1:A:430:TRP:CZ2	2.18	0.79
1:A:567:LYS:CE	1:A:568:PRO:HD2	2.12	0.79
1:A:563:PRO:HG3	1:A:572:TRP:CZ2	2.17	0.79
2:B:661:LEU:HD11	2:B:684:LEU:HD21	1.64	0.79
12:L:32:ALA:CB	12:L:55:ILE:HG13	2.12	0.79
12:L:60:ARG:HG2	12:L:61:THR:H	1.46	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:29:LEU:HD12	7:G:82:PHE:CZ	2.18	0.79
1:A:172:PRO:HB3	1:A:185:TRP:CD2	2.18	0.79
1:A:981:LEU:HD21	1:A:1039:LYS:HA	1.65	0.79
2:B:221:ASN:OD1	2:B:242:SER:HA	1.83	0.79
1:A:1241:ARG:O	1:A:1242:VAL:HG23	1.83	0.79
1:A:69:THR:O	1:A:71:GLN:N	2.16	0.79
5:E:117:THR:HG22	5:E:119:SER:N	1.96	0.78
7:G:9:LEU:HD12	7:G:10:ASN:H	1.48	0.78
2:B:942:ARG:HH22	14:T:23:BRU:H5"	1.47	0.78
5:E:117:THR:HB	5:E:120:ALA:HB2	1.65	0.78
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.65	0.78
1:A:535:THR:HG21	1:A:616:VAL:HA	1.66	0.78
7:G:14:HIS:CD2	7:G:16:SER:H	2.01	0.78
2:B:758:PHE:CE2	2:B:1044:ALA:HA	2.18	0.78
2:B:613:VAL:HG22	2:B:628:THR:HA	1.66	0.78
7:G:128:PRO:O	7:G:138:THR:HG23	1.84	0.78
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.65	0.78
2:B:126:SER:OG	2:B:172:ILE:HD11	1.84	0.78
1:A:710:LEU:HD12	1:A:710:LEU:H	1.47	0.78
8:H:59:ILE:HG22	8:H:60:ALA:N	1.97	0.78
2:B:294:ASP:H	9:I:12:ASN:ND2	1.81	0.78
4:D:203:SER:OG	4:D:206:GLU:HB2	1.83	0.78
7:G:106:MET:HG2	7:G:107:LYS:N	1.97	0.78
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.14	0.78
2:B:583:ASN:HD21	2:B:628:THR:CG2	1.95	0.78
1:A:49:LYS:HZ1	1:A:61:ILE:N	1.81	0.78
1:A:665:GLY:O	1:A:667:GLY:N	2.16	0.78
1:A:53:LEU:CD2	1:A:54:ASN:H	1.89	0.78
1:A:265:LYS:HE3	1:A:265:LYS:CA	2.13	0.78
4:D:159:THR:O	4:D:163:VAL:HG23	1.83	0.78
1:A:1291:VAL:HG22	1:A:1292:PRO:HD2	1.66	0.78
2:B:542:MET:HG2	2:B:747:MET:HE3	1.64	0.77
8:H:95:TYR:CE2	8:H:97:MET:HG3	2.18	0.77
4:D:130:LEU:HD13	4:D:142:LYS:HD3	1.65	0.77
5:E:90:VAL:HA	5:E:120:ALA:HB2	1.65	0.77
7:G:129:SER:HB3	7:G:138:THR:OG1	1.84	0.77
2:B:167:ILE:HG22	2:B:453:ILE:HD12	1.67	0.77
2:B:516:ASN:N	2:B:516:ASN:HD22	1.81	0.77
4:D:14:ARG:HB3	4:D:14:ARG:NH1	1.98	0.77
2:B:955:THR:HG22	2:B:956:THR:O	1.83	0.77
4:D:71:LYS:HA	4:D:74:GLN:CG	2.14	0.77
2:B:465:ASN:HD22	2:B:465:ASN:N	1.81	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:547:VAL:HG12	2:B:612:GLU:OE2	1.85	0.77
5:E:117:THR:HB	5:E:120:ALA:CB	2.15	0.77
2:B:1072:MET:HE3	2:B:1085:ILE:HB	1.67	0.77
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.65	0.77
2:B:25:ILE:HD11	2:B:653:VAL:O	1.85	0.77
3:C:253:LYS:O	3:C:256:ALA:HB3	1.84	0.77
10:J:1:MET:N	10:J:57:ILE:H	1.82	0.77
5:E:124:VAL:HG13	5:E:132:ILE:CG1	2.14	0.77
4:D:202:ILE:HD13	4:D:207:LEU:HB2	1.65	0.77
1:A:1135:ARG:HG2	1:A:1136:SER:N	2.00	0.77
2:B:745:PRO:O	2:B:748:ILE:HG12	1.85	0.77
8:H:127:GLY:O	8:H:128:ASN:HB2	1.83	0.77
3:C:45:ALA:HA	3:C:72:LEU:HD12	1.66	0.77
1:A:1227:ILE:HG22	1:A:1228:TRP:H	1.49	0.77
7:G:115:MET:HB3	7:G:116:PRO:HD2	1.65	0.76
1:A:1261:LYS:O	1:A:1264:GLU:HB3	1.85	0.76
2:B:589:VAL:HG12	2:B:590:HIS:H	1.50	0.76
2:B:987:LYS:HE3	15:P:11:G:O2'	1.85	0.76
1:A:1030:ARG:HG2	1:A:1034:GLU:OE2	1.86	0.76
1:A:666:ILE:N	2:B:1026:LEU:HD13	2.00	0.76
5:E:22:MET:HE1	5:E:26:ARG:NH2	2.01	0.76
2:B:193:LYS:NZ	12:L:32:ALA:HB1	1.99	0.76
2:B:824:ILE:HG12	10:J:48:ARG:NH1	2.01	0.76
14:T:27:DC:H42	15:P:2:A:H61	1.30	0.76
5:E:198:ILE:HD11	5:E:212:ARG:HG3	1.65	0.76
2:B:796:LEU:HD21	2:B:821:GLN:HE21	1.50	0.76
5:E:22:MET:HE3	5:E:26:ARG:HE	1.50	0.76
8:H:100:THR:HG23	8:H:138:GLU:HA	1.68	0.76
13:N:5:DC:H2''	13:N:6:DT:OP2	1.84	0.76
2:B:327:ARG:NH2	2:B:371:GLU:HG2	2.00	0.76
1:A:427:GLN:HG3	1:A:430:TRP:CE2	2.21	0.76
1:A:1214:GLU:O	1:A:1218:GLN:HG2	1.85	0.76
1:A:63:ARG:HA	1:A:74:MET:HE2	1.68	0.76
1:A:675:THR:O	1:A:679:ILE:HG13	1.85	0.76
2:B:254:LEU:HD12	2:B:272:THR:O	1.85	0.76
1:A:1409:LEU:HD13	2:B:1207:LEU:HD11	1.66	0.76
2:B:261:ARG:HB3	2:B:261:ARG:NH1	1.98	0.76
2:B:975:GLN:HG2	2:B:976:ILE:N	2.00	0.76
1:A:913:LEU:HD12	1:A:914:GLU:N	1.99	0.76
2:B:603:LEU:HD12	2:B:609:ILE:HG23	1.67	0.75
12:L:49:LYS:O	12:L:50:ASP:HB2	1.85	0.75
1:A:388:LEU:O	1:A:392:VAL:HG23	1.87	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1206:ASP:HB3	1:A:1274:ARG:NH2	1.99	0.75
2:B:654:ARG:H	2:B:657:HIS:HD2	1.31	0.75
2:B:565:PRO:HB2	2:B:567:GLU:HG2	1.67	0.75
2:B:882:THR:CG2	2:B:884:ARG:H	2.00	0.75
4:D:167:LEU:HD21	4:D:214:LEU:HD21	1.69	0.75
1:A:1385:THR:HG22	1:A:1386:ARG:N	2.01	0.75
2:B:278:GLN:HG2	2:B:279:ASP:N	2.00	0.75
8:H:84:ALA:HB1	8:H:87:ARG:HB2	1.69	0.75
1:A:1158:PRO:HG2	1:A:1159:ARG:HE	1.49	0.75
1:A:372:LYS:HA	1:A:435:HIS:ND1	2.00	0.75
2:B:839:MET:HE3	2:B:1010:LEU:HD21	1.67	0.75
7:G:21:ARG:NH1	7:G:24:GLN:HB2	2.01	0.75
8:H:104:PHE:CZ	8:H:136:LYS:HA	2.20	0.75
2:B:351:TYR:O	2:B:355:ILE:HG13	1.86	0.75
2:B:483:LEU:HD11	2:B:491:THR:HG23	1.68	0.75
1:A:524:VAL:HG12	1:A:525:GLN:H	1.49	0.75
2:B:272:THR:HG23	2:B:279:ASP:OD1	1.87	0.75
3:C:98:VAL:C	3:C:99:LEU:HD23	2.07	0.75
2:B:955:THR:HG22	2:B:956:THR:N	2.02	0.75
2:B:806:THR:H	2:B:809:MET:HE3	1.52	0.74
2:B:345:LYS:HG2	2:B:346:GLU:N	1.99	0.74
3:C:123:ASN:ND2	3:C:125:MET:HG2	2.01	0.74
2:B:112:LEU:HD12	2:B:113:TYR:H	1.52	0.74
3:C:259:LEU:HD21	11:K:91:CYS:HB3	1.69	0.74
2:B:593:PRO:HG2	2:B:617:ARG:NH2	2.02	0.74
2:B:408:LEU:O	2:B:412:LEU:HD12	1.87	0.74
1:A:1033:GLN:HA	1:A:1036:ARG:HH12	1.52	0.74
8:H:130:ARG:HD3	8:H:130:ARG:N	2.02	0.74
2:B:710:LEU:CA	2:B:733:HIS:HB3	2.18	0.74
5:E:144:ILE:HG13	5:E:145:THR:N	2.03	0.74
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.23	0.74
3:C:115:SER:HB3	3:C:141:GLY:O	1.86	0.74
1:A:886:ILE:HG23	1:A:887:GLY:N	2.03	0.74
2:B:549:THR:HB	2:B:628:THR:OG1	1.87	0.74
1:A:709:THR:HG22	1:A:710:LEU:H	1.53	0.74
1:A:399:HIS:O	1:A:401:GLY:N	2.20	0.74
9:I:85:PHE:HD2	9:I:85:PHE:H	1.35	0.74
3:C:99:LEU:HD23	3:C:99:LEU:N	2.02	0.74
1:A:868:TYR:HD2	1:A:1058:VAL:HG21	1.50	0.74
1:A:722:LEU:HD21	1:A:794:PRO:HB3	1.68	0.74
2:B:848:ARG:HH22	2:B:996:ARG:HD3	1.53	0.74
5:E:147:HIS:HB3	5:E:150:VAL:HG23	1.69	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:H:130:ARG:HH11	8:H:130:ARG:H	1.35	0.74
11:K:46:ILE:O	11:K:50:LEU:HB2	1.88	0.74
1:A:821:ARG:HB2	1:A:821:ARG:HH11	1.53	0.74
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.51	0.74
2:B:642:ASP:HB3	2:B:649:LYS:CD	2.18	0.74
15:P:5:C:O2'	15:P:6:A:H5'	1.88	0.74
2:B:1039:GLY:HA2	10:J:51:LEU:HD21	1.66	0.74
4:D:71:LYS:HA	4:D:74:GLN:HG3	1.70	0.74
2:B:68:THR:HG22	2:B:91:SER:HA	1.70	0.74
1:A:399:HIS:CB	1:A:400:PRO:HD3	2.18	0.73
7:G:125:SER:OG	7:G:128:PRO:HA	1.88	0.73
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.69	0.73
1:A:288:ALA:HA	1:A:291:GLU:OE1	1.89	0.73
2:B:637:LEU:HD12	2:B:693:ILE:HD11	1.69	0.73
1:A:407:ARG:HG2	1:A:430:TRP:CZ2	2.23	0.73
2:B:114:PRO:HG2	2:B:115:GLN:H	1.54	0.73
2:B:508:LEU:HD13	2:B:510:LYS:CE	2.14	0.73
8:H:89:LEU:O	8:H:91:ASP:N	2.22	0.73
1:A:12:ARG:HB3	2:B:1218:THR:CG2	2.18	0.73
1:A:828:ALA:HB2	2:B:530:GLY:HA2	1.69	0.73
12:L:55:ILE:O	12:L:56:LEU:HB2	1.88	0.73
8:H:139:ASN:O	8:H:140:ALA:HB2	1.89	0.73
11:K:65:HIS:HD2	11:K:67:PHE:H	1.36	0.73
1:A:308:ILE:HG22	1:A:309:ALA:H	1.51	0.73
3:C:3:GLU:HG2	3:C:4:GLU:HG3	1.70	0.73
1:A:399:HIS:HB3	1:A:400:PRO:CD	2.18	0.73
2:B:918:ILE:HG21	2:B:935:ARG:NH2	2.03	0.73
2:B:622:LYS:HE2	9:I:59:VAL:CG2	2.19	0.73
2:B:110:HIS:HB3	12:L:54:ARG:HH22	1.51	0.73
1:A:93:VAL:CG2	1:A:301:ALA:HA	2.17	0.73
3:C:183:TRP:O	3:C:185:LYS:N	2.21	0.73
1:A:49:LYS:HZ1	1:A:61:ILE:HG13	1.54	0.73
12:L:53:HIS:HB3	12:L:55:ILE:CD1	2.18	0.73
3:C:189:THR:HG22	3:C:190:ASP:N	2.01	0.73
2:B:557:PHE:HD2	2:B:557:PHE:O	1.72	0.73
1:A:549:MET:HE3	1:A:656:TRP:CD1	2.21	0.73
12:L:30:ILE:O	12:L:56:LEU:HD23	1.88	0.73
2:B:999:MET:HA	2:B:999:MET:CE	2.18	0.73
4:D:193:THR:HG21	7:G:167:TYR:CD1	2.24	0.73
2:B:219:ALA:HB2	2:B:405:ARG:NH1	2.03	0.73
1:A:898:ARG:HD2	1:A:899:VAL:N	2.04	0.73
4:D:7:THR:O	4:D:9:GLN:N	2.21	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1329:THR:HG22	1:A:1331:SER:N	2.03	0.73
3:C:22:LEU:HG	3:C:25:VAL:HG21	1.71	0.73
4:D:23:ASN:N	4:D:23:ASN:ND2	2.33	0.73
4:D:4:SER:O	4:D:5:THR:HB	1.88	0.73
1:A:157:ASP:OD2	1:A:159:THR:HB	1.88	0.73
5:E:207:ARG:NH1	5:E:207:ARG:HB3	2.03	0.73
9:I:7:CYS:HB3	9:I:14:LEU:HD21	1.68	0.73
1:A:1121:GLU:HG2	1:A:1122:PRO:HD2	1.71	0.73
1:A:35:ILE:HA	1:A:52:GLY:O	1.89	0.73
2:B:800:GLN:HB3	10:J:52:THR:HG22	1.71	0.72
10:J:23:ASN:C	10:J:25:LEU:H	1.93	0.72
2:B:842:ASN:ND2	2:B:845:SER:H	1.86	0.72
2:B:186:GLU:HG3	10:J:62:ARG:HH22	1.52	0.72
14:T:16:DT:H2''	14:T:17:DT:C5'	2.20	0.72
11:K:12:LEU:HD12	11:K:37:LYS:HG2	1.71	0.72
2:B:1201:LYS:HE2	2:B:1205:GLN:OE1	1.89	0.72
2:B:865:LYS:NZ	2:B:869:SER:HA	2.04	0.72
6:F:103:MET:HE1	7:G:66:GLY:H	1.53	0.72
2:B:134:LYS:HE2	2:B:164:LYS:NZ	2.04	0.72
5:E:164:LEU:HD13	5:E:211:TYR:CE2	2.25	0.72
1:A:66:LYS:HD3	1:A:67:CYS:N	2.05	0.72
7:G:1:MET:SD	7:G:2:PHE:N	2.62	0.72
2:B:653:VAL:HG23	2:B:689:LEU:HB3	1.70	0.72
3:C:189:THR:HG22	3:C:190:ASP:H	1.53	0.72
3:C:167:HIS:CD2	12:L:70:ARG:HB3	2.24	0.72
2:B:1072:MET:CE	2:B:1085:ILE:HB	2.20	0.72
1:A:236:LEU:HD11	1:A:304:MET:HE1	1.71	0.72
3:C:209:TYR:H	3:C:209:TYR:HD1	1.35	0.72
1:A:102:VAL:CG1	1:A:211:PHE:HE1	2.02	0.72
2:B:800:GLN:HB3	10:J:52:THR:HG21	1.69	0.72
4:D:23:ASN:ND2	4:D:23:ASN:H	1.88	0.72
1:A:1149:ALA:HB2	9:I:47:GLU:HA	1.72	0.72
2:B:515:HIS:CD2	2:B:517:THR:HG23	2.25	0.72
11:K:45:LEU:HG	11:K:94:ILE:HD13	1.71	0.72
1:A:310:GLY:O	1:A:312:PRO:HD2	1.88	0.72
8:H:11:GLN:HA	8:H:53:ASP:O	1.89	0.72
2:B:705:MET:H	2:B:710:LEU:HD12	1.54	0.72
1:A:70:CYS:O	1:A:72:GLU:HG2	1.89	0.72
1:A:767:GLN:NE2	1:A:774:ARG:HB3	2.05	0.72
4:D:160:VAL:O	4:D:164:ILE:HG13	1.89	0.72
1:A:425:GLN:N	1:A:425:GLN:OE1	2.22	0.72
1:A:666:ILE:CD1	1:A:667:GLY:H	2.02	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:248:SER:H	2:B:418:LYS:HZ3	1.35	0.72
2:B:953:LEU:HD21	2:B:965:LYS:HB2	1.72	0.72
7:G:21:ARG:HD2	7:G:24:GLN:HB3	1.72	0.72
1:A:858:ASN:ND2	1:A:860:LEU:H	1.88	0.72
1:A:34:LYS:HZ1	1:A:57:ARG:NH2	1.87	0.72
12:L:55:ILE:HD13	12:L:55:ILE:H	1.55	0.72
1:A:1387:HIS:O	1:A:1391:ARG:HD3	1.90	0.72
2:B:824:ILE:HG12	10:J:48:ARG:HH12	1.53	0.72
3:C:7:GLN:HG3	11:K:104:ASN:HD22	1.53	0.72
1:A:1205:LYS:O	1:A:1207:LEU:HG	1.89	0.72
2:B:644:GLU:OE2	2:B:646:LEU:HB2	1.90	0.71
2:B:435:THR:C	2:B:437:GLU:H	1.93	0.71
2:B:44:VAL:HG21	2:B:199:MET:O	1.90	0.71
2:B:549:THR:HG22	2:B:550:ASP:N	2.05	0.71
3:C:79:GLN:HE21	3:C:127:ARG:HD3	1.55	0.71
5:E:124:VAL:HA	5:E:132:ILE:HD12	1.71	0.71
8:H:62:SER:O	8:H:63:LEU:HG	1.89	0.71
1:A:1438:THR:HB	2:B:1144:ALA:HB3	1.71	0.71
8:H:102:TYR:OH	8:H:122:LEU:HD22	1.89	0.71
7:G:111:THR:CG2	7:G:114:LEU:HD13	2.20	0.71
12:L:32:ALA:HB2	12:L:55:ILE:HG13	1.73	0.71
2:B:758:PHE:CE1	2:B:1027:ILE:HG22	2.25	0.71
1:A:37:PHE:HB2	1:A:52:GLY:HA3	1.72	0.71
1:A:305:ASP:OD2	1:A:326:ARG:HD3	1.90	0.71
1:A:135:PHE:CD1	1:A:222:LEU:HD22	2.24	0.71
1:A:1118:VAL:CG2	1:A:1306:LEU:HB2	2.20	0.71
10:J:64:ASN:HB3	10:J:65:PRO:HD2	1.73	0.71
3:C:76:ASP:OD2	3:C:128:ASN:N	2.24	0.71
1:A:960:ILE:O	1:A:963:ILE:HG22	1.90	0.71
2:B:1096:ARG:O	2:B:1097:HIS:HB2	1.91	0.71
2:B:345:LYS:CG	2:B:346:GLU:H	1.99	0.71
1:A:503:GLN:HE21	6:F:90:ARG:HH22	1.34	0.71
1:A:381:THR:HG22	1:A:383:TYR:N	2.03	0.71
3:C:56:THR:HG22	3:C:57:VAL:H	1.54	0.71
1:A:344:ARG:NH1	1:A:344:ARG:HB3	2.06	0.71
2:B:248:SER:H	2:B:418:LYS:NZ	1.88	0.71
2:B:1031:LEU:HD11	2:B:1042:GLY:HA3	1.73	0.71
5:E:100:ILE:HG23	5:E:105:PHE:HB2	1.72	0.71
1:A:821:ARG:HB2	1:A:821:ARG:NH1	2.06	0.71
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.73	0.71
1:A:335:ARG:NH1	2:B:1202:LEU:HD13	2.05	0.70
2:B:860:MET:HG3	2:B:965:LYS:HG2	1.72	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:H:24:CYS:HB2	8:H:44:VAL:HG21	1.72	0.70
3:C:66:ARG:NH2	10:J:3:VAL:O	2.24	0.70
1:A:670:ILE:HG23	1:A:805:LEU:HD21	1.73	0.70
4:D:24:ALA:CB	4:D:26:THR:HG23	2.21	0.70
2:B:424:LEU:O	2:B:428:ILE:HG13	1.90	0.70
11:K:68:PHE:HD1	11:K:70:ARG:HH12	1.39	0.70
5:E:197:LYS:HE2	5:E:199:ILE:HD11	1.73	0.70
9:I:71:SER:OG	9:I:83:ASN:HB2	1.92	0.70
3:C:220:ASP:CG	3:C:223:ALA:HB2	2.11	0.70
1:A:1424:VAL:HG11	2:B:1139:ILE:CD1	2.20	0.70
9:I:34:TYR:CD2	9:I:35:VAL:N	2.60	0.70
1:A:268:ASP:HB3	1:A:299:HIS:ND1	2.05	0.70
7:G:34:VAL:HG11	7:G:74:TYR:CE1	2.21	0.70
2:B:983:ARG:NH1	2:B:1028:GLU:OE1	2.24	0.70
2:B:243:ALA:HA	2:B:250:PHE:O	1.91	0.70
2:B:890:TYR:O	2:B:893:LEU:HB2	1.91	0.70
1:A:1244:ARG:HB2	1:A:1245:PRO:CD	2.22	0.70
2:B:842:ASN:ND2	2:B:845:SER:OG	2.24	0.70
1:A:1148:ILE:HD11	1:A:1198:ASP:HA	1.74	0.70
1:A:444:PHE:HB3	1:A:458:HIS:HD2	1.56	0.70
2:B:705:MET:N	2:B:710:LEU:HD12	2.05	0.70
9:I:55:THR:HG23	9:I:86:PHE:HZ	1.55	0.70
2:B:980:PHE:HE1	2:B:990:ILE:HD11	1.56	0.70
1:A:763:ALA:O	1:A:803:SER:HB3	1.91	0.70
3:C:11:ARG:HH12	3:C:205:LYS:NZ	1.90	0.70
2:B:361:LEU:HD21	2:B:377:PHE:CD2	2.27	0.70
2:B:600:LEU:O	2:B:609:ILE:HD11	1.92	0.70
2:B:616:ILE:HG12	2:B:697:GLU:HA	1.72	0.70
2:B:29:ASP:HB3	2:B:658:ILE:CD1	2.22	0.70
12:L:27:LEU:HD13	12:L:37:LYS:HD2	1.74	0.70
3:C:93:ASP:OD1	3:C:122:SER:HB2	1.92	0.70
1:A:1081:LEU:HD11	1:A:1098:VAL:H	1.55	0.70
1:A:244:PRO:HB2	1:A:245:PRO:CD	2.18	0.70
2:B:859:TYR:CZ	2:B:941:LEU:HD12	2.26	0.70
1:A:828:ALA:CB	2:B:530:GLY:HA2	2.21	0.70
2:B:681:TRP:HA	2:B:684:LEU:HD12	1.74	0.70
4:D:71:LYS:HG2	4:D:74:GLN:HG3	1.74	0.70
12:L:38:LEU:HD11	12:L:49:LYS:HE2	1.74	0.70
2:B:235:SER:C	2:B:236:HIS:HD2	1.95	0.70
1:A:1004:ASN:ND2	5:E:167:ARG:HD2	2.07	0.70
3:C:143:LEU:HD21	3:C:146:LYS:HE2	1.73	0.70
9:I:55:THR:HG21	9:I:109:ILE:HD13	1.73	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:1122:ARG:HB3	14:T:22:DC:OP1	1.92	0.70
5:E:202:SER:OG	5:E:204:THR:HG22	1.90	0.70
4:D:190:GLU:O	4:D:193:THR:HG22	1.92	0.70
4:D:208:GLU:O	4:D:212:LYS:HG3	1.92	0.70
9:I:50:THR:HG23	9:I:52:ILE:HG12	1.73	0.70
1:A:866:PHE:O	1:A:867:ILE:HD12	1.91	0.70
2:B:345:LYS:O	2:B:347:LYS:HG2	1.92	0.69
1:A:567:LYS:HE3	1:A:568:PRO:CG	2.21	0.69
1:A:883:LEU:HD11	1:A:1017:LEU:HD11	1.73	0.69
8:H:4:THR:HA	8:H:60:ALA:CB	2.17	0.69
1:A:1436:ILE:O	1:A:1437:GLY:C	2.30	0.69
11:K:107:THR:O	11:K:111:LEU:HG	1.92	0.69
3:C:186:LEU:CD2	3:C:225:ALA:HB2	2.22	0.69
1:A:567:LYS:CG	1:A:568:PRO:HD2	2.22	0.69
1:A:500:GLU:O	1:A:504:LEU:HB2	1.93	0.69
2:B:217:ARG:HE	2:B:405:ARG:HB2	1.57	0.69
1:A:982:THR:HB	1:A:985:ASP:H	1.56	0.69
1:A:53:LEU:CD2	1:A:54:ASN:N	2.50	0.69
1:A:1155:ASP:OD2	1:A:1161:THR:HA	1.93	0.69
11:K:55:LYS:HB3	11:K:81:TYR:HD1	1.57	0.69
5:E:90:VAL:HB	5:E:117:THR:HG21	1.73	0.69
5:E:23:VAL:HG13	5:E:78:LEU:HD13	1.74	0.69
7:G:51:TYR:O	7:G:54:ILE:HG13	1.91	0.69
3:C:89:GLU:O	3:C:90:ASP:HB3	1.93	0.69
2:B:882:THR:CG2	2:B:934:LYS:O	2.41	0.69
3:C:16:ASP:C	3:C:240:VAL:HG11	2.12	0.69
2:B:839:MET:HE1	2:B:980:PHE:HB2	1.75	0.69
5:E:164:LEU:HD22	5:E:211:TYR:CD2	2.27	0.69
6:F:86:THR:HG23	6:F:89:GLU:OE1	1.92	0.69
9:I:102:VAL:HG22	9:I:109:ILE:HG12	1.73	0.69
8:H:130:ARG:HH11	8:H:130:ARG:CB	2.05	0.69
9:I:76:PRO:HD2	9:I:108:HIS:HD2	1.57	0.69
8:H:58:THR:HB	8:H:143:LEU:HD13	1.73	0.69
1:A:351:THR:HG22	2:B:1103:ILE:CA	2.23	0.69
1:A:1291:VAL:HG22	1:A:1292:PRO:CD	2.23	0.69
1:A:898:ARG:HD2	1:A:899:VAL:H	1.57	0.69
1:A:443:LEU:HD12	2:B:1146:PHE:CE2	2.28	0.69
1:A:916:GLY:O	1:A:919:ILE:HG22	1.93	0.69
12:L:30:ILE:HG22	12:L:31:CYS:N	2.07	0.69
4:D:23:ASN:N	4:D:23:ASN:HD22	1.91	0.69
3:C:186:LEU:HD21	3:C:225:ALA:HB2	1.74	0.69
1:A:105:CYS:SG	1:A:139:TRP:HA	2.32	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.75	0.69
1:A:7:SER:OG	2:B:1161:HIS:HE1	1.75	0.69
2:B:957:ASN:HD21	2:B:961:LEU:HB2	1.58	0.69
2:B:1002:THR:OG1	2:B:1006:ILE:HG13	1.93	0.69
3:C:133:ILE:HD12	3:C:237:SER:N	2.08	0.69
1:A:1420:ASP:O	1:A:1421:CYS:HB2	1.93	0.69
2:B:60:GLN:O	2:B:63:ILE:HG22	1.93	0.69
1:A:249:SER:O	1:A:250:ILE:HG13	1.91	0.69
1:A:1095:THR:HG21	1:A:1112:LYS:CB	2.23	0.68
2:B:1084:GLN:HG2	3:C:201:TRP:CZ2	2.28	0.68
2:B:405:ARG:NE	2:B:629:ASP:OD2	2.26	0.68
5:E:32:GLN:HG3	5:E:36:GLU:OE2	1.93	0.68
1:A:512:VAL:HA	1:A:519:PRO:HA	1.75	0.68
8:H:76:THR:O	8:H:77:ARG:HB2	1.92	0.68
2:B:805:THR:HG22	2:B:806:THR:N	2.07	0.68
1:A:1312:ASN:ND2	1:A:1315:GLU:HG3	2.08	0.68
7:G:21:ARG:HD2	7:G:24:GLN:CB	2.23	0.68
1:A:444:PHE:HB3	1:A:458:HIS:CD2	2.27	0.68
6:F:109:VAL:HG12	6:F:110:ASP:N	2.05	0.68
1:A:853:ASP:O	1:A:854:ASN:HB2	1.92	0.68
1:A:323:LYS:N	1:A:323:LYS:HD2	2.04	0.68
1:A:741:ASN:HD22	1:A:742:ASN:N	1.90	0.68
7:G:115:MET:HG2	7:G:163:ILE:HD11	1.74	0.68
10:J:12:LYS:O	10:J:14:VAL:HG23	1.93	0.68
1:A:567:LYS:CB	1:A:568:PRO:CD	2.69	0.68
1:A:567:LYS:HB3	8:H:95:TYR:HA	1.74	0.68
1:A:1254:ALA:O	1:A:1255:GLU:HB2	1.92	0.68
1:A:1255:GLU:HG2	1:A:1258:HIS:HD2	1.58	0.68
4:D:50:LEU:HD11	7:G:4:ILE:HD11	1.74	0.68
3:C:147:LEU:HB2	3:C:151:GLN:HB2	1.74	0.68
2:B:737:THR:CG2	9:I:66:PRO:HA	2.23	0.68
2:B:987:LYS:HD3	2:B:987:LYS:H	1.57	0.68
1:A:167:CYS:HB2	1:A:169:ASN:ND2	2.08	0.68
2:B:891:ASP:C	2:B:893:LEU:H	1.97	0.68
2:B:873:THR:O	2:B:914:LYS:HA	1.93	0.68
14:T:11:DA:H2''	14:T:12:DG:H5'	1.75	0.68
5:E:124:VAL:N	5:E:125:PRO:HD2	2.09	0.68
1:A:55:ASP:CG	1:A:55:ASP:O	2.29	0.68
1:A:62:ASP:O	1:A:63:ARG:C	2.30	0.68
14:T:10:DA:H2''	14:T:11:DA:C8	2.29	0.68
1:A:1121:GLU:CG	1:A:1122:PRO:HD2	2.22	0.68
1:A:1188:GLN:OE1	1:A:1241:ARG:HD2	1.93	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1100:ARG:HH21	1:A:1351:GLU:CG	2.06	0.68
7:G:116:PRO:HG2	7:G:119:LEU:CB	2.24	0.68
11:K:65:HIS:CD2	11:K:67:PHE:H	2.11	0.68
1:A:1029:ARG:HG3	1:A:1029:ARG:HH11	1.59	0.68
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.75	0.68
5:E:31:THR:HG23	5:E:34:GLU:HB2	1.74	0.68
6:F:96:THR:O	6:F:100:GLN:HG3	1.93	0.68
2:B:23:ALA:HB1	2:B:24:PRO:HD2	1.76	0.68
1:A:154:SER:HB3	1:A:162:VAL:CG2	2.24	0.68
12:L:48:CYS:HB3	12:L:51:CYS:O	1.93	0.68
4:D:24:ALA:HB3	4:D:26:THR:CG2	2.24	0.68
2:B:237:VAL:HG22	2:B:257:LYS:HA	1.75	0.68
1:A:709:THR:HG23	9:I:94:ASP:HA	1.75	0.68
1:A:107:CYS:SG	1:A:148:CYS:HB2	2.34	0.68
1:A:1127:ASP:CG	1:A:1130:GLN:HB2	2.13	0.68
2:B:464:GLY:O	2:B:477:ALA:HA	1.94	0.68
1:A:117:GLU:H	1:A:117:GLU:CD	1.96	0.68
2:B:232:SER:HA	14:T:11:DA:OP1	1.93	0.67
2:B:43:LEU:HD11	2:B:811:TYR:O	1.94	0.67
1:A:709:THR:HB	1:A:712:GLU:H	1.59	0.67
1:A:1158:PRO:HG2	1:A:1159:ARG:NE	2.09	0.67
1:A:858:ASN:C	1:A:858:ASN:HD22	1.98	0.67
1:A:152:VAL:CG1	1:A:153:PRO:HD2	2.24	0.67
10:J:27:GLU:O	10:J:29:GLU:N	2.28	0.67
2:B:705:MET:H	2:B:710:LEU:CD1	2.07	0.67
4:D:59:ILE:HG21	4:D:145:MET:SD	2.35	0.67
1:A:284:ALA:O	1:A:286:HIS:N	2.28	0.67
2:B:589:VAL:HG12	2:B:590:HIS:N	2.10	0.67
1:A:34:LYS:HZ2	1:A:57:ARG:NH2	1.90	0.67
10:J:3:VAL:HG21	10:J:18:TRP:CB	2.22	0.67
1:A:369:SER:HB3	11:K:2:ASN:OD1	1.93	0.67
1:A:66:LYS:HZ3	1:A:68:GLN:N	1.83	0.67
2:B:863:GLU:O	2:B:961:LEU:HD13	1.94	0.67
8:H:81:PRO:CB	8:H:82:PRO:HD2	2.24	0.67
1:A:683:ILE:HD13	1:A:801:GLU:CG	2.24	0.67
1:A:886:ILE:HG23	1:A:887:GLY:H	1.58	0.67
1:A:1323:ASP:OD1	1:A:1325:THR:HG22	1.94	0.67
3:C:254:LYS:O	3:C:258:ILE:HD13	1.94	0.67
1:A:1187:GLN:HA	1:A:1244:ARG:HB3	1.76	0.67
2:B:846:ILE:CG2	2:B:974:PRO:HG2	2.23	0.67
5:E:69:ILE:HD12	5:E:69:ILE:N	2.09	0.67
1:A:743:VAL:O	1:A:747:VAL:HG23	1.94	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:F:89:GLU:O	6:F:93:ILE:HD12	1.94	0.67
1:A:524:VAL:HG12	1:A:525:GLN:N	2.10	0.67
1:A:946:VAL:HG12	1:A:947:PHE:CD2	2.30	0.67
2:B:399:ASP:OD2	2:B:510:LYS:HB2	1.95	0.67
1:A:718:VAL:O	1:A:722:LEU:HD12	1.95	0.67
4:D:32:GLU:OE1	7:G:41:LYS:HE2	1.94	0.67
8:H:30:SER:HB2	8:H:36:CYS:HB3	1.77	0.67
2:B:863:GLU:OE2	2:B:873:THR:HA	1.94	0.67
9:I:55:THR:HG23	9:I:86:PHE:CZ	2.30	0.67
2:B:68:THR:HG22	2:B:91:SER:HB3	1.77	0.67
2:B:291:ILE:HD13	2:B:300:HIS:CD2	2.30	0.67
9:I:116:ASN:C	9:I:117:LYS:HD2	2.15	0.67
1:A:809:THR:OG1	1:A:812:GLU:HG3	1.94	0.67
2:B:899:ILE:HG22	2:B:900:ALA:O	1.95	0.67
4:D:119:ARG:HG3	4:D:119:ARG:HH11	1.60	0.66
5:E:94:LYS:O	5:E:98:ILE:HG13	1.95	0.66
9:I:80:SER:OG	9:I:105:SER:HB2	1.95	0.66
2:B:515:HIS:H	2:B:518:HIS:HD2	1.43	0.66
9:I:50:THR:HG22	9:I:51:ASN:N	2.10	0.66
1:A:567:LYS:CB	8:H:95:TYR:HA	2.24	0.66
1:A:382:PRO:CA	1:A:428:TYR:HE2	2.07	0.66
9:I:55:THR:O	9:I:55:THR:HG22	1.94	0.66
2:B:1187:ASN:O	2:B:1188:LYS:CB	2.42	0.66
1:A:925:LEU:HD13	1:A:983:ILE:CG2	2.24	0.66
1:A:332:LYS:O	1:A:333:GLU:HB2	1.94	0.66
3:C:47:ASP:HA	12:L:69:ALA:HB3	1.78	0.66
8:H:95:TYR:HE2	8:H:97:MET:CG	2.06	0.66
9:I:58:VAL:HG13	9:I:62:ILE:HD13	1.78	0.66
1:A:1223:ASP:HA	1:A:1243:VAL:HG11	1.76	0.66
2:B:917:PRO:O	2:B:918:ILE:HG13	1.95	0.66
1:A:684:ALA:O	1:A:687:LYS:HB2	1.94	0.66
1:A:688:LYS:HD2	1:A:691:LEU:HD23	1.77	0.66
2:B:251:ILE:HG22	2:B:251:ILE:O	1.96	0.66
2:B:778:MET:CE	2:B:1094:ARG:HD3	2.24	0.66
9:I:8:ARG:HG3	9:I:34:TYR:CE1	2.30	0.66
1:A:122:MET:HA	1:A:141:LEU:CD1	2.25	0.66
1:A:55:ASP:N	1:A:56:PRO:HD3	2.10	0.66
3:C:124:LEU:HD21	3:C:129:ILE:O	1.95	0.66
4:D:185:CYS:O	4:D:211:LEU:HD22	1.94	0.66
9:I:76:PRO:HD2	9:I:108:HIS:CD2	2.29	0.66
3:C:161:LYS:O	3:C:170:TRP:NE1	2.27	0.66
8:H:89:LEU:C	8:H:91:ASP:N	2.47	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:29:LEU:HD22	4:D:29:LEU:N	2.10	0.66
6:F:82:THR:CG2	6:F:84:TYR:H	2.09	0.66
6:F:69:LEU:HD13	6:F:71:GLU:OE1	1.96	0.66
1:A:547:LEU:HD13	11:K:58:PHE:CD1	2.31	0.66
10:J:44:TYR:HA	10:J:47:ARG:HB2	1.77	0.66
3:C:184:ASN:OD1	3:C:187:LYS:HA	1.94	0.66
1:A:866:PHE:C	1:A:867:ILE:HD12	2.15	0.66
1:A:446:ARG:HB3	1:A:478:TYR:HB3	1.77	0.66
8:H:58:THR:HG22	8:H:59:ILE:H	1.60	0.66
1:A:7:SER:HB3	2:B:1193:GLN:HE22	1.60	0.66
1:A:563:PRO:HD3	8:H:79:TRP:CD1	2.31	0.66
1:A:942:PHE:HE1	5:E:207:ARG:HD3	1.58	0.66
1:A:346:ASP:HB3	2:B:1108:ARG:H	1.60	0.66
2:B:558:LEU:CD2	2:B:596:LEU:HD11	2.26	0.66
2:B:394:ASP:N	2:B:394:ASP:OD2	2.23	0.66
2:B:110:HIS:HB2	12:L:54:ARG:NH2	2.10	0.66
5:E:19:VAL:O	5:E:23:VAL:HG23	1.95	0.66
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.78	0.66
5:E:48:ASP:HB3	5:E:54:GLN:NE2	2.10	0.66
2:B:69:LEU:HB3	2:B:429:PHE:HE1	1.61	0.66
1:A:50:ILE:C	1:A:52:GLY:H	1.98	0.66
2:B:1099:VAL:HG13	2:B:1100:ASP:N	2.11	0.66
1:A:1027:ALA:O	1:A:1031:VAL:HG23	1.96	0.66
1:A:503:GLN:NE2	6:F:90:ARG:HH22	1.93	0.66
1:A:264:PHE:HB3	1:A:265:LYS:HZ1	1.61	0.66
1:A:23:SER:HA	1:A:233:TRP:CD1	2.31	0.66
7:G:27:LYS:HD3	7:G:51:TYR:CE2	2.31	0.66
2:B:1060:ARG:CZ	3:C:202:PRO:HG3	2.25	0.66
4:D:54:GLU:O	4:D:58:VAL:HG23	1.95	0.66
2:B:882:THR:HG23	2:B:884:ARG:CB	2.24	0.65
1:A:914:GLU:HB2	1:A:979:SER:O	1.96	0.65
1:A:1424:VAL:HG11	2:B:1139:ILE:HD13	1.75	0.65
8:H:82:PRO:C	8:H:84:ALA:H	1.98	0.65
7:G:111:THR:HG23	7:G:114:LEU:HD13	1.77	0.65
9:I:4:PHE:HE2	9:I:14:LEU:O	1.79	0.65
3:C:35:ARG:NH1	11:K:41:THR:OG1	2.29	0.65
2:B:1115:THR:O	2:B:1116:ARG:HB2	1.94	0.65
2:B:37:PHE:CE1	2:B:41:LYS:HG3	2.31	0.65
4:D:156:ASP:O	4:D:158:GLU:N	2.30	0.65
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.77	0.65
12:L:30:ILE:O	12:L:56:LEU:HA	1.95	0.65
9:I:6:PHE:N	9:I:6:PHE:CD1	2.64	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:654:ARG:HH11	2:B:654:ARG:HG3	1.61	0.65
2:B:654:ARG:H	2:B:657:HIS:CD2	2.12	0.65
2:B:902:GLY:O	12:L:65:VAL:HG11	1.97	0.65
1:A:1152:ILE:HD13	1:A:1260:LEU:HD23	1.78	0.65
1:A:471:ASN:OD1	1:A:472:LEU:N	2.30	0.65
8:H:43:ASN:ND2	8:H:46:LEU:HD12	2.11	0.65
9:I:85:PHE:CD1	9:I:99:LEU:HD13	2.31	0.65
1:A:1313:LEU:O	1:A:1315:GLU:N	2.30	0.65
2:B:1124:ARG:HH11	2:B:1124:ARG:HB3	1.60	0.65
10:J:27:GLU:O	10:J:29:GLU:HG3	1.95	0.65
2:B:1001:PHE:CE2	3:C:34:ARG:NE	2.65	0.65
1:A:122:MET:HA	1:A:141:LEU:HD11	1.79	0.65
2:B:882:THR:HG21	2:B:934:LYS:O	1.95	0.65
3:C:172:PRO:O	3:C:235:VAL:HG23	1.95	0.65
10:J:3:VAL:HA	10:J:53:HIS:CE1	2.32	0.65
12:L:32:ALA:HB3	12:L:55:ILE:HG13	1.77	0.65
2:B:65:GLU:OE1	2:B:418:LYS:HE3	1.97	0.65
1:A:1255:GLU:HG2	1:A:1258:HIS:CD2	2.31	0.65
7:G:27:LYS:HG2	7:G:54:ILE:HD12	1.77	0.65
1:A:1149:ALA:CB	9:I:47:GLU:HA	2.26	0.65
1:A:1195:LEU:HD11	1:A:1267:MET:CE	2.27	0.65
5:E:56:LYS:HZ2	5:E:85:GLU:HG3	1.62	0.65
7:G:1:MET:SD	7:G:79:PHE:CD1	2.90	0.65
3:C:73:GLN:HE21	3:C:75:MET:N	1.93	0.65
2:B:189:LEU:O	2:B:192:LEU:N	2.29	0.65
1:A:709:THR:HG22	1:A:710:LEU:N	2.10	0.65
8:H:109:LYS:HG2	8:H:110:ASP:OD1	1.96	0.65
12:L:28:LYS:HB3	12:L:39:SER:HB2	1.79	0.65
3:C:34:ARG:NH1	3:C:35:ARG:HG2	2.12	0.65
1:A:66:LYS:O	1:A:67:CYS:HB2	1.96	0.65
2:B:243:ALA:CB	2:B:251:ILE:HD13	2.21	0.65
4:D:12:ARG:HH11	4:D:12:ARG:HG2	1.61	0.65
5:E:17:ARG:O	5:E:20:LYS:HB2	1.97	0.65
2:B:978:ASP:OD2	2:B:1098:MET:HG2	1.96	0.65
2:B:516:ASN:ND2	2:B:516:ASN:N	2.44	0.65
1:A:341:MET:HE1	2:B:1135:ARG:NH1	2.12	0.65
1:A:90:VAL:HG11	1:A:297:GLN:HA	1.77	0.65
4:D:66:ARG:HD2	4:D:133:THR:HB	1.78	0.65
1:A:102:VAL:HB	1:A:211:PHE:CE1	2.32	0.65
2:B:193:LYS:HZ2	12:L:32:ALA:HB1	1.60	0.65
6:F:82:THR:HG22	6:F:84:TYR:N	2.09	0.65
1:A:1313:LEU:HD23	1:A:1338:VAL:HG21	1.77	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:176:PRO:O	5:E:212:ARG:HA	1.97	0.65
11:K:63:VAL:O	11:K:63:VAL:HG23	1.95	0.65
1:A:868:TYR:CD2	1:A:1058:VAL:HG21	2.31	0.65
1:A:67:CYS:C	1:A:68:GLN:HG3	2.17	0.65
4:D:124:GLU:CD	4:D:124:GLU:H	2.00	0.65
2:B:955:THR:CG2	2:B:956:THR:N	2.60	0.65
1:A:1130:GLN:O	1:A:1134:ILE:HG13	1.97	0.65
1:A:903:ASN:HD22	1:A:904:THR:H	1.45	0.65
7:G:27:LYS:HE2	7:G:54:ILE:HB	1.78	0.65
2:B:944:THR:HG21	2:B:1122:ARG:NH2	2.12	0.65
1:A:37:PHE:N	1:A:37:PHE:CD1	2.64	0.65
1:A:567:LYS:HZ3	8:H:46:LEU:HB2	1.61	0.65
1:A:7:SER:HB3	2:B:1193:GLN:NE2	2.11	0.65
2:B:879:ARG:CD	2:B:879:ARG:H	2.10	0.65
2:B:879:ARG:NH2	2:B:885:MET:CE	2.60	0.65
2:B:1037:LEU:HD21	2:B:1064:TYR:HE1	1.62	0.65
2:B:378:LEU:HD12	2:B:378:LEU:O	1.97	0.65
2:B:579:ARG:HA	2:B:589:VAL:HG13	1.78	0.65
6:F:118:LEU:O	6:F:122:MET:HG3	1.96	0.65
12:L:53:HIS:O	12:L:55:ILE:HD13	1.97	0.65
2:B:25:ILE:CG2	2:B:658:ILE:HD12	2.27	0.65
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.79	0.65
4:D:56:ARG:HA	4:D:148:LEU:HD13	1.78	0.64
2:B:102:VAL:CG2	2:B:112:LEU:HB2	2.27	0.64
12:L:55:ILE:HG12	12:L:56:LEU:N	2.11	0.64
5:E:98:ILE:HA	5:E:101:GLN:HB3	1.79	0.64
1:A:1352:VAL:O	1:A:1355:VAL:HG12	1.96	0.64
7:G:116:PRO:HD2	7:G:119:LEU:HD23	1.79	0.64
2:B:90:ILE:HD11	2:B:432:MET:SD	2.38	0.64
1:A:250:ILE:HG22	1:A:250:ILE:O	1.96	0.64
1:A:977:LYS:HB3	1:A:978:PRO:HD2	1.78	0.64
3:C:244:VAL:O	3:C:248:ILE:HG13	1.98	0.64
1:A:904:THR:O	1:A:904:THR:HG22	1.97	0.64
2:B:294:ASP:O	2:B:296:GLU:N	2.30	0.64
8:H:25:ARG:HA	8:H:41:ASP:HA	1.79	0.64
9:I:55:THR:HG22	9:I:58:VAL:HG21	1.79	0.64
4:D:156:ASP:C	4:D:158:GLU:H	2.01	0.64
1:A:961:ARG:HG2	1:A:965:GLN:HE21	1.62	0.64
2:B:639:ILE:HG22	2:B:641:GLU:HG2	1.79	0.64
2:B:708:GLU:HG3	2:B:709:ASP:H	1.63	0.64
7:G:59:GLY:HA3	7:G:70:PHE:CD2	2.33	0.64
3:C:165:LYS:O	11:K:6:ARG:NH1	2.31	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:144:THR:O	4:D:148:LEU:HB2	1.97	0.64
1:A:390:GLN:NE2	1:A:394:ASN:HD22	1.95	0.64
3:C:31:ASN:OD1	3:C:34:ARG:HD3	1.97	0.64
1:A:55:ASP:C	1:A:57:ARG:N	2.47	0.64
4:D:119:ARG:NH1	4:D:119:ARG:HG3	2.12	0.64
2:B:102:VAL:HG22	2:B:112:LEU:HD22	1.79	0.64
8:H:84:ALA:CB	8:H:87:ARG:HD2	2.27	0.64
7:G:9:LEU:HD12	7:G:10:ASN:N	2.13	0.64
1:A:356:ASP:OD2	11:K:65:HIS:HE1	1.81	0.64
2:B:56:ASP:HB3	2:B:57:TYR:CD1	2.32	0.64
1:A:347:PHE:HE2	1:A:375:THR:HG23	1.61	0.64
1:A:573:SER:O	1:A:576:GLN:HB2	1.97	0.64
2:B:885:MET:HA	2:B:936:ASP:CB	2.26	0.64
2:B:98:THR:HG23	2:B:127:GLY:O	1.98	0.64
2:B:1159:ARG:NH1	2:B:1159:ARG:HB3	2.12	0.64
7:G:111:THR:O	7:G:114:LEU:N	2.28	0.64
1:A:535:THR:CG2	1:A:616:VAL:HA	2.27	0.64
1:A:35:ILE:O	1:A:35:ILE:HG22	1.96	0.64
14:T:18:DC:H2"	14:T:19:DT:OP2	1.97	0.64
5:E:127:ILE:O	5:E:127:ILE:HG13	1.96	0.64
2:B:597:MET:HA	2:B:597:MET:CE	2.27	0.64
1:A:1445:ILE:HD11	7:G:68:ALA:HB1	1.80	0.64
1:A:1444:MET:HG3	7:G:59:GLY:O	1.97	0.64
4:D:66:ARG:O	4:D:70:PHE:HB2	1.98	0.64
2:B:916:THR:HB	2:B:935:ARG:HD2	1.80	0.64
2:B:1181:GLU:HB2	2:B:1188:LYS:HG3	1.79	0.64
4:D:145:MET:O	4:D:149:THR:HB	1.96	0.64
5:E:144:ILE:HG13	5:E:145:THR:H	1.61	0.64
1:A:596:THR:O	1:A:598:LEU:N	2.31	0.64
1:A:153:PRO:HD3	1:A:161:LEU:HD13	1.77	0.64
5:E:128:PRO:HA	5:E:129:PRO:C	2.18	0.64
8:H:44:VAL:HG13	8:H:48:PRO:HA	1.78	0.64
10:J:1:MET:N	10:J:56:LEU:N	2.46	0.64
7:G:116:PRO:HG2	7:G:119:LEU:HB3	1.78	0.64
2:B:515:HIS:H	2:B:518:HIS:CD2	2.16	0.64
1:A:858:ASN:HD21	1:A:860:LEU:HB2	1.63	0.64
3:C:196:ASP:OD2	3:C:199:LYS:HE3	1.98	0.64
2:B:882:THR:C	2:B:884:ARG:H	2.00	0.64
5:E:78:LEU:HD21	5:E:80:VAL:HG23	1.80	0.64
1:A:1258:HIS:O	1:A:1262:LYS:HE3	1.97	0.64
2:B:408:LEU:O	2:B:411:PRO:HD2	1.97	0.64
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.79	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:426:LYS:O	2:B:426:LYS:HG3	1.97	0.64
2:B:364:ILE:O	2:B:365:THR:HB	1.97	0.63
1:A:794:PRO:HG2	1:A:795:GLU:OE2	1.98	0.63
3:C:120:ILE:CD1	3:C:124:LEU:HD11	2.27	0.63
7:G:112:LYS:HA	7:G:115:MET:CE	2.28	0.63
5:E:48:ASP:CG	5:E:49:SER:H	2.01	0.63
1:A:478:TYR:O	1:A:479:ASN:HB2	1.97	0.63
4:D:138:ASN:HB3	4:D:141:LEU:HB3	1.80	0.63
3:C:100:THR:HG21	3:C:102:GLN:HE21	1.64	0.63
5:E:28:TYR:C	5:E:65:THR:HG22	2.19	0.63
1:A:590:ARG:O	1:A:591:PHE:HB2	1.98	0.63
2:B:29:ASP:HB3	2:B:658:ILE:HD13	1.79	0.63
1:A:1341:ILE:HD12	1:A:1379:GLY:O	1.97	0.63
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.81	0.63
2:B:805:THR:HA	2:B:809:MET:HE1	1.80	0.63
2:B:221:ASN:O	2:B:222:ILE:HG13	1.99	0.63
4:D:35:LEU:HD11	4:D:173:HIS:CD2	2.33	0.63
2:B:879:ARG:NH2	2:B:885:MET:HE2	2.14	0.63
2:B:289:LEU:HD13	2:B:375:ALA:CB	2.25	0.63
2:B:996:ARG:HH12	3:C:175:ALA:H	1.46	0.63
3:C:236:GLY:O	3:C:238:ILE:N	2.31	0.63
2:B:95:ILE:CG1	2:B:130:VAL:HG22	2.29	0.63
2:B:95:ILE:HG13	2:B:130:VAL:HG22	1.78	0.63
1:A:984:LYS:HG2	1:A:988:LEU:HD11	1.80	0.63
11:K:55:LYS:HB3	11:K:81:TYR:CD1	2.33	0.63
7:G:87:VAL:HG23	7:G:103:VAL:HG21	1.79	0.63
4:D:179:GLN:OE1	4:D:179:GLN:HA	1.97	0.63
9:I:58:VAL:HG13	9:I:62:ILE:CD1	2.29	0.63
1:A:1107:VAL:CG1	1:A:1107:VAL:O	2.45	0.63
1:A:1387:HIS:CE1	13:N:4:DA:H5'	2.33	0.63
2:B:558:LEU:HD11	2:B:596:LEU:HD21	1.79	0.63
2:B:798:TYR:CE2	3:C:62:PHE:CE2	2.82	0.63
1:A:185:TRP:CE3	1:A:185:TRP:N	2.65	0.63
1:A:335:ARG:HH12	2:B:1206:GLU:CD	2.02	0.63
4:D:13:ARG:C	4:D:15:LEU:H	2.02	0.63
11:K:54:ARG:HG2	11:K:54:ARG:HH11	1.63	0.63
8:H:56:THR:HB	8:H:145:ARG:HG2	1.79	0.63
1:A:1223:ASP:HA	1:A:1243:VAL:CG1	2.28	0.63
1:A:1187:GLN:CB	1:A:1244:ARG:HG2	2.25	0.63
4:D:123:LEU:O	4:D:127:ASP:HB2	1.99	0.63
1:A:1094:VAL:HG13	1:A:1113:THR:CG2	2.28	0.63
3:C:11:ARG:HH12	3:C:205:LYS:CE	2.11	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:579:ARG:HH11	2:B:579:ARG:HG2	1.64	0.63
1:A:710:LEU:HD12	1:A:710:LEU:N	2.14	0.63
2:B:1034:VAL:HG12	2:B:1035:ALA:N	2.14	0.63
4:D:190:GLU:C	4:D:193:THR:HG22	2.19	0.63
1:A:441:PRO:HD2	1:A:498:ARG:NH2	2.13	0.63
2:B:577:ALA:HB1	2:B:589:VAL:CG1	2.17	0.63
1:A:1444:MET:HE1	6:F:135:ARG:HB2	1.79	0.63
1:A:1313:LEU:C	1:A:1315:GLU:H	2.02	0.63
2:B:839:MET:CE	2:B:1010:LEU:HD21	2.28	0.63
1:A:37:PHE:HD1	1:A:37:PHE:N	1.97	0.63
2:B:56:ASP:HB3	2:B:57:TYR:HD1	1.63	0.63
2:B:259:TYR:HB2	2:B:268:THR:HG23	1.80	0.63
1:A:134:ARG:HD2	1:A:221:SER:O	1.98	0.63
5:E:84:ASP:O	5:E:86:PRO:HD3	1.97	0.63
2:B:999:MET:HE3	2:B:999:MET:HA	1.80	0.63
11:K:31:VAL:HG12	11:K:32:VAL:N	2.13	0.63
1:A:308:ILE:HG22	1:A:309:ALA:N	2.13	0.63
2:B:35:SER:HA	2:B:811:TYR:HE2	1.63	0.63
7:G:91:VAL:HG23	7:G:141:SER:O	1.98	0.63
1:A:875:ALA:HA	1:A:878:ILE:HD12	1.81	0.62
3:C:163:ILE:HG13	3:C:165:LYS:H	1.64	0.62
2:B:995:ARG:NH1	3:C:165:LYS:HG2	2.14	0.62
12:L:53:HIS:HB3	12:L:55:ILE:HD11	1.80	0.62
1:A:390:GLN:O	1:A:394:ASN:HB2	1.99	0.62
3:C:179:GLU:HG2	3:C:180:TYR:N	2.14	0.62
1:A:347:PHE:H	2:B:1107:ALA:HA	1.63	0.62
5:E:213:ILE:HG12	5:E:214:CYS:H	1.64	0.62
7:G:20:PRO:HD2	7:G:21:ARG:H	1.64	0.62
2:B:891:ASP:O	2:B:893:LEU:N	2.32	0.62
2:B:1001:PHE:CE1	2:B:1073:TYR:HB2	2.34	0.62
2:B:756:ILE:O	2:B:759:PRO:HD3	1.98	0.62
11:K:82:ASP:OD1	11:K:84:LYS:N	2.32	0.62
1:A:714:PHE:O	1:A:718:VAL:HG23	2.00	0.62
1:A:754:SER:N	1:A:757:ASN:HD22	1.96	0.62
1:A:1018:PHE:O	1:A:1021:LEU:HB3	1.98	0.62
1:A:145:LYS:HE3	1:A:145:LYS:HA	1.81	0.62
1:A:11:LEU:HB2	2:B:1193:GLN:HG2	1.81	0.62
2:B:987:LYS:HG3	15:P:11:G:O2'	1.99	0.62
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.34	0.62
12:L:61:THR:HG22	12:L:62:LYS:N	2.15	0.62
1:A:443:LEU:HD12	2:B:1146:PHE:CZ	2.34	0.62
2:B:637:LEU:CD2	2:B:742:GLU:HA	2.30	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1239:ARG:HH22	1:A:1241:ARG:HH22	1.45	0.62
1:A:694:THR:O	1:A:698:GLN:HG3	1.98	0.62
2:B:168:GLY:HA2	2:B:454:THR:OG1	2.00	0.62
1:A:831:THR:CG2	1:A:832:ALA:H	2.13	0.62
1:A:1420:ASP:OD2	1:A:1420:ASP:N	2.31	0.62
2:B:293:PRO:HG2	2:B:296:GLU:HB3	1.81	0.62
2:B:654:ARG:N	2:B:657:HIS:HD2	1.96	0.62
10:J:9:SER:HB2	10:J:45:CYS:HB2	1.82	0.62
8:H:77:ARG:HG2	8:H:78:SER:H	1.63	0.62
9:I:44:TYR:CD1	9:I:45:ARG:N	2.68	0.62
1:A:266:LEU:HD21	1:A:303:TYR:CE1	2.34	0.62
1:A:367:PRO:HG2	1:A:370:ILE:HD12	1.81	0.62
2:B:616:ILE:HD12	2:B:616:ILE:N	2.14	0.62
8:H:11:GLN:O	8:H:28:ALA:HB1	2.00	0.62
2:B:844:SER:O	2:B:847:ASP:HB2	2.00	0.62
10:J:3:VAL:HA	10:J:53:HIS:ND1	2.14	0.62
1:A:596:THR:C	1:A:598:LEU:H	2.03	0.62
12:L:26:THR:CG2	12:L:27:LEU:N	2.63	0.62
2:B:948:ILE:HG22	2:B:949:VAL:O	1.99	0.62
5:E:157:SER:O	5:E:159:ASP:N	2.33	0.62
2:B:345:LYS:N	2:B:347:LYS:HE2	2.15	0.62
1:A:41:MET:HB2	1:A:49:LYS:HA	1.81	0.62
2:B:957:ASN:O	2:B:959:ASP:N	2.33	0.62
2:B:954:VAL:O	12:L:55:ILE:O	2.16	0.62
1:A:1171:GLN:O	1:A:1174:PHE:HB2	2.00	0.62
9:I:93:LYS:HD3	9:I:93:LYS:N	2.15	0.62
3:C:34:ARG:HH11	3:C:35:ARG:HG2	1.64	0.62
4:D:192:LYS:HD2	4:D:199:ASN:HA	1.81	0.62
3:C:92:CYS:SG	3:C:94:LYS:HB3	2.40	0.62
2:B:582:VAL:HG23	2:B:626:ILE:HB	1.80	0.62
1:A:718:VAL:HG12	1:A:722:LEU:HD11	1.81	0.62
1:A:106:VAL:HG12	1:A:107:CYS:N	2.15	0.62
1:A:590:ARG:HG2	1:A:604:GLY:HA2	1.80	0.62
2:B:466:TRP:O	2:B:468:GLU:N	2.33	0.62
1:A:984:LYS:HG2	1:A:988:LEU:CD1	2.30	0.62
1:A:868:TYR:CZ	1:A:1064:VAL:HG11	2.35	0.62
1:A:1189:SER:O	1:A:1241:ARG:HD3	1.99	0.62
3:C:148:ARG:H	3:C:151:GLN:HG3	1.65	0.62
3:C:235:VAL:HG13	10:J:13:VAL:HG22	1.82	0.62
2:B:115:GLN:HG2	2:B:193:LYS:HB2	1.82	0.62
2:B:57:TYR:N	2:B:57:TYR:HD1	1.98	0.62
5:E:99:HIS:O	5:E:103:LYS:HG2	1.99	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:782:ARG:NH2	2:B:699:GLU:O	2.33	0.62
1:A:1218:GLN:O	1:A:1221:LYS:HG3	2.00	0.62
2:B:642:ASP:CA	2:B:649:LYS:HA	2.30	0.62
1:A:75:ASN:HD22	2:B:1116:ARG:NH1	1.97	0.62
1:A:873:MET:C	1:A:1058:VAL:HG23	2.19	0.61
2:B:615:MET:CB	2:B:626:ILE:HG12	2.29	0.61
2:B:707:PRO:HG2	2:B:708:GLU:N	2.13	0.61
1:A:1170:ILE:HD12	1:A:1170:ILE:N	2.13	0.61
7:G:112:LYS:HA	7:G:115:MET:HE3	1.80	0.61
9:I:84:VAL:O	9:I:84:VAL:HG13	2.00	0.61
7:G:132:SER:HB3	7:G:135:ASP:H	1.65	0.61
2:B:879:ARG:NE	2:B:879:ARG:H	1.97	0.61
2:B:996:ARG:NH2	3:C:38:ILE:HG23	2.15	0.61
3:C:205:LYS:HG2	3:C:205:LYS:O	2.00	0.61
2:B:1130:PHE:HZ	2:B:1138:MET:HG2	1.65	0.61
2:B:570:VAL:HG21	2:B:573:GLN:CD	2.20	0.61
1:A:69:THR:O	1:A:71:GLN:HG3	2.01	0.61
1:A:774:ARG:HB2	1:A:797:LYS:O	2.01	0.61
10:J:44:TYR:H	10:J:44:TYR:HD2	1.48	0.61
4:D:4:SER:O	4:D:5:THR:CB	2.47	0.61
2:B:305:VAL:HG12	2:B:305:VAL:O	1.99	0.61
2:B:617:ARG:HA	2:B:624:LEU:HD12	1.83	0.61
8:H:5:LEU:HG	8:H:60:ALA:HA	1.83	0.61
1:A:661:GLY:HA3	2:B:1081:LEU:HD22	1.81	0.61
2:B:953:LEU:CD2	2:B:965:LYS:HB2	2.30	0.61
1:A:23:SER:HB3	1:A:233:TRP:CZ2	2.35	0.61
4:D:195:ILE:CG2	4:D:198:LEU:HG	2.31	0.61
2:B:465:ASN:N	2:B:465:ASN:ND2	2.45	0.61
9:I:50:THR:CG2	9:I:52:ILE:HG12	2.30	0.61
9:I:44:TYR:HD1	9:I:45:ARG:N	1.98	0.61
1:A:150:THR:HG23	1:A:166:GLY:HA2	1.81	0.61
1:A:2:VAL:HG22	1:A:3:GLY:H	1.66	0.61
7:G:26:LEU:HD11	7:G:70:PHE:CD1	2.35	0.61
10:J:1:MET:H1	10:J:56:LEU:N	1.98	0.61
4:D:12:ARG:NH1	4:D:14:ARG:HA	2.15	0.61
1:A:768:GLN:CG	1:A:816:HIS:HA	2.28	0.61
1:A:288:ALA:HA	1:A:291:GLU:CG	2.30	0.61
1:A:1150:SER:HB3	1:A:1195:LEU:CD2	2.31	0.61
9:I:101:PHE:N	9:I:101:PHE:CD1	2.68	0.61
2:B:218:SER:CB	2:B:241:ARG:HH12	2.14	0.61
6:F:90:ARG:HD3	6:F:155:LEU:CD1	2.22	0.61
6:F:103:MET:O	6:F:104:ASN:HB2	2.01	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:898:ARG:HD3	1:A:933:TYR:CD1	2.36	0.61
1:A:482:PHE:CE1	2:B:836:GLU:HB2	2.35	0.61
2:B:906:SER:HA	2:B:946:ASN:HB2	1.82	0.61
4:D:207:LEU:O	4:D:207:LEU:HD12	2.00	0.61
2:B:290:GLY:O	2:B:292:ILE:HG13	2.01	0.61
3:C:11:ARG:HH12	3:C:205:LYS:HE2	1.66	0.61
6:F:109:VAL:HG11	6:F:123:LYS:HG2	1.81	0.61
3:C:50:GLU:OE1	12:L:64:LEU:HD13	2.00	0.61
2:B:637:LEU:HD11	2:B:703:ILE:HD13	1.81	0.61
8:H:38:LEU:HD12	8:H:124:ARG:O	2.01	0.61
2:B:797:TYR:HE1	2:B:854:LEU:CD2	2.13	0.61
2:B:899:ILE:HG21	2:B:949:VAL:HG21	1.83	0.61
2:B:283:VAL:HG21	2:B:317:CYS:O	2.00	0.61
2:B:39:ARG:CZ	2:B:665:GLU:HG2	2.30	0.61
1:A:517:ASN:HD22	1:A:1364:ASN:HD22	1.47	0.61
2:B:360:PHE:CD2	2:B:361:LEU:HB2	2.35	0.61
1:A:1445:ILE:HD12	1:A:1445:ILE:N	2.08	0.61
1:A:691:LEU:O	1:A:694:THR:HB	2.01	0.61
3:C:123:ASN:HD21	3:C:125:MET:HA	1.64	0.61
1:A:16:GLU:OE1	4:D:13:ARG:NH2	2.32	0.61
1:A:1227:ILE:HG22	1:A:1228:TRP:N	2.15	0.61
1:A:1141:THR:CG2	1:A:1205:LYS:HD3	2.31	0.61
2:B:309:GLN:CD	9:I:52:ILE:HD11	2.21	0.61
10:J:14:VAL:HG12	10:J:14:VAL:O	2.01	0.61
2:B:123:THR:OG1	2:B:458:LYS:HE2	2.01	0.61
1:A:1241:ARG:O	1:A:1242:VAL:CG2	2.48	0.61
9:I:86:PHE:CE1	9:I:100:PHE:HB2	2.36	0.61
2:B:1096:ARG:O	2:B:1097:HIS:CB	2.48	0.61
2:B:57:TYR:CD1	2:B:57:TYR:N	2.68	0.61
3:C:147:LEU:HD23	3:C:147:LEU:N	2.16	0.60
2:B:847:ASP:C	2:B:849:GLY:H	2.02	0.60
3:C:166:GLU:C	11:K:6:ARG:NH1	2.54	0.60
3:C:66:ARG:NH1	10:J:2:ILE:CG2	2.63	0.60
2:B:313:MET:HE3	2:B:386:LEU:HD22	1.82	0.60
1:A:353:ILE:HG21	1:A:487:MET:HG3	1.81	0.60
1:A:537:ARG:NH1	8:H:120:GLY:O	2.34	0.60
1:A:1244:ARG:HB2	1:A:1245:PRO:HD2	1.82	0.60
2:B:288:ALA:O	2:B:331:LEU:HD11	2.00	0.60
6:F:90:ARG:NH1	6:F:94:LEU:HD11	2.15	0.60
2:B:912:ILE:O	2:B:938:SER:HB3	2.01	0.60
8:H:58:THR:HG22	8:H:59:ILE:N	2.15	0.60
1:A:1308:THR:CG2	1:A:1309:ASP:N	2.62	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:733:ALA:O	1:A:737:LEU:HG	2.01	0.60
2:B:1124:ARG:NH1	2:B:1124:ARG:HB3	2.16	0.60
3:C:31:ASN:O	3:C:35:ARG:HG3	2.01	0.60
8:H:143:LEU:N	8:H:143:LEU:HD12	2.17	0.60
1:A:66:LYS:NZ	1:A:68:GLN:N	2.46	0.60
7:G:123:ALA:C	7:G:125:SER:H	2.04	0.60
1:A:1385:THR:HG22	1:A:1386:ARG:H	1.67	0.60
1:A:469:ARG:NH2	2:B:991:GLY:O	2.35	0.60
1:A:870:GLU:HB2	5:E:204:THR:HG21	1.82	0.60
9:I:73:ARG:HD2	9:I:101:PHE:CE2	2.35	0.60
7:G:55:ASP:OD1	7:G:57:GLN:HG3	2.02	0.60
1:A:54:ASN:HB3	1:A:247:ARG:HH22	1.67	0.60
2:B:37:PHE:HE1	2:B:41:LYS:HG3	1.64	0.60
4:D:155:ARG:HD3	4:D:221:TYR:CE1	2.37	0.60
3:C:97:VAL:HG12	3:C:99:LEU:CD2	2.32	0.60
6:F:75:PRO:O	6:F:77:ASP:O	2.19	0.60
1:A:219:PHE:HE1	1:A:230:ARG:HE	1.48	0.60
1:A:289:ILE:HG22	1:A:290:GLU:N	2.16	0.60
2:B:235:SER:OG	2:B:236:HIS:CD2	2.54	0.60
1:A:869:GLY:O	5:E:204:THR:HG21	2.01	0.60
3:C:181:ASP:CG	3:C:186:LEU:HD13	2.21	0.60
2:B:284:ILE:HD13	2:B:324:ILE:HD12	1.84	0.60
7:G:126:ASN:C	7:G:126:ASN:HD22	2.05	0.60
9:I:61:ASP:C	9:I:63:GLY:H	2.05	0.60
3:C:242:GLN:C	3:C:244:VAL:H	2.05	0.60
7:G:115:MET:HB3	7:G:116:PRO:CD	2.32	0.60
1:A:1342:GLU:CG	5:E:198:ILE:HD13	2.32	0.60
11:K:94:ILE:O	11:K:98:LEU:HG	2.00	0.60
9:I:46:HIS:CE1	9:I:48:LEU:HD23	2.37	0.60
2:B:205:ILE:N	2:B:205:ILE:HD12	2.17	0.60
4:D:130:LEU:HD13	4:D:142:LYS:CD	2.32	0.60
12:L:38:LEU:O	12:L:39:SER:HB3	2.02	0.60
6:F:130:ILE:HB	6:F:148:VAL:HG21	1.83	0.60
1:A:302:THR:HA	1:A:305:ASP:O	2.02	0.60
3:C:177:GLU:CG	3:C:231:ASN:HB3	2.29	0.60
1:A:870:GLU:HG2	5:E:208:TYR:CG	2.36	0.60
2:B:309:GLN:HG3	9:I:52:ILE:HD12	1.84	0.60
2:B:558:LEU:HD21	2:B:596:LEU:HD11	1.84	0.60
7:G:85:GLU:HG2	7:G:87:VAL:HG13	1.83	0.60
2:B:781:PHE:HE2	2:B:795:ILE:HD11	1.65	0.60
5:E:37:LEU:CD1	5:E:41:ASP:HB2	2.31	0.60
1:A:718:VAL:O	1:A:721:PHE:HB2	2.01	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:J:5:VAL:HG12	10:J:6:ARG:CG	2.32	0.60
1:A:351:THR:CG2	2:B:1103:ILE:HG13	2.32	0.60
8:H:84:ALA:O	8:H:85:GLY:C	2.41	0.60
5:E:192:ARG:HG3	5:E:192:ARG:HH11	1.67	0.60
1:A:1070:GLN:O	1:A:1074:GLU:HB2	2.02	0.60
1:A:23:SER:HA	1:A:233:TRP:NE1	2.16	0.60
8:H:65:LEU:H	8:H:65:LEU:HD23	1.66	0.60
2:B:1039:GLY:HA2	10:J:51:LEU:CD2	2.32	0.60
10:J:21:TYR:HB2	10:J:39:LEU:CD1	2.32	0.60
1:A:100:LYS:HE2	1:A:104:GLU:OE2	2.01	0.60
3:C:33:LEU:O	3:C:33:LEU:HD12	2.01	0.60
1:A:1202:MET:CE	1:A:1212:VAL:HG21	2.31	0.60
2:B:557:PHE:O	2:B:557:PHE:CD2	2.53	0.60
1:A:1161:THR:HG21	1:A:1163:ILE:HD12	1.83	0.60
1:A:1193:LEU:HD12	1:A:1194:ARG:N	2.17	0.60
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.37	0.60
2:B:126:SER:CB	2:B:172:ILE:HD11	2.32	0.60
1:A:1312:ASN:O	1:A:1316:VAL:HG23	2.01	0.60
1:A:1342:GLU:HG3	5:E:198:ILE:HG21	1.83	0.60
1:A:946:VAL:HG22	5:E:201:LYS:HD2	1.82	0.60
5:E:99:HIS:CE1	5:E:103:LYS:HG3	2.37	0.60
