



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 06:27 am GMT

PDB ID : 1Y77  
Title : Complete RNA Polymerase II elongation complex with substrate analogue GMPCPP  
Authors : Kettenberger, H.; Armache, K.-J.; Cramer, P.  
Deposited on : 2004-12-08  
Resolution : 4.50 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](mailto: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.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (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

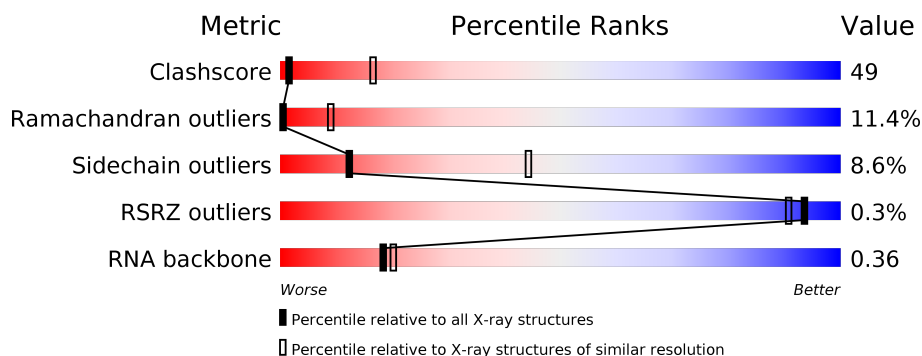
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.50 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.



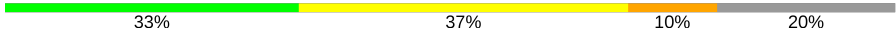

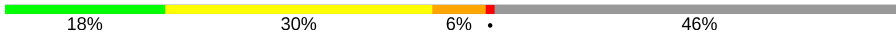
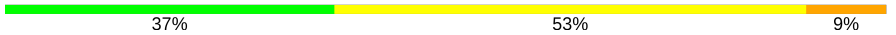
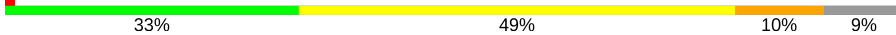
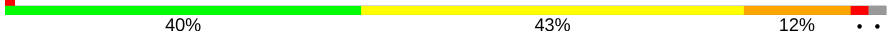
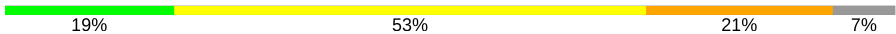
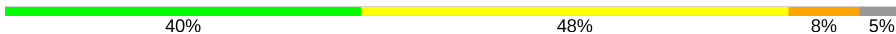

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	1029 (5.30-3.70)
Ramachandran outliers	110173	1025 (5.30-3.66)
Sidechain outliers	110143	1006 (5.30-3.66)
RSRZ outliers	101464	1015 (5.30-3.64)
RNA backbone	2435	1038 (6.00-2.90)

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  $\geq 3$ , 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	T	19	<div> <div>21%</div> <div>21% 58% 21%</div> </div>
2	N	7	<div> <div>14%</div> <div>86%</div> </div>
3	P	10	<div> <div>80% 10% 10%</div> </div>
4	A	1733	<div> <div>27% 43% 10% 18%</div> </div>
5	B	1224	<div> <div>29% 48% 13% 9%</div> </div>
6	C	318	<div> <div>23% 47% 12% 16%</div> </div>

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Mol	Chain	Length	Quality of chain
7	D	221	
8	E	215	
9	F	155	
10	G	171	
11	H	146	
12	I	122	
13	J	70	
14	K	120	
15	L	70	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	G2P	B	1308	X	-	-	-

## 2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 31835 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 DNA chain called 5'-D(P\*AP\*GP\*TP\*AP\*CP\*TP\*TP\*AP\*CP\*T\*CP\*GP\*CP\*CP\*TP\*GP\*GP\*TP\*CP\*TP\*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	19	Total	C	N	O	P	21	0	0
			388	185	67	117	19			

- Molecule 2 is a DNA chain called 5'-D(\*AP\*AP\*GP\*TP\*AP\*CP\*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	7	Total	C	N	O	P	20	0	0
			141	69	27	39	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	10	Total	C	N	O	P	0	0	0
			214	97	44	64	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1416	Total	C	N	O	S	0	0	0
			11140	7021	1946	2111	62			

- Molecule 5 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	1112	Total	C	N	O	S	0	0	0
			8836	5594	1548	1639	55			

- Molecule 6 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

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

- Molecule 7 is a protein called DNA-directed RNA polymerase II 32 kDa polypeptide.

