



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 06:31 am 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 X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

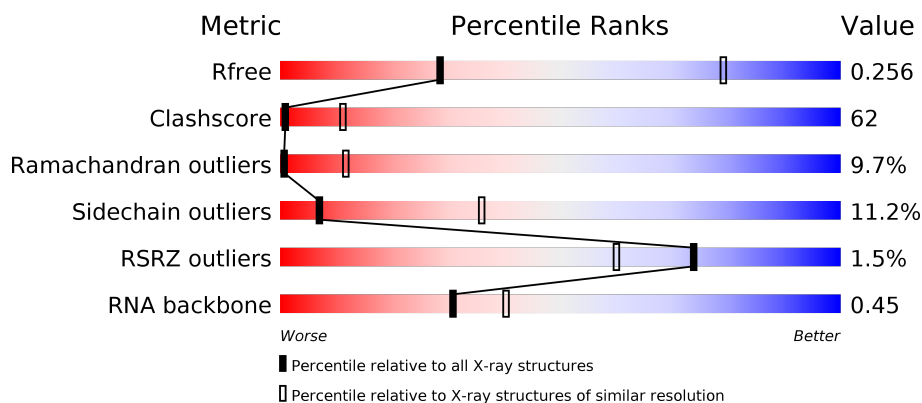
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.65 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.






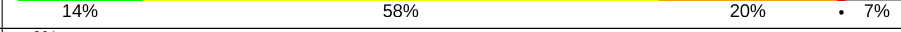
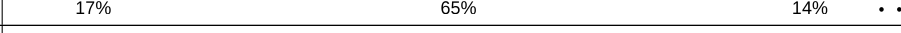

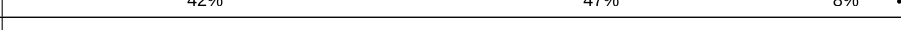
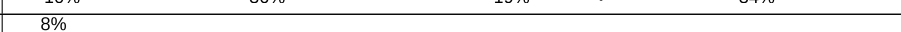
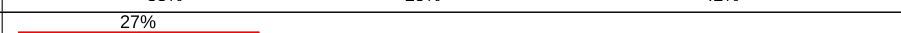


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1134 (3.82-3.50)
Clashscore	112137	1267 (3.82-3.50)
Ramachandran outliers	110173	1219 (3.82-3.50)
Sidechain outliers	110143	1218 (3.82-3.50)
RSRZ outliers	101464	1160 (3.82-3.50)
RNA backbone	2435	1004 (4.40-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	1733	<div> <div></div> <div> <div>23%</div> <div>47%</div> <div>10%</div> <div>•</div> <div>18%</div> </div> </div>
2	B	1224	<div> <div></div> <div> <div>23%</div> <div>52%</div> <div>14%</div> <div>•</div> <div>9%</div> </div> </div>
3	C	347	<div> <div>18%</div> <div>47%</div> <div>11%</div> <div>•</div> <div>23%</div> </div>
4	D	221	<div> <div>23%</div> <div>45%</div> <div>12%</div> <div>•</div> <div>19%</div> </div>

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Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	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 hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	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		

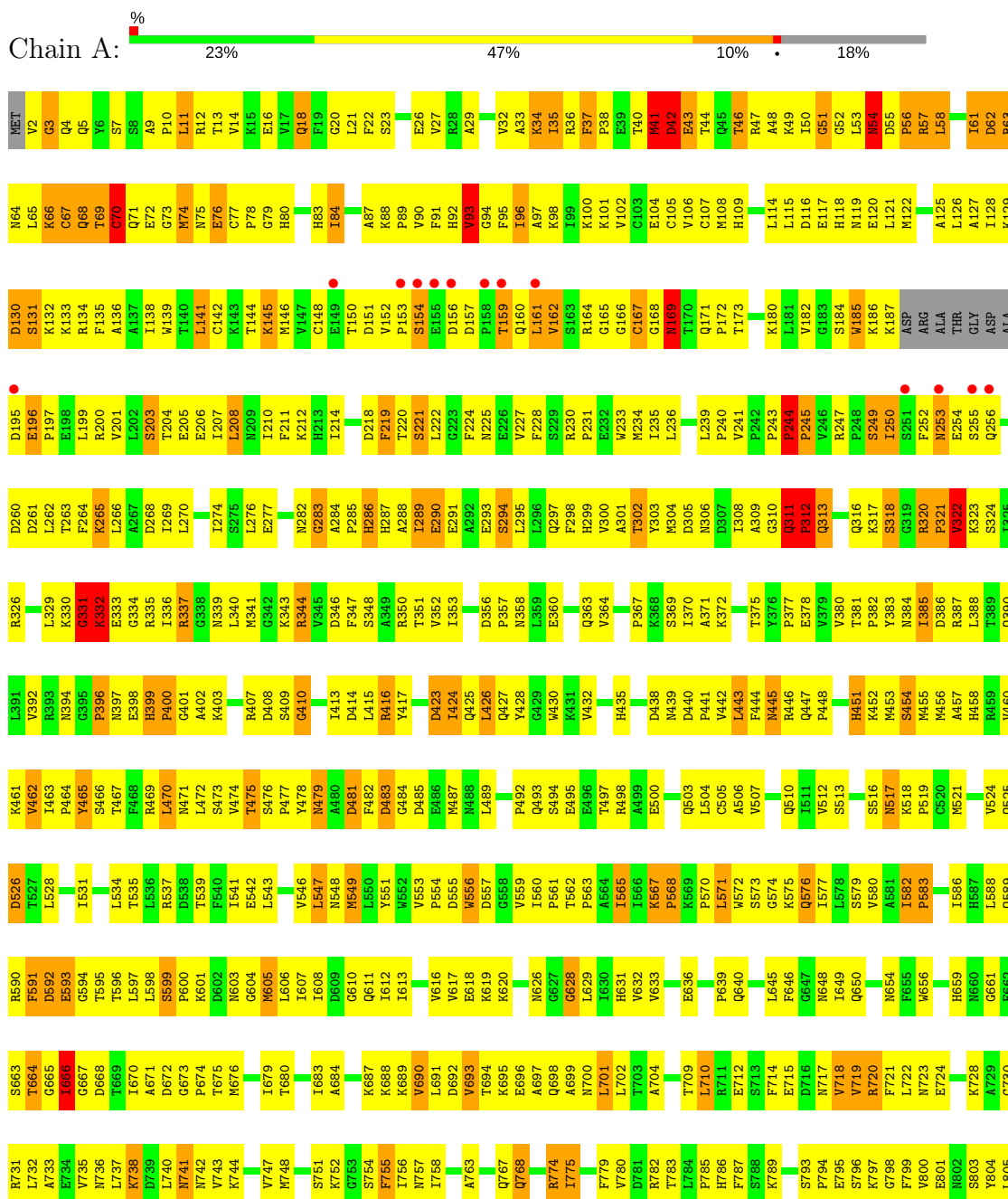
- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

3 Residue-property plots

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

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

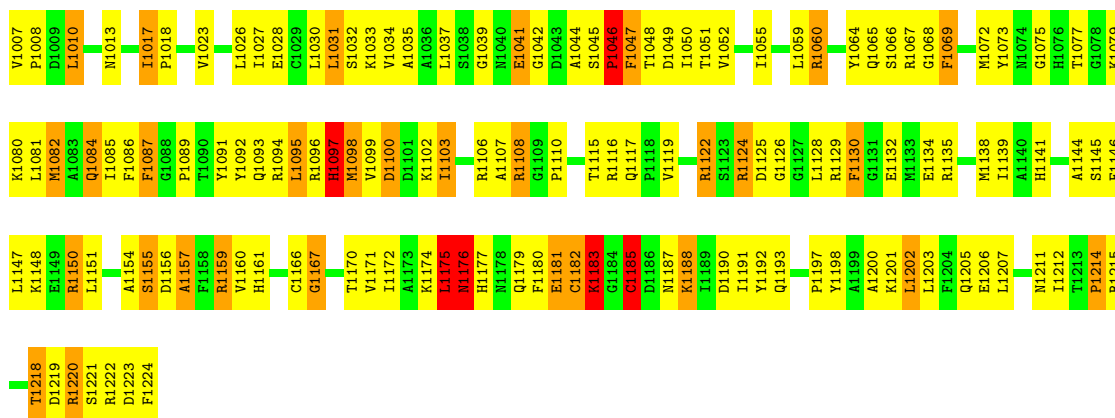


THR	SER	THR	SER	THR	GLY	GLN	GLU	F1389	T1325	E1263	M1202	E1139	T1077	Q1011	R940	Q872	R806
PRO	PRO	PRO	PRO	PRO	GLY	LYS	LYS	M1390	R1326	E1264	N1203	H1140	Q1078	R1012	K941	M873	R809
THR	THR	THR	THR	THR	THR	ILE	ILE	R1391	T1329	M1265	D1204	T1141	M1079	V1015	L943	D874	T800
PRO	PRO	PRO	PRO	PRO	GLY	THR	THR	M1393	T1330	M1266	K1205	K1145	T1080	L1016	R944	A875	Q811
PRO	PRO	PRO	PRO	PRO	THR	THR	THR	M1394	T1331	M1267	D1206	S1144	L1081	L1017	R945	E876	E812
PRO	PRO	PRO	PRO	PRO	THR	THR	THR	M1395	F1332	M1268	L1207	S1146	THR	F1018	V946	I877	F813
PRO	PRO	PRO	PRO	PRO	THR	THR	THR	M1396	F1333	E1269	T1208	T1147	THR	C1019	F947	I878	F814
PRO	PRO	PRO	PRO	PRO	THR	THR	THR	M1397	D1334	M1270	M1209	T1148	THR	C1020	S882	S882	F815
PRO	PRO	PRO	PRO	PRO	THR	THR	THR	M1398	D1335	M1271	G1210	T1149	THR	L1021	A952	D884	L883
PRO	PRO	PRO	PRO	PRO	THR	THR	THR	M1399	M1336	Q1211	Q1212	A1149	THR	L1022	N953	D894	A817
PRO	PRO	PRO	PRO	PRO	THR	THR	THR	C1400	E1337	Q1213	G1213	S1150	THR	R1023	W954	T885	M818
PRO	PRO	PRO	PRO	PRO	THR	THR	THR	S1401	E1338	R1274	E1214	E1151	THR	S1024	G819	I886	G819
PRO	PRO	PRO	PRO	PRO	THR	THR	THR	F1402	L1339	V1275	R1214	T1152	THR	R1025	V958	G887	G820
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PRO	PRO	PRO	PRO	PRO	THR	THR	THR	T1405	E1342	M1278	I1217	D1155	THR	R1028	R961	D890	G823
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PRO	PRO	PRO	PRO	PRO	THR	THR	THR	F1407	G1344	R1281	F1220	R1159	THR	R1030	I963	I825	I825
PRO	PRO	PRO	PRO	PRO	THR	THR	THR	L1408	R1345	V1282	K1221	S1160	THR	V1031	I964	R836	R826
PRO	PRO	PRO	PRO	PRO	THR	THR	THR	L1409	R1346	M1283	M1222	T1161	THR	V1032	Q965	Y897	T827
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PRO	PRO	PRO	PRO	PRO	THR	THR	THR	D1420	I1355	P1292	D1231	Q1171	THR	L1105	K977	D838	D838
PRO	PRO	PRO	PRO	PRO	THR	THR	THR	C1421	I1356	S1293	N1232	H1173	THR	T907	P978	R839	R839
PRO	PRO	PRO	PRO	PRO	THR	THR	THR	D1422	D1359	T1295	D1233	F1174	THR	F1042	S979	R840	R840
PRO	PRO	PRO	PRO	PRO	THR	THR	THR	G1423	Y1362	E1296	L1236	S1175	THR	V1045	D980	V850	V850
PRO	PRO	PRO	PRO	PRO	THR	THR	THR	V1424	V1363	G1297	I1237	LEU	THR	L1046	L981	H851	H851
PRO	PRO	PRO	PRO	PRO	THR	THR	THR	S1425	M1364	V1298	I1238	LEU	THR	S1047	P910	K843	K843
PRO	PRO	PRO	PRO	PRO	THR	THR	THR	E1426	N1365	V1299	N1239	ASP	THR	N1048	I983	A844	A844
PRO	PRO	PRO	PRO	PRO	THR	THR	THR	I1429	R1366	K1300	C1240	GLU	THR	I1049	K984	L845	L845
PRO	PRO	PRO	PRO	PRO	THR	THR	THR	Q1432	R1367	M1304	V1241	GLU	THR	F1053	D985	E846	E846
PRO	PRO	PRO	PRO	PRO	THR	THR	THR	L1436	M1368	V1305	R1243	ALA	THR	L1054	V987	G916	G916
PRO	PRO	PRO	PRO	PRO	THR	THR	THR	G1437	A1369	L1306	R1244	GLN	THR	R1055	L988	I919	I919
PRO	PRO	PRO	PRO	PRO	THR	THR	THR	L1438	L1370	E1307	P1245	THR	THR	L1056	D982	L920	L920
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PRO	PRO	PRO	PRO	PRO	THR	THR	THR	V1374	V1373	V1310	LEU	Q1187	THR	E1062	E995	L923	L923
PRO	PRO	PRO	PRO	PRO	THR	THR	THR	M1375	V1374	V1311	ASP	Q1188	THR	M1063	N996	K924	K924
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PRO	PRO	PRO	PRO	PRO	THR	THR	THR	F1441	T1376	L1313	GLU	P1190	THR	G1065	L998	Q926	Q926
PRO	PRO	PRO	PRO	PRO	THR	THR	THR	D1442	T1377	S1314	THR	W1191	THR	G1065	V999	V927	V927
PRO	PRO	PRO	PRO	PRO	THR	THR	THR	V1443	Q1378	E1315	GLU	L1192	THR	V1066	L1000	L928	L928
PRO	PRO	PRO	PRO	PRO	THR	THR	THR	M1444	G1379	V1316	THR	L1193	THR	V1067	L1001	L929	L929
PRO	PRO	PRO	PRO	PRO	THR	THR	THR	L1445	G1380	M1317	E1254	R1194	THR	G1002	G1002	K864	K864
PRO	PRO	PRO	PRO	PRO	THR	THR	THR	L1450	L1381	T1318	E1255	R1195	THR	S1071	K1003	Q933	Q933
PRO	PRO	PRO	PRO	PRO	THR	THR	THR	V1451	V1384	V1319	D1257	E1196	THR	S1071	K1003	Q933	Q933
PRO	PRO	PRO	PRO	PRO	THR	THR	THR	T1452	T1385	P1320	M1258	L1197	THR	E1005	F1005	T867	T867
PRO	PRO	PRO	PRO	PRO	THR	THR	THR	Y1453	T1386	G1321	M1259	L1197	THR	G1073	I1006	L936	L936
PRO	PRO	PRO	PRO	PRO	THR	THR	THR	M1454	H1387	I1322	L1260	R1199	THR	A1074	N1009	Y937	Y937
PRO	PRO	PRO	PRO	PRO	THR	THR	THR	P1455	G1388	D1323	K1261	A1200	THR	P1075	K938	E870	E870
PRO	PRO	PRO	PRO	PRO	THR	THR	THR			P1324	K1262	A1201	THR	A1076	A1010	D871	D871

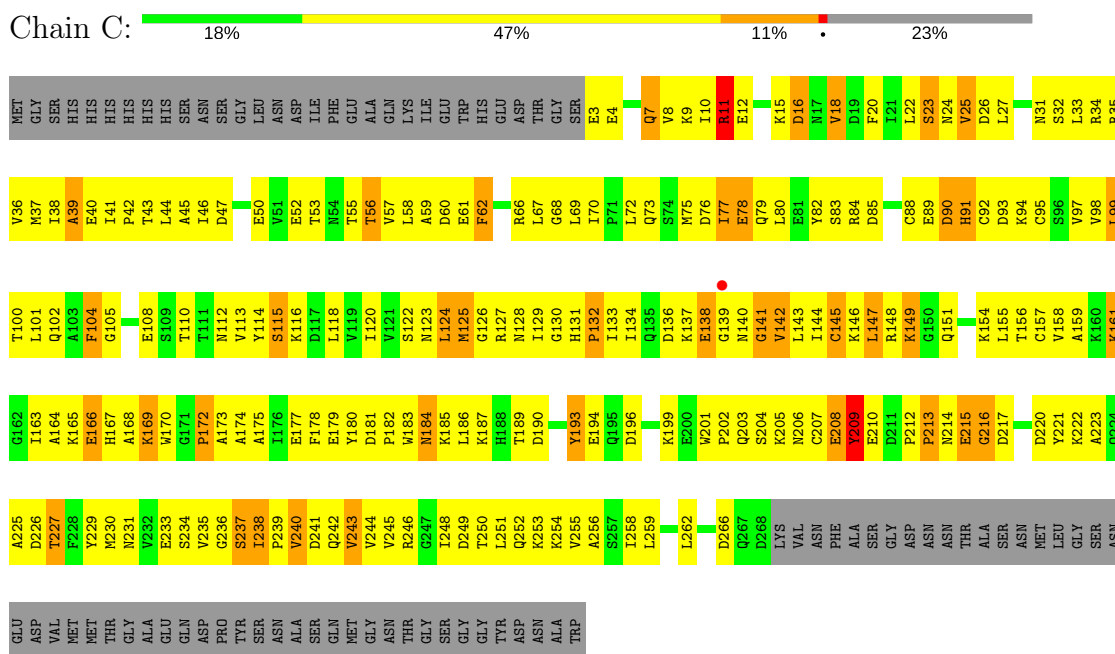
• Molecule 2: DNA-directed RNA polymerase II subunit RPB2



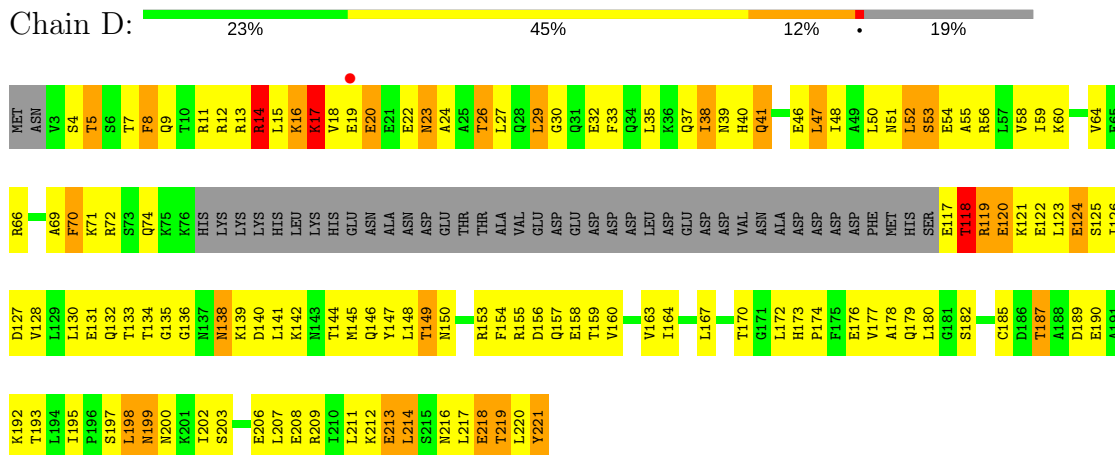
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Y948	R884	L883	N822	F758	I693	G631	P571	R504	ASP	T380	V318	V256	L189	G127	C64	SER
Y949	R885	A823	A823	P759	D694	R632	H572	ASP	PHE	N381	E319	K257	Y190	F128	E65	ASP
D950	K886	A695	I824	D760	G573	V633	H573	GLY	ASN	K382	D320	K258	G191	F129	D66	LEU
G951	H887	E696	V825	H761	E696	R635	S574	LYS	MET	N383	V323	Q260	L192	V130	S67	ALA
V952	G888	E697	A826	N762	E697	R636	P575	L508	LEU	R384	I324	R261	E194	D131	T68	ASN
L953	T889	E698	I827	Q763	E698	P636	D576	A509	L446	L385	Q325	E262	E195	V132	L69	SER
Y954	S700	E699	Y830	S764	E699	L637	A577	K510	A447	L386	Q326	E263	G196	K133	I70	GLU
T955	D891	S700	Y830	P765	S700	F638	T578	K511	L448	L387	D326	G263	P196	K134	LEU	LYS
T956	K892	L701	G832	N767	L701	I639	R579	R512	N449	C388	R327	S264	M199	ARG	GLN	TYR
N957	L893	L702	Y833	T768	L702	V640	V580	Q513	A389	E328	R327	S265	M199	THR	GLN	TYR
Q958	N834	L703	Y833	T769	L703	E641	F581	L514	L390	E328	R329	A266	F203	TYR	LEU	ASP
D959	N834	A704	Y834	Y769	A704	D642	V582	H515	D391	E328	L331	R267	I204	ALA	GLN	GLU
D960	Q835	W705	Q835	Q770	W705	D643	N583	N516	R392	E328	L331	R267	I204	ALA	GLN	ASP
D961	E936	Q706	Q835	S771	Q706	E644	N583	N516	R392	E328	L331	R267	I204	ALA	GLN	ASP
D962	E936	Q707	Q835	A772	Q707	S645	N583	N516	R392	E328	L331	R267	I204	ALA	GLN	ASP
D963	E936	Q707	Q835	A772	Q707	S645	N583	N516	R392	E328	L331	R267	I204	ALA	GLN	ASP
D964	E936	Q707	Q835	A772	Q707	S645	N583	N516	R392	E328	L331	R267	I204	ALA	GLN	ASP
D965	E936	Q707	Q835	A772	Q707	S645	N583	N516	R392	E328	L331	R267	I204	ALA	GLN	ASP
D966	E936	Q707	Q835	A772	Q707	S645	N583	N516	R392	E328	L331	R267	I204	ALA	GLN	ASP
D967	E936	Q707	Q835	A772	Q707	S645	N583	N516	R392	E328	L331	R267	I204	ALA	GLN	ASP
D968	E936	Q707	Q835	A772	Q707	S645	N583	N516	R392	E328	L331	R267	I204	ALA	GLN	ASP
D969	E936	Q707	Q835	A772	Q707	S645	N583	N516	R392	E328	L331	R267	I204	ALA	GLN	ASP
D970	E936	Q707	Q835	A772	Q707	S645	N583	N516	R392	E328	L331	R267	I204	ALA	GLN	ASP
D971	E936	Q707	Q835	A772	Q707	S645	N583	N516	R392	E328	L331	R267	I204	ALA	GLN	ASP
D972	E936	Q707	Q835	A772	Q707	S645	N583	N516	R392	E328	L331	R267	I204	ALA	GLN	ASP
D973	E936	Q707	Q835	A772	Q707	S645	N583	N516	R392	E328	L331	R267	I204	ALA	GLN	ASP
D974	E936	Q707	Q835	A772	Q707	S645	N583	N516	R392	E328	L331	R267	I204	ALA	GLN	ASP
D975	E936	Q707	Q835	A772	Q707	S645	N583	N516	R392	E328	L331	R267	I204	ALA	GLN	ASP
D976	E936	Q707	Q835	A772	Q707	S645	N583	N516	R392	E328	L331	R267	I204	ALA	GLN	ASP
D977	E936	Q707	Q835	A772	Q707	S645	N583	N516	R392	E328	L331	R267	I204	ALA	GLN	ASP
D978	E936	Q707	Q835	A772	Q707	S645	N583	N516	R392	E328	L331	R267	I204	ALA	GLN	ASP
D979	E936	Q707	Q835	A772	Q707	S645	N583	N516	R392	E328	L331	R267	I204	ALA	GLN	ASP
D980	E936	Q707	Q835	A772	Q707	S645	N583	N516	R392	E328	L331	R267	I204	ALA	GLN	ASP
D981	E936	Q707	Q835	A772	Q707	S645	N583	N516	R392	E328	L331	R267	I204	ALA	GLN	ASP
D982	E936	Q707	Q835	A772	Q707	S645	N583	N516	R392	E328	L331	R267	I204	ALA	GLN	ASP
D983	E936	Q707	Q835	A772	Q707	S645	N583	N516	R392	E328	L331	R267	I204	ALA	GLN	ASP
D984	E936	Q707	Q835	A772	Q707	S645	N583	N516	R392	E328	L331	R267	I204	ALA	GLN	ASP
D985	E936	Q707	Q835	A772	Q707	S645	N583	N516	R392	E328	L331	R267	I204	ALA	GLN	ASP
D986	E936	Q707	Q835	A772	Q707	S645	N583	N516	R392	E328	L331	R267	I204	ALA	GLN	ASP
D987	E936	Q707	Q835	A772	Q707	S645	N583	N516	R392	E328	L331	R267	I204	ALA	GLN	ASP
D988	E936	Q707	Q835	A772	Q707	S645	N583	N516	R392	E328	L331	R267	I204	ALA	GLN	ASP
D989	E936	Q707	Q835	A772	Q707	S645	N583	N516	R392	E328	L331	R267	I204	ALA	GLN	ASP
D990	E936	Q707	Q835	A772	Q707	S645	N583	N516	R392	E328	L331	R267	I204	ALA	GLN	ASP
D991	E936	Q707	Q835	A772	Q707	S645	N583	N516	R392	E328	L331	R267	I204	ALA	GLN	ASP
D992	E936	Q707	Q835	A772	Q707	S645	N583	N516	R392	E328	L331	R267	I204	ALA	GLN	ASP
D993	E936	Q707	Q835	A772	Q707	S645	N583	N516	R392	E328	L331	R267	I204	ALA	GLN	ASP
D994	E936	Q707	Q835	A772	Q707	S645	N583	N516	R392	E328	L331	R267	I204	ALA	GLN	ASP
D995	E936	Q707	Q835	A772	Q707	S645	N583	N516	R392	E328	L331	R267	I204	ALA	GLN	ASP
D996	E936	Q707	Q835	A772	Q707	S645	N583	N516	R392	E328	L331	R267	I204	ALA	GLN	ASP
D997	E936	Q707	Q835	A772	Q707	S645	N583	N516	R392	E328	L331	R267	I204	ALA	GLN	ASP
D998	E936	Q707	Q835	A772	Q707	S645	N583	N516	R392	E328	L331	R267	I204	ALA	GLN	ASP
D999	E936	Q707	Q835	A772	Q707	S645	N583	N516	R392	E328	L331	R267	I204	ALA	GLN	ASP
F1000	E936	Q707	Q835	A772	Q707	S645	N583	N516	R392	E328	L331	R267	I204	ALA	GLN	ASP
F1001	E936	Q707	Q835	A772	Q707	S645	N583	N516	R392	E328	L331	R267	I204	ALA	GLN	ASP
F1002	E936	Q707	Q835	A772	Q707	S645	N583	N516	R392	E328	L331	R267	I204	ALA	GLN	ASP
A1003	E936	Q707	Q835	A772	Q707	S645	N583	N516	R392	E328	L331	R267	I204	ALA	GLN	ASP
E1004	E936	Q707	Q835	A772	Q707	S645	N583	N516	R392	E328	L331	R267	I204	ALA	GLN	ASP
G1005	E936	Q707	Q835	A772	Q707	S645	N583	N516	R392	E328	L331	R267	I204	ALA	GLN	ASP
I1006	E936	Q707	Q835	A772	Q707	S645	N583	N516	R392	E328	L331	R267	I204	ALA	GLN	ASP



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

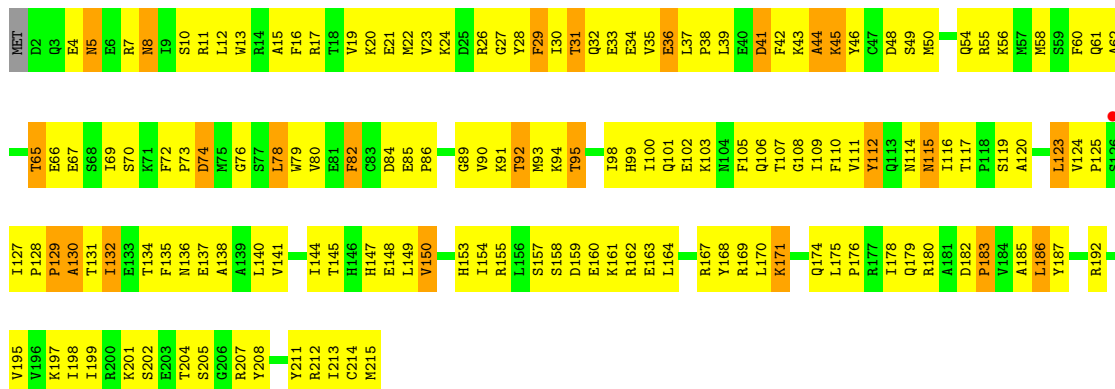
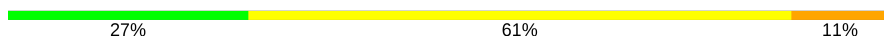


- Molecule 4: DNA-directed RNA polymerase II subunit RPB4



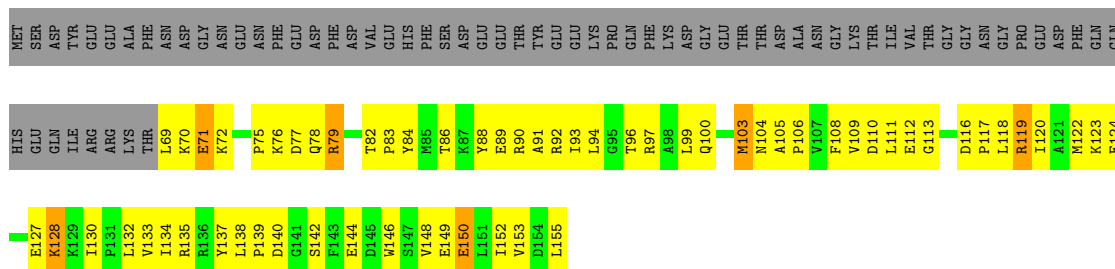
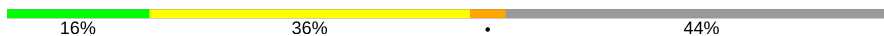
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:



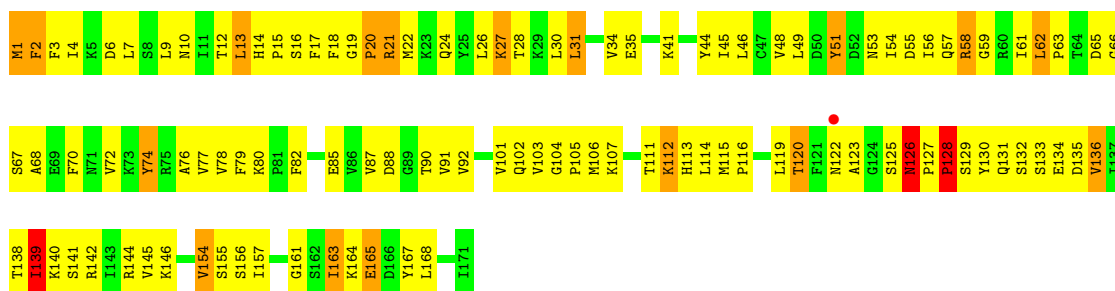
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:



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

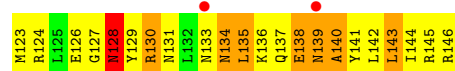
Chain G:



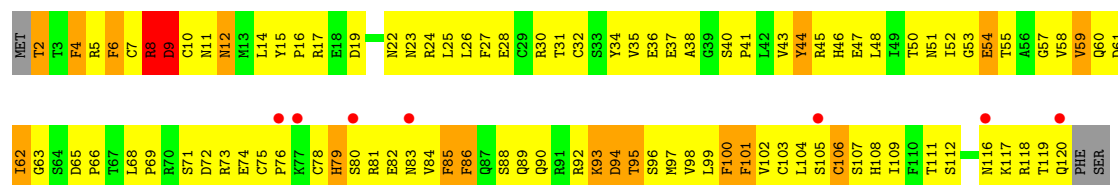
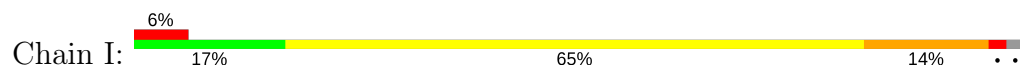
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:

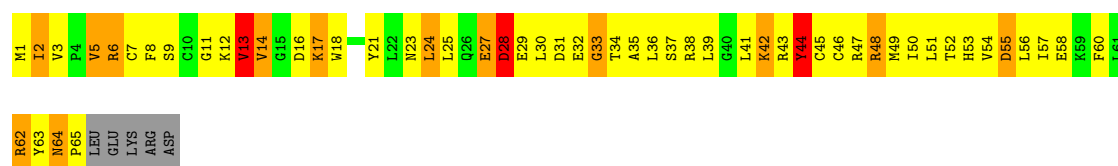
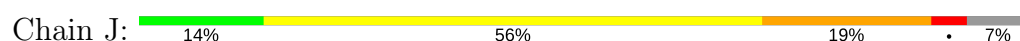




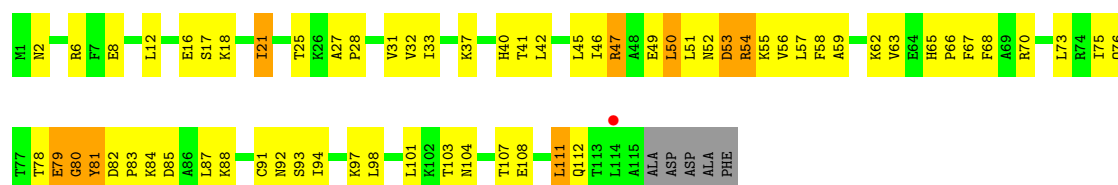
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



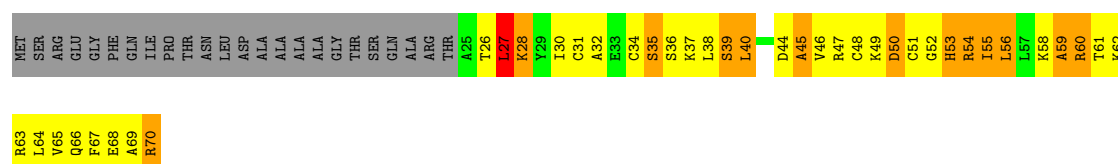
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



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



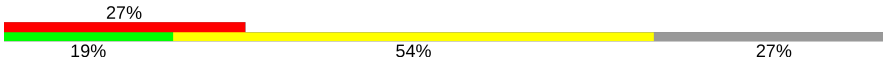
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

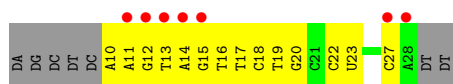


- Molecule 13: 5'-D(*AP*CP*TP*AP*CP*TP*TP*GP*AP*GP*CP*T)-3'



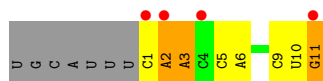
- Molecule 14: 5'-D(*AP*GP*CP*TP*C*AP*AP*GP*TP*AP*GP*TP*TP*CP*TP*GP*CP*C
P*(BRU)P*GP*GP*TP*CP*AP*TP*T)-3'

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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	3.21 (at 3.67Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.210 , 0.253 0.213 , 0.256	Depositor DCC
R_{free} test set	2674 reflections (2.01%)	DCC
Wilson B-factor (Å ²)	88.8	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 113.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
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
F_o, F_c correlation	0.90	EDS
Total number of atoms	31961	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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
10	J	532	0	542	112	0
11	K	924	0	934	105	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 62.