3:C:182:PRO:HD2	3:C:210:GLU:OE1	2.01	0.60
1:A:1144:LYS:HB2	1:A:1268:LEU:O	2.01	0.60
2:B:559:SER:CA	2:B:563:MET:HB3	2.10	0.59
4:D:29:LEU:HD12	7:G:82:PHE:CE2	2.37	0.59
6:F:103:MET:HE2	7:G:66:GLY:H	1.66	0.59
1:A:754:SER:H	1:A:757:ASN:ND2	1.98	0.59
5:E:212:ARG:HH11	5:E:212:ARG:HG3	1.67	0.59
1:A:899:VAL:HB	1:A:929:LEU:HD12	1.83	0.59
2:B:260:GLY:O	2:B:267:ARG:NH1	2.34	0.59
8:H:59:ILE:O	8:H:60:ALA:HB3	2.01	0.59
1:A:385:ILE:HD11	1:A:426:LEU:HB2	1.82	0.59
2:B:872:GLU:CD	2:B:914:LYS:HE3	2.23	0.59
11:K:21:ILE:HG22	11:K:31:VAL:HG11	1.84	0.59
3:C:7:GLN:HG3	11:K:104:ASN:ND2	2.17	0.59
2:B:1177:HIS:HB3	2:B:1179:GLN:HE21	1.67	0.59
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.84	0.59
1:A:380:VAL:HG13	1:A:385:ILE:HG12	1.83	0.59
4:D:128:VAL:C	4:D:130:LEU:N	2.54	0.59
2:B:68:THR:HA	2:B:90:ILE:O	2.02	0.59
4:D:9:GLN:HG3	4:D:9:GLN:O	2.03	0.59
2:B:1031:LEU:HD11	2:B:1042:GLY:CA	2.32	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1148:ILE:HG12	1:A:1198:ASP:HB2	1.83	0.59
3:C:35:ARG:NH1	11:K:41:THR:H	2.00	0.59
2:B:781:PHE:HD2	2:B:781:PHE:H	1.49	0.59
5:E:136:ASN:OD1	5:E:138:ALA:N	2.35	0.59
2:B:797:TYR:O	10:J:1:MET:HG2	2.02	0.59
4:D:153:ARG:C	4:D:154:PHE:CD2	2.76	0.59
4:D:156:ASP:C	4:D:158:GLU:N	2.54	0.59
4:D:56:ARG:HD3	4:D:149:THR:HA	1.84	0.59
1:A:186:LYS:O	1:A:187:LYS:HB2	2.01	0.59
8:H:30:SER:CB	8:H:36:CYS:HB3	2.32	0.59
2:B:347:LYS:HG3	2:B:348:ARG:H	1.67	0.59
2:B:868:MET:O	2:B:870:ILE:HG13	2.01	0.59
2:B:1007:VAL:CG2	2:B:1008:PRO:HD2	2.32	0.59
3:C:258:ILE:HD11	11:K:42:LEU:HD21	1.83	0.59
1:A:353:ILE:HD12	1:A:470:LEU:HD21	1.85	0.59
4:D:51:ASN:O	4:D:52:LEU:O	2.20	0.59
3:C:208:GLU:O	3:C:210:GLU:N	2.36	0.59
2:B:745:PRO:O	2:B:747:MET:N	2.36	0.59
1:A:567:LYS:HD2	8:H:95:TYR:CG	2.38	0.59
1:A:87:ALA:CB	1:A:276:LEU:HD23	2.27	0.59
7:G:49:LEU:HG	7:G:76:ALA:HA	1.84	0.59
2:B:1102:LYS:O	2:B:1103:ILE:C	2.41	0.59
1:A:102:VAL:HG11	1:A:211:PHE:HE1	1.68	0.59
1:A:1094:VAL:HG13	1:A:1113:THR:HG21	1.84	0.59
2:B:120:ARG:NH1	12:L:54:ARG:HH11	2.01	0.59
1:A:464:PRO:HG2	1:A:465:TYR:HD1	1.68	0.59
2:B:1031:LEU:O	2:B:1031:LEU:HD12	2.03	0.59
1:A:447:GLN:NE2	14:T:20:DG:H4'	2.17	0.59
2:B:549:THR:HG22	2:B:550:ASP:H	1.66	0.59
1:A:567:LYS:HD2	8:H:95:TYR:HA	1.84	0.59
1:A:666:ILE:HD11	2:B:1086:PHE:HE1	1.67	0.59
2:B:248:SER:N	2:B:418:LYS:HZ3	2.00	0.59
11:K:57:LEU:HB2	11:K:76:GLN:HG2	1.84	0.59
2:B:1084:GLN:NE2	2:B:1084:GLN:N	2.51	0.59
2:B:297:ILE:HG22	2:B:298:LEU:HD22	1.85	0.59
2:B:332:ASP:OD1	2:B:348:ARG:HD2	2.03	0.59
2:B:708:GLU:O	2:B:710:LEU:N	2.36	0.59
2:B:999:MET:HB3	2:B:1007:VAL:HG21	1.85	0.59
1:A:671:ALA:O	1:A:676:MET:HE2	2.02	0.59
1:A:981:LEU:CD2	1:A:1039:LYS:HA	2.32	0.59
1:A:964:ILE:O	1:A:967:ALA:HB3	2.03	0.59
1:A:1325:THR:HG22	1:A:1326:ARG:HG3	1.82	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:240:ILE:CG2	2:B:254:LEU:HB3	2.33	0.59
1:A:88:LYS:HG3	1:A:276:LEU:HD21	1.85	0.59
15:P:10:U:H5'	15:P:11:G:C3'	2.33	0.59
6:F:69:LEU:HB3	6:F:71:GLU:OE2	2.02	0.59
2:B:911:ILE:HD11	2:B:941:LEU:CD1	2.31	0.59
1:A:444:PHE:CB	1:A:458:HIS:HD2	2.16	0.59
2:B:732:SER:HB2	2:B:734:HIS:NE2	2.18	0.59
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.43	0.59
2:B:562:GLY:HA3	2:B:590:HIS:ND1	2.17	0.59
2:B:579:ARG:CB	2:B:586:TRP:HE1	2.16	0.59
5:E:135:PHE:HD2	5:E:140:LEU:HD21	1.67	0.59
2:B:1084:GLN:HE21	2:B:1084:GLN:N	2.01	0.59
1:A:476:SER:OG	1:A:477:PRO:HD3	2.03	0.59
7:G:90:THR:HG22	7:G:91:VAL:O	2.03	0.59
1:A:416:ARG:HH11	1:A:417:TYR:HE1	1.51	0.59
3:C:69:LEU:HD12	3:C:69:LEU:N	2.17	0.58
10:J:57:ILE:HA	10:J:60:PHE:HD2	1.66	0.58
1:A:925:LEU:HD13	1:A:983:ILE:HG21	1.83	0.58
2:B:975:GLN:O	2:B:990:ILE:HD12	2.02	0.58
2:B:429:PHE:HD1	2:B:432:MET:HE3	1.68	0.58
11:K:18:LYS:NZ	11:K:37:LYS:O	2.35	0.58
6:F:109:VAL:HG21	6:F:124:GLU:HA	1.84	0.58
2:B:360:PHE:HD2	2:B:361:LEU:HB2	1.68	0.58
3:C:40:GLU:HA	3:C:163:ILE:HD12	1.85	0.58
7:G:34:VAL:CG1	7:G:45:ILE:HG21	2.32	0.58
9:I:19:ASP:HB3	9:I:24:ARG:HG2	1.85	0.58
5:E:92:THR:O	5:E:95:THR:HB	2.03	0.58
1:A:1161:THR:C	1:A:1163:ILE:H	2.07	0.58
1:A:1239:ARG:HH12	1:A:1241:ARG:HH12	1.50	0.58
3:C:97:VAL:HG12	3:C:99:LEU:HD21	1.85	0.58
4:D:17:LYS:HD2	4:D:18:VAL:HG13	1.84	0.58
1:A:1259:MET:HA	1:A:1262:LYS:CD	2.33	0.58
1:A:683:ILE:HG21	1:A:801:GLU:HG3	1.85	0.58
9:I:116:ASN:O	9:I:117:LYS:HD2	2.03	0.58
2:B:246:LYS:HA	2:B:249:ARG:CZ	2.33	0.58
5:E:93:MET:CG	5:E:123:LEU:HD12	2.34	0.58
11:K:65:HIS:HD2	11:K:67:PHE:N	2.01	0.58
1:A:1286:LYS:HB2	1:A:1304:TRP:CZ3	2.39	0.58
1:A:186:LYS:NZ	1:A:197:PRO:HD3	2.18	0.58
2:B:353:LYS:O	2:B:357:GLN:HG2	2.03	0.58
8:H:42:ILE:HG23	8:H:95:TYR:CE1	2.39	0.58
4:D:120:GLU:OE1	4:D:120:GLU:O	2.22	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1094:VAL:CG2	1:A:1113:THR:HG21	2.29	0.58
2:B:801:LYS:O	10:J:52:THR:CG2	2.51	0.58
1:A:1308:THR:HG23	1:A:1310:GLY:H	1.69	0.58
2:B:65:GLU:HG3	2:B:66:ASP:N	2.14	0.58
2:B:953:LEU:O	2:B:953:LEU:HD23	2.04	0.58
11:K:49:GLU:HG3	11:K:94:ILE:HG13	1.85	0.58
1:A:203:SER:O	1:A:206:GLU:HB3	2.03	0.58
1:A:288:ALA:HA	1:A:291:GLU:CD	2.24	0.58
2:B:235:SER:C	2:B:236:HIS:CD2	2.77	0.58
1:A:857:ARG:NH1	6:F:139:PRO:HB2	2.19	0.58
2:B:295:GLY:H	2:B:298:LEU:HD23	1.69	0.58
3:C:32:SER:O	3:C:36:VAL:HG23	2.03	0.58
1:A:1444:MET:CE	6:F:135:ARG:HB2	2.34	0.58
1:A:666:ILE:HD11	2:B:1067:ARG:O	2.03	0.58
1:A:1074:GLU:HB3	1:A:1075:PRO:HD3	1.85	0.58
1:A:332:LYS:HD3	1:A:333:GLU:HG2	1.85	0.58
5:E:213:ILE:HG12	5:E:214:CYS:N	2.18	0.58
1:A:1120:LEU:O	1:A:1323:ASP:HB2	2.03	0.58
7:G:58:ARG:HH11	7:G:58:ARG:HG3	1.68	0.58
1:A:503:GLN:NE2	6:F:90:ARG:NH2	2.48	0.58
1:A:256:GLN:NE2	2:B:935:ARG:HH12	2.01	0.58
2:B:1187:ASN:HD21	2:B:1190:ASP:HB3	1.69	0.58
3:C:177:GLU:HG3	3:C:231:ASN:ND2	2.18	0.58
8:H:81:PRO:HB3	8:H:82:PRO:HD2	1.85	0.58
9:I:80:SER:HB2	9:I:103:CYS:SG	2.43	0.58
1:A:1066:VAL:O	1:A:1070:GLN:HG3	2.04	0.58
1:A:710:LEU:CD1	1:A:710:LEU:H	2.15	0.58
3:C:114:TYR:CD2	3:C:140:ASN:CB	2.86	0.58
2:B:871:THR:HG22	2:B:872:GLU:O	2.04	0.58
2:B:955:THR:CG2	2:B:956:THR:H	2.17	0.58
9:I:78:CYS:SG	9:I:106:CYS:SG	3.01	0.58
2:B:468:GLU:OE1	2:B:470:LYS:HE3	2.04	0.58
2:B:217:ARG:C	2:B:217:ARG:HD2	2.24	0.58
1:A:1241:ARG:O	1:A:1242:VAL:CB	2.52	0.58
1:A:1438:THR:O	6:F:92:ARG:NH1	2.37	0.58
1:A:265:LYS:O	1:A:269:ILE:HG13	2.02	0.58
10:J:1:MET:H2	10:J:57:ILE:H	1.51	0.58
2:B:906:SER:O	2:B:941:LEU:HD23	2.04	0.58
9:I:8:ARG:HG3	9:I:34:TYR:HE1	1.66	0.58
5:E:198:ILE:CD1	5:E:212:ARG:HG3	2.34	0.58
1:A:119:ASN:O	1:A:122:MET:HB3	2.04	0.58
4:D:52:LEU:HD21	4:D:147:TYR:HE2	1.68	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:36:VAL:HG21	3:C:251:LEU:HB2	1.85	0.58
2:B:398:ARG:HB2	2:B:398:ARG:NH1	2.19	0.58
1:A:567:LYS:CB	8:H:96:VAL:H	2.05	0.57
4:D:35:LEU:H	4:D:35:LEU:HD12	1.68	0.57
3:C:124:LEU:O	3:C:127:ARG:HG2	2.03	0.57
2:B:758:PHE:HE1	2:B:1027:ILE:HG22	1.69	0.57
11:K:79:GLU:HG3	11:K:80:GLY:N	2.19	0.57
1:A:1340:GLY:HA2	5:E:183:PRO:HD2	1.86	0.57
1:A:1353:TYR:CD2	1:A:1353:TYR:C	2.77	0.57
1:A:1208:THR:HB	1:A:1211:GLN:CG	2.16	0.57
8:H:40:LEU:HD13	8:H:123:MET:CE	2.31	0.57
10:J:57:ILE:O	10:J:60:PHE:HB2	2.04	0.57
4:D:118:THR:O	4:D:121:LYS:N	2.29	0.57
4:D:163:VAL:O	4:D:167:LEU:HG	2.04	0.57
5:E:15:ALA:O	5:E:19:VAL:HG23	2.03	0.57
5:E:78:LEU:HD23	5:E:78:LEU:C	2.23	0.57
5:E:124:VAL:HA	5:E:132:ILE:CD1	2.33	0.57
3:C:226:ASP:O	3:C:227:THR:HB	2.04	0.57
1:A:129:LYS:O	1:A:130:ASP:HB2	2.04	0.57
2:B:254:LEU:HD11	2:B:273:LEU:HD23	1.85	0.57
1:A:63:ARG:HA	1:A:74:MET:CE	2.33	0.57
2:B:891:ASP:C	2:B:893:LEU:N	2.55	0.57
1:A:628:GLY:O	1:A:632:VAL:HG23	2.03	0.57
5:E:153:HIS:O	5:E:154:ILE:HG13	2.04	0.57
2:B:996:ARG:HH21	3:C:38:ILE:HG23	1.69	0.57
5:E:147:HIS:CD2	5:E:149:LEU:H	2.21	0.57
1:A:102:VAL:HB	1:A:211:PHE:CZ	2.39	0.57
4:D:123:LEU:CD1	4:D:149:THR:HG21	2.33	0.57
2:B:758:PHE:CE1	2:B:1027:ILE:CG2	2.87	0.57
1:A:851:HIS:O	1:A:853:ASP:N	2.37	0.57
1:A:855:THR:HG21	1:A:857:ARG:NE	2.20	0.57
1:A:833:GLU:O	1:A:837:ILE:HG13	2.04	0.57
2:B:273:LEU:CB	2:B:276:ILE:HD12	2.26	0.57
1:A:265:LYS:HE3	1:A:265:LYS:HA	1.85	0.57
1:A:322:VAL:CG1	1:A:322:VAL:O	2.53	0.57
1:A:49:LYS:HE2	1:A:61:ILE:HD12	1.85	0.57
1:A:1339:LEU:HD13	5:E:147:HIS:CD2	2.40	0.57
3:C:101:LEU:HD13	3:C:118:LEU:HD23	1.86	0.57
12:L:30:ILE:HG22	12:L:31:CYS:H	1.69	0.57
2:B:1202:LEU:O	2:B:1206:GLU:HG3	2.04	0.57
14:T:16:DT:H1'	14:T:17:DT:H5''	1.86	0.57
2:B:25:ILE:HG21	2:B:658:ILE:HD12	1.86	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:483:LEU:HD11	2:B:491:THR:CG2	2.33	0.57
2:B:411:PRO:O	2:B:414:ALA:HB3	2.04	0.57
2:B:121:ASN:HA	2:B:207:GLY:HA2	1.85	0.57
1:A:196:GLU:HG2	1:A:197:PRO:HD2	1.87	0.57
1:A:317:LYS:O	1:A:318:SER:CB	2.52	0.57
1:A:399:HIS:O	1:A:400:PRO:C	2.40	0.57
2:B:914:LYS:HG2	2:B:937:ALA:HB3	1.87	0.57
1:A:1116:LEU:HB3	1:A:1308:THR:CG2	2.32	0.57
7:G:13:LEU:HD22	7:G:17:PHE:HB2	1.85	0.57
1:A:1237:ILE:HG22	1:A:1238:ILE:N	2.19	0.57
2:B:707:PRO:CG	2:B:708:GLU:H	2.15	0.57
4:D:47:LEU:HD11	7:G:3:PHE:CD2	2.40	0.57
3:C:238:ILE:HG22	3:C:243:VAL:HG23	1.87	0.57
2:B:168:GLY:N	2:B:450:ALA:HB1	2.16	0.57
1:A:903:ASN:ND2	1:A:904:THR:N	2.52	0.57
1:A:446:ARG:HB2	1:A:487:MET:SD	2.44	0.57
1:A:438:ASP:O	1:A:439:ASN:HB2	2.05	0.57
5:E:67:GLU:O	5:E:70:SER:N	2.37	0.57
2:B:807:ARG:HG2	2:B:1045:SER:OG	2.05	0.57
1:A:567:LYS:CD	1:A:568:PRO:HD2	2.34	0.57
10:J:2:ILE:HG12	10:J:57:ILE:HD12	1.86	0.57
3:C:238:ILE:HG23	3:C:242:GLN:HB2	1.85	0.57
2:B:129:PHE:HD2	2:B:166:PHE:HA	1.70	0.57
15:P:2:A:H2'	15:P:3:A:H8	1.70	0.57
2:B:326:ASP:OD2	2:B:328:GLU:HB3	2.05	0.57
7:G:21:ARG:CZ	7:G:24:GLN:HB2	2.35	0.57
1:A:853:ASP:OD1	1:A:855:THR:HB	2.04	0.57
2:B:222:ILE:H	2:B:240:ILE:CD1	2.17	0.57
2:B:865:LYS:HZ3	2:B:869:SER:HA	1.69	0.57
3:C:177:GLU:HG3	3:C:231:ASN:CB	2.32	0.57
3:C:99:LEU:HD12	3:C:118:LEU:HD13	1.87	0.57
8:H:130:ARG:HH11	8:H:130:ARG:N	2.00	0.57
2:B:992:ILE:HG12	2:B:993:THR:N	2.20	0.57
1:A:1037:LEU:HD22	1:A:1041:ALA:HB1	1.86	0.57
10:J:27:GLU:C	10:J:29:GLU:H	2.08	0.57
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.37	0.57
1:A:1370:LEU:O	1:A:1374:VAL:HG23	2.05	0.57
2:B:176:SER:O	2:B:182:SER:HB3	2.05	0.57
2:B:222:ILE:HD11	2:B:627:PHE:CZ	2.40	0.57
1:A:372:LYS:HA	1:A:435:HIS:CE1	2.39	0.57
5:E:56:LYS:NZ	5:E:84:ASP:H	2.03	0.57
4:D:128:VAL:C	4:D:130:LEU:H	2.07	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:56:THR:HG21	3:C:145:CYS:SG	2.45	0.57
1:A:679:ILE:HG12	1:A:732:LEU:HD12	1.86	0.57
2:B:110:HIS:CB	12:L:54:ARG:NH2	2.64	0.57
8:H:130:ARG:H	8:H:130:ARG:NH1	2.01	0.57
2:B:810:GLU:HA	2:B:815:ARG:NH2	2.20	0.57
7:G:106:MET:HG3	7:G:157:ILE:O	2.04	0.57
4:D:7:THR:HG23	4:D:7:THR:O	2.03	0.57
1:A:1166:ASP:OD2	1:A:1239:ARG:HD2	2.05	0.56
4:D:47:LEU:HD13	4:D:48:ILE:N	2.19	0.56
2:B:865:LYS:O	2:B:866:TYR:HD1	1.88	0.56
14:T:15:DG:H2"	14:T:16:DT:H6	1.70	0.56
3:C:259:LEU:CD2	11:K:91:CYS:HB3	2.35	0.56
5:E:30:ILE:HG22	5:E:31:THR:O	2.05	0.56
4:D:52:LEU:O	4:D:54:GLU:N	2.35	0.56
2:B:431:TYR:CD1	2:B:447:ALA:HB2	2.40	0.56
2:B:916:THR:HB	2:B:935:ARG:CG	2.35	0.56
2:B:778:MET:HE1	2:B:1094:ARG:HD3	1.87	0.56
1:A:897:TYR:HB3	1:A:936:LEU:CD1	2.35	0.56
9:I:14:LEU:HA	9:I:28:GLU:O	2.06	0.56
2:B:68:THR:HG22	2:B:91:SER:CB	2.34	0.56
10:J:23:ASN:C	10:J:25:LEU:N	2.57	0.56
1:A:1045:VAL:O	1:A:1049:ILE:HG13	2.05	0.56
1:A:982:THR:C	1:A:984:LYS:H	2.07	0.56
1:A:457:ALA:HB3	1:A:506:ALA:HA	1.86	0.56
2:B:20:ASP:C	2:B:22:SER:H	2.09	0.56
9:I:10:CYS:SG	9:I:32:CYS:HB3	2.44	0.56
1:A:54:ASN:HA	1:A:58:LEU:HD12	1.86	0.56
2:B:637:LEU:HB2	2:B:693:ILE:HD11	1.86	0.56
8:H:12:VAL:HG13	8:H:26:ILE:HD11	1.87	0.56
1:A:380:VAL:HG12	1:A:428:TYR:HA	1.86	0.56
7:G:139:ILE:CG2	7:G:140:LYS:N	2.68	0.56
9:I:118:ARG:NH1	9:I:120:GLN:HB2	2.20	0.56
3:C:124:LEU:O	3:C:126:GLY:N	2.38	0.56
5:E:145:THR:HG21	5:E:187:TYR:CE2	2.41	0.56
2:B:822:ASN:ND2	10:J:52:THR:HG21	2.20	0.56
2:B:859:TYR:OH	2:B:941:LEU:HD12	2.05	0.56
1:A:23:SER:HB3	1:A:233:TRP:CE2	2.40	0.56
1:A:596:THR:C	1:A:598:LEU:N	2.58	0.56
1:A:831:THR:CG2	1:A:832:ALA:N	2.65	0.56
9:I:7:CYS:SG	9:I:8:ARG:O	2.64	0.56
1:A:963:ILE:HD13	1:A:1049:ILE:HG12	1.87	0.56
3:C:254:LYS:HE2	11:K:42:LEU:HD13	1.86	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:477:PRO:HG2	1:A:521:MET:HG2	1.87	0.56
2:B:295:GLY:O	2:B:299:GLU:HG3	2.06	0.56
11:K:93:SER:OG	11:K:97:LYS:HE3	2.06	0.56
4:D:134:THR:HG22	4:D:135:GLY:N	2.20	0.56
1:A:875:ALA:HA	1:A:878:ILE:CD1	2.36	0.56
6:F:94:LEU:HD22	6:F:122:MET:HG2	1.87	0.56
1:A:57:ARG:O	1:A:68:GLN:HG2	2.06	0.56
2:B:850:LEU:HD12	2:B:851:PHE:N	2.20	0.56
2:B:885:MET:HA	2:B:936:ASP:HB3	1.87	0.56
1:A:698:GLN:NE2	9:I:99:LEU:HD11	2.21	0.56
10:J:1:MET:H1	10:J:57:ILE:H	1.53	0.56
2:B:293:PRO:HG2	2:B:296:GLU:CB	2.36	0.56
7:G:20:PRO:CD	7:G:21:ARG:H	2.18	0.56
2:B:186:GLU:HG3	10:J:62:ARG:NH2	2.18	0.56
2:B:300:HIS:O	2:B:303:TYR:HE2	1.87	0.56
2:B:308:TRP:CH2	9:I:45:ARG:HG2	2.41	0.56
2:B:805:THR:HA	2:B:809:MET:CE	2.35	0.56
1:A:868:TYR:OH	1:A:1366:ARG:HD3	2.05	0.56
2:B:276:ILE:CG2	2:B:336:ARG:HB2	2.36	0.56
8:H:26:ILE:HG22	8:H:40:LEU:O	2.05	0.56
1:A:381:THR:HG23	1:A:382:PRO:CD	2.32	0.56
7:G:34:VAL:HG13	7:G:45:ILE:HG21	1.88	0.56
7:G:48:VAL:HG13	7:G:74:TYR:HD1	1.69	0.56
2:B:918:ILE:HD12	2:B:935:ARG:NH1	2.21	0.56
8:H:84:ALA:CB	8:H:87:ARG:HB2	2.34	0.56
1:A:1317:MET:O	1:A:1322:ILE:HD11	2.04	0.56
11:K:88:LYS:O	11:K:91:CYS:HB2	2.04	0.56
2:B:1156:ASP:O	2:B:1157:ALA:O	2.23	0.56
2:B:459:TYR:CZ	2:B:469:GLN:HG2	2.41	0.56
3:C:33:LEU:O	3:C:37:MET:HG3	2.05	0.56
6:F:111:LEU:O	6:F:113:GLY:N	2.32	0.56
2:B:553:PRO:HG2	2:B:554:ILE:HD12	1.87	0.56
2:B:542:MET:HE3	2:B:747:MET:HG3	1.87	0.56
2:B:254:LEU:HD23	2:B:381:MET:HE3	1.87	0.56
3:C:221:TYR:CE1	3:C:222:LYS:HG3	2.41	0.56
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	1.86	0.56
1:A:69:THR:HG21	2:B:1174:LYS:HZ2	1.71	0.56
2:B:886:LYS:NZ	2:B:936:ASP:OD1	2.39	0.56
2:B:798:TYR:HE2	3:C:62:PHE:CZ	2.23	0.56
2:B:189:LEU:HD13	2:B:196:PRO:HA	1.88	0.56
1:A:591:PHE:HA	1:A:595:THR:CG2	2.35	0.56
2:B:990:ILE:HG22	2:B:991:GLY:N	2.21	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1159:ARG:HD2	1:A:1159:ARG:N	2.21	0.56
2:B:68:THR:HG22	2:B:91:SER:CA	2.35	0.56
1:A:1006:ILE:HD11	5:E:163:GLU:HG3	1.87	0.56
5:E:157:SER:C	5:E:159:ASP:H	2.09	0.56
2:B:39:ARG:NH2	2:B:665:GLU:HG2	2.20	0.56
1:A:129:LYS:O	1:A:130:ASP:CB	2.53	0.56
1:A:239:LEU:HD12	1:A:240:PRO:HD2	1.87	0.56
2:B:1017:ILE:HB	2:B:1018:PRO:HD3	1.88	0.56
7:G:138:THR:CG2	7:G:139:ILE:N	2.49	0.56
2:B:865:LYS:HZ2	2:B:869:SER:HA	1.69	0.56
10:J:53:HIS:CD2	10:J:53:HIS:C	2.77	0.56
4:D:14:ARG:NH1	4:D:16:LYS:HD2	2.21	0.56
2:B:120:ARG:NH1	12:L:54:ARG:HD2	2.20	0.56
1:A:1316:VAL:HG12	1:A:1316:VAL:O	2.05	0.56
1:A:285:PRO:HG2	1:A:288:ALA:HB3	1.88	0.56
1:A:973:ILE:HD13	1:A:1037:LEU:HA	1.88	0.56
3:C:73:GLN:NE2	3:C:75:MET:H	2.00	0.56
1:A:332:LYS:O	1:A:334:GLY:N	2.38	0.56
2:B:303:TYR:N	2:B:303:TYR:CD2	2.74	0.56
2:B:750:GLY:O	2:B:751:VAL:C	2.44	0.56
2:B:359:GLU:O	2:B:362:PRO:HD3	2.05	0.56
2:B:284:ILE:HD13	2:B:333:PHE:CD2	2.41	0.56
2:B:26:THR:HB	2:B:708:GLU:OE1	2.06	0.56
5:E:147:HIS:HB3	5:E:150:VAL:CG2	2.36	0.56
1:A:1033:GLN:HA	1:A:1036:ARG:NH1	2.19	0.56
2:B:204:ILE:C	2:B:205:ILE:HD12	2.26	0.56
2:B:254:LEU:HD23	2:B:381:MET:CE	2.36	0.56
2:B:615:MET:HB3	2:B:626:ILE:CG1	2.30	0.56
2:B:842:ASN:O	2:B:846:ILE:HG13	2.06	0.56
1:A:787:PHE:HE1	1:A:796:SER:HA	1.70	0.56
7:G:87:VAL:HB	7:G:103:VAL:HG11	1.87	0.56
5:E:179:GLN:HA	5:E:179:GLN:OE1	2.06	0.56
5:E:112:TYR:CE1	5:E:136:ASN:HA	2.41	0.55
2:B:1174:LYS:O	2:B:1176:ASN:N	2.39	0.55
3:C:235:VAL:HG21	10:J:6:ARG:NH2	2.21	0.55
2:B:129:PHE:CE2	2:B:166:PHE:CD1	2.94	0.55
5:E:164:LEU:CD2	5:E:211:TYR:CD2	2.88	0.55
5:E:171:LYS:HG2	5:E:174:GLN:CD	2.26	0.55
1:A:108:MET:HB3	1:A:210:ILE:CD1	2.36	0.55
8:H:12:VAL:CG1	8:H:26:ILE:HD11	2.36	0.55
2:B:705:MET:HA	2:B:705:MET:CE	2.35	0.55
1:A:34:LYS:HZ1	1:A:57:ARG:HH21	1.55	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:56:PRO:O	1:A:57:ARG:CG	2.52	0.55
2:B:847:ASP:C	2:B:849:GLY:N	2.59	0.55
1:A:427:GLN:HB2	1:A:430:TRP:CD1	2.41	0.55
3:C:243:VAL:HG12	3:C:243:VAL:O	2.06	0.55
1:A:335:ARG:NH1	2:B:1206:GLU:OE1	2.38	0.55
10:J:7:CYS:HA	10:J:49:MET:HE3	1.88	0.55
2:B:186:GLU:CG	10:J:62:ARG:HH22	2.19	0.55
3:C:226:ASP:O	3:C:227:THR:CB	2.53	0.55
2:B:430:ARG:HB3	2:B:434:ARG:NH2	2.21	0.55
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.88	0.55
3:C:114:TYR:CD2	3:C:140:ASN:HB3	2.41	0.55
3:C:100:THR:CG2	3:C:102:GLN:HE21	2.18	0.55
1:A:1168:GLU:O	1:A:1171:GLN:OE1	2.24	0.55
1:A:590:ARG:HB3	1:A:605:MET:N	2.22	0.55
2:B:810:GLU:HA	2:B:815:ARG:HH22	1.71	0.55
12:L:61:THR:HG22	12:L:63:ARG:H	1.71	0.55
2:B:429:PHE:CD1	2:B:432:MET:HE3	2.41	0.55
4:D:50:LEU:HD21	7:G:4:ILE:HD12	1.87	0.55
2:B:1115:THR:HG22	2:B:1117:GLN:H	1.70	0.55
1:A:341:MET:CE	2:B:1135:ARG:NH1	2.70	0.55
7:G:101:VAL:HG12	7:G:102:GLN:N	2.21	0.55
5:E:169:ARG:HB3	6:F:140:ASP:OD2	2.07	0.55
8:H:12:VAL:CG1	8:H:51:ALA:HA	2.36	0.55
2:B:999:MET:HB3	2:B:1007:VAL:CG2	2.36	0.55
1:A:1345:ARG:HG2	1:A:1372:VAL:HG12	1.87	0.55
1:A:1348:LEU:HD23	1:A:1372:VAL:HG13	1.89	0.55
2:B:20:ASP:O	2:B:22:SER:N	2.35	0.55
2:B:1050:ILE:HG22	2:B:1051:THR:N	2.21	0.55
2:B:711:GLU:HB2	2:B:712:PRO:CD	2.36	0.55
1:A:571:LEU:CD2	8:H:46:LEU:HD11	2.36	0.55
2:B:1161:HIS:NE2	2:B:1175:LEU:HD21	2.22	0.55
2:B:842:ASN:HD21	2:B:844:SER:HB2	1.72	0.55
1:A:979:SER:OG	1:A:980:ASP:N	2.38	0.55
1:A:1308:THR:HG23	1:A:1309:ASP:H	1.69	0.55
1:A:616:VAL:HG12	1:A:617:VAL:N	2.21	0.55
2:B:315:LYS:N	2:B:316:PRO:HD2	2.22	0.55
6:F:128:LYS:HD3	6:F:149:GLU:O	2.06	0.55
1:A:780:VAL:O	1:A:782:ARG:HG2	2.07	0.55
1:A:567:LYS:HB3	8:H:95:TYR:CA	2.36	0.55
6:F:94:LEU:HD21	6:F:122:MET:HA	1.89	0.55
5:E:56:LYS:HZ3	5:E:84:ASP:H	1.54	0.55
1:A:598:LEU:HA	8:H:122:LEU:HD13	1.87	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:I:6:PHE:HA	9:I:14:LEU:HG	1.89	0.55
1:A:311:GLN:O	1:A:313:GLN:N	2.40	0.55
9:I:73:ARG:O	9:I:81:ARG:HA	2.07	0.55
2:B:360:PHE:CD2	2:B:360:PHE:C	2.80	0.55
2:B:1174:LYS:O	2:B:1175:LEU:C	2.44	0.55
5:E:82:PHE:N	5:E:82:PHE:CD1	2.74	0.55
12:L:38:LEU:HG	12:L:39:SER:H	1.71	0.55
3:C:189:THR:CG2	3:C:190:ASP:N	2.70	0.55
3:C:10:ILE:HG13	11:K:108:GLU:HB3	1.87	0.55
1:A:870:GLU:HG2	5:E:208:TYR:CD2	2.41	0.55
1:A:853:ASP:OD1	1:A:855:THR:HG22	2.07	0.55
2:B:281:PRO:HB3	2:B:320:ASP:OD2	2.06	0.55
4:D:39:ASN:HD22	4:D:41:GLN:HB2	1.71	0.55
1:A:1076:ALA:HA	1:A:1079:MET:CE	2.37	0.55
2:B:704:ALA:HB2	2:B:738:PHE:CD2	2.42	0.55
2:B:240:ILE:HG21	2:B:381:MET:HE1	1.88	0.55
2:B:549:THR:CG2	2:B:550:ASP:N	2.70	0.55
7:G:74:TYR:H	7:G:74:TYR:HD2	1.55	0.55
7:G:129:SER:CB	7:G:138:THR:OG1	2.55	0.55
2:B:916:THR:O	2:B:935:ARG:HG2	2.07	0.55
1:A:925:LEU:HD13	1:A:983:ILE:HG22	1.88	0.55
4:D:14:ARG:CZ	4:D:16:LYS:HD2	2.37	0.55
8:H:83:GLN:C	8:H:85:GLY:H	2.10	0.55
1:A:590:ARG:HG3	1:A:591:PHE:N	2.21	0.55
5:E:124:VAL:N	5:E:125:PRO:CD	2.70	0.55
1:A:1385:THR:CG2	1:A:1386:ARG:N	2.69	0.55
8:H:128:ASN:ND2	8:H:131:ASN:OD1	2.39	0.55
1:A:1029:ARG:CG	1:A:1029:ARG:HH11	2.20	0.55
1:A:266:LEU:HD21	1:A:303:TYR:CZ	2.41	0.55
2:B:1045:SER:O	2:B:1048:THR:HG23	2.06	0.55
1:A:1244:ARG:NE	1:A:1245:PRO:HD2	2.05	0.55
1:A:399:HIS:CB	1:A:400:PRO:CD	2.78	0.55
1:A:401:GLY:C	1:A:435:HIS:HD2	2.09	0.55
8:H:139:ASN:O	8:H:140:ALA:CB	2.54	0.55
1:A:1030:ARG:CG	1:A:1034:GLU:OE2	2.53	0.55
1:A:899:VAL:CG1	1:A:929:LEU:HD12	2.37	0.55
1:A:443:LEU:O	1:A:489:LEU:HD12	2.06	0.55
1:A:1120:LEU:HD23	1:A:1304:TRP:O	2.06	0.55
1:A:75:ASN:ND2	2:B:1116:ARG:NH1	2.54	0.55
1:A:940:ARG:O	1:A:944:ARG:HG3	2.06	0.55
10:J:16:ASP:OD1	10:J:16:ASP:N	2.34	0.55
3:C:91:HIS:ND1	3:C:158:VAL:HG11	2.21	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:I:22:ASN:O	9:I:23:ASN:HB2	2.07	0.55
1:A:1402:PHE:CE2	1:A:1403:GLU:HG3	2.42	0.55
2:B:857:ARG:HH21	2:B:942:ARG:CZ	2.20	0.55
10:J:31:ASP:OD1	10:J:34:THR:OG1	2.25	0.55
1:A:79:GLY:HA3	1:A:243:PRO:CG	2.36	0.55
8:H:63:LEU:HD11	8:H:141:TYR:CD2	2.42	0.55
1:A:1105:LEU:HD22	1:A:1384:VAL:HG21	1.89	0.55
1:A:579:SER:HA	1:A:582:ILE:HG13	1.87	0.55
1:A:62:ASP:O	1:A:64:ASN:N	2.40	0.54
2:B:852:ARG:HH22	12:L:70:ARG:C	2.10	0.54
1:A:407:ARG:HG2	1:A:430:TRP:CH2	2.42	0.54
4:D:220:LEU:HD22	4:D:221:TYR:H	1.66	0.54
1:A:211:PHE:O	1:A:214:ILE:HG13	2.07	0.54
1:A:225:ASN:ND2	1:A:227:VAL:H	2.05	0.54
1:A:1116:LEU:H	1:A:1308:THR:HG22	1.71	0.54
1:A:331:GLY:O	1:A:332:LYS:O	2.24	0.54
4:D:71:LYS:HA	4:D:74:GLN:CB	2.36	0.54
2:B:91:SER:OG	2:B:133:LYS:HB2	2.07	0.54
2:B:235:SER:O	2:B:236:HIS:HD2	1.88	0.54
3:C:91:HIS:HD2	3:C:91:HIS:O	1.90	0.54
1:A:1287:TYR:CD1	1:A:1305:VAL:HG21	2.42	0.54
1:A:738:LYS:HG3	1:A:740:LEU:HG	1.88	0.54
3:C:138:GLU:OE1	3:C:138:GLU:N	2.40	0.54
1:A:689:LYS:HE2	1:A:721:PHE:CE2	2.41	0.54
4:D:155:ARG:HD3	4:D:221:TYR:CZ	2.43	0.54
2:B:1068:GLY:O	2:B:1069:PHE:O	2.25	0.54
11:K:50:LEU:HD11	11:K:75:ILE:CD1	2.37	0.54
1:A:288:ALA:HA	1:A:291:GLU:HG3	1.88	0.54
1:A:1110:ASN:H	1:A:1110:ASN:HD22	1.55	0.54
3:C:116:LYS:HD3	3:C:140:ASN:HA	1.90	0.54
1:A:264:PHE:C	1:A:265:LYS:HE3	2.27	0.54
1:A:463:ILE:HB	1:A:464:PRO:HD2	1.90	0.54
1:A:962:ARG:O	1:A:964:ILE:N	2.41	0.54
2:B:90:ILE:CD1	2:B:432:MET:SD	2.94	0.54
11:K:108:GLU:O	11:K:112:GLN:HG2	2.07	0.54
10:J:14:VAL:CG1	10:J:50:ILE:HD11	2.37	0.54
11:K:52:ASN:O	11:K:54:ARG:N	2.40	0.54
6:F:111:LEU:C	6:F:113:GLY:H	2.08	0.54
5:E:21:GLU:O	5:E:24:LYS:HG2	2.08	0.54
8:H:33:GLN:C	8:H:35:GLN:H	2.10	0.54
1:A:744:LYS:HG2	1:A:748:MET:HE2	1.88	0.54
1:A:133:LYS:O	1:A:136:ALA:HB3	2.06	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:868:TYR:CZ	1:A:1366:ARG:HD3	2.42	0.54
2:B:222:ILE:HD11	2:B:627:PHE:HZ	1.72	0.54
3:C:43:THR:CG2	3:C:44:LEU:N	2.70	0.54
1:A:541:ILE:HG22	1:A:546:VAL:HG23	1.88	0.54
7:G:119:LEU:HD12	7:G:120:THR:H	1.72	0.54
2:B:1182:CYS:SG	2:B:1185:CYS:HB2	2.47	0.54
1:A:311:GLN:O	1:A:312:PRO:C	2.45	0.54
1:A:1161:THR:C	1:A:1163:ILE:N	2.61	0.54
2:B:288:ALA:HA	2:B:331:LEU:HD12	1.90	0.54
1:A:668:ASP:HB3	1:A:741:ASN:ND2	2.17	0.54
15:P:2:A:H2'	15:P:3:A:C8	2.43	0.54
1:A:472:LEU:O	1:A:475:THR:HB	2.07	0.54
4:D:69:ALA:HB2	4:D:72:ARG:NH2	2.22	0.54
8:H:1:MET:O	8:H:1:MET:HG2	2.07	0.54
2:B:520:GLY:H	2:B:748:ILE:HG22	1.73	0.54
2:B:563:MET:SD	2:B:580:VAL:HG11	2.48	0.54
2:B:332:ASP:O	2:B:334:ILE:N	2.33	0.54
7:G:1:MET:SD	7:G:79:PHE:CE1	3.01	0.54
2:B:936:ASP:OD1	2:B:937:ALA:N	2.41	0.54
4:D:156:ASP:HB2	4:D:159:THR:OG1	2.08	0.54
1:A:1259:MET:HE3	1:A:1263:ILE:HG13	1.89	0.54
2:B:427:ASP:HA	2:B:430:ARG:HD2	1.87	0.54
2:B:345:LYS:HA	2:B:348:ARG:HE	1.72	0.54
3:C:143:LEU:HG	3:C:143:LEU:O	2.08	0.54
1:A:320:ARG:NE	1:A:323:LYS:NZ	2.55	0.54
7:G:126:ASN:C	7:G:126:ASN:ND2	2.60	0.54
10:J:1:MET:O	10:J:2:ILE:O	2.26	0.54
2:B:642:ASP:H	2:B:649:LYS:HE3	1.72	0.54
2:B:653:VAL:HA	2:B:657:HIS:CD2	2.43	0.54
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.42	0.54
2:B:313:MET:CE	2:B:386:LEU:HD22	2.37	0.54
1:A:75:ASN:O	1:A:76:GLU:CB	2.56	0.54
4:D:209:ARG:HG2	4:D:209:ARG:HH11	1.72	0.54
2:B:487:THR:HG22	2:B:490:SER:H	1.73	0.54
3:C:8:VAL:HG12	3:C:9:LYS:N	2.22	0.54
2:B:580:VAL:HG22	2:B:624:LEU:HB3	1.89	0.54
8:H:8:ASP:OD2	8:H:9:ILE:N	2.40	0.54
2:B:616:ILE:HG23	2:B:700:SER:OG	2.08	0.54
1:A:1236:LEU:C	1:A:1237:ILE:HG13	2.27	0.54
3:C:146:LYS:C	3:C:147:LEU:HD23	2.28	0.54
8:H:84:ALA:C	8:H:86:ASP:N	2.58	0.54
1:A:744:LYS:HG2	1:A:748:MET:CE	2.38	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:8:VAL:HG12	3:C:9:LYS:H	1.72	0.54
8:H:9:ILE:HD13	8:H:146:ARG:HH12	1.72	0.54
1:A:1244:ARG:HE	1:A:1245:PRO:CD	2.07	0.54
1:A:399:HIS:CG	1:A:400:PRO:N	2.74	0.54
4:D:130:LEU:O	4:D:132:GLN:N	2.37	0.54
4:D:35:LEU:HD12	4:D:35:LEU:N	2.23	0.54
2:B:866:TYR:CB	2:B:870:ILE:HB	2.36	0.54
2:B:914:LYS:HE2	2:B:937:ALA:HB1	1.90	0.54
1:A:541:ILE:HD11	1:A:656:TRP:CD1	2.42	0.54
11:K:31:VAL:HG12	11:K:32:VAL:H	1.72	0.54
8:H:130:ARG:HB3	8:H:134:ASN:H	1.73	0.54
2:B:69:LEU:HB3	2:B:429:PHE:CE1	2.40	0.54
1:A:833:GLU:HG3	1:A:1102:LYS:HE2	1.90	0.54
2:B:118:ARG:HH22	2:B:194:GLU:CD	2.11	0.54
2:B:637:LEU:HD22	2:B:741:CYS:O	2.07	0.54
1:A:1191:TRP:CZ3	9:I:43:VAL:HG21	2.43	0.54
2:B:644:GLU:HB3	2:B:648:HIS:O	2.07	0.54
1:A:1074:GLU:HB3	1:A:1075:PRO:CD	2.38	0.54
9:I:7:CYS:HB2	9:I:34:TYR:CG	2.43	0.54
8:H:127:GLY:O	8:H:128:ASN:CB	2.53	0.54
2:B:327:ARG:HH21	2:B:371:GLU:HG2	1.70	0.54
11:K:67:PHE:C	11:K:68:PHE:HD2	2.11	0.54
2:B:185:THR:O	2:B:186:GLU:C	2.46	0.54
2:B:398:ARG:NH1	2:B:398:ARG:CB	2.71	0.54
2:B:794:ASN:ND2	2:B:794:ASN:N	2.56	0.54
2:B:590:HIS:NE2	2:B:592:ASN:O	2.40	0.53
3:C:137:LYS:HB3	3:C:138:GLU:OE1	2.07	0.53
2:B:557:PHE:CD2	2:B:557:PHE:C	2.81	0.53
5:E:192:ARG:NH1	5:E:192:ARG:HG3	2.23	0.53
1:A:464:PRO:HG2	1:A:465:TYR:CD1	2.43	0.53
12:L:61:THR:CG2	12:L:63:ARG:HG3	2.37	0.53
2:B:435:THR:C	2:B:437:GLU:N	2.60	0.53
9:I:101:PHE:H	9:I:101:PHE:HD1	1.56	0.53
1:A:416:ARG:HG3	1:A:417:TYR:CD1	2.43	0.53
3:C:251:LEU:O	3:C:255:VAL:HG23	2.08	0.53
4:D:117:GLU:HG2	4:D:122:GLU:OE2	2.08	0.53
4:D:130:LEU:C	4:D:132:GLN:H	2.11	0.53
10:J:53:HIS:NE2	10:J:55:ASP:HA	2.24	0.53
2:B:192:LEU:O	2:B:193:LYS:HB2	2.08	0.53
1:A:942:PHE:CE1	5:E:207:ARG:HD3	2.40	0.53
1:A:962:ARG:O	1:A:965:GLN:N	2.41	0.53
4:D:208:GLU:HA	4:D:211:LEU:HD12	1.90	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:209:GLU:OE2	2:B:485:ARG:NE	2.36	0.53
3:C:114:TYR:CD2	3:C:140:ASN:HB2	2.43	0.53
5:E:112:TYR:O	5:E:137:GLU:HG3	2.08	0.53
9:I:62:ILE:HG12	9:I:62:ILE:O	2.08	0.53
3:C:66:ARG:NH1	3:C:144:ILE:O	2.42	0.53
3:C:239:PRO:O	3:C:242:GLN:N	2.42	0.53
2:B:801:LYS:O	10:J:52:THR:HG23	2.08	0.53
2:B:831:SER:HB3	2:B:994:TYR:OH	2.09	0.53
1:A:335:ARG:O	1:A:339:ASN:HB2	2.08	0.53
5:E:108:GLY:O	5:E:132:ILE:HG22	2.09	0.53
1:A:1121:GLU:HB2	1:A:1321:GLY:O	2.08	0.53
1:A:1147:THR:HB	9:I:48:LEU:CD1	2.38	0.53
1:A:890:ASP:H	1:A:1296:GLY:HA3	1.73	0.53
8:H:37:LYS:HD2	8:H:126:GLU:OE2	2.09	0.53
1:A:205:GLU:CD	1:A:205:GLU:H	2.11	0.53
5:E:90:VAL:HA	5:E:120:ALA:CB	2.36	0.53
4:D:155:ARG:HD3	4:D:221:TYR:OH	2.07	0.53
3:C:100:THR:HG22	3:C:101:LEU:N	2.23	0.53
1:A:93:VAL:CG1	1:A:301:ALA:HB1	2.37	0.53
4:D:13:ARG:O	4:D:15:LEU:N	2.42	0.53
12:L:58:LYS:O	12:L:59:ALA:O	2.27	0.53
1:A:547:LEU:HD21	1:A:560:ILE:HD13	1.90	0.53
2:B:63:ILE:HD12	2:B:421:PHE:CE2	2.44	0.53
1:A:965:GLN:HA	1:A:968:GLN:HG3	1.89	0.53
1:A:50:ILE:O	1:A:52:GLY:N	2.40	0.53
11:K:12:LEU:HG	11:K:16:GLU:HB2	1.90	0.53
2:B:1180:PHE:HB3	2:B:1191:ILE:HD13	1.89	0.53
1:A:481:ASP:OD1	1:A:485:ASP:OD2	2.25	0.53
2:B:637:LEU:HD21	2:B:742:GLU:OE2	2.09	0.53
1:A:1186:ASP:O	1:A:1187:GLN:CB	2.53	0.53
2:B:871:THR:HG22	2:B:872:GLU:N	2.23	0.53
2:B:872:GLU:OE1	2:B:914:LYS:HE3	2.07	0.53
2:B:1065:GLN:HB3	2:B:1069:PHE:O	2.09	0.53
4:D:149:THR:CG2	4:D:150:ASN:N	2.72	0.53
12:L:34:CYS:SG	12:L:34:CYS:O	2.67	0.53
3:C:189:THR:CG2	3:C:190:ASP:H	2.21	0.53
1:A:853:ASP:OD1	1:A:855:THR:N	2.42	0.53
2:B:398:ARG:CB	2:B:398:ARG:HH11	2.21	0.53
6:F:111:LEU:C	6:F:113:GLY:N	2.62	0.53
9:I:82:GLU:HB3	9:I:104:LEU:HD12	1.91	0.53
1:A:1343:ALA:O	1:A:1346:ALA:HB3	2.08	0.53
1:A:1202:MET:HE1	1:A:1212:VAL:HG21	1.89	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:864:LYS:HG3	2:B:872:GLU:OE1	2.09	0.53
2:B:770:GLN:CD	2:B:983:ARG:HA	2.27	0.53
3:C:177:GLU:O	3:C:230:MET:HA	2.09	0.53
1:A:665:GLY:C	1:A:666:ILE:HD12	2.28	0.53
1:A:549:MET:SD	1:A:577:ILE:CD1	2.96	0.53
1:A:93:VAL:HG21	1:A:301:ALA:O	2.08	0.53
1:A:356:ASP:OD1	1:A:358:ASN:N	2.42	0.53
1:A:50:ILE:C	1:A:52:GLY:N	2.62	0.53
1:A:458:HIS:CE1	1:A:507:VAL:HG21	2.43	0.53
9:I:50:THR:CG2	9:I:51:ASN:N	2.71	0.53
2:B:291:ILE:HD13	2:B:300:HIS:NE2	2.23	0.53
1:A:184:SER:CB	1:A:199:LEU:HD23	2.39	0.53
1:A:270:LEU:O	1:A:274:ILE:HG13	2.08	0.53
2:B:222:ILE:N	2:B:240:ILE:CD1	2.72	0.53
1:A:590:ARG:NH2	1:A:620:LYS:HB2	2.23	0.53
1:A:1130:GLN:HA	1:A:1133:LEU:HD12	1.91	0.53
1:A:1341:ILE:HG23	1:A:1342:GLU:N	2.23	0.53
5:E:129:PRO:O	5:E:130:ALA:C	2.47	0.53
2:B:728:ARG:HH12	2:B:1047:PHE:HB3	1.73	0.53
1:A:350:ARG:HB2	2:B:1128:LEU:CD1	2.39	0.53
2:B:557:PHE:HD2	2:B:557:PHE:C	2.11	0.53
8:H:13:SER:HB3	8:H:27:GLU:O	2.09	0.53
3:C:241:ASP:O	3:C:245:VAL:HG23	2.09	0.53
1:A:666:ILE:CD1	1:A:667:GLY:N	2.72	0.53
2:B:1059:LEU:HD23	2:B:1065:GLN:O	2.09	0.53
1:A:1313:LEU:HD23	1:A:1338:VAL:CG2	2.39	0.53
5:E:161:LYS:HD2	5:E:195:VAL:HG23	1.91	0.53
4:D:193:THR:HG21	7:G:167:TYR:HD1	1.73	0.53
1:A:1325:THR:O	5:E:148:GLU:HB2	2.08	0.53
9:I:111:THR:OG1	9:I:112:SER:N	2.42	0.53
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.91	0.53
2:B:58:THR:O	2:B:62:ILE:HG13	2.08	0.53
2:B:755:ILE:HG22	2:B:755:ILE:O	2.09	0.53
2:B:376:PHE:CZ	2:B:569:TYR:HB3	2.44	0.53
2:B:363:HIS:O	2:B:364:ILE:HB	2.09	0.53
2:B:331:LEU:CD2	2:B:353:LYS:HG2	2.38	0.53
4:D:47:LEU:HD13	4:D:48:ILE:H	1.74	0.53
2:B:619:ILE:HG22	2:B:620:ARG:N	2.24	0.53
3:C:43:THR:HG22	3:C:44:LEU:N	2.24	0.53
2:B:102:VAL:HG23	2:B:112:LEU:HB2	1.89	0.53
7:G:119:LEU:HD12	7:G:120:THR:N	2.24	0.53
2:B:292:ILE:HD11	2:B:327:ARG:H	1.74	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:J:23:ASN:O	10:J:25:LEU:N	2.42	0.53
2:B:558:LEU:HD22	2:B:596:LEU:HD11	1.91	0.53
8:H:133:ASN:O	8:H:135:LEU:N	2.41	0.53
1:A:786:HIS:CD2	1:A:786:HIS:N	2.74	0.53
2:B:640:VAL:HG22	2:B:651:LEU:HD23	1.89	0.53
3:C:148:ARG:N	3:C:151:GLN:HG3	2.23	0.53
1:A:719:VAL:HG13	1:A:723:ASN:ND2	2.24	0.53
3:C:123:ASN:C	3:C:125:MET:H	2.12	0.53
3:C:120:ILE:HD11	3:C:130:GLY:O	2.08	0.53
1:A:659:HIS:O	2:B:1081:LEU:HD23	2.09	0.53
2:B:763:GLN:HG2	2:B:765:PRO:CD	2.35	0.53
1:A:828:ALA:C	1:A:831:THR:HG22	2.30	0.53
2:B:185:THR:H	2:B:188:ASP:HB2	1.73	0.53
2:B:31:TRP:CZ2	2:B:807:ARG:HB2	2.44	0.52
2:B:806:THR:HA	2:B:1045:SER:OG	2.09	0.52
2:B:278:GLN:CG	2:B:279:ASP:N	2.58	0.52
1:A:1191:TRP:HZ3	9:I:43:VAL:HG21	1.73	0.52
2:B:244:LEU:O	2:B:249:ARG:HG3	2.08	0.52
1:A:385:ILE:CD1	1:A:426:LEU:HB2	2.39	0.52
2:B:882:THR:HG22	2:B:883:LEU:N	2.24	0.52
2:B:619:ILE:O	2:B:622:LYS:N	2.34	0.52
3:C:18:VAL:O	3:C:20:PHE:HD2	1.92	0.52
1:A:102:VAL:CB	1:A:211:PHE:HE1	2.22	0.52
1:A:337:ARG:HD3	1:A:839:ARG:NH2	2.24	0.52
5:E:178:ILE:HG22	5:E:213:ILE:O	2.08	0.52
12:L:26:THR:HG23	12:L:27:LEU:H	1.73	0.52
1:A:853:ASP:OD1	1:A:855:THR:CB	2.56	0.52
3:C:258:ILE:N	3:C:258:ILE:HD12	2.24	0.52
1:A:1009:ASN:CG	1:A:1012:ARG:HH12	2.13	0.52
1:A:377:PRO:HD3	1:A:493:GLN:OE1	2.08	0.52
2:B:875:GLU:O	2:B:877:PRO:HD3	2.08	0.52
3:C:123:ASN:ND2	3:C:125:MET:HA	2.24	0.52
1:A:154:SER:CB	1:A:162:VAL:CG2	2.87	0.52
7:G:115:MET:HA	7:G:163:ILE:HG13	1.91	0.52
1:A:710:LEU:HD22	9:I:96:SER:HA	1.90	0.52
6:F:109:VAL:CG1	6:F:110:ASP:N	2.72	0.52
2:B:816:GLU:O	2:B:817:LEU:HD23	2.09	0.52
8:H:91:ASP:O	8:H:93:TYR:N	2.39	0.52
8:H:27:GLU:HG2	8:H:39:THR:HA	1.90	0.52
3:C:104:PHE:HD2	3:C:105:GLY:N	2.07	0.52
1:A:306:ASN:ND2	1:A:322:VAL:HG12	2.25	0.52
2:B:1175:LEU:O	2:B:1176:ASN:HB2	2.10	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:692:ASP:O	1:A:694:THR:N	2.42	0.52
1:A:168:GLY:O	1:A:169:ASN:C	2.47	0.52
1:A:897:TYR:HB3	1:A:936:LEU:HD12	1.92	0.52
2:B:294:ASP:C	2:B:296:GLU:H	2.12	0.52
2:B:874:PHE:HA	2:B:913:GLY:O	2.09	0.52
2:B:758:PHE:CZ	2:B:1044:ALA:HA	2.44	0.52
1:A:1006:ILE:CD1	5:E:163:GLU:HG3	2.39	0.52
1:A:851:HIS:HB2	1:A:855:THR:HG22	1.92	0.52
1:A:152:VAL:HG12	1:A:153:PRO:HD2	1.90	0.52
5:E:157:SER:C	5:E:159:ASP:N	2.62	0.52
1:A:1402:PHE:CG	1:A:1403:GLU:HG2	2.44	0.52
3:C:39:ALA:O	3:C:164:ALA:HB3	2.09	0.52
1:A:132:LYS:HE3	1:A:1411:GLU:HG3	1.90	0.52
1:A:1215:ARG:NH1	1:A:1272:THR:O	2.43	0.52
8:H:106:GLU:O	8:H:108:SER:N	2.32	0.52
2:B:708:GLU:O	2:B:709:ASP:C	2.48	0.52
1:A:12:ARG:NH1	2:B:1218:THR:HB	2.25	0.52
3:C:123:ASN:HD22	3:C:125:MET:HG2	1.74	0.52
5:E:61:GLN:NE2	5:E:105:PHE:CE2	2.78	0.52
2:B:1202:LEU:HD22	2:B:1206:GLU:CD	2.30	0.52
1:A:16:GLU:HB3	1:A:1418:LEU:HD11	1.91	0.52
12:L:60:ARG:HG2	12:L:61:THR:N	2.21	0.52
1:A:886:ILE:CG2	1:A:887:GLY:N	2.71	0.52
2:B:134:LYS:HE2	2:B:164:LYS:HZ3	1.72	0.52
1:A:851:HIS:HB2	1:A:855:THR:CG2	2.39	0.52
8:H:40:LEU:HB2	8:H:123:MET:HE2	1.91	0.52
3:C:148:ARG:NH1	10:J:64:ASN:HA	2.24	0.52
2:B:865:LYS:C	2:B:866:TYR:HD1	2.13	0.52
1:A:666:ILE:HD12	1:A:667:GLY:N	2.21	0.52
1:A:774:ARG:O	1:A:775:ILE:C	2.47	0.52
7:G:88:ASP:HB3	7:G:144:ARG:CA	2.32	0.52
7:G:106:MET:CG	7:G:107:LYS:N	2.72	0.52
1:A:356:ASP:OD1	1:A:358:ASN:HB2	2.09	0.52
2:B:1116:ARG:HD2	2:B:1198:TYR:CD1	2.44	0.52
1:A:626:ASN:O	1:A:631:HIS:CD2	2.62	0.52
1:A:555:ASP:O	1:A:556:TRP:C	2.48	0.52
1:A:864:ILE:HG22	1:A:865:GLN:HG3	1.91	0.52
2:B:373:ARG:NH2	2:B:587:HIS:HA	2.24	0.52
2:B:549:THR:CG2	2:B:550:ASP:H	2.23	0.52
1:A:1161:THR:OG1	1:A:1239:ARG:NH2	2.43	0.52
1:A:13:THR:HB	1:A:1432:GLN:NE2	2.25	0.52
4:D:47:LEU:HD11	7:G:3:PHE:HD2	1.74	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:866:TYR:HB3	2:B:870:ILE:HD12	1.90	0.52
1:A:102:VAL:HG21	1:A:234:MET:HE1	1.91	0.52
2:B:193:LYS:HZ1	12:L:32:ALA:HB1	1.75	0.52
2:B:901:PRO:HD2	12:L:59:ALA:O	2.10	0.52
4:D:71:LYS:CG	4:D:74:GLN:HG3	2.40	0.52
2:B:383:ASN:O	2:B:387:LEU:HD12	2.10	0.52
1:A:1397:LEU:HB2	1:A:1426:GLU:OE1	2.10	0.52
15:P:1:C:H2'	15:P:1:C:O2	2.10	0.52
1:A:54:ASN:N	1:A:54:ASN:HD22	2.07	0.52
1:A:1218:GLN:O	1:A:1221:LYS:HE3	2.10	0.52
8:H:9:ILE:HG12	8:H:56:THR:HA	1.92	0.52
2:B:245:GLU:HG2	2:B:246:LYS:HG3	1.90	0.52
3:C:18:VAL:HG23	3:C:240:VAL:HB	1.89	0.52
1:A:598:LEU:O	1:A:599:SER:C	2.47	0.52
2:B:1095:LEU:HD12	2:B:1095:LEU:N	2.15	0.52
1:A:1385:THR:HG21	1:A:1387:HIS:CD2	2.45	0.52
3:C:184:ASN:OD1	3:C:187:LYS:CA	2.58	0.52
2:B:313:MET:O	2:B:316:PRO:HD2	2.09	0.52
2:B:1115:THR:HG22	2:B:1117:GLN:N	2.24	0.52
2:B:819:ALA:O	2:B:1093:GLN:HG2	2.09	0.52
1:A:1200:ALA:HA	1:A:1203:ASN:HD22	1.74	0.52
1:A:252:PHE:O	1:A:256:GLN:NE2	2.42	0.52
14:T:15:DG:H2''	14:T:16:DT:C6	2.45	0.52
2:B:282:ILE:CG2	2:B:382:ILE:HD11	2.40	0.52
2:B:282:ILE:HD12	2:B:382:ILE:HD13	1.91	0.52
7:G:87:VAL:O	7:G:87:VAL:HG23	2.08	0.52
1:A:92:HIS:O	1:A:94:GLY:N	2.42	0.52
1:A:305:ASP:OD1	1:A:306:ASN:N	2.43	0.52
3:C:242:GLN:C	3:C:244:VAL:N	2.63	0.52
1:A:35:ILE:CD1	1:A:241:VAL:HG11	2.40	0.52
1:A:963:ILE:HD11	1:A:1048:ASN:HB3	1.92	0.52
6:F:138:LEU:HB2	6:F:142:SER:HB2	1.90	0.52
3:C:249:ASP:O	3:C:252:GLN:HB3	2.09	0.52
1:A:1445:ILE:HD12	7:G:59:GLY:O	2.10	0.52
1:A:34:LYS:HB2	1:A:36:ARG:NH2	2.25	0.52
7:G:139:ILE:HG23	7:G:140:LYS:N	2.24	0.52
3:C:233:GLU:CG	3:C:234:SER:H	2.23	0.52
10:J:3:VAL:N	10:J:53:HIS:HE1	2.08	0.52
3:C:22:LEU:HD22	3:C:230:MET:CE	2.40	0.52
2:B:773:MET:CE	2:B:985:GLY:HA2	2.39	0.52
12:L:52:GLY:O	12:L:53:HIS:C	2.48	0.52
8:H:104:PHE:CD2	8:H:114:VAL:HG12	2.44	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:K:73:LEU:HD21	11:K:75:ILE:HD11	1.92	0.52
4:D:5:THR:O	4:D:5:THR:HG23	2.10	0.52
11:K:107:THR:HG22	11:K:108:GLU:N	2.24	0.52
1:A:152:VAL:HG13	1:A:153:PRO:HD2	1.91	0.52
3:C:168:ALA:O	3:C:170:TRP:N	2.42	0.52
4:D:147:TYR:OH	7:G:103:VAL:HG13	2.10	0.52
2:B:498:THR:O	2:B:536:VAL:HA	2.09	0.52
1:A:440:ASP:O	1:A:460:VAL:HG23	2.11	0.52
2:B:787:VAL:HG12	2:B:787:VAL:O	2.10	0.52
2:B:276:ILE:HG23	2:B:336:ARG:HB2	1.91	0.51
2:B:519:TRP:C	2:B:519:TRP:CD1	2.83	0.51
1:A:64:ASN:O	1:A:65:LEU:C	2.48	0.51
9:I:53:GLY:O	9:I:89:GLN:HB2	2.10	0.51
5:E:147:HIS:HD2	5:E:149:LEU:H	1.58	0.51
1:A:715:GLU:OE1	1:A:774:ARG:HD3	2.10	0.51
7:G:116:PRO:HG2	7:G:119:LEU:HB2	1.92	0.51
2:B:429:PHE:HA	2:B:432:MET:CE	2.39	0.51
1:A:1230:GLU:O	1:A:1232:ASN:N	2.43	0.51
2:B:745:PRO:C	2:B:747:MET:N	2.63	0.51
2:B:806:THR:HB	2:B:809:MET:HG3	1.92	0.51
2:B:638:PHE:HB3	2:B:651:LEU:HD22	1.92	0.51
1:A:69:THR:C	1:A:71:GLN:N	2.60	0.51
2:B:1007:VAL:HG22	2:B:1008:PRO:CD	2.37	0.51
5:E:207:ARG:CB	5:E:207:ARG:NH1	2.71	0.51
1:A:697:ALA:HB2	1:A:702:LEU:CD1	2.39	0.51
1:A:988:LEU:O	1:A:992:ASP:HB2	2.10	0.51
6:F:127:GLU:O	6:F:128:LYS:C	2.48	0.51
9:I:44:TYR:CD1	9:I:44:TYR:C	2.83	0.51
1:A:1412:ALA:HA	1:A:1417:GLU:OE2	2.10	0.51
1:A:528:LEU:O	1:A:531:ILE:HG22	2.11	0.51
2:B:1166:CYS:O	2:B:1166:CYS:SG	2.69	0.51
2:B:360:PHE:HE2	2:B:361:LEU:HD13	1.75	0.51
2:B:640:VAL:HG12	2:B:640:VAL:O	2.10	0.51
5:E:136:ASN:OD1	5:E:137:GLU:N	2.43	0.51
2:B:707:PRO:O	2:B:708:GLU:O	2.28	0.51
1:A:68:GLN:O	1:A:68:GLN:OE1	2.27	0.51
1:A:722:LEU:H	1:A:722:LEU:HD12	1.75	0.51
3:C:239:PRO:HB2	3:C:241:ASP:OD1	2.10	0.51
5:E:78:LEU:CA	5:E:107:THR:HB	2.34	0.51
7:G:51:TYR:C	7:G:51:TYR:CD2	2.84	0.51
1:A:999:VAL:HG12	1:A:1000:LEU:HD12	1.92	0.51
3:C:179:GLU:HG2	3:C:180:TYR:H	1.74	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:31:ASN:O	3:C:34:ARG:HB3	2.11	0.51
1:A:1268:LEU:O	1:A:1269:GLU:HG3	2.10	0.51
8:H:135:LEU:HB3	8:H:137:GLN:HG2	1.92	0.51
1:A:974:ASP:C	1:A:976:THR:H	2.14	0.51
2:B:745:PRO:C	2:B:747:MET:H	2.13	0.51
1:A:500:GLU:OE2	1:A:1438:THR:HG21	2.11	0.51
1:A:382:PRO:HD3	1:A:428:TYR:CD2	2.45	0.51
1:A:688:LYS:CD	1:A:691:LEU:HD23	2.41	0.51
9:I:53:GLY:O	9:I:55:THR:N	2.44	0.51
1:A:1329:THR:H	1:A:1335:ILE:HD11	1.75	0.51
1:A:1435:PRO:O	1:A:1436:ILE:HG13	2.10	0.51
12:L:58:LYS:HG2	12:L:58:LYS:O	2.10	0.51
2:B:1031:LEU:HB2	2:B:1055:ILE:CD1	2.40	0.51
5:E:31:THR:HG1	5:E:34:GLU:H	1.57	0.51
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.93	0.51
2:B:398:ARG:HB3	2:B:398:ARG:HH11	1.76	0.51
12:L:66:GLN:HG2	12:L:67:PHE:N	2.25	0.51
8:H:10:PHE:CD1	8:H:10:PHE:N	2.78	0.51
1:A:1208:THR:O	1:A:1212:VAL:HG23	2.11	0.51
2:B:708:GLU:HG3	2:B:709:ASP:N	2.25	0.51
1:A:688:LYS:HA	1:A:691:LEU:HB3	1.93	0.51
1:A:720:ARG:HG2	1:A:720:ARG:O	2.11	0.51
1:A:351:THR:HG22	2:B:1103:ILE:HG13	1.91	0.51
1:A:915:SER:O	1:A:919:ILE:HB	2.10	0.51
3:C:118:LEU:HB2	3:C:132:PRO:HG2	1.93	0.51
5:E:94:LYS:CE	5:E:98:ILE:HD11	2.33	0.51
2:B:976:ILE:O	2:B:990:ILE:HB	2.10	0.51
1:A:889:SER:CB	1:A:1297:GLU:HG3	2.38	0.51
1:A:696:GLU:OE2	1:A:702:LEU:HD21	2.09	0.51
1:A:982:THR:C	1:A:984:LYS:N	2.64	0.51
1:A:75:ASN:O	1:A:76:GLU:HB2	2.10	0.51
1:A:414:ASP:OD1	1:A:416:ARG:HG2	2.10	0.51
7:G:58:ARG:NH1	7:G:58:ARG:HG3	2.25	0.51
1:A:108:MET:HB3	1:A:210:ILE:HD11	1.91	0.51
1:A:1299:VAL:HG12	1:A:1300:LYS:N	2.26	0.51
2:B:67:SER:HB2	2:B:92:PHE:HD1	1.76	0.51
1:A:247:ARG:NH1	1:A:263:THR:HG23	2.25	0.51
2:B:640:VAL:O	2:B:641:GLU:C	2.48	0.51
1:A:69:THR:C	1:A:71:GLN:H	2.13	0.51
2:B:1069:PHE:HA	2:B:1085:ILE:O	2.09	0.51
2:B:642:ASP:HB3	2:B:649:LYS:CG	2.39	0.51
1:A:332:LYS:O	1:A:333:GLU:CB	2.57	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:195:ILE:HG22	4:D:195:ILE:O	2.10	0.51
9:I:34:TYR:CE2	9:I:36:GLU:HB3	2.46	0.51
2:B:69:LEU:HD13	2:B:429:PHE:HD1	1.75	0.51
3:C:186:LEU:N	3:C:186:LEU:HD12	2.25	0.51
7:G:91:VAL:HG12	7:G:92:VAL:N	2.24	0.51
1:A:1402:PHE:CD1	1:A:1403:GLU:HG2	2.46	0.51
2:B:569:TYR:CE1	2:B:589:VAL:HG21	2.46	0.51
2:B:637:LEU:HD12	2:B:693:ILE:CD1	2.38	0.51
1:A:1155:ASP:OD2	1:A:1161:THR:HG23	2.10	0.51
5:E:56:LYS:HZ3	5:E:84:ASP:N	2.09	0.51
1:A:33:ALA:HA	1:A:57:ARG:NH1	2.25	0.51
2:B:770:GLN:HG2	2:B:983:ARG:O	2.11	0.51
2:B:996:ARG:HH12	3:C:175:ALA:N	2.09	0.51
2:B:861:ASP:OD1	2:B:862:GLN:N	2.44	0.51
2:B:1095:LEU:CD1	2:B:1095:LEU:H	2.15	0.51
1:A:650:GLN:HB3	1:A:654:ASN:HD21	1.76	0.51
2:B:980:PHE:CE2	2:B:1094:ARG:HG3	2.46	0.51
6:F:119:ARG:HG3	6:F:119:ARG:NH1	2.19	0.51
14:T:22:DC:H2"	14:T:23:BRU:OP2	2.10	0.51
2:B:130:VAL:HG23	2:B:167:ILE:HD13	1.92	0.51
11:K:68:PHE:N	11:K:68:PHE:CD2	2.75	0.51
1:A:445:ASN:HB2	1:A:454:SER:O	2.10	0.51
1:A:445:ASN:CB	1:A:455:MET:HG2	2.41	0.51
4:D:8:PHE:CD2	7:G:6:ASP:HB2	2.46	0.51
1:A:125:ALA:C	1:A:127:ALA:H	2.14	0.51
1:A:567:LYS:NZ	8:H:46:LEU:HB2	2.26	0.51
1:A:49:LYS:HD3	1:A:55:ASP:HB3	1.93	0.51
9:I:86:PHE:HE1	9:I:100:PHE:HB2	1.76	0.51
12:L:30:ILE:CG2	12:L:31:CYS:N	2.74	0.51
1:A:737:LEU:HD22	1:A:741:ASN:OD1	2.11	0.51
2:B:839:MET:CE	2:B:980:PHE:HB2	2.40	0.51
2:B:1182:CYS:O	2:B:1183:LYS:C	2.49	0.51
2:B:565:PRO:HB2	2:B:567:GLU:CG	2.40	0.51
2:B:46:GLN:HE21	2:B:539:LEU:HD12	1.76	0.51
11:K:68:PHE:HD1	11:K:70:ARG:NH1	2.05	0.51
3:C:183:TRP:CH2	3:C:203:GLN:NE2	2.78	0.51
1:A:1450:LEU:HG	7:G:19:GLY:O	2.11	0.51
1:A:447:GLN:HE22	14:T:20:DG:H4'	1.76	0.51
9:I:75:CYS:SG	9:I:79:HIS:N	2.84	0.51
1:A:483:ASP:O	2:B:979:LYS:HE3	2.11	0.51
2:B:555:ILE:HG22	2:B:556:THR:N	2.26	0.51
5:E:10:SER:O	5:E:13:TRP:HB3	2.11	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:168:TYR:HB3	5:E:170:LEU:HG	1.92	0.51
2:B:37:PHE:HD2	2:B:542:MET:SD	2.34	0.51
3:C:140:ASN:O	3:C:141:GLY:O	2.29	0.51
2:B:557:PHE:CE1	2:B:603:LEU:HD11	2.46	0.51
4:D:128:VAL:O	4:D:130:LEU:N	2.44	0.51
2:B:875:GLU:HG3	2:B:877:PRO:HD3	1.92	0.51
1:A:1054:LEU:HD13	6:F:84:TYR:OH	2.11	0.51
8:H:100:THR:HG22	8:H:101:ALA:N	2.26	0.51
1:A:332:LYS:C	1:A:334:GLY:N	2.52	0.51
1:A:1386:ARG:O	1:A:1391:ARG:HD2	2.10	0.51
2:B:307:ASP:OD2	2:B:310:MET:HB2	2.09	0.51
2:B:899:ILE:CG2	2:B:949:VAL:HG21	2.41	0.51
2:B:834:ASN:O	2:B:838:SER:O	2.29	0.51