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

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

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

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

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

- Molecule 10 is a protein called DNA-directed RNA polymerase II 19 kDa polypeptide.

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

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

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

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit 9.

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

- Molecule 13 is a protein called DNA-directed RNA polymerases I/II/III subunit 10.

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

- Molecule 14 is a protein called DNA-directed RNA polymerase II 13.6 kDa polypeptide.

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

- Molecule 15 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

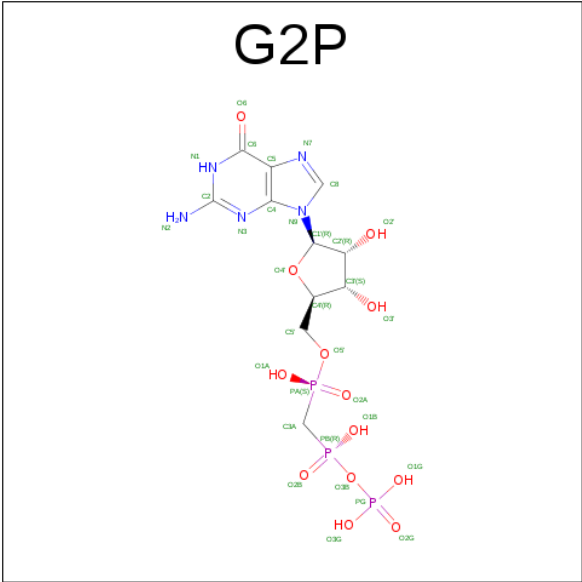
- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

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	A	1	Total	Mg	0	0
			1	1		

- Molecule 18 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: G2P) (formula: C<sub>11</sub>H<sub>18</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).

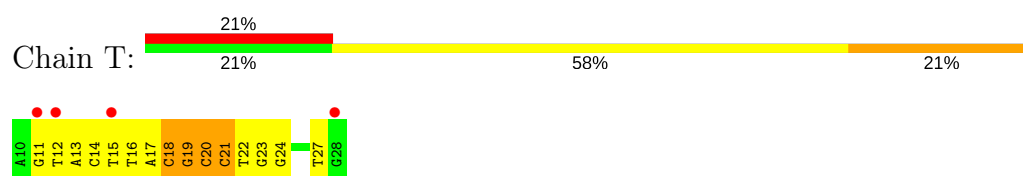


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	B	1	Total	C	N	O	P	32	0
			32	11	5	13	3		

### 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.

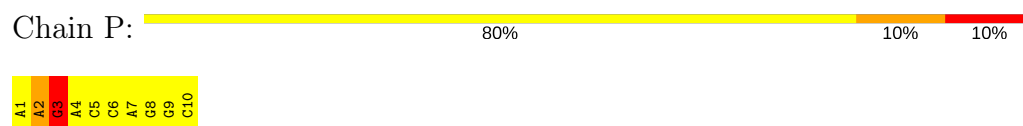
- Molecule 1: 5'-D(P\*AP\*GP\*TP\*AP\*CP\*TP\*TP\*AP\*CP\*T\*CP\*GP\*CP\*CP\*TP\*GP\*GP\*T P\*CP\*TP\*G)-3'