All (3920) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B: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:1206:ASP:HB3	1:A:1274:ARG:HH22	1.19	1.04
1:A:567:LYS:HB3	8:H:96:VAL:H	1.21	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:273:LEU:HB2	2:B:276:ILE:HD12	1.40	1.03
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:139:ILE:HG23	7:G:140:LYS:HG3	1.46	0.97
7:G:34:VAL:HG11	7:G:74:TYR:HE1	1.30	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
2:B:1187:ASN:O	2:B:1188:LYS:HB2	1.64	0.95
2:B:243:ALA:HB2	2:B:251:ILE:HD13	1.45	0.95
10:J:53:HIS:HD2	10:J:54:VAL:N	1.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:510:LYS:HG3	2:B:511:PRO:CD	1.96	0.93
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:1329:THR:HG22	1:A:1331:SER:H	1.30	0.93
1:A:66:LYS:HZ3	1:A:68:GLN:H	1.01	0.93
1:A:629:LEU:O	1:A:633:VAL:HG23	1.69	0.93
3:C:177:GLU:HG3	3:C:231:ASN:HB3	1.51	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: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
1:A:182:VAL:HG22	1:A:201:VAL:HA	1.52	0.91
5:E:22:MET:HE1	5:E:26:ARG:HH21	1.34	0.91
1:A:1063:MET:SD	1:A:1436:ILE:HG12	2.10	0.91
1:A:154:SER:HB3	1:A:162:VAL:HG21	1.50	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:114:PRO:HG3	2:B:181:LEU:HD11	1.53	0.90
2:B:241:ARG:HA	2:B:253:THR:HG22	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
1:A:107:CYS:HA	1:A:171:GLN:NE2	1.85	0.90
15:P:10:U:H5'	15:P:11:G:O3'	1.71	0.90
1:A:381:THR:HG23	1:A:382:PRO:HD2	1.54	0.90
4:D:24:ALA:HB3	4:D:26:THR:HG23	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:59:ILE:HG22	8:H:60:ALA:H	1.37	0.90
8:H:84:ALA:HB2	8:H:87:ARG:HD2	1.54	0.89
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
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
8:H:17:PRO:HB3	8:H:24:CYS:SG	2.12	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:107:CYS:HA	1:A:171:GLN:HE22	1.37	0.89
1:A:779:PHE:HE1	1:A:785:PRO:HD3	1.38	0.89
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.54	0.88
2:B:830:TYR:CE2	2:B:1000:PRO:HD3	2.08	0.88
4:D:220:LEU:HD23	4:D:221:TYR:H	1.36	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
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
11:K:21:ILE:HG23	11:K:33:ILE:HG12	1.56	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
1:A:55:ASP:C	1:A:57:ARG:H	1.75	0.87
2:B:603:LEU:HD13	2:B:608:ASP:HB2	1.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:1107:VAL:HG12	1:A:1107:VAL:O	1.76	0.85
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.12	0.85
7:G:26:LEU:CD1	7:G:56:ILE:HD11	2.05	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
1:A:668:ASP:HB3	1:A:741:ASN:HD21	1.41	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: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
1:A:225:ASN:ND2	1:A:228:PHE:H	1.73	0.83
2:B:841:MET:HG2	2:B:846:ILE:HD11	1.60	0.83
1:A:698:GLN:HA	9:I:97:MET:O	1.78	0.83
1:A:1259:MET:HA	1:A:1262:LYS:HD2	1.60	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
4:D:23:ASN:H	4:D:23:ASN:HD22	1.24	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
1:A:503:GLN:HE21	6:F:90:ARG:NH2	1.76	0.83
1:A:534:LEU:O	1:A:574:GLY:HA3	1.77	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:1224:LEU:HD11	1:A:1240:CYS:HB3	1.60	0.83
1:A:167:CYS:HB2	1:A:169:ASN:HD21	1.43	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:425:THR:HA	2:B:428:ILE:HD12	1.59	0.82
1:A:1293:SER:OG	1:A:1295:THR:HG23	1.79	0.82
2:B:882:THR:HG21	2:B:935:ARG:HA	1.62	0.82
2:B:110:HIS:CB	12:L:54:ARG:HH22	1.92	0.82
7:G:122:ASN:ND2	7:G:125:SER:HB3	1.93	0.82
1:A:40:THR:HG22	1:A:41:MET:HG3	1.62	0.82
2:B:559:SER:HA	2:B:563:MET:CB	2.07	0.82
1:A:1348:LEU:O	1:A:1352:VAL:HG23	1.78	0.82
1:A:14:VAL:H	1:A:1432:GLN:NE2	1.77	0.82
2:B:351:TYR:CE1	2:B:355:ILE:HD11	2.13	0.82
2:B:1065:GLN:HE21	2:B:1067:ARG:N	1.76	0.82
5:E:56:LYS:NZ	5:E:85:GLU:HG3	1.94	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
1:A:1312:ASN:HD21	1:A:1315:GLU:HG3	1.45	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
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
7:G:15:PRO:HA	7:G:18:PHE:CE1	2.15	0.82
10:J:5:VAL:HG12	10:J:6:ARG:HG3	1.60	0.82
2:B:1095:LEU:HD12	2:B:1095:LEU:H	1.45	0.81
1:A:831:THR:HG23	1:A:832:ALA:H	1.44	0.81
2:B:798:TYR:HE2	3:C:62:PHE:CE2	1.97	0.81
1:A:1420:ASP:HB2	1:A:1422:ARG:HG3	1.61	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
2:B:815:ARG:HD3	2:B:1041:GLU:OE2	1.79	0.81
1:A:390:GLN:HE21	1:A:394:ASN:HD22	1.27	0.81
8:H:101:ALA:HB2	8:H:116:TYR:CE2	2.15	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
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
8:H:40:LEU:HD13	8:H:123:MET:HE3	1.60	0.81
1:A:903:ASN:HD22	1:A:904:THR:N	1.78	0.81
2:B:642:ASP:HA	2:B:649:LYS:HA	1.62	0.81
5:E:124:VAL:HG13	5:E:132:ILE:HG13	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1387:HIS:HA	1:A:1391:ARG:HH11	1.45	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
8:H:130:ARG:HB2	8:H:130:ARG:HH11	1.45	0.81
1:A:666:ILE:H	2:B:1026:LEU:HD13	1.44	0.80
2:B:577:ALA:CB	2:B:589:VAL:HG11	2.10	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
1:A:754:SER:H	1:A:757:ASN:HD22	1.29	0.80
2:B:579:ARG:HB2	2:B:586:TRP:HE1	1.45	0.80
1:A:889:SER:HB3	1:A:1297:GLU:HG3	1.64	0.80
1:A:332:LYS:C	1:A:334:GLY:H	1.85	0.80
1:A:683:ILE:HD13	1:A:801:GLU:HG3	1.63	0.80
1:A:896:ARG:HD3	1:A:897:TYR:CE1	2.16	0.80
3:C:177:GLU:HG3	3:C:231:ASN:HD22	1.45	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
2:B:613:VAL:HG13	2:B:627:PHE:O	1.82	0.80
9:I:6:PHE:HB3	9:I:12:ASN:O	1.82	0.80
14:T:16:DT:H2''	14:T:17:DT:H5'	1.62	0.80
14:T:15:DG:H2'	14:T:16:DT:H71	1.63	0.80
1:A:901:LEU:HD22	1:A:919:ILE:HG23	1.64	0.80
2:B:278:GLN:CG	2:B:279:ASP:H	1.93	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
1:A:697:ALA:HB2	1:A:702:LEU:HD12	1.64	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:GLN:HG3	1:A:430:TRP:CZ2	2.18	0.79
1:A:563:PRO:HG3	1:A:572:TRP:CZ2	2.17	0.79
1:A:567:LYS:CE	1:A:568:PRO:HD2	2.12	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
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
4:D:29:LEU:HD12	7:G:82:PHE:CZ	2.18	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
2:B:221:ASN:OD1	2:B:242:SER:HA	1.83	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
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
5:E:117:THR:HB	5:E:120:ALA:HB2	1.65	0.78
2:B:758:PHE:CE2	2:B:1044:ALA:HA	2.18	0.78
7:G:14:HIS:CD2	7:G:16:SER:H	2.01	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
1:A:710:LEU:HD12	1:A:710:LEU:H	1.47	0.78
2:B:126:SER:OG	2:B:172:ILE:HD11	1.84	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
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
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.14	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
2:B:583:ASN:HD21	2:B:628:THR:CG2	1.95	0.78
1:A:1291:VAL:HG22	1:A:1292:PRO:HD2	1.66	0.78
1:A:265:LYS:HE3	1:A:265:LYS:CA	2.13	0.78
1:A:53:LEU:CD2	1:A:54:ASN:H	1.89	0.78
4:D:159:THR:O	4:D:163:VAL:HG23	1.83	0.78
2:B:542:MET:HG2	2:B:747:MET:HE3	1.64	0.77
4:D:130:LEU:HD13	4:D:142:LYS:HD3	1.65	0.77
8:H:95:TYR:CE2	8:H:97:MET:HG3	2.18	0.77
5:E:90:VAL:HA	5:E:120:ALA:HB2	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:465:ASN:HD22	2:B:465:ASN:N	1.81	0.77
2:B:955:THR:HG22	2:B:956:THR:O	1.83	0.77
4:D:14:ARG:HB3	4:D:14:ARG:NH1	1.98	0.77
4:D:71:LYS:HA	4:D:74:GLN:CG	2.14	0.77
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
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.65	0.77
2:B:1072:MET:HE3	2:B:1085:ILE:HB	1.67	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
1:A:1135:ARG:HG2	1:A:1136:SER:N	2.00	0.77
4:D:202:ILE:HD13	4:D:207:LEU:HB2	1.65	0.77
5:E:124:VAL:HG13	5:E:132:ILE:CG1	2.14	0.77
10:J:1:MET:N	10:J:57:ILE:H	1.82	0.77
1:A:1227:ILE:HG22	1:A:1228:TRP:H	1.49	0.77
2:B:745:PRO:O	2:B:748:ILE:HG12	1.85	0.77
3:C:45:ALA:HA	3:C:72:LEU:HD12	1.66	0.77
8:H:127:GLY:O	8:H:128:ASN:HB2	1.83	0.77
1:A:1261:LYS:O	1:A:1264:GLU:HB3	1.85	0.76
7:G:115:MET:HB3	7:G:116:PRO:HD2	1.65	0.76
1:A:1030:ARG:HG2	1:A:1034:GLU:OE2	1.86	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:666:ILE:N	2:B:1026:LEU:HD13	2.00	0.76
2:B:824:ILE:HG12	10:J:48:ARG:NH1	2.01	0.76
5:E:198:ILE:HD11	5:E:212:ARG:HG3	1.65	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
14:T:27:DC:H42	15:P:2:A:H61	1.30	0.76
2:B:327:ARG:NH2	2:B:371:GLU:HG2	2.00	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
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:675:THR:O	1:A:679:ILE:HG13	1.85	0.76
1:A:63:ARG:HA	1:A:74:MET:HE2	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1409:LEU:HD13	2:B:1207:LEU:HD11	1.66	0.76
2:B:254:LEU:HD12	2:B:272:THR:O	1.85	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
1:A:388:LEU:O	1:A:392:VAL:HG23	1.87	0.75
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:1206:ASP:HB3	1:A:1274:ARG:NH2	1.99	0.75
2:B:565:PRO:HB2	2:B:567:GLU:HG2	1.67	0.75
2:B:654:ARG:H	2:B:657:HIS:HD2	1.31	0.75
1:A:1385:THR:HG22	1:A:1386:ARG:N	2.01	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:1158:PRO:HG2	1:A:1159:ARG:HE	1.49	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: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
2:B:955:THR:HG22	2:B:956:THR:N	2.02	0.75
3:C:98:VAL:C	3:C:99:LEU:HD23	2.07	0.75
2:B:112:LEU:HD12	2:B:113:TYR:H	1.52	0.74
2:B:345:LYS:HG2	2:B:346:GLU:N	1.99	0.74
2:B:806:THR:H	2:B:809:MET:HE3	1.52	0.74
3:C:123:ASN:ND2	3:C:125:MET:HG2	2.01	0.74
3:C:259:LEU:HD21	11:K:91:CYS:HB3	1.69	0.74
1:A:1033:GLN:HA	1:A:1036:ARG:HH12	1.52	0.74
2:B:408:LEU:O	2:B:412:LEU:HD12	1.87	0.74
2:B:593:PRO:HG2	2:B:617:ARG:NH2	2.02	0.74
8:H:130:ARG:HD3	8:H:130:ARG:N	2.02	0.74
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.23	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:886:ILE:HG23	1:A:887:GLY:N	2.03	0.74
3:C:115:SER:HB3	3:C:141:GLY:O	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:THR:HG22	1:A:710:LEU:H	1.53	0.74
2:B:549:THR:HB	2:B:628:THR:OG1	1.87	0.74
1:A:399:HIS:O	1:A:401:GLY:N	2.20	0.74
3:C:99:LEU:HD23	3:C:99:LEU:N	2.02	0.74
9:I:85:PHE:HD2	9:I:85:PHE:H	1.35	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
1:A:821:ARG:HB2	1:A:821:ARG:HH11	1.53	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
8:H:130:ARG:H	8:H:130:ARG:HH11	1.35	0.74
11:K:46:ILE:O	11:K:50:LEU:HB2	1.88	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
2:B:1039:GLY:HA2	10:J:51:LEU:HD21	1.66	0.74
15:P:5:C:O2'	15:P:6:A:H5'	1.88	0.74
2:B:68:THR:HG22	2:B:91:SER:HA	1.70	0.74
4:D:71:LYS:HA	4:D:74:GLN:HG3	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
1:A:288:ALA:HA	1:A:291:GLU:OE1	1.89	0.73
10:J:64:ASN:HB3	10:J:65:PRO:HD3	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:637:LEU:HD12	2:B:693:ILE:HD11	1.69	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
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: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
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
12:L:55:ILE:O	12:L:56:LEU:HB2	1.88	0.73
1:A:399:HIS:HB3	1:A:400:PRO:CD	2.18	0.73
1:A:93:VAL:CG2	1:A:301:ALA:HA	2.17	0.73
2:B:110:HIS:HB3	12:L:54:ARG:HH22	1.51	0.73
2:B:622:LYS:HE2	9:I:59:VAL:CG2	2.19	0.73
2:B:918:ILE:HG21	2:B:935:ARG:NH2	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:189:THR:HG22	3:C:190:ASP:N	2.01	0.73
12:L:53:HIS:HB3	12:L:55:ILE:CD1	2.18	0.73
1:A:549:MET:HE3	1:A:656:TRP:CD1	2.21	0.73
1:A:898:ARG:HD2	1:A:899:VAL:N	2.04	0.73
2:B:219:ALA:HB2	2:B:405:ARG:NH1	2.03	0.73
2:B:557:PHE:O	2:B:557:PHE:HD2	1.72	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
4:D:7:THR:O	4:D:9:GLN:N	2.21	0.73
12:L:30:ILE:O	12:L:56:LEU:HD23	1.88	0.73
1:A:1329:THR:HG22	1:A:1331:SER:N	2.03	0.73
1:A:157:ASP:OD2	1:A:159:THR:HB	1.88	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: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
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
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:186:GLU:HG3	10:J:62:ARG:HH22	1.52	0.72
2:B:842:ASN:ND2	2:B:845:SER:H	1.86	0.72
2:B:1201:LYS:HE2	2:B:1205:GLN:OE1	1.89	0.72
11:K:12:LEU:HD12	11:K:37:LYS:HG2	1.71	0.72
14:T:16:DT:H2''	14:T:17:DT:C5'	2.20	0.72
2:B:134:LYS:HE2	2:B:164:LYS:NZ	2.04	0.72
2:B:865:LYS:NZ	2:B:869:SER:HA	2.04	0.72
5:E:164:LEU:HD13	5:E:211:TYR:CE2	2.25	0.72
6:F:103:MET:HE1	7:G:66:GLY:H	1.53	0.72
1:A:66:LYS:HD3	1:A:67:CYS:N	2.05	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
7:G:1:MET:SD	7:G:2:PHE:N	2.62	0.72
1:A:236:LEU:HD11	1:A:304:MET:HE1	1.71	0.72
2:B:1072:MET:CE	2:B:1085:ILE:HB	2.20	0.72
3:C:167:HIS:CD2	12:L:70:ARG:HB3	2.24	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
1:A:310:GLY:O	1:A:312:PRO:HD2	1.88	0.72
2:B:515:HIS:CD2	2:B:517:THR:HG23	2.25	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:800:GLN:HB3	10:J:52:THR:HG21	1.69	0.72
11:K:45:LEU:HG	11:K:94:ILE:HD13	1.71	0.72
1:A:425:GLN:N	1:A:425:GLN:OE1	2.22	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
2:B:705:MET:H	2:B:710:LEU:HD12	1.54	0.72
4:D:160:VAL:O	4:D:164:ILE:HG13	1.89	0.72
8:H:11:GLN:HA	8:H:53:ASP:O	1.89	0.72
1:A:666:ILE:CD1	1:A:667:GLY:H	2.02	0.72
1:A:858:ASN:ND2	1:A:860:LEU:H	1.88	0.72
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:1205:LYS:O	1:A:1207:LEU:HG	1.89	0.72
1:A:1387:HIS:O	1:A:1391:ARG:HD3	1.90	0.72
1:A:34:LYS:HZ1	1:A:57:ARG:NH2	1.87	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
12:L:55:ILE:HD13	12:L:55:ILE:H	1.55	0.72
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:644:GLU:OE2	2:B:646:LEU:HB2	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
7:G:111:THR:CG2	7:G:114:LEU:HD13	2.20	0.71
8:H:102:TYR:OH	8:H:122:LEU:HD22	1.89	0.71
1:A:37:PHE:HB2	1:A:52:GLY:HA3	1.72	0.71
2:B:758:PHE:CE1	2:B:1027:ILE:HG22	2.25	0.71
12:L:32:ALA:HB2	12:L:55:ILE:HG13	1.73	0.71
1:A:1118:VAL:CG2	1:A:1306:LEU:HB2	2.20	0.71
1:A:135:PHE:CD1	1:A:222:LEU:HD22	2.24	0.71
1:A:305:ASP:OD2	1:A:326:ARG:HD3	1.90	0.71
1:A:960:ILE:O	1:A:963:ILE:HG22	1.90	0.71
3:C:76:ASP:OD2	3:C:128:ASN:N	2.24	0.71
10:J:64:ASN:HB3	10:J:65:PRO:HD2	1.73	0.71
2:B:1096:ARG:O	2:B:1097:HIS:HB2	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:THR:HG22	1:A:383:TYR:N	2.03	0.71
2:B:345:LYS:CG	2:B:346:GLU:H	1.99	0.71
3:C:56:THR:HG22	3:C:57:VAL:H	1.54	0.71
1:A:503:GLN:HE21	6:F:90:ARG:HH22	1.34	0.71
1:A:344:ARG:NH1	1:A:344:ARG:HB3	2.06	0.71
2:B:1031:LEU:HD11	2:B:1042:GLY:HA3	1.73	0.71
2:B:248:SER:H	2:B:418:LYS:NZ	1.88	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
5:E:100:ILE:HG23	5:E:105:PHE:HB2	1.72	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
1:A:670:ILE:HG23	1:A:805:LEU:HD21	1.73	0.70
2:B:424:LEU:O	2:B:428:ILE:HG13	1.90	0.70
3:C:220:ASP:CG	3:C:223:ALA:HB2	2.11	0.70
4:D:24:ALA:CB	4:D:26:THR:HG23	2.21	0.70
5:E:197:LYS:HE2	5:E:199:ILE:HD11	1.73	0.70
8:H:24:CYS:HB2	8:H:44:VAL:HG21	1.72	0.70
9:I:71:SER:OG	9:I:83:ASN:HB2	1.92	0.70
3:C:66:ARG:NH2	10:J:3:VAL:O	2.24	0.70
11:K:68:PHE:HD1	11:K:70:ARG:HH12	1.39	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
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
2:B:983:ARG:NH1	2:B:1028:GLU:OE1	2.24	0.70
7:G:34:VAL:HG11	7:G:74:TYR:CE1	2.21	0.70
1:A:1148:ILE:HD11	1:A:1198:ASP:HA	1.74	0.70
1:A:1244:ARG:HB2	1:A:1245:PRO:CD	2.22	0.70
1:A:444:PHE:HB3	1:A:458:HIS:HD2	1.56	0.70
2:B:842:ASN:ND2	2:B:845:SER:OG	2.24	0.70
1:A:763:ALA:O	1:A:803:SER:HB3	1.91	0.70
2:B:705:MET:N	2:B:710:LEU:HD12	2.05	0.70
2:B:980:PHE:HE1	2:B:990:ILE:HD11	1.56	0.70
3:C:11:ARG:HH12	3:C:205:LYS:NZ	1.90	0.70
9:I:55:THR:HG23	9:I:86:PHE:HZ	1.55	0.70
1:A:1081:LEU:HD11	1:A:1098:VAL:H	1.55	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:29:ASP:HB3	2:B:658:ILE:CD1	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:616:ILE:HG12	2:B:697:GLU:HA	1.72	0.70
3:C:93:ASP:OD1	3:C:122:SER:HB2	1.92	0.70
12:L:27:LEU:HD13	12:L:37:LYS:HD2	1.74	0.70
1:A:244:PRO:HB2	1:A:245:PRO:CD	2.18	0.70
1:A:828:ALA:CB	2:B:530:GLY:HA2	2.21	0.70
2:B:235:SER:C	2:B:236:HIS:HD2	1.95	0.70
2:B:681:TRP:HA	2:B:684:LEU:HD12	1.74	0.70
2:B:859:TYR:CZ	2:B:941:LEU:HD12	2.26	0.70
4:D:71:LYS:HG2	4:D:74:GLN:HG3	1.74	0.70
1:A:1004:ASN:ND2	5:E:167:ARG:HD2	2.07	0.70
12:L:38:LEU:HD11	12:L:49:LYS:HE2	1.74	0.70
2:B:1122:ARG:HB3	14:T:22:DC:OP1	1.92	0.70
3:C:143:LEU:HD21	3:C:146:LYS:HE2	1.73	0.70
5:E:202:SER:OG	5:E:204:THR:HG22	1.90	0.70
9:I:55:THR:HG21	9:I:109:ILE:HD13	1.73	0.70
1:A:866:PHE:O	1:A:867:ILE:HD12	1.91	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:883:LEU:HD11	1:A:1017:LEU:HD11	1.73	0.69
1:A:567:LYS:HE3	1:A:568:PRO:CG	2.21	0.69
2:B:345:LYS:O	2:B:347:LYS:HG2	1.92	0.69
1:A:1436:ILE:O	1:A:1437:GLY:C	2.30	0.69
3:C:186:LEU:CD2	3:C:225:ALA:HB2	2.22	0.69
8:H:4:THR:HA	8:H:60:ALA:CB	2.17	0.69
11:K:107:THR:O	11:K:111:LEU:HG	1.92	0.69
1:A:500:GLU:O	1:A:504:LEU:HB2	1.93	0.69
1:A:567:LYS:CG	1:A:568:PRO:HD2	2.22	0.69
1:A:982:THR:HB	1:A:985:ASP:H	1.56	0.69
2:B:217:ARG:HE	2:B:405:ARG:HB2	1.57	0.69
1:A:1155:ASP:OD2	1:A:1161:THR:HA	1.93	0.69
1:A:53:LEU:CD2	1:A:54:ASN:N	2.50	0.69
11:K:55:LYS:HB3	11:K:81:TYR:HD1	1.57	0.69
3:C:89:GLU:O	3:C:90:ASP:HB3	1.93	0.69
5:E:23:VAL:HG13	5:E:78:LEU:HD13	1.74	0.69
5:E:90:VAL:HB	5:E:117:THR:HG21	1.73	0.69
7:G:51:TYR:O	7:G:54:ILE:HG13	1.91	0.69
2:B:839:MET:HE1	2:B:980:PHE:HB2	1.75	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
5:E:164:LEU:HD22	5:E:211:TYR:CD2	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:86:THR:HG23	6:F:89:GLU:OE1	1.92	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
9:I:102:VAL:HG22	9:I:109:ILE:HG12	1.73	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:1291:VAL:HG22	1:A:1292:PRO:CD	2.23	0.69
1:A:351:THR:HG22	2:B:1103:ILE:CA	2.23	0.69
8:H:58:THR:HB	8:H:143:LEU:HD13	1.73	0.69
1:A:105:CYS:SG	1:A:139:TRP:HA	2.32	0.69
1:A:916:GLY:O	1:A:919:ILE:HG22	1.93	0.69
3:C:186:LEU:HD21	3:C:225:ALA:HB2	1.74	0.69
4:D:23:ASN:N	4:D:23:ASN:HD22	1.91	0.69
12:L:30:ILE:HG22	12:L:31:CYS:N	2.07	0.69
1:A:1420:ASP:O	1:A:1421:CYS:HB2	1.93	0.69
1:A:249:SER:O	1:A:250:ILE:HG13	1.91	0.69
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.75	0.69
2:B:1002:THR:OG1	2:B:1006:ILE:HG13	1.93	0.69
1:A:7:SER:OG	2:B:1161:HIS:HE1	1.75	0.69
2:B:60:GLN:O	2:B:63:ILE:HG22	1.93	0.69
2:B:957:ASN:HD21	2:B:961:LEU:HB2	1.58	0.69
3:C:133:ILE:HD12	3:C:237:SER:N	2.08	0.69
1:A:1095:THR:HG21	1:A:1112:LYS:CB	2.23	0.68
1:A:512:VAL:HA	1:A:519:PRO:HA	1.75	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
8:H:76:THR:O	8:H:77:ARG:HB2	1.92	0.68
1:A:1312:ASN:ND2	1:A:1315:GLU:HG3	2.08	0.68
1:A:444:PHE:HB3	1:A:458:HIS:CD2	2.27	0.68
1:A:853:ASP:O	1:A:854:ASN:HB2	1.92	0.68
2:B:805:THR:HG22	2:B:806:THR:N	2.07	0.68
6:F:109:VAL:HG12	6:F:110:ASP:N	2.05	0.68
7:G:21:ARG:HD2	7:G:24:GLN:CB	2.23	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: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
1:A:567:LYS:CB	1:A:568:PRO:CD	2.69	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LYS:HB3	8:H:95:TYR:HA	1.74	0.68
4:D:50:LEU:HD11	7:G:4:ILE:HD11	1.74	0.68
1:A:167:CYS:HB2	1:A:169:ASN:ND2	2.08	0.68
2:B:737:THR:CG2	9:I:66:PRO:HA	2.23	0.68
2:B:891:ASP:C	2:B:893:LEU:H	1.97	0.68
2:B:987:LYS:HD3	2:B:987:LYS:H	1.57	0.68
3:C:147:LEU:HB2	3:C:151:GLN:HB2	1.74	0.68
2:B:873:THR:O	2:B:914:LYS:HA	1.93	0.68
5:E:124:VAL:N	5:E:125:PRO:HD2	2.09	0.68
14:T:11:DA:H2''	14:T:12:DG:H5'	1.75	0.68
1:A:1121:GLU:CG	1:A:1122:PRO:HD2	2.22	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:1029:ARG:HG3	1:A:1029:ARG:HH11	1.59	0.68
1:A:1188:GLN:OE1	1:A:1241:ARG:HD2	1.93	0.68
1:A:1100:ARG:HH21	1:A:1351:GLU:CG	2.06	0.68
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.75	0.68
2:B:23:ALA:HB1	2:B:24:PRO:HD2	1.76	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
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:154:SER:HB3	1:A:162:VAL:CG2	2.24	0.68
2:B:237:VAL:HG22	2:B:257:LYS:HA	1.75	0.68
4:D:24:ALA:HB3	4:D:26:THR:CG2	2.24	0.68
1:A:709:THR:HG23	9:I:94:ASP:HA	1.75	0.68
12:L:48:CYS:HB3	12:L:51:CYS:O	1.93	0.68
1:A:1127:ASP:CG	1:A:1130:GLN:HB2	2.13	0.68
1:A:117:GLU:H	1:A:117:GLU:CD	1.96	0.68
1:A:107:CYS:SG	1:A:148:CYS:HB2	2.34	0.68
2:B:464:GLY:O	2:B:477:ALA:HA	1.94	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:1158:PRO:HG2	1:A:1159:ARG:NE	2.09	0.67
1:A:152:VAL:CG1	1:A:153:PRO:HD2	2.24	0.67
1:A:709:THR:HB	1:A:712:GLU:H	1.59	0.67
1:A:858:ASN:C	1:A:858:ASN:HD22	1.98	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
1:A:284:ALA:O	1:A:286:HIS:N	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:59:ILE:HG21	4:D:145:MET:SD	2.35	0.67
1:A:34:LYS:HZ2	1:A:57:ARG:NH2	1.90	0.67
1:A:369:SER:HB3	11:K:2:ASN:OD1	1.93	0.67
2:B:589:VAL:HG12	2:B:590:HIS:N	2.10	0.67
10:J:3:VAL:HG21	10:J:18:TRP:CB	2.22	0.67
1:A:1323:ASP:OD1	1:A:1325:THR:HG22	1.94	0.67
1:A:66:LYS:HZ3	1:A:68:GLN:N	1.83	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
2:B:863:GLU:O	2:B:961:LEU:HD13	1.94	0.67
3:C:254:LYS:O	3:C:258:ILE:HD13	1.94	0.67
8:H:81:PRO:CB	8:H:82:PRO:HD2	2.24	0.67
1:A:1187:GLN:HA	1:A:1244:ARG:HB3	1.76	0.67
1:A:743:VAL:O	1:A:747:VAL:HG23	1.94	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: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
6:F:89:GLU:O	6:F:93:ILE:HD12	1.94	0.67
1:A:718:VAL:O	1:A:722:LEU:HD12	1.95	0.67
2:B:399:ASP:OD2	2:B:510:LYS:HB2	1.95	0.67
4:D:32:GLU:OE1	7:G:41:LYS:HE2	1.94	0.67
1:A:809:THR:OG1	1:A:812:GLU:HG3	1.94	0.67
2:B:291:ILE:HD13	2:B:300:HIS:CD2	2.30	0.67
2:B:68:THR:HG22	2:B:91:SER:HB3	1.77	0.67
2:B:863:GLU:OE2	2:B:873:THR:HA	1.94	0.67
2:B:899:ILE:HG22	2:B:900:ALA:O	1.95	0.67
8:H:30:SER:HB2	8:H:36:CYS:HB3	1.77	0.67
9:I:116:ASN:C	9:I:117:LYS:HD2	2.15	0.67
9:I:55:THR:HG23	9:I:86:PHE:CZ	2.30	0.67
2:B:515:HIS:H	2:B:518:HIS:HD2	1.43	0.66
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
9:I:50:THR:HG22	9:I:51:ASN:N	2.10	0.66
1:A:332:LYS:O	1:A:333:GLU:HB2	1.94	0.66
1:A:382:PRO:CA	1:A:428:TYR:HE2	2.07	0.66
1:A:567:LYS:CB	8:H:95:TYR:HA	2.24	0.66
1:A:925:LEU:HD13	1:A:983:ILE:CG2	2.24	0.66
2:B:1187:ASN:O	2:B:1188:LYS:CB	2.42	0.66
3:C:47:ASP:HA	12:L:69:ALA:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:55:THR:O	9:I:55:THR:HG22	1.94	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
1:A:122:MET:HA	1:A:141:LEU:CD1	2.25	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
2:B:917:PRO:O	2:B:918:ILE:HG13	1.95	0.66
9:I:8:ARG:HG3	9:I:34:TYR:CE1	2.30	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
3:C:161:LYS:O	3:C:170:TRP:NE1	2.27	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
1:A:446:ARG:HB3	1:A:478:TYR:HB3	1.77	0.66
1:A:866:PHE:C	1:A:867:ILE:HD12	2.15	0.66
3:C:184:ASN:OD1	3:C:187:LYS:HA	1.94	0.66
4:D:29:LEU:HD22	4:D:29:LEU:N	2.10	0.66
6:F:69:LEU:HD13	6:F:71:GLU:OE1	1.96	0.66
6:F:82:THR:CG2	6:F:84:TYR:H	2.09	0.66
8:H:89:LEU:C	8:H:91:ASP:N	2.47	0.66
10:J:44:TYR:HA	10:J:47:ARG:HB2	1.77	0.66
1:A:547:LEU:HD13	11:K:58:PHE:CD1	2.31	0.66
1:A:563:PRO:HD3	8:H:79:TRP:CD1	2.31	0.66
1:A:7:SER:HB3	2:B:1193:GLN:HE22	1.60	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:394:ASP:N	2:B:394:ASP:OD2	2.23	0.66
2:B:558:LEU:CD2	2:B:596:LEU:HD11	2.26	0.66
8:H:58:THR:HG22	8:H:59:ILE:H	1.60	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
2:B:110:HIS:HB2	12:L:54:ARG:NH2	2.10	0.66
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.78	0.66
2:B:69:LEU:HB3	2:B:429:PHE:HE1	1.61	0.66
5:E:19:VAL:O	5:E:23:VAL:HG23	1.95	0.66
5:E:48:ASP:HB3	5:E:54:GLN:NE2	2.10	0.66
1:A:1027:ALA:O	1:A:1031:VAL:HG23	1.96	0.66
1:A:23:SER:HA	1:A:233:TRP:CD1	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:PHE:HB3	1:A:265:LYS:HZ1	1.61	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
1:A:503:GLN:NE2	6:F:90:ARG:HH22	1.93	0.66
7:G:27:LYS:HD3	7:G:51:TYR:CE2	2.31	0.66
1:A:1424:VAL:HG11	2:B:1139:ILE:HD13	1.75	0.65
1:A:914:GLU:HB2	1:A:979:SER:O	1.96	0.65
2:B:1115:THR:O	2:B:1116:ARG:HB2	1.94	0.65
2:B:882:THR:HG23	2:B:884:ARG:CB	2.24	0.65
7:G:111:THR:HG23	7:G:114:LEU:HD13	1.77	0.65
8:H:82:PRO:C	8:H:84:ALA:H	1.98	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
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
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.77	0.65
2:B:37:PHE:CE1	2:B:41:LYS:HG3	2.31	0.65
2:B:654:ARG:H	2:B:657:HIS:CD2	2.12	0.65
2:B:654:ARG:HG3	2:B:654:ARG:HH11	1.61	0.65
4:D:156:ASP:O	4:D:158:GLU:N	2.30	0.65
9:I:6:PHE:N	9:I:6:PHE:CD1	2.64	0.65
12:L:30:ILE:O	12:L:56:LEU:HA	1.95	0.65
2:B:902:GLY:O	12:L:65:VAL:HG11	1.97	0.65
1:A:1313:LEU:O	1:A:1315:GLU:N	2.30	0.65
1:A:122:MET:HA	1:A:141:LEU:HD11	1.79	0.65
2:B:1001:PHE:CE2	3:C:34:ARG:NE	2.65	0.65
2:B:1124:ARG:HB3	2:B:1124:ARG:HH11	1.60	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
10:J:27:GLU:O	10:J:29:GLU:HG3	1.95	0.65
1:A:1149:ALA:CB	9:I:47:GLU:HA	2.26	0.65
1:A:1255:GLU:HG2	1:A:1258:HIS:CD2	2.31	0.65