3:C:70:ILE:HG12	3:C:142:VAL:HG11	1.93	0.51
1:A:583:PRO:O	1:A:610:GLY:HA3	2.11	0.51
2:B:31:TRP:CE3	2:B:34:ILE:HD12	2.46	0.51
2:B:593:PRO:O	2:B:595:ARG:N	2.43	0.51
2:B:361:LEU:O	2:B:363:HIS:O	2.29	0.51
1:A:88:LYS:HD3	1:A:293:GLU:CD	2.31	0.51
4:D:47:LEU:CD1	4:D:48:ILE:N	2.74	0.51
7:G:48:VAL:HA	7:G:76:ALA:HB2	1.93	0.51
1:A:691:LEU:O	1:A:691:LEU:HD12	2.11	0.51
2:B:1072:MET:HB2	2:B:1085:ILE:HD13	1.92	0.51
11:K:21:ILE:HG22	11:K:31:VAL:CG1	2.40	0.51
5:E:69:ILE:HD12	5:E:69:ILE:H	1.74	0.51
1:A:335:ARG:CZ	2:B:1202:LEU:HD13	2.41	0.51
8:H:62:SER:OG	8:H:63:LEU:N	2.43	0.51
1:A:1041:ALA:O	1:A:1045:VAL:HG23	2.11	0.51
2:B:1099:VAL:HG13	2:B:1100:ASP:H	1.76	0.51
2:B:1221:SER:O	2:B:1223:ASP:N	2.43	0.51
1:A:610:GLY:O	1:A:611:GLN:NE2	2.45	0.51
2:B:402:GLY:CA	2:B:695:ALA:HB3	2.41	0.51
1:A:43:GLU:HG3	1:A:46:THR:HB	1.93	0.51
2:B:606:LYS:HD2	2:B:608:ASP:OD2	2.10	0.50
3:C:104:PHE:HD2	3:C:105:GLY:H	1.57	0.50
1:A:7:SER:OG	2:B:1161:HIS:CE1	2.61	0.50
2:B:996:ARG:NH1	3:C:175:ALA:H	2.09	0.50
7:G:14:HIS:HD2	7:G:16:SER:OG	1.94	0.50
5:E:22:MET:HE3	5:E:26:ARG:NE	2.22	0.50
2:B:830:TYR:O	2:B:831:SER:C	2.49	0.50
1:A:1254:ALA:O	1:A:1255:GLU:CB	2.58	0.50
2:B:658:ILE:HG22	2:B:662:MET:HE2	1.93	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:326:ASP:OD1	2:B:329:THR:HB	2.10	0.50
1:A:1118:VAL:HG23	1:A:1306:LEU:HB2	1.93	0.50
1:A:946:VAL:HG22	5:E:201:LYS:CD	2.41	0.50
2:B:39:ARG:HH21	2:B:665:GLU:CD	2.15	0.50
6:F:111:LEU:HD12	6:F:111:LEU:N	2.25	0.50
2:B:230:ALA:HB3	2:B:231:PRO:HD3	1.93	0.50
1:A:1453:TYR:O	1:A:1454:MET:HB3	2.12	0.50
2:B:393:LYS:HA	2:B:393:LYS:HE3	1.93	0.50
2:B:213:ILE:HD12	2:B:497:ARG:HB3	1.93	0.50
1:A:1444:MET:HE1	6:F:135:ARG:NE	2.26	0.50
2:B:879:ARG:HD2	2:B:879:ARG:H	1.76	0.50
2:B:983:ARG:HH11	2:B:1091:TYR:HB3	1.75	0.50
4:D:217:LEU:O	4:D:219:THR:N	2.44	0.50
4:D:220:LEU:CD2	4:D:221:TYR:N	2.63	0.50
4:D:53:SER:C	4:D:55:ALA:N	2.65	0.50
4:D:53:SER:H	4:D:148:LEU:CD2	2.24	0.50
2:B:504:ARG:NH2	14:T:15:DG:O6	2.43	0.50
2:B:661:LEU:HD23	2:B:679:TYR:O	2.11	0.50
11:K:53:ASP:OD1	11:K:55:LYS:HB2	2.12	0.50
4:D:52:LEU:HD12	4:D:182:SER:HB2	1.93	0.50
2:B:205:ILE:N	2:B:205:ILE:CD1	2.74	0.50
2:B:1197:PRO:O	2:B:1200:ALA:N	2.34	0.50
1:A:84:ILE:O	1:A:84:ILE:HG22	2.10	0.50
2:B:223:VAL:HG11	2:B:381:MET:HG2	1.93	0.50
2:B:616:ILE:CG1	2:B:697:GLU:HA	2.40	0.50
1:A:268:ASP:HB3	1:A:299:HIS:CE1	2.46	0.50
4:D:46:GLU:HG2	4:D:47:LEU:N	2.26	0.50
4:D:60:LYS:HE3	4:D:126:ILE:CD1	2.33	0.50
2:B:642:ASP:O	2:B:644:GLU:N	2.38	0.50
5:E:65:THR:O	5:E:69:ILE:CD1	2.59	0.50
2:B:911:ILE:HG22	2:B:966:VAL:HG21	1.94	0.50
1:A:605:MET:HE1	1:A:612:ILE:HG12	1.93	0.50
1:A:332:LYS:H	1:A:337:ARG:HB2	1.77	0.50
1:A:1387:HIS:HA	1:A:1391:ARG:NH1	2.23	0.50
5:E:178:ILE:HB	5:E:212:ARG:HB3	1.94	0.50
2:B:212:LEU:HD23	2:B:480:SER:HB2	1.93	0.50
5:E:129:PRO:HG2	5:E:130:ALA:H	1.75	0.50
1:A:108:MET:SD	1:A:210:ILE:HD13	2.52	0.50
3:C:91:HIS:O	3:C:91:HIS:CD2	2.64	0.50
1:A:1220:PHE:O	1:A:1221:LYS:HB2	2.11	0.50
2:B:376:PHE:CZ	2:B:569:TYR:HD2	2.29	0.50
2:B:365:THR:OG1	2:B:367:LEU:HG	2.11	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:847:ASP:O	2:B:849:GLY:N	2.44	0.50
1:A:672:ASP:CG	1:A:674:PRO:HD2	2.32	0.50
2:B:827:ILE:O	2:B:1085:ILE:HG23	2.11	0.50
1:A:1332:PHE:CE1	1:A:1348:LEU:HD13	2.46	0.50
2:B:687:GLU:O	2:B:689:LEU:HG	2.11	0.50
10:J:36:LEU:HB2	10:J:47:ARG:HH12	1.76	0.50
1:A:886:ILE:CG2	1:A:952:ALA:HB2	2.41	0.50
1:A:285:PRO:O	1:A:287:HIS:N	2.44	0.50
6:F:97:ARG:HD3	6:F:130:ILE:HG23	1.94	0.50
1:A:196:GLU:HG2	1:A:197:PRO:CD	2.41	0.50
5:E:182:ASP:HB3	5:E:185:ALA:CB	2.41	0.50
1:A:1211:GLN:O	1:A:1214:GLU:HB2	2.12	0.50
8:H:55:LEU:HD22	8:H:144:ILE:CG2	2.42	0.50
1:A:1187:GLN:HB2	1:A:1244:ARG:CG	2.30	0.50
1:A:568:PRO:HB2	3:C:221:TYR:CZ	2.46	0.50
1:A:51:GLY:C	1:A:56:PRO:HB3	2.32	0.50
2:B:622:LYS:CE	9:I:59:VAL:HG22	2.31	0.50
2:B:113:TYR:CD2	2:B:192:LEU:HD22	2.47	0.50
1:A:115:LEU:HD13	1:A:141:LEU:HD13	1.93	0.50
14:T:18:DC:H3'	14:T:18:DC:OP1	2.11	0.50
1:A:1208:THR:HG22	1:A:1210:GLY:H	1.76	0.50
1:A:298:PHE:O	1:A:302:THR:HB	2.12	0.50
2:B:882:THR:CG2	2:B:884:ARG:N	2.66	0.50
4:D:153:ARG:O	4:D:154:PHE:HD2	1.95	0.50
1:A:901:LEU:HA	1:A:907:THR:OG1	2.11	0.50
2:B:233:PRO:HG2	2:B:234:ILE:HD13	1.94	0.50
1:A:1138:ILE:HG21	1:A:1316:VAL:HG13	1.93	0.50
1:A:964:ILE:HD13	1:A:1035:TYR:CE1	2.46	0.50
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.47	0.50
2:B:259:TYR:HD1	2:B:259:TYR:H	1.59	0.50
1:A:1011:GLN:NE2	1:A:1015:VAL:HG21	2.26	0.50
2:B:1017:ILE:H	2:B:1018:PRO:CD	2.24	0.50
2:B:59:LEU:HD12	2:B:417:PHE:CD2	2.47	0.50
1:A:608:ILE:HD12	1:A:613:ILE:CD1	2.42	0.50
10:J:24:LEU:O	10:J:30:LEU:HB2	2.11	0.50
1:A:1212:VAL:O	1:A:1216:ILE:HG13	2.11	0.50
3:C:138:GLU:HB2	3:C:140:ASN:ND2	2.26	0.50
1:A:1244:ARG:CB	1:A:1245:PRO:CD	2.88	0.50
1:A:12:ARG:NH2	2:B:1192:TYR:CZ	2.79	0.50
1:A:1111:MET:O	1:A:1112:LYS:O	2.30	0.50
2:B:678:GLU:HG2	2:B:679:TYR:N	2.26	0.50
1:A:886:ILE:CG2	1:A:887:GLY:H	2.23	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:213:PRO:HG2	3:C:214:ASN:H	1.76	0.50
1:A:858:ASN:ND2	1:A:858:ASN:C	2.65	0.50
1:A:460:VAL:HG12	1:A:461:LYS:N	2.26	0.50
2:B:258:LEU:HG	2:B:258:LEU:O	2.11	0.50
1:A:53:LEU:C	1:A:54:ASN:HD22	2.15	0.50
2:B:335:GLY:O	2:B:336:ARG:HG3	2.12	0.50
2:B:345:LYS:C	2:B:346:GLU:HG3	2.31	0.50
2:B:357:GLN:O	2:B:366:GLN:HA	2.11	0.50
1:A:269:ILE:HG23	1:A:300:VAL:HG23	1.94	0.50
2:B:705:MET:HB3	2:B:706:GLN:OE1	2.12	0.50
1:A:65:LEU:O	1:A:66:LYS:C	2.50	0.50
2:B:842:ASN:HD22	2:B:845:SER:N	2.04	0.50
7:G:3:PHE:HB2	7:G:78:VAL:HG23	1.94	0.50
1:A:690:VAL:HG12	1:A:691:LEU:N	2.26	0.50
3:C:242:GLN:O	3:C:244:VAL:N	2.45	0.50
2:B:292:ILE:HD13	2:B:326:ASP:HA	1.93	0.50
5:E:211:TYR:CD1	5:E:211:TYR:N	2.79	0.50
1:A:475:THR:CG2	1:A:476:SER:N	2.75	0.50
5:E:37:LEU:HD11	5:E:41:ASP:HB2	1.93	0.50
1:A:1202:MET:HE1	1:A:1212:VAL:CG2	2.42	0.50
2:B:639:ILE:HD11	2:B:691:GLU:HB3	1.94	0.50
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.92	0.50
1:A:51:GLY:O	1:A:56:PRO:HB3	2.12	0.50
1:A:666:ILE:HD11	2:B:1086:PHE:CE1	2.46	0.50
5:E:27:GLY:O	5:E:65:THR:HG23	2.12	0.50
1:A:590:ARG:HH22	1:A:620:LYS:HB2	1.77	0.50
1:A:1313:LEU:C	1:A:1315:GLU:N	2.65	0.50
2:B:429:PHE:HA	2:B:432:MET:HE3	1.93	0.50
2:B:134:LYS:HE2	2:B:164:LYS:HZ1	1.77	0.50
1:A:115:LEU:HG	1:A:142:CYS:HB3	1.94	0.50
1:A:482:PHE:CD1	2:B:836:GLU:HB2	2.46	0.50
1:A:1214:GLU:C	1:A:1218:GLN:HE21	2.16	0.49
1:A:427:GLN:O	1:A:428:TYR:C	2.49	0.49
2:B:1187:ASN:OD1	2:B:1190:ASP:N	2.45	0.49
3:C:73:GLN:HB3	3:C:131:HIS:H	1.77	0.49
1:A:629:LEU:HD11	1:A:645:LEU:HD21	1.94	0.49
2:B:987:LYS:HE3	15:P:11:G:H1'	1.94	0.49
1:A:146:MET:HA	1:A:171:GLN:HB2	1.94	0.49
5:E:100:ILE:CG2	5:E:105:PHE:HB2	2.41	0.49
7:G:51:TYR:HD2	7:G:51:TYR:C	2.16	0.49
1:A:1003:LYS:O	1:A:1004:ASN:HB3	2.11	0.49
9:I:50:THR:HB	9:I:92:ARG:HH22	1.77	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:21:LEU:HD11	1:A:1414:ALA:HA	1.94	0.49
1:A:22:PHE:HB2	2:B:1211:ASN:OD1	2.12	0.49
1:A:1280:GLU:O	1:A:1281:ARG:O	2.30	0.49
9:I:119:THR:O	9:I:119:THR:HG22	2.11	0.49
1:A:40:THR:HB	1:A:41:MET:CE	2.41	0.49
4:D:29:LEU:N	4:D:29:LEU:CD2	2.74	0.49
2:B:882:THR:C	2:B:884:ARG:N	2.66	0.49
4:D:144:THR:HG21	7:G:46:LEU:HD13	1.92	0.49
4:D:12:ARG:NH1	4:D:12:ARG:HG2	2.26	0.49
8:H:82:PRO:C	8:H:84:ALA:N	2.64	0.49
2:B:839:MET:HE3	2:B:1010:LEU:CD2	2.39	0.49
5:E:48:ASP:CG	5:E:49:SER:N	2.64	0.49
6:F:109:VAL:HG12	6:F:110:ASP:H	1.75	0.49
1:A:108:MET:HA	1:A:210:ILE:HD13	1.93	0.49
1:A:40:THR:HB	1:A:41:MET:HE2	1.94	0.49
2:B:916:THR:HB	2:B:935:ARG:CD	2.41	0.49
9:I:118:ARG:HH12	9:I:120:GLN:HB2	1.77	0.49
3:C:97:VAL:HG21	3:C:129:ILE:HG22	1.93	0.49
2:B:654:ARG:O	2:B:656:GLY:N	2.46	0.49
3:C:46:ILE:HD13	3:C:157:CYS:SG	2.52	0.49
10:J:32:GLU:O	10:J:34:THR:N	2.45	0.49
10:J:48:ARG:HE	10:J:49:MET:HE2	1.78	0.49
2:B:211:VAL:HG23	2:B:483:LEU:HB2	1.93	0.49
1:A:153:PRO:CD	1:A:161:LEU:HD13	2.41	0.49
1:A:336:ILE:HD13	1:A:340:LEU:HD12	1.93	0.49
4:D:209:ARG:NH1	4:D:209:ARG:HG2	2.27	0.49
4:D:8:PHE:CE2	7:G:6:ASP:HB2	2.48	0.49
8:H:40:LEU:HD23	8:H:42:ILE:HD11	1.93	0.49
1:A:1206:ASP:O	1:A:1274:ARG:NH2	2.44	0.49
3:C:105:GLY:O	3:C:149:LYS:O	2.31	0.49
1:A:382:PRO:N	1:A:428:TYR:HE2	2.10	0.49
2:B:996:ARG:HH22	3:C:175:ALA:H	1.60	0.49
2:B:167:ILE:HD12	2:B:167:ILE:N	2.27	0.49
1:A:287:HIS:ND1	1:A:290:GLU:HG2	2.28	0.49
1:A:809:THR:H	1:A:812:GLU:HB2	1.77	0.49
1:A:1349:TYR:CD2	1:A:1349:TYR:C	2.86	0.49
2:B:363:HIS:O	2:B:364:ILE:CB	2.61	0.49
1:A:55:ASP:OD2	1:A:55:ASP:O	2.31	0.49
4:D:35:LEU:HA	4:D:47:LEU:HB2	1.92	0.49
3:C:239:PRO:O	3:C:241:ASP:N	2.45	0.49
1:A:670:ILE:HD12	2:B:1067:ARG:NH2	2.27	0.49
5:E:61:GLN:HG3	5:E:78:LEU:O	2.11	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:I:88:SER:C	9:I:90:GLN:H	2.15	0.49
2:B:910:VAL:HG11	2:B:938:SER:HB3	1.94	0.49
4:D:71:LYS:HA	4:D:74:GLN:HB2	1.93	0.49
2:B:287:ARG:HG3	2:B:292:ILE:HA	1.93	0.49
3:C:215:GLU:O	3:C:217:ASP:N	2.46	0.49
1:A:946:VAL:CG2	5:E:201:LYS:HD2	2.42	0.49
4:D:20:GLU:H	4:D:20:GLU:CD	2.16	0.49
1:A:1129:GLU:OE2	1:A:1132:LYS:HD2	2.12	0.49
2:B:254:LEU:HD22	2:B:361:LEU:HD12	1.94	0.49
1:A:49:LYS:HZ1	1:A:61:ILE:H	1.57	0.49
1:A:56:PRO:O	1:A:57:ARG:NH1	2.45	0.49
2:B:995:ARG:HH12	3:C:165:LYS:HG2	1.77	0.49
1:A:380:VAL:CG1	1:A:385:ILE:HG12	2.42	0.49
2:B:575:PRO:HG2	2:B:576:ASP:H	1.76	0.49
4:D:153:ARG:HB3	4:D:154:PHE:CE2	2.48	0.49
6:F:69:LEU:HB2	6:F:72:LYS:HD2	1.95	0.49
2:B:25:ILE:CD1	2:B:653:VAL:O	2.60	0.49
2:B:185:THR:O	2:B:188:ASP:N	2.46	0.49
11:K:49:GLU:HG3	11:K:94:ILE:CG1	2.42	0.49
1:A:888:GLY:O	1:A:940:ARG:NH2	2.45	0.49
5:E:168:TYR:CB	5:E:170:LEU:HG	2.42	0.49
7:G:165:GLU:HB2	7:G:168:LEU:HD12	1.94	0.49
1:A:343:LYS:HZ2	2:B:1151:LEU:HG	1.76	0.49
2:B:240:ILE:HG23	2:B:254:LEU:HB3	1.94	0.49
2:B:603:LEU:HD13	2:B:608:ASP:CB	2.35	0.49
2:B:849:GLY:O	2:B:850:LEU:C	2.51	0.49
2:B:1065:GLN:NE2	2:B:1066:SER:N	2.61	0.49
4:D:149:THR:HG22	4:D:150:ASN:N	2.27	0.49
2:B:874:PHE:HB3	2:B:896:ASP:O	2.12	0.49
12:L:61:THR:HG22	12:L:62:LYS:H	1.78	0.49
3:C:33:LEU:HD12	3:C:37:MET:HG3	1.95	0.49
8:H:135:LEU:CB	8:H:137:GLN:HG2	2.43	0.49
2:B:579:ARG:N	2:B:589:VAL:HG13	2.28	0.49
2:B:579:ARG:CA	2:B:589:VAL:HG13	2.42	0.49
2:B:603:LEU:HD12	2:B:609:ILE:CG2	2.41	0.49
8:H:12:VAL:HG11	8:H:51:ALA:HA	1.95	0.49
1:A:265:LYS:CA	1:A:265:LYS:CE	2.86	0.49
1:A:382:PRO:HD3	1:A:428:TYR:CE2	2.47	0.49
1:A:774:ARG:NH1	1:A:797:LYS:HG3	2.27	0.49
2:B:129:PHE:HA	2:B:165:VAL:O	2.13	0.49
11:K:50:LEU:HD11	11:K:75:ILE:HD13	1.94	0.49
1:A:820:GLY:O	1:A:822:GLU:N	2.45	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:217:ARG:NE	2:B:405:ARG:HB2	2.26	0.49
1:A:846:GLU:OE1	1:A:1425:SER:OG	2.29	0.49
1:A:2:VAL:HG22	1:A:3:GLY:N	2.26	0.49
2:B:281:PRO:O	2:B:283:VAL:N	2.45	0.49
2:B:711:GLU:HB2	2:B:712:PRO:HD2	1.94	0.49
15:P:9:C:OP2	15:P:9:C:H6	1.96	0.49
2:B:542:MET:CE	2:B:747:MET:HG3	2.43	0.49
8:H:93:TYR:HB3	8:H:144:ILE:O	2.12	0.49
8:H:44:VAL:CG1	8:H:48:PRO:HA	2.41	0.49
3:C:167:HIS:N	11:K:6:ARG:NH1	2.61	0.49
1:A:256:GLN:HE21	2:B:935:ARG:HH12	1.60	0.49
3:C:144:ILE:HG22	3:C:145:CYS:N	2.28	0.49
10:J:53:HIS:CD2	10:J:54:VAL:C	2.86	0.49
4:D:118:THR:CB	4:D:121:LYS:HB3	2.43	0.49
1:A:337:ARG:HD2	2:B:1132:GLU:OE1	2.13	0.49
9:I:7:CYS:C	9:I:8:ARG:O	2.51	0.49
1:A:993:LEU:HD22	1:A:1046:LEU:CD2	2.42	0.49
2:B:59:LEU:HD12	2:B:417:PHE:CE2	2.48	0.49
2:B:277:LYS:HG2	2:B:336:ARG:HB3	1.94	0.49
1:A:1187:GLN:HG2	1:A:1188:GLN:N	2.28	0.49
5:E:119:SER:O	5:E:123:LEU:HD21	2.13	0.49
1:A:306:ASN:HD22	1:A:322:VAL:HG12	1.78	0.49
1:A:70:CYS:HA	2:B:1174:LYS:HG2	1.94	0.49
1:A:919:ILE:HG12	1:A:925:LEU:HD12	1.95	0.49
4:D:120:GLU:HA	4:D:123:LEU:HD23	1.95	0.49
1:A:1436:ILE:O	1:A:1439:GLY:N	2.27	0.49
2:B:179:CYS:SG	2:B:181:LEU:HB2	2.53	0.49
12:L:34:CYS:HB3	12:L:51:CYS:SG	2.53	0.49
8:H:82:PRO:HG2	8:H:83:GLN:H	1.78	0.49
1:A:1293:SER:OG	1:A:1294:PRO:HD2	2.13	0.49
2:B:815:ARG:HB2	2:B:815:ARG:NH1	2.28	0.49
13:N:4:DA:H2"	13:N:5:DC:C6	2.48	0.49
2:B:129:PHE:CE2	2:B:166:PHE:HD1	2.31	0.49
1:A:378:GLU:OE2	1:A:387:ARG:NH2	2.46	0.49
1:A:853:ASP:C	1:A:853:ASP:OD1	2.51	0.49
1:A:639:PRO:HG2	1:A:640:GLN:HE21	1.77	0.49
3:C:15:LYS:HG2	3:C:15:LYS:O	2.12	0.49
1:A:321:PRO:O	1:A:322:VAL:CB	2.60	0.48
1:A:12:ARG:CB	2:B:1218:THR:HG22	2.29	0.48
3:C:166:GLU:C	11:K:6:ARG:HH11	2.16	0.48
2:B:866:TYR:O	2:B:867:GLY:C	2.50	0.48
2:B:879:ARG:N	2:B:879:ARG:CD	2.75	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:14:ARG:NH2	4:D:16:LYS:HD2	2.28	0.48
5:E:79:TRP:HB2	5:E:105:PHE:CE1	2.47	0.48
2:B:1094:ARG:HH21	2:B:1098:MET:HG2	1.78	0.48
2:B:753:ALA:O	2:B:756:ILE:HG13	2.13	0.48
1:A:482:PHE:HB2	2:B:838:SER:OG	2.13	0.48
3:C:82:TYR:O	3:C:83:SER:C	2.50	0.48
9:I:2:THR:HG23	9:I:2:THR:O	2.13	0.48
2:B:641:GLU:C	2:B:643:ASP:H	2.16	0.48
2:B:247:GLY:H	2:B:249:ARG:HH21	1.61	0.48
5:E:112:TYR:CD1	5:E:112:TYR:C	2.86	0.48
8:H:44:VAL:HG12	8:H:44:VAL:O	2.13	0.48
4:D:136:GLY:HA2	4:D:142:LYS:NZ	2.28	0.48
10:J:53:HIS:HD2	10:J:54:VAL:C	2.17	0.48
5:E:22:MET:CE	5:E:26:ARG:NH2	2.67	0.48
1:A:774:ARG:CZ	1:A:797:LYS:HB2	2.43	0.48
12:L:34:CYS:SG	12:L:51:CYS:SG	3.11	0.48
2:B:839:MET:HG3	2:B:1010:LEU:HD23	1.94	0.48
2:B:405:ARG:NE	2:B:632:ARG:HG2	2.27	0.48
5:E:157:SER:OG	5:E:160:GLU:HG3	2.13	0.48
1:A:482:PHE:HD1	2:B:838:SER:HG	1.61	0.48
1:A:1280:GLU:O	1:A:1281:ARG:C	2.51	0.48
2:B:183:GLU:O	2:B:184:ALA:O	2.30	0.48
2:B:218:SER:HB3	2:B:241:ARG:HH12	1.77	0.48
9:I:61:ASP:O	9:I:63:GLY:N	2.47	0.48
3:C:238:ILE:HD11	3:C:246:ARG:NH1	2.28	0.48
1:A:666:ILE:HG23	2:B:1026:LEU:HB3	1.95	0.48
2:B:642:ASP:CB	2:B:649:LYS:HA	2.44	0.48
1:A:144:THR:O	1:A:146:MET:HG3	2.12	0.48
1:A:463:ILE:CD1	1:A:469:ARG:HG3	2.43	0.48
2:B:976:ILE:HD13	2:B:992:ILE:HA	1.95	0.48
9:I:17:ARG:HG3	9:I:28:GLU:HG2	1.95	0.48
7:G:30:LEU:HD23	7:G:54:ILE:HD13	1.95	0.48
12:L:61:THR:HG22	12:L:63:ARG:HG3	1.93	0.48
12:L:27:LEU:HD13	12:L:37:LYS:CD	2.43	0.48
11:K:45:LEU:HG	11:K:94:ILE:CD1	2.41	0.48
1:A:883:LEU:CD1	1:A:1017:LEU:HD11	2.40	0.48
3:C:89:GLU:O	3:C:90:ASP:CB	2.60	0.48
2:B:1001:PHE:CD2	3:C:34:ARG:NH2	2.81	0.48
7:G:87:VAL:CG2	7:G:103:VAL:HG21	2.44	0.48
1:A:336:ILE:HD11	2:B:1203:LEU:HD22	1.94	0.48
3:C:167:HIS:N	11:K:6:ARG:HH12	2.11	0.48
1:A:901:LEU:HD23	1:A:907:THR:OG1	2.12	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:925:LEU:C	1:A:927:VAL:N	2.66	0.48
3:C:177:GLU:CG	3:C:231:ASN:HD22	2.20	0.48
2:B:766:ARG:HH11	2:B:769:TYR:HD1	1.61	0.48
2:B:120:ARG:NH1	12:L:54:ARG:NH1	2.60	0.48
1:A:1315:GLU:C	1:A:1317:MET:H	2.17	0.48
12:L:36:SER:O	12:L:37:LYS:C	2.51	0.48
2:B:282:ILE:HG21	2:B:382:ILE:HD11	1.95	0.48
2:B:384:ARG:HA	2:B:387:LEU:HD13	1.96	0.48
11:K:54:ARG:HG2	11:K:54:ARG:NH1	2.27	0.48
8:H:56:THR:O	8:H:144:ILE:HA	2.14	0.48
8:H:4:THR:CA	8:H:60:ALA:HB2	2.23	0.48
1:A:381:THR:CG2	1:A:382:PRO:HD2	2.35	0.48
1:A:255:SER:OG	2:B:918:ILE:CG2	2.61	0.48
1:A:720:ARG:O	1:A:724:GLU:HB2	2.12	0.48
2:B:797:TYR:C	2:B:798:TYR:HD2	2.17	0.48
1:A:200:ARG:HG2	1:A:201:VAL:N	2.28	0.48
12:L:31:CYS:SG	12:L:34:CYS:N	2.86	0.48
2:B:416:LEU:HD12	2:B:466:TRP:CE2	2.49	0.48
3:C:35:ARG:NH1	11:K:41:THR:N	2.60	0.48
2:B:521:LEU:HB3	2:B:633:VAL:HG11	1.95	0.48
1:A:1057:VAL:HG12	1:A:1058:VAL:N	2.29	0.48
1:A:264:PHE:HB3	1:A:265:LYS:NZ	2.28	0.48
1:A:320:ARG:NE	1:A:323:LYS:HZ2	2.12	0.48
1:A:34:LYS:HZ2	1:A:57:ARG:HH22	1.59	0.48
1:A:65:LEU:O	1:A:71:GLN:HA	2.13	0.48
7:G:7:LEU:HB2	7:G:74:TYR:CE2	2.49	0.48
2:B:882:THR:HG23	2:B:884:ARG:CA	2.44	0.48
3:C:56:THR:HG22	3:C:57:VAL:N	2.26	0.48
3:C:133:ILE:CD1	3:C:236:GLY:C	2.82	0.48
1:A:1094:VAL:HG13	1:A:1113:THR:HB	1.96	0.48
2:B:644:GLU:C	2:B:646:LEU:H	2.17	0.48
2:B:831:SER:CB	2:B:994:TYR:OH	2.61	0.48
2:B:860:MET:CG	2:B:965:LYS:HG2	2.42	0.48
7:G:115:MET:O	7:G:164:LYS:HD3	2.14	0.48
9:I:12:ASN:HA	9:I:12:ASN:HD22	1.53	0.48
2:B:412:LEU:HB3	2:B:466:TRP:NE1	2.28	0.48
1:A:1029:ARG:NH1	1:A:1029:ARG:CG	2.77	0.48
1:A:20:GLY:O	1:A:21:LEU:HD23	2.13	0.48
5:E:7:ARG:HG3	5:E:8:ASN:H	1.77	0.48
1:A:663:SER:OG	1:A:664:THR:N	2.43	0.48
1:A:49:LYS:CD	1:A:55:ASP:HB3	2.44	0.48
4:D:40:HIS:CE1	7:G:7:LEU:O	2.65	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:126:ILE:HD13	4:D:145:MET:HE2	1.95	0.48
4:D:17:LYS:C	4:D:17:LYS:HD2	2.33	0.48
2:B:190:TYR:CE1	2:B:196:PRO:HG3	2.49	0.48
2:B:1000:PRO:O	2:B:1007:VAL:HG23	2.14	0.48
7:G:88:ASP:CB	7:G:144:ARG:HA	2.34	0.48
2:B:896:ASP:OD2	12:L:58:LYS:HE3	2.14	0.48
8:H:61:SER:O	8:H:62:SER:HB2	2.14	0.48
2:B:1115:THR:O	2:B:1116:ARG:CB	2.59	0.48
2:B:360:PHE:CE2	2:B:361:LEU:HD13	2.49	0.48
2:B:284:ILE:HG21	2:B:333:PHE:HD2	1.79	0.48
8:H:24:CYS:HB2	8:H:44:VAL:CG2	2.43	0.48
2:B:957:ASN:O	2:B:958:GLN:C	2.52	0.48
4:D:155:ARG:HB3	4:D:155:ARG:HH11	1.79	0.48
1:A:593:GLU:C	1:A:595:THR:H	2.15	0.48
1:A:1127:ASP:HB3	1:A:1130:GLN:HB3	1.94	0.48
1:A:1134:ILE:O	1:A:1138:ILE:HG12	2.13	0.48
2:B:515:HIS:HD2	2:B:517:THR:OG1	1.97	0.48
11:K:111:LEU:N	11:K:111:LEU:HD23	2.29	0.48
1:A:477:PRO:CG	1:A:521:MET:HG2	2.44	0.48
2:B:434:ARG:O	2:B:436:VAL:HG23	2.13	0.48
4:D:39:ASN:ND2	4:D:41:GLN:HB2	2.28	0.48
1:A:526:ASP:HB2	2:B:835:GLN:OE1	2.14	0.48
1:A:26:GLU:O	1:A:29:ALA:HB3	2.14	0.48
2:B:1170:THR:O	2:B:1172:ILE:HD13	2.13	0.48
12:L:46:VAL:O	12:L:46:VAL:HG12	2.14	0.48
1:A:396:PRO:HB3	1:A:402:ALA:O	2.13	0.48
8:H:5:LEU:CG	8:H:60:ALA:HA	2.44	0.48
8:H:9:ILE:HG23	8:H:55:LEU:C	2.34	0.48
1:A:9:ALA:O	1:A:10:PRO:C	2.52	0.48
2:B:1072:MET:HB2	2:B:1085:ILE:CD1	2.44	0.48
4:D:123:LEU:CD2	4:D:149:THR:HG21	2.44	0.48
11:K:21:ILE:CG2	11:K:33:ILE:HG12	2.37	0.48
1:A:896:ARG:HD3	1:A:897:TYR:CZ	2.48	0.48
3:C:213:PRO:O	3:C:214:ASN:HB3	2.14	0.48
2:B:405:ARG:HD2	2:B:631:GLY:O	2.14	0.48
3:C:186:LEU:N	3:C:186:LEU:CD1	2.77	0.48
1:A:239:LEU:HD12	1:A:239:LEU:HA	1.59	0.48
10:J:24:LEU:HA	10:J:28:ASP:HB2	1.96	0.48
2:B:1154:ALA:O	2:B:1155:SER:HB2	2.13	0.48
2:B:360:PHE:HD2	2:B:360:PHE:C	2.16	0.48
2:B:701:ILE:HG13	2:B:702:LEU:N	2.29	0.48
3:C:105:GLY:HA3	3:C:149:LYS:O	2.14	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:49:LYS:NZ	1:A:61:ILE:N	2.58	0.48
7:G:31:LEU:HD13	7:G:35:GLU:HG3	1.96	0.48
4:D:154:PHE:CE2	4:D:218:GLU:HA	2.49	0.48
3:C:236:GLY:C	3:C:238:ILE:N	2.66	0.48
11:K:101:LEU:HD23	11:K:101:LEU:O	2.13	0.48
2:B:100:PRO:HG3	2:B:172:ILE:HD12	1.96	0.48
7:G:111:THR:O	7:G:112:LYS:C	2.52	0.48
7:G:111:THR:O	7:G:113:HIS:N	2.47	0.48
1:A:821:ARG:HD2	1:A:825:ILE:HD11	1.96	0.48
11:K:8:GLU:O	11:K:37:LYS:HD2	2.14	0.48
11:K:53:ASP:C	11:K:55:LYS:H	2.18	0.48
9:I:82:GLU:HB3	9:I:104:LEU:CG	2.44	0.48
8:H:135:LEU:HD13	8:H:137:GLN:NE2	2.29	0.48
4:D:27:LEU:HD11	4:D:197:SER:HB3	1.96	0.48
3:C:84:ARG:HG3	3:C:85:ASP:OD1	2.14	0.48
2:B:1219:ASP:C	2:B:1219:ASP:OD1	2.51	0.48
1:A:1025:ARG:HG3	1:A:1025:ARG:HH11	1.79	0.48
8:H:47:PHE:HB3	8:H:95:TYR:HD1	1.78	0.47
2:B:935:ARG:HG3	2:B:935:ARG:O	2.12	0.47
1:A:208:LEU:HD22	1:A:212:LYS:HD2	1.96	0.47
2:B:644:GLU:HA	2:B:644:GLU:OE1	2.14	0.47
2:B:425:THR:HA	2:B:428:ILE:CD1	2.39	0.47
1:A:595:THR:C	1:A:596:THR:HG23	2.34	0.47
1:A:1319:VAL:HG12	1:A:1320:PRO:O	2.14	0.47
2:B:975:GLN:CG	2:B:976:ILE:N	2.74	0.47
1:A:899:VAL:CB	1:A:929:LEU:HD12	2.44	0.47
1:A:443:LEU:HD21	1:A:455:MET:HB3	1.96	0.47
3:C:35:ARG:HH12	11:K:41:THR:H	1.62	0.47
2:B:1223:ASP:O	2:B:1224:PHE:CB	2.60	0.47
1:A:1169:ILE:O	1:A:1169:ILE:HG22	2.15	0.47
5:E:138:ALA:HA	5:E:141:VAL:HG23	1.95	0.47
1:A:7:SER:C	1:A:9:ALA:H	2.17	0.47
2:B:875:GLU:O	2:B:877:PRO:CD	2.62	0.47
9:I:55:THR:HG22	9:I:58:VAL:CG2	2.44	0.47
1:A:645:LEU:HG	1:A:649:ILE:CD1	2.44	0.47
1:A:1278:ASN:O	1:A:1310:GLY:HA3	2.13	0.47
5:E:49:SER:OG	5:E:50:MET:N	2.47	0.47
6:F:119:ARG:HH11	6:F:119:ARG:CG	2.21	0.47
12:L:26:THR:CG2	12:L:27:LEU:H	2.27	0.47
7:G:21:ARG:HD2	7:G:24:GLN:HB2	1.93	0.47
2:B:313:MET:HE2	2:B:390:LEU:HD11	1.95	0.47
14:T:19:DT:OP1	14:T:19:DT:H3'	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:195:ASP:O	1:A:196:GLU:HB3	2.14	0.47
2:B:431:TYR:CG	2:B:447:ALA:HB2	2.49	0.47
2:B:434:ARG:O	2:B:436:VAL:N	2.46	0.47
10:J:16:ASP:OD1	10:J:17:LYS:HD2	2.14	0.47
1:A:1285:MET:O	1:A:1305:VAL:N	2.39	0.47
8:H:11:GLN:O	8:H:28:ALA:CB	2.61	0.47
8:H:41:ASP:O	8:H:42:ILE:HG13	2.15	0.47
10:J:2:ILE:HG12	10:J:57:ILE:CD1	2.44	0.47
4:D:17:LYS:CD	4:D:18:VAL:HG13	2.43	0.47
2:B:1097:HIS:H	2:B:1098:MET:HE2	1.80	0.47
1:A:90:VAL:HG12	1:A:91:PHE:N	2.29	0.47
1:A:537:ARG:HB2	8:H:20:TYR:CE2	2.50	0.47
1:A:186:LYS:HZ1	1:A:197:PRO:HD3	1.77	0.47
14:T:13:DT:H2"	14:T:14:DA:C8	2.48	0.47
1:A:1394:THR:HG21	1:A:1398:MET:SD	2.53	0.47
7:G:45:ILE:HA	7:G:78:VAL:HG12	1.95	0.47
2:B:882:THR:CG2	2:B:883:LEU:N	2.78	0.47
3:C:235:VAL:CG1	10:J:13:VAL:HG13	2.44	0.47
3:C:66:ARG:NH2	10:J:5:VAL:HG23	2.28	0.47
4:D:220:LEU:HD23	4:D:221:TYR:N	2.17	0.47
1:A:106:VAL:CG1	1:A:107:CYS:N	2.77	0.47
5:E:61:GLN:HG2	5:E:62:ALA:N	2.29	0.47
2:B:101:MET:HB3	2:B:109:THR:CG2	2.45	0.47
2:B:47:GLN:O	2:B:173:MET:HE1	2.14	0.47
1:A:963:ILE:HD11	1:A:1048:ASN:CB	2.44	0.47
6:F:109:VAL:HG13	6:F:127:GLU:OE1	2.14	0.47
1:A:494:SER:O	1:A:498:ARG:HG2	2.14	0.47
1:A:262:LEU:O	1:A:266:LEU:HG	2.14	0.47
1:A:350:ARG:CB	2:B:1128:LEU:HD11	2.45	0.47
5:E:182:ASP:HB3	5:E:185:ALA:HB2	1.96	0.47
2:B:55:VAL:HG13	2:B:97:VAL:HG21	1.97	0.47
2:B:635:ARG:HB2	2:B:636:PRO:HD2	1.95	0.47
2:B:638:PHE:HD2	2:B:690:VAL:HG22	1.79	0.47
2:B:635:ARG:NH1	2:B:742:GLU:OE2	2.48	0.47
1:A:500:GLU:OE1	2:B:1145:SER:N	2.48	0.47
2:B:997:GLU:H	2:B:997:GLU:HG3	1.41	0.47
2:B:878:GLN:O	2:B:879:ARG:C	2.53	0.47
2:B:918:ILE:CG2	2:B:935:ARG:NH2	2.74	0.47
1:A:719:VAL:HG12	1:A:720:ARG:N	2.29	0.47
1:A:698:GLN:HE21	9:I:99:LEU:HD21	1.78	0.47
5:E:145:THR:HG21	5:E:187:TYR:CD2	2.50	0.47
2:B:642:ASP:CA	2:B:649:LYS:HG3	2.43	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:113:TYR:CE2	2:B:192:LEU:HD21	2.50	0.47
2:B:167:ILE:HG22	2:B:453:ILE:CD1	2.41	0.47
12:L:26:THR:HG22	12:L:27:LEU:N	2.30	0.47
2:B:291:ILE:CD1	2:B:300:HIS:NE2	2.77	0.47
1:A:843:LYS:HD3	1:A:846:GLU:OE2	2.14	0.47
1:A:90:VAL:CG1	1:A:297:GLN:HA	2.42	0.47
1:A:38:PRO:HA	1:A:270:LEU:HD23	1.96	0.47
1:A:849:MET:HE1	1:A:1061:GLY:HA2	1.96	0.47
3:C:193:TYR:HD1	3:C:193:TYR:O	1.97	0.47
7:G:136:VAL:O	7:G:136:VAL:HG12	2.14	0.47
2:B:31:TRP:CZ3	2:B:34:ILE:HD12	2.49	0.47
2:B:849:GLY:O	2:B:852:ARG:HG3	2.14	0.47
7:G:123:ALA:O	7:G:125:SER:N	2.48	0.47
2:B:798:TYR:CE2	3:C:62:PHE:HE2	2.30	0.47
3:C:22:LEU:CD2	3:C:230:MET:HE2	2.45	0.47
1:A:1332:PHE:H	1:A:1332:PHE:HD2	1.63	0.47
2:B:29:ASP:CB	2:B:658:ILE:HD13	2.44	0.47
1:A:1341:ILE:CG2	1:A:1342:GLU:N	2.78	0.47
1:A:960:ILE:HA	1:A:963:ILE:HG22	1.97	0.47
1:A:456:MET:HE3	1:A:474:VAL:CG2	2.45	0.47
1:A:316:GLN:O	1:A:317:LYS:C	2.51	0.47
2:B:560:GLU:O	2:B:561:TRP:CD1	2.68	0.47
2:B:34:ILE:HG12	2:B:542:MET:HE1	1.97	0.47
1:A:1166:ASP:O	1:A:1167:GLU:C	2.52	0.47
2:B:331:LEU:HD23	2:B:353:LYS:HG2	1.97	0.47
5:E:112:TYR:CE1	5:E:136:ASN:HB2	2.50	0.47
1:A:1441:PHE:HE1	6:F:92:ARG:HG2	1.79	0.47
1:A:269:ILE:HG12	1:A:299:HIS:HB3	1.97	0.47
1:A:69:THR:HB	2:B:1174:LYS:HZ3	1.79	0.47
1:A:795:GLU:CD	1:A:795:GLU:H	2.17	0.47
3:C:59:ALA:O	3:C:62:PHE:HB3	2.13	0.47
2:B:996:ARG:HH12	3:C:174:ALA:HA	1.80	0.47
3:C:44:LEU:HD21	3:C:159:ALA:CB	2.44	0.47
3:C:73:GLN:NE2	3:C:75:MET:N	2.62	0.47
3:C:131:HIS:O	3:C:133:ILE:N	2.48	0.47
1:A:1424:VAL:HG13	1:A:1436:ILE:CD1	2.45	0.47
8:H:81:PRO:CB	8:H:82:PRO:CD	2.92	0.47
8:H:82:PRO:O	8:H:84:ALA:N	2.33	0.47
2:B:126:SER:HA	2:B:169:ARG:HH12	1.79	0.47
2:B:789:MET:HE2	2:B:965:LYS:HB2	1.96	0.47
2:B:952:VAL:HG12	2:B:953:LEU:N	2.30	0.47
2:B:860:MET:SD	2:B:963:PHE:HE1	2.37	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:233:TRP:C	1:A:235:ILE:H	2.16	0.47
9:I:95:THR:HG22	9:I:96:SER:O	2.15	0.47
2:B:129:PHE:CD2	2:B:166:PHE:HA	2.49	0.47
2:B:654:ARG:O	2:B:657:HIS:N	2.47	0.47
2:B:654:ARG:NH1	2:B:654:ARG:HG3	2.29	0.47
12:L:27:LEU:O	12:L:28:LYS:HB2	2.13	0.47
1:A:898:ARG:HD3	1:A:933:TYR:CE1	2.50	0.47
1:A:79:GLY:H	2:B:1205:GLN:HE22	1.63	0.47
2:B:515:HIS:NE2	2:B:517:THR:HG23	2.30	0.47
1:A:1048:ASN:HD22	1:A:1048:ASN:N	2.12	0.47
2:B:1073:TYR:HE2	3:C:180:TYR:CE2	2.32	0.47
1:A:453:MET:HB3	1:A:477:PRO:HB3	1.96	0.47
1:A:993:LEU:CD2	1:A:1022:LEU:HD11	2.45	0.47
1:A:1353:TYR:HD2	1:A:1353:TYR:C	2.17	0.47
8:H:98:TYR:C	8:H:118:PHE:HD2	2.16	0.47
1:A:551:TYR:CE2	11:K:62:LYS:HE2	2.50	0.47
2:B:526:GLU:HG3	2:B:771:SER:HB3	1.96	0.47
1:A:953:ASN:C	1:A:954:TRP:CD1	2.88	0.47
1:A:814:PHE:O	1:A:814:PHE:CD2	2.67	0.47
2:B:37:PHE:HE1	2:B:41:LYS:CG	2.28	0.47
2:B:641:GLU:O	2:B:643:ASP:N	2.46	0.47
2:B:706:GLN:NE2	2:B:730:ARG:HD3	2.29	0.47
1:A:385:ILE:HG22	1:A:386:ASP:N	2.30	0.47
2:B:878:GLN:HA	2:B:885:MET:HE1	1.97	0.47
9:I:100:PHE:CD1	9:I:100:PHE:N	2.83	0.47
12:L:53:HIS:C	12:L:55:ILE:HD13	2.34	0.47
2:B:98:THR:O	2:B:126:SER:HB2	2.14	0.47
1:A:23:SER:CB	1:A:233:TRP:NE1	2.78	0.47
1:A:904:THR:O	1:A:904:THR:CG2	2.62	0.47
2:B:1183:LYS:HE3	2:B:1183:LYS:O	2.14	0.47
12:L:60:ARG:HH21	12:L:65:VAL:CG2	2.28	0.47
10:J:7:CYS:SG	10:J:49:MET:HE3	2.55	0.47
1:A:442:VAL:CG2	1:A:489:LEU:HD11	2.45	0.47
2:B:735:ALA:HB3	2:B:738:PHE:CE1	2.50	0.47
2:B:376:PHE:HB3	2:B:566:LEU:HD21	1.96	0.47
1:A:1166:ASP:OD2	1:A:1239:ARG:CD	2.62	0.47
2:B:848:ARG:HD3	10:J:11:GLY:HA2	1.97	0.47
2:B:1181:GLU:H	2:B:1188:LYS:HA	1.80	0.47
12:L:30:ILE:CG2	12:L:31:CYS:H	2.28	0.47
2:B:126:SER:HB3	2:B:172:ILE:HD11	1.97	0.47
2:B:992:ILE:HG12	2:B:993:THR:H	1.79	0.47
2:B:412:LEU:HB3	2:B:466:TRP:CZ2	2.50	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:1167:GLY:O	2:B:1215:ARG:HA	2.15	0.47
1:A:180:LYS:NZ	1:A:294:SER:HB3	2.30	0.47
1:A:1283:VAL:HG12	1:A:1284:MET:N	2.29	0.47
5:E:162:ARG:HB3	5:E:162:ARG:CZ	2.45	0.47
2:B:562:GLY:HA3	2:B:590:HIS:CE1	2.50	0.47
8:H:15:VAL:HG22	8:H:26:ILE:CD1	2.45	0.47
4:D:139:LYS:HG3	4:D:140:ASP:OD1	2.15	0.47
3:C:101:LEU:HD13	3:C:118:LEU:CD2	2.45	0.47
8:H:84:ALA:HA	8:H:87:ARG:HG3	1.96	0.47
14:T:15:DG:C8	14:T:16:DT:C7	2.98	0.47
2:B:63:ILE:HD12	2:B:421:PHE:CD2	2.49	0.47
1:A:960:ILE:HA	1:A:963:ILE:CG2	2.45	0.47
2:B:307:ASP:OD1	2:B:309:GLN:HB2	2.15	0.47
1:A:90:VAL:HG12	1:A:297:GLN:NE2	2.30	0.47
10:J:21:TYR:HB2	10:J:39:LEU:HD11	1.96	0.47
2:B:430:ARG:HB3	2:B:434:ARG:CZ	2.45	0.47
4:D:39:ASN:ND2	4:D:41:GLN:H	2.13	0.47
1:A:483:ASP:HA	2:B:988:GLY:HA2	1.96	0.47
1:A:1410:PHE:HD2	2:B:1212:ILE:HD12	1.80	0.47
3:C:80:LEU:HD11	3:C:95:CYS:C	2.35	0.47
1:A:785:PRO:HG2	1:A:786:HIS:CD2	2.51	0.46
2:B:360:PHE:O	2:B:361:LEU:C	2.53	0.46
1:A:71:GLN:C	1:A:73:GLY:H	2.17	0.46
9:I:58:VAL:HG12	9:I:58:VAL:O	2.15	0.46
2:B:797:TYR:HE1	2:B:854:LEU:HD21	1.80	0.46
4:D:155:ARG:NE	4:D:221:TYR:CE1	2.83	0.46
4:D:15:LEU:O	4:D:15:LEU:HD12	2.15	0.46
1:A:590:ARG:NH1	1:A:590:ARG:HG2	2.29	0.46
1:A:1315:GLU:C	1:A:1317:MET:N	2.68	0.46
2:B:528:PRO:HG2	2:B:532:ALA:O	2.15	0.46
2:B:466:TRP:N	2:B:475:SER:OG	2.48	0.46
3:C:196:ASP:HB3	3:C:199:LYS:HD2	1.96	0.46
1:A:1208:THR:HG22	1:A:1210:GLY:N	2.29	0.46
2:B:706:GLN:HB2	2:B:709:ASP:HB2	1.97	0.46
7:G:126:ASN:HD22	7:G:127:PRO:N	2.13	0.46
2:B:649:LYS:HD3	2:B:736:THR:O	2.14	0.46
2:B:189:LEU:CD1	2:B:196:PRO:HA	2.45	0.46
5:E:78:LEU:HD21	5:E:80:VAL:CG2	2.45	0.46
2:B:777:ALA:HA	2:B:1095:LEU:HA	1.97	0.46
11:K:12:LEU:HD12	11:K:37:LYS:CG	2.44	0.46
2:B:269:ILE:O	2:B:282:ILE:HG12	2.15	0.46
1:A:1081:LEU:HD21	1:A:1097:GLY:HA3	1.96	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:K:79:GLU:C	11:K:81:TYR:H	2.19	0.46
11:K:55:LYS:HB2	11:K:81:TYR:CE1	2.49	0.46
10:J:41:LEU:HD11	10:J:50:ILE:HG13	1.97	0.46
2:B:1130:PHE:CE1	2:B:1134:GLU:HB3	2.51	0.46
1:A:1349:TYR:O	1:A:1350:LYS:C	2.52	0.46
2:B:970:THR:HG22	2:B:971:THR:N	2.30	0.46
1:A:934:LYS:O	1:A:937:VAL:HG12	2.16	0.46
5:E:12:LEU:HD22	5:E:55:ARG:CZ	2.46	0.46
8:H:12:VAL:HA	8:H:28:ALA:HB2	1.97	0.46
8:H:94:ASP:O	8:H:95:TYR:HB2	2.15	0.46
1:A:504:LEU:HD13	6:F:91:ALA:CB	2.44	0.46
1:A:398:GLU:O	1:A:399:HIS:O	2.34	0.46
1:A:49:LYS:HZ3	1:A:61:ILE:HG13	1.78	0.46
1:A:407:ARG:CD	1:A:413:ILE:HD11	2.40	0.46
4:D:154:PHE:N	4:D:154:PHE:CD2	2.82	0.46
4:D:219:THR:HG23	4:D:220:LEU:O	2.16	0.46
2:B:952:VAL:HG22	2:B:966:VAL:HG13	1.96	0.46
6:F:116:ASP:OD1	6:F:117:PRO:N	2.48	0.46
2:B:25:ILE:HD13	2:B:653:VAL:HG12	1.96	0.46
12:L:59:ALA:O	12:L:60:ARG:O	2.34	0.46
2:B:944:THR:HG21	2:B:1122:ARG:CZ	2.45	0.46
8:H:109:LYS:HD3	8:H:111:LEU:HD11	1.96	0.46
2:B:416:LEU:HD12	2:B:466:TRP:CZ2	2.50	0.46
2:B:696:GLU:O	2:B:699:GLU:HB2	2.15	0.46
1:A:196:GLU:HG2	1:A:197:PRO:N	2.31	0.46
6:F:111:LEU:HD12	6:F:111:LEU:H	1.80	0.46
8:H:9:ILE:HG23	8:H:55:LEU:O	2.15	0.46
2:B:604:ARG:C	2:B:606:LYS:H	2.19	0.46
3:C:221:TYR:CD1	3:C:222:LYS:HG3	2.50	0.46
1:A:690:VAL:CG1	1:A:691:LEU:N	2.78	0.46
9:I:62:ILE:HD11	9:I:86:PHE:CE2	2.50	0.46
11:K:33:ILE:HD13	11:K:87:LEU:HD22	1.96	0.46
1:A:1420:ASP:CB	1:A:1422:ARG:HG3	2.41	0.46
2:B:96:TYR:N	2:B:129:PHE:O	2.38	0.46
2:B:653:VAL:CG2	2:B:689:LEU:HB3	2.44	0.46
2:B:63:ILE:HA	2:B:421:PHE:CE2	2.51	0.46
10:J:48:ARG:HE	10:J:49:MET:CE	2.28	0.46
11:K:85:ASP:O	11:K:88:LYS:HB2	2.15	0.46
3:C:10:ILE:HG22	3:C:11:ARG:O	2.16	0.46
2:B:236:HIS:CE1	2:B:389:ALA:HA	2.50	0.46
10:J:14:VAL:HG12	10:J:50:ILE:HD11	1.97	0.46
1:A:1076:ALA:HA	1:A:1079:MET:HG3	1.96	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:350:ARG:HB2	2:B:1128:LEU:HD11	1.97	0.46
2:B:602:THR:HA	2:B:605:ARG:HB2	1.97	0.46
1:A:1166:ASP:HA	1:A:1169:ILE:HD12	1.97	0.46
1:A:1197:LEU:HD11	1:A:1238:ILE:HD11	1.96	0.46
1:A:401:GLY:C	1:A:435:HIS:CD2	2.89	0.46
1:A:244:PRO:CB	1:A:245:PRO:CD	2.91	0.46
2:B:293:PRO:C	2:B:294:ASP:O	2.51	0.46
2:B:792:MET:H	2:B:857:ARG:HA	1.79	0.46
3:C:209:TYR:N	3:C:209:TYR:CD1	2.75	0.46
11:K:53:ASP:HB3	11:K:56:VAL:HG23	1.97	0.46
1:A:1289:ARG:NH1	1:A:1326:ARG:NH1	2.63	0.46
1:A:100:LYS:O	1:A:104:GLU:HG3	2.16	0.46
1:A:108:MET:O	1:A:109:HIS:HB3	2.15	0.46
2:B:427:ASP:OD1	2:B:430:ARG:HD2	2.16	0.46
1:A:751:SER:O	1:A:752:LYS:HG2	2.16	0.46
1:A:699:ALA:HB3	1:A:701:LEU:HG	1.96	0.46
2:B:254:LEU:CD1	2:B:273:LEU:HD23	2.45	0.46
2:B:347:LYS:CG	2:B:348:ARG:H	2.29	0.46
1:A:295:LEU:O	1:A:298:PHE:HB3	2.16	0.46
4:D:138:ASN:C	4:D:140:ASP:N	2.67	0.46
9:I:61:ASP:C	9:I:63:GLY:N	2.67	0.46
10:J:3:VAL:N	10:J:53:HIS:CE1	2.84	0.46
4:D:155:ARG:NE	4:D:221:TYR:HE1	2.14	0.46
1:A:728:LYS:O	1:A:732:LEU:HG	2.15	0.46
1:A:767:GLN:NE2	1:A:774:ARG:CB	2.77	0.46
6:F:103:MET:HE1	7:G:66:GLY:N	2.24	0.46
2:B:294:ASP:H	9:I:12:ASN:HD22	1.57	0.46
2:B:910:VAL:CG1	2:B:938:SER:HB3	2.46	0.46
2:B:1001:PHE:CZ	2:B:1073:TYR:HB2	2.50	0.46
1:A:121:LEU:O	1:A:121:LEU:HD23	2.16	0.46
3:C:196:ASP:CB	3:C:199:LYS:HD2	2.45	0.46
2:B:430:ARG:NH1	2:B:430:ARG:HG2	2.31	0.46
2:B:417:PHE:O	2:B:420:LEU:HB2	2.16	0.46
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.49	0.46
1:A:1155:ASP:OD2	1:A:1162:VAL:N	2.48	0.46
2:B:918:ILE:HD12	2:B:935:ARG:CZ	2.45	0.46
2:B:914:LYS:HE2	2:B:937:ALA:CB	2.45	0.46
1:A:675:THR:HB	1:A:736:ASN:OD1	2.15	0.46
1:A:577:ILE:HA	1:A:580:VAL:HG23	1.98	0.46
2:B:860:MET:HE2	2:B:965:LYS:HE2	1.98	0.46
2:B:527:THR:OG1	2:B:528:PRO:HD2	2.15	0.46
9:I:8:ARG:H	9:I:8:ARG:HG3	1.59	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:284:ALA:HB1	1:A:289:ILE:HD12	1.97	0.46
2:B:282:ILE:CD1	2:B:382:ILE:HD13	2.46	0.46
1:A:492:PRO:HB2	1:A:497:THR:HG22	1.96	0.46
2:B:311:LEU:O	2:B:314:LEU:N	2.49	0.46
2:B:265:SER:O	2:B:266:ALA:HB3	2.16	0.46
2:B:37:PHE:CD2	2:B:542:MET:SD	3.09	0.46
6:F:90:ARG:O	6:F:91:ALA:C	2.55	0.46
10:J:3:VAL:HA	10:J:53:HIS:HD1	1.80	0.46
7:G:14:HIS:HD2	7:G:16:SER:CB	2.29	0.46
1:A:1423:GLY:O	1:A:1424:VAL:C	2.54	0.46
1:A:592:ASP:N	1:A:595:THR:OG1	2.49	0.46
1:A:1420:ASP:O	1:A:1421:CYS:CB	2.62	0.46
1:A:898:ARG:O	1:A:1029:ARG:NH1	2.48	0.46
1:A:80:HIS:H	1:A:243:PRO:CB	2.28	0.46
2:B:131:ASP:HA	2:B:164:LYS:HB3	1.98	0.46
1:A:851:HIS:C	1:A:853:ASP:H	2.19	0.46
1:A:853:ASP:OD1	1:A:855:THR:CG2	2.63	0.46
2:B:1116:ARG:NE	2:B:1198:TYR:CE1	2.84	0.46
1:A:1394:THR:CG2	1:A:1398:MET:SD	3.04	0.46
7:G:154:VAL:HG12	7:G:155:SER:N	2.30	0.46
2:B:593:PRO:O	2:B:594:ALA:C	2.54	0.46
1:A:871:ASP:OD2	1:A:873:MET:HB2	2.16	0.46
2:B:582:VAL:HG22	2:B:626:ILE:HG22	1.98	0.46
5:E:56:LYS:NZ	5:E:84:ASP:N	2.63	0.46
4:D:123:LEU:HD13	4:D:149:THR:HG21	1.97	0.46
4:D:14:ARG:O	4:D:16:LYS:N	2.40	0.46
1:A:185:TRP:HE3	1:A:185:TRP:N	1.98	0.46
6:F:69:LEU:HD22	6:F:71:GLU:OE2	2.15	0.46
7:G:112:LYS:HA	7:G:115:MET:HE2	1.98	0.46
1:A:897:TYR:CD2	1:A:936:LEU:HD13	2.51	0.46
10:J:32:GLU:CD	10:J:32:GLU:H	2.18	0.46
10:J:9:SER:OG	10:J:48:ARG:NH2	2.48	0.46
1:A:1195:LEU:HD11	1:A:1267:MET:HE1	1.95	0.46
2:B:525:ALA:O	2:B:768:THR:HG23	2.16	0.46
6:F:79:ARG:NH2	6:F:150:GLU:OE1	2.35	0.46
6:F:79:ARG:HG2	6:F:144:GLU:HB3	1.97	0.46
3:C:23:SER:O	3:C:24:ASN:HB3	2.16	0.46
5:E:186:LEU:HA	5:E:186:LEU:HD23	1.71	0.46
2:B:356:LEU:HD23	2:B:360:PHE:CD1	2.51	0.46
2:B:582:VAL:O	2:B:582:VAL:HG12	2.14	0.46
8:H:15:VAL:HG13	8:H:26:ILE:HD12	1.98	0.46
8:H:11:GLN:C	8:H:28:ALA:HB1	2.35	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:710:LEU:HA	2:B:733:HIS:CB	2.29	0.46
12:L:70:ARG:HG2	12:L:70:ARG:HH11	1.81	0.46
2:B:878:GLN:HB2	2:B:879:ARG:NH1	2.30	0.46
1:A:793:SER:HB2	1:A:794:PRO:HD2	1.98	0.46
3:C:100:THR:CG2	3:C:101:LEU:N	2.79	0.46
1:A:648:ASN:O	1:A:649:ILE:C	2.55	0.46
1:A:645:LEU:HG	1:A:649:ILE:HD11	1.98	0.46
2:B:773:MET:HE1	2:B:985:GLY:HA2	1.98	0.46
2:B:102:VAL:HG22	2:B:112:LEU:HB2	1.96	0.46
5:E:19:VAL:HG11	5:E:80:VAL:HG11	1.98	0.46
2:B:169:ARG:CB	2:B:454:THR:HG23	2.45	0.46
1:A:575:LYS:HB3	1:A:612:ILE:CG2	2.46	0.46
5:E:108:GLY:HA3	5:E:132:ILE:HG23	1.98	0.46
2:B:980:PHE:HD2	2:B:1094:ARG:HA	1.81	0.46
2:B:1034:VAL:O	2:B:1037:LEU:N	2.48	0.46
2:B:1033:LYS:HA	2:B:1089:PRO:HD2	1.98	0.46
2:B:792:MET:O	2:B:793:ALA:HB2	2.16	0.46
1:A:356:ASP:OD2	11:K:65:HIS:CE1	2.65	0.46
1:A:898:ARG:HA	1:A:933:TYR:CD1	2.51	0.46
2:B:295:GLY:N	2:B:298:LEU:HD23	2.29	0.46
1:A:738:LYS:NZ	3:C:194:GLU:O	2.48	0.46
4:D:8:PHE:CG	4:D:38:ILE:O	2.69	0.46
1:A:1362:TYR:CD1	1:A:1363:VAL:N	2.84	0.46
2:B:1045:SER:HB3	2:B:1046:PRO:HD2	1.98	0.45
2:B:582:VAL:O	2:B:582:VAL:CG1	2.63	0.45
8:H:123:MET:HE3	8:H:142:LEU:HD21	1.98	0.45
1:A:321:PRO:O	1:A:322:VAL:HG12	2.16	0.45
4:D:64:VAL:C	4:D:66:ARG:N	2.68	0.45
2:B:866:TYR:CB	2:B:870:ILE:HD12	2.47	0.45
1:A:698:GLN:O	9:I:98:VAL:HA	2.16	0.45
2:B:797:TYR:HE1	2:B:854:LEU:HD23	1.81	0.45
2:B:112:LEU:HD12	2:B:113:TYR:N	2.27	0.45
1:A:741:ASN:C	1:A:741:ASN:HD22	2.16	0.45
1:A:233:TRP:C	1:A:235:ILE:N	2.69	0.45
11:K:47:ARG:HH11	11:K:47:ARG:CB	2.23	0.45
12:L:38:LEU:O	12:L:39:SER:CB	2.63	0.45
1:A:282:ASN:O	1:A:284:ALA:N	2.48	0.45
1:A:153:PRO:HD3	1:A:161:LEU:CD1	2.46	0.45
1:A:474:VAL:HG22	1:A:478:TYR:HE1	1.81	0.45
1:A:138:ILE:HD12	1:A:221:SER:O	2.16	0.45
1:A:639:PRO:HG2	1:A:640:GLN:N	2.31	0.45
2:B:210:LYS:HD3	2:B:482:VAL:HG22	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:134:ILE:HG21	3:C:139:GLY:HA2	1.97	0.45
2:B:1106:ARG:HD3	2:B:1126:GLY:C	2.36	0.45
8:H:123:MET:HE3	8:H:142:LEU:CD2	2.47	0.45
10:J:3:VAL:CA	10:J:53:HIS:CE1	2.98	0.45
1:A:329:LEU:HD21	2:B:1206:GLU:OE1	2.16	0.45
1:A:332:LYS:HB3	1:A:337:ARG:NE	2.31	0.45
1:A:806:ARG:O	2:B:761:HIS:HE1	1.99	0.45
2:B:567:GLU:HA	2:B:567:GLU:OE1	2.16	0.45
1:A:1081:LEU:CD2	1:A:1097:GLY:HA3	2.46	0.45
3:C:34:ARG:HG2	3:C:35:ARG:N	2.31	0.45
4:D:146:GLN:O	4:D:147:TYR:C	2.55	0.45
2:B:1180:PHE:HB3	2:B:1191:ILE:CD1	2.47	0.45
7:G:12:THR:HG23	7:G:67:SER:HB3	1.98	0.45
1:A:1064:VAL:HG12	1:A:1064:VAL:O	2.14	0.45
2:B:244:LEU:HD13	2:B:366:GLN:HE22	1.81	0.45
1:A:61:ILE:HG22	1:A:62:ASP:N	2.31	0.45
7:G:123:ALA:C	7:G:125:SER:N	2.70	0.45
7:G:129:SER:CB	7:G:138:THR:HG1	2.29	0.45
9:I:55:THR:OG1	9:I:100:PHE:HD2	1.99	0.45
3:C:75:MET:HB3	3:C:128:ASN:HB3	1.98	0.45
1:A:207:ILE:O	1:A:208:LEU:C	2.55	0.45
9:I:105:SER:O	9:I:106:CYS:CB	2.52	0.45
1:A:858:ASN:HD22	1:A:860:LEU:H	1.62	0.45
1:A:867:ILE:HD11	1:A:1000:LEU:HD21	1.97	0.45
2:B:1130:PHE:CD2	2:B:1150:ARG:HG2	2.52	0.45
1:A:856:THR:HG22	1:A:856:THR:O	2.16	0.45
1:A:492:PRO:O	1:A:493:GLN:NE2	2.49	0.45
2:B:314:LEU:O	2:B:318:VAL:HG23	2.16	0.45
2:B:722:ASP:HB3	2:B:723:VAL:H	1.62	0.45
1:A:41:MET:O	1:A:42:ASP:C	2.55	0.45
7:G:1:MET:SD	7:G:1:MET:C	2.95	0.45
9:I:85:PHE:HD1	9:I:99:LEU:HD13	1.75	0.45
1:A:768:GLN:NE2	1:A:816:HIS:ND1	2.64	0.45
5:E:135:PHE:HD2	5:E:140:LEU:CD2	2.28	0.45
1:A:452:LYS:HB3	2:B:1141:HIS:CE1	2.52	0.45
1:A:335:ARG:HH12	2:B:1202:LEU:HD22	1.81	0.45
1:A:1141:THR:HG21	1:A:1205:LYS:HD3	1.98	0.45
1:A:1048:ASN:O	1:A:1049:ILE:C	2.53	0.45
2:B:1099:VAL:CG1	2:B:1100:ASP:N	2.78	0.45
1:A:164:ARG:HG3	1:A:165:GLY:N	2.32	0.45
1:A:1203:ASN:O	1:A:1204:ASP:C	2.55	0.45
1:A:608:ILE:HG13	1:A:613:ILE:HD12	1.99	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:500:THR:HA	2:B:501:PRO:HD2	1.75	0.45
2:B:591:ARG:O	2:B:592:ASN:C	2.55	0.45
1:A:1187:GLN:CA	1:A:1244:ARG:HB3	2.45	0.45
2:B:345:LYS:C	2:B:347:LYS:H	2.20	0.45
1:A:1444:MET:O	6:F:133:VAL:N	2.47	0.45
1:A:255:SER:OG	2:B:918:ILE:HG21	2.16	0.45
1:A:211:PHE:HA	1:A:214:ILE:HG13	1.98	0.45
1:A:1435:PRO:HA	1:A:1439:GLY:O	2.17	0.45
1:A:774:ARG:NH2	1:A:797:LYS:HB2	2.31	0.45
2:B:120:ARG:HH11	12:L:54:ARG:HH11	1.63	0.45
12:L:52:GLY:O	12:L:54:ARG:N	2.50	0.45
1:A:146:MET:CA	1:A:171:GLN:HB2	2.47	0.45
2:B:66:ASP:OD1	2:B:422:LYS:HE2	2.15	0.45
8:H:100:THR:OG1	8:H:138:GLU:HG2	2.16	0.45
2:B:412:LEU:CD2	2:B:479:VAL:HG11	2.45	0.45
1:A:35:ILE:HD13	1:A:241:VAL:HG11	1.98	0.45
3:C:204:SER:C	3:C:206:ASN:N	2.69	0.45
1:A:993:LEU:HD23	1:A:1022:LEU:HD21	1.99	0.45
1:A:447:GLN:HA	1:A:448:PRO:C	2.37	0.45
1:A:1110:ASN:HD22	1:A:1110:ASN:N	2.14	0.45
5:E:4:GLU:HB3	5:E:7:ARG:HE	1.81	0.45
1:A:95:PHE:O	1:A:96:ILE:C	2.55	0.45
2:B:27:ALA:O	2:B:28:GLU:C	2.55	0.45
2:B:604:ARG:CA	2:B:609:ILE:HG13	2.47	0.45
2:B:288:ALA:HA	2:B:331:LEU:CD1	2.46	0.45
4:D:35:LEU:H	4:D:35:LEU:CD1	2.29	0.45
2:B:848:ARG:HA	3:C:69:LEU:HD21	1.98	0.45
3:C:99:LEU:HD22	3:C:120:ILE:HG12	1.98	0.45
1:A:549:MET:SD	1:A:577:ILE:HD12	2.57	0.45
2:B:642:ASP:C	2:B:644:GLU:H	2.18	0.45
2:B:120:ARG:CG	2:B:955:THR:HG21	2.46	0.45
5:E:69:ILE:CD1	5:E:69:ILE:N	2.79	0.45
2:B:101:MET:HB2	2:B:169:ARG:HH22	1.82	0.45
1:A:332:LYS:CD	1:A:333:GLU:HG2	2.47	0.45
1:A:1173:HIS:CD2	1:A:1227:ILE:HG23	2.52	0.45
2:B:46:GLN:HB2	2:B:408:LEU:HD21	1.98	0.45
7:G:17:PHE:C	7:G:19:GLY:H	2.20	0.45
1:A:1454:MET:HG3	1:A:1454:MET:O	2.17	0.45
1:A:96:ILE:HG22	1:A:97:ALA:N	2.32	0.45
1:A:1395:GLY:HA3	1:A:1419:ASP:OD2	2.16	0.45
1:A:1266:THR:O	1:A:1270:ASN:HB2	2.17	0.45
2:B:1214:PRO:HG2	2:B:1214:PRO:O	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1194:ARG:NH2	1:A:1237:ILE:HD13	2.31	0.45
1:A:1242:VAL:CG1	1:A:1243:VAL:N	2.43	0.45
5:E:90:VAL:CA	5:E:120:ALA:HB2	2.40	0.45
1:A:1062:GLU:HG2	6:F:88:TYR:OH	2.17	0.45
5:E:56:LYS:CE	5:E:84:ASP:H	2.29	0.45
6:F:77:ASP:O	6:F:78:GLN:CB	2.49	0.45
5:E:145:THR:HG21	5:E:187:TYR:CZ	2.51	0.45
8:H:138:GLU:O	8:H:139:ASN:C	2.55	0.45
2:B:679:TYR:HE1	2:B:687:GLU:OE2	1.98	0.45
2:B:729:ILE:HG22	2:B:729:ILE:O	2.16	0.45
1:A:860:LEU:HA	1:A:860:LEU:HD23	1.81	0.45
5:E:204:THR:HG23	5:E:205:SER:N	2.32	0.45
5:E:129:PRO:O	5:E:130:ALA:O	2.35	0.45
8:H:20:TYR:O	8:H:22:LYS:N	2.50	0.45
5:E:92:THR:HG22	5:E:92:THR:O	2.15	0.45
2:B:431:TYR:CE1	2:B:447:ALA:HB2	2.52	0.45
1:A:492:PRO:CB	1:A:497:THR:HG22	2.47	0.45
3:C:249:ASP:O	3:C:250:THR:C	2.55	0.45
1:A:125:ALA:O	1:A:127:ALA:N	2.50	0.45
2:B:799:PRO:HB2	2:B:818:PRO:HG2	1.98	0.45
2:B:856:PHE:N	2:B:856:PHE:CD1	2.84	0.45
3:C:229:TYR:CD1	3:C:229:TYR:N	2.84	0.45
8:H:7:ASP:O	8:H:8:ASP:HB2	2.17	0.45
5:E:112:TYR:HB3	5:E:116:ILE:HD11	1.99	0.45
4:D:138:ASN:ND2	7:G:35:GLU:HB3	2.19	0.45
1:A:709:THR:HG21	9:I:93:LYS:O	2.16	0.45
3:C:185:LYS:HE2	3:C:213:PRO:HA	1.99	0.45
11:K:17:SER:O	11:K:18:LYS:C	2.50	0.45
11:K:37:LYS:HA	11:K:37:LYS:HD3	1.88	0.45
2:B:1177:HIS:CB	2:B:1179:GLN:HE21	2.29	0.45
3:C:193:TYR:C	3:C:193:TYR:CD1	2.89	0.45
2:B:1119:VAL:O	2:B:1126:GLY:HA3	2.15	0.45
2:B:880:THR:O	2:B:880:THR:HG22	2.17	0.45
1:A:1277:GLU:C	1:A:1279:ILE:H	2.20	0.45
1:A:565:ILE:HG22	1:A:565:ILE:O	2.17	0.45
2:B:621:GLU:HG3	2:B:621:GLU:O	2.17	0.45
1:A:785:PRO:HG2	1:A:786:HIS:HD2	1.81	0.45
2:B:349:ILE:O	2:B:353:LYS:HG3	2.17	0.45
1:A:55:ASP:N	1:A:56:PRO:CD	2.78	0.45
1:A:687:LYS:O	1:A:690:VAL:HG12	2.16	0.45
1:A:692:ASP:O	1:A:693:VAL:C	2.55	0.45
3:C:20:PHE:C	3:C:20:PHE:CD1	2.90	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:769:TYR:HB3	2:B:987:LYS:NZ	2.31	0.45
1:A:1116:LEU:N	1:A:1308:THR:CG2	2.73	0.45
1:A:1115:SER:C	1:A:1308:THR:HG22	2.38	0.45
2:B:531:GLN:HG3	2:B:532:ALA:H	1.82	0.45
1:A:1387:HIS:NE2	13:N:4:DA:H5'	2.32	0.45
1:A:50:ILE:HG22	1:A:52:GLY:N	2.32	0.45
11:K:12:LEU:HD21	11:K:17:SER:C	2.37	0.45
10:J:27:GLU:C	10:J:29:GLU:N	2.67	0.45