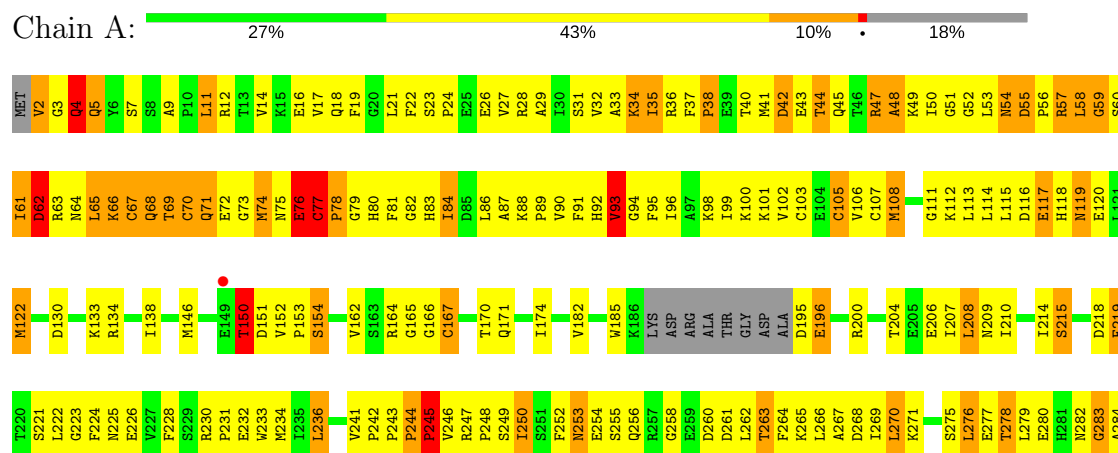
- Molecule 2: 5'-D(\*AP\*AP\*GP\*TP\*AP\*CP\*T)-3'



- Molecule 3: 5'-R(\*AP\*AP\*GP\*AP\*CP\*CP\*AP\*GP\*GP\*C)-3'



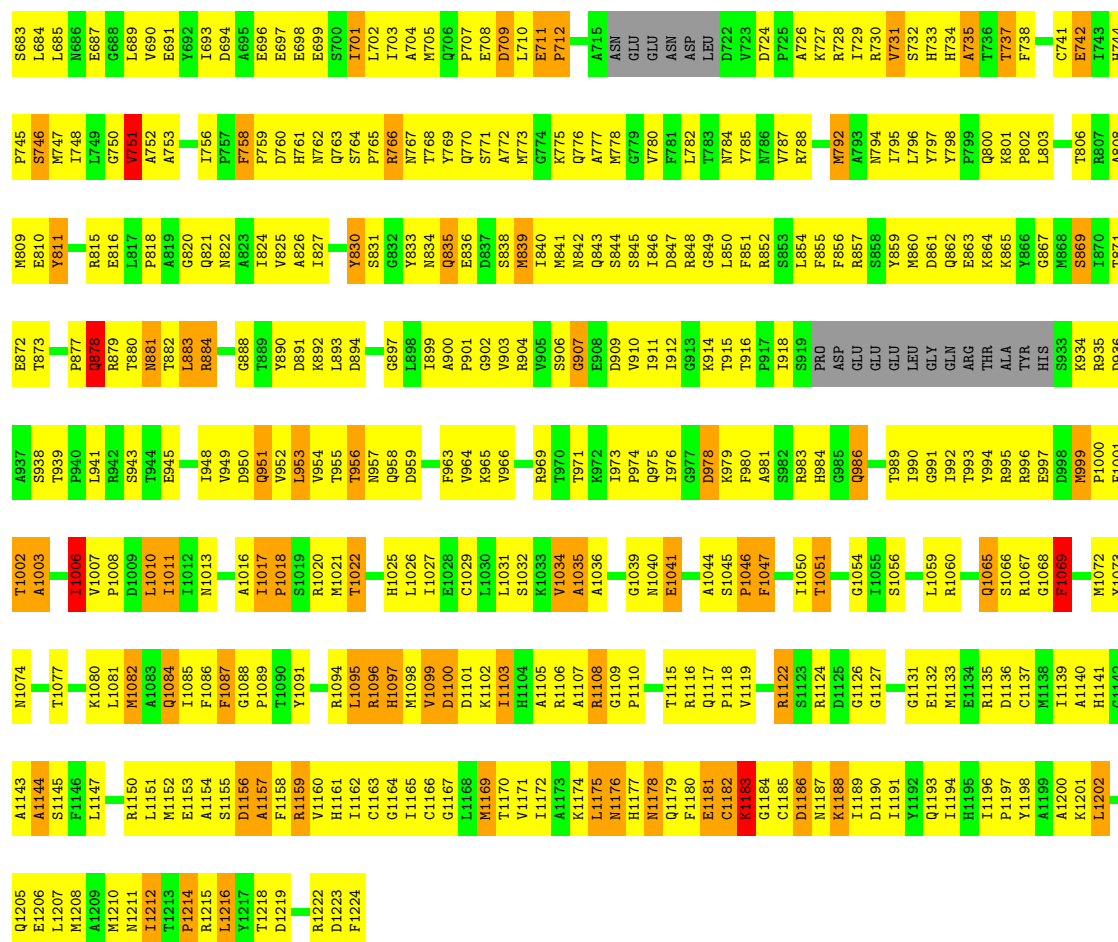
- Molecule 4: DNA-directed RNA polymerase II largest subunit