1:A:1195:LEU:HD11	1:A:1267:MET:CE	2.27	0.65
2:B:65:GLU:OE1	2:B:418:LYS:HE3	1.97	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
7:G:27:LYS:HG2	7:G:54:ILE:HD12	1.77	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
1:A:709:THR:HG22	1:A:710:LEU:N	2.10	0.65
2:B:189:LEU:O	2:B:192:LEU:N	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:34:ARG:NH1	3:C:35:ARG:HG2	2.12	0.65
3:C:73:GLN:HE21	3:C:75:MET:N	1.93	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
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
1:A:90:VAL:HG11	1:A:297:GLN:HA	1.77	0.65
1:A:66:LYS:O	1:A:67:CYS:HB2	1.96	0.65
2:B:978:ASP:OD2	2:B:1098:MET:HG2	1.96	0.65
1:A:341:MET:HE1	2:B:1135:ARG:NH1	2.12	0.65
2:B:243:ALA:CB	2:B:251:ILE:HD13	2.21	0.65
2:B:516:ASN:ND2	2:B:516:ASN:N	2.44	0.65
4:D:12:ARG:HG2	4:D:12:ARG:HH11	1.61	0.65
5:E:17:ARG:O	5:E:20:LYS:HB2	1.97	0.65
1:A:102:VAL:HB	1:A:211:PHE:CE1	2.32	0.65
1:A:1313:LEU:HD23	1:A:1338:VAL:HG21	1.77	0.65
2:B:193:LYS:HZ2	12:L:32:ALA:HB1	1.60	0.65
4:D:66:ARG:HD2	4:D:133:THR:HB	1.78	0.65
5:E:176:PRO:O	5:E:212:ARG:HA	1.97	0.65
6:F:82:THR:HG22	6:F:84:TYR:N	2.09	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:1130:GLN:O	1:A:1134:ILE:HG13	1.97	0.65
1:A:37:PHE:N	1:A:37:PHE:CD1	2.64	0.65
1:A:67:CYS:C	1:A:68:GLN:HG3	2.17	0.65
1:A:903:ASN:HD22	1:A:904:THR:H	1.45	0.65
2:B:944:THR:HG21	2:B:1122:ARG:NH2	2.12	0.65
2:B:955:THR:CG2	2:B:956:THR:N	2.60	0.65
4:D:124:GLU:CD	4:D:124:GLU:H	2.00	0.65
7:G:27:LYS:HE2	7:G:54:ILE:HB	1.78	0.65
2:B:1037:LEU:HD21	2:B:1064:TYR:HE1	1.62	0.65
1:A:7:SER:HB3	2:B:1193:GLN:NE2	2.11	0.65
2:B:378:LEU:HD12	2:B:378:LEU:O	1.97	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
1:A:567:LYS:HZ3	8:H:46:LEU:HB2	1.61	0.65
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.79	0.65
2:B:25:ILE:CG2	2:B:658:ILE:HD12	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1352:VAL:O	1:A:1355:VAL:HG12	1.96	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
2:B:102:VAL:CG2	2:B:112:LEU:HB2	2.27	0.64
2:B:90:ILE:HD11	2:B:432:MET:SD	2.38	0.64
4:D:56:ARG:HA	4:D:148:LEU:HD13	1.78	0.64
5:E:98:ILE:HA	5:E:101:GLN:HB3	1.79	0.64
7:G:116:PRO:HD2	7:G:119:LEU:HD23	1.79	0.64
12:L:55:ILE:HG12	12:L:56:LEU:N	2.11	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
3:C:244:VAL:O	3:C:248:ILE:HG13	1.98	0.64
1:A:961:ARG:HG2	1:A:965:GLN:HE21	1.62	0.64
4:D:156:ASP:C	4:D:158:GLU:H	2.01	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
1:A:390:GLN:NE2	1:A:394:ASN:HD22	1.95	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
3:C:31:ASN:OD1	3:C:34:ARG:HD3	1.97	0.64
4:D:144:THR:O	4:D:148:LEU:HB2	1.97	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
1:A:55:ASP:C	1:A:57:ARG:N	2.47	0.64
2:B:102:VAL:HG22	2:B:112:LEU:HD22	1.79	0.64
2:B:56:ASP:HB3	2:B:57:TYR:CD1	2.32	0.64
4:D:119:ARG:NH1	4:D:119:ARG:HG3	2.12	0.64
7:G:9:LEU:HD12	7:G:10:ASN:N	2.13	0.64
8:H:84:ALA:CB	8:H:87:ARG:HD2	2.27	0.64
1:A:356:ASP:OD2	11:K:65:HIS:HE1	1.81	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
1:A:35:ILE:HG22	1:A:35:ILE:O	1.96	0.64
1:A:535:THR:CG2	1:A:616:VAL:HA	2.27	0.64
2:B:1159:ARG:NH1	2:B:1159:ARG:HB3	2.12	0.64
2:B:98:THR:HG23	2:B:127:GLY:O	1.98	0.64
2:B:885:MET:HA	2:B:936:ASP:CB	2.26	0.64
5:E:127:ILE:O	5:E:127:ILE:HG13	1.96	0.64
7:G:111:THR:O	7:G:114:LEU:N	2.28	0.64
14:T:18:DC:H2"	14:T:19:DT:OP2	1.97	0.64
1:A:153:PRO:HD3	1:A:161:LEU:HD13	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:596:THR:O	1:A:598:LEU:N	2.31	0.64
2:B:1181:GLU:HB2	2:B:1188:LYS:HG3	1.79	0.64
2:B:597:MET:HA	2:B:597:MET:CE	2.27	0.64
2:B:916:THR:HB	2:B:935:ARG:HD2	1.80	0.64
4:D:145:MET:O	4:D:149:THR:HB	1.96	0.64
4:D:66:ARG:O	4:D:70:PHE:HB2	1.98	0.64
5:E:128:PRO:HA	5:E:129:PRO:C	2.18	0.64
5:E:144:ILE:HG13	5:E:145:THR:H	1.61	0.64
1:A:1444:MET:HG3	7:G:59:GLY:O	1.97	0.64
1:A:1445:ILE:HD11	7:G:68:ALA:HB1	1.80	0.64
1:A:858:ASN:HD21	1:A:860:LEU:HB2	1.63	0.64
2:B:515:HIS:H	2:B:518:HIS:CD2	2.16	0.64
3:C:196:ASP:OD2	3:C:199:LYS:HE3	1.98	0.64
7:G:116:PRO:HG2	7:G:119:LEU:HB3	1.78	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
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:426:LYS:O	2:B:426:LYS:HG3	1.97	0.64
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.79	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:478:TYR:O	1:A:479:ASN:HB2	1.97	0.63
1:A:794:PRO:HG2	1:A:795:GLU:OE2	1.98	0.63
2:B:364:ILE:O	2:B:365:THR:HB	1.97	0.63
3:C:120:ILE:CD1	3:C:124:LEU:HD11	2.27	0.63
5:E:48:ASP:CG	5:E:49:SER:H	2.01	0.63
7:G:112:LYS:HA	7:G:115:MET:CE	2.28	0.63
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.81	0.63
1:A:1341:ILE:HD12	1:A:1379:GLY:O	1.97	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
3:C:100:THR:HG21	3:C:102:GLN:HE21	1.64	0.63
4:D:138:ASN:HB3	4:D:141:LEU:HB3	1.80	0.63
5:E:28:TYR:C	5:E:65:THR:HG22	2.19	0.63
1:A:984:LYS:HG2	1:A:988:LEU:HD11	1.80	0.63
2:B:95:ILE:CG1	2:B:130:VAL:HG22	2.29	0.63
2:B:221:ASN:O	2:B:222:ILE:HG13	1.99	0.63
2:B:289:LEU:HD13	2:B:375:ALA:CB	2.25	0.63
2:B:805:THR:HA	2:B:809:MET:HE1	1.80	0.63
2:B:879:ARG:NH2	2:B:885:MET:HE2	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:ILE:HG13	2:B:130:VAL:HG22	1.78	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
4:D:35:LEU:HD11	4:D:173:HIS:CD2	2.33	0.63
4:D:179:GLN:OE1	4:D:179:GLN:HA	1.97	0.63
7:G:87:VAL:HG23	7:G:103:VAL:HG21	1.79	0.63
11:K:55:LYS:HB3	11:K:81:TYR:CD1	2.33	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
9:I:58:VAL:HG13	9:I:62:ILE:CD1	2.29	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
2:B:798:TYR:CE2	3:C:62:PHE:CE2	2.82	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
1:A:1094:VAL:HG13	1:A:1113:THR:CG2	2.28	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
3:C:11:ARG:HH12	3:C:205:LYS:CE	2.11	0.63
4:D:123:LEU:O	4:D:127:ASP:HB2	1.99	0.63
8:H:56:THR:HB	8:H:145:ARG:HG2	1.79	0.63
1:A:441:PRO:HD2	1:A:498:ARG:NH2	2.13	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
2:B:579:ARG:HH11	2:B:579:ARG:HG2	1.64	0.63
4:D:190:GLU:C	4:D:193:THR:HG22	2.19	0.63
1:A:1313:LEU:C	1:A:1315:GLU:H	2.02	0.63
1:A:134:ARG:HD2	1:A:221:SER:O	1.98	0.63
1:A:37:PHE:HD1	1:A:37:PHE:N	1.97	0.63
2:B:839:MET:CE	2:B:1010:LEU:HD21	2.28	0.63
2:B:259:TYR:HB2	2:B:268:THR:HG23	1.80	0.63
2:B:577:ALA:HB1	2:B:589:VAL:CG1	2.17	0.63
2:B:56:ASP:HB3	2:B:57:TYR:HD1	1.63	0.63
1:A:1444:MET:HE1	6:F:135:ARG:HB2	1.79	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
2:B:999:MET:HE3	2:B:999:MET:HA	1.80	0.63
5:E:84:ASP:O	5:E:86:PRO:HD3	1.97	0.63
7:G:91:VAL:HG23	7:G:141:SER:O	1.98	0.63
11:K:31:VAL:HG12	11:K:32:VAL:N	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:PHE:H	2:B:1107:ALA:HA	1.63	0.62
1:A:390:GLN:O	1:A:394:ASN:HB2	1.99	0.62
1:A:875:ALA:HA	1:A:878:ILE:HD12	1.81	0.62
2:B:995:ARG:NH1	3:C:165:LYS:HG2	2.14	0.62
3:C:163:ILE:HG13	3:C:165:LYS:H	1.64	0.62
3:C:179:GLU:HG2	3:C:180:TYR:N	2.14	0.62
12:L:53:HIS:HB3	12:L:55:ILE:HD11	1.80	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
2:B:891:ASP:O	2:B:893:LEU:N	2.32	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
11:K:82:ASP:OD1	11:K:84:LYS:N	2.32	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: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:11:LEU:HB2	2:B:1193:GLN:HG2	1.81	0.62
1:A:443:LEU:HD12	2:B:1146:PHE:CZ	2.34	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
2:B:987:LYS:HG3	15:P:11:G:O2'	1.99	0.62
1:A:1239:ARG:HH22	1:A:1241:ARG:HH22	1.45	0.62
1:A:1420:ASP:OD2	1:A:1420:ASP:N	2.31	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
1:A:694:THR:O	1:A:698:GLN:HG3	1.98	0.62
1:A:831:THR:CG2	1:A:832:ALA:H	2.13	0.62
2:B:293:PRO:HG2	2:B:296:GLU:HB3	1.81	0.62
2:B:168:GLY:HA2	2:B:454:THR:OG1	2.00	0.62
2:B:637:LEU:CD2	2:B:742:GLU:HA	2.30	0.62
2:B:654:ARG:N	2:B:657:HIS:HD2	1.96	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
10:J:9:SER:HB2	10:J:45:CYS:HB2	1.82	0.62
1:A:596:THR:C	1:A:598:LEU:H	2.03	0.62
2:B:616:ILE:HD12	2:B:616:ILE:N	2.14	0.62
2:B:844:SER:O	2:B:847:ASP:HB2	2.00	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
8:H:11:GLN:O	8:H:28:ALA:HB1	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:3:VAL:HA	10:J:53:HIS:ND1	2.14	0.62
12:L:26:THR:CG2	12:L:27:LEU:N	2.63	0.62
1:A:1171:GLN:O	1:A:1174:PHE:HB2	2.00	0.62
1:A:41:MET:HB2	1:A:49:LYS:HA	1.81	0.62
2:B:345:LYS:N	2:B:347:LYS:HE2	2.15	0.62
2:B:957:ASN:O	2:B:959:ASP:N	2.33	0.62
3:C:34:ARG:HH11	3:C:35:ARG:HG2	1.64	0.62
3:C:92:CYS:SG	3:C:94:LYS:HB3	2.40	0.62
4:D:192:LYS:HD2	4:D:199:ASN:HA	1.81	0.62
9:I:93:LYS:HD3	9:I:93:LYS:N	2.15	0.62
2:B:954:VAL:O	12:L:55:ILE:O	2.16	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
1:A:718:VAL:HG12	1:A:722:LEU:HD11	1.81	0.62
1:A:984:LYS:HG2	1:A:988:LEU:CD1	2.30	0.62
2:B:466:TRP:O	2:B:468:GLU:N	2.33	0.62
2:B:582:VAL:HG23	2:B:626:ILE:HB	1.80	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
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
1:A:782:ARG:NH2	2:B:699:GLU:O	2.33	0.62
3:C:148:ARG:H	3:C:151:GLN:HG3	1.65	0.62
5:E:99:HIS:O	5:E:103:LYS:HG2	1.99	0.62
3:C:235:VAL:HG13	10:J:13:VAL:HG22	1.82	0.62
1:A:1218:GLN:O	1:A:1221:LYS:HG3	2.00	0.62
1:A:75:ASN:HD22	2:B:1116:ARG:NH1	1.97	0.62
2:B:642:ASP:CA	2:B:649:LYS:HA	2.30	0.62
1:A:873:MET:C	1:A:1058:VAL:HG23	2.19	0.61
1:A:1170:ILE:N	1:A:1170:ILE:HD12	2.13	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
7:G:112:LYS:HA	7:G:115:MET:HE3	1.80	0.61
7:G:132:SER:HB3	7:G:135:ASP:H	1.65	0.61
9:I:84:VAL:O	9:I:84:VAL:HG13	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
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
1:A:69:THR:O	1:A:71:GLN:HG3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:774:ARG:HB2	1:A:797:LYS:O	2.01	0.61
2:B:305:VAL:HG12	2:B:305:VAL:O	1.99	0.61
4:D:4:SER:O	4:D:5:THR:CB	2.47	0.61
10:J:44:TYR:HD2	10:J:44:TYR:H	1.48	0.61
1:A:150:THR:HG23	1:A:166:GLY:HA2	1.81	0.61
1:A:23:SER:HB3	1:A:233:TRP:CZ2	2.35	0.61
1:A:2:VAL:HG22	1:A:3:GLY:H	1.66	0.61
1:A:661:GLY:HA3	2:B:1081:LEU:HD22	1.81	0.61
2:B:465:ASN:N	2:B:465:ASN:ND2	2.45	0.61
2:B:617:ARG:HA	2:B:624:LEU:HD12	1.83	0.61
2:B:953:LEU:CD2	2:B:965:LYS:HB2	2.30	0.61
4:D:195:ILE:CG2	4:D:198:LEU:HG	2.31	0.61
8:H:5:LEU:HG	8:H:60:ALA:HA	1.83	0.61
9:I:44:TYR:HD1	9:I:45:ARG:N	1.98	0.61
9:I:50:THR:CG2	9:I:52:ILE:HG12	2.30	0.61
1:A:1150:SER:HB3	1:A:1195:LEU:CD2	2.31	0.61
1:A:288:ALA:HA	1:A:291:GLU:CG	2.30	0.61
1:A:768:GLN:CG	1:A:816:HIS:HA	2.28	0.61
4:D:12:ARG:NH1	4:D:14:ARG:HA	2.15	0.61
7:G:26:LEU:HD11	7:G:70:PHE:CD1	2.35	0.61
9:I:101:PHE:N	9:I:101:PHE:CD1	2.68	0.61
10:J:1:MET:H1	10:J:56:LEU:N	1.98	0.61
1:A:482:PHE:CE1	2:B:836:GLU:HB2	2.35	0.61
1:A:898:ARG:HD3	1:A:933:TYR:CD1	2.36	0.61
2:B:218:SER:CB	2:B:241:ARG:HH12	2.14	0.61
6:F:103:MET:O	6:F:104:ASN:HB2	2.01	0.61
6:F:90:ARG:HD3	6:F:155:LEU:CD1	2.22	0.61
2:B:290:GLY:O	2:B:292:ILE:HG13	2.01	0.61
2:B:906:SER:HA	2:B:946:ASN:HB2	1.82	0.61
3:C:11:ARG:HH12	3:C:205:LYS:HE2	1.66	0.61
3:C:50:GLU:OE1	12:L:64:LEU:HD13	2.00	0.61
4:D:207:LEU:O	4:D:207:LEU:HD12	2.00	0.61
6:F:109:VAL:HG11	6:F:123:LYS:HG2	1.81	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
2:B:637:LEU:HD11	2:B:703:ILE:HD13	1.81	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
8:H:38:LEU:HD12	8:H:124:ARG:O	2.01	0.61
1:A:1141:THR:CG2	1:A:1205:LYS:HD3	2.31	0.61
1:A:1227:ILE:HG22	1:A:1228:TRP:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1445:ILE:HD12	1:A:1445:ILE:N	2.08	0.61
1:A:517:ASN:HD22	1:A:1364:ASN:HD22	1.47	0.61
1:A:691:LEU:O	1:A:694:THR:HB	2.01	0.61
2:B:309:GLN:CD	9:I:52:ILE:HD11	2.21	0.61
2:B:360:PHE:CD2	2:B:361:LEU:HB2	2.35	0.61
2:B:123:THR:OG1	2:B:458:LYS:HE2	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
10:J:14:VAL:HG12	10:J:14:VAL:O	2.01	0.61
1:A:1241:ARG:O	1:A:1242:VAL:CG2	2.48	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
9:I:86:PHE:CE1	9:I:100:PHE:HB2	2.36	0.61
1:A:353:ILE:HG21	1:A:487:MET:HG3	1.81	0.60
2:B:313:MET:HE3	2:B:386:LEU:HD22	1.82	0.60
2:B:847:ASP:C	2:B:849:GLY:H	2.02	0.60
3:C:147:LEU:N	3:C:147:LEU:HD23	2.16	0.60
1:A:537:ARG:NH1	8:H:120:GLY:O	2.34	0.60
3:C:66:ARG:NH1	10:J:2:ILE:CG2	2.63	0.60
3:C:166:GLU:C	11:K:6:ARG:NH1	2.54	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
2:B:912:ILE:O	2:B:938:SER:HB3	2.01	0.60
6:F:90:ARG:NH1	6:F:94:LEU:HD11	2.15	0.60
1:A:1308:THR:CG2	1:A:1309:ASP:N	2.62	0.60
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:58:THR:HG22	8:H:59:ILE:N	2.15	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:66:LYS:NZ	1:A:68:GLN:N	2.46	0.60
1:A:870:GLU:HB2	5:E:204:THR:HG21	1.82	0.60
7:G:123:ALA:C	7:G:125:SER:H	2.04	0.60
7:G:55:ASP:OD1	7:G:57:GLN:HG3	2.02	0.60
8:H:143:LEU:N	8:H:143:LEU:HD12	2.17	0.60
9:I:73:ARG:HD2	9:I:101:PHE:CE2	2.35	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
1:A:54:ASN:HB3	1:A:247:ARG:HH22	1.67	0.60
1:A:869:GLY:O	5:E:204:THR:HG21	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:235:SER:OG	2:B:236:HIS:CD2	2.54	0.60
2:B:37:PHE:HE1	2:B:41:LYS:HG3	1.64	0.60
3:C:181:ASP:CG	3:C:186:LEU:HD13	2.21	0.60
3:C:97:VAL:HG12	3:C:99:LEU:CD2	2.32	0.60
4:D:155:ARG:HD3	4:D:221:TYR:CE1	2.37	0.60
6:F:75:PRO:O	6:F:77:ASP:O	2.19	0.60
1:A:1342:GLU:CG	5:E:198:ILE:HD13	2.32	0.60
2:B:205:ILE:N	2:B:205:ILE:HD12	2.17	0.60
2:B:284:ILE:HD13	2:B:324:ILE:HD12	1.84	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
7:G:126:ASN:C	7:G:126:ASN:HD22	2.05	0.60
9:I:46:HIS:CE1	9:I:48:LEU:HD23	2.37	0.60
9:I:61:ASP:C	9:I:63:GLY:H	2.05	0.60
11:K:94:ILE:O	11:K:98:LEU:HG	2.00	0.60
4:D:130:LEU:HD13	4:D:142:LYS:CD	2.32	0.60
6:F:130:ILE:HB	6:F:148:VAL:HG21	1.83	0.60
12:L:38:LEU:O	12:L:39:SER:HB3	2.02	0.60
1:A:302:THR:HA	1:A:305:ASP:O	2.02	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
2:B:781:PHE:HE2	2:B:795:ILE:HD11	1.65	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
5:E:37:LEU:CD1	5:E:41:ASP:HB2	2.31	0.60
7:G:85:GLU:HG2	7:G:87:VAL:HG13	1.83	0.60
1:A:100:LYS:HE2	1:A:104:GLU:OE2	2.01	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
1:A:718:VAL:O	1:A:721:PHE:HB2	2.01	0.60
1:A:351:THR:CG2	2:B:1103:ILE:HG13	2.32	0.60
3:C:33:LEU:O	3:C:33:LEU:HD12	2.01	0.60
5:E:192:ARG:HG3	5:E:192:ARG:HH11	1.67	0.60
8:H:65:LEU:H	8:H:65:LEU:HD23	1.66	0.60
8:H:84:ALA:O	8:H:85:GLY:C	2.41	0.60
10:J:21:TYR:HB2	10:J:39:LEU:CD1	2.32	0.60
2:B:1039:GLY:HA2	10:J:51:LEU:CD2	2.32	0.60
10:J:5:VAL:HG12	10:J:6:ARG:CG	2.32	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:1202:MET:CE	1:A:1212:VAL:HG21	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1144:LYS:HB2	1:A:1268:LEU:O	2.01	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:1441:PHE:CZ	6:F:89:GLU:HA	2.37	0.60
1:A:946:VAL:HG22	5:E:201:LYS:HD2	1.82	0.60
2:B:126:SER:CB	2:B:172:ILE:HD11	2.32	0.60
2:B:557:PHE:O	2:B:557:PHE:CD2	2.53	0.60
3:C:182:PRO:HD2	3:C:210:GLU:OE1	2.01	0.60
5:E:99:HIS:CE1	5:E:103:LYS:HG3	2.37	0.60
1:A:754:SER:H	1:A:757:ASN:ND2	1.98	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
2:B:559:SER:CA	2:B:563:MET:HB3	2.10	0.59
5:E:212:ARG:HH11	5:E:212:ARG:HG3	1.67	0.59
6:F:103:MET:HE2	7:G:66:GLY:H	1.66	0.59
4:D:29:LEU:HD12	7:G:82:PHE:CE2	2.37	0.59
1:A:385:ILE:HD11	1:A:426:LEU:HB2	1.82	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
2:B:872:GLU:CD	2:B:914:LYS:HE3	2.23	0.59
8:H:59:ILE:O	8:H:60:ALA:HB3	2.01	0.59
3:C:7:GLN:HG3	11:K:104:ASN:ND2	2.17	0.59
11:K:21:ILE:HG22	11:K:31:VAL:HG11	1.84	0.59
1:A:1148:ILE:HG12	1:A:1198:ASP:HB2	1.83	0.59
1:A:380:VAL:HG13	1:A:385:ILE:HG12	1.83	0.59
2:B:1031:LEU:HD11	2:B:1042:GLY:CA	2.32	0.59
2:B:68:THR:HA	2:B:90:ILE:O	2.02	0.59
2:B:781:PHE:HD2	2:B:781:PHE:H	1.49	0.59
3:C:35:ARG:NH1	11:K:41:THR:H	2.00	0.59
4:D:128:VAL:C	4:D:130:LEU:N	2.54	0.59
4:D:9:GLN:HG3	4:D:9:GLN:O	2.03	0.59
1:A:186:LYS:O	1:A:187:LYS:HB2	2.01	0.59
4:D:56:ARG:HD3	4:D:149:THR:HA	1.84	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
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
1:A:353:ILE:HD12	1:A:470:LEU:HD21	1.85	0.59
2:B:1007:VAL:CG2	2:B:1008:PRO:HD2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:208:GLU:O	3:C:210:GLU:N	2.36	0.59
3:C:258:ILE:HD11	11:K:42:LEU:HD21	1.83	0.59
4:D:51:ASN:O	4:D:52:LEU:O	2.20	0.59
8:H:30:SER:CB	8:H:36:CYS:HB3	2.32	0.59
1:A:1094:VAL:HG13	1:A:1113:THR:HG21	1.84	0.59
1:A:102:VAL:HG11	1:A:211:PHE:HE1	1.68	0.59
1:A:87:ALA:CB	1:A:276:LEU:HD23	2.27	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
2:B:1102:LYS:O	2:B:1103:ILE:C	2.41	0.59
2:B:120:ARG:NH1	12:L:54:ARG:HH11	2.01	0.59
2:B:745:PRO:O	2:B:747:MET:N	2.36	0.59
7:G:49:LEU:HG	7:G:76:ALA:HA	1.84	0.59
1:A:567:LYS:HD2	8:H:95:TYR:CG	2.38	0.59
1:A:447:GLN:NE2	14:T:20:DG:H4'	2.17	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:1084:GLN:NE2	2:B:1084:GLN:N	2.51	0.59
2:B:248:SER:N	2:B:418:LYS:HZ3	2.00	0.59
2:B:297:ILE:HG22	2:B:298:LEU:HD22	1.85	0.59
2:B:549:THR:HG22	2:B:550:ASP:H	1.66	0.59
11:K:57:LEU:HB2	11:K:76:GLN:HG2	1.84	0.59
1:A:1325:THR:HG22	1:A:1326:ARG:HG3	1.82	0.59
1:A:671:ALA:O	1:A:676:MET:HE2	2.02	0.59
1:A:964:ILE:O	1:A:967:ALA:HB3	2.03	0.59
1:A:981:LEU:CD2	1:A:1039:LYS:HA	2.32	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:1015:VAL:HG12	1:A:1019:CYS:SG	2.43	0.59
1:A:444:PHE:CB	1:A:458:HIS:HD2	2.16	0.59
1:A:88:LYS:HG3	1:A:276:LEU:HD21	1.85	0.59
2:B:240:ILE:CG2	2:B:254:LEU:HB3	2.33	0.59
2:B:732:SER:HB2	2:B:734:HIS:NE2	2.18	0.59
2:B:911:ILE:HD11	2:B:941:LEU:CD1	2.31	0.59
6:F:69:LEU:HB3	6:F:71:GLU:OE2	2.02	0.59
15:P:10:U:H5'	15:P:11:G:C3'	2.33	0.59
1:A:416:ARG:HH11	1:A:417:TYR:HE1	1.51	0.59
1:A:476:SER:OG	1:A:477:PRO:HD3	2.03	0.59
2:B:1084:GLN:HE21	2:B:1084:GLN:N	2.01	0.59
2:B:562:GLY:HA3	2:B:590:HIS:ND1	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:G:90:THR:HG22	7:G:91:VAL:O	2.03	0.59
1:A:925:LEU:HD13	1:A:983:ILE:HG21	1.83	0.58
2:B:429:PHE:HD1	2:B:432:MET:HE3	1.68	0.58
2:B:975:GLN:O	2:B:990:ILE:HD12	2.02	0.58
3:C:69:LEU:HD12	3:C:69:LEU:N	2.17	0.58
6:F:109:VAL:HG21	6:F:124:GLU:HA	1.84	0.58
10:J:57:ILE:HA	10:J:60:PHE:HD2	1.66	0.58
11:K:18:LYS:NZ	11:K:37:LYS:O	2.35	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
5:E:92:THR:O	5:E:95:THR:HB	2.03	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
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
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
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
9:I:116:ASN:O	9:I:117:LYS:HD2	2.03	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: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:1094:VAL:CG2	1:A:1113:THR:HG21	2.29	0.58
1:A:1308:THR:HG23	1:A:1310:GLY:H	1.69	0.58
1:A:203:SER:O	1:A:206:GLU:HB3	2.03	0.58
2:B:353:LYS:O	2:B:357:GLN:HG2	2.03	0.58
2:B:65:GLU:HG3	2:B:66:ASP:N	2.14	0.58
2:B:801:LYS:O	10:J:52:THR:CG2	2.51	0.58
2:B:953:LEU:O	2:B:953:LEU:HD23	2.04	0.58
4:D:120:GLU:OE1	4:D:120:GLU:O	2.22	0.58
8:H:42:ILE:HG23	8:H:95:TYR:CE1	2.39	0.58
11:K:49:GLU:HG3	11:K:94:ILE:HG13	1.85	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:857:ARG:NH1	6:F:139:PRO:HB2	2.19	0.58
1:A:1074:GLU:HB3	1:A:1075:PRO:HD3	1.85	0.58
1:A:1120:LEU:O	1:A:1323:ASP:HB2	2.03	0.58
1:A:1444:MET:CE	6:F:135:ARG:HB2	2.34	0.58
1:A:332:LYS:HD3	1:A:333:GLU:HG2	1.85	0.58
1:A:666:ILE:HD11	2:B:1067:ARG:O	2.03	0.58
5:E:213:ILE:HG12	5:E:214:CYS:N	2.18	0.58
7:G:58:ARG:HH11	7:G:58:ARG:HG3	1.68	0.58
1:A:1066:VAL:O	1:A:1070:GLN:HG3	2.04	0.58
1:A:256:GLN:NE2	2:B:935:ARG:HH12	2.01	0.58
1:A:710:LEU:CD1	1:A:710:LEU:H	2.15	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
1:A:503:GLN:NE2	6:F:90:ARG:NH2	2.48	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
2:B:217:ARG:C	2:B:217:ARG:HD2	2.24	0.58
2:B:468:GLU:OE1	2:B:470:LYS:HE3	2.04	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
3:C:114:TYR:CD2	3:C:140:ASN:CB	2.86	0.58
9:I:78:CYS:SG	9:I:106:CYS:SG	3.01	0.58
1:A:119:ASN:O	1:A:122:MET:HB3	2.04	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
2:B:398:ARG:HB2	2:B:398:ARG:NH1	2.19	0.58
2:B:906:SER:O	2:B:941:LEU:HD23	2.04	0.58
3:C:36:VAL:HG21	3:C:251:LEU:HB2	1.85	0.58
4:D:52:LEU:HD21	4:D:147:TYR:HE2	1.68	0.58
5:E:198:ILE:CD1	5:E:212:ARG:HG3	2.34	0.58
9:I:8:ARG:HG3	9:I:34:TYR:HE1	1.66	0.58
10:J:1:MET:H2	10:J:57:ILE:H	1.51	0.58
1:A:1353:TYR:CD2	1:A:1353:TYR:C	2.77	0.57
2:B:758:PHE:HE1	2:B:1027:ILE:HG22	1.69	0.57
3:C:124:LEU:O	3:C:127:ARG:HG2	2.03	0.57
4:D:35:LEU:H	4:D:35:LEU:HD12	1.68	0.57
1:A:1340:GLY:HA2	5:E:183:PRO:HD2	1.86	0.57
1:A:567:LYS:CB	8:H:96:VAL:H	2.05	0.57
11:K:79:GLU:HG3	11:K:80:GLY:N	2.19	0.57
1:A:1208:THR:HB	1:A:1211:GLN:CG	2.16	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:LYS:O	1:A:130:ASP:HB2	2.04	0.57
3:C:226:ASP:O	3:C:227:THR:HB	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:124:VAL:HA	5:E:132:ILE:CD1	2.33	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
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
1:A:628:GLY:O	1:A:632:VAL:HG23	2.03	0.57
1:A:63:ARG:HA	1:A:74:MET:CE	2.33	0.57
2:B:254:LEU:HD11	2:B:273:LEU:HD23	1.85	0.57
2:B:891:ASP:C	2:B:893:LEU:N	2.55	0.57
5:E:153:HIS:O	5:E:154:ILE:HG13	2.04	0.57
1:A:102:VAL:HB	1:A:211:PHE:CZ	2.39	0.57
1:A:833:GLU:O	1:A:837:ILE:HG13	2.04	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
2:B:758:PHE:CE1	2:B:1027:ILE:CG2	2.87	0.57
2:B:996:ARG:HH21	3:C:38:ILE:HG23	1.69	0.57
4:D:123:LEU:CD1	4:D:149:THR:HG21	2.33	0.57
5:E:147:HIS:CD2	5:E:149:LEU:H	2.21	0.57
1:A:196:GLU:HG2	1:A:197:PRO:HD2	1.87	0.57
1:A:265:LYS:HE3	1:A:265:LYS:HA	1.85	0.57
1:A:317:LYS:O	1:A:318:SER:CB	2.52	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
2:B:1202:LEU:O	2:B:1206:GLU:HG3	2.04	0.57
2:B:121:ASN:HA	2:B:207:GLY:HA2	1.85	0.57
2:B:273:LEU:CB	2:B:276:ILE:HD12	2.26	0.57
2:B:411:PRO:O	2:B:414:ALA:HB3	2.04	0.57
2:B:483:LEU:HD11	2:B:491:THR:CG2	2.33	0.57
2:B:25:ILE:HG21	2:B:658:ILE:HD12	1.86	0.57
3:C:101:LEU:HD13	3:C:118:LEU:HD23	1.86	0.57
1:A:1339:LEU:HD13	5:E:147:HIS:CD2	2.40	0.57
12:L:30:ILE:HG22	12:L:31:CYS:H	1.69	0.57
14:T:16:DT:H1'	14:T:17:DT:H5''	1.86	0.57
1:A:1116:LEU:HB3	1:A:1308:THR:CG2	2.32	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
7:G:13:LEU:HD22	7:G:17:PHE:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1237:ILE:HG22	1:A:1238:ILE:N	2.19	0.57
1:A:438:ASP:O	1:A:439:ASN:HB2	2.05	0.57
1:A:446:ARG:HB2	1:A:487:MET:SD	2.44	0.57
1:A:903:ASN:ND2	1:A:904:THR:N	2.52	0.57
2:B:168:GLY:N	2:B:450:ALA:HB1	2.16	0.57
2:B:707:PRO:CG	2:B:708:GLU:H	2.15	0.57
3:C:238:ILE:HG22	3:C:243:VAL:HG23	1.87	0.57
4:D:47:LEU:HD11	7:G:3:PHE:CD2	2.40	0.57
5:E:67:GLU:O	5:E:70:SER:N	2.37	0.57
1:A:567:LYS:CD	1:A:568:PRO:HD2	2.34	0.57
1:A:853:ASP:OD1	1:A:855:THR:HB	2.04	0.57
2:B:129:PHE:HD2	2:B:166:PHE:HA	1.70	0.57
2:B:326:ASP:OD2	2:B:328:GLU:HB3	2.05	0.57
2:B:807:ARG:HG2	2:B:1045:SER:OG	2.05	0.57
3:C:238:ILE:HG23	3:C:242:GLN:HB2	1.85	0.57
7:G:21:ARG:CZ	7:G:24:GLN:HB2	2.35	0.57
10:J:2:ILE:HG12	10:J:57:ILE:HD12	1.86	0.57
15:P:2:A:H2'	15:P:3:A:H8	1.70	0.57
1:A:1037:LEU:HD22	1:A:1041:ALA:HB1	1.86	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:H	2:B:240:ILE:CD1	2.17	0.57
2:B:865:LYS:HZ3	2:B:869:SER:HA	1.69	0.57
2:B:992:ILE:HG12	2:B:993:THR:N	2.20	0.57
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.37	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:N	8:H:130:ARG:HH11	2.00	0.57
10:J:27:GLU:C	10:J:29:GLU:H	2.08	0.57
1:A:372:LYS:HA	1:A:435:HIS:CE1	2.39	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
2:B:222:ILE:HD11	2:B:627:PHE:CZ	2.40	0.57
2:B:810:GLU:HA	2:B:815:ARG:NH2	2.20	0.57
3:C:56:THR:HG21	3:C:145:CYS:SG	2.45	0.57
4:D:128:VAL:C	4:D:130:LEU:H	2.07	0.57
4:D:7:THR:HG23	4:D:7:THR:O	2.03	0.57
5:E:56:LYS:NZ	5:E:84:ASP:H	2.03	0.57
7:G:106:MET:HG3	7:G:157:ILE:O	2.04	0.57
8:H:130:ARG:H	8:H:130:ARG:NH1	2.01	0.57
1:A:1166:ASP:OD2	1:A:1239:ARG:HD2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:431:TYR:CD1	2:B:447:ALA:HB2	2.40	0.56
2:B:865:LYS:O	2:B:866:TYR:HD1	1.88	0.56
3:C:259:LEU:CD2	11:K:91:CYS:HB3	2.35	0.56
4:D:47:LEU:HD13	4:D:48:ILE:N	2.19	0.56
4:D:52:LEU:O	4:D:54:GLU:N	2.35	0.56
5:E:30:ILE:HG22	5:E:31:THR:O	2.05	0.56
14:T:15:DG:H2"	14:T:16:DT:H6	1.70	0.56
1:A:1045:VAL:O	1:A:1049:ILE:HG13	2.05	0.56
1:A:457:ALA:HB3	1:A:506:ALA:HA	1.86	0.56
1:A:897:TYR:HB3	1:A:936:LEU:CD1	2.35	0.56
1:A:982:THR:C	1:A:984:LYS:H	2.07	0.56
2:B:778:MET:HE1	2:B:1094:ARG:HD3	1.87	0.56
2:B:20:ASP:C	2:B:22:SER:H	2.09	0.56
2:B:68:THR:HG22	2:B:91:SER:CB	2.34	0.56
2:B:916:THR:HB	2:B:935:ARG:CG	2.35	0.56
9:I:14:LEU:HA	9:I:28:GLU:O	2.06	0.56
9:I:10:CYS:SG	9:I:32:CYS:HB3	2.44	0.56
10:J:23:ASN:C	10:J:25:LEU:N	2.57	0.56
1:A:380:VAL:HG12	1:A:428:TYR:HA	1.86	0.56
1:A:477:PRO:HG2	1:A:521:MET:HG2	1.87	0.56
1:A:54:ASN:HA	1:A:58:LEU:HD12	1.86	0.56
1:A:831:THR:CG2	1:A:832:ALA:N	2.65	0.56
1:A:963:ILE:HD13	1:A:1049:ILE:HG12	1.87	0.56
2:B:859:TYR:OH	2:B:941:LEU:HD12	2.05	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