1:A:416:ARG:HG3	1:A:417:TYR:CE1	2.52	0.45
5:E:154:ILE:HG22	5:E:155:ARG:O	2.17	0.45
1:A:108:MET:O	1:A:109:HIS:CB	2.63	0.45
2:B:370:PHE:CD2	2:B:373:ARG:HD2	2.52	0.45
10:J:30:LEU:HD11	10:J:38:ARG:NH1	2.32	0.45
3:C:193:TYR:HD1	3:C:193:TYR:C	2.21	0.45
8:H:55:LEU:HD22	8:H:144:ILE:HG22	1.99	0.45
1:A:1161:THR:CG2	1:A:1163:ILE:HD12	2.46	0.45
12:L:54:ARG:HG3	12:L:54:ARG:H	1.43	0.45
2:B:100:PRO:HB2	2:B:180:TYR:HE1	1.82	0.45
7:G:113:HIS:CD2	7:G:113:HIS:H	2.34	0.45
2:B:69:LEU:HD13	2:B:429:PHE:CD1	2.52	0.45
2:B:889:THR:HG23	2:B:891:ASP:N	2.32	0.45
1:A:1081:LEU:HD11	1:A:1097:GLY:HA3	1.98	0.45
2:B:811:TYR:N	2:B:811:TYR:CD1	2.84	0.45
1:A:1199:ARG:O	1:A:1203:ASN:ND2	2.50	0.45
1:A:1072:ILE:HG23	1:A:1356:ILE:HD11	1.99	0.45
1:A:798:GLY:HA2	1:A:815:PHE:HD1	1.81	0.45
2:B:203:PHE:N	2:B:203:PHE:CD1	2.85	0.45
2:B:805:THR:CG2	2:B:806:THR:H	2.20	0.44
6:F:89:GLU:OE2	6:F:134:ILE:HG21	2.16	0.44
4:D:29:LEU:HB3	7:G:82:PHE:CE2	2.52	0.44
1:A:692:ASP:C	1:A:694:THR:N	2.68	0.44
10:J:53:HIS:CD2	10:J:55:ASP:N	2.85	0.44
2:B:1072:MET:O	2:B:1081:LEU:HB2	2.17	0.44
2:B:486:TYR:HD1	2:B:775:LYS:O	2.00	0.44
1:A:451:HIS:HA	1:A:1070:GLN:OE1	2.16	0.44
4:D:13:ARG:C	4:D:15:LEU:N	2.68	0.44
1:A:605:MET:HE1	1:A:607:ILE:HG12	1.98	0.44
1:A:330:LYS:O	1:A:334:GLY:HA3	2.17	0.44
7:G:111:THR:O	7:G:111:THR:HG23	2.17	0.44
2:B:294:ASP:H	9:I:12:ASN:HD21	1.60	0.44
10:J:62:ARG:HG2	10:J:62:ARG:O	2.17	0.44
2:B:458:LYS:O	2:B:459:TYR:C	2.55	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:I:40:SER:OG	9:I:41:PRO:HD2	2.17	0.44
1:A:1208:THR:HA	1:A:1231:ASP:OD1	2.17	0.44
8:H:2:SER:OG	8:H:3:ASN:N	2.50	0.44
2:B:958:GLN:C	2:B:960:GLY:H	2.20	0.44
9:I:100:PHE:N	9:I:100:PHE:HD1	2.15	0.44
1:A:1335:ILE:HG23	1:A:1339:LEU:HD12	1.98	0.44
3:C:79:GLN:HE21	3:C:127:ARG:CD	2.27	0.44
2:B:1072:MET:HE3	2:B:1085:ILE:CB	2.44	0.44
1:A:335:ARG:NH1	2:B:1206:GLU:CD	2.68	0.44
2:B:412:LEU:HB3	2:B:466:TRP:CE2	2.52	0.44
11:K:55:LYS:HB2	11:K:81:TYR:HE1	1.82	0.44
6:F:97:ARG:NH2	6:F:108:PHE:CE1	2.86	0.44
5:E:128:PRO:HA	5:E:129:PRO:O	2.17	0.44
3:C:67:LEU:HA	3:C:70:ILE:CD1	2.48	0.44
2:B:1106:ARG:HD2	2:B:1125:ASP:O	2.17	0.44
3:C:68:GLY:O	3:C:169:LYS:HB2	2.17	0.44
1:A:352:VAL:O	1:A:467:THR:HB	2.17	0.44
2:B:806:THR:CG2	2:B:808:ALA:HB3	2.47	0.44
2:B:579:ARG:HG2	2:B:579:ARG:NH1	2.30	0.44
8:H:4:THR:O	8:H:5:LEU:HD23	2.17	0.44
4:D:173:HIS:ND1	4:D:174:PRO:HD2	2.33	0.44
2:B:1002:THR:HG23	2:B:1087:PHE:HE1	1.81	0.44
3:C:124:LEU:O	3:C:125:MET:C	2.55	0.44
1:A:102:VAL:HB	1:A:211:PHE:HE1	1.77	0.44
1:A:1111:MET:HG3	1:A:1114:PRO:HB3	2.00	0.44
2:B:987:LYS:HE3	15:P:11:G:C2'	2.46	0.44
1:A:1170:ILE:HG22	1:A:1174:PHE:CZ	2.52	0.44
2:B:234:ILE:HG21	2:B:237:VAL:HG23	1.98	0.44
4:D:51:ASN:OD1	4:D:54:GLU:HB2	2.17	0.44
1:A:1147:THR:HB	9:I:48:LEU:HD12	1.98	0.44
5:E:33:GLU:C	5:E:35:VAL:N	2.71	0.44
1:A:224:PHE:CD2	1:A:231:PRO:HG3	2.52	0.44
2:B:263:GLY:O	2:B:264:SER:C	2.55	0.44
2:B:593:PRO:C	2:B:595:ARG:N	2.71	0.44
2:B:637:LEU:HD22	2:B:742:GLU:HA	2.00	0.44
1:A:1161:THR:HG22	1:A:1163:ILE:HG13	1.98	0.44
1:A:264:PHE:CB	1:A:265:LYS:NZ	2.81	0.44
1:A:12:ARG:NH2	2:B:1192:TYR:CE2	2.85	0.44
7:G:1:MET:SD	7:G:79:PHE:HD1	2.39	0.44
3:C:69:LEU:HB3	10:J:6:ARG:HD3	1.99	0.44
2:B:1003:ALA:HA	3:C:178:PHE:O	2.17	0.44
1:A:1094:VAL:HG13	1:A:1113:THR:CB	2.48	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:100:ILE:HG23	5:E:105:PHE:CD1	2.53	0.44
8:H:100:THR:CG2	8:H:101:ALA:N	2.81	0.44
1:A:939:ASP:O	1:A:942:PHE:HB3	2.18	0.44
1:A:121:LEU:HD22	1:A:141:LEU:HD21	2.00	0.44
2:B:485:ARG:HG3	2:B:781:PHE:HD1	1.83	0.44
1:A:833:GLU:OE2	1:A:1102:LYS:HE3	2.17	0.44
2:B:67:SER:HB2	2:B:92:PHE:CD1	2.52	0.44
9:I:74:GLU:O	9:I:74:GLU:HG3	2.17	0.44
5:E:74:ASP:N	5:E:74:ASP:OD1	2.50	0.44
6:F:135:ARG:HG2	6:F:137:TYR:CE1	2.52	0.44
1:A:49:LYS:HZ1	1:A:61:ILE:CG1	2.26	0.44
2:B:879:ARG:N	2:B:879:ARG:HD2	2.33	0.44
9:I:59:VAL:C	9:I:61:ASP:H	2.21	0.44
1:A:1424:VAL:HG11	2:B:1139:ILE:HD11	1.98	0.44
2:B:114:PRO:O	2:B:115:GLN:C	2.55	0.44
1:A:1100:ARG:O	1:A:1100:ARG:HD2	2.17	0.44
7:G:114:LEU:HD23	7:G:161:GLY:O	2.16	0.44
1:A:755:PHE:O	1:A:757:ASN:N	2.51	0.44
2:B:650:GLU:HG3	2:B:654:ARG:HH21	1.83	0.44
1:A:378:GLU:CD	1:A:387:ARG:HH22	2.21	0.44
2:B:408:LEU:HB3	2:B:409:ALA:H	1.69	0.44
1:A:858:ASN:ND2	1:A:860:LEU:HB2	2.32	0.44
1:A:1037:LEU:HD13	1:A:1042:PHE:HA	2.00	0.44
1:A:336:ILE:CD1	2:B:1203:LEU:HD22	2.47	0.44
1:A:1019:CYS:O	1:A:1020:CYS:C	2.56	0.44
1:A:377:PRO:O	1:A:377:PRO:HG2	2.18	0.44
5:E:89:GLY:C	5:E:91:LYS:H	2.20	0.44
8:H:99:GLY:HA3	8:H:117:SER:O	2.17	0.44
2:B:273:LEU:HD22	2:B:360:PHE:CD1	2.52	0.44
1:A:1237:ILE:CG2	1:A:1238:ILE:N	2.79	0.44
5:E:111:VAL:HG12	5:E:137:GLU:HG2	1.99	0.44
1:A:384:ASN:O	1:A:385:ILE:C	2.55	0.44
3:C:174:ALA:O	3:C:175:ALA:HB3	2.18	0.44
4:D:155:ARG:CD	4:D:221:TYR:CE1	3.00	0.44
1:A:1311:VAL:HG21	1:A:1329:THR:HG23	2.00	0.44
6:F:82:THR:HA	6:F:83:PRO:HD3	1.71	0.44
8:H:102:TYR:N	8:H:102:TYR:CD2	2.86	0.44
5:E:124:VAL:HG13	5:E:132:ILE:CB	2.47	0.44
9:I:88:SER:HB3	9:I:95:THR:HG21	2.00	0.44
6:F:119:ARG:CG	6:F:119:ARG:NH1	2.78	0.44
1:A:388:LEU:HD13	1:A:432:VAL:CG2	2.48	0.44
1:A:821:ARG:HG2	2:B:514:LEU:H	1.82	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:183:TRP:CZ3	3:C:203:GLN:NE2	2.86	0.44
1:A:1081:LEU:CD1	1:A:1098:VAL:H	2.29	0.44
7:G:91:VAL:CG1	7:G:92:VAL:N	2.80	0.44
2:B:781:PHE:N	2:B:781:PHE:CD2	2.83	0.44
5:E:33:GLU:C	5:E:35:VAL:H	2.19	0.44
1:A:317:LYS:O	1:A:318:SER:HB3	2.18	0.44
3:C:91:HIS:C	3:C:91:HIS:CD2	2.91	0.44
1:A:730:GLY:O	1:A:731:ARG:C	2.56	0.44
2:B:225:VAL:HG11	2:B:385:LEU:HA	1.99	0.44
4:D:180:LEU:HD23	4:D:180:LEU:HA	1.89	0.44
1:A:1166:ASP:CG	1:A:1194:ARG:HE	2.21	0.44
1:A:568:PRO:HB2	3:C:221:TYR:CE1	2.52	0.44
1:A:321:PRO:O	1:A:322:VAL:HB	2.16	0.44
5:E:56:LYS:CE	5:E:84:ASP:HB2	2.29	0.44
7:G:1:MET:HE2	7:G:3:PHE:CE1	2.53	0.44
5:E:78:LEU:HD11	5:E:109:ILE:HD12	1.99	0.44
2:B:860:MET:HG2	2:B:861:ASP:N	2.32	0.44
8:H:65:LEU:CD2	8:H:65:LEU:N	2.64	0.44
1:A:378:GLU:OE1	1:A:388:LEU:HD21	2.17	0.44
1:A:1118:VAL:HG23	1:A:1118:VAL:O	2.18	0.44
1:A:973:ILE:CD1	1:A:1037:LEU:HA	2.47	0.44
3:C:208:GLU:C	3:C:210:GLU:H	2.20	0.44
1:A:173:THR:HG22	1:A:184:SER:OG	2.18	0.44
1:A:818:MET:HB3	1:A:818:MET:HE2	1.89	0.44
1:A:935:GLN:NE2	1:A:938:LYS:HD2	2.32	0.44
3:C:114:TYR:HB3	3:C:140:ASN:O	2.18	0.44
2:B:599:THR:O	2:B:603:LEU:HB2	2.18	0.44
8:H:26:ILE:CD1	8:H:49:VAL:HG11	2.48	0.44
1:A:722:LEU:HD23	1:A:799:PHE:CD1	2.53	0.44
1:A:666:ILE:HD12	1:A:666:ILE:N	2.33	0.44
5:E:78:LEU:HD23	5:E:79:TRP:N	2.33	0.44
2:B:860:MET:HG3	2:B:965:LYS:CG	2.44	0.44
2:B:906:SER:O	2:B:907:GLY:C	2.56	0.44
1:A:337:ARG:HD2	2:B:1132:GLU:CD	2.38	0.44
5:E:46:TYR:O	5:E:54:GLN:HB2	2.18	0.44
2:B:758:PHE:HB3	2:B:761:HIS:HD2	1.82	0.44
1:A:117:GLU:N	1:A:117:GLU:CD	2.68	0.44
1:A:836:TYR:N	14:T:18:DC:H5'	2.33	0.44
11:K:83:PRO:O	11:K:84:LYS:C	2.56	0.44
1:A:482:PHE:C	1:A:484:GLY:H	2.20	0.44
1:A:1410:PHE:HD2	2:B:1212:ILE:CD1	2.30	0.44
2:B:1110:PRO:O	2:B:1119:VAL:HG13	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:817:ALA:O	1:A:818:MET:C	2.54	0.44
2:B:33:VAL:O	2:B:36:ALA:HB3	2.17	0.44
2:B:597:MET:SD	2:B:617:ARG:HB2	2.57	0.44
2:B:603:LEU:CD1	2:B:609:ILE:HG23	2.43	0.44
1:A:1161:THR:O	1:A:1163:ILE:N	2.51	0.44
1:A:382:PRO:HB3	1:A:428:TYR:CE2	2.53	0.44
9:I:55:THR:OG1	9:I:100:PHE:CD2	2.70	0.44
2:B:770:GLN:OE1	2:B:983:ARG:CA	2.53	0.44
3:C:233:GLU:CG	3:C:234:SER:N	2.80	0.44
4:D:216:ASN:C	4:D:218:GLU:N	2.68	0.44
5:E:114:ASN:O	5:E:115:ASN:CB	2.54	0.44
2:B:351:TYR:CD1	2:B:355:ILE:HD11	2.52	0.44
1:A:889:SER:C	1:A:891:ALA:N	2.69	0.44
14:T:16:DT:C2'	14:T:17:DT:C5'	2.94	0.44
6:F:116:ASP:C	6:F:116:ASP:OD1	2.56	0.44
2:B:661:LEU:C	2:B:663:ALA:N	2.70	0.44
1:A:884:ASP:HB2	1:A:1024:SER:OG	2.18	0.44
3:C:3:GLU:N	11:K:104:ASN:HD21	2.15	0.44
2:B:309:GLN:OE1	9:I:52:ILE:HD11	2.18	0.44
6:F:120:ILE:O	6:F:124:GLU:HG3	2.18	0.44
4:D:51:ASN:C	4:D:52:LEU:O	2.55	0.44
1:A:1144:LYS:HA	1:A:1268:LEU:HD22	2.00	0.44
1:A:277:GLU:HG2	1:A:277:GLU:O	2.18	0.44
8:H:6:PHE:CD2	8:H:6:PHE:C	2.91	0.44
2:B:376:PHE:CE2	2:B:569:TYR:HD2	2.35	0.43
8:H:143:LEU:C	8:H:144:ILE:HG13	2.38	0.43
1:A:1241:ARG:O	1:A:1242:VAL:HB	2.17	0.43
8:H:123:MET:CE	8:H:142:LEU:HD21	2.47	0.43
1:A:265:LYS:HA	1:A:265:LYS:CE	2.48	0.43
7:G:138:THR:HG22	7:G:139:ILE:HB	2.00	0.43
9:I:69:PRO:HG2	9:I:85:PHE:CD2	2.52	0.43
7:G:18:PHE:HA	7:G:22:MET:CE	2.48	0.43
8:H:130:ARG:HH11	8:H:130:ARG:CA	2.31	0.43
1:A:1259:MET:CE	1:A:1263:ILE:HG13	2.48	0.43
1:A:683:ILE:HG21	1:A:801:GLU:CG	2.48	0.43
1:A:844:ALA:O	1:A:845:LEU:HD23	2.18	0.43
3:C:33:LEU:C	3:C:33:LEU:HD12	2.37	0.43
2:B:526:GLU:OE1	2:B:752:ALA:CB	2.66	0.43
8:H:92:ASP:C	8:H:93:TYR:CD1	2.91	0.43
2:B:240:ILE:HD12	2:B:241:ARG:N	2.33	0.43
2:B:273:LEU:HD12	2:B:280:ILE:HD12	2.00	0.43
2:B:604:ARG:NH1	2:B:691:GLU:OE2	2.42	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:571:LEU:HD22	8:H:46:LEU:CD1	2.41	0.43
1:A:306:ASN:O	1:A:306:ASN:OD1	2.36	0.43
1:A:34:LYS:NZ	1:A:57:ARG:HH21	2.10	0.43
7:G:138:THR:O	7:G:140:LYS:N	2.51	0.43
1:A:693:VAL:HG21	1:A:721:PHE:HE1	1.82	0.43
10:J:57:ILE:HA	10:J:60:PHE:CD2	2.50	0.43
10:J:60:PHE:O	10:J:63:TYR:HD1	2.01	0.43
2:B:1002:THR:O	2:B:1004:GLU:N	2.50	0.43
3:C:44:LEU:HD21	3:C:159:ALA:HB1	2.00	0.43
7:G:14:HIS:CE1	7:G:15:PRO:HD2	2.53	0.43
1:A:1319:VAL:O	1:A:1322:ILE:HG12	2.17	0.43
2:B:235:SER:O	2:B:236:HIS:CD2	2.69	0.43
1:A:347:PHE:CD1	1:A:347:PHE:N	2.87	0.43
1:A:495:GLU:O	1:A:498:ARG:HG3	2.17	0.43
1:A:528:LEU:HD23	1:A:751:SER:HA	2.01	0.43
2:B:880:THR:O	2:B:881:ASN:HB2	2.17	0.43
5:E:42:PHE:O	5:E:43:LYS:C	2.57	0.43
2:B:604:ARG:O	2:B:606:LYS:N	2.51	0.43
2:B:284:ILE:CD1	2:B:324:ILE:HD12	2.48	0.43
5:E:111:VAL:O	5:E:111:VAL:HG12	2.18	0.43
8:H:40:LEU:CD2	8:H:42:ILE:HD11	2.48	0.43
2:B:885:MET:HA	2:B:936:ASP:HB2	1.98	0.43
5:E:82:PHE:N	5:E:82:PHE:HD1	2.17	0.43
6:F:69:LEU:O	6:F:70:LYS:HB2	2.19	0.43
2:B:1033:LYS:O	2:B:1037:LEU:HG	2.18	0.43
10:J:47:ARG:C	10:J:49:MET:N	2.69	0.43
2:B:50:SER:OG	2:B:411:PRO:HD3	2.17	0.43
1:A:1118:VAL:HG22	1:A:1306:LEU:HB2	1.99	0.43
1:A:857:ARG:CZ	6:F:139:PRO:HG3	2.48	0.43
1:A:341:MET:CE	1:A:843:LYS:NZ	2.82	0.43
1:A:184:SER:HB3	1:A:199:LEU:HD23	1.99	0.43
1:A:184:SER:HB2	1:A:199:LEU:HD23	2.00	0.43
1:A:528:LEU:HD23	1:A:751:SER:CA	2.48	0.43
6:F:76:LYS:O	6:F:79:ARG:HD3	2.17	0.43
2:B:604:ARG:HA	2:B:609:ILE:HG13	1.99	0.43
2:B:604:ARG:O	2:B:607:GLY:N	2.51	0.43
7:G:26:LEU:HA	7:G:26:LEU:HD23	1.73	0.43
1:A:717:ASN:O	1:A:718:VAL:C	2.56	0.43
1:A:787:PHE:CE1	1:A:796:SER:HA	2.50	0.43
3:C:52:GLU:OE2	3:C:154:LYS:HD2	2.18	0.43
2:B:1004:GLU:HG3	10:J:42:LYS:HZ1	1.82	0.43
3:C:22:LEU:HD11	11:K:101:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:207:ILE:CG2	1:A:211:PHE:CE2	3.02	0.43
2:B:778:MET:HE3	2:B:1094:ARG:HD3	2.00	0.43
1:A:709:THR:CG2	1:A:710:LEU:H	2.28	0.43
2:B:69:LEU:HD22	2:B:429:PHE:CE1	2.53	0.43
2:B:546:SER:OG	2:B:631:GLY:N	2.51	0.43
4:D:7:THR:HG21	4:D:32:GLU:CD	2.38	0.43
1:A:973:ILE:HD11	1:A:1041:ALA:CB	2.48	0.43
2:B:1001:PHE:CE2	3:C:34:ARG:CZ	3.02	0.43
1:A:1267:MET:HA	1:A:1271:ILE:HD12	2.00	0.43
5:E:35:VAL:C	5:E:37:LEU:H	2.22	0.43
1:A:1230:GLU:C	1:A:1232:ASN:N	2.72	0.43
1:A:1280:GLU:HB3	1:A:1281:ARG:H	1.64	0.43
1:A:1399:ARG:HB3	1:A:1408:ILE:HD13	2.00	0.43
3:C:58:LEU:N	3:C:58:LEU:HD23	2.33	0.43
10:J:8:PHE:CD2	10:J:8:PHE:N	2.86	0.43
2:B:887:HIS:N	2:B:887:HIS:CD2	2.85	0.43
1:A:1193:LEU:HD12	1:A:1193:LEU:C	2.38	0.43
2:B:261:ARG:HH11	2:B:261:ARG:CB	2.09	0.43
5:E:116:ILE:HG22	5:E:120:ALA:HB3	2.00	0.43
8:H:40:LEU:HG	8:H:42:ILE:HG13	2.00	0.43
1:A:298:PHE:HD2	1:A:299:HIS:HD2	1.67	0.43
2:B:846:ILE:HG23	2:B:974:PRO:CG	2.31	0.43
4:D:33:PHE:CE1	7:G:80:LYS:HD3	2.52	0.43
4:D:219:THR:CG2	4:D:220:LEU:O	2.67	0.43
1:A:1345:ARG:HD2	1:A:1373:ASP:OD1	2.18	0.43
1:A:1389:PHE:C	1:A:1391:ARG:H	2.22	0.43
1:A:709:THR:OG1	1:A:712:GLU:HG3	2.17	0.43
5:E:46:TYR:CD2	5:E:58:MET:HG3	2.54	0.43
2:B:95:ILE:CB	2:B:130:VAL:HG22	2.48	0.43
10:J:7:CYS:CA	10:J:49:MET:HE3	2.47	0.43
5:E:161:LYS:HD2	5:E:195:VAL:CG2	2.49	0.43
12:L:38:LEU:HG	12:L:39:SER:N	2.33	0.43
4:D:187:THR:C	4:D:189:ASP:N	2.70	0.43
2:B:269:ILE:CG2	2:B:282:ILE:HD13	2.49	0.43
2:B:312:GLU:O	2:B:315:LYS:HB2	2.19	0.43
3:C:31:ASN:HA	3:C:34:ARG:HB3	1.99	0.43
11:K:40:HIS:O	11:K:41:THR:C	2.57	0.43
1:A:1015:VAL:CG1	1:A:1019:CYS:SG	3.06	0.43
5:E:153:HIS:C	5:E:154:ILE:HG13	2.39	0.43
1:A:1336:MET:CE	1:A:1381:LEU:HG	2.49	0.43
1:A:1077:THR:HB	1:A:1078:GLN:HE21	1.84	0.43
2:B:218:SER:HA	2:B:404:LYS:HA	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:11:LEU:CD2	1:A:11:LEU:O	2.61	0.43
1:A:47:ARG:NH1	1:A:254:GLU:HG2	2.34	0.43
1:A:794:PRO:C	1:A:796:SER:H	2.22	0.43
2:B:1201:LYS:HE2	2:B:1205:GLN:CD	2.39	0.43
3:C:220:ASP:OD1	3:C:223:ALA:HB2	2.18	0.43
9:I:50:THR:CG2	9:I:51:ASN:H	2.32	0.43
1:A:836:TYR:CD2	1:A:840:ARG:HD2	2.54	0.43
1:A:2:VAL:CG1	2:B:1157:ALA:O	2.67	0.43
9:I:82:GLU:HB3	9:I:104:LEU:HG	2.01	0.43
1:A:343:LYS:NZ	2:B:1151:LEU:O	2.51	0.43
1:A:1376:THR:O	1:A:1377:THR:C	2.56	0.43
3:C:136:ASP:OD2	3:C:137:LYS:N	2.52	0.43
2:B:222:ILE:C	2:B:240:ILE:HD13	2.39	0.43
2:B:605:ARG:NE	2:B:639:ILE:HD13	2.33	0.43
8:H:15:VAL:HG22	8:H:26:ILE:HD11	2.00	0.43
4:D:29:LEU:HD12	7:G:82:PHE:CE1	2.52	0.43
4:D:35:LEU:HD11	4:D:173:HIS:NE2	2.33	0.43
2:B:883:LEU:O	2:B:885:MET:N	2.52	0.43
10:J:3:VAL:HG21	10:J:18:TRP:CG	2.54	0.43
10:J:1:MET:HB2	10:J:56:LEU:HD12	1.99	0.43
4:D:119:ARG:HD2	4:D:221:TYR:CG	2.53	0.43
4:D:155:ARG:NH1	4:D:155:ARG:CB	2.82	0.43
1:A:351:THR:HG21	2:B:1103:ILE:HG13	2.00	0.43
4:D:53:SER:H	4:D:148:LEU:HD22	1.84	0.43
1:A:774:ARG:HG3	1:A:797:LYS:HB3	2.01	0.43
1:A:804:TYR:OH	2:B:763:GLN:HA	2.19	0.43
1:A:1308:THR:HG21	1:A:1310:GLY:O	2.19	0.43
1:A:1074:GLU:N	1:A:1075:PRO:HD2	2.34	0.43
8:H:130:ARG:HD3	8:H:130:ARG:H	1.79	0.43
1:A:1124:HIS:HB2	1:A:1130:GLN:HG2	2.01	0.43
7:G:20:PRO:CD	7:G:21:ARG:N	2.82	0.43
2:B:46:GLN:HB2	2:B:408:LEU:CD2	2.48	0.43
2:B:46:GLN:OE1	2:B:47:GLN:N	2.50	0.43
1:A:289:ILE:CG2	1:A:290:GLU:N	2.80	0.43
11:K:55:LYS:CB	11:K:81:TYR:CD1	3.01	0.43
1:A:833:GLU:CG	1:A:1102:LYS:HE2	2.48	0.43
4:D:38:ILE:HG12	4:D:38:ILE:H	1.47	0.43
1:A:396:PRO:HG2	1:A:397:ASN:OD1	2.19	0.43
2:B:821:GLN:OE1	2:B:850:LEU:CD1	2.67	0.43
1:A:382:PRO:CB	1:A:428:TYR:HE2	2.32	0.43
2:B:1023:VAL:O	2:B:1026:LEU:HB2	2.18	0.43
4:D:53:SER:HA	4:D:56:ARG:HB3	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:766:ARG:NH1	2:B:769:TYR:CE1	2.87	0.43
1:A:218:ASP:O	1:A:219:PHE:C	2.56	0.43
1:A:141:LEU:HD23	1:A:141:LEU:HA	1.86	0.43
2:B:1198:TYR:O	2:B:1198:TYR:CD2	2.72	0.43
2:B:259:TYR:N	2:B:259:TYR:CD1	2.87	0.43
2:B:570:VAL:HG21	2:B:573:GLN:NE2	2.34	0.43
2:B:317:CYS:O	2:B:320:ASP:HB3	2.19	0.43
1:A:239:LEU:HA	1:A:240:PRO:HD2	1.82	0.43
1:A:108:MET:CB	1:A:210:ILE:HD13	2.49	0.43
3:C:142:VAL:H	10:J:16:ASP:HB3	1.83	0.43
1:A:565:ILE:O	1:A:570:PRO:HA	2.19	0.43
1:A:360:GLU:HB2	1:A:363:GLN:HG3	2.01	0.43
1:A:785:PRO:O	2:B:702:LEU:HD12	2.18	0.43
1:A:1189:SER:HB2	1:A:1256:GLU:OE1	2.18	0.43
1:A:69:THR:HG22	2:B:1174:LYS:HD3	2.01	0.43
7:G:1:MET:HE1	7:G:80:LYS:H	1.83	0.43
3:C:22:LEU:HD22	3:C:230:MET:HE2	1.99	0.43
3:C:99:LEU:CD2	3:C:99:LEU:N	2.74	0.43
1:A:889:SER:HA	1:A:1297:GLU:N	2.33	0.43
3:C:184:ASN:ND2	3:C:189:THR:HB	2.34	0.43
11:K:12:LEU:HD12	11:K:12:LEU:HA	1.88	0.43
1:A:1450:LEU:CD1	6:F:108:PHE:CZ	3.02	0.43
11:K:41:THR:HG22	11:K:42:LEU:N	2.33	0.43
2:B:308:TRP:CZ3	9:I:45:ARG:HG2	2.54	0.43
3:C:41:ILE:HA	3:C:42:PRO:HD3	1.90	0.43
2:B:460:ALA:O	2:B:462:ALA:N	2.52	0.43
2:B:376:PHE:CE1	2:B:569:TYR:HB3	2.53	0.43
5:E:112:TYR:C	5:E:112:TYR:HD1	2.21	0.43
4:D:138:ASN:O	4:D:142:LYS:HG2	2.19	0.43
4:D:173:HIS:CG	4:D:174:PRO:HD2	2.54	0.43
7:G:49:LEU:HD21	7:G:77:VAL:HG23	2.00	0.43
4:D:118:THR:O	4:D:119:ARG:C	2.57	0.43
1:A:919:ILE:CG1	1:A:925:LEU:HD12	2.49	0.43
4:D:12:ARG:HH12	4:D:14:ARG:HA	1.81	0.43
1:A:151:ASP:HA	1:A:162:VAL:O	2.19	0.43
1:A:1115:SER:OG	1:A:1116:LEU:N	2.51	0.43
2:B:479:VAL:O	2:B:480:SER:HB3	2.17	0.43
11:K:79:GLU:HG3	11:K:80:GLY:H	1.83	0.43
2:B:1224:PHE:CE1	5:E:171:LYS:HG3	2.54	0.43
1:A:1110:ASN:ND2	1:A:1110:ASN:N	2.66	0.43
5:E:24:LYS:HB2	5:E:24:LYS:HE3	1.88	0.43
3:C:24:ASN:O	3:C:24:ASN:CG	2.55	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:423:ASP:OD1	1:A:424:ILE:N	2.52	0.43
8:H:42:ILE:O	8:H:44:VAL:HG23	2.18	0.42
8:H:94:ASP:N	8:H:94:ASP:OD1	2.51	0.42
1:A:504:LEU:HD21	6:F:88:TYR:HD2	1.83	0.42
1:A:71:GLN:O	1:A:73:GLY:N	2.45	0.42
3:C:167:HIS:CA	11:K:6:ARG:HH12	2.32	0.42
2:B:576:ASP:HB3	2:B:622:LYS:NZ	2.34	0.42
3:C:235:VAL:HG21	10:J:6:ARG:HH22	1.83	0.42
2:B:822:ASN:HD22	10:J:52:THR:HG21	1.83	0.42
5:E:135:PHE:CD2	5:E:140:LEU:HD21	2.52	0.42
1:A:1035:TYR:N	1:A:1035:TYR:CD2	2.85	0.42
3:C:214:ASN:O	3:C:217:ASP:OD2	2.36	0.42
1:A:78:PRO:CB	2:B:1201:LYS:HE3	2.49	0.42
1:A:114:LEU:HB2	1:A:142:CYS:HB2	2.01	0.42
4:D:51:ASN:O	4:D:52:LEU:C	2.55	0.42
9:I:82:GLU:HB3	9:I:104:LEU:CD1	2.49	0.42
1:A:1153:TYR:HA	9:I:41:PRO:O	2.19	0.42
2:B:604:ARG:NH2	2:B:613:VAL:O	2.41	0.42
10:J:64:ASN:CB	10:J:65:PRO:CD	2.78	0.42
1:A:67:CYS:O	1:A:68:GLN:HG3	2.19	0.42
1:A:690:VAL:CG2	1:A:718:VAL:HG13	2.48	0.42
3:C:101:LEU:CD1	3:C:118:LEU:HD23	2.47	0.42
1:A:463:ILE:HD11	1:A:469:ARG:HG3	2.01	0.42
1:A:754:SER:O	1:A:757:ASN:HB2	2.19	0.42
1:A:636:GLU:OE2	1:A:962:ARG:NH1	2.52	0.42
2:B:1207:LEU:HD23	2:B:1207:LEU:HA	1.73	0.42
2:B:405:ARG:CD	2:B:631:GLY:O	2.67	0.42
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.34	0.42
10:J:14:VAL:CG1	10:J:14:VAL:O	2.66	0.42
1:A:353:ILE:HG21	1:A:487:MET:HE3	2.01	0.42
1:A:1152:ILE:HG23	1:A:1260:LEU:CD2	2.49	0.42
1:A:482:PHE:CB	2:B:838:SER:OG	2.66	0.42
1:A:583:PRO:HG2	1:A:586:ILE:HG13	2.01	0.42
1:A:26:GLU:O	1:A:27:VAL:C	2.57	0.42
1:A:849:MET:CE	1:A:1061:GLY:HA2	2.49	0.42
2:B:785:TYR:CD1	2:B:786:ASN:N	2.87	0.42
2:B:522:VAL:CG1	2:B:537:LYS:HB3	2.50	0.42
2:B:522:VAL:HG11	2:B:537:LYS:HB3	2.01	0.42
11:K:27:ALA:HB1	11:K:28:PRO:HD2	2.02	0.42
1:A:874:ASP:N	1:A:1058:VAL:HG23	2.34	0.42
2:B:636:PRO:O	2:B:636:PRO:HG2	2.20	0.42
1:A:264:PHE:CB	1:A:265:LYS:HZ1	2.31	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:843:GLN:HA	2:B:846:ILE:HD12	1.99	0.42
7:G:125:SER:O	7:G:126:ASN:HB2	2.20	0.42
3:C:97:VAL:CG1	3:C:99:LEU:HD21	2.48	0.42
2:B:233:PRO:HD3	14:T:11:DA:OP1	2.18	0.42
1:A:806:ARG:HH12	2:B:729:ILE:CD1	2.33	0.42
7:G:21:ARG:HH11	7:G:24:GLN:HB2	1.81	0.42
2:B:473:MET:C	2:B:475:SER:H	2.23	0.42
3:C:183:TRP:CZ2	3:C:212:PRO:HG3	2.54	0.42
1:A:829:VAL:O	1:A:830:LYS:C	2.57	0.42
1:A:443:LEU:CD1	2:B:1146:PHE:CE2	3.01	0.42
11:K:63:VAL:O	11:K:63:VAL:CG2	2.66	0.42
7:G:101:VAL:CG1	7:G:102:GLN:N	2.83	0.42
2:B:370:PHE:HD2	2:B:373:ARG:HD2	1.83	0.42
2:B:1220:ARG:NH1	2:B:1220:ARG:HB3	2.34	0.42
8:H:59:ILE:CG2	8:H:60:ALA:N	2.70	0.42
8:H:89:LEU:CD1	8:H:91:ASP:OD1	2.68	0.42
1:A:1191:TRP:CD1	1:A:1256:GLU:HB2	2.54	0.42
1:A:722:LEU:HB3	1:A:799:PHE:CD1	2.54	0.42
3:C:66:ARG:HH21	10:J:5:VAL:HG23	1.85	0.42
2:B:172:ILE:HD13	2:B:178:ASN:ND2	2.24	0.42
1:A:1332:PHE:N	1:A:1332:PHE:CD2	2.86	0.42
10:J:34:THR:O	10:J:35:ALA:C	2.57	0.42
10:J:46:CYS:O	10:J:49:MET:HB3	2.20	0.42
2:B:412:LEU:HD21	2:B:479:VAL:HG11	2.02	0.42
1:A:1081:LEU:CD1	1:A:1097:GLY:HA3	2.49	0.42
4:D:8:PHE:HZ	4:D:37:GLN:CD	2.23	0.42
2:B:788:ARG:O	2:B:967:ARG:NH1	2.53	0.42
2:B:1079:LYS:HA	3:C:27:LEU:HD21	2.01	0.42
1:A:1001:ARG:O	1:A:1002:GLY:C	2.57	0.42
1:A:116:ASP:C	1:A:118:HIS:N	2.71	0.42
5:E:5:ASN:ND2	5:E:5:ASN:O	2.52	0.42
2:B:700:SER:O	2:B:701:ILE:HG22	2.20	0.42
2:B:244:LEU:CD2	2:B:366:GLN:NE2	2.82	0.42
6:F:88:TYR:O	6:F:89:GLU:C	2.58	0.42
4:D:138:ASN:C	4:D:140:ASP:H	2.23	0.42
4:D:213:GLU:O	4:D:217:LEU:HG	2.18	0.42
1:A:674:PRO:HG2	1:A:675:THR:H	1.84	0.42
1:A:548:ASN:O	1:A:549:MET:C	2.57	0.42
1:A:1263:ILE:O	1:A:1263:ILE:HG22	2.19	0.42
2:B:530:GLY:O	2:B:531:GLN:C	2.57	0.42
1:A:1385:THR:CG2	1:A:1386:ARG:H	2.29	0.42
12:L:61:THR:CG2	12:L:62:LYS:N	2.82	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:384:ARG:HB3	2:B:384:ARG:HE	1.34	0.42
2:B:431:TYR:CG	2:B:447:ALA:CB	3.02	0.42
5:E:13:TRP:CZ3	5:E:39:LEU:HB2	2.54	0.42
1:A:364:VAL:O	1:A:364:VAL:HG13	2.17	0.42
1:A:517:ASN:ND2	1:A:1364:ASN:HD22	2.16	0.42
2:B:600:LEU:HD13	2:B:626:ILE:HD11	2.02	0.42
2:B:604:ARG:HG3	2:B:611:PRO:HA	2.01	0.42
2:B:345:LYS:HA	2:B:348:ARG:NE	2.33	0.42
2:B:244:LEU:CD1	2:B:366:GLN:HE22	2.32	0.42
1:A:66:LYS:HD3	1:A:67:CYS:H	1.84	0.42
4:D:138:ASN:O	4:D:140:ASP:N	2.52	0.42
2:B:1065:GLN:CD	2:B:1066:SER:N	2.73	0.42
5:E:22:MET:HG3	5:E:187:TYR:CD1	2.55	0.42
1:A:774:ARG:CZ	1:A:797:LYS:CB	2.98	0.42
1:A:816:HIS:HE2	2:B:764:SER:H	1.68	0.42
2:B:831:SER:HB2	2:B:833:TYR:CD1	2.54	0.42
2:B:1202:LEU:HD22	2:B:1206:GLU:OE2	2.19	0.42
9:I:93:LYS:H	9:I:93:LYS:CD	2.12	0.42
1:A:889:SER:OG	1:A:891:ALA:HB3	2.20	0.42
3:C:46:ILE:HG13	3:C:72:LEU:HD11	2.02	0.42
2:B:51:PHE:CD2	2:B:173:MET:HB3	2.55	0.42
1:A:283:GLY:O	1:A:285:PRO:CD	2.67	0.42
3:C:11:ARG:NH2	3:C:206:ASN:OD1	2.52	0.42
3:C:204:SER:C	3:C:206:ASN:H	2.23	0.42
1:A:993:LEU:CD2	1:A:1022:LEU:HD21	2.49	0.42
1:A:555:ASP:O	1:A:556:TRP:O	2.36	0.42
1:A:639:PRO:CD	1:A:640:GLN:H	2.32	0.42
5:E:89:GLY:C	5:E:91:LYS:N	2.72	0.42
6:F:132:LEU:HD23	6:F:132:LEU:HA	1.82	0.42
2:B:597:MET:CE	2:B:624:LEU:HD21	2.49	0.42
8:H:39:THR:O	8:H:123:MET:HG3	2.19	0.42
6:F:133:VAL:HG13	6:F:146:TRP:O	2.19	0.42
2:B:995:ARG:CB	2:B:997:GLU:OE2	2.67	0.42
1:A:385:ILE:CG2	1:A:386:ASP:N	2.82	0.42
7:G:35:GLU:HG2	7:G:48:VAL:HG23	2.02	0.42
9:I:99:LEU:C	9:I:100:PHE:HD1	2.23	0.42
11:K:47:ARG:O	11:K:47:ARG:HD2	2.19	0.42
2:B:1082:MET:HA	3:C:189:THR:HA	2.02	0.42
2:B:386:LEU:O	2:B:387:LEU:C	2.55	0.42
2:B:889:THR:CG2	2:B:891:ASP:HB2	2.50	0.42
2:B:56:ASP:CB	2:B:57:TYR:HD1	2.32	0.42
2:B:123:THR:HA	2:B:204:ILE:O	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:130:ASP:O	1:A:131:SER:C	2.58	0.42
2:B:1050:ILE:CG2	2:B:1051:THR:N	2.82	0.42
1:A:626:ASN:O	1:A:631:HIS:HD2	2.02	0.42
2:B:526:GLU:OE1	2:B:752:ALA:HB3	2.20	0.42
1:A:1371:LEU:HD12	1:A:1375:MET:HG3	2.00	0.42
3:C:136:ASP:CB	3:C:141:GLY:H	2.33	0.42
2:B:637:LEU:HA	2:B:637:LEU:HD23	1.80	0.42
8:H:27:GLU:HG2	8:H:38:LEU:O	2.20	0.42
1:A:244:PRO:CB	1:A:245:PRO:HD3	2.31	0.42
1:A:719:VAL:O	1:A:721:PHE:N	2.53	0.42
1:A:1339:LEU:HD13	5:E:147:HIS:CG	2.55	0.42
3:C:44:LEU:HD13	3:C:129:ILE:HG23	2.01	0.42
12:L:34:CYS:O	12:L:35:SER:C	2.58	0.42
12:L:34:CYS:CB	12:L:51:CYS:HG	2.32	0.42
8:H:83:GLN:CD	8:H:87:ARG:NH2	2.73	0.42
5:E:180:ARG:HH21	5:E:192:ARG:HB2	1.85	0.42
5:E:61:GLN:HB2	5:E:79:TRP:HE3	1.85	0.42
5:E:78:LEU:HB2	5:E:107:THR:HG21	2.02	0.42
2:B:100:PRO:HG2	2:B:124:TYR:CE1	2.55	0.42
1:A:219:PHE:O	1:A:222:LEU:N	2.51	0.42
2:B:992:ILE:HD11	11:K:66:PRO:HB2	2.00	0.42
1:A:709:THR:CG2	1:A:710:LEU:N	2.80	0.42
2:B:1182:CYS:C	2:B:1183:LYS:HE3	2.40	0.42
2:B:44:VAL:HG11	2:B:495:LEU:HD13	2.02	0.42
5:E:167:ARG:HD3	5:E:167:ARG:HA	1.78	0.42
11:K:78:THR:HG22	11:K:79:GLU:N	2.35	0.42
6:F:97:ARG:NH2	6:F:108:PHE:HE1	2.17	0.42
2:B:558:LEU:HD11	2:B:596:LEU:CD2	2.48	0.42
9:I:25:LEU:HG	9:I:38:ALA:HB2	2.02	0.42
7:G:53:ASN:HD22	7:G:53:ASN:N	2.15	0.42
1:A:758:ILE:H	1:A:758:ILE:HG13	1.72	0.42
2:B:597:MET:HE2	2:B:597:MET:HA	2.01	0.42
2:B:638:PHE:CD2	2:B:690:VAL:HG22	2.54	0.42
2:B:973:ILE:HG23	2:B:974:PRO:HD2	2.02	0.42
2:B:885:MET:HG2	2:B:936:ASP:HB2	2.02	0.42
1:A:692:ASP:O	1:A:695:LYS:N	2.53	0.42
4:D:155:ARG:HB3	4:D:155:ARG:NH1	2.34	0.42
3:C:248:ILE:CD1	11:K:101:LEU:HD22	2.49	0.42
1:A:913:LEU:CD1	1:A:914:GLU:N	2.78	0.42
2:B:859:TYR:CD1	2:B:859:TYR:N	2.88	0.42
8:H:138:GLU:OE1	8:H:138:GLU:C	2.58	0.42
1:A:903:ASN:ND2	1:A:903:ASN:C	2.73	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:124:VAL:H	5:E:125:PRO:HD2	1.82	0.42
1:A:1297:GLU:OE1	1:A:1297:GLU:N	2.53	0.42
1:A:683:ILE:HG21	1:A:801:GLU:CD	2.40	0.42
4:D:71:LYS:C	4:D:74:GLN:H	2.23	0.42
1:A:1225:PHE:CE2	1:A:1227:ILE:HD11	2.55	0.42
10:J:32:GLU:O	10:J:33:GLY:C	2.57	0.42
1:A:870:GLU:CB	5:E:204:THR:HG21	2.49	0.42
1:A:845:LEU:O	1:A:846:GLU:C	2.58	0.42
7:G:132:SER:HB3	7:G:135:ASP:N	2.32	0.42
2:B:39:ARG:NH2	2:B:665:GLU:CD	2.73	0.42
2:B:779:GLY:O	2:B:795:ILE:HA	2.20	0.42
4:D:8:PHE:HZ	4:D:37:GLN:NE2	2.17	0.42
1:A:923:LEU:HD23	1:A:923:LEU:HA	1.88	0.42
2:B:580:VAL:CG2	2:B:624:LEU:HB3	2.49	0.42
1:A:850:VAL:HG21	1:A:1058:VAL:HG11	2.01	0.42
8:H:3:ASN:CG	8:H:4:THR:H	2.24	0.42
2:B:365:THR:O	2:B:365:THR:HG23	2.20	0.42
8:H:40:LEU:HD22	8:H:123:MET:CE	2.50	0.42
8:H:12:VAL:HB	8:H:52:GLN:N	2.34	0.42
1:A:65:LEU:O	1:A:66:LYS:O	2.38	0.42
1:A:10:PRO:HG2	2:B:1192:TYR:HD2	1.85	0.42
3:C:38:ILE:H	3:C:38:ILE:HG13	1.61	0.42
3:C:22:LEU:HB2	3:C:230:MET:CE	2.50	0.42
4:D:16:LYS:O	4:D:18:VAL:N	2.50	0.42
5:E:22:MET:O	5:E:26:ARG:HG2	2.20	0.42
2:B:642:ASP:N	2:B:649:LYS:HG3	2.35	0.42
2:B:644:GLU:C	2:B:646:LEU:N	2.73	0.42
1:A:148:CYS:HB3	1:A:167:CYS:O	2.19	0.42
1:A:547:LEU:HD21	1:A:560:ILE:CD1	2.50	0.42
2:B:1124:ARG:NH2	15:P:2:A:OP2	2.52	0.42
11:K:53:ASP:HB3	11:K:56:VAL:CG2	2.50	0.42
1:A:442:VAL:HB	1:A:489:LEU:HD11	2.01	0.42
1:A:700:ASN:C	1:A:701:LEU:HD23	2.40	0.42
2:B:512:ARG:HG2	2:B:512:ARG:HH11	1.83	0.42
2:B:594:ALA:HA	2:B:617:ARG:NH1	2.35	0.41
8:H:9:ILE:HA	8:H:55:LEU:O	2.20	0.41
2:B:377:PHE:C	2:B:379:GLY:N	2.72	0.41
1:A:1189:SER:OG	1:A:1191:TRP:HB2	2.20	0.41
2:B:865:LYS:HD3	2:B:866:TYR:H	1.85	0.41
1:A:718:VAL:HG12	1:A:722:LEU:CD1	2.50	0.41
4:D:218:GLU:O	4:D:219:THR:C	2.58	0.41
4:D:124:GLU:N	4:D:124:GLU:CD	2.71	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:19:VAL:HG22	5:E:140:LEU:HD12	2.00	0.41
8:H:110:ASP:O	8:H:128:ASN:OD1	2.38	0.41
1:A:884:ASP:OD2	1:A:1030:ARG:NH2	2.53	0.41
10:J:47:ARG:NH1	10:J:47:ARG:HG2	2.34	0.41
3:C:215:GLU:O	3:C:216:GLY:C	2.57	0.41
2:B:44:VAL:O	2:B:45:SER:C	2.59	0.41
1:A:740:LEU:HD12	1:A:740:LEU:C	2.41	0.41
1:A:1451:VAL:C	1:A:1453:TYR:N	2.73	0.41
4:D:27:LEU:CD1	4:D:197:SER:HB3	2.50	0.41
1:A:1025:ARG:HG3	1:A:1025:ARG:NH1	2.33	0.41
2:B:557:PHE:HE1	2:B:603:LEU:HD11	1.84	0.41
3:C:113:VAL:HG23	3:C:147:LEU:HD21	2.01	0.41
5:E:56:LYS:HZ1	5:E:85:GLU:HG3	1.82	0.41
7:G:122:ASN:HB2	7:G:131:GLN:NE2	2.35	0.41
3:C:69:LEU:O	10:J:6:ARG:HD2	2.20	0.41
3:C:22:LEU:HD22	3:C:230:MET:HE1	2.01	0.41
1:A:821:ARG:CB	1:A:821:ARG:HH11	2.27	0.41
1:A:150:THR:O	1:A:150:THR:HG22	2.20	0.41
1:A:1102:LYS:O	1:A:1106:ASN:ND2	2.53	0.41
3:C:88:CYS:SG	3:C:91:HIS:HA	2.61	0.41
1:A:877:HIS:C	1:A:878:ILE:HG13	2.40	0.41
1:A:41:MET:O	1:A:42:ASP:O	2.38	0.41
2:B:850:LEU:HD12	2:B:850:LEU:C	2.39	0.41
1:A:253:ASN:HB3	1:A:254:GLU:H	1.70	0.41
1:A:1127:ASP:O	1:A:1128:GLN:C	2.58	0.41
1:A:1314:SER:C	1:A:1315:GLU:HG2	2.41	0.41
4:D:7:THR:HG21	4:D:32:GLU:OE2	2.20	0.41
1:A:77:CYS:C	1:A:78:PRO:O	2.58	0.41
1:A:1037:LEU:HD11	1:A:1045:VAL:HG21	2.00	0.41
11:K:79:GLU:O	11:K:81:TYR:N	2.54	0.41
4:D:50:LEU:HD21	7:G:4:ILE:CD1	2.49	0.41
1:A:347:PHE:HE2	1:A:375:THR:CG2	2.32	0.41
2:B:570:VAL:HA	2:B:571:PRO:HD2	1.82	0.41
1:A:150:THR:HA	1:A:165:GLY:O	2.20	0.41
2:B:430:ARG:HG2	2:B:430:ARG:HH11	1.84	0.41
1:A:481:ASP:O	1:A:485:ASP:HB2	2.21	0.41
5:E:7:ARG:HG3	5:E:8:ASN:N	2.35	0.41
1:A:260:ASP:OD1	1:A:261:ASP:N	2.53	0.41
1:A:553:VAL:HA	1:A:554:PRO:HD2	1.90	0.41
1:A:54:ASN:HB3	1:A:247:ARG:NH2	2.33	0.41
7:G:26:LEU:O	7:G:28:THR:N	2.52	0.41
4:D:29:LEU:H	4:D:29:LEU:CD2	2.33	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:G:126:ASN:HA	7:G:127:PRO:HA	1.95	0.41
3:C:234:SER:OG	3:C:235:VAL:N	2.54	0.41
4:D:118:THR:HB	4:D:121:LYS:HB3	2.00	0.41
3:C:44:LEU:CD2	3:C:159:ALA:HB1	2.50	0.41
6:F:105:ALA:HB1	6:F:106:PRO:CD	2.50	0.41
2:B:766:ARG:NH1	2:B:769:TYR:CD1	2.87	0.41
2:B:114:PRO:HG2	2:B:115:GLN:N	2.30	0.41
1:A:332:LYS:HB3	1:A:337:ARG:CZ	2.50	0.41
1:A:697:ALA:CB	1:A:702:LEU:HD12	2.41	0.41
10:J:34:THR:O	10:J:37:SER:N	2.54	0.41
10:J:36:LEU:HD12	10:J:47:ARG:NH1	2.35	0.41
5:E:195:VAL:HG22	5:E:213:ILE:HG13	2.01	0.41
11:K:68:PHE:CD1	11:K:70:ARG:NH1	2.81	0.41
1:A:348:SER:HA	1:A:489:LEU:O	2.21	0.41
1:A:855:THR:HG21	1:A:857:ARG:HE	1.85	0.41
2:B:615:MET:C	2:B:616:ILE:HD12	2.41	0.41
8:H:38:LEU:HD12	8:H:38:LEU:HA	1.84	0.41
1:A:382:PRO:N	1:A:428:TYR:CE2	2.89	0.41
1:A:382:PRO:CD	1:A:428:TYR:CE2	3.04	0.41
2:B:877:PRO:O	2:B:878:GLN:HB3	2.20	0.41
2:B:936:ASP:CG	2:B:937:ALA:N	2.74	0.41
2:B:1002:THR:OG1	2:B:1006:ILE:CG1	2.66	0.41
6:F:106:PRO:HG2	7:G:18:PHE:C	2.41	0.41
4:D:124:GLU:HA	4:D:127:ASP:HB2	2.01	0.41
1:A:767:GLN:NE2	1:A:768:GLN:O	2.53	0.41
1:A:774:ARG:CZ	1:A:797:LYS:HG3	2.51	0.41
8:H:84:ALA:O	8:H:86:ASP:N	2.53	0.41
9:I:78:CYS:O	9:I:80:SER:N	2.53	0.41
11:K:47:ARG:NH1	11:K:47:ARG:HB3	2.23	0.41
10:J:37:SER:OG	10:J:47:ARG:NH2	2.53	0.41
12:L:27:LEU:N	12:L:27:LEU:HD23	2.36	0.41
2:B:313:MET:CE	2:B:386:LEU:HB3	2.50	0.41
1:A:830:LYS:HG3	1:A:1098:VAL:HG21	2.02	0.41
9:I:60:GLN:OE1	9:I:107:SER:OG	2.35	0.41
1:A:557:ASP:O	1:A:559:VAL:HG23	2.20	0.41
2:B:1175:LEU:O	2:B:1176:ASN:CB	2.66	0.41
1:A:255:SER:OG	2:B:918:ILE:HD13	2.20	0.41
9:I:62:ILE:HD11	9:I:86:PHE:HE2	1.86	0.41
4:D:153:ARG:C	4:D:154:PHE:HD2	2.24	0.41
3:C:124:LEU:C	3:C:126:GLY:N	2.74	0.41
3:C:73:GLN:CB	3:C:131:HIS:H	2.34	0.41
1:A:665:GLY:O	1:A:666:ILE:C	2.59	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:113:TYR:CE2	2:B:192:LEU:CD2	3.03	0.41
8:H:83:GLN:O	8:H:85:GLY:N	2.54	0.41
2:B:94:LYS:HZ3	2:B:96:TYR:HE2	1.66	0.41
2:B:63:ILE:HG12	2:B:130:VAL:HG21	2.03	0.41
1:A:392:VAL:HG13	1:A:415:LEU:HD11	2.03	0.41
2:B:515:HIS:O	2:B:518:HIS:HB2	2.20	0.41
1:A:425:GLN:HG2	1:A:425:GLN:O	2.20	0.41
3:C:258:ILE:N	3:C:258:ILE:CD1	2.83	0.41
9:I:46:HIS:CE1	9:I:48:LEU:CD2	3.03	0.41
1:A:1147:THR:O	9:I:48:LEU:HD12	2.20	0.41
9:I:73:ARG:NH1	9:I:101:PHE:CZ	2.89	0.41
1:A:1454:MET:HA	1:A:1455:PRO:HD2	1.94	0.41
2:B:54:PHE:CZ	2:B:59:LEU:HD13	2.56	0.41
4:D:170:THR:HB	4:D:172:LEU:HG	2.02	0.41
1:A:516:SER:O	1:A:517:ASN:C	2.59	0.41
3:C:138:GLU:HB2	3:C:140:ASN:HD21	1.86	0.41
2:B:361:LEU:N	2:B:362:PRO:CD	2.84	0.41
2:B:618:ASP:O	2:B:622:LYS:N	2.53	0.41
4:D:154:PHE:HE1	4:D:163:VAL:HG11	1.85	0.41
4:D:156:ASP:HB2	4:D:159:THR:HG1	1.84	0.41
2:B:1002:THR:O	2:B:1003:ALA:C	2.59	0.41
2:B:1003:ALA:O	3:C:177:GLU:HA	2.21	0.41
1:A:219:PHE:HB2	1:A:220:THR:H	1.46	0.41
1:A:593:GLU:HB3	1:A:594:GLY:H	1.48	0.41
4:D:198:LEU:O	4:D:200:ASN:N	2.54	0.41
11:K:85:ASP:O	11:K:88:LYS:N	2.54	0.41
1:A:820:GLY:O	1:A:823:GLY:N	2.54	0.41
11:K:51:LEU:CD1	11:K:59:ALA:HB3	2.51	0.41
2:B:1001:PHE:CD1	2:B:1001:PHE:C	2.94	0.41
1:A:946:VAL:HG12	1:A:947:PHE:CE2	2.56	0.41
9:I:45:ARG:HG3	9:I:46:HIS:N	2.36	0.41
1:A:396:PRO:HB3	1:A:403:LYS:HA	2.02	0.41
7:G:104:GLY:HA3	7:G:105:PRO:HD2	1.93	0.41
9:I:16:PRO:HB3	9:I:27:PHE:CE2	2.56	0.41
2:B:707:PRO:CG	2:B:708:GLU:N	2.75	0.41
9:I:54:GLU:HB3	9:I:100:PHE:HE2	1.85	0.41
10:J:2:ILE:C	10:J:53:HIS:CE1	2.94	0.41
4:D:150:ASN:HB3	7:G:142:ARG:NH2	2.36	0.41
4:D:24:ALA:C	4:D:26:THR:H	2.24	0.41
1:A:93:VAL:HG21	1:A:301:ALA:HA	2.01	0.41
1:A:451:HIS:O	1:A:452:LYS:C	2.58	0.41
2:B:976:ILE:CD1	2:B:992:ILE:HA	2.51	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:I:88:SER:C	9:I:90:GLN:N	2.74	0.41
5:E:45:LYS:HD3	5:E:46:TYR:CE1	2.56	0.41
5:E:175:LEU:HA	5:E:176:PRO:HD3	1.81	0.41
2:B:1084:GLN:OE1	3:C:189:THR:CG2	2.69	0.41
6:F:97:ARG:NE	6:F:124:GLU:OE1	2.54	0.41
1:A:800:VAL:HA	1:A:812:GLU:OE2	2.20	0.41
1:A:120:GLU:C	1:A:122:MET:N	2.73	0.41
1:A:473:SER:O	1:A:521:MET:HB3	2.21	0.41
1:A:1195:LEU:HD11	1:A:1267:MET:HE3	2.01	0.41
2:B:259:TYR:O	2:B:260:GLY:O	2.39	0.41
2:B:205:ILE:O	2:B:207:GLY:N	2.54	0.41
1:A:460:VAL:CG1	1:A:461:LYS:N	2.83	0.41
1:A:343:LYS:NZ	2:B:1151:LEU:HG	2.35	0.41
1:A:639:PRO:CG	1:A:640:GLN:N	2.83	0.41
1:A:1356:ILE:HD12	1:A:1368:MET:SD	2.60	0.41
1:A:1273:LEU:CD1	1:A:1273:LEU:N	2.84	0.41
6:F:152:ILE:HG22	6:F:153:VAL:N	2.35	0.41
2:B:593:PRO:HG2	2:B:617:ARG:CZ	2.50	0.41
1:A:298:PHE:CD2	1:A:299:HIS:HD2	2.38	0.41
1:A:40:THR:C	1:A:41:MET:HG3	2.41	0.41
4:D:66:ARG:NH2	7:G:31:LEU:HD11	2.35	0.41
2:B:918:ILE:HG21	2:B:935:ARG:HH22	1.83	0.41
1:A:690:VAL:HG11	1:A:794:PRO:HD3	2.03	0.41
9:I:54:GLU:OE1	9:I:118:ARG:NH2	2.53	0.41
10:J:57:ILE:HG23	10:J:58:GLU:N	2.35	0.41
3:C:133:ILE:CD1	3:C:237:SER:N	2.82	0.41
3:C:154:LYS:HE3	3:C:154:LYS:HB2	1.85	0.41
3:C:177:GLU:HB2	3:C:231:ASN:HB3	2.02	0.41
1:A:805:LEU:CD1	2:B:1052:VAL:HG21	2.51	0.41
11:K:31:VAL:CG1	11:K:32:VAL:N	2.81	0.41
2:B:789:MET:HE2	2:B:965:LYS:CB	2.51	0.41
1:A:1345:ARG:HG2	1:A:1372:VAL:CG1	2.49	0.41
1:A:575:LYS:HB3	1:A:612:ILE:HG21	2.01	0.41
6:F:116:ASP:HB3	6:F:119:ARG:HB2	2.02	0.41
2:B:25:ILE:HG21	2:B:658:ILE:CD1	2.49	0.41
2:B:912:ILE:O	2:B:938:SER:CB	2.67	0.41
2:B:913:GLY:HA2	2:B:938:SER:OG	2.20	0.41
8:H:128:ASN:C	8:H:128:ASN:HD22	2.23	0.41
2:B:326:ASP:OD1	2:B:329:THR:CB	2.68	0.41
2:B:467:GLY:N	2:B:475:SER:OG	2.54	0.41
1:A:820:GLY:O	1:A:821:ARG:C	2.58	0.41
2:B:1084:GLN:HE21	2:B:1084:GLN:H	1.67	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:401:PHE:HB2	2:B:517:THR:OG1	2.20	0.41
2:B:435:THR:HG22	2:B:437:GLU:C	2.41	0.41
1:A:1038:THR:H	1:A:1041:ALA:HB3	1.85	0.41
6:F:138:LEU:HA	6:F:138:LEU:HD23	1.84	0.41
2:B:1073:TYR:CE2	2:B:1080:LYS:HG3	2.56	0.41
1:A:479:ASN:HA	1:A:479:ASN:HD22	1.62	0.41
5:E:99:HIS:ND1	5:E:103:LYS:HG3	2.36	0.41
2:B:571:PRO:HG2	2:B:572:HIS:H	1.86	0.41
4:D:122:GLU:HA	4:D:125:SER:HB3	2.02	0.41
1:A:526:ASP:OD1	2:B:1013:ASN:ND2	2.52	0.41
2:B:969:ARG:HD2	3:C:61:GLU:OE2	2.21	0.41
1:A:1279:ILE:O	1:A:1279:ILE:HG22	2.21	0.41
1:A:559:VAL:O	1:A:561:PRO:HD3	2.20	0.41
7:G:145:VAL:HG12	7:G:146:LYS:N	2.36	0.41
7:G:44:TYR:OH	7:G:156:SER:HB2	2.20	0.41
9:I:15:TYR:CD1	9:I:30:ARG:HD2	2.56	0.41
1:A:542:GLU:HG2	1:A:542:GLU:H	1.63	0.41
2:B:333:PHE:O	2:B:334:ILE:HG13	2.20	0.41
7:G:59:GLY:CA	7:G:70:PHE:CD2	3.04	0.41
1:A:64:ASN:O	1:A:66:LYS:N	2.54	0.41
7:G:1:MET:CE	7:G:80:LYS:O	2.69	0.41
1:A:722:LEU:HD23	1:A:799:PHE:CG	2.56	0.41
2:B:798:TYR:CE2	3:C:62:PHE:CZ	3.07	0.41
2:B:251:ILE:O	2:B:251:ILE:CG2	2.67	0.41
3:C:22:LEU:HD11	11:K:101:LEU:HD11	2.03	0.41
1:A:1116:LEU:HG	1:A:1308:THR:HB	2.03	0.41
8:H:130:ARG:N	8:H:130:ARG:CD	2.80	0.41
1:A:1138:ILE:HG13	1:A:1139:GLU:N	2.36	0.41
1:A:650:GLN:HB3	1:A:654:ASN:ND2	2.36	0.41
2:B:1032:SER:HB3	2:B:1089:PRO:HG2	2.03	0.41
12:L:49:LYS:O	12:L:50:ASP:CB	2.58	0.41
2:B:186:GLU:OE2	2:B:186:GLU:HA	2.21	0.41
5:E:164:LEU:HD22	5:E:211:TYR:HD2	1.77	0.41
2:B:205:ILE:HG12	2:B:461:LEU:HB3	2.03	0.41
1:A:1053:PHE:O	1:A:1056:SER:N	2.54	0.41
1:A:996:ASN:O	1:A:998:LEU:N	2.49	0.41
1:A:371:ALA:HB2	1:A:462:VAL:HG13	2.03	0.41
7:G:61:ILE:HG22	7:G:62:LEU:O	2.21	0.41
2:B:806:THR:HG21	2:B:808:ALA:HB3	2.03	0.40
8:H:8:ASP:OD1	8:H:30:SER:OG	2.31	0.40
2:B:333:PHE:O	2:B:334:ILE:CG1	2.69	0.40
3:C:239:PRO:O	3:C:240:VAL:C	2.59	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:1026:LEU:HA	2:B:1026:LEU:HD23	1.86	0.40
4:D:53:SER:HA	4:D:56:ARG:CB	2.51	0.40
5:E:98:ILE:HG22	5:E:102:GLU:HG3	2.03	0.40
1:A:683:ILE:HG21	1:A:801:GLU:OE1	2.21	0.40
12:L:38:LEU:CG	12:L:39:SER:N	2.83	0.40
2:B:390:LEU:O	2:B:391:ASP:C	2.59	0.40
5:E:29:PHE:HD1	5:E:30:ILE:N	2.19	0.40
1:A:152:VAL:HG12	1:A:153:PRO:CD	2.51	0.40
1:A:347:PHE:CE2	2:B:1107:ALA:HB1	2.56	0.40
4:D:134:THR:CG2	4:D:135:GLY:N	2.84	0.40
5:E:11:ARG:C	5:E:13:TRP:N	2.74	0.40
1:A:909:ASP:OD1	1:A:911:SER:N	2.46	0.40
1:A:786:HIS:HE1	2:B:519:TRP:CZ2	2.39	0.40
2:B:276:ILE:HG22	2:B:336:ARG:HB2	2.02	0.40
1:A:34:LYS:CB	1:A:36:ARG:NH2	2.85	0.40
2:B:854:LEU:HD23	2:B:854:LEU:HA	1.91	0.40
10:J:53:HIS:HD2	10:J:54:VAL:H	1.58	0.40
4:D:154:PHE:HA	4:D:219:THR:HB	2.02	0.40
3:C:44:LEU:HD23	3:C:44:LEU:C	2.42	0.40
1:A:546:VAL:HG21	1:A:572:TRP:HB2	2.03	0.40
2:B:769:TYR:HA	15:P:11:G:H22	1.87	0.40
12:L:44:ASP:O	12:L:45:ALA:HB3	2.21	0.40
2:B:955:THR:HG23	12:L:54:ARG:O	2.21	0.40
6:F:84:TYR:N	6:F:84:TYR:CD1	2.90	0.40
1:A:598:LEU:HA	8:H:122:LEU:CD1	2.48	0.40
1:A:897:TYR:CD1	1:A:897:TYR:N	2.89	0.40
9:I:8:ARG:O	9:I:9:ASP:HB2	2.21	0.40
2:B:473:MET:HE3	2:B:474:SER:N	2.37	0.40
3:C:3:GLU:HB3	11:K:104:ASN:OD1	2.21	0.40
4:D:190:GLU:O	4:D:193:THR:CG2	2.67	0.40
2:B:186:GLU:HB3	2:B:187:SER:H	1.71	0.40
11:K:49:GLU:C	11:K:51:LEU:N	2.75	0.40
2:B:1031:LEU:HB2	2:B:1055:ILE:HD13	2.03	0.40
1:A:857:ARG:NH1	6:F:139:PRO:CB	2.84	0.40
1:A:101:LYS:HA	1:A:104:GLU:OE1	2.22	0.40
1:A:752:LYS:HD3	1:A:752:LYS:HA	1.77	0.40
7:G:62:LEU:HD13	7:G:62:LEU:HA	1.89	0.40
2:B:104:GLU:OE2	12:L:47:ARG:NH2	2.55	0.40
1:A:589:GLN:HG3	1:A:606:LEU:HD13	2.04	0.40
2:B:224:GLN:HA	2:B:396:ASP:OD2	2.20	0.40
2:B:624:LEU:HA	2:B:624:LEU:HD12	1.57	0.40
8:H:43:ASN:C	8:H:45:GLU:H	2.24	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:47:ARG:CZ	1:A:254:GLU:HG2	2.51	0.40
1:A:665:GLY:HA2	2:B:1026:LEU:CD2	2.50	0.40
4:D:126:ILE:HD13	4:D:145:MET:CE	2.50	0.40
1:A:1170:ILE:CD1	1:A:1170:ILE:H	2.16	0.40
1:A:604:GLY:O	1:A:605:MET:HB2	2.21	0.40
1:A:1134:ILE:HG13	1:A:1134:ILE:H	1.66	0.40
9:I:5:ARG:CZ	9:I:36:GLU:OE1	2.69	0.40
2:B:687:GLU:O	2:B:688:GLY:C	2.59	0.40
1:A:1030:ARG:NH1	1:A:1035:TYR:OH	2.54	0.40
1:A:524:VAL:CG1	1:A:525:GLN:H	2.25	0.40
2:B:629:ASP:HB3	2:B:632:ARG:HE	1.86	0.40
2:B:282:ILE:HG21	2:B:382:ILE:CD1	2.51	0.40
1:A:1006:ILE:HD12	5:E:167:ARG:CG	2.50	0.40
1:A:984:LYS:HG2	1:A:988:LEU:HD12	2.02	0.40
6:F:109:VAL:CG2	6:F:124:GLU:HA	2.51	0.40
3:C:77:ILE:HG23	3:C:161:LYS:HE3	2.03	0.40
11:K:92:ASN:O	11:K:93:SER:C	2.60	0.40
2:B:1221:SER:C	2:B:1223:ASP:H	2.25	0.40
1:A:738:LYS:H	1:A:738:LYS:HD3	1.85	0.40
8:H:37:LYS:H	8:H:126:GLU:HB2	1.87	0.40
2:B:58:THR:HG22	2:B:62:ILE:HD11	2.02	0.40
2:B:969:ARG:HG2	2:B:970:THR:N	2.36	0.40
2:B:970:THR:CG2	2:B:971:THR:N	2.84	0.40
4:D:176:GLU:O	4:D:178:ALA:N	2.54	0.40
1:A:600:PRO:HG2	1:A:601:LYS:H	1.87	0.40
1:A:1333:ILE:H	1:A:1333:ILE:HG12	1.48	0.40
1:A:409:SER:O	1:A:410:GLY:C	2.59	0.40
2:B:345:LYS:CG	2:B:346:GLU:N	2.70	0.40
3:C:148:ARG:CG	3:C:149:LYS:H	2.34	0.40
1:A:276:LEU:HD13	1:A:293:GLU:HA	2.03	0.40
1:A:381:THR:C	1:A:383:TYR:N	2.73	0.40
4:D:173:HIS:O	4:D:177:VAL:HG23	2.21	0.40
7:G:80:LYS:O	7:G:82:PHE:CE1	2.75	0.40
2:B:871:THR:CG2	2:B:872:GLU:N	2.85	0.40
1:A:253:ASN:ND2	2:B:884:ARG:HD2	2.35	0.40
2:B:620:ARG:NH1	9:I:68:LEU:HD21	2.37	0.40
1:A:154:SER:C	1:A:156:ASP:H	2.25	0.40
1:A:135:PHE:HD1	1:A:222:LEU:HD22	1.79	0.40
1:A:588:LEU:HD23	1:A:607:ILE:HD12	2.02	0.40
2:B:129:PHE:HE2	2:B:166:PHE:CD1	2.38	0.40
2:B:327:ARG:HH22	2:B:371:GLU:HG2	1.79	0.40
4:D:187:THR:HB	4:D:190:GLU:H	1.86	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:185:THR:N	2:B:188:ASP:OD2	2.55	0.40
1:A:1120:LEU:HD12	1:A:1120:LEU:C	2.42	0.40
1:A:1104:ILE:O	1:A:1106:ASN:N	2.55	0.40
11:K:93:SER:O	11:K:97:LYS:HG3	2.21	0.40
2:B:231:PRO:HG2	2:B:231:PRO:O	2.21	0.40
1:A:1334:ASP:O	1:A:1336:MET:N	2.54	0.40
2:B:950:ASP:HB3	2:B:967:ARG:O	2.21	0.40
1:A:89:PRO:HG2	1:A:204:THR:HB	2.04	0.40
5:E:60:PHE:CD1	5:E:60:PHE:C	2.95	0.40
2:B:655:LYS:HA	2:B:655:LYS:HD2	1.90	0.40
2:B:273:LEU:HA	2:B:274:PRO:HD2	1.95	0.40
2:B:557:PHE:CZ	2:B:603:LEU:HG	2.56	0.40
8:H:12:VAL:HG11	8:H:15:VAL:HG22	2.03	0.40
2:B:796:LEU:HD12	2:B:852:ARG:O	2.21	0.40
2:B:878:GLN:HB2	2:B:879:ARG:HH11	1.87	0.40
3:C:238:ILE:CG2	3:C:242:GLN:HB2	2.50	0.40
1:A:208:LEU:C	1:A:208:LEU:CD2	2.90	0.40
2:B:1030:LEU:HD11	2:B:1059:LEU:HD22	2.04	0.40
2:B:773:MET:C	2:B:775:LYS:N	2.74	0.40
5:E:80:VAL:HG12	5:E:82:PHE:CE1	2.57	0.40
1:A:671:ALA:CB	1:A:676:MET:HG3	2.40	0.40
1:A:599:SER:HB2	1:A:603:ASN:H	1.87	0.40
2:B:515:HIS:CD2	2:B:517:THR:CG2	3.02	0.40
2:B:390:LEU:O	2:B:392:ARG:HG3	2.21	0.40
9:I:50:THR:H	9:I:92:ARG:HH12	1.69	0.40
1:A:249:SER:O	1:A:250:ILE:CG1	2.66	0.40
6:F:138:LEU:HB3	6:F:139:PRO:HD2	2.03	0.40
2:B:570:VAL:HB	2:B:573:GLN:HB3	2.02	0.40
2:B:286:PHE:HB3	2:B:297:ILE:HG12	2.02	0.40
1:A:856:THR:HG21	1:A:1370:LEU:HD21	2.04	0.40
2:B:1017:ILE:H	2:B:1018:PRO:HD2	1.87	0.40
8:H:118:PHE:O	8:H:119:GLY:C	2.60	0.40
1:A:699:ALA:O	1:A:700:ASN:HB3	2.22	0.40
2:B:825:VAL:HG21	2:B:1092:TYR:HE1	1.87	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	1408/1733 (81%)	1012 (72%)	262 (19%)	134 (10%)	1	20
2	B	1089/1224 (89%)	779 (72%)	201 (18%)	109 (10%)	1	17
3	C	264/347 (76%)	186 (70%)	51 (19%)	27 (10%)	1	17
4	D	175/221 (79%)	121 (69%)	39 (22%)	15 (9%)	1	23
5	E	212/215 (99%)	154 (73%)	42 (20%)	16 (8%)	2	28
6	F	85/155 (55%)	69 (81%)	14 (16%)	2 (2%)	9	62
7	G	169/171 (99%)	145 (86%)	13 (8%)	11 (6%)	2	33
8	H	132/146 (90%)	85 (64%)	23 (17%)	24 (18%)	0	4
9	I	117/122 (96%)	79 (68%)	29 (25%)	9 (8%)	1	26
10	J	63/70 (90%)	39 (62%)	11 (18%)	13 (21%)	0	3
11	K	113/120 (94%)	87 (77%)	22 (20%)	4 (4%)	6	53
12	L	44/70 (63%)	23 (52%)	9 (20%)	12 (27%)	0	1
All	All	3871/4594 (84%)	2779 (72%)	716 (18%)	376 (10%)	1	19