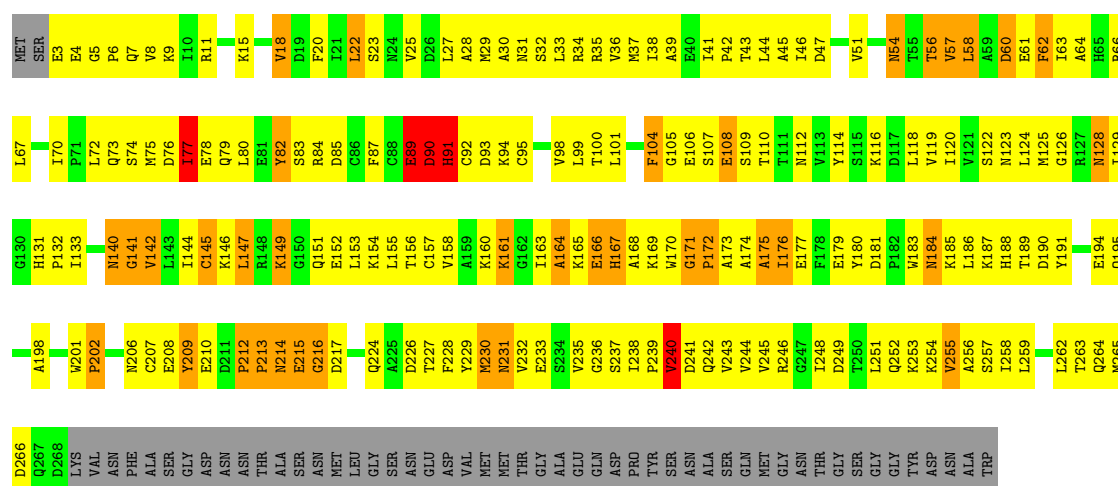
L1339	G1340	I1341	E1342	A1343	G1344	R1345	A1346	A1347	L1348	Y1349	G1350	E1351	V1352	V1355	D1359	Y1362	V1363	M1364	Y1365	R1366	H1367	M1368	A1369	W1370	V1371	V1372	D1373	V1374	M1375	T1376	T1377	L1378	G1379	G1380	L1381	V1384	T1385	R1386	H1387	G1388	F1389	N1390	N1393	T1394	G1395	A1396	L1397	M1398	R1399	G1400	S1401	F1402	E1403	E1404	
L1197	D1198	M1202	K1205	D1206	L1207	T1208	M1209	G1210	G1211	G1212	G1213	E1214	E1215	I1216	Y1217	P1218	F1219	K1221	P1222	D1223	L1224	F1225	V1226	I1227	W1228	D1233	L1236	I1237	L1238	R1239	G1240	R1241	V1242	V1243	ARG	PRO	LYS	SER	LEU	ASP	T1322	P1324	R1326	I1327	Y1328	T1329	M1330	F1332	D1333	D1334	I1335	F1336	E1337	V1338	
L1268	I1271	R1274	I1279	E1280	R1281	V1282	G1283	M1284	R1289	V1290	V1291	S1292	P1293	P1294	T1295	G1296	E1297	Y1298	R1299	K1300	E1303	W1304	V1305	L1306	F1307	T1308	D1309	M1312	L1313	S1314	E1315	V1316	V1319	P1320	G1321	I1322	P1324	R1326	I1327	Y1328	T1329	M1330	F1332	D1333	D1334	I1335	F1336	E1337	V1338						
A1131	K1132	T1133	S1135	A1137	T1141	T1147	I1148	A1149	S1150	E1151	I1152	Y1153	Y1154	D1155	P1156	F1157	K1158	R1159	S1160	L1161	V1162	P1163	E1165	D1166	F1167	E1168	I1169	T1170	L1171	R1172	H1173	F1174	S1175	L1176	ASP	GLU	GLU	ALA	GLN	SER	PHE	ASP	Q1187	E1255	E1256	K1261	E1264	M1265	T1266	E1267					
P1060	M1063	V1064	L1067	I1072	G1073	P1074	A1076	M1079	T1080	L1081	ASN	THR	PHE	HIS	PHE	ALA	GLY	VAL	ALA	L1022	R1023	S1024	K1092	K1093	V1094	T1095	S1096	G1097	V1098	P1099	R1100	E1103	Y1105	M1106	V1107	M1110	M1111	T1113	P1114	S1115	L1116	T1117	V1118	L1119	L1120	E1121	P1122	G1123	H1124	D1127	Q1130				
E946	D947	I948	Y952	D953	R954	T955	R956	R957	N958	S959	G961	N962	L964	K965	F966	I967	Y968	G969	E970	D971	M972	N973	D974	A975	H976	H977	I978	Q981	S982	D983	T984	I986	G987	D989	R996	V999	L990	L991	S992	L993	S994	T995	P996	F997	G998	H999	I990	E991	S992	L993					
R782	T783	L784	P785	H786	K789	P794	S795	T796	K797	G798	F799	V800	E801	N802	S803	Y804	L805	G806	G807	L808	T809	P810	G811	E812	F813	R814	F815	H816	A817	M818	G819	G820	R821	E822	G823	L824	T825	T827	A828	V829	K830	T831	E833	G834	G835	Y836	D837	S838	L839	E840	R841	P842	K843	A844	L845
E846	D847	I848	Y852	D853	R854	T855	R856	R857	N858	S859	G861	N862	L864	K865	F866	I867	Y868	G869	E870	D871	M872	N873	D874	A875	H876	H877	I878	Q881	S882	D883	T884	I886	G887	D890	R896	V899	L900	L901	S902	N903	T904	D905	H906	T907	R908	L909	D910	P911	S912	L913					
E914	T919	G921	R922	Q926	L929	E932	Y933	Y934	Q935	L936	Y937	K938	R939	E940	F941	L942	D943	F947	Y948	D949	W954	A1027	P1028	V1029	S1030	G1031	R1032	V1033	E1034	Y1035	R1036	L1037	T1038	Q1039	A1040	Q968	Q969	T970	F971	K977	P978	S979	D980	L981	T982	F1053	K984	L1054	D985	I986	V987	N996	L997		
L998	Y999	R1000	G1002	M1004	E1005	I1006	T1007	Q1008	A1009	L1010	Q1011	T1012	R1013	ASN	THR	PHE	HIS	VAL	ALA	L1022	R1023	S1024	K1092	K1093	V1094	T1095	S1096	G1097	V1098	P1099	R1100	E1103	Y1105	M1106	V1107	M1110	M1111	T1113	P1114	S1115	L1116	T1117	V1118	L1119	L1120	E1121	P1122	G1123	H1124	D1127	Q1130				
L1197	D1198	M1202	K1205	D1206	L1207	T1208	M1209	G1210	G1211	G1212	G1213	E1214	E1215	I1216	Y1217	P1218	F1219	K1221	P1222	D1223	L1224	F1225	V1226	I1227	W1228	D1233	L1236	I1237	L1238	R1239	G1240	R1241	V1242	V1243	ARG	PRO	LYS	SER	LEU	ASP	T1322	P1324	R1326	I1327	Y1328	T1329	M1330	F1332	D1333	D1334	I1335	F1336	E1337	V1338	
L1268	I1271	R1274	I1279	E1280	R1281	V1282	G1283	M1284	R1289	V1290	V1291	S1292	P1293	P1294	T1295	G1296	E1297	Y1298	R1299	K1300	E1303	W1304	V1305	L1306	F1307	T1308	D1309	M1312	L1313	S1314	E1315	V1316	V1319	P1320	G1321	I1322	P1324	R1326	I1327	Y1328	T1329	M1330	F1332	D1333	D1334	I1335	F1336	E1337	V1338						