8:H:12:VAL:HG13	8:H:26:ILE:HD11	1.87	0.56
2:B:822:ASN:ND2	10:J:52:THR:HG21	2.20	0.56
11:K:93:SER:OG	11:K:97:LYS:HE3	2.06	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
2:B:295:GLY:O	2:B:299:GLU:HG3	2.06	0.56
2:B:637:LEU:HB2	2:B:693:ILE:HD11	1.86	0.56
3:C:254:LYS:HE2	11:K:42:LEU:HD13	1.86	0.56
4:D:134:THR:HG22	4:D:135:GLY:N	2.20	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
9:I:7:CYS:SG	9:I:8:ARG:O	2.64	0.56
1:A:57:ARG:O	1:A:68:GLN:HG2	2.06	0.56
1:A:698:GLN:NE2	9:I:99:LEU:HD11	2.21	0.56
1:A:875:ALA:HA	1:A:878:ILE:CD1	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:293:PRO:HG2	2:B:296:GLU:CB	2.36	0.56
2:B:300:HIS:O	2:B:303:TYR:HE2	1.87	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
6:F:94:LEU:HD22	6:F:122:MET:HG2	1.87	0.56
7:G:20:PRO:CD	7:G:21:ARG:H	2.18	0.56
2:B:308:TRP:CH2	9:I:45:ARG:HG2	2.41	0.56
10:J:1:MET:H1	10:J:57:ILE:H	1.53	0.56
2:B:186:GLU:HG3	10:J:62:ARG:NH2	2.18	0.56
1:A:1317:MET:O	1:A:1322:ILE:HD11	2.04	0.56
1:A:381:THR:HG23	1:A:382:PRO:CD	2.32	0.56
1:A:868:TYR:OH	1:A:1366:ARG:HD3	2.05	0.56
2:B:1156:ASP:O	2:B:1157:ALA:O	2.23	0.56
2:B:276:ILE:CG2	2:B:336:ARG:HB2	2.36	0.56
2:B:459:TYR:CZ	2:B:469:GLN:HG2	2.41	0.56
2:B:553:PRO:HG2	2:B:554:ILE:HD12	1.87	0.56
2:B:805:THR:HA	2:B:809:MET:CE	2.35	0.56
2:B:918:ILE:HD12	2:B:935:ARG:NH1	2.21	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
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
8:H:26:ILE:HG22	8:H:40:LEU:O	2.05	0.56
8:H:84:ALA:CB	8:H:87:ARG:HB2	2.34	0.56
11:K:88:LYS:O	11:K:91:CYS:HB2	2.04	0.56
1:A:1159:ARG:HD2	1:A:1159:ARG:N	2.21	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
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	1.86	0.56
1:A:591:PHE:HA	1:A:595:THR:CG2	2.35	0.56
2:B:1017:ILE:HB	2:B:1018:PRO:HD3	1.88	0.56
1:A:69:THR:HG21	2:B:1174:LYS:HZ2	1.71	0.56
2:B:189:LEU:HD13	2:B:196:PRO:HA	1.88	0.56
2:B:254:LEU:HD23	2:B:381:MET:HE3	1.87	0.56
2:B:39:ARG:NH2	2:B:665:GLU:HG2	2.20	0.56
2:B:68:THR:HG22	2:B:91:SER:CA	2.35	0.56
2:B:542:MET:HE3	2:B:747:MET:HG3	1.87	0.56
2:B:798:TYR:HE2	3:C:62:PHE:CZ	2.23	0.56
2:B:886:LYS:NZ	2:B:936:ASP:OD1	2.39	0.56
2:B:990:ILE:HG22	2:B:991:GLY:N	2.21	0.56
3:C:221:TYR:CE1	3:C:222:LYS:HG3	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:157:SER:C	5:E:159:ASP:H	2.09	0.56
1:A:1006:ILE:HD11	5:E:163:GLU:HG3	1.87	0.56
1:A:1316:VAL:O	1:A:1316:VAL:HG12	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
2:B:120:ARG:NH1	12:L:54:ARG:HD2	2.20	0.56
2:B:865:LYS:HZ2	2:B:869:SER:HA	1.69	0.56
4:D:14:ARG:NH1	4:D:16:LYS:HD2	2.21	0.56
7:G:138:THR:CG2	7:G:139:ILE:N	2.49	0.56
10:J:53:HIS:CD2	10:J:53:HIS:C	2.77	0.56
1:A:332:LYS:O	1:A:334:GLY:N	2.38	0.56
2:B:303:TYR:CD2	2:B:303:TYR:N	2.74	0.56
2:B:750:GLY:O	2:B:751:VAL:C	2.44	0.56
3:C:73:GLN:NE2	3:C:75:MET:H	2.00	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:284:ILE:HD13	2:B:333:PHE:CD2	2.41	0.56
2:B:359:GLU:O	2:B:362:PRO:HD3	2.05	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:787:PHE:HE1	1:A:796:SER:HA	1.70	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
5:E:179:GLN:HA	5:E:179:GLN:OE1	2.06	0.56
7:G:87:VAL:HB	7:G:103:VAL:HG11	1.87	0.56
1:A:108:MET:HB3	1:A:210:ILE:CD1	2.36	0.55
2:B:1174:LYS:O	2:B:1176:ASN:N	2.39	0.55
2:B:129:PHE:CE2	2:B:166:PHE:CD1	2.94	0.55
5:E:112:TYR:CE1	5:E:136:ASN:HA	2.41	0.55
5:E:171:LYS:HG2	5:E:174:GLN:CD	2.26	0.55
5:E:164:LEU:CD2	5:E:211:TYR:CD2	2.88	0.55
3:C:235:VAL:HG21	10:J:6:ARG:NH2	2.21	0.55
1:A:427:GLN:HB2	1:A:430:TRP:CD1	2.41	0.55
1:A:56:PRO:O	1:A:57:ARG:CG	2.52	0.55
1:A:34:LYS:HZ1	1:A:57:ARG:HH21	1.55	0.55
1:A:335:ARG:NH1	2:B:1206:GLU:OE1	2.38	0.55
2:B:186:GLU:CG	10:J:62:ARG:HH22	2.19	0.55
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.88	0.55
2:B:430:ARG:HB3	2:B:434:ARG:NH2	2.21	0.55
2:B:705:MET:HA	2:B:705:MET:CE	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:847:ASP:C	2:B:849:GLY:N	2.59	0.55
3:C:226:ASP:O	3:C:227:THR:CB	2.53	0.55
3:C:243:VAL:HG12	3:C:243:VAL:O	2.06	0.55
8:H:12:VAL:CG1	8:H:26:ILE:HD11	2.36	0.55
10:J:7:CYS:HA	10:J:49:MET:HE3	1.88	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: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
2:B:429:PHE:CD1	2:B:432:MET:HE3	2.41	0.55
2:B:810:GLU:HA	2:B:815:ARG:HH22	1.71	0.55
3:C:100:THR:CG2	3:C:102:GLN:HE21	2.18	0.55
3:C:114:TYR:CD2	3:C:140:ASN:HB3	2.41	0.55
4:D:50:LEU:HD21	7:G:4:ILE:HD12	1.87	0.55
5:E:169:ARG:HB3	6:F:140:ASP:OD2	2.07	0.55
7:G:101:VAL:HG12	7:G:102:GLN:N	2.21	0.55
12:L:61:THR:HG22	12:L:63:ARG:H	1.71	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:999:MET:HB3	2:B:1007:VAL:CG2	2.36	0.55
2:B:1050:ILE:HG22	2:B:1051:THR:N	2.21	0.55
2:B:20:ASP:O	2:B:22:SER:N	2.35	0.55
2:B:711:GLU:HB2	2:B:712:PRO:CD	2.36	0.55
8:H:12:VAL:CG1	8:H:51:ALA:HA	2.36	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
1:A:780:VAL:O	1:A:782:ARG:HG2	2.07	0.55
1:A:979:SER:OG	1:A:980:ASP:N	2.38	0.55
2:B:1161:HIS:NE2	2:B:1175:LEU:HD21	2.22	0.55
2:B:315:LYS:N	2:B:316:PRO:HD2	2.22	0.55
2:B:842:ASN:HD21	2:B:844:SER:HB2	1.72	0.55
6:F:128:LYS:HD3	6:F:149:GLU:O	2.06	0.55
1:A:571:LEU:CD2	8:H:46:LEU:HD11	2.36	0.55
1:A:311:GLN:O	1:A:313:GLN:N	2.40	0.55
5:E:56:LYS:HZ3	5:E:84:ASP:H	1.54	0.55
6:F:94:LEU:HD21	6:F:122:MET:HA	1.89	0.55
1:A:598:LEU:HA	8:H:122:LEU:HD13	1.87	0.55
1:A:567:LYS:HB3	8:H:95:TYR:CA	2.36	0.55
9:I:6:PHE:HA	9:I:14:LEU:HG	1.89	0.55
9:I:73:ARG:O	9:I:81:ARG:HA	2.07	0.55
1:A:1076:ALA:HA	1:A:1079:MET:CE	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:853:ASP:OD1	1:A:855:THR:HG22	2.07	0.55
2:B:1174:LYS:O	2:B:1175:LEU:C	2.44	0.55
2:B:281:PRO:HB3	2:B:320:ASP:OD2	2.06	0.55
2:B:360:PHE:CD2	2:B:360:PHE:C	2.80	0.55
2:B:704:ALA:HB2	2:B:738:PHE:CD2	2.42	0.55
3:C:189:THR:CG2	3:C:190:ASP:N	2.70	0.55
4:D:39:ASN:HD22	4:D:41:GLN:HB2	1.71	0.55
1:A:870:GLU:HG2	5:E:208:TYR:CD2	2.41	0.55
5:E:82:PHE:CD1	5:E:82:PHE:N	2.74	0.55
3:C:10:ILE:HG13	11:K:108:GLU:HB3	1.87	0.55
12:L:38:LEU:HG	12:L:39:SER:H	1.71	0.55
1:A:1029:ARG:HH11	1:A:1029:ARG:CG	2.20	0.55
1:A:1385:THR:CG2	1:A:1386:ARG:N	2.69	0.55
1:A:266:LEU:HD21	1:A:303:TYR:CZ	2.41	0.55
1:A:590:ARG:HG3	1:A:591:PHE:N	2.21	0.55
1:A:925:LEU:HD13	1:A:983:ILE:HG22	1.88	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
2:B:916:THR:O	2:B:935:ARG:HG2	2.07	0.55
4:D:14:ARG:CZ	4:D:16:LYS:HD2	2.37	0.55
5:E:124:VAL:N	5:E:125:PRO:CD	2.70	0.55
7:G:129:SER:CB	7:G:138:THR:OG1	2.55	0.55
7:G:74:TYR:H	7:G:74:TYR:HD2	1.55	0.55
8:H:128:ASN:ND2	8:H:131:ASN:OD1	2.39	0.55
8:H:83:GLN:C	8:H:85:GLY:H	2.10	0.55
1:A:1030:ARG:CG	1:A:1034:GLU:OE2	2.53	0.55
1:A:1120:LEU:HD23	1:A:1304:TRP:O	2.06	0.55
1:A:1244:ARG:NE	1:A:1245:PRO:HD2	2.05	0.55
1:A:1402:PHE:CE2	1:A:1403:GLU:HG3	2.42	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
1:A:443:LEU:O	1:A:489:LEU:HD12	2.06	0.55
1:A:75:ASN:ND2	2:B:1116:ARG:NH1	2.54	0.55
1:A:899:VAL:CG1	1:A:929:LEU:HD12	2.37	0.55
1:A:940:ARG:O	1:A:944:ARG:HG3	2.06	0.55
2:B:1045:SER:O	2:B:1048:THR:HG23	2.06	0.55
3:C:91:HIS:ND1	3:C:158:VAL:HG11	2.21	0.55
8:H:139:ASN:O	8:H:140:ALA:CB	2.54	0.55
9:I:22:ASN:O	9:I:23:ASN:HB2	2.07	0.55
10:J:16:ASP:OD1	10:J:16:ASP:N	2.34	0.55
1:A:1105:LEU:HD22	1:A:1384:VAL:HG21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:GLY:HA3	1:A:243:PRO:CG	2.36	0.55
1:A:579:SER:HA	1:A:582:ILE:HG13	1.87	0.55
2:B:857:ARG:HH21	2:B:942:ARG:CZ	2.20	0.55
8:H:63:LEU:HD11	8:H:141:TYR:CD2	2.42	0.55
10:J:31:ASP:OD1	10:J:34:THR:OG1	2.25	0.55
1:A:1287:TYR:CD1	1:A:1305:VAL:HG21	2.42	0.54
1:A:1116:LEU:H	1:A:1308:THR:HG22	1.71	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:331:GLY:O	1:A:332:LYS:O	2.24	0.54
1:A:407:ARG:HG2	1:A:430:TRP:CH2	2.42	0.54
1:A:62:ASP:O	1:A:64:ASN:N	2.40	0.54
1:A:738:LYS:HG3	1:A:740:LEU:HG	1.88	0.54
2:B:235:SER:O	2:B:236:HIS:HD2	1.88	0.54
2:B:852:ARG:HH22	12:L:70:ARG:C	2.10	0.54
2:B:91:SER:OG	2:B:133:LYS:HB2	2.07	0.54
3:C:91:HIS:HD2	3:C:91:HIS:O	1.90	0.54
4:D:220:LEU:HD22	4:D:221:TYR:H	1.66	0.54
4:D:71:LYS:HA	4:D:74:GLN:CB	2.36	0.54
1:A:1110:ASN:H	1:A:1110:ASN:HD22	1.55	0.54
1:A:288:ALA:HA	1:A:291:GLU:HG3	1.88	0.54
1:A:689:LYS:HE2	1:A:721:PHE:CE2	2.41	0.54
2:B:1068:GLY:O	2:B:1069:PHE:O	2.25	0.54
3:C:138:GLU:OE1	3:C:138:GLU:N	2.40	0.54
4:D:155:ARG:HD3	4:D:221:TYR:CZ	2.43	0.54
11:K:50:LEU:HD11	11:K:75:ILE:CD1	2.37	0.54
1:A:133:LYS:O	1:A:136:ALA:HB3	2.06	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:744:LYS:HG2	1:A:748:MET:HE2	1.88	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
3:C:116:LYS:HD3	3:C:140:ASN:HA	1.90	0.54
5:E:21:GLU:O	5:E:24:LYS:HG2	2.08	0.54
6:F:111:LEU:C	6:F:113:GLY:H	2.08	0.54
8:H:33:GLN:C	8:H:35:GLN:H	2.10	0.54
10:J:14:VAL:CG1	10:J:50:ILE:HD11	2.37	0.54
11:K:108:GLU:O	11:K:112:GLN:HG2	2.07	0.54
11:K:52:ASN:O	11:K:54:ARG:N	2.40	0.54
1:A:311:GLN:O	1:A:312:PRO:C	2.45	0.54
1:A:541:ILE:HG22	1:A:546:VAL:HG23	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:868:TYR:CZ	1:A:1366:ARG:HD3	2.42	0.54
2:B:1182:CYS:SG	2:B:1185:CYS:HB2	2.47	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
7:G:119:LEU:HD12	7:G:120:THR:H	1.72	0.54
1:A:1161:THR:C	1:A:1163:ILE:N	2.61	0.54
1:A:472:LEU:O	1:A:475:THR:HB	2.07	0.54
1:A:668:ASP:HB3	1:A:741:ASN:ND2	2.17	0.54
2:B:288:ALA:HA	2:B:331:LEU:HD12	1.90	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
15:P:2:A:H2'	15:P:3:A:C8	2.43	0.54
1:A:1259:MET:HE3	1:A:1263:ILE:HG13	1.89	0.54
2:B:332:ASP:O	2:B:334:ILE:N	2.33	0.54
2:B:427:ASP:HA	2:B:430:ARG:HD2	1.87	0.54
2:B:563:MET:SD	2:B:580:VAL:HG11	2.48	0.54
2:B:520:GLY:H	2:B:748:ILE:HG22	1.73	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
7:G:1:MET:SD	7:G:79:PHE:CE1	3.01	0.54
1:A:320:ARG:NE	1:A:323:LYS:NZ	2.55	0.54
1:A:75:ASN:O	1:A:76:GLU:CB	2.56	0.54
2:B:345:LYS:HA	2:B:348:ARG:HE	1.72	0.54
2:B:313:MET:CE	2:B:386:LEU:HD22	2.37	0.54
2:B:487:THR:HG22	2:B:490:SER:H	1.73	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:143:LEU:HG	3:C:143:LEU:O	2.08	0.54
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.42	0.54
3:C:8:VAL:HG12	3:C:9:LYS:N	2.22	0.54
4:D:209:ARG:HG2	4:D:209:ARG:HH11	1.72	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
1:A:1236:LEU:C	1:A:1237:ILE:HG13	2.27	0.54
1:A:744:LYS:HG2	1:A:748:MET:CE	2.38	0.54
2:B:580:VAL:HG22	2:B:624:LEU:HB3	1.89	0.54
2:B:616:ILE:HG23	2:B:700:SER:OG	2.08	0.54
3:C:146:LYS:C	3:C:147:LEU:HD23	2.28	0.54
3:C:8:VAL:HG12	3:C:9:LYS:H	1.72	0.54
8:H:84:ALA:C	8:H:86:ASP:N	2.58	0.54
8:H:8:ASP:OD2	8:H:9:ILE:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:541:ILE:HD11	1:A:656:TRP:CD1	2.42	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:69:LEU:HB3	2:B:429:PHE:CE1	2.40	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
4:D:130:LEU:O	4:D:132:GLN:N	2.37	0.54
4:D:35:LEU:N	4:D:35:LEU:HD12	2.23	0.54
8:H:130:ARG:HB3	8:H:134:ASN:H	1.73	0.54
8:H:9:ILE:HD13	8:H:146:ARG:HH12	1.72	0.54
11:K:31:VAL:HG12	11:K:32:VAL:H	1.72	0.54
1:A:1074:GLU:HB3	1:A:1075:PRO:CD	2.38	0.54
2:B:185:THR:O	2:B:186:GLU:C	2.46	0.54
2:B:327:ARG:HH21	2:B:371:GLU:HG2	1.70	0.54
2:B:398:ARG:NH1	2:B:398:ARG:CB	2.71	0.54
2:B:637:LEU:HD22	2:B:741:CYS:O	2.07	0.54
2:B:644:GLU:HB3	2:B:648:HIS:O	2.07	0.54
2:B:794:ASN:ND2	2:B:794:ASN:N	2.56	0.54
8:H:127:GLY:O	8:H:128:ASN:CB	2.53	0.54
9:I:7:CYS:HB2	9:I:34:TYR:CG	2.43	0.54
1:A:1191:TRP:CZ3	9:I:43:VAL:HG21	2.43	0.54
11:K:67:PHE:C	11:K:68:PHE:HD2	2.11	0.54
1:A:416:ARG:HG3	1:A:417:TYR:CD1	2.43	0.53
1:A:464:PRO:HG2	1:A:465:TYR:CD1	2.43	0.53
2:B:435:THR:C	2:B:437:GLU:N	2.60	0.53
2:B:557:PHE:C	2:B:557:PHE:CD2	2.81	0.53
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
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
5:E:192:ARG:NH1	5:E:192:ARG:HG3	2.23	0.53
9:I:101:PHE:H	9:I:101:PHE:HD1	1.56	0.53
12:L:61:THR:CG2	12:L:63:ARG:HG3	2.37	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
2:B:192:LEU:O	2:B:193:LYS:HB2	2.08	0.53
2:B:209:GLU:OE2	2:B:485:ARG:NE	2.36	0.53
4:D:130:LEU:C	4:D:132:GLN:H	2.11	0.53
4:D:208:GLU:HA	4:D:211:LEU:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:53:HIS:NE2	10:J:55:ASP:HA	2.24	0.53
1:A:1147:THR:HB	9:I:48:LEU:CD1	2.38	0.53
1:A:1121:GLU:HB2	1:A:1321:GLY:O	2.08	0.53
1:A:205:GLU:CD	1:A:205:GLU:H	2.11	0.53
1:A:335:ARG:O	1:A:339:ASN:HB2	2.08	0.53
1:A:890:ASP:H	1:A:1296:GLY:HA3	1.73	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
3:C:114:TYR:CD2	3:C:140:ASN:HB2	2.43	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
5:E:112:TYR:O	5:E:137:GLU:HG3	2.08	0.53
5:E:108:GLY:O	5:E:132:ILE:HG22	2.09	0.53
8:H:37:LYS:HD2	8:H:126:GLU:OE2	2.09	0.53
9:I:62:ILE:HG12	9:I:62:ILE:O	2.08	0.53
1:A:93:VAL:CG1	1:A:301:ALA:HB1	2.37	0.53
1:A:481:ASP:OD1	1:A:485:ASP:OD2	2.25	0.53
1:A:50:ILE:O	1:A:52:GLY:N	2.40	0.53
1:A:547:LEU:HD21	1:A:560:ILE:HD13	1.90	0.53
1:A:965:GLN:HA	1:A:968:GLN:HG3	1.89	0.53
2:B:1180:PHE:HB3	2:B:1191:ILE:HD13	1.89	0.53
2:B:63:ILE:HD12	2:B:421:PHE:CE2	2.44	0.53
3:C:100:THR:HG22	3:C:101:LEU:N	2.23	0.53
4:D:13:ARG:O	4:D:15:LEU:N	2.42	0.53
4:D:155:ARG:HD3	4:D:221:TYR:OH	2.07	0.53
5:E:90:VAL:HA	5:E:120:ALA:CB	2.36	0.53
11:K:12:LEU:HG	11:K:16:GLU:HB2	1.90	0.53
12:L:58:LYS:O	12:L:59:ALA:O	2.27	0.53
1:A:1186:ASP:O	1:A:1187:GLN:CB	2.53	0.53
1:A:1343:ALA:O	1:A:1346:ALA:HB3	2.08	0.53
1:A:853:ASP:OD1	1:A:855:THR:N	2.42	0.53
2:B:1065:GLN:HB3	2:B:1069:PHE:O	2.09	0.53
2:B:398:ARG:CB	2:B:398:ARG:HH11	2.21	0.53
2:B:637:LEU:HD21	2:B:742:GLU:OE2	2.09	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
3:C:189:THR:CG2	3:C:190:ASP:H	2.21	0.53
4:D:149:THR:CG2	4:D:150:ASN:N	2.72	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
12:L:34:CYS:SG	12:L:34:CYS:O	2.67	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1202:MET:HE1	1:A:1212:VAL:HG21	1.89	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
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:458:HIS:CE1	1:A:507:VAL:HG21	2.43	0.53
1:A:50:ILE:C	1:A:52:GLY:N	2.62	0.53
1:A:549:MET:SD	1:A:577:ILE:CD1	2.96	0.53
1:A:665:GLY:C	1:A:666:ILE:HD12	2.28	0.53
2:B:291:ILE:HD13	2:B:300:HIS:NE2	2.23	0.53
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
9:I:50:THR:CG2	9:I:51:ASN:N	2.71	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
1:A:350:ARG:HB2	2:B:1128:LEU:CD1	2.39	0.53
1:A:590:ARG:NH2	1:A:620:LYS:HB2	2.23	0.53
2:B:728:ARG:HH12	2:B:1047:PHE:HB3	1.73	0.53
2:B:222:ILE:N	2:B:240:ILE:CD1	2.72	0.53
5:E:129:PRO:O	5:E:130:ALA:C	2.47	0.53
1:A:1313:LEU:HD23	1:A:1338:VAL:CG2	2.39	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
2:B:557:PHE:C	2:B:557:PHE:HD2	2.11	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
3:C:241:ASP:O	3:C:245:VAL:HG23	2.09	0.53
3:C:39:ALA:HA	3:C:164:ALA:HB3	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
5:E:161:LYS:HD2	5:E:195:VAL:HG23	1.91	0.53
8:H:13:SER:HB3	8:H:27:GLU:O	2.09	0.53
9:I:111:THR:OG1	9:I:112:SER:N	2.42	0.53
2:B:102:VAL:HG23	2:B:112:LEU:HB2	1.89	0.53
2:B:292:ILE:HD11	2:B:327:ARG:H	1.74	0.53
2:B:331:LEU:CD2	2:B:353:LYS:HG2	2.38	0.53
2:B:363:HIS:O	2:B:364:ILE:HB	2.09	0.53
2:B:376:PHE:CZ	2:B:569:TYR:HB3	2.44	0.53
2:B:558:LEU:HD22	2:B:596:LEU:HD11	1.91	0.53
2:B:619:ILE:HG22	2:B:620:ARG:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:43:THR:HG22	3:C:44:LEU:N	2.24	0.53
4:D:47:LEU:HD13	4:D:48:ILE:H	1.74	0.53
7:G:119:LEU:HD12	7:G:120:THR:N	2.24	0.53
8:H:133:ASN:O	8:H:135:LEU:N	2.41	0.53
10:J:23:ASN:O	10:J:25:LEU:N	2.42	0.53
1:A:659:HIS:O	2:B:1081:LEU:HD23	2.09	0.53
1:A:719:VAL:HG13	1:A:723:ASN:ND2	2.24	0.53
1:A:786:HIS:CD2	1:A:786:HIS:N	2.74	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:640:VAL:HG22	2:B:651:LEU:HD23	1.89	0.53
2:B:763:GLN:HG2	2:B:765:PRO:CD	2.35	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
3:C:148:ARG:N	3:C:151:GLN:HG3	2.23	0.53
1:A:1009:ASN:CG	1:A:1012:ARG:HH12	2.13	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
1:A:377:PRO:HD3	1:A:493:GLN:OE1	2.08	0.52
1:A:385:ILE:CD1	1:A:426:LEU:HB2	2.39	0.52
1:A:853:ASP:OD1	1:A:855:THR:CB	2.56	0.52
2:B:806:THR:HA	2:B:1045:SER:OG	2.09	0.52
2:B:244:LEU:O	2:B:249:ARG:HG3	2.08	0.52
2:B:278:GLN:CG	2:B:279:ASP:N	2.58	0.52
2:B:31:TRP:CZ2	2:B:807:ARG:HB2	2.44	0.52
2:B:619:ILE:O	2:B:622:LYS:N	2.34	0.52
2:B:882:THR:HG22	2:B:883:LEU:N	2.24	0.52
3:C:18:VAL:O	3:C:20:PHE:HD2	1.92	0.52
3:C:258:ILE:N	3:C:258:ILE:HD12	2.24	0.52
5:E:178:ILE:HG22	5:E:213:ILE:O	2.08	0.52
1:A:1191:TRP:HZ3	9:I:43:VAL:HG21	1.73	0.52
12:L:26:THR:HG23	12:L:27:LEU:H	1.73	0.52
1:A:154:SER:CB	1:A:162:VAL:CG2	2.87	0.52
2:B:816:GLU:O	2:B:817:LEU:HD23	2.09	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
6:F:109:VAL:CG1	6:F:110:ASP:N	2.72	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
1:A:1006:ILE:CD1	5:E:163:GLU:HG3	2.39	0.52
1:A:1215:ARG:NH1	1:A:1272:THR:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1402:PHE:CG	1:A:1403:GLU:HG2	2.44	0.52
1:A:132:LYS:HE3	1:A:1411:GLU:HG3	1.90	0.52
1:A:152:VAL:HG12	1:A:153:PRO:HD2	1.90	0.52
1:A:168:GLY:O	1:A:169:ASN:C	2.47	0.52
1:A:306:ASN:ND2	1:A:322:VAL:HG12	2.25	0.52
1:A:692:ASP:O	1:A:694:THR:N	2.42	0.52
1:A:851:HIS:HB2	1:A:855:THR:HG22	1.92	0.52
1:A:897:TYR:HB3	1:A:936:LEU:HD12	1.92	0.52
2:B:1175:LEU:O	2:B:1176:ASN:HB2	2.10	0.52
2:B:294:ASP:C	2:B:296:GLU:H	2.12	0.52
2:B:758:PHE:CZ	2:B:1044:ALA:HA	2.44	0.52
2:B:874:PHE:HA	2:B:913:GLY:O	2.09	0.52
3:C:104:PHE:HD2	3:C:105:GLY:N	2.07	0.52
3:C:39:ALA:O	3:C:164:ALA:HB3	2.09	0.52
5:E:157:SER:C	5:E:159:ASP:N	2.62	0.52
8:H:106:GLU:O	8:H:108:SER:N	2.32	0.52
8:H:27:GLU:HG2	8:H:39:THR:HA	1.90	0.52
8:H:91:ASP:O	8:H:93:TYR:N	2.39	0.52
1:A:16:GLU:HB3	1:A:1418:LEU:HD11	1.91	0.52
1:A:851:HIS:HB2	1:A:855:THR:CG2	2.39	0.52
1:A:886:ILE:CG2	1:A:887:GLY:N	2.71	0.52
2:B:1202:LEU:HD22	2:B:1206:GLU:CD	2.30	0.52
1:A:12:ARG:NH1	2:B:1218:THR:HB	2.25	0.52
2:B:134:LYS:HE2	2:B:164:LYS:HZ3	1.72	0.52
2:B:708:GLU:O	2:B:709:ASP:C	2.48	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
12:L:60:ARG:HG2	12:L:61:THR:N	2.21	0.52
1:A:356:ASP:OD1	1:A:358:ASN:HB2	2.09	0.52
1:A:555:ASP:O	1:A:556:TRP:C	2.48	0.52
1:A:626:ASN:O	1:A:631:HIS:CD2	2.62	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
1:A:864:ILE:HG22	1:A:865:GLN:HG3	1.91	0.52
2:B:1116:ARG:HD2	2:B:1198:TYR:CD1	2.44	0.52
2:B:373:ARG:NH2	2:B:587:HIS:HA	2.24	0.52
2:B:865:LYS:C	2:B:866:TYR:HD1	2.13	0.52
3:C:148:ARG:NH1	10:J:64:ASN:HA	2.24	0.52
7:G:106:MET:CG	7:G:107:LYS:N	2.72	0.52
7:G:88:ASP:HB3	7:G:144:ARG:CA	2.32	0.52
8:H:40:LEU:HB2	8:H:123:MET:HE2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1161:THR:OG1	1:A:1239:ARG:NH2	2.43	0.52
1:A:1397:LEU:HB2	1:A:1426:GLU:OE1	2.10	0.52
1:A:13:THR:HB	1:A:1432:GLN:NE2	2.25	0.52
1:A:102:VAL:HG21	1:A:234:MET:HE1	1.91	0.52
2:B:383:ASN:O	2:B:387:LEU:HD12	2.10	0.52
2:B:549:THR:CG2	2:B:550:ASP:H	2.23	0.52
2:B:866:TYR:HB3	2:B:870:ILE:HD12	1.90	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
4:D:47:LEU:HD11	7:G:3:PHE:HD2	1.74	0.52
2:B:193:LYS:HZ1	12:L:32:ALA:HB1	1.75	0.52
15:P:1:C:H2'	15:P:1:C:O2	2.10	0.52
1:A:1200:ALA:HA	1:A:1203:ASN:HD22	1.74	0.52
1:A:1218:GLN:O	1:A:1221:LYS:HE3	2.10	0.52
1:A:1385:THR:HG21	1:A:1387:HIS:CD2	2.45	0.52
1:A:54:ASN:N	1:A:54:ASN:HD22	2.07	0.52
1:A:598:LEU:O	1:A:599:SER:C	2.47	0.52
2:B:819:ALA:O	2:B:1093:GLN:HG2	2.09	0.52
2:B:1095:LEU:HD12	2:B:1095:LEU:N	2.15	0.52
2:B:1115:THR:HG22	2:B:1117:GLN:N	2.24	0.52
2:B:245:GLU:HG2	2:B:246:LYS:HG3	1.90	0.52
2:B:313:MET:O	2:B:316:PRO:HD2	2.09	0.52
3:C:184:ASN:OD1	3:C:187:LYS:CA	2.58	0.52
3:C:18:VAL:HG23	3:C:240:VAL:HB	1.89	0.52
8:H:9:ILE:HG12	8:H:56:THR:HA	1.92	0.52
1:A:252:PHE:O	1:A:256:GLN:NE2	2.42	0.52
1:A:92:HIS:O	1:A:94:GLY:N	2.42	0.52
2:B:282:ILE:HD12	2:B:382:ILE:HD13	1.91	0.52
2:B:282:ILE:CG2	2:B:382:ILE:HD11	2.40	0.52
7:G:87:VAL:O	7:G:87:VAL:HG23	2.08	0.52
14:T:15:DG:H2''	14:T:16:DT:C6	2.45	0.52
1:A:35:ILE:CD1	1:A:241:VAL:HG11	2.40	0.52
1:A:305:ASP:OD1	1:A:306:ASN:N	2.43	0.52
1:A:963:ILE:HD11	1:A:1048:ASN:HB3	1.92	0.52
3:C:242:GLN:C	3:C:244:VAL:N	2.63	0.52
3:C:249:ASP:O	3:C:252:GLN:HB3	2.09	0.52
6:F:138:LEU:HB2	6:F:142:SER:HB2	1.90	0.52
1:A:1445:ILE:HD12	7:G:59:GLY:O	2.10	0.52
1:A:152:VAL:HG13	1:A:153:PRO:HD2	1.91	0.52
1:A:34:LYS:HB2	1:A:36:ARG:NH2	2.25	0.52
1:A:440:ASP:O	1:A:460:VAL:HG23	2.11	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:498:THR:O	2:B:536:VAL:HA	2.09	0.52
2:B:787:VAL:HG12	2:B:787:VAL:O	2.10	0.52
2:B:773:MET:CE	2:B:985:GLY:HA2	2.39	0.52
3:C:168:ALA:O	3:C:170:TRP:N	2.42	0.52
3:C:22:LEU:HD22	3:C:230:MET:CE	2.40	0.52
3:C:233:GLU:CG	3:C:234:SER:H	2.23	0.52
4:D:5:THR:O	4:D:5:THR:HG23	2.10	0.52
4:D:147:TYR:OH	7:G:103:VAL:HG13	2.10	0.52
7:G:139:ILE:HG23	7:G:140:LYS:N	2.24	0.52
8:H:104:PHE:CD2	8:H:114:VAL:HG12	2.44	0.52
10:J:3:VAL:N	10:J:53:HIS:HE1	2.08	0.52
11:K:107:THR:HG22	11:K:108:GLU:N	2.24	0.52
11:K:73:LEU:HD21	11:K:75:ILE:HD11	1.92	0.52
12:L:52:GLY:O	12:L:53:HIS:C	2.48	0.52
1:A:1230:GLU:O	1:A:1232:ASN:N	2.43	0.51
1:A:64:ASN:O	1:A:65:LEU:C	2.48	0.51
1:A:715:GLU:OE1	1:A:774:ARG:HD3	2.10	0.51
2:B:276:ILE:HG23	2:B:336:ARG:HB2	1.91	0.51
2:B:429:PHE:HA	2:B:432:MET:CE	2.39	0.51
2:B:519:TRP:C	2:B:519:TRP:CD1	2.83	0.51
5:E:147:HIS:HD2	5:E:149:LEU:H	1.58	0.51
7:G:116:PRO:HG2	7:G:119:LEU:HB2	1.92	0.51
9:I:53:GLY:O	9:I:89:GLN:HB2	2.10	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
1:A:697:ALA:HB2	1:A:702:LEU:CD1	2.39	0.51
1:A:69:THR:C	1:A:71:GLN:N	2.60	0.51
1:A:988:LEU:O	1:A:992:ASP:HB2	2.10	0.51
2:B:1007:VAL:HG22	2:B:1008:PRO:CD	2.37	0.51
2:B:1166:CYS:O	2:B:1166:CYS:SG	2.69	0.51
2:B:638:PHE:HB3	2:B:651:LEU:HD22	1.92	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
5:E:207:ARG:CB	5:E:207:ARG:NH1	2.71	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:999:VAL:HG12	1:A:1000:LEU:HD12	1.92	0.51
1:A:1268:LEU:O	1:A:1269:GLU:HG3	2.10	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
1:A:974:ASP:C	1:A:976:THR:H	2.14	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:707:PRO:O	2:B:708:GLU:O	2.28	0.51
3:C:179:GLU:HG2	3:C:180:TYR:H	1.74	0.51
3:C:239:PRO:HB2	3:C:241:ASP:OD1	2.10	0.51
3:C:31:ASN:O	3:C:34:ARG:HB3	2.11	0.51
5:E:78:LEU:CA	5:E:107:THR:HB	2.34	0.51
5:E:136:ASN:OD1	5:E:137:GLU:N	2.43	0.51
7:G:51:TYR:C	7:G:51:TYR:CD2	2.84	0.51
8:H:135:LEU:HB3	8:H:137:GLN:HG2	1.92	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
1:A:382:PRO:HD3	1:A:428:TYR:CD2	2.45	0.51
1:A:500:GLU:OE2	1:A:1438:THR:HG21	2.11	0.51
1:A:688:LYS:CD	1:A:691:LEU:HD23	2.41	0.51
2:B:1031:LEU:HB2	2:B:1055:ILE:CD1	2.40	0.51
2:B:398:ARG:HB3	2:B:398:ARG:HH11	1.76	0.51
2:B:745:PRO:C	2:B:747:MET:H	2.13	0.51
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.93	0.51
5:E:31:THR:HG1	5:E:34:GLU:H	1.57	0.51
8:H:10:PHE:CD1	8:H:10:PHE:N	2.78	0.51
9:I:53:GLY:O	9:I:55:THR:N	2.44	0.51
12:L:58:LYS:HG2	12:L:58:LYS:O	2.10	0.51
12:L:66:GLN:HG2	12:L:67:PHE:N	2.25	0.51
1:A:108:MET:HB3	1:A:210:ILE:HD11	1.91	0.51
1:A:1208:THR:O	1:A:1212:VAL:HG23	2.11	0.51
1:A:889:SER:CB	1:A:1297:GLU:HG3	2.38	0.51
1:A:1299:VAL:HG12	1:A:1300:LYS:N	2.26	0.51
1:A:414:ASP:OD1	1:A:416:ARG:HG2	2.10	0.51
1:A:688:LYS:HA	1:A:691:LEU:HB3	1.93	0.51
1:A:696:GLU:OE2	1:A:702:LEU:HD21	2.09	0.51
1:A:720:ARG:HG2	1:A:720:ARG:O	2.11	0.51
1:A:75:ASN:O	1:A:76:GLU:HB2	2.10	0.51
1:A:915:SER:O	1:A:919:ILE:HB	2.10	0.51
1:A:982:THR:C	1:A:984:LYS:N	2.64	0.51
1:A:351:THR:HG22	2:B:1103:ILE:HG13	1.91	0.51
2:B:67:SER:HB2	2:B:92:PHE:HD1	1.76	0.51
2:B:708:GLU:HG3	2:B:709:ASP:N	2.25	0.51
2:B:976:ILE:O	2:B:990: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:58:ARG:NH1	7:G:58:ARG:HG3	2.25	0.51
1:A:1402:PHE:CD1	1:A:1403:GLU:HG2	2.46	0.51
1:A:247:ARG:NH1	1:A:263:THR:HG23	2.25	0.51
1:A:332:LYS:O	1:A:333:GLU:CB	2.57	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:69:LEU:HD13	2:B:429:PHE:HD1	1.75	0.51
2:B:640:VAL:O	2:B:641:GLU:C	2.48	0.51
2:B:642:ASP:HB3	2:B:649:LYS:CG	2.39	0.51
3:C:186:LEU:N	3:C:186:LEU:HD12	2.25	0.51
4:D:195:ILE:HG22	4:D:195:ILE:O	2.10	0.51
7:G:91:VAL:HG12	7:G:92:VAL:N	2.24	0.51
9:I:34:TYR:CE2	9:I:36:GLU:HB3	2.46	0.51
1:A:1155:ASP:OD2	1:A:1161:THR:HG23	2.10	0.51
1:A:125:ALA:C	1:A:127:ALA:H	2.14	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
1:A:33:ALA:HA	1:A:57:ARG:NH1	2.25	0.51
1:A:650:GLN:HB3	1:A:654:ASN:HD21	1.76	0.51
2:B:1095:LEU:CD1	2:B:1095:LEU:H	2.15	0.51
2:B:130:VAL:HG23	2:B:167:ILE:HD13	1.92	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
2:B:770:GLN:HG2	2:B:983:ARG:O	2.11	0.51
2:B:861:ASP:OD1	2:B:862:GLN:N	2.44	0.51
2:B:980:PHE:CE2	2:B:1094:ARG:HG3	2.46	0.51
2:B:996:ARG:HH12	3:C:175:ALA:N	2.09	0.51
5:E:56:LYS:HZ3	5:E:84:ASP:N	2.09	0.51
6:F:119:ARG:HG3	6:F:119:ARG:NH1	2.19	0.51
4:D:8:PHE:CD2	7:G:6:ASP:HB2	2.46	0.51
11:K:68:PHE:N	11:K:68:PHE:CD2	2.75	0.51
14:T:22:DC:H2''	14:T:23:BRU:OP2	2.10	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
1:A:49:LYS:HD3	1:A:55:ASP:HB3	1.93	0.51
1:A:567:LYS:NZ	8:H:46:LEU:HB2	2.26	0.51
1:A:737:LEU:HD22	1:A:741:ASN:OD1	2.11	0.51
2:B:1182:CYS:O	2:B:1183:LYS:C	2.49	0.51