All (376) 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	54	ASN
1	A	57	ARG
1	A	58	LEU
1	A	62	ASP
1	A	63	ARG
1	A	67	CYS
1	A	70	CYS
1	A	128	ILE
1	A	130	ASP

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Mol	Chain	Res	Type
1	A	154	SER
1	A	167	CYS
1	A	250	ILE
1	A	286	HIS
1	A	311	GLN
1	A	312	PRO
1	A	332	LYS
1	A	399	HIS
1	A	423	ASP
1	A	567	LYS
1	A	666	ILE
1	A	1112	LYS
1	A	1114	PRO
1	A	1120	LEU
1	A	1124	HIS
1	A	1223	ASP
1	A	1233	ASP
1	A	1242	VAL
1	A	1255	GLU
1	A	1281	ARG
1	A	1314	SER
1	A	1405	THR
2	B	21	GLU
2	B	67	SER
2	B	68	THR
2	B	108	VAL
2	B	184	ALA
2	B	186	GLU
2	B	282	ILE
2	B	365	THR
2	B	367	LEU
2	B	435	THR
2	B	467	GLY
2	B	619	ILE
2	B	708	GLU
2	B	709	ASP
2	B	731	VAL
2	B	850	LEU
2	B	879	ARG
2	B	907	GLY
2	B	958	GLN
2	B	1041	GLU