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E946	D947	I948	Y952	D953	R954	T955	R956	R957	N958	S959	G961	N962	L964	K965	F966	I967	Y968	G969	E970	D971	M972	N973	D974	A975	H976	H977	I978	Q981	S982	D983	T984	I986	G987	D989	R996	V999	L990	L991	S992	L993	S994	T995	P996	F997	G998	H999	I990	E991	S992	L993					
R782	T783	L784	P785	H786	K789	P794	S795	T796	K797	G798	F799	V800	E801	N802	S803	Y804	L805	G806	G807	L808	T809	P810	G811	E812	F813	R814	F815	H816	A817	M818	G819	G820	R821	E822	G823	L824	T825	T827	A828	V829	K830	T831	E833	G834	G835	Y836	D837	S838	L839	E840	R841	P842	K843	A844	L845
E846	D847	I848	Y852	D853	R854	T855	R856	R857	N858	S859	G861	N862	L864	K865	F866	I867	Y868	G869	E870	D871	M872	N873	D874	A875	H876	H877	I878	Q881	S882	D883	T884	I886	G887	D890	R896	V899	L900	L901	S902	N903	T904	D905	H906	T907	R908	L909	D910	P911	S912	L913					
E914	T919	G921	R922	Q926	L929	E932	Y933	Y934	Q935	L936	Y937	K938	R939	E940	F941	L942	D943	F947	Y948	D949	W954	A1027	P1028	V1029	S1030	G1031	R1032	V1033	E1034	Y1035	R1036	L1037	T1038	Q1039	A1040	Q968	Q969	T970	F971	K977	P978	S979	D980	L981	T982	F1053	K984	L1054	D985	I986	V987	N996	L997		
L998	Y999	R1000	G1002	M1004	E1005	I1006	T1007	Q1008	A1009	L1010	Q1011	T1012	R1013	ASN	THR	PHE	HIS	VAL	ALA	L1022	R1023	S1024	K1092	K1093	V1094	T1095	S1096	G1097	V1098	P1099	R1100	E1103	Y1105	M1106	V1107	M1110	M1111	T1113	P1114	S1115	L1116	T1117	V1118	L1119	L1120	E1121	P1122	G1123	H1124	D1127	Q1130				
L1197	D1198	M1202	K1205	D1206	L1207	T1208	M1209	G1210	G1211	G1212	G1213	E1214	E1215	I1216	Y1217	P1218	F1219	K1221	P1222	D1223	L1224	F1225	V1226	I1227	W1228	D1233	L1236	I1237	L1238	R1239	G1240	R1241	V1242	V1243	ARG	PRO	LYS	SER	LEU	ASP	T1322	P1324	R1326	I1327	Y1328	T1329	M1330	F1332	D1333	D1334	I1335	F1336	E1337	V1338	
L1268	I1271	R1274	I1279	E1280	R1281	V1282	G1283	M1284	R1289	V1290	V1291	S1292	P1293	P1294	T1295	G1296	E1297	Y1298	R1299	K1300	E1303	W1304	V1305	L1306	F1307	T1308	D1309	M1312	L1313	S1314	E1315	V1316	V1319	P1320	G1321	I1322	P1324	R1326	I1327	Y1328	T1329	M1330	F1332	D1333	D1334	I1335	F1336	E1337	V1338						
A1131	K1132	T1133	S1135	A1137	T1141	T1147	I1148	A1149	S1150	E1151	I1152	Y1153	Y1154	D1155	P1156	F1157	K1158	R1159	S1160	L1161	V1162	P1163	E1165	D1166	F1167	E1168	I1169	T1170	L1171	R1172	H1173	F1174	S1175	L1176	ASP	GLU	GLU	ALA	GLN	SER	PHE	ASP	Q1187	E1255	E1256	K1261	E1264	M1265	T1266	E1267					
P1060	M1063	V1064	L1067	I1072	G1073	P1074	A1076	M1079	T1080	L1081	ASN	THR	PHE	HIS	PHE	ALA	GLY	VAL	ALA	L1022	R1023	S1024	K1092	K1093	V1094	T1095	S1096	G1097	V1098	P1099	R1100	E1103	Y1105	M1106	V1107	M1110	M1111	T1113	P1114	S1115	L1116	T1117	V1118	L1119	L1120	E1121	P1122	G1123	H1124	D1127	Q1130				
E946	D947	I948	Y952	D953	R954	T955	R956	R957	N958	S959	G961	N962	L964	K965	F966	I967	Y968	G969	E970	D971	M972	N973	D974	A975	H976	H977	I978	Q981	S982	D983	T984	I986	G987	D989	R996	V999	L990	L991	S992	L993	S994	T995	P996	F997	G998	H999	I990	E991	S992	L993					
R782	T783	L784	P785	H786	K789	P794	S795	T796	K797	G798	F799	V800	E801	N802	S803	Y804	L805	G806	G807	L808	T809	P810	G811	E812	F813	R814	F815	H816	A817	M818	G819	G820	R821	E822	G823	L824	T825	T827	A828	V829	K830	T831	E833	G834	G835	Y836	D837	S838	L839	E840	R841	P842	K843	A844	L845
E846	D847	I848	Y852	D853	R854	T855	R856	R857	N858	S859	G861	N862	L864	K865	F866	I867	Y868	G869	E870	D871	M872	N873	D874	A875	H876	H877	I878	Q881	S882	D883	T884	I886	G887	D890	R896	V899	L900	L901	S902	N903	T904	D905	H906	T907	R908	L909	D910	P911	S912	L913					
E914	T919	G921	R922	Q926	L929	E932	Y933	Y934	Q935	L936	Y937	K938	R939	E940	F941	L942	D943	F947	Y948	D949	W954	A1027	P1028	V1029	S1030	G1031	R1032	V1033	E1034	Y1035	R1036	L1037	T1038	Q1039	A1040	Q968	Q969	T970	F971	K977	P978	S979	D980	L981	T982	F1053	K984	L1054	D985	I986	V987	N996	L997		
L998	Y999	R1000	G																																																				