2:B:46:GLN:HE21	2:B:539:LEU:HD12	1.76	0.51
2:B:555:ILE:HG22	2:B:556:THR:N	2.26	0.51
2:B:565:PRO:HB2	2:B:567:GLU:CG	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:ASP:O	2:B:979:LYS:HE3	2.11	0.51
2:B:839:MET:CE	2:B:980:PHE:HB2	2.40	0.51
3:C:183:TRP:CH2	3:C:203:GLN:NE2	2.78	0.51
5:E:10:SER:O	5:E:13:TRP:HB3	2.11	0.51
5:E:168:TYR:HB3	5:E:170:LEU:HG	1.92	0.51
9:I:86:PHE:HE1	9:I:100:PHE:HB2	1.76	0.51
9:I:75:CYS:SG	9:I:79:HIS:N	2.84	0.51
11:K:68:PHE:HD1	11:K:70:ARG:NH1	2.05	0.51
12:L:30:ILE:CG2	12:L:31:CYS:N	2.74	0.51
1:A:1054:LEU:HD13	6:F:84:TYR:OH	2.11	0.51
1:A:1386:ARG:O	1:A:1391:ARG:HD2	2.10	0.51
1:A:332:LYS:C	1:A:334:GLY:N	2.52	0.51
1:A:583:PRO:O	1:A:610:GLY:HA3	2.11	0.51
2:B:307:ASP:OD2	2:B:310:MET:HB2	2.09	0.51
2:B:37:PHE:HD2	2:B:542:MET:SD	2.34	0.51
2:B:557:PHE:CE1	2:B:603:LEU:HD11	2.46	0.51
2:B:834:ASN:O	2:B:838:SER:O	2.29	0.51
2:B:875:GLU:HG3	2:B:877:PRO:HD3	1.92	0.51
2:B:899:ILE:CG2	2:B:949:VAL:HG21	2.41	0.51
3:C:140:ASN:O	3:C:141:GLY:O	2.29	0.51
3:C:70:ILE:HG12	3:C:142:VAL:HG11	1.93	0.51
4:D:128:VAL:O	4:D:130:LEU:N	2.44	0.51
8:H:100:THR:HG22	8:H:101:ALA:N	2.26	0.51
1:A:1041:ALA:O	1:A:1045:VAL:HG23	2.11	0.51
1:A:88:LYS:HD3	1:A:293:GLU:CD	2.31	0.51
1:A:335:ARG:CZ	2:B:1202:LEU:HD13	2.41	0.51
1:A:43:GLU:HG3	1:A:46:THR:HB	1.93	0.51
1:A:610:GLY:O	1:A:611:GLN:NE2	2.45	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
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
2:B:31:TRP:CE3	2:B:34:ILE:HD12	2.46	0.51
2:B:361:LEU:O	2:B:363:HIS:O	2.29	0.51
2:B:593:PRO:O	2:B:595:ARG:N	2.43	0.51
2:B:402:GLY:CA	2:B:695:ALA:HB3	2.41	0.51
4:D:47:LEU:CD1	4:D:48:ILE:N	2.74	0.51
5:E:69:ILE:HD12	5:E:69:ILE:H	1.74	0.51
7:G:48:VAL:HA	7:G:76:ALA:HB2	1.93	0.51
8:H:62:SER:OG	8:H:63:LEU:N	2.43	0.51
11:K:21:ILE:HG22	11:K:31:VAL:CG1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1118:VAL:HG23	1:A:1306:LEU:HB2	1.93	0.50
1:A:1254:ALA:O	1:A:1255:GLU:CB	2.58	0.50
1:A:1453:TYR:O	1:A:1454:MET:HB3	2.12	0.50
1:A:7:SER:OG	2:B:1161:HIS:CE1	2.61	0.50
1:A:946:VAL:HG22	5:E:201:LYS:CD	2.41	0.50
2:B:213:ILE:HD12	2:B:497:ARG:HB3	1.93	0.50
2:B:230:ALA:HB3	2:B:231:PRO:HD3	1.93	0.50
2:B:326:ASP:OD1	2:B:329:THR:HB	2.10	0.50
2:B:393:LYS:HA	2:B:393:LYS:HE3	1.93	0.50
2:B:606:LYS:HD2	2:B:608:ASP:OD2	2.10	0.50
2:B:658:ILE:HG22	2:B:662:MET:HE2	1.93	0.50
2:B:39:ARG:HH21	2:B:665:GLU:CD	2.15	0.50
2:B:830:TYR:O	2:B:831:SER:C	2.49	0.50
2:B:996:ARG:NH1	3:C:175:ALA:H	2.09	0.50
3:C:104:PHE:HD2	3:C:105:GLY:H	1.57	0.50
5:E:22:MET:HE3	5:E:26:ARG:NE	2.22	0.50
6:F:111:LEU:HD12	6:F:111:LEU:N	2.25	0.50
7:G:14:HIS:HD2	7:G:16:SER:OG	1.94	0.50
1:A:1444:MET:HE1	6:F:135:ARG:NE	2.26	0.50
1:A:84:ILE:O	1:A:84:ILE:HG22	2.10	0.50
2:B:983:ARG:HH11	2:B:1091:TYR:HB3	1.75	0.50
2:B:1197:PRO:O	2:B:1200:ALA:N	2.34	0.50
2:B:205:ILE:N	2:B:205:ILE:CD1	2.74	0.50
2:B:661:LEU:HD23	2:B:679:TYR:O	2.11	0.50
2:B:879:ARG:HD2	2:B:879:ARG:H	1.76	0.50
4:D:53:SER:H	4:D:148:LEU:CD2	2.24	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:52:LEU:HD12	4:D:182:SER:HB2	1.93	0.50
4:D:53:SER:C	4:D:55:ALA:N	2.65	0.50
11:K:53:ASP:OD1	11:K:55:LYS:HB2	2.12	0.50
2:B:504:ARG:NH2	14:T:15:DG:O6	2.43	0.50
1:A:1387:HIS:HA	1:A:1391:ARG:NH1	2.23	0.50
1:A:108:MET:SD	1:A:210:ILE:HD13	2.52	0.50
1:A:268:ASP:HB3	1:A:299:HIS:CE1	2.46	0.50
1:A:332:LYS:H	1:A:337:ARG:HB2	1.77	0.50
1:A:605:MET:HE1	1:A:612:ILE:HG12	1.93	0.50
2:B:223:VAL:HG11	2:B:381:MET:HG2	1.93	0.50
2:B:212:LEU:HD23	2:B:480:SER:HB2	1.93	0.50
2:B:642:ASP:O	2:B:644:GLU:N	2.38	0.50
2:B:616:ILE:CG1	2:B:697:GLU:HA	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:911:ILE:HG22	2:B:966:VAL:HG21	1.94	0.50
3:C:91:HIS:O	3:C:91:HIS:CD2	2.64	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
5:E:129:PRO:HG2	5:E:130:ALA:H	1.75	0.50
5:E:178:ILE:HB	5:E:212:ARG:HB3	1.94	0.50
5:E:65:THR:O	5:E:69:ILE:CD1	2.59	0.50
1:A:1220:PHE:O	1:A:1221:LYS:HB2	2.11	0.50
1:A:1332:PHE:CE1	1:A:1348:LEU:HD13	2.46	0.50
1:A:196:GLU:HG2	1:A:197:PRO:CD	2.41	0.50
1:A:285:PRO:O	1:A:287:HIS:N	2.44	0.50
1:A:672:ASP:CG	1:A:674:PRO:HD2	2.32	0.50
1:A:886:ILE:CG2	1:A:952:ALA:HB2	2.41	0.50
2:B:827:ILE:O	2:B:1085:ILE:HG23	2.11	0.50
2:B:365:THR:OG1	2:B:367:LEU:HG	2.11	0.50
2:B:376:PHE:CZ	2:B:569:TYR:HD2	2.29	0.50
2:B:687:GLU:O	2:B:689:LEU:HG	2.11	0.50
2:B:847:ASP:O	2:B:849:GLY:N	2.44	0.50
5:E:182:ASP:HB3	5:E:185:ALA:CB	2.41	0.50
6:F:97:ARG:HD3	6:F:130:ILE:HG23	1.94	0.50
10:J:36:LEU:HB2	10:J:47:ARG:HH12	1.76	0.50
1:A:1187:GLN:HB2	1:A:1244:ARG:CG	2.30	0.50
1:A:1211:GLN:O	1:A:1214:GLU:HB2	2.12	0.50
1:A:115:LEU:HD13	1:A:141:LEU:HD13	1.93	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:113:TYR:CD2	2:B:192:LEU:HD22	2.47	0.50
8:H:55:LEU:HD22	8:H:144:ILE:CG2	2.42	0.50
2:B:622:LYS:CE	9:I:59:VAL:HG22	2.31	0.50
14:T:18:DC:H3'	14:T:18:DC:OP1	2.11	0.50
1:A:1011:GLN:NE2	1:A:1015:VAL:HG21	2.26	0.50
1:A:964:ILE:HD13	1:A:1035:TYR:CE1	2.46	0.50
1:A:1208:THR:HG22	1:A:1210:GLY:H	1.76	0.50
1:A:1138:ILE:HG21	1:A:1316:VAL:HG13	1.93	0.50
1:A:298:PHE:O	1:A:302:THR:HB	2.12	0.50
1:A:608:ILE:HD12	1:A:613:ILE:CD1	2.42	0.50
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.47	0.50
1:A:901:LEU:HA	1:A:907:THR:OG1	2.11	0.50
2:B:1017:ILE:H	2:B:1018:PRO:CD	2.24	0.50
2:B:233:PRO:HG2	2:B:234:ILE:HD13	1.94	0.50
2:B:259:TYR:HD1	2:B:259:TYR:H	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:59:LEU:HD12	2:B:417:PHE:CD2	2.47	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
10:J:24:LEU:O	10:J:30:LEU:HB2	2.11	0.50
1:A:1111:MET:O	1:A:1112:LYS:O	2.30	0.50
1:A:1212:VAL:O	1:A:1216:ILE:HG13	2.11	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:460:VAL:HG12	1:A:461:LYS:N	2.26	0.50
1:A:858:ASN:ND2	1:A:858:ASN:C	2.65	0.50
1:A:886:ILE:CG2	1:A:887:GLY:H	2.23	0.50
2:B:258:LEU:HG	2:B:258:LEU:O	2.11	0.50
2:B:678:GLU:HG2	2:B:679:TYR:N	2.26	0.50
3:C:138:GLU:HB2	3:C:140:ASN:ND2	2.26	0.50
3:C:213:PRO:HG2	3:C:214:ASN:H	1.76	0.50
1:A:269:ILE:HG23	1:A:300:VAL:HG23	1.94	0.50
1:A:475:THR:CG2	1:A:476:SER:N	2.75	0.50
1:A:53:LEU:C	1:A:54:ASN:HD22	2.15	0.50
1:A:65:LEU:O	1:A:66:LYS:C	2.50	0.50
1:A:690:VAL:HG12	1:A:691:LEU:N	2.26	0.50
2:B:292:ILE:HD13	2:B:326:ASP:HA	1.93	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
2:B:705:MET:HB3	2:B:706:GLN:OE1	2.12	0.50
2:B:842:ASN:HD22	2:B:845:SER:N	2.04	0.50
3:C:242:GLN:O	3:C:244:VAL:N	2.45	0.50
5:E:211:TYR:CD1	5:E:211:TYR:N	2.79	0.50
5:E:37:LEU:HD11	5:E:41:ASP:HB2	1.93	0.50
7:G:3:PHE:HB2	7:G:78:VAL:HG23	1.94	0.50
1:A:115:LEU:HG	1:A:142:CYS:HB3	1.94	0.50
1:A:1202:MET:HE1	1:A:1212:VAL:CG2	2.42	0.50
1:A:1313:LEU:C	1:A:1315:GLU:N	2.65	0.50
1:A:51:GLY:O	1:A:56:PRO:HB3	2.12	0.50
1:A:590:ARG:HH22	1:A:620:LYS:HB2	1.77	0.50
1:A:666:ILE:HD11	2:B:1086:PHE:CE1	2.46	0.50
2:B:134:LYS:HE2	2:B:164:LYS:HZ1	1.77	0.50
2:B:429:PHE:HA	2:B:432:MET:HE3	1.93	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:482:PHE:CD1	2:B:836:GLU:HB2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:27:GLY:O	5:E:65:THR:HG23	2.12	0.50
1:A:1003:LYS:O	1:A:1004:ASN:HB3	2.11	0.49
1:A:1214:GLU:C	1:A:1218:GLN:HE21	2.16	0.49
1:A:1280:GLU:O	1:A:1281:ARG:O	2.30	0.49
1:A:146:MET:HA	1:A:171:GLN:HB2	1.94	0.49
1:A:21:LEU:HD11	1:A:1414:ALA:HA	1.94	0.49
1:A:427:GLN:O	1:A:428:TYR:C	2.49	0.49
1:A:629:LEU:HD11	1:A:645:LEU:HD21	1.94	0.49
2:B:1187:ASN:OD1	2:B:1190:ASP:N	2.45	0.49
1:A:22:PHE:HB2	2:B:1211:ASN:OD1	2.12	0.49
2:B:987:LYS:HE3	15:P:11:G:H1'	1.94	0.49
3:C:73:GLN:HB3	3:C:131:HIS:H	1.77	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
9:I:119:THR:O	9:I:119:THR:HG22	2.11	0.49
9:I:50:THR:HB	9:I:92:ARG:HH22	1.77	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:CE	2.41	0.49
2:B:839:MET:HE3	2:B:1010:LEU:CD2	2.39	0.49
2:B:882:THR:C	2:B:884:ARG:N	2.66	0.49
4:D:12:ARG:HG2	4:D:12:ARG:NH1	2.26	0.49
4:D:144:THR:HG21	7:G:46:LEU:HD13	1.92	0.49
4:D:29:LEU:N	4:D:29:LEU:CD2	2.74	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
8:H:82:PRO:C	8:H:84:ALA:N	2.64	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
1:A:40:THR:HB	1:A:41:MET:HE2	1.94	0.49
2:B:211:VAL:HG23	2:B:483:LEU:HB2	1.93	0.49
2:B:654:ARG:O	2:B:656:GLY:N	2.46	0.49
2:B:916:THR:HB	2:B:935:ARG:CD	2.41	0.49
3:C:97:VAL:HG21	3:C:129:ILE:HG22	1.93	0.49
3:C:46:ILE:HD13	3:C:157:CYS:SG	2.52	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
9:I:118:ARG:HH12	9:I:120:GLN:HB2	1.77	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
1:A:1206:ASP:O	1:A:1274:ARG:NH2	2.44	0.49
1:A:1349:TYR:CD2	1:A:1349:TYR:C	2.86	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:HIS:ND1	1:A:290:GLU:HG2	2.28	0.49
1:A:382:PRO:N	1:A:428:TYR:HE2	2.10	0.49
1:A:809:THR:H	1:A:812:GLU:HB2	1.77	0.49
2:B:167:ILE:HD12	2:B:167:ILE:N	2.27	0.49
2:B:996:ARG:HH22	3:C:175:ALA:H	1.60	0.49
3:C:105:GLY:O	3:C:149:LYS:O	2.31	0.49
8:H:40:LEU:HD23	8:H:42:ILE:HD11	1.93	0.49
1:A:1129:GLU:OE2	1:A:1132:LYS:HD2	2.12	0.49
1:A:55:ASP:OD2	1:A:55:ASP:O	2.31	0.49
1:A:670:ILE:HD12	2:B:1067:ARG:NH2	2.27	0.49
1:A:946:VAL:CG2	5:E:201:LYS:HD2	2.42	0.49
2:B:287:ARG:HG3	2:B:292:ILE:HA	1.93	0.49
2:B:363:HIS:O	2:B:364:ILE:CB	2.61	0.49
2:B:910:VAL:HG11	2:B:938:SER:HB3	1.94	0.49
3:C:215:GLU:O	3:C:217:ASP:N	2.46	0.49
3:C:239:PRO:O	3:C:241:ASP:N	2.45	0.49
4:D:20:GLU:H	4:D:20:GLU:CD	2.16	0.49
4:D:35:LEU:HA	4:D:47:LEU:HB2	1.92	0.49
4:D:71:LYS:HA	4:D:74:GLN:HB2	1.93	0.49
5:E:61:GLN:HG3	5:E:78:LEU:O	2.11	0.49
9:I:88:SER:C	9:I:90:GLN:H	2.15	0.49
1:A:343:LYS:HZ2	2:B:1151:LEU:HG	1.76	0.49
1:A:380:VAL:CG1	1:A:385:ILE:HG12	2.42	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
1:A:888:GLY:O	1:A:940:ARG:NH2	2.45	0.49
2:B:185:THR:O	2:B:188:ASP:N	2.46	0.49
2:B:254:LEU:HD22	2:B:361:LEU:HD12	1.94	0.49
2:B:575:PRO:HG2	2:B:576:ASP:H	1.76	0.49
2:B:25:ILE:CD1	2:B:653:VAL:O	2.60	0.49
2:B:995:ARG:HH12	3:C:165:LYS:HG2	1.77	0.49
4:D:153:ARG:HB3	4:D:154:PHE:CE2	2.48	0.49
5:E:168:TYR:CB	5:E:170:LEU:HG	2.42	0.49
6:F:69:LEU:HB2	6:F:72:LYS:HD2	1.95	0.49
7:G:165:GLU:HB2	7:G:168:LEU:HD12	1.94	0.49
11:K:49:GLU:HG3	11:K:94:ILE:CG1	2.42	0.49
2:B:1065:GLN:NE2	2:B:1066:SER:N	2.61	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:874:PHE:HB3	2:B:896:ASP:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:33:LEU:HD12	3:C:37:MET:HG3	1.95	0.49
4:D:149:THR:HG22	4:D:150:ASN:N	2.27	0.49
8:H:135:LEU:CB	8:H:137:GLN:HG2	2.43	0.49
12:L:61:THR:HG22	12:L:62:LYS:H	1.78	0.49
1:A:265:LYS:CA	1:A:265:LYS:CE	2.86	0.49
1:A:2:VAL:HG22	1:A:3:GLY:N	2.26	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
1:A:820:GLY:O	1:A:822:GLU:N	2.45	0.49
1:A:846:GLU:OE1	1:A:1425:SER:OG	2.29	0.49
2:B:129:PHE:HA	2:B:165:VAL:O	2.13	0.49
2:B:217:ARG:NE	2:B:405:ARG:HB2	2.26	0.49
2:B:281:PRO:O	2:B:283:VAL:N	2.45	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
2:B:711:GLU:HB2	2:B:712:PRO:HD2	1.94	0.49
8:H:12:VAL:HG11	8:H:51:ALA:HA	1.95	0.49
11:K:50:LEU:HD11	11:K:75:ILE:HD13	1.94	0.49
15:P:9:C:OP2	15:P:9:C:H6	1.96	0.49
1:A:256:GLN:HE21	2:B:935:ARG:HH12	1.60	0.49
1:A:337:ARG:HD2	2:B:1132:GLU:OE1	2.13	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:542:MET:CE	2:B:747:MET:HG3	2.43	0.49
3:C:144:ILE:HG22	3:C:145:CYS:N	2.28	0.49
3:C:167:HIS:N	11:K:6:ARG:NH1	2.61	0.49
4:D:118:THR:CB	4:D:121:LYS:HB3	2.43	0.49
8:H:44:VAL:CG1	8:H:48:PRO:HA	2.41	0.49
8:H:93:TYR:HB3	8:H:144:ILE:O	2.12	0.49
9:I:7:CYS:C	9:I:8:ARG:O	2.51	0.49
10:J:53:HIS:CD2	10:J:54:VAL:C	2.86	0.49
1:A:1187:GLN:HG2	1:A:1188:GLN:N	2.28	0.49
1:A:1293:SER:OG	1:A:1294:PRO:HD2	2.13	0.49
1:A:1436:ILE:O	1:A:1439:GLY:N	2.27	0.49
1:A:306:ASN:HD22	1:A:322:VAL:HG12	1.78	0.49
1:A:378:GLU:OE2	1:A:387:ARG:NH2	2.46	0.49
1:A:639:PRO:HG2	1:A:640:GLN:HE21	1.77	0.49
1:A:853:ASP:C	1:A:853:ASP:OD1	2.51	0.49
1:A:919:ILE:HG12	1:A:925:LEU:HD12	1.95	0.49
1:A:70:CYS:HA	2:B:1174:LYS:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:129:PHE:CE2	2:B:166:PHE:HD1	2.31	0.49
2:B:179:CYS:SG	2:B:181:LEU:HB2	2.53	0.49
2:B:277:LYS:HG2	2:B:336:ARG:HB3	1.94	0.49
2:B:815:ARG:HB2	2:B:815:ARG:NH1	2.28	0.49
3:C:15:LYS:HG2	3:C:15:LYS:O	2.12	0.49
4:D:120:GLU:HA	4:D:123:LEU:HD23	1.95	0.49
5:E:119:SER:O	5:E:123:LEU:HD21	2.13	0.49
8:H:82:PRO:HG2	8:H:83:GLN:H	1.78	0.49
12:L:34:CYS:HB3	12:L:51:CYS:SG	2.53	0.49
13:N:4:DA:H2"	13:N:5:DC:C6	2.48	0.49
1:A:321:PRO:O	1:A:322:VAL:CB	2.60	0.48
1:A:482:PHE:HB2	2:B:838:SER:OG	2.13	0.48
2:B:1094:ARG:HH21	2:B:1098:MET:HG2	1.78	0.48
1:A:12:ARG:CB	2:B:1218:THR:HG22	2.29	0.48
2:B:753:ALA:O	2:B:756:ILE:HG13	2.13	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
3:C:166:GLU:C	11:K:6:ARG:HH11	2.16	0.48
3:C:82:TYR:O	3:C:83:SER:C	2.50	0.48
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
9:I:2:THR:HG23	9:I:2:THR:O	2.13	0.48
1:A:1280:GLU:O	1:A:1281:ARG:C	2.51	0.48
1:A:774:ARG:CZ	1:A:797:LYS:HB2	2.43	0.48
2:B:839:MET:HG3	2:B:1010:LEU:HD23	1.94	0.48
2:B:183:GLU:O	2:B:184:ALA:O	2.30	0.48
2:B:247:GLY:H	2:B:249:ARG:HH21	1.61	0.48
2:B:405:ARG:NE	2:B:632:ARG:HG2	2.27	0.48
2:B:641:GLU:C	2:B:643:ASP:H	2.16	0.48
1:A:482:PHE:HD1	2:B:838:SER:HG	1.61	0.48
4:D:136:GLY:HA2	4:D:142:LYS:NZ	2.28	0.48
5:E:112:TYR:CD1	5:E:112:TYR:C	2.86	0.48
5:E:157:SER:OG	5:E:160:GLU:HG3	2.13	0.48
5:E:22:MET:CE	5:E:26:ARG:NH2	2.67	0.48
8:H:44:VAL:HG12	8:H:44:VAL:O	2.13	0.48
10:J:53:HIS:HD2	10:J:54:VAL:C	2.17	0.48
12:L:34:CYS:SG	12:L:51:CYS:SG	3.11	0.48
1:A:144:THR:O	1:A:146:MET:HG3	2.12	0.48
1:A:336:ILE:HD11	2:B:1203:LEU:HD22	1.94	0.48
1:A:463:ILE:CD1	1:A:469:ARG:HG3	2.43	0.48
1:A:666:ILE:HG23	2:B:1026:LEU:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:883:LEU:CD1	1:A:1017:LEU:HD11	2.40	0.48
2:B:1001:PHE:CD2	3:C:34:ARG:NH2	2.81	0.48
2:B:218:SER:HB3	2:B:241:ARG:HH12	1.77	0.48
2:B:642:ASP:CB	2:B:649:LYS:HA	2.44	0.48
2:B:976:ILE:HD13	2:B:992:ILE:HA	1.95	0.48
3:C:238:ILE:HD11	3:C:246:ARG:NH1	2.28	0.48
3:C:89:GLU:O	3:C:90:ASP:CB	2.60	0.48
7:G:30:LEU:HD23	7:G:54:ILE:HD13	1.95	0.48
7:G:87:VAL:CG2	7:G:103:VAL:HG21	2.44	0.48
9:I:17:ARG:HG3	9:I:28:GLU:HG2	1.95	0.48
9:I:61:ASP:O	9:I:63:GLY:N	2.47	0.48
11:K:45:LEU:HG	11:K:94:ILE:CD1	2.41	0.48
12:L:27:LEU:HD13	12:L:37:LYS:CD	2.43	0.48
12:L:61:THR:HG22	12:L:63:ARG:HG3	1.93	0.48
1:A:1315:GLU:C	1:A:1317:MET:H	2.17	0.48
1:A:901:LEU:HD23	1:A:907:THR:OG1	2.12	0.48
1:A:925:LEU:C	1:A:927:VAL:N	2.66	0.48
2:B:120:ARG:NH1	12:L:54:ARG:NH1	2.60	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
2:B:766:ARG:HH11	2:B:769:TYR:HD1	1.61	0.48
3:C:167:HIS:N	11:K:6:ARG:HH12	2.11	0.48
3:C:177:GLU:CG	3:C:231:ASN:HD22	2.20	0.48
11:K:54:ARG:HG2	11:K:54:ARG:NH1	2.27	0.48
12:L:36:SER:O	12:L:37:LYS:C	2.51	0.48
1:A:200:ARG:HG2	1:A:201:VAL:N	2.28	0.48
1:A:255:SER:OG	2:B:918:ILE:CG2	2.61	0.48
1:A:381:THR:CG2	1:A:382:PRO:HD2	2.35	0.48
1:A:720:ARG:O	1:A:724:GLU:HB2	2.12	0.48
2:B:416:LEU:HD12	2:B:466:TRP:CE2	2.49	0.48
2:B:521:LEU:HB3	2:B:633:VAL:HG11	1.95	0.48
2:B:797:TYR:C	2:B:798:TYR:HD2	2.17	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
3:C:35:ARG:NH1	11:K:41:THR:N	2.60	0.48
12:L:31:CYS:SG	12:L:34:CYS:N	2.86	0.48
1:A:1029:ARG:NH1	1:A:1029:ARG:CG	2.77	0.48
1:A:1057:VAL:HG12	1:A:1058:VAL:N	2.29	0.48
1:A:1094:VAL:HG13	1:A:1113:THR:HB	1.96	0.48
1:A:20:GLY:O	1:A:21:LEU:HD23	2.13	0.48
1:A:264:PHE:HB3	1:A:265:LYS:NZ	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:663:SER:OG	1:A:664:THR:N	2.43	0.48
2:B:412:LEU:HB3	2:B:466:TRP:NE1	2.28	0.48
2:B:644:GLU:C	2:B:646:LEU:H	2.17	0.48
2:B:882:THR:HG23	2:B:884:ARG:CA	2.44	0.48
2:B:860:MET:CG	2:B:965:LYS:HG2	2.42	0.48
2:B:831:SER:CB	2:B:994:TYR:OH	2.61	0.48
3:C:133:ILE:CD1	3:C:236:GLY:C	2.82	0.48
3:C:56:THR:HG22	3:C:57:VAL:N	2.26	0.48
5:E:7:ARG:HG3	5:E:8:ASN:H	1.77	0.48
7:G:115:MET:O	7:G:164:LYS:HD3	2.14	0.48
7:G:7:LEU:HB2	7:G:74:TYR:CE2	2.49	0.48
9:I:12:ASN:HA	9:I:12:ASN:HD22	1.53	0.48
1:A:49:LYS:CD	1:A:55:ASP:HB3	2.44	0.48
2:B:1000:PRO:O	2:B:1007:VAL:HG23	2.14	0.48
2:B:1115:THR:O	2:B:1116:ARG:CB	2.59	0.48
2:B:190:TYR:CE1	2:B:196:PRO:HG3	2.49	0.48
2:B:896:ASP:OD2	12:L:58:LYS:HE3	2.14	0.48
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
4:D:40:HIS:CE1	7:G:7:LEU:O	2.65	0.48
7:G:88:ASP:CB	7:G:144:ARG:HA	2.34	0.48
8:H:61:SER:O	8:H:62:SER:HB2	2.14	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
1:A:26:GLU:O	1:A:29:ALA:HB3	2.14	0.48
1:A:396:PRO:HB3	1:A:402:ALA:O	2.13	0.48
1:A:477:PRO:CG	1:A:521:MET:HG2	2.44	0.48
1:A:526:ASP:HB2	2:B:835:GLN:OE1	2.14	0.48
1:A:593:GLU:C	1:A:595:THR:H	2.15	0.48
2:B:1170:THR:O	2:B:1172:ILE:HD13	2.13	0.48
2:B:284:ILE:HG21	2:B:333:PHE:HD2	1.79	0.48
2:B:360:PHE:CE2	2:B:361:LEU:HD13	2.49	0.48
2:B:434:ARG:O	2:B:436:VAL:HG23	2.13	0.48
2:B:515:HIS:HD2	2:B:517:THR:OG1	1.97	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
4:D:39:ASN:ND2	4:D:41:GLN:HB2	2.28	0.48
8:H:24:CYS:HB2	8:H:44:VAL:CG2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:111:LEU:N	11:K:111:LEU:HD23	2.29	0.48
12:L:46:VAL:O	12:L:46:VAL:HG12	2.14	0.48
1:A:239:LEU:HD12	1:A:239:LEU:HA	1.59	0.48
1:A:896:ARG:HD3	1:A:897:TYR:CZ	2.48	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
2:B:1154:ALA:O	2:B:1155:SER:HB2	2.13	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
3:C:213:PRO:O	3:C:214:ASN:HB3	2.14	0.48
4:D:123:LEU:CD2	4:D:149:THR:HG21	2.44	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
10:J:24:LEU:HA	10:J:28:ASP:HB2	1.96	0.48
11:K:21:ILE:CG2	11:K:33:ILE:HG12	2.37	0.48
1:A:1025:ARG:HG3	1:A:1025:ARG:HH11	1.79	0.48
1:A:49:LYS:NZ	1:A:61:ILE:N	2.58	0.48
1:A:821:ARG:HD2	1:A:825:ILE:HD11	1.96	0.48
2:B:100:PRO:HG3	2:B:172:ILE:HD12	1.96	0.48
2:B:1219:ASP:C	2:B:1219:ASP:OD1	2.51	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
3:C:236:GLY:C	3:C:238:ILE:N	2.66	0.48
3:C:84:ARG:HG3	3:C:85:ASP:OD1	2.14	0.48
4:D:154:PHE:CE2	4:D:218:GLU:HA	2.49	0.48
4:D:27:LEU:HD11	4:D:197:SER:HB3	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
7:G:31:LEU:HD13	7:G:35:GLU:HG3	1.96	0.48
8:H:135:LEU:HD13	8:H:137:GLN:NE2	2.29	0.48
9:I:82:GLU:HB3	9:I:104:LEU:CG	2.44	0.48
11:K:101:LEU:HD23	11:K:101:LEU:O	2.13	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
1:A:1319:VAL:HG12	1:A:1320:PRO:O	2.14	0.47
1:A:208:LEU:HD22	1:A:212:LYS:HD2	1.96	0.47
1:A:443:LEU:HD21	1:A:455:MET:HB3	1.96	0.47
1:A:595:THR:C	1:A:596:THR:HG23	2.34	0.47
1:A:899:VAL:CB	1:A:929:LEU:HD12	2.44	0.47
2:B:1223:ASP:O	2:B:1224:PHE:CB	2.60	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:425:THR:HA	2:B:428:ILE:CD1	2.39	0.47
2:B:644:GLU:HA	2:B:644:GLU:OE1	2.14	0.47
2:B:935:ARG:HG3	2:B:935:ARG:O	2.12	0.47
2:B:975:GLN:CG	2:B:976:ILE:N	2.74	0.47
3:C:35:ARG:HH12	11:K:41:THR:H	1.62	0.47
8:H:47:PHE:HB3	8:H:95:TYR:HD1	1.78	0.47
1:A:1169:ILE:O	1:A:1169:ILE:HG22	2.15	0.47
1:A:1278:ASN:O	1:A:1310:GLY:HA3	2.13	0.47
1:A:1285:MET:O	1:A:1305:VAL:N	2.39	0.47
1:A:195:ASP:O	1:A:196:GLU:HB3	2.14	0.47
1:A:645:LEU:HG	1:A:649:ILE:CD1	2.44	0.47
1:A:7:SER:C	1:A:9:ALA:H	2.17	0.47
2:B:313:MET:HE2	2:B:390:LEU:HD11	1.95	0.47
2:B:434:ARG:O	2:B:436:VAL:N	2.46	0.47
2:B:431:TYR:CG	2:B:447:ALA:HB2	2.49	0.47
2:B:875:GLU:O	2:B:877:PRO:CD	2.62	0.47
5:E:138:ALA:HA	5:E:141:VAL:HG23	1.95	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
7:G:21:ARG:HD2	7:G:24:GLN:HB2	1.93	0.47
9:I:55:THR:HG22	9:I:58:VAL:CG2	2.44	0.47
10:J:16:ASP:OD1	10:J:17:LYS:HD2	2.14	0.47
12:L:26:THR:CG2	12:L:27:LEU:H	2.27	0.47
14:T:19:DT:OP1	14:T:19:DT:H3'	2.14	0.47
1:A:1394:THR:HG21	1:A:1398:MET:SD	2.53	0.47
1:A:186:LYS:HZ1	1:A:197:PRO:HD3	1.77	0.47
1:A:537:ARG:HB2	8:H:20:TYR:CE2	2.50	0.47
1:A:90:VAL:HG12	1:A:91:PHE:N	2.29	0.47
2:B:1097:HIS:H	2:B:1098:MET:HE2	1.80	0.47
4:D:17:LYS:CD	4:D:18:VAL:HG13	2.43	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
14:T:13:DT:H2''	14:T:14:DA:C8	2.48	0.47
1:A:963:ILE:HD11	1:A:1048:ASN:CB	2.44	0.47
1:A:106:VAL:CG1	1:A:107:CYS:N	2.77	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
1:A:494:SER:O	1:A:498:ARG:HG2	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:55:VAL:HG13	2:B:97:VAL:HG21	1.97	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
5:E:182:ASP:HB3	5:E:185:ALA:HB2	1.96	0.47
5:E:61:GLN:HG2	5:E:62:ALA:N	2.29	0.47
6:F:109:VAL:HG13	6:F:127:GLU:OE1	2.14	0.47
7:G:45:ILE:HA	7:G:78:VAL:HG12	1.95	0.47
1:A:38:PRO:HA	1:A:270:LEU:HD23	1.96	0.47
1:A:719:VAL:HG12	1:A:720:ARG:N	2.29	0.47
1:A:843:LYS:HD3	1:A:846:GLU:OE2	2.14	0.47
1:A:849:MET:HE1	1:A:1061:GLY:HA2	1.96	0.47
1:A:90:VAL:CG1	1:A:297:GLN:HA	2.42	0.47
2:B:113:TYR:CE2	2:B:192:LEU:HD21	2.50	0.47
1:A:500:GLU:OE1	2:B:1145:SER:N	2.48	0.47
2:B:167:ILE:HG22	2:B:453:ILE:CD1	2.41	0.47
2:B:291:ILE:CD1	2:B:300:HIS:NE2	2.77	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:642:ASP:CA	2:B:649:LYS:HG3	2.43	0.47
2:B:635:ARG:NH1	2:B:742:GLU:OE2	2.48	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
2:B:997:GLU:H	2:B:997:GLU:HG3	1.41	0.47
3:C:193:TYR:HD1	3:C:193:TYR:O	1.97	0.47
5:E:145:THR:HG21	5:E:187:TYR:CD2	2.50	0.47
7:G:136:VAL:O	7:G:136:VAL:HG12	2.14	0.47
1:A:698:GLN:HE21	9:I:99:LEU:HD21	1.78	0.47
12:L:26:THR:HG22	12:L:27:LEU:N	2.30	0.47
1:A:1332:PHE:H	1:A:1332:PHE:HD2	1.63	0.47
1:A:1341:ILE:CG2	1:A:1342:GLU:N	2.78	0.47
1:A:316:GLN:O	1:A:317:LYS:C	2.51	0.47
1:A:456:MET:HE3	1:A:474:VAL:CG2	2.45	0.47
1:A:960:ILE:HA	1:A:963:ILE:HG22	1.97	0.47
2:B:29:ASP:CB	2:B:658:ILE:HD13	2.44	0.47
2:B:31:TRP:CZ3	2:B:34:ILE:HD12	2.49	0.47
2:B:560:GLU:O	2:B:561:TRP:CD1	2.68	0.47
2:B:849:GLY:O	2:B:852:ARG:HG3	2.14	0.47
3:C:22:LEU:CD2	3:C:230:MET:HE2	2.45	0.47
2:B:798:TYR:CE2	3:C:62:PHE:HE2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:123:ALA:O	7:G:125:SER:N	2.48	0.47
1:A:1048:ASN:HD22	1:A:1048:ASN:N	2.12	0.47
1:A:1166:ASP:O	1:A:1167:GLU:C	2.52	0.47
1:A:1353:TYR:HD2	1:A:1353:TYR:C	2.17	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:453:MET:HB3	1:A:477:PRO:HB3	1.96	0.47
1:A:79:GLY:H	2:B:1205:GLN:HE22	1.63	0.47
1:A:898:ARG:HD3	1:A:933:TYR:CE1	2.50	0.47
1:A:993:LEU:CD2	1:A:1022:LEU:HD11	2.45	0.47
1:A:69:THR:HB	2:B:1174:LYS:HZ3	1.79	0.47
2:B:34:ILE:HG12	2:B:542:MET:HE1	1.97	0.47
2:B:654:ARG:O	2:B:657:HIS:N	2.47	0.47
2:B:789:MET:HE2	2:B:965:LYS:HB2	1.96	0.47
3:C:44:LEU:HD21	3:C:159:ALA:CB	2.44	0.47
2:B:1073:TYR:HE2	3:C:180:TYR:CE2	2.32	0.47
3:C:59:ALA:O	3:C:62:PHE:HB3	2.13	0.47
3:C:73:GLN:NE2	3:C:75:MET:N	2.62	0.47
5:E:112:TYR:CE1	5:E:136:ASN:HB2	2.50	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
8:H:98:TYR:C	8:H:118:PHE:HD2	2.16	0.47
9:I:95:THR:HG22	9:I:96:SER:O	2.15	0.47
12:L:27:LEU:O	12:L:28:LYS:HB2	2.13	0.47
1:A:1424:VAL:HG13	1:A:1436:ILE:CD1	2.45	0.47
1:A:233:TRP:C	1:A:235:ILE:H	2.16	0.47
1:A:795:GLU:CD	1:A:795:GLU:H	2.17	0.47
1:A:814:PHE:O	1:A:814:PHE:CD2	2.67	0.47
1:A:953:ASN:C	1:A:954:TRP:CD1	2.88	0.47
2:B:129:PHE:CD2	2:B:166:PHE:HA	2.49	0.47
2:B:126:SER:HA	2:B:169:ARG:HH12	1.79	0.47
2:B:331:LEU:HD23	2:B:353:LYS:HG2	1.97	0.47
2:B:515:HIS:NE2	2:B:517:THR:HG23	2.30	0.47
2:B:526:GLU:HG3	2:B:771:SER:HB3	1.96	0.47
2:B:654:ARG:NH1	2:B:654:ARG:HG3	2.29	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
2:B:996:ARG:HH12	3:C:174:ALA:HA	1.80	0.47
3:C:131:HIS:O	3:C:133:ILE:N	2.48	0.47
1:A:551:TYR:CE2	11:K:62:LYS:HE2	2.50	0.47
1:A:23:SER:CB	1:A:233:TRP:NE1	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:ILE:HG22	1:A:386:ASP:N	2.30	0.47
1:A:442:VAL:CG2	1:A:489:LEU:HD11	2.45	0.47
1:A:904:THR:CG2	1:A:904:THR:O	2.62	0.47
2:B:1183:LYS:HE3	2:B:1183:LYS:O	2.14	0.47
2:B:98:THR:O	2:B:126:SER:HB2	2.14	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
2:B:735:ALA:HB3	2:B:738:PHE:CE1	2.50	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
10:J:7:CYS:SG	10:J:49:MET:HE3	2.55	0.47
12:L:53:HIS:C	12:L:55:ILE:HD13	2.34	0.47
12:L:60:ARG:HH21	12:L:65:VAL:CG2	2.28	0.47
1:A:1166:ASP:OD2	1:A:1239:ARG:CD	2.62	0.47
1:A:1283:VAL:HG12	1:A:1284:MET:N	2.29	0.47
1:A:180:LYS:NZ	1:A:294:SER:HB3	2.30	0.47
2:B:1167:GLY:O	2:B:1215:ARG:HA	2.15	0.47
2:B:1181:GLU:H	2:B:1188:LYS:HA	1.80	0.47
2:B:126:SER:HB3	2:B:172:ILE:HD11	1.97	0.47
2:B:412:LEU:HB3	2:B:466:TRP:CZ2	2.50	0.47
2:B:376:PHE:HB3	2:B:566:LEU:HD21	1.96	0.47
2:B:992:ILE:HG12	2:B:993:THR:H	1.79	0.47
5:E:162:ARG:HB3	5:E:162:ARG:CZ	2.45	0.47
2:B:848:ARG:HD3	10:J:11:GLY:HA2	1.97	0.47
12:L:30:ILE:CG2	12:L:31:CYS:H	2.28	0.47
1:A:90:VAL:HG12	1:A:297:GLN:NE2	2.30	0.47
1:A:483:ASP:HA	2:B:988:GLY:HA2	1.96	0.47
1:A:960:ILE:HA	1:A:963:ILE:CG2	2.45	0.47
1:A:1410:PHE:HD2	2:B:1212:ILE:HD12	1.80	0.47
2:B:307:ASP:OD1	2:B:309:GLN:HB2	2.15	0.47
2:B:63:ILE:HD12	2:B:421:PHE:CD2	2.49	0.47
2:B:430:ARG:HB3	2:B:434:ARG:CZ	2.45	0.47
2:B:562:GLY:HA3	2:B:590:HIS:CE1	2.50	0.47
3:C:101:LEU:HD13	3:C:118:LEU:CD2	2.45	0.47
3:C:80:LEU:HD11	3:C:95:CYS:C	2.35	0.47
4:D:139:LYS:HG3	4:D:140:ASP:OD1	2.15	0.47
4:D:39:ASN:ND2	4:D:41:GLN:H	2.13	0.47
8:H:15:VAL:HG22	8:H:26:ILE:CD1	2.45	0.47
8:H:84:ALA:HA	8:H:87:ARG:HG3	1.96	0.47
10:J:21:TYR:HB2	10:J:39:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:15:DG:C8	14:T:16:DT:C7	2.98	0.47
1:A:1315:GLU:C	1:A:1317:MET:N	2.68	0.46
1:A:590:ARG:NH1	1:A:590:ARG:HG2	2.29	0.46