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Mol	Chain	Res	Type
2	B	1046	PRO
2	B	1069	PHE
2	B	1097	HIS
2	B	1103	ILE
2	B	1108	ARG
2	B	1155	SER
2	B	1157	ALA
2	B	1181	GLU
2	B	1188	LYS
2	B	1222	ARG
3	C	56	THR
3	C	90	ASP
3	C	110	THR
3	C	125	MET
3	C	141	GLY
3	C	149	LYS
3	C	161	LYS
3	C	184	ASN
3	C	209	TYR
3	C	215	GLU
3	C	216	GLY
3	C	237	SER
4	D	5	THR
4	D	8	PHE
4	D	17	LYS
4	D	52	LEU
4	D	198	LEU
4	D	218	GLU
5	E	45	LYS
5	E	74	ASP
5	E	106	GLN
5	E	115	ASN
7	G	112	LYS
7	G	139	ILE
8	H	62	SER
8	H	77	ARG
8	H	82	PRO
8	H	108	SER
8	H	128	ASN
8	H	134	ASN
8	H	140	ALA
9	I	11	ASN

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Mol	Chain	Res	Type
9	I	79	HIS
10	J	2	ILE
10	J	28	ASP
10	J	42	LYS
10	J	55	ASP
10	J	64	ASN
12	L	50	ASP
12	L	53	HIS
12	L	59	ALA
12	L	60	ARG
1	A	5	GLN
1	A	76	GLU
1	A	93	VAL
1	A	126	LEU
1	A	249	SER
1	A	253	ASN
1	A	318	SER
1	A	400	PRO
1	A	410	GLY
1	A	424	ILE
1	A	556	TRP
1	A	576	GLN
1	A	591	PHE
1	A	592	ASP
1	A	597	LEU
1	A	628	GLY
1	A	718	VAL
1	A	821	ARG
1	A	846	GLU
1	A	852	TYR
1	A	884	ASP
1	A	885	THR
1	A	891	ALA
1	A	963	ILE
1	A	968	GLN
1	A	986	ILE
1	A	1002	GLY
1	A	1123	GLY
1	A	1127	ASP
1	A	1139	GLU
1	A	1187	GLN
1	A	1231	ASP