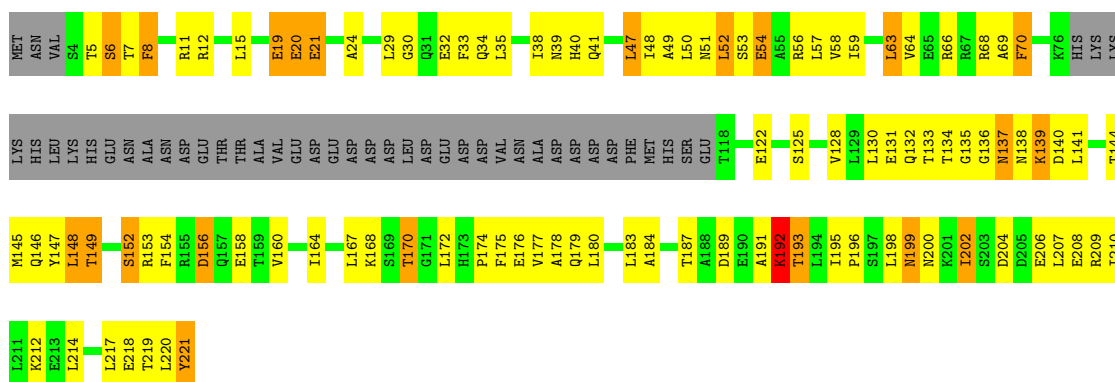
- Molecule 6: DNA-directed RNA polymerase II 45 kDa polypeptide