1:A:71:GLN:C	1:A:73:GLY:H	2.17	0.46
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
2:B:466:TRP:N	2:B:475:SER:OG	2.48	0.46
2:B:528:PRO:HG2	2:B:532:ALA:O	2.15	0.46
2:B:797:TYR:HE1	2:B:854:LEU:HD21	1.80	0.46
3:C:196:ASP:HB3	3:C:199:LYS:HD2	1.96	0.46
4:D:15:LEU:O	4:D:15:LEU:HD12	2.15	0.46
4:D:155:ARG:NE	4:D:221:TYR:CE1	2.83	0.46
9:I:58:VAL:HG12	9:I:58:VAL:O	2.15	0.46
1:A:1081:LEU:HD21	1:A:1097:GLY:HA3	1.96	0.46
1:A:1208:THR:HG22	1:A:1210:GLY:N	2.29	0.46
1:A:1349:TYR:O	1:A:1350:LYS:C	2.52	0.46
1:A:934:LYS:O	1:A:937:VAL:HG12	2.16	0.46
2:B:1130:PHE:CE1	2:B:1134:GLU:HB3	2.51	0.46
2:B:189:LEU:CD1	2:B:196:PRO:HA	2.45	0.46
2:B:269:ILE:O	2:B:282:ILE:HG12	2.15	0.46
2:B:649:LYS:HD3	2:B:736:THR:O	2.14	0.46
2:B:706:GLN:HB2	2:B:709:ASP:HB2	1.97	0.46
2:B:777:ALA:HA	2:B:1095:LEU:HA	1.97	0.46
2:B:970:THR:HG22	2:B:971:THR:N	2.30	0.46
5:E:12:LEU:HD22	5:E:55:ARG:CZ	2.46	0.46
5:E:78:LEU:HD21	5:E:80:VAL:CG2	2.45	0.46
7:G:126:ASN:HD22	7:G:127:PRO:N	2.13	0.46
10:J:41:LEU:HD11	10:J:50:ILE:HG13	1.97	0.46
11:K:12:LEU:HD12	11:K:37:LYS:CG	2.44	0.46
11:K:55:LYS:HB2	11:K:81:TYR:CE1	2.49	0.46
11:K:79:GLU:C	11:K:81:TYR:H	2.19	0.46
1:A:196:GLU:HG2	1:A:197:PRO:N	2.31	0.46
1:A:398:GLU:O	1:A:399:HIS:O	2.34	0.46
1:A:407:ARG:CD	1:A:413:ILE:HD11	2.40	0.46
1:A:49:LYS:HZ3	1:A:61:ILE:HG13	1.78	0.46
2:B:944:THR:HG21	2:B:1122:ARG:CZ	2.45	0.46
2:B:416:LEU:HD12	2:B:466:TRP:CZ2	2.50	0.46
2:B:25:ILE:HD13	2:B:653:VAL:HG12	1.96	0.46
2:B:696:GLU:O	2:B:699:GLU:HB2	2.15	0.46
2:B:952:VAL:HG22	2:B:966:VAL:HG13	1.96	0.46
4:D:154:PHE:N	4:D:154:PHE:CD2	2.82	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:219:THR:HG23	4:D:220:LEU:O	2.16	0.46
6:F:111:LEU:HD12	6:F:111:LEU:H	1.80	0.46
6:F:116:ASP:OD1	6:F:117:PRO:N	2.48	0.46
1:A:504:LEU:HD13	6:F:91:ALA:CB	2.44	0.46
8:H:109:LYS:HD3	8:H:111:LEU:HD11	1.96	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
12:L:59:ALA:O	12:L:60:ARG:O	2.34	0.46
1:A:1076:ALA:HA	1:A:1079:MET:HG3	1.96	0.46
1:A:1420:ASP:CB	1:A:1422:ARG:HG3	2.41	0.46
1:A:690:VAL:CG1	1:A:691:LEU:N	2.78	0.46
1:A:350:ARG:HB2	2:B:1128:LEU:HD11	1.97	0.46
2:B:96:TYR:N	2:B:129:PHE:O	2.38	0.46
2:B:236:HIS:CE1	2:B:389:ALA:HA	2.50	0.46
2:B:63:ILE:HA	2:B:421:PHE:CE2	2.51	0.46
2:B:604:ARG:C	2:B:606:LYS:H	2.19	0.46
2:B:653:VAL:CG2	2:B:689:LEU:HB3	2.44	0.46
3:C:10:ILE:HG22	3:C:11:ARG:O	2.16	0.46
3:C:221:TYR:CD1	3:C:222:LYS:HG3	2.50	0.46
8:H:9:ILE:HG23	8:H:55:LEU:O	2.15	0.46
9:I:62:ILE:HD11	9:I:86:PHE:CE2	2.50	0.46
10:J:14:VAL:HG12	10:J:50:ILE:HD11	1.97	0.46
10:J:48:ARG:HE	10:J:49:MET:CE	2.28	0.46
11:K:33:ILE:HD13	11:K:87:LEU:HD22	1.96	0.46
11:K:85:ASP:O	11:K:88:LYS:HB2	2.15	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
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:1289:ARG:NH1	1:A:1326:ARG:NH1	2.63	0.46
1:A:244:PRO:CB	1:A:245:PRO:CD	2.91	0.46
1:A:401:GLY:C	1:A:435:HIS:CD2	2.89	0.46
1:A:699:ALA:HB3	1:A:701:LEU:HG	1.96	0.46
1:A:751:SER:O	1:A:752:LYS:HG2	2.16	0.46
2:B:293:PRO:C	2:B:294:ASP:O	2.51	0.46
2:B:427:ASP:OD1	2:B:430:ARG:HD2	2.16	0.46
2:B:602:THR:HA	2:B:605:ARG:HB2	1.97	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:121:LEU:O	1:A:121:LEU:HD23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:LEU:O	1:A:298:PHE:HB3	2.16	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
2:B:1001:PHE:CZ	2:B:1073:TYR:HB2	2.50	0.46
2:B:254:LEU:CD1	2:B:273:LEU:HD23	2.45	0.46
2:B:294:ASP:H	9:I:12:ASN:HD22	1.57	0.46
2:B:347:LYS:CG	2:B:348:ARG:H	2.29	0.46
2:B:417:PHE:O	2:B:420:LEU:HB2	2.16	0.46
2:B:430:ARG:NH1	2:B:430:ARG:HG2	2.31	0.46
2:B:910:VAL:CG1	2:B:938:SER:HB3	2.46	0.46
3:C:196:ASP:CB	3:C:199:LYS:HD2	2.45	0.46
4:D:138:ASN:C	4:D:140:ASP:N	2.67	0.46
4:D:155:ARG:NE	4:D:221:TYR:HE1	2.14	0.46
6:F:103:MET:HE1	7:G:66:GLY:N	2.24	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
1:A:1155:ASP:OD2	1:A:1162:VAL:N	2.48	0.46
1:A:284:ALA:HB1	1:A:289:ILE:HD12	1.97	0.46
1:A:492:PRO:HB2	1:A:497:THR:HG22	1.96	0.46
1:A:577:ILE:HA	1:A:580:VAL:HG23	1.98	0.46
1:A:675:THR:HB	1:A:736:ASN:OD1	2.15	0.46
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.49	0.46
2:B:265:SER:O	2:B:266:ALA:HB3	2.16	0.46
2:B:311:LEU:O	2:B:314:LEU:N	2.49	0.46
2:B:282:ILE:CD1	2:B:382:ILE:HD13	2.46	0.46
2:B:527:THR:OG1	2:B:528:PRO:HD2	2.15	0.46
2:B:860:MET:HE2	2:B:965:LYS:HE2	1.98	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
9:I:8:ARG:HG3	9:I:8:ARG:H	1.59	0.46
1:A:1394:THR:CG2	1:A:1398:MET:SD	3.04	0.46
1:A:1420:ASP:O	1:A:1421:CYS:CB	2.62	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:80:HIS:H	1:A:243:PRO:CB	2.28	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
1:A:898:ARG:O	1:A:1029:ARG:NH1	2.48	0.46
2:B:1116:ARG:NE	2:B:1198:TYR:CE1	2.84	0.46
2:B:131:ASP:HA	2:B:164:LYS:HB3	1.98	0.46
2:B:37:PHE:CD2	2:B:542:MET:SD	3.09	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:90:ARG:O	6:F:91:ALA:C	2.55	0.46
7:G:14:HIS:HD2	7:G:16:SER:CB	2.29	0.46
7:G:154:VAL:HG12	7:G:155:SER:N	2.30	0.46
10:J:3:VAL:HA	10:J:53:HIS:HD1	1.80	0.46
1:A:1195:LEU:HD11	1:A:1267:MET:HE1	1.95	0.46
1:A:185:TRP:HE3	1:A:185:TRP:N	1.98	0.46
1:A:871:ASP:OD2	1:A:873:MET:HB2	2.16	0.46
1:A:897:TYR:CD2	1:A:936:LEU:HD13	2.51	0.46
2:B:525:ALA:O	2:B:768:THR:HG23	2.16	0.46
2:B:593:PRO:O	2:B:594:ALA:C	2.54	0.46
2:B:582:VAL:HG22	2:B:626:ILE:HG22	1.98	0.46
3:C:23:SER:O	3:C:24:ASN:HB3	2.16	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
5:E:186:LEU:HA	5:E:186:LEU:HD23	1.71	0.46
5:E:56:LYS:NZ	5:E:84:ASP:N	2.63	0.46
6:F:79:ARG:HG2	6:F:144:GLU:HB3	1.97	0.46
6:F:79:ARG:NH2	6:F:150:GLU:OE1	2.35	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
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:1362:TYR:CD1	1:A:1363:VAL:N	2.84	0.46
1:A:356:ASP:OD2	11:K:65:HIS:CE1	2.65	0.46
1:A:575:LYS:HB3	1:A:612:ILE:CG2	2.46	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
1:A:793:SER:HB2	1:A:794:PRO:HD2	1.98	0.46
1:A:898:ARG:HA	1:A:933:TYR:CD1	2.51	0.46
2:B:102:VAL:HG22	2:B:112:LEU:HB2	1.96	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:295:GLY:N	2:B:298:LEU:HD23	2.29	0.46
2:B:356:LEU:HD23	2:B:360:PHE:CD1	2.51	0.46
2:B:169:ARG:CB	2:B:454:THR:HG23	2.45	0.46
2:B:582:VAL:O	2:B:582:VAL:HG12	2.14	0.46
2:B:710:LEU:HA	2:B:733:HIS:CB	2.29	0.46
2:B:792:MET:O	2:B:793:ALA:HB2	2.16	0.46
2:B:878:GLN:HB2	2:B:879:ARG:NH1	2.30	0.46
2:B:980:PHE:HD2	2:B:1094:ARG:HA	1.81	0.46
2:B:773:MET:HE1	2:B:985:GLY:HA2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:100:THR:CG2	3:C:101:LEU:N	2.79	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
5:E:108:GLY:HA3	5:E:132:ILE:HG23	1.98	0.46
5:E:19:VAL:HG11	5:E:80:VAL:HG11	1.98	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
12:L:70:ARG:HG2	12:L:70:ARG:HH11	1.81	0.46
1:A:153:PRO:HD3	1:A:161:LEU:CD1	2.46	0.45
1:A:138:ILE:HD12	1:A:221:SER:O	2.16	0.45
1:A:233:TRP:C	1:A:235:ILE:N	2.69	0.45
1:A:282:ASN:O	1:A:284:ALA:N	2.48	0.45
1:A:321:PRO:O	1:A:322:VAL:HG12	2.16	0.45
1:A:474:VAL:HG22	1:A:478:TYR:HE1	1.81	0.45
1:A:639:PRO:HG2	1:A:640:GLN:N	2.31	0.45
1:A:741:ASN:C	1:A:741:ASN:HD22	2.16	0.45
2:B:1045:SER:HB3	2:B:1046:PRO:HD2	1.98	0.45
2:B:1106:ARG:HD3	2:B:1126:GLY:C	2.36	0.45
2:B:112:LEU:HD12	2:B:113:TYR:N	2.27	0.45
2:B:210:LYS:HD3	2:B:482:VAL:HG22	1.98	0.45
2:B:582:VAL:O	2:B:582:VAL:CG1	2.63	0.45
2:B:797:TYR:HE1	2:B:854:LEU:HD23	1.81	0.45
2:B:866:TYR:CB	2:B:870:ILE:HD12	2.47	0.45
3:C:134:ILE:HG21	3:C:139:GLY:HA2	1.97	0.45
4:D:64:VAL:C	4:D:66:ARG:N	2.68	0.45
8:H:123:MET:HE3	8:H:142:LEU:HD21	1.98	0.45
1:A:698:GLN:O	9:I:98:VAL:HA	2.16	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:1081:LEU:CD2	1:A:1097:GLY:HA3	2.46	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:1180:PHE:HB3	2:B:1191:ILE:CD1	2.47	0.45
1:A:329:LEU:HD21	2:B:1206:GLU:OE1	2.16	0.45
2:B:567:GLU:HA	2:B:567:GLU:OE1	2.16	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
7:G:12:THR:HG23	7:G:67:SER:HB3	1.98	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:1064:VAL:HG12	1:A:1064:VAL:O	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:ILE:O	1:A:208:LEU:C	2.55	0.45
1:A:492:PRO:O	1:A:493:GLN:NE2	2.49	0.45
1:A:61:ILE:HG22	1:A:62:ASP:N	2.31	0.45
1:A:856:THR:HG22	1:A:856:THR:O	2.16	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
2:B:244:LEU:HD13	2:B:366:GLN:HE22	1.81	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
3:C:75:MET:HB3	3:C:128:ASN:HB3	1.98	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:105:SER:O	9:I:106:CYS:CB	2.52	0.45
9:I:55:THR:OG1	9:I:100:PHE:HD2	1.99	0.45
1:A:1048:ASN:O	1:A:1049:ILE:C	2.53	0.45
1:A:1203:ASN:O	1:A:1204:ASP:C	2.55	0.45
1:A:1141:THR:HG21	1:A:1205:LYS:HD3	1.98	0.45
1:A:164:ARG:HG3	1:A:165:GLY:N	2.32	0.45
1:A:335:ARG:HH12	2:B:1202:LEU:HD22	1.81	0.45
1:A:41:MET:O	1:A:42:ASP:C	2.55	0.45
1:A:452:LYS:HB3	2:B:1141:HIS:CE1	2.52	0.45
1:A:608:ILE:HG13	1:A:613:ILE:HD12	1.99	0.45
1:A:768:GLN:NE2	1:A:816:HIS:ND1	2.64	0.45
2:B:1099:VAL:CG1	2:B:1100:ASP:N	2.78	0.45
2:B:500:THR:HA	2:B:501:PRO:HD2	1.75	0.45
5:E:135:PHE:HD2	5:E:140:LEU:CD2	2.28	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:1110:ASN:HD22	1:A:1110:ASN:N	2.14	0.45
1:A:1187:GLN:CA	1:A:1244:ARG:HB3	2.45	0.45
1:A:1435:PRO:HA	1:A:1439:GLY:O	2.17	0.45
1:A:1444:MET:O	6:F:133:VAL:N	2.47	0.45
1:A:146:MET:CA	1:A:171:GLN:HB2	2.47	0.45
1:A:211:PHE:HA	1:A:214:ILE:HG13	1.98	0.45
1:A:35:ILE:HD13	1:A:241:VAL:HG11	1.98	0.45
1:A:447:GLN:HA	1:A:448:PRO:C	2.37	0.45
1:A:774:ARG:NH2	1:A:797:LYS:HB2	2.31	0.45
1:A:95:PHE:O	1:A:96:ILE:C	2.55	0.45
1:A:993:LEU:HD23	1:A:1022:LEU:HD21	1.99	0.45
2:B:120:ARG:HH11	12:L:54:ARG:HH11	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:27:ALA:O	2:B:28:GLU:C	2.55	0.45
2:B:345:LYS:C	2:B:347:LYS:H	2.20	0.45
2:B:412:LEU:CD2	2:B:479:VAL:HG11	2.45	0.45
2:B:591:ARG:O	2:B:592:ASN:C	2.55	0.45
2:B:66:ASP:OD1	2:B:422:LYS:HE2	2.15	0.45
1:A:255:SER:OG	2:B:918:ILE:HG21	2.16	0.45
3:C:204:SER:C	3:C:206:ASN:N	2.69	0.45
5:E:4:GLU:HB3	5:E:7:ARG:HE	1.81	0.45
8:H:100:THR:OG1	8:H:138:GLU:HG2	2.16	0.45
12:L:52:GLY:O	12:L:54:ARG:N	2.50	0.45
1:A:1173:HIS:CD2	1:A:1227:ILE:HG23	2.52	0.45
1:A:1266:THR:O	1:A:1270:ASN:HB2	2.17	0.45
1:A:1395:GLY:HA3	1:A:1419:ASP:OD2	2.16	0.45
1:A:1454:MET:HG3	1:A:1454:MET:O	2.17	0.45
1:A:332:LYS:CD	1:A:333:GLU:HG2	2.47	0.45
1:A:549:MET:SD	1:A:577:ILE:HD12	2.57	0.45
1:A:96:ILE:HG22	1:A:97:ALA:N	2.32	0.45
2:B:1214:PRO:O	2:B:1214:PRO:HG2	2.16	0.45
2:B:101:MET:HB2	2:B:169:ARG:HH22	1.82	0.45
2:B:288:ALA:HA	2:B:331:LEU:CD1	2.46	0.45
2:B:46:GLN:HB2	2:B:408:LEU:HD21	1.98	0.45
2:B:604:ARG:CA	2:B:609:ILE:HG13	2.47	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
3:C:99:LEU:HD22	3:C:120:ILE:HG12	1.98	0.45
2:B:848:ARG:HA	3:C:69:LEU:HD21	1.98	0.45
4:D:35:LEU:H	4:D:35:LEU:CD1	2.29	0.45
5:E:69:ILE:CD1	5:E:69:ILE:N	2.79	0.45
7:G:17:PHE:C	7:G:19:GLY:H	2.20	0.45
1:A:1062:GLU:HG2	6:F:88:TYR:OH	2.17	0.45
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
1:A:125:ALA:O	1:A:127:ALA:N	2.50	0.45
1:A:492:PRO:CB	1:A:497:THR:HG22	2.47	0.45
1:A:860:LEU:HA	1:A:860:LEU:HD23	1.81	0.45
2:B:431:TYR:CE1	2:B:447:ALA:HB2	2.52	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:249:ASP:O	3:C:250:THR:C	2.55	0.45
5:E:90:VAL:CA	5:E:120:ALA:HB2	2.40	0.45
5:E:129:PRO:O	5:E:130:ALA:O	2.35	0.45
5:E:145:THR:HG21	5:E:187:TYR:CZ	2.51	0.45
5:E:204:THR:HG23	5:E:205:SER:N	2.32	0.45
5:E:56:LYS:CE	5:E:84:ASP:H	2.29	0.45
5:E:92:THR:HG22	5:E:92:THR:O	2.15	0.45
6:F:77:ASP:O	6:F:78:GLN:CB	2.49	0.45
8:H:138:GLU:O	8:H:139:ASN:C	2.55	0.45
8:H:20:TYR:O	8:H:22:LYS:N	2.50	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
1:A:709:THR:HG21	9:I:93:LYS:O	2.16	0.45
2:B:1119:VAL:O	2:B:1126:GLY:HA3	2.15	0.45
2:B:1177:HIS:CB	2:B:1179:GLN:HE21	2.29	0.45
2:B:621:GLU:HG3	2:B:621:GLU:O	2.17	0.45
2:B:880:THR:O	2:B:880:THR:HG22	2.17	0.45
3:C:193:TYR:C	3:C:193:TYR:CD1	2.89	0.45
3:C:185:LYS:HE2	3:C:213:PRO:HA	1.99	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
8:H:7:ASP:O	8:H:8:ASP:HB2	2.17	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
1:A:108:MET:O	1:A:109:HIS:CB	2.63	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
1:A:416:ARG:HG3	1:A:417:TYR:CE1	2.52	0.45
1:A:50:ILE:HG22	1:A:52:GLY:N	2.32	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
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
2:B:370:PHE:CD2	2:B:373:ARG:HD2	2.52	0.45
2:B:531:GLN:HG3	2:B:532:ALA:H	1.82	0.45
2:B:769:TYR:HB3	2:B:987:LYS:NZ	2.31	0.45
3:C:193:TYR:HD1	3:C:193:TYR:C	2.21	0.45
3:C:20:PHE:C	3:C:20:PHE:CD1	2.90	0.45
5:E:154:ILE:HG22	5:E:155:ARG:O	2.17	0.45
10:J:27:GLU:C	10:J:29:GLU:N	2.67	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:30:LEU:HD11	10:J:38:ARG:NH1	2.32	0.45
11:K:12:LEU:HD21	11:K:17:SER:C	2.37	0.45
1:A:1387:HIS:NE2	13:N:4:DA:H5'	2.32	0.45
1:A:1081:LEU:HD11	1:A:1097:GLY:HA3	1.98	0.45
1:A:1161:THR:CG2	1:A:1163:ILE:HD12	2.46	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:100:PRO:HB2	2:B:180:TYR:HE1	1.82	0.45
2:B:203:PHE:N	2:B:203:PHE:CD1	2.85	0.45
2:B:69:LEU:HD13	2:B:429:PHE:CD1	2.52	0.45
2:B:811:TYR:N	2:B:811:TYR:CD1	2.84	0.45
2:B:889:THR:HG23	2:B:891:ASP:N	2.32	0.45
7:G:113:HIS:CD2	7:G:113:HIS:H	2.34	0.45
8:H:55:LEU:HD22	8:H:144:ILE:HG22	1.99	0.45
12:L:54:ARG:HG3	12:L:54:ARG:H	1.43	0.45
1:A:451:HIS:HA	1:A:1070:GLN:OE1	2.16	0.44
1:A:330:LYS:O	1:A:334:GLY:HA3	2.17	0.44
1:A:605:MET:HE1	1:A:607:ILE:HG12	1.98	0.44
1:A:692:ASP:C	1:A:694:THR:N	2.68	0.44
2:B:1072:MET:O	2:B:1081:LEU:HB2	2.17	0.44
2:B:294:ASP:H	9:I:12:ASN:HD21	1.60	0.44
2:B:458:LYS:O	2:B:459:TYR:C	2.55	0.44
2:B:486:TYR:HD1	2:B:775:LYS:O	2.00	0.44
2:B:805:THR:CG2	2:B:806:THR:H	2.20	0.44
4:D:13:ARG:C	4:D:15:LEU:N	2.68	0.44
4:D:29:LEU:HB3	7:G:82:PHE:CE2	2.52	0.44
6:F:89:GLU:OE2	6:F:134:ILE:HG21	2.16	0.44
7:G:111:THR:O	7:G:111:THR:HG23	2.17	0.44
9:I:40:SER:OG	9:I:41:PRO:HD2	2.17	0.44
10:J:53:HIS:CD2	10:J:55:ASP:N	2.85	0.44
10:J:62:ARG:HG2	10:J:62:ARG:O	2.17	0.44
1:A:1208:THR:HA	1:A:1231:ASP:OD1	2.17	0.44
1:A:1335:ILE:HG23	1:A:1339:LEU:HD12	1.98	0.44
1:A:335:ARG:NH1	2:B:1206:GLU:CD	2.68	0.44
1:A:352:VAL:O	1:A:467:THR:HB	2.17	0.44
2:B:1072:MET:HE3	2:B:1085:ILE:CB	2.44	0.44
2:B:1106:ARG:HD2	2:B:1125:ASP:O	2.17	0.44
2:B:412:LEU:HB3	2:B:466:TRP:CE2	2.52	0.44
2:B:958:GLN:C	2:B:960:GLY:H	2.20	0.44
3:C:68:GLY:O	3:C:169:LYS:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:67:LEU:HA	3:C:70:ILE:CD1	2.48	0.44
3:C:79:GLN:HE21	3:C:127:ARG:CD	2.27	0.44
5:E:128:PRO:HA	5:E:129:PRO:O	2.17	0.44
6:F:97:ARG:NH2	6:F:108:PHE:CE1	2.86	0.44
8:H:2:SER:OG	8:H:3:ASN:N	2.50	0.44
9:I:100:PHE:N	9:I:100:PHE:HD1	2.15	0.44
11:K:55:LYS:HB2	11:K:81:TYR:HE1	1.82	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
1:A:1170:ILE:HG22	1:A:1174:PHE:CZ	2.52	0.44
1:A:224:PHE:CD2	1:A:231:PRO:HG3	2.52	0.44
2:B:1002:THR:HG23	2:B:1087:PHE:HE1	1.81	0.44
2:B:234:ILE:HG21	2:B:237:VAL:HG23	1.98	0.44
2:B:263:GLY:O	2:B:264:SER:C	2.55	0.44
2:B:579:ARG:HG2	2:B:579:ARG:NH1	2.30	0.44
2:B:806:THR:CG2	2:B:808:ALA:HB3	2.47	0.44
2:B:987:LYS:HE3	15:P:11:G:C2'	2.46	0.44
3:C:124:LEU:O	3:C:125:MET:C	2.55	0.44
4:D:173:HIS:ND1	4:D:174:PRO:HD2	2.33	0.44
4:D:51:ASN:OD1	4:D:54:GLU:HB2	2.17	0.44
5:E:33:GLU:C	5:E:35:VAL:N	2.71	0.44
8:H:4:THR:O	8:H:5:LEU:HD23	2.17	0.44
1:A:1147:THR:HB	9:I:48:LEU:HD12	1.98	0.44
1:A:1094:VAL:HG13	1:A:1113:THR:CB	2.48	0.44
1:A:833:GLU:OE2	1:A:1102:LYS:HE3	2.17	0.44
1:A:1161:THR:HG22	1:A:1163:ILE:HG13	1.98	0.44
1:A:121:LEU:HD22	1:A:141:LEU:HD21	2.00	0.44
1:A:264:PHE:CB	1:A:265:LYS:NZ	2.81	0.44
1:A:939:ASP:O	1:A:942:PHE:HB3	2.18	0.44
1:A:12:ARG:NH2	2:B:1192:TYR:CE2	2.85	0.44
2:B:485:ARG:HG3	2:B:781:PHE:HD1	1.83	0.44
2:B:593:PRO:C	2:B:595:ARG:N	2.71	0.44
2:B:67:SER:HB2	2:B:92:PHE:CD1	2.52	0.44
2:B:637:LEU:HD22	2:B:742:GLU:HA	2.00	0.44
2:B:1003:ALA:HA	3:C:178:PHE:O	2.17	0.44
3:C:69:LEU:HB3	10:J:6:ARG:HD3	1.99	0.44
5:E:100:ILE:HG23	5:E:105:PHE:CD1	2.53	0.44
5:E:74:ASP:N	5:E:74:ASP:OD1	2.50	0.44
7:G:1:MET:SD	7:G:79:PHE:HD1	2.39	0.44
8:H:100:THR:CG2	8:H:101:ALA:N	2.81	0.44
9:I:74:GLU:O	9:I:74:GLU:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1019:CYS:O	1:A:1020:CYS:C	2.56	0.44
1:A:1037:LEU:HD13	1:A:1042:PHE:HA	2.00	0.44
1:A:1100:ARG:O	1:A:1100:ARG:HD2	2.17	0.44
1:A:1424:VAL:HG11	2:B:1139:ILE:HD11	1.98	0.44
1:A:336:ILE:CD1	2:B:1203:LEU:HD22	2.47	0.44
1:A:377:PRO:O	1:A:377:PRO:HG2	2.18	0.44
1:A:378:GLU:CD	1:A:387:ARG:HH22	2.21	0.44
1:A:49:LYS:HZ1	1:A:61:ILE:CG1	2.26	0.44
1:A:755:PHE:O	1:A:757:ASN:N	2.51	0.44
1:A:858:ASN:ND2	1:A:860:LEU:HB2	2.32	0.44
2:B:114:PRO:O	2:B:115:GLN:C	2.55	0.44
2:B:408:LEU:HB3	2:B:409:ALA:H	1.69	0.44
2:B:650:GLU:HG3	2:B:654:ARG:HH21	1.83	0.44
2:B:879:ARG:N	2:B:879:ARG:HD2	2.33	0.44
5:E:89:GLY:C	5:E:91:LYS:H	2.20	0.44
6:F:135:ARG:HG2	6:F:137:TYR:CE1	2.52	0.44
7:G:114:LEU:HD23	7:G:161:GLY:O	2.16	0.44
8:H:99:GLY:HA3	8:H:117:SER:O	2.17	0.44
9:I:59:VAL:C	9:I:61:ASP:H	2.21	0.44
1:A:1081:LEU:CD1	1:A:1098:VAL:H	2.29	0.44
1:A:1237:ILE:CG2	1:A:1238:ILE:N	2.79	0.44
1:A:1311:VAL:HG21	1:A:1329:THR:HG23	2.00	0.44
1:A:317:LYS:O	1:A:318:SER:HB3	2.18	0.44
1:A:384:ASN:O	1:A:385:ILE:C	2.55	0.44
1:A:388:LEU:HD13	1:A:432:VAL:CG2	2.48	0.44
1:A:730:GLY:O	1:A:731:ARG:C	2.56	0.44
1:A:821:ARG:HG2	2:B:514:LEU:H	1.82	0.44
2:B:225:VAL:HG11	2:B:385:LEU:HA	1.99	0.44
2:B:273:LEU:HD22	2:B:360:PHE:CD1	2.52	0.44
2:B:781:PHE:N	2:B:781:PHE:CD2	2.83	0.44
3:C:174:ALA:O	3:C:175:ALA:HB3	2.18	0.44
3:C:183:TRP:CZ3	3:C:203:GLN:NE2	2.86	0.44
3:C:91:HIS:C	3:C:91:HIS:CD2	2.91	0.44
4:D:180:LEU:HD23	4:D:180:LEU:HA	1.89	0.44
4:D:155:ARG:CD	4:D:221:TYR:CE1	3.00	0.44
5:E:124:VAL:HG13	5:E:132:ILE:CB	2.47	0.44
5:E:111:VAL:HG12	5:E:137:GLU:HG2	1.99	0.44
5:E:33:GLU:C	5:E:35:VAL:H	2.19	0.44
6:F:119:ARG:CG	6:F:119:ARG:NH1	2.78	0.44
6:F:82:THR:HA	6:F:83:PRO:HD3	1.71	0.44
7:G:91:VAL:CG1	7:G:92:VAL:N	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:102:TYR:N	8:H:102:TYR:CD2	2.86	0.44
9:I:88:SER:HB3	9:I:95:THR:HG21	2.00	0.44
1:A:973:ILE:CD1	1:A:1037:LEU:HA	2.47	0.44
1:A:1118:VAL:HG23	1:A:1118:VAL:O	2.18	0.44
1:A:1166:ASP:CG	1:A:1194:ARG:HE	2.21	0.44
1:A:173:THR:HG22	1:A:184:SER:OG	2.18	0.44
1:A:321:PRO:O	1:A:322:VAL:HB	2.16	0.44
1:A:378:GLU:OE1	1:A:388:LEU:HD21	2.17	0.44
1:A:568:PRO:HB2	3:C:221:TYR:CE1	2.52	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
2:B:860:MET:HG2	2:B:861:ASP:N	2.32	0.44
3:C:208:GLU:C	3:C:210:GLU:H	2.20	0.44
5:E:78:LEU:HD11	5:E:109:ILE:HD12	1.99	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
8:H:65:LEU:CD2	8:H:65:LEU:N	2.64	0.44
1:A:117:GLU:N	1:A:117:GLU:CD	2.68	0.44
1:A:1410:PHE:HD2	2:B:1212:ILE:CD1	2.30	0.44
1:A:337:ARG:HD2	2:B:1132:GLU:CD	2.38	0.44
1:A:482:PHE:C	1:A:484:GLY:H	2.20	0.44
1:A:666:ILE:HD12	1:A:666:ILE:N	2.33	0.44
1:A:722:LEU:HD23	1:A:799:PHE:CD1	2.53	0.44
1:A:817:ALA:O	1:A:818:MET:C	2.54	0.44
1:A:836:TYR:N	14:T:18:DC:H5'	2.33	0.44
2:B:1110:PRO:O	2:B:1119:VAL:HG13	2.17	0.44
2:B:33:VAL:O	2:B:36:ALA:HB3	2.17	0.44
2:B:599:THR:O	2:B:603:LEU:HB2	2.18	0.44
2:B:758:PHE:HB3	2:B:761:HIS:HD2	1.82	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
3:C:114:TYR:HB3	3:C:140:ASN:O	2.18	0.44
5:E:46:TYR:O	5:E:54:GLN:HB2	2.18	0.44
5:E:78:LEU:HD23	5:E:79:TRP:N	2.33	0.44
8:H:26:ILE:CD1	8:H:49:VAL:HG11	2.48	0.44
11:K:83:PRO:O	11:K:84:LYS:C	2.56	0.44
1:A:1144:LYS:HA	1:A:1268:LEU:HD22	2.00	0.44
1:A:1161:THR:O	1:A:1163:ILE:N	2.51	0.44
1:A:277:GLU:O	1:A:277:GLU:HG2	2.18	0.44
1:A:382:PRO:HB3	1:A:428:TYR:CE2	2.53	0.44
1:A:884:ASP:HB2	1:A:1024:SER:OG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:889:SER:C	1:A:891:ALA:N	2.69	0.44
2:B:351:TYR:CD1	2:B:355:ILE:HD11	2.52	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
2:B:661:LEU:C	2:B:663:ALA:N	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
3:C:3:GLU:N	11:K:104:ASN:HD21	2.15	0.44
4:D:216:ASN:C	4:D:218:GLU:N	2.68	0.44
4:D:51:ASN:C	4:D:52:LEU:O	2.55	0.44
5:E:114:ASN:O	5:E:115:ASN:CB	2.54	0.44
6:F:116:ASP:C	6:F:116:ASP:OD1	2.56	0.44
6:F:120:ILE:O	6:F:124:GLU:HG3	2.18	0.44
8:H:6:PHE:CD2	8:H:6:PHE:C	2.91	0.44
2:B:309:GLN:OE1	9:I:52:ILE:HD11	2.18	0.44
9:I:55:THR:OG1	9:I:100:PHE:CD2	2.70	0.44
14:T:16:DT:C2'	14:T:17:DT:C5'	2.94	0.44
1:A:1241:ARG:O	1:A:1242:VAL:HB	2.17	0.43
1:A:1259:MET:CE	1:A:1263:ILE:HG13	2.48	0.43
1:A:265:LYS:HA	1:A:265:LYS:CE	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
2:B:376:PHE:CE2	2:B:569:TYR:HD2	2.35	0.43
2:B:526:GLU:OE1	2:B:752:ALA:CB	2.66	0.43
3:C:33:LEU:C	3:C:33:LEU:HD12	2.37	0.43
7:G:138:THR:HG22	7:G:139:ILE:HB	2.00	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
8:H:123:MET:CE	8:H:142:LEU:HD21	2.47	0.43
8:H:143:LEU:C	8:H:144:ILE:HG13	2.38	0.43
9:I:69:PRO:HG2	9:I:85:PHE:CD2	2.52	0.43
1:A:1319:VAL:O	1:A:1322:ILE:HG12	2.17	0.43
1:A:306:ASN:O	1:A:306:ASN:OD1	2.36	0.43
1:A:347:PHE:CD1	1:A:347:PHE:N	2.87	0.43
1:A:34:LYS:NZ	1:A:57:ARG:HH21	2.10	0.43
1:A:495:GLU:O	1:A:498:ARG:HG3	2.17	0.43
1:A:571:LEU:HD22	8:H:46:LEU:CD1	2.41	0.43
1:A:693:VAL:HG21	1:A:721:PHE:HE1	1.82	0.43
1:A:528:LEU:HD23	1:A:751:SER:HA	2.01	0.43
2:B:1002:THR:O	2:B:1004:GLU:N	2.50	0.43
2:B:235:SER:O	2:B:236:HIS:CD2	2.69	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:880:THR:O	2:B:881:ASN:HB2	2.17	0.43
3:C:44:LEU:HD21	3:C:159:ALA:HB1	2.00	0.43
5:E:42:PHE:O	5:E:43:LYS:C	2.57	0.43
7:G:138:THR:O	7:G:140:LYS:N	2.51	0.43
7:G:14:HIS:CE1	7:G:15:PRO:HD2	2.53	0.43
8:H:92:ASP:C	8:H:93:TYR:CD1	2.91	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
1:A:1118:VAL:HG22	1:A:1306:LEU:HB2	1.99	0.43
1:A:184:SER:HB2	1:A:199:LEU:HD23	2.00	0.43
1:A:184:SER:HB3	1:A:199:LEU:HD23	1.99	0.43
1:A:528:LEU:HD23	1:A:751:SER:CA	2.48	0.43
1:A:341:MET:CE	1:A:843:LYS:NZ	2.82	0.43
2:B:1033:LYS:O	2:B:1037:LEU:HG	2.18	0.43
2:B:284:ILE:CD1	2:B:324:ILE:HD12	2.48	0.43
2:B:50:SER:OG	2:B:411:PRO:HD3	2.17	0.43
2:B:604:ARG:O	2:B:606:LYS:N	2.51	0.43
2:B:885:MET:HA	2:B:936:ASP:HB2	1.98	0.43
5:E:111:VAL:O	5:E:111:VAL:HG12	2.18	0.43
5:E:82:PHE:N	5:E:82:PHE:HD1	2.17	0.43
1:A:857:ARG:CZ	6:F:139:PRO:HG3	2.48	0.43
6:F:69:LEU:O	6:F:70:LYS:HB2	2.19	0.43
6:F:76:LYS:O	6:F:79:ARG:HD3	2.17	0.43
8:H:40:LEU:CD2	8:H:42:ILE:HD11	2.48	0.43
10:J:47:ARG:C	10:J:49:MET:N	2.69	0.43
1:A:1230:GLU:C	1:A:1232:ASN:N	2.72	0.43
1:A:1267:MET:HA	1:A:1271:ILE:HD12	2.00	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
1:A:207:ILE:CG2	1:A:211:PHE:CE2	3.02	0.43
1:A:709:THR:CG2	1:A:710:LEU:H	2.28	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
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
2:B:1004:GLU:HG3	10:J:42:LYS:HZ1	1.82	0.43
2:B:778:MET:HE3	2:B:1094:ARG:HD3	2.00	0.43
2:B:546:SER:OG	2:B:631:GLY:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:604:ARG:O	2:B:607:GLY:N	2.51	0.43
2:B:604:ARG:HA	2:B:609:ILE:HG13	1.99	0.43
2:B:69:LEU:HD22	2:B:429:PHE:CE1	2.53	0.43
2:B:887:HIS:N	2:B:887:HIS:CD2	2.85	0.43
3:C:22:LEU:HD11	11:K:101:LEU:HD21	2.00	0.43
3:C:52:GLU:OE2	3:C:154:LYS:HD2	2.18	0.43
3:C:58:LEU:N	3:C:58:LEU:HD23	2.33	0.43
4:D:7:THR:HG21	4:D:32:GLU:CD	2.38	0.43
5:E:35:VAL:C	5:E:37:LEU:H	2.22	0.43
7:G:26:LEU:HA	7:G:26:LEU:HD23	1.73	0.43
10:J:8:PHE:CD2	10:J:8:PHE:N	2.86	0.43
1:A:1015:VAL:CG1	1:A:1019:CYS:SG	3.06	0.43
1:A:1077:THR:HB	1:A:1078:GLN:HE21	1.84	0.43
1:A:1193:LEU:HD12	1:A:1193:LEU:C	2.38	0.43
1:A:1345:ARG:HD2	1:A:1373:ASP:OD1	2.18	0.43
1:A:1336:MET:CE	1:A:1381:LEU:HG	2.49	0.43
1:A:1389:PHE:C	1:A:1391:ARG:H	2.22	0.43
1:A:298:PHE:HD2	1:A:299:HIS:HD2	1.67	0.43
1:A:709:THR:OG1	1:A:712:GLU:HG3	2.17	0.43
2:B:261:ARG:HH11	2:B:261:ARG:CB	2.09	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
2:B:846:ILE:HG23	2:B:974:PRO:CG	2.31	0.43
2:B:95:ILE:CB	2:B:130:VAL:HG22	2.48	0.43
3:C:31:ASN:HA	3:C:34:ARG:HB3	1.99	0.43
4:D:187:THR:C	4:D:189:ASP:N	2.70	0.43
4:D:219:THR:CG2	4:D:220:LEU:O	2.67	0.43
5:E:116:ILE:HG22	5:E:120:ALA:HB3	2.00	0.43
5:E:153:HIS:C	5:E:154:ILE:HG13	2.39	0.43
5:E:161:LYS:HD2	5:E:195:VAL:CG2	2.49	0.43
5:E:46:TYR:CD2	5:E:58:MET:HG3	2.54	0.43
4:D:33:PHE:CE1	7:G:80:LYS:HD3	2.52	0.43
8:H:40:LEU:HG	8:H:42:ILE:HG13	2.00	0.43
10:J:7:CYS:CA	10:J:49:MET:HE3	2.47	0.43
11:K:40:HIS:O	11:K:41:THR:C	2.57	0.43
12:L:38:LEU:HG	12:L:39:SER:N	2.33	0.43
1:A:11:LEU:CD2	1:A:11:LEU:O	2.61	0.43
1:A:1376:THR:O	1:A:1377:THR:C	2.56	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
1:A:836:TYR:CD2	1:A:840:ARG:HD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:LYS:NZ	2:B:1151:LEU:O	2.51	0.43
1:A:2:VAL:CG1	2:B:1157:ALA:O	2.67	0.43
2:B:1201:LYS:HE2	2:B:1205:GLN:CD	2.39	0.43
2:B:218:SER:HA	2:B:404:LYS:HA	2.00	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
9:I:82:GLU:HB3	9:I:104:LEU:HG	2.01	0.43
1:A:1074:GLU:N	1:A:1075:PRO:HD2	2.34	0.43
1:A:1124:HIS:HB2	1:A:1130:GLN:HG2	2.01	0.43
1:A:1308:THR:HG21	1:A:1310:GLY:O	2.19	0.43
1:A:289:ILE:CG2	1:A:290:GLU:N	2.80	0.43
1:A:396:PRO:HG2	1:A:397:ASN:OD1	2.19	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:833:GLU:CG	1:A:1102:LYS:HE2	2.48	0.43