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Mol	Chain	Res	Type
1	A	1280	GLU
1	A	1309	ASP
1	A	1438	THR
2	B	58	THR
2	B	65	GLU
2	B	100	PRO
2	B	221	ASN
2	B	249	ARG
2	B	258	LEU
2	B	259	TYR
2	B	260	GLY
2	B	295	GLY
2	B	333	PHE
2	B	334	ILE
2	B	448	ILE
2	B	461	LEU
2	B	466	TRP
2	B	468	GLU
2	B	474	SER
2	B	501	PRO
2	B	575	PRO
2	B	591	ARG
2	B	642	ASP
2	B	643	ASP
2	B	655	LYS
2	B	746	SER
2	B	751	VAL
2	B	792	MET
2	B	869	SER
2	B	943	SER
2	B	1175	LEU
2	B	1176	ASN
2	B	1214	PRO
3	C	60	ASP
3	C	173	ALA
3	C	240	VAL
4	D	14	ARG
4	D	19	GLU
4	D	119	ARG
4	D	131	GLU
4	D	199	ASN
5	E	36	GLU

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Mol	Chain	Res	Type
5	E	130	ALA
5	E	158	SER
7	G	63	PRO
7	G	154	VAL
8	H	12	VAL
8	H	17	PRO
8	H	21	ASN
8	H	32	THR
8	H	51	ALA
8	H	59	ILE
8	H	84	ALA
8	H	90	ALA
8	H	92	ASP
8	H	95	TYR
8	H	107	VAL
9	I	54	GLU
9	I	57	GLY
9	I	106	CYS
10	J	6	ARG
10	J	17	LYS
10	J	33	GLY
10	J	62	ARG
11	K	53	ASP
11	K	80	GLY
12	L	28	LYS
12	L	40	LEU
12	L	54	ARG
1	A	51	GLY
1	A	61	ILE
1	A	66	LYS
1	A	74	MET
1	A	131	SER
1	A	169	ASN
1	A	219	PHE
1	A	283	GLY
1	A	313	GLN
1	A	322	VAL
1	A	426	LEU
1	A	517	ASN
1	A	755	PHE
1	A	975	HIS
1	A	1122	PRO