Chain C:  23% 47% 12% 1% 16%

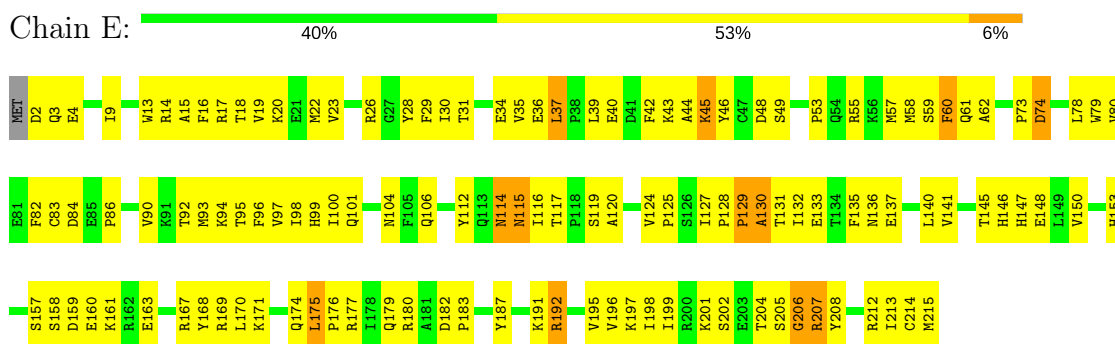


- Molecule 7: DNA-directed RNA polymerase II 32 kDa polypeptide