1:A:351:THR:HG21	2:B:1103:ILE:HG13	2.00	0.43
2:B:222:ILE:C	2:B:240:ILE:HD13	2.39	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
2:B:605:ARG:NE	2:B:639:ILE:HD13	2.33	0.43
2:B:883:LEU:O	2:B:885:MET:N	2.52	0.43
3:C:136:ASP:OD2	3:C:137:LYS:N	2.52	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
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
4:D:38:ILE:HG12	4:D:38:ILE:H	1.47	0.43
4:D:53:SER:H	4:D:148:LEU:HD22	1.84	0.43
7:G:20:PRO:CD	7:G:21:ARG:N	2.82	0.43
8:H:130:ARG:H	8:H:130:ARG:HD3	1.79	0.43
8:H:15:VAL:HG22	8:H:26:ILE:HD11	2.00	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
11:K:55:LYS:CB	11:K:81:TYR:CD1	3.01	0.43
1:A:141:LEU:HD23	1:A:141:LEU:HA	1.86	0.43
1:A:108:MET:CB	1:A:210:ILE:HD13	2.49	0.43
1:A:218:ASP:O	1:A:219:PHE:C	2.56	0.43
1:A:239:LEU:HA	1:A:240:PRO:HD2	1.82	0.43
1:A:360:GLU:HB2	1:A:363:GLN:HG3	2.01	0.43
1:A:382:PRO:CB	1:A:428:TYR:HE2	2.32	0.43
1:A:565:ILE:O	1:A:570:PRO:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1023:VAL:O	2:B:1026:LEU:HB2	2.18	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:317:CYS:O	2:B:320:ASP:HB3	2.19	0.43
2:B:570:VAL:HG21	2:B:573:GLN:NE2	2.34	0.43
2:B:766:ARG:NH1	2:B:769:TYR:CE1	2.87	0.43
2:B:821:GLN:OE1	2:B:850:LEU:CD1	2.67	0.43
3:C:142:VAL:H	10:J:16:ASP:HB3	1.83	0.43
4:D:53:SER:HA	4:D:56:ARG:HB3	2.00	0.43
1:A:1189:SER:HB2	1:A:1256:GLU:OE1	2.18	0.43
1:A:1450:LEU:CD1	6:F:108:PHE:CZ	3.02	0.43
1:A:889:SER:HA	1:A:1297:GLU:N	2.33	0.43
1:A:69:THR:HG22	2:B:1174:LYS:HD3	2.01	0.43
2:B:460:ALA:O	2:B:462:ALA:N	2.52	0.43
1:A:785:PRO:O	2:B:702:LEU:HD12	2.18	0.43
3:C:184:ASN:ND2	3:C:189:THR:HB	2.34	0.43
3:C:22:LEU:HD22	3:C:230:MET:HE2	1.99	0.43
3:C:41:ILE:HA	3:C:42:PRO:HD3	1.90	0.43
3:C:99:LEU:CD2	3:C:99:LEU:N	2.74	0.43
7:G:1:MET:HE1	7:G:80:LYS:H	1.83	0.43
2:B:308:TRP:CZ3	9:I:45:ARG:HG2	2.54	0.43
11:K:12:LEU:HD12	11:K:12:LEU:HA	1.88	0.43
11:K:41:THR:HG22	11:K:42:LEU:N	2.33	0.43
1:A:1110:ASN:ND2	1:A:1110:ASN:N	2.66	0.43
1:A:1115:SER:OG	1:A:1116:LEU:N	2.51	0.43
1:A:151:ASP:HA	1:A:162:VAL:O	2.19	0.43
1:A:423:ASP:OD1	1:A:424:ILE:N	2.52	0.43
1:A:919:ILE:CG1	1:A:925:LEU:HD12	2.49	0.43
2:B:479:VAL:O	2:B:480:SER:HB3	2.17	0.43
2:B:376:PHE:CE1	2:B:569:TYR:HB3	2.53	0.43
3:C:24:ASN:O	3:C:24:ASN:CG	2.55	0.43
4:D:118:THR:O	4:D:119:ARG:C	2.57	0.43
4:D:12:ARG:HH12	4:D:14:ARG:HA	1.81	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
5:E:112:TYR:C	5:E:112:TYR:HD1	2.21	0.43
2:B:1224:PHE:CE1	5:E:171:LYS:HG3	2.54	0.43
5:E:24:LYS:HB2	5:E:24:LYS:HE3	1.88	0.43
7:G:49:LEU:HD21	7:G:77:VAL:HG23	2.00	0.43
11:K:79:GLU:HG3	11:K:80:GLY:H	1.83	0.43
1:A:1035:TYR:N	1:A:1035:TYR:CD2	2.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1153:TYR:HA	9:I:41:PRO:O	2.19	0.42
1:A:114:LEU:HB2	1:A:142:CYS:HB2	2.01	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
1:A:78:PRO:CB	2:B:1201:LYS:HE3	2.49	0.42
2:B:576:ASP:HB3	2:B:622:LYS:NZ	2.34	0.42
3:C:167:HIS:CA	11:K:6:ARG:HH12	2.32	0.42
3:C:214:ASN:O	3:C:217:ASP:OD2	2.36	0.42
3:C:235:VAL:HG21	10:J:6:ARG:HH22	1.83	0.42
4:D:51:ASN:O	4:D:52:LEU:C	2.55	0.42
5:E:135:PHE:CD2	5:E:140:LEU:HD21	2.52	0.42
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
9:I:82:GLU:HB3	9:I:104:LEU:CD1	2.49	0.42
2:B:822:ASN:HD22	10:J:52:THR:HG21	1.83	0.42
1:A:849:MET:CE	1:A:1061:GLY:HA2	2.49	0.42
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.34	0.42
1:A:1152:ILE:HG23	1:A:1260:LEU:CD2	2.49	0.42
1:A:26:GLU:O	1:A:27:VAL:C	2.57	0.42
1:A:463:ILE:HD11	1:A:469:ARG:HG3	2.01	0.42
1:A:353:ILE:HG21	1:A:487:MET:HE3	2.01	0.42
1:A:583:PRO:HG2	1:A:586:ILE:HG13	2.01	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
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: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
2:B:604:ARG:NH2	2:B:613:VAL:O	2.41	0.42
2:B:405:ARG:CD	2:B:631:GLY:O	2.67	0.42
2:B:785:TYR:CD1	2:B:786:ASN:N	2.87	0.42
1:A:482:PHE:CB	2:B:838:SER:OG	2.66	0.42
3:C:101:LEU:CD1	3:C:118:LEU:HD23	2.47	0.42
10:J:14:VAL:CG1	10:J:14:VAL:O	2.66	0.42
10:J:64:ASN:CB	10:J:65:PRO:CD	2.78	0.42
11:K:27:ALA:HB1	11:K:28:PRO:HD2	2.02	0.42
1:A:264:PHE:CB	1:A:265:LYS:HZ1	2.31	0.42
1:A:806:ARG:HH12	2:B:729:ILE:CD1	2.33	0.42
1:A:829:VAL:O	1:A:830:LYS:C	2.57	0.42
1:A:874:ASP:N	1:A:1058:VAL:HG23	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:LEU:CD1	2:B:1146:PHE:CE2	3.01	0.42
2:B:1220:ARG:NH1	2:B:1220:ARG:HB3	2.34	0.42
2:B:370:PHE:HD2	2:B:373:ARG:HD2	1.83	0.42
2:B:473:MET:C	2:B:475:SER:H	2.23	0.42
2:B:636:PRO:O	2:B:636:PRO:HG2	2.20	0.42
2:B:843:GLN:HA	2:B:846:ILE:HD12	1.99	0.42
3:C:183:TRP:CZ2	3:C:212:PRO:HG3	2.54	0.42
3:C:97:VAL:CG1	3:C:99:LEU:HD21	2.48	0.42
7:G:101:VAL:CG1	7:G:102:GLN:N	2.83	0.42
7:G:125:SER:O	7:G:126:ASN:HB2	2.20	0.42
7:G:21:ARG:HH11	7:G:24:GLN:HB2	1.81	0.42
11:K:63:VAL:O	11:K:63:VAL:CG2	2.66	0.42
2:B:233:PRO:HD3	14:T:11:DA:OP1	2.18	0.42
1:A:1001:ARG:O	1:A:1002:GLY:C	2.57	0.42
1:A:1081:LEU:CD1	1:A:1097:GLY:HA3	2.49	0.42
1:A:116:ASP:C	1:A:118:HIS:N	2.71	0.42
1:A:1191:TRP:CD1	1:A:1256:GLU:HB2	2.54	0.42
1:A:1332:PHE:N	1:A:1332:PHE:CD2	2.86	0.42
1:A:722:LEU:HB3	1:A:799:PHE:CD1	2.54	0.42
2:B:1079:LYS:HA	3:C:27:LEU:HD21	2.01	0.42
2:B:172:ILE:HD13	2:B:178:ASN:ND2	2.24	0.42
2:B:412:LEU:HD21	2:B:479:VAL:HG11	2.02	0.42
2:B:788:ARG:O	2:B:967:ARG:NH1	2.53	0.42
4:D:8:PHE:HZ	4:D:37:GLN:CD	2.23	0.42
5:E:5:ASN:ND2	5:E:5:ASN:O	2.52	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
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
3:C:66:ARG:HH21	10:J:5:VAL:HG23	1.85	0.42
1:A:1263:ILE:O	1:A:1263:ILE:HG22	2.19	0.42
1:A:1385:THR:CG2	1:A:1386:ARG:H	2.29	0.42
1:A:364:VAL:O	1:A:364:VAL:HG13	2.17	0.42
1:A:548:ASN:O	1:A:549:MET:C	2.57	0.42
1:A:674:PRO:HG2	1:A:675:THR:H	1.84	0.42
2:B:244:LEU:CD2	2:B:366:GLN:NE2	2.82	0.42
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
2:B:530:GLY:O	2:B:531:GLN:C	2.57	0.42
2:B:700:SER:O	2:B:701:ILE:HG22	2.20	0.42
4:D:138:ASN:C	4:D:140:ASP:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:213:GLU:O	4:D:217:LEU:HG	2.18	0.42
5:E:13:TRP:CZ3	5:E:39:LEU:HB2	2.54	0.42
6:F:88:TYR:O	6:F:89:GLU:C	2.58	0.42
12:L:61:THR:CG2	12:L:62:LYS:N	2.82	0.42
1:A:993:LEU:CD2	1:A:1022:LEU:HD21	2.49	0.42
1:A:517:ASN:ND2	1:A:1364:ASN:HD22	2.16	0.42
1:A:283:GLY:O	1:A:285:PRO:CD	2.67	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
1:A:66:LYS:HD3	1:A:67:CYS:H	1.84	0.42
1:A:774:ARG:CZ	1:A:797:LYS:CB	2.98	0.42
1:A:889:SER:OG	1:A:891:ALA:HB3	2.20	0.42
2:B:1065:GLN:CD	2:B:1066:SER:N	2.73	0.42
2:B:1202:LEU:HD22	2:B:1206:GLU:OE2	2.19	0.42
2:B:51:PHE:CD2	2:B:173:MET:HB3	2.55	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
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
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
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
3:C:46:ILE:HG13	3:C:72:LEU:HD11	2.02	0.42
4:D:138:ASN:O	4:D:140:ASP:N	2.52	0.42
5:E:22:MET:HG3	5:E:187:TYR:CD1	2.55	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
9:I:93:LYS:H	9:I:93:LYS:CD	2.12	0.42
1:A:130:ASP:O	1:A:131:SER:C	2.58	0.42
1:A:1371:LEU:HD12	1:A:1375:MET:HG3	2.00	0.42
1:A:385:ILE:CG2	1:A:386:ASP:N	2.82	0.42
1:A:626:ASN:O	1:A:631:HIS:HD2	2.02	0.42
2:B:1050:ILE:CG2	2:B:1051:THR:N	2.82	0.42
2:B:1082:MET:HA	3:C:189:THR:HA	2.02	0.42
2:B:123:THR:HA	2:B:204:ILE:O	2.19	0.42
2:B:386:LEU:O	2:B:387:LEU:C	2.55	0.42
2:B:56:ASP:CB	2:B:57:TYR:HD1	2.32	0.42
2:B:597:MET:CE	2:B:624:LEU:HD21	2.49	0.42
2:B:526:GLU:OE1	2:B:752:ALA:HB3	2.20	0.42
2:B:889:THR:CG2	2:B:891:ASP:HB2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:995:ARG:CB	2:B:997:GLU:OE2	2.67	0.42
6:F:133:VAL:HG13	6:F:146:TRP:O	2.19	0.42
7:G:35:GLU:HG2	7:G:48:VAL:HG23	2.02	0.42
8:H:39:THR:O	8:H:123:MET:HG3	2.19	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
1:A:1339:LEU:HD13	5:E:147:HIS:CG	2.55	0.42
1:A:219:PHE:O	1:A:222:LEU:N	2.51	0.42
1:A:244:PRO:CB	1:A:245:PRO:HD3	2.31	0.42
1:A:709:THR:CG2	1:A:710:LEU:N	2.80	0.42
1:A:719:VAL:O	1:A:721:PHE:N	2.53	0.42
1:A:758:ILE:H	1:A:758:ILE:HG13	1.72	0.42
2:B:1182:CYS:C	2:B:1183:LYS:HE3	2.40	0.42
2:B:100:PRO:HG2	2:B:124:TYR:CE1	2.55	0.42
2:B:44:VAL:HG11	2:B:495:LEU:HD13	2.02	0.42
2:B:558:LEU:HD11	2:B:596:LEU:CD2	2.48	0.42
2:B:637:LEU:HD23	2:B:637:LEU:HA	1.80	0.42
3:C:136:ASP:CB	3:C:141:GLY:H	2.33	0.42
3:C:44:LEU:HD13	3:C:129:ILE:HG23	2.01	0.42
5:E:167:ARG:HD3	5:E:167:ARG:HA	1.78	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
6:F:97:ARG:NH2	6:F:108:PHE:HE1	2.17	0.42
7:G:53:ASN:HD22	7:G:53:ASN:N	2.15	0.42
8:H:27:GLU:HG2	8:H:38:LEU:O	2.20	0.42
8:H:83:GLN:CD	8:H:87:ARG:NH2	2.73	0.42
9:I:25:LEU:HG	9:I:38:ALA:HB2	2.02	0.42
2:B:992:ILE:HD11	11:K:66:PRO:HB2	2.00	0.42
11:K:78:THR:HG22	11:K:79:GLU:N	2.35	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
1:A:1225:PHE:CE2	1:A:1227:ILE:HD11	2.55	0.42
1:A:1297:GLU:OE1	1:A:1297:GLU:N	2.53	0.42
1:A:692:ASP:O	1:A:695:LYS:N	2.53	0.42
1:A:683:ILE:HG21	1:A:801:GLU:CD	2.40	0.42
1:A:845:LEU:O	1:A:846:GLU:C	2.58	0.42
1:A:903:ASN:ND2	1:A:903:ASN:C	2.73	0.42
1:A:913:LEU:CD1	1:A:914:GLU:N	2.78	0.42
1:A:923:LEU:HD23	1:A:923:LEU:HA	1.88	0.42
2:B:597:MET:HE2	2:B:597:MET:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:638:PHE:CD2	2:B:690:VAL:HG22	2.54	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
2:B:859:TYR:CD1	2:B:859:TYR:N	2.88	0.42
2:B:885:MET:HG2	2:B:936:ASP:HB2	2.02	0.42
2:B:973:ILE:HG23	2:B:974:PRO:HD2	2.02	0.42
4:D:155:ARG:HB3	4:D:155:ARG:NH1	2.34	0.42
4:D:71:LYS:C	4:D:74:GLN:H	2.23	0.42
4:D:8:PHE:HZ	4:D:37:GLN:NE2	2.17	0.42
5:E:124:VAL:H	5:E:125:PRO:HD2	1.82	0.42
1:A:870:GLU:CB	5:E:204:THR:HG21	2.49	0.42
7:G:132:SER:HB3	7:G:135:ASP:N	2.32	0.42
8:H:138:GLU:C	8:H:138:GLU:OE1	2.58	0.42
10:J:32:GLU:O	10:J:33:GLY:C	2.57	0.42
3:C:248:ILE:CD1	11:K:101:LEU:HD22	2.49	0.42
1:A:148:CYS:HB3	1:A:167:CYS:O	2.19	0.42
1:A:442:VAL:HB	1:A:489:LEU:HD11	2.01	0.42
1:A:547:LEU:HD21	1:A:560:ILE:CD1	2.50	0.42
1:A:65:LEU:O	1:A:66:LYS:O	2.38	0.42
1:A:700:ASN:C	1:A:701:LEU:HD23	2.40	0.42
1:A:850:VAL:HG21	1:A:1058:VAL:HG11	2.01	0.42
1:A:10:PRO:HG2	2:B:1192:TYR:HD2	1.85	0.42
2:B:365:THR:O	2:B:365:THR:HG23	2.20	0.42
2:B:512:ARG:HG2	2:B:512:ARG:HH11	1.83	0.42
2:B:580:VAL:CG2	2:B:624:LEU:HB3	2.49	0.42
2:B:644:GLU:C	2:B:646:LEU:N	2.73	0.42
2:B:642:ASP:N	2:B:649:LYS:HG3	2.35	0.42
3:C:22:LEU:HB2	3:C:230:MET:CE	2.50	0.42
3:C:38:ILE:H	3:C:38:ILE:HG13	1.61	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
8:H:12:VAL:HB	8:H:52:GLN:N	2.34	0.42
8:H:3:ASN:CG	8:H:4:THR:H	2.24	0.42
8:H:40:LEU:HD22	8:H:123:MET:CE	2.50	0.42
11:K:53:ASP:HB3	11:K:56:VAL:CG2	2.50	0.42
2:B:1124:ARG:NH2	15:P:2:A:OP2	2.52	0.42
1:A:1025:ARG:HG3	1:A:1025:ARG:NH1	2.33	0.41
1:A:884:ASP:OD2	1:A:1030:ARG:NH2	2.53	0.41
1:A:1189:SER:OG	1:A:1191:TRP:HB2	2.20	0.41
1:A:1451:VAL:C	1:A:1453:TYR:N	2.73	0.41
1:A:718:VAL:HG12	1:A:722:LEU:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:740:LEU:HD12	1:A:740:LEU:C	2.41	0.41
2:B:377:PHE:C	2:B:379:GLY:N	2.72	0.41
2:B:44:VAL:O	2:B:45:SER:C	2.59	0.41
2:B:594:ALA:HA	2:B:617:ARG:NH1	2.35	0.41
2:B:865:LYS:HD3	2:B:866:TYR:H	1.85	0.41
3:C:215:GLU:O	3:C:216:GLY:C	2.57	0.41
4:D:124:GLU:N	4:D:124:GLU:CD	2.71	0.41
4:D:27:LEU:CD1	4:D:197:SER:HB3	2.50	0.41
4:D:218:GLU:O	4:D:219:THR:C	2.58	0.41
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
8:H:9:ILE:HA	8:H:55:LEU:O	2.20	0.41
10:J:47:ARG:NH1	10:J:47:ARG:HG2	2.34	0.41
1:A:1102:LYS:O	1:A:1106:ASN:ND2	2.53	0.41
1:A:150:THR:O	1:A:150:THR:HG22	2.20	0.41
1:A:821:ARG:CB	1:A:821:ARG:HH11	2.27	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
3:C:22:LEU:HD22	3:C:230:MET:HE1	2.01	0.41
3:C:69:LEU:O	10:J:6:ARG:HD2	2.20	0.41
3:C:88:CYS:SG	3:C:91:HIS:HA	2.61	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
1:A:1037:LEU:HD11	1:A:1045:VAL:HG21	2.00	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
1:A:150:THR:HA	1:A:165:GLY:O	2.20	0.41
1:A:253:ASN:HB3	1:A:254:GLU:H	1.70	0.41
1:A:260:ASP:OD1	1:A:261:ASP:N	2.53	0.41
1:A:347:PHE:HE2	1:A:375:THR:CG2	2.32	0.41
1:A:41:MET:O	1:A:42:ASP:O	2.38	0.41
1:A:481:ASP:O	1:A:485:ASP:HB2	2.21	0.41
1:A:553:VAL:HA	1:A:554:PRO:HD2	1.90	0.41
1:A:77:CYS:C	1:A:78:PRO:O	2.58	0.41
1:A:877:HIS:C	1:A:878:ILE:HG13	2.40	0.41
2:B:430:ARG:HG2	2:B:430:ARG:HH11	1.84	0.41
2:B:570:VAL:HA	2:B:571:PRO:HD2	1.82	0.41
2:B:850:LEU:HD12	2:B:850:LEU:C	2.39	0.41
4:D:7:THR:HG21	4:D:32:GLU:OE2	2.20	0.41
4:D:50:LEU:HD21	7:G:4:ILE:CD1	2.49	0.41
5:E:7:ARG:HG3	5:E:8:ASN:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:79:GLU:O	11:K:81:TYR:N	2.54	0.41
1:A:332:LYS:HB3	1:A:337:ARG:CZ	2.50	0.41
1:A:348:SER:HA	1:A:489:LEU:O	2.21	0.41
1:A:54:ASN:HB3	1:A:247:ARG:NH2	2.33	0.41
1:A:697:ALA:CB	1:A:702:LEU:HD12	2.41	0.41
1:A:855:THR:HG21	1:A:857:ARG:HE	1.85	0.41
2:B:114:PRO:HG2	2:B:115:GLN:N	2.30	0.41
2:B:766:ARG:NH1	2:B:769:TYR:CD1	2.87	0.41
3:C:234:SER:OG	3:C:235:VAL:N	2.54	0.41
3:C:44:LEU:CD2	3:C:159:ALA:HB1	2.50	0.41
4:D:118:THR:HB	4:D:121:LYS:HB3	2.00	0.41
4:D:29:LEU:H	4:D:29:LEU:CD2	2.33	0.41
5:E:195:VAL:HG22	5:E:213:ILE:HG13	2.01	0.41
6:F:105:ALA:HB1	6:F:106:PRO:CD	2.50	0.41
7:G:126:ASN:HA	7:G:127:PRO:HA	1.95	0.41
7:G:26:LEU:O	7:G:28:THR:N	2.52	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
11:K:68:PHE:CD1	11:K:70:ARG:NH1	2.81	0.41
1:A:830:LYS:HG3	1:A:1098:VAL:HG21	2.02	0.41
1:A:382:PRO:CD	1:A:428:TYR:CE2	3.04	0.41
1:A:382:PRO:N	1:A:428:TYR:CE2	2.89	0.41
1:A:557:ASP:O	1:A:559:VAL:HG23	2.20	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
2:B:1002:THR:OG1	2:B:1006:ILE:CG1	2.66	0.41
2:B:313:MET:CE	2:B:386:LEU:HB3	2.50	0.41
2:B:615:MET:C	2:B:616:ILE:HD12	2.41	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
4:D:124:GLU:HA	4:D:127:ASP:HB2	2.01	0.41
6:F:106:PRO:HG2	7:G:18:PHE:C	2.41	0.41
8:H:38:LEU:HD12	8:H:38:LEU:HA	1.84	0.41
8:H:84:ALA:O	8:H:86:ASP:N	2.53	0.41
9:I:60:GLN:OE1	9:I:107:SER:OG	2.35	0.41
9:I:78:CYS:O	9:I:80:SER:N	2.53	0.41
10:J:37:SER:OG	10:J:47:ARG:NH2	2.53	0.41
11:K:47:ARG:NH1	11:K:47:ARG:HB3	2.23	0.41
12:L:27:LEU:N	12:L:27:LEU:HD23	2.36	0.41
1:A:1454:MET:HA	1:A:1455:PRO:HD2	1.94	0.41
1:A:255:SER:OG	2:B:918:ILE:HD13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:VAL:HG13	1:A:415:LEU:HD11	2.03	0.41
1:A:425:GLN:HG2	1:A:425:GLN:O	2.20	0.41
1:A:665:GLY:O	1:A:666:ILE:C	2.59	0.41
2:B:1175:LEU:O	2:B:1176:ASN:CB	2.66	0.41
2:B:63:ILE:HG12	2:B:130:VAL:HG21	2.03	0.41
2:B:113:TYR:CE2	2:B:192:LEU:CD2	3.03	0.41
2:B:515:HIS:O	2:B:518:HIS:HB2	2.20	0.41
2:B:54:PHE:CZ	2:B:59:LEU:HD13	2.56	0.41
2:B:94:LYS:HZ3	2:B:96:TYR:HE2	1.66	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
3:C:258:ILE:N	3:C:258:ILE:CD1	2.83	0.41
4:D:153:ARG:C	4:D:154:PHE:HD2	2.24	0.41
4:D:170:THR:HB	4:D:172:LEU:HG	2.02	0.41
8:H:83:GLN:O	8:H:85:GLY:N	2.54	0.41
9:I:73:ARG:NH1	9:I:101:PHE:CZ	2.89	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:62:ILE:HD11	9:I:86:PHE:HE2	1.86	0.41
1:A:219:PHE:HB2	1:A:220:THR:H	1.46	0.41
1:A:396:PRO:HB3	1:A:403:LYS:HA	2.02	0.41
1:A:516:SER:O	1:A:517:ASN:C	2.59	0.41
1:A:593:GLU:HB3	1:A:594:GLY:H	1.48	0.41
1:A:820:GLY:O	1:A:823:GLY:N	2.54	0.41
1:A:946:VAL:HG12	1:A:947:PHE:CE2	2.56	0.41
2:B:1001:PHE:CD1	2:B:1001:PHE:C	2.94	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
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
3:C:138:GLU:HB2	3:C:140:ASN:HD21	1.86	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
4:D:198:LEU:O	4:D:200:ASN:N	2.54	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
9:I:45:ARG:HG3	9:I:46:HIS:N	2.36	0.41
11:K:51:LEU:CD1	11:K:59:ALA:HB3	2.51	0.41
11:K:85:ASP:O	11:K:88:LYS:N	2.54	0.41
1:A:1195:LEU:HD11	1:A:1267:MET:HE3	2.01	0.41
1:A:120:GLU:C	1:A:122:MET:N	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1273:LEU:CD1	1:A:1273:LEU:N	2.84	0.41
1:A:1356:ILE:HD12	1:A:1368:MET:SD	2.60	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
1:A:460:VAL:CG1	1:A:461:LYS:N	2.83	0.41
1:A:473:SER:O	1:A:521:MET:HB3	2.21	0.41
1:A:639:PRO:CG	1:A:640:GLN:N	2.83	0.41
1:A:800:VAL:HA	1:A:812:GLU:OE2	2.20	0.41
2:B:1084:GLN:OE1	3:C:189:THR:CG2	2.69	0.41
1:A:343:LYS:NZ	2:B:1151:LEU:HG	2.35	0.41
2:B:205:ILE:O	2:B:207:GLY:N	2.54	0.41
2:B:259:TYR:O	2:B:260:GLY:O	2.39	0.41
2:B:707:PRO:CG	2:B:708:GLU:N	2.75	0.41
2:B:976:ILE:CD1	2:B:992:ILE:HA	2.51	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
5:E:175:LEU:HA	5:E:176:PRO:HD3	1.81	0.41
5:E:45:LYS:HD3	5:E:46:TYR:CE1	2.56	0.41
6:F:152:ILE:HG22	6:F:153:VAL:N	2.35	0.41
6:F:97:ARG:NE	6:F:124:GLU:OE1	2.54	0.41
9:I:54:GLU:HB3	9:I:100:PHE:HE2	1.85	0.41
9:I:88:SER:C	9:I:90:GLN:N	2.74	0.41
10:J:2:ILE:C	10:J:53:HIS:CE1	2.94	0.41
1:A:1038:THR:H	1:A:1041:ALA:HB3	1.85	0.41
1:A:1279:ILE:O	1:A:1279:ILE:HG22	2.21	0.41
1:A:298:PHE:CD2	1:A:299:HIS:HD2	2.38	0.41
1:A:479:ASN:HA	1:A:479:ASN:HD22	1.62	0.41
1:A:526:ASP:OD1	2:B:1013:ASN:ND2	2.52	0.41
1:A:559:VAL:O	1:A:561:PRO:HD3	2.20	0.41
1:A:575:LYS:HB3	1:A:612:ILE:HG21	2.01	0.41
1:A:690:VAL:HG11	1:A:794:PRO:HD3	2.03	0.41
1:A:805:LEU:CD1	2:B:1052:VAL:HG21	2.51	0.41
2:B:1073:TYR:CE2	2:B:1080:LYS:HG3	2.56	0.41
2:B:25:ILE:HG21	2:B:658:ILE:CD1	2.49	0.41
2:B:467:GLY:N	2:B:475:SER:OG	2.54	0.41
2:B:918:ILE:HG21	2:B:935:ARG:HH22	1.83	0.41
3:C:133:ILE:CD1	3:C:237:SER:N	2.82	0.41
4:D:122:GLU:HA	4:D:125:SER:HB3	2.02	0.41
4:D:66:ARG:NH2	7:G:31:LEU:HD11	2.35	0.41
5:E:99:HIS:ND1	5:E:103:LYS:HG3	2.36	0.41
6:F:116:ASP:HB3	6:F:119:ARG:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:138:LEU:HA	6:F:138:LEU:HD23	1.84	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
8:H:128:ASN:C	8:H:128:ASN:HD22	2.23	0.41
9:I:15:TYR:CD1	9:I:30:ARG:HD2	2.56	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
1:A:1345:ARG:HG2	1:A:1372:VAL:CG1	2.49	0.41
1:A:40:THR:C	1:A:41:MET:HG3	2.41	0.41
1:A:542:GLU:HG2	1:A:542:GLU:H	1.63	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
2:B:326:ASP:OD1	2:B:329:THR:CB	2.68	0.41
2:B:435:THR:HG22	2:B:437:GLU:C	2.41	0.41
2:B:401:PHE:HB2	2:B:517:THR:OG1	2.20	0.41
2:B:571:PRO:HG2	2:B:572:HIS:H	1.86	0.41
2:B:593:PRO:HG2	2:B:617:ARG:CZ	2.50	0.41
2:B:789:MET:HE2	2:B:965:LYS:CB	2.51	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
2:B:969:ARG:HD2	3:C:61:GLU:OE2	2.21	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
11:K:31:VAL:CG1	11:K:32:VAL:N	2.81	0.41
1:A:1053:PHE:O	1:A:1056:SER:N	2.54	0.41
1:A:1138:ILE:HG13	1:A:1139:GLU:N	2.36	0.41
1:A:1116:LEU:HG	1:A:1308:THR:HB	2.03	0.41
1:A:371:ALA:HB2	1:A:462:VAL:HG13	2.03	0.41
1:A:64:ASN:O	1:A:66:LYS:N	2.54	0.41
1:A:650:GLN:HB3	1:A:654:ASN:ND2	2.36	0.41
1:A:722:LEU:HD23	1:A:799:PHE:CG	2.56	0.41
1:A:996:ASN:O	1:A:998:LEU:N	2.49	0.41
2:B:1032:SER:HB3	2:B:1089:PRO:HG2	2.03	0.41
2:B:186:GLU:OE2	2:B:186:GLU:HA	2.21	0.41
2:B:251:ILE:O	2:B:251:ILE:CG2	2.67	0.41
2:B:333:PHE:O	2:B:334:ILE:HG13	2.20	0.41
2:B:205:ILE:HG12	2:B:461:LEU:HB3	2.03	0.41
2:B:798:TYR:CE2	3:C:62:PHE:CZ	3.07	0.41
5:E:164:LEU:HD22	5:E:211:TYR:HD2	1.77	0.41
7:G:61:ILE:HG22	7:G:62:LEU:O	2.21	0.41
7:G:59:GLY:CA	7:G:70:PHE:CD2	3.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:1:MET:CE	7:G:80:LYS:O	2.69	0.41
8:H:130:ARG:N	8:H:130:ARG:CD	2.80	0.41
3:C:22:LEU:HD11	11:K:101:LEU:HD11	2.03	0.41
12:L:49:LYS:O	12:L:50:ASP:CB	2.58	0.41
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
1:A:683:ILE:HG21	1:A:801:GLU:OE1	2.21	0.40
1:A:909:ASP:OD1	1:A:911:SER:N	2.46	0.40
2:B:1026:LEU:HA	2:B:1026:LEU:HD23	1.86	0.40
2:B:333:PHE:O	2:B:334:ILE:CG1	2.69	0.40
2:B:390:LEU:O	2:B:391:ASP:C	2.59	0.40
2:B:806:THR:HG21	2:B:808:ALA:HB3	2.03	0.40
3:C:239:PRO:O	3:C:240:VAL:C	2.59	0.40
4:D:134:THR:CG2	4:D:135:GLY:N	2.84	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
5:E:11:ARG:C	5:E:13:TRP:N	2.74	0.40
5:E:29:PHE:HD1	5:E:30:ILE:N	2.19	0.40
8:H:8:ASP:OD1	8:H:30:SER:OG	2.31	0.40
12:L:38:LEU:CG	12:L:39:SER:N	2.83	0.40
1:A:101:LYS:HA	1:A:104:GLU:OE1	2.22	0.40
1:A:34:LYS:CB	1:A:36:ARG:NH2	2.85	0.40
1:A:546:VAL:HG21	1:A:572:TRP:HB2	2.03	0.40
1:A:589:GLN:HG3	1:A:606:LEU:HD13	2.04	0.40
1:A:598:LEU:HA	8:H:122:LEU:CD1	2.48	0.40
1:A:752:LYS:HD3	1:A:752:LYS:HA	1.77	0.40
1:A:786:HIS:HE1	2:B:519:TRP:CZ2	2.39	0.40
1:A:857:ARG:NH1	6:F:139:PRO:CB	2.84	0.40
1:A:897:TYR:CD1	1:A:897:TYR:N	2.89	0.40
2:B:104:GLU:OE2	12:L:47:ARG:NH2	2.55	0.40
2:B:1031:LEU:HB2	2:B:1055:ILE:HD13	2.03	0.40
2:B:186:GLU:HB3	2:B:187:SER:H	1.71	0.40
2:B:276:ILE:HG22	2:B:336:ARG:HB2	2.02	0.40
2:B:224:GLN:HA	2:B:396:ASP:OD2	2.20	0.40
2:B:473:MET:HE3	2:B:474:SER:N	2.37	0.40
2:B:854:LEU:HD23	2:B:854:LEU:HA	1.91	0.40
3:C:3:GLU:HB3	11:K:104:ASN:OD1	2.21	0.40
3:C:44:LEU:HD23	3:C:44:LEU:C	2.42	0.40
4:D:190:GLU:O	4:D:193:THR:CG2	2.67	0.40
4:D:154:PHE:HA	4:D:219:THR:HB	2.02	0.40
6:F:84:TYR:CD1	6:F:84:TYR:N	2.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:62:LEU:HD13	7:G:62:LEU:HA	1.89	0.40
9:I:8:ARG:O	9:I:9:ASP:HB2	2.21	0.40
10:J:53:HIS:HD2	10:J:54:VAL:H	1.58	0.40
11:K:49:GLU:C	11:K:51:LEU:N	2.75	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
2:B:769:TYR:HA	15:P:11:G:H22	1.87	0.40
1:A:1006:ILE:HD12	5:E:167:ARG:CG	2.50	0.40
1:A:1030:ARG:NH1	1:A:1035:TYR:OH	2.54	0.40
1:A:1134:ILE:HG13	1:A:1134:ILE:H	1.66	0.40
1:A:1170:ILE:CD1	1:A:1170:ILE:H	2.16	0.40
1:A:1333:ILE:H	1:A:1333:ILE:HG12	1.48	0.40
1:A:47:ARG:CZ	1:A:254:GLU:HG2	2.51	0.40
1:A:409:SER:O	1:A:410:GLY:C	2.59	0.40
1:A:524:VAL:CG1	1:A:525:GLN:H	2.25	0.40
1:A:600:PRO:HG2	1:A:601:LYS:H	1.87	0.40
1:A:604:GLY:O	1:A:605:MET:HB2	2.21	0.40
1:A:738:LYS:H	1:A:738:LYS:HD3	1.85	0.40
1:A:984:LYS:HG2	1:A:988:LEU:HD12	2.02	0.40
1:A:665:GLY:HA2	2:B:1026:LEU:CD2	2.50	0.40
2:B:1221:SER:C	2:B:1223:ASP:H	2.25	0.40
2:B:282:ILE:HG21	2:B:382:ILE:CD1	2.51	0.40
2:B:624:LEU:HA	2:B:624:LEU:HD12	1.57	0.40
2:B:629:ASP:HB3	2:B:632:ARG:HE	1.86	0.40
2:B:58:THR:HG22	2:B:62:ILE:HD11	2.02	0.40
2:B:687:GLU:O	2:B:688:GLY:C	2.59	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
3:C:77:ILE:HG23	3:C:161:LYS:HE3	2.03	0.40
4:D:126:ILE:HD13	4:D:145:MET:CE	2.50	0.40
4:D:176:GLU:O	4:D:178:ALA:N	2.54	0.40
6:F:109:VAL:CG2	6:F:124:GLU:HA	2.51	0.40
8:H:37:LYS:H	8:H:126:GLU:HB2	1.87	0.40
8:H:43:ASN:C	8:H:45:GLU:H	2.24	0.40
9:I:5:ARG:CZ	9:I:36:GLU:OE1	2.69	0.40
11:K:92:ASN:O	11:K:93:SER:C	2.60	0.40
1:A:1104:ILE:O	1:A:1106:ASN:N	2.55	0.40
1:A:1120:LEU:HD12	1:A:1120:LEU:C	2.42	0.40
1:A:1334:ASP:O	1:A:1336:MET:N	2.54	0.40
1:A:154:SER:C	1:A:156:ASP:H	2.25	0.40
1:A:89:PRO:HG2	1:A:204:THR:HB	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:PHE:HD1	1:A:222:LEU:HD22	1.79	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
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:185:THR:N	2:B:188:ASP:OD2	2.55	0.40
2:B:231:PRO:HG2	2:B:231:PRO:O	2.21	0.40
2:B:345:LYS:CG	2:B:346:GLU:N	2.70	0.40
2:B:327:ARG:HH22	2:B:371:GLU:HG2	1.79	0.40
2:B:655:LYS:HA	2:B:655:LYS:HD2	1.90	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:950:ASP:HB3	2:B:967:ARG:O	2.21	0.40
3:C:148:ARG:CG	3:C:149:LYS:H	2.34	0.40
4:D:173:HIS:O	4:D:177:VAL:HG23	2.21	0.40
4:D:187:THR:HB	4:D:190:GLU:H	1.86	0.40
5:E:60:PHE:CD1	5:E:60:PHE:C	2.95	0.40
7:G:80:LYS:O	7:G:82:PHE:CE1	2.75	0.40
2:B:620:ARG:NH1	9:I:68:LEU:HD21	2.37	0.40
11:K:93:SER:O	11:K:97:LYS:HG3	2.21	0.40
1:A:208:LEU:C	1:A:208:LEU:CD2	2.90	0.40
1:A:249:SER:O	1:A:250:ILE:CG1	2.66	0.40
1:A:599:SER:HB2	1:A:603:ASN:H	1.87	0.40
1:A:671:ALA:CB	1:A:676:MET:HG3	2.40	0.40
1:A:699:ALA:O	1:A:700:ASN:HB3	2.22	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
2:B:1030:LEU:HD11	2:B:1059:LEU:HD22	2.04	0.40
2:B:825:VAL:HG21	2:B:1092:TYR:HE1	1.87	0.40
2:B:273:LEU:HA	2:B:274:PRO:HD2	1.95	0.40
2:B:286:PHE:HB3	2:B:297:ILE:HG12	2.02	0.40
2:B:390:LEU:O	2:B:392:ARG:HG3	2.21	0.40
2:B:515:HIS:CD2	2:B:517:THR:CG2	3.02	0.40
2:B:570:VAL:HB	2:B:573:GLN:HB3	2.02	0.40
2:B:557:PHE:CZ	2:B:603:LEU:HG	2.56	0.40
2:B:773:MET:C	2:B:775:LYS:N	2.74	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
5:E:80:VAL:HG12	5:E:82:PHE:CE1	2.57	0.40
6:F:138:LEU:HB3	6:F:139:PRO:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:118:PHE:O	8:H:119:GLY:C	2.60	0.40
8:H:12:VAL:HG11	8:H:15:VAL:HG22	2.03	0.40
9:I:50:THR:H	9:I:92:ARG:HH12	1.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1408/1733 (81%)	1012 (72%)	262 (19%)	134 (10%)	1	12
2	B	1089/1224 (89%)	779 (72%)	201 (18%)	109 (10%)	1	11
3	C	264/347 (76%)	186 (70%)	51 (19%)	27 (10%)	1	11
4	D	175/221 (79%)	121 (69%)	39 (22%)	15 (9%)	1	14
5	E	212/215 (99%)	154 (73%)	42 (20%)	16 (8%)	1	17
6	F	85/155 (55%)	69 (81%)	14 (16%)	2 (2%)	7	46
7	G	169/171 (99%)	145 (86%)	13 (8%)	11 (6%)	1	22
8	H	132/146 (90%)	85 (64%)	23 (17%)	24 (18%)	0	2
9	I	117/122 (96%)	79 (68%)	29 (25%)	9 (8%)	1	17
10	J	63/70 (90%)	39 (62%)	11 (18%)	13 (21%)	0	2
11	K	113/120 (94%)	87 (77%)	22 (20%)	4 (4%)	4	38
12	L	44/70 (63%)	23 (52%)	9 (20%)	12 (27%)	0	0
All	All	3871/4594 (84%)	2779 (72%)	716 (18%)	376 (10%)	1	12