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Mol	Chain	Res	Type
1	A	1206	ASP
1	A	1221	LYS
1	A	1308	THR
1	A	1378	GLN
1	A	1390	ASN
2	B	24	PRO
2	B	27	ALA
2	B	206	ASN
2	B	309	GLN
2	B	531	GLN
2	B	561	TRP
2	B	594	ALA
2	B	605	ARG
2	B	641	GLU
2	B	711	GLU
2	B	728	ARG
2	B	734	HIS
2	B	752	ALA
2	B	881	ASN
2	B	892	LYS
2	B	906	SER
2	B	959	ASP
2	B	1003	ALA
2	B	1100	ASP
3	C	132	PRO
3	C	169	LYS
3	C	172	PRO
3	C	208	GLU
4	D	157	GLN
5	E	76	GLY
6	F	128	LYS
7	G	2	PHE
7	G	20	PRO
8	H	44	VAL
8	H	63	LEU
9	I	8	ARG
9	I	9	ASP
10	J	14	VAL
10	J	24	LEU
12	L	27	LEU
12	L	35	SER
1	A	69	THR

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Mol	Chain	Res	Type
1	A	159	THR
1	A	294	SER
1	A	331	GLY
1	A	466	SER
1	A	510	GLN
1	A	526	ASP
1	A	789	LYS
1	A	875	ALA
1	A	1278	ASN
2	B	114	PRO
2	B	257	LYS
2	B	264	SER
2	B	277	LYS
2	B	294	ASP
2	B	509	ALA
2	B	680	THR
2	B	810	GLU
2	B	848	ARG
2	B	937	ALA
2	B	1017	ILE
2	B	1082	MET
3	C	11	ARG
3	C	142	VAL
3	C	213	PRO
3	C	227	THR
3	C	243	VAL
4	D	118	THR
5	E	95	THR
5	E	129	PRO
7	G	27	LYS
7	G	136	VAL
8	H	81	PRO
8	H	139	ASN
9	I	62	ILE
11	K	54	ARG
11	K	79	GLU
12	L	39	SER
1	A	35	ILE
1	A	42	ASP
1	A	244	PRO
1	A	465	TYR
1	A	543	LEU

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Mol	Chain	Res	Type
1	A	619	LYS
1	A	673	GLY
1	A	693	VAL
1	A	704	ALA
1	A	720	ARG
1	A	958	VAL
1	A	995	GLU
1	A	1067	LEU
1	A	1105	LEU
1	A	1158	PRO
1	A	1244	ARG
1	A	1270	ASN
1	A	1365	TYR
1	A	1454	MET
2	B	45	SER
2	B	245	GLU
2	B	291	ILE
2	B	449	ASN
2	B	460	ALA
2	B	738	PHE
2	B	878	GLN
2	B	1075	GLY
2	B	1171	VAL
2	B	1183	LYS
3	C	12	GLU
4	D	30	GLY
4	D	53	SER
5	E	66	GLU
5	E	73	PRO
5	E	92	THR
6	F	150	GLU
8	H	8	ASP
9	I	95	THR
10	J	27	GLU
12	L	45	ALA
12	L	56	LEU
1	A	599	SER
1	A	605	MET
1	A	922	ASP
1	A	1211	GLN
2	B	793	ALA
3	C	78	GLU

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Mol	Chain	Res	Type
5	E	38	PRO
5	E	44	ALA
10	J	13	VAL
1	A	1437	GLY
2	B	818	PRO
2	B	1167	GLY
5	E	183	PRO
8	H	47	PHE
1	A	719	VAL
1	A	1335	ILE
2	B	593	PRO
7	G	126	ASN
1	A	775	ILE
2	B	707	PRO
2	B	764	SER
2	B	867	GLY
7	G	163	ILE
1	A	84	ILE
1	A	568	PRO
1	A	583	PRO
1	A	756	ILE
1	A	973	ILE
2	B	364	ILE
3	C	18	VAL
7	G	128	PRO
1	A	96	ILE
1	A	1006	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	1241/1520 (82%)	1109 (89%)	132 (11%)	10	46
2	B	963/1061 (91%)	841 (87%)	122 (13%)	6	35
3	C	234/299 (78%)	206 (88%)	28 (12%)	7	38
4	D	161/200 (80%)	139 (86%)	22 (14%)	5	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	196/197 (100%)	180 (92%)	16 (8%)	17	62
6	F	77/137 (56%)	73 (95%)	4 (5%)	32	79
7	G	152/152 (100%)	137 (90%)	15 (10%)	11	50
8	H	120/128 (94%)	104 (87%)	16 (13%)	6	33
9	I	113/116 (97%)	97 (86%)	16 (14%)	5	30
10	J	60/65 (92%)	55 (92%)	5 (8%)	16	61
11	K	99/102 (97%)	92 (93%)	7 (7%)	21	69
12	L	40/57 (70%)	36 (90%)	4 (10%)	11	50
All	All	3456/4034 (86%)	3069 (89%)	387 (11%)	9	42

All (387) 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	42	ASP
1	A	46	THR
1	A	54	ASN
1	A	68	GLN
1	A	70	CYS
1	A	83	HIS
1	A	93	VAL
1	A	141	LEU
1	A	145	LYS
1	A	160	GLN
1	A	161	LEU
1	A	162	VAL
1	A	169	ASN
1	A	185	TRP
1	A	196	GLU
1	A	203	SER
1	A	208	LEU
1	A	221	SER
1	A	244	PRO
1	A	245	PRO

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Mol	Chain	Res	Type
1	A	265	LYS
1	A	289	ILE
1	A	290	GLU
1	A	302	THR
1	A	312	PRO
1	A	320	ARG
1	A	321	PRO
1	A	322	VAL
1	A	324	SER
1	A	332	LYS
1	A	337	ARG
1	A	344	ARG
1	A	385	ILE
1	A	396	PRO
1	A	408	ASP
1	A	416	ARG
1	A	443	LEU
1	A	445	ASN
1	A	451	HIS
1	A	454	SER
1	A	462	VAL
1	A	470	LEU
1	A	475	THR
1	A	479	ASN
1	A	481	ASP
1	A	483	ASP
1	A	505	CYS
1	A	513	SER
1	A	518	LYS
1	A	539	THR
1	A	547	LEU
1	A	549	MET
1	A	562	THR
1	A	565	ILE
1	A	571	LEU
1	A	582	ILE
1	A	593	GLU
1	A	618	GLU
1	A	664	THR
1	A	666	ILE
1	A	680	THR
1	A	690	VAL

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Mol	Chain	Res	Type
1	A	701	LEU
1	A	710	LEU
1	A	735	VAL
1	A	738	LYS
1	A	741	ASN
1	A	768	GLN
1	A	774	ARG
1	A	810	PRO
1	A	821	ARG
1	A	822	GLU
1	A	827	THR
1	A	838	GLN
1	A	858	ASN
1	A	871	ASP
1	A	882	SER
1	A	903	ASN
1	A	906	HIS
1	A	920	LEU
1	A	923	LEU
1	A	941	LYS
1	A	961	ARG
1	A	978	PRO
1	A	983	ILE
1	A	992	ASP
1	A	1009	ASN
1	A	1029	ARG
1	A	1048	ASN
1	A	1067	LEU
1	A	1096	SER
1	A	1116	LEU
1	A	1120	LEU
1	A	1122	PRO
1	A	1124	HIS
1	A	1135	ARG
1	A	1146	VAL
1	A	1170	ILE
1	A	1171	GLN
1	A	1193	LEU
1	A	1217	LYS
1	A	1222	ASN
1	A	1257	ASP
1	A	1265	ASN

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Mol	Chain	Res	Type
1	A	1276	VAL
1	A	1280	GLU
1	A	1288	ASP
1	A	1291	VAL
1	A	1295	THR
1	A	1297	GLU
1	A	1308	THR
1	A	1315	GLU
1	A	1325	THR
1	A	1333	ILE
1	A	1349	TYR
1	A	1353	TYR
1	A	1359	ASP
1	A	1368	MET
1	A	1370	LEU
1	A	1371	LEU
1	A	1393	ASN
1	A	1394	THR
1	A	1400	CYS
1	A	1420	ASP
1	A	1442	ASP
1	A	1445	ILE
2	B	21	GLU
2	B	25	ILE
2	B	37	PHE
2	B	46	GLN
2	B	57	TYR
2	B	91	SER
2	B	98	THR
2	B	128	LEU
2	B	167	ILE
2	B	194	GLU
2	B	217	ARG
2	B	222	ILE
2	B	225	VAL
2	B	249	ARG
2	B	261	ARG
2	B	262	GLU
2	B	272	THR
2	B	297	ILE
2	B	298	LEU
2	B	303	TYR

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Mol	Chain	Res	Type
2	B	323	VAL
2	B	348	ARG
2	B	360	PHE
2	B	361	LEU
2	B	364	ILE
2	B	371	GLU
2	B	376	PHE
2	B	378	LEU
2	B	393	LYS
2	B	394	ASP
2	B	401	PHE
2	B	416	LEU
2	B	425	THR
2	B	427	ASP
2	B	429	PHE
2	B	446	LEU
2	B	455	SER
2	B	465	ASN
2	B	466	TRP
2	B	473	MET
2	B	476	ARG
2	B	485	ARG
2	B	487	THR
2	B	493	SER
2	B	502	ILE
2	B	513	GLN
2	B	516	ASN
2	B	529	GLU
2	B	557	PHE
2	B	558	LEU
2	B	568	ASP
2	B	570	VAL
2	B	576	ASP
2	B	582	VAL
2	B	597	MET
2	B	603	LEU
2	B	615	MET
2	B	635	ARG
2	B	636	PRO
2	B	682	SER
2	B	691	GLU
2	B	693	ILE

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Mol	Chain	Res	Type
2	B	705	MET
2	B	730	ARG
2	B	737	THR
2	B	742	GLU
2	B	748	ILE
2	B	776	GLN
2	B	781	PHE
2	B	786	ASN
2	B	790	ASP
2	B	794	ASN
2	B	797	TYR
2	B	805	THR
2	B	830	TYR
2	B	835	GLN
2	B	839	MET
2	B	859	TYR
2	B	878	GLN
2	B	879	ARG
2	B	882	THR
2	B	883	LEU
2	B	884	ARG
2	B	889	THR
2	B	909	ASP
2	B	939	THR
2	B	944	THR
2	B	953	LEU
2	B	956	THR
2	B	959	ASP
2	B	966	VAL
2	B	987	LYS
2	B	997	GLU
2	B	999	MET
2	B	1010	LEU
2	B	1031	LEU
2	B	1046	PRO
2	B	1047	PHE
2	B	1049	ASP
2	B	1060	ARG
2	B	1077	THR
2	B	1084	GLN
2	B	1087	PHE
2	B	1095	LEU

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Mol	Chain	Res	Type
2	B	1097	HIS
2	B	1098	MET
2	B	1122	ARG
2	B	1124	ARG
2	B	1129	ARG
2	B	1147	LEU
2	B	1148	LYS
2	B	1150	ARG
2	B	1159	ARG
2	B	1160	VAL
2	B	1175	LEU
2	B	1176	ASN
2	B	1182	CYS
2	B	1183	LYS
2	B	1185	CYS
2	B	1202	LEU
2	B	1218	THR
2	B	1220	ARG
3	C	7	GLN
3	C	11	ARG
3	C	16	ASP
3	C	23	SER
3	C	25	VAL
3	C	26	ASP
3	C	53	THR
3	C	55	THR
3	C	62	PHE
3	C	77	ILE
3	C	78	GLU
3	C	91	HIS
3	C	99	LEU
3	C	104	PHE
3	C	108	GLU
3	C	115	SER
3	C	124	LEU
3	C	138	GLU
3	C	145	CYS
3	C	147	LEU
3	C	155	LEU
3	C	156	THR
3	C	166	GLU
3	C	193	TYR

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Mol	Chain	Res	Type
3	C	209	TYR
3	C	238	ILE
3	C	262	LEU
3	C	266	ASP
4	D	11	ARG
4	D	14	ARG
4	D	16	LYS
4	D	17	LYS
4	D	20	GLU
4	D	22	GLU
4	D	23	ASN
4	D	29	LEU
4	D	38	ILE
4	D	41	GLN
4	D	47	LEU
4	D	70	PHE
4	D	118	THR
4	D	120	GLU
4	D	124	GLU
4	D	138	ASN
4	D	149	THR
4	D	187	THR
4	D	213	GLU
4	D	214	LEU
4	D	219	THR
4	D	221	TYR
5	E	5	ASN
5	E	8	ASN
5	E	29	PHE
5	E	31	THR
5	E	41	ASP
5	E	65	THR
5	E	72	PHE
5	E	78	LEU
5	E	82	PHE
5	E	110	PHE
5	E	112	TYR
5	E	123	LEU
5	E	131	THR
5	E	132	ILE
5	E	134	THR
5	E	150	VAL

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Mol	Chain	Res	Type
6	F	79	ARG
6	F	103	MET
6	F	112	GLU
6	F	119	ARG
7	G	1	MET
7	G	13	LEU
7	G	21	ARG
7	G	31	LEU
7	G	51	TYR
7	G	58	ARG
7	G	62	LEU
7	G	74	TYR
7	G	120	THR
7	G	126	ASN
7	G	128	PRO
7	G	133	SER
7	G	134	GLU
7	G	139	ILE
7	G	165	GLU
8	H	10	PHE
8	H	14	GLU
8	H	17	PRO
8	H	53	ASP
8	H	65	LEU
8	H	88	SER
8	H	89	LEU
8	H	91	ASP
8	H	94	ASP
8	H	102	TYR
8	H	128	ASN
8	H	129	TYR
8	H	130	ARG
8	H	135	LEU
8	H	138	GLU
8	H	143	LEU
9	I	2	THR
9	I	4	PHE
9	I	6	PHE
9	I	8	ARG
9	I	9	ASP
9	I	12	ASN
9	I	31	THR

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Mol	Chain	Res	Type
9	I	44	TYR
9	I	59	VAL
9	I	72	ASP
9	I	85	PHE
9	I	86	PHE
9	I	93	LYS
9	I	94	ASP
9	I	100	PHE
9	I	101	PHE
10	J	13	VAL
10	J	28	ASP
10	J	43	ARG
10	J	44	TYR
10	J	48	ARG
11	K	21	ILE
11	K	25	THR
11	K	47	ARG
11	K	50	LEU
11	K	81	TYR
11	K	103	THR
11	K	111	LEU
12	L	27	LEU
12	L	55	ILE
12	L	68	GLU
12	L	70	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (106) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	68	GLN
1	A	71	GLN
1	A	75	ASN
1	A	169	ASN
1	A	171	GLN
1	A	225	ASN
1	A	253	ASN
1	A	256	GLN
1	A	282	ASN
1	A	306	ASN
1	A	316	GLN
1	A	339	ASN

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Mol	Chain	Res	Type
1	A	390	GLN
1	A	435	HIS
1	A	447	GLN
1	A	451	HIS
1	A	479	ASN
1	A	493	GLN
1	A	503	GLN
1	A	517	ASN
1	A	611	GLN
1	A	640	GLN
1	A	654	ASN
1	A	723	ASN
1	A	741	ASN
1	A	745	GLN
1	A	757	ASN
1	A	768	GLN
1	A	786	HIS
1	A	858	ASN
1	A	903	ASN
1	A	926	GLN
1	A	935	GLN
1	A	965	GLN
1	A	994	GLN
1	A	1048	ASN
1	A	1078	GLN
1	A	1110	ASN
1	A	1140	HIS
1	A	1203	ASN
1	A	1211	GLN
1	A	1218	GLN
1	A	1258	HIS
1	A	1265	ASN
1	A	1312	ASN
1	A	1393	ASN
1	A	1432	GLN
2	B	53	GLN
2	B	60	GLN
2	B	115	GLN
2	B	178	ASN
2	B	236	HIS
2	B	366	GLN
2	B	383	ASN

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Mol	Chain	Res	Type
2	B	465	ASN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	657	HIS
2	B	667	GLN
2	B	794	ASN
2	B	842	ASN
2	B	862	GLN
2	B	887	HIS
2	B	957	ASN
2	B	1065	GLN
2	B	1076	HIS
2	B	1161	HIS
2	B	1179	GLN
2	B	1193	GLN
3	C	7	GLN
3	C	65	HIS
3	C	73	GLN
3	C	79	GLN
3	C	91	HIS
3	C	102	GLN
3	C	112	ASN
3	C	123	ASN
3	C	135	GLN
3	C	140	ASN
3	C	231	ASN
4	D	23	ASN
4	D	39	ASN
4	D	40	HIS
4	D	41	GLN
4	D	138	ASN
5	E	54	GLN
5	E	61	GLN
5	E	101	GLN
5	E	104	ASN
5	E	147	HIS
7	G	14	HIS
7	G	53	ASN
7	G	113	HIS
7	G	122	ASN
7	G	126	ASN

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Mol	Chain	Res	Type
7	G	131	GLN
8	H	128	ASN
8	H	131	ASN
9	I	12	ASN
9	I	46	HIS
9	I	108	HIS
10	J	53	HIS
11	K	65	HIS
11	K	89	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	10/18 (55%)	2 (20%)	1 (10%)

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	P	3	A
15	P	11	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
15	P	2	A

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z  > 2$
14	BRU	T	23	15,14	19,21,22	3.79	3 (15%)	22,30,33	1.78	3 (13%)

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
14	BRU	T	23	15,14	-	0/5/21/22	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	23	BRU	BR-C5	-15.72	1.50	1.90
14	T	23	BRU	C4-C5	3.22	1.45	1.39
14	T	23	BRU	P-OP1	2.66	1.49	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	23	BRU	C5-C6-N1	6.08	123.67	119.67
14	T	23	BRU	C6-N1-C2	-4.38	121.16	122.41
14	T	23	BRU	BR-C5-C6	2.54	123.02	117.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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.

## 5.7 Other polymers ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1418/1733 (81%)	0.02	7 (0%) 88 72	23, 70, 112, 141	0
2	B	1109/1224 (90%)	0.05	4 (0%) 90 77	23, 81, 123, 141	0
3	C	266/347 (76%)	0.01	0 100 100	34, 69, 105, 119	0
4	D	179/221 (80%)	0.12	1 (0%) 86 68	37, 79, 118, 131	0
5	E	214/215 (99%)	0.21	0 100 100	41, 97, 129, 137	0
6	F	87/155 (56%)	-0.20	0 100 100	19, 46, 77, 86	0
7	G	171/171 (100%)	0.06	0 100 100	48, 64, 104, 113	0
8	H	136/146 (93%)	0.48	1 (0%) 84 65	80, 106, 127, 135	0
9	I	119/122 (97%)	0.32	3 (2%) 54 33	65, 100, 125, 143	0
10	J	65/70 (92%)	-0.15	0 100 100	49, 65, 92, 105	0
11	K	115/120 (95%)	0.03	0 100 100	34, 73, 93, 122	0
12	L	46/70 (65%)	0.23	0 100 100	48, 108, 125, 132	0
13	N	7/12 (58%)	1.67	2 (28%) 1 1	135, 140, 151, 157	0
14	T	19/26 (73%)	1.66	7 (36%) 1 1	117, 142, 155, 155	0
15	P	11/18 (61%)	1.36	2 (18%) 2 2	125, 133, 152, 156	0
All	All	3962/4650 (85%)	0.08	27 (0%) 84 65	19, 76, 122, 157	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	T	28	DA	4.7
15	P	1	C	4.1
14	T	13	DT	3.4
2	B	868	MET	2.9
1	A	155	GLU	2.8
14	T	14	DA	2.8
1	A	1455	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
14	T	23	BRU	2.8
2	B	733	HIS	2.7
14	T	27	DC	2.7
4	D	19	GLU	2.6
14	T	11	DA	2.5
1	A	158	PRO	2.4
1	A	256	GLN	2.3
13	N	3	DT	2.3
1	A	1188	GLN	2.2
1	A	1081	LEU	2.2
14	T	12	DG	2.2
2	B	918	ILE	2.2
13	N	1	DA	2.1
9	I	76	PRO	2.1
9	I	77	LYS	2.1
9	I	120	GLN	2.1
15	P	2	A	2.1
1	A	253	ASN	2.1
8	H	36	CYS	2.1
2	B	250	PHE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
14	BRU	T	23	20/21	0.34	2.74	136,142,145,146	0

## 6.3 Carbohydrates ⓘ

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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
16	ZN	J	1066	1/1	0.20	0.39	53,53,53,53	0
16	ZN	B	2225	1/1	0.16	-0.73	30,30,30,30	0
17	MG	P	2458	1/1	0.24	-0.73	180,180,180,180	0
16	ZN	C	1269	1/1	0.10	-1.41	40,40,40,40	0
16	ZN	A	2457	1/1	0.12	-1.60	31,31,31,31	0
16	ZN	L	1071	1/1	0.05	-1.82	100,100,100,100	0
16	ZN	I	1121	1/1	0.08	-2.18	76,76,76,76	0
16	ZN	I	1122	1/1	0.12	-2.37	135,135,135,135	0
16	ZN	A	2456	1/1	0.06	-3.91	88,88,88,88	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.