All (376) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLN

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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%)	8	38
2	B	963/1061 (91%)	841 (87%)	122 (13%)	5	29
3	C	234/299 (78%)	206 (88%)	28 (12%)	6	32
4	D	161/200 (80%)	139 (86%)	22 (14%)	4	27
5	E	196/197 (100%)	180 (92%)	16 (8%)	13	50
6	F	77/137 (56%)	73 (95%)	4 (5%)	27	66
7	G	152/152 (100%)	137 (90%)	15 (10%)	9	41
8	H	120/128 (94%)	104 (87%)	16 (13%)	4	28
9	I	113/116 (97%)	97 (86%)	16 (14%)	4	26
10	J	60/65 (92%)	55 (92%)	5 (8%)	13	49
11	K	99/102 (97%)	92 (93%)	7 (7%)	17	56
12	L	40/57 (70%)	36 (90%)	4 (10%)	9	41
All	All	3456/4034 (86%)	3069 (89%)	387 (11%)	7	36

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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%)	0

All (2) RNA backbone outliers are listed below:

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

There are no RNA pucker outliers to report.

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	13,21,22	4.23	3 (23%)	16,30,33	3.87	3 (18%)

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	-	0/3/21/22	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	-13.78	1.50	1.90
14	T	23	BRU	C4-N3	3.32	1.39	1.33
14	T	23	BRU	C4-C5	5.36	1.45	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	23	BRU	C5-C4-N3	-6.76	115.55	123.64
14	T	23	BRU	C5-C6-N1	2.81	123.67	119.56
14	T	23	BRU	C4-N3-C2	13.41	126.89	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	T	23	BRU	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1418/1733 (81%)	-0.13	16 (1%) 80 67	23, 70, 112, 141	0
2	B	1109/1224 (90%)	-0.11	15 (1%) 75 62	23, 81, 123, 141	0
3	C	266/347 (76%)	-0.16	1 (0%) 92 87	34, 69, 105, 119	0
4	D	179/221 (80%)	-0.04	1 (0%) 89 82	37, 79, 118, 131	0
5	E	214/215 (99%)	0.12	1 (0%) 90 84	41, 97, 129, 137	0
6	F	87/155 (56%)	-0.40	0 100 100	19, 46, 77, 86	0
7	G	171/171 (100%)	-0.07	1 (0%) 89 82	48, 64, 104, 113	0
8	H	136/146 (93%)	0.47	3 (2%) 62 47	80, 106, 127, 135	0
9	I	119/122 (97%)	0.29	7 (5%) 23 15	65, 100, 125, 143	0
10	J	65/70 (92%)	-0.36	0 100 100	49, 65, 92, 105	0
11	K	115/120 (95%)	-0.10	1 (0%) 84 73	34, 73, 93, 122	0
12	L	46/70 (65%)	0.20	0 100 100	48, 108, 125, 132	0
13	N	7/12 (58%)	1.65	1 (14%) 3 3	135, 140, 151, 157	0
14	T	18/26 (69%)	1.45	7 (38%) 0 1	117, 144, 155, 155	0
15	P	11/18 (61%)	1.72	4 (36%) 0 1	125, 133, 152, 156	0
All	All	3961/4650 (85%)	-0.06	58 (1%) 74 60	19, 76, 121, 157	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
15	P	1	C	4.0
1	A	1455	PRO	3.9
2	B	733	HIS	3.8
14	T	28	DA	3.8
1	A	255	SER	3.6
1	A	253	ASN	3.3
1	A	155	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	256	GLN	3.1
1	A	158	PRO	2.9
1	A	1257	ASP	2.9
9	I	76	PRO	2.8
2	B	868	MET	2.8
4	D	19	GLU	2.8
14	T	13	DT	2.8
2	B	919	SER	2.8
1	A	154	SER	2.7
15	P	4	C	2.6
2	B	918	ILE	2.5
9	I	83	ASN	2.5
8	H	139	ASN	2.5
14	T	27	DC	2.5
9	I	116	ASN	2.4
13	N	3	DT	2.4
5	E	126	SER	2.4
1	A	1188	GLN	2.4
2	B	349	ILE	2.4
2	B	470	LYS	2.4
9	I	120	GLN	2.3
14	T	14	DA	2.3
1	A	156	ASP	2.3
1	A	195	ASP	2.3
14	T	11	DA	2.3
7	G	122	ASN	2.3
1	A	153	PRO	2.3
1	A	159	THR	2.3
2	B	250	PHE	2.3
2	B	433	GLN	2.3
15	P	11	G	2.2
2	B	871	THR	2.2
1	A	161	LEU	2.2
3	C	139	GLY	2.2
2	B	715	ALA	2.2
8	H	36	CYS	2.2
11	K	114	LEU	2.1
14	T	12	DG	2.1
2	B	249	ARG	2.1
9	I	80	SER	2.1
1	A	251	SER	2.1
2	B	882	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	149	GLU	2.1
2	B	346	GLU	2.1
14	T	15	DG	2.1
9	I	77	LYS	2.1
2	B	883	LEU	2.0
9	I	105	SER	2.0
8	H	133	ASN	2.0
2	B	265	SER	2.0
15	P	2	A	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
14	BRU	T	23	20/21	0.67	0.37	-	136,142,145,146	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
17	MG	P	2458	1/1	0.84	0.32	0.21	180,180,180,180	0
16	ZN	J	1066	1/1	1.00	0.20	-0.46	53,53,53,53	0
16	ZN	B	2225	1/1	0.99	0.17	-0.70	30,30,30,30	0
16	ZN	C	1269	1/1	1.00	0.10	-1.58	40,40,40,40	0
16	ZN	A	2457	1/1	1.00	0.13	-1.69	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
16	ZN	L	1071	1/1	0.98	0.05	-1.93	100,100,100,100	0
16	ZN	I	1121	1/1	0.99	0.08	-2.35	76,76,76,76	0
16	ZN	I	1122	1/1	0.95	0.14	-2.65	135,135,135,135	0
16	ZN	A	2456	1/1	0.97	0.07	-4.04	88,88,88,88	0

6.5 Other polymers [i](#)

There are no such residues in this entry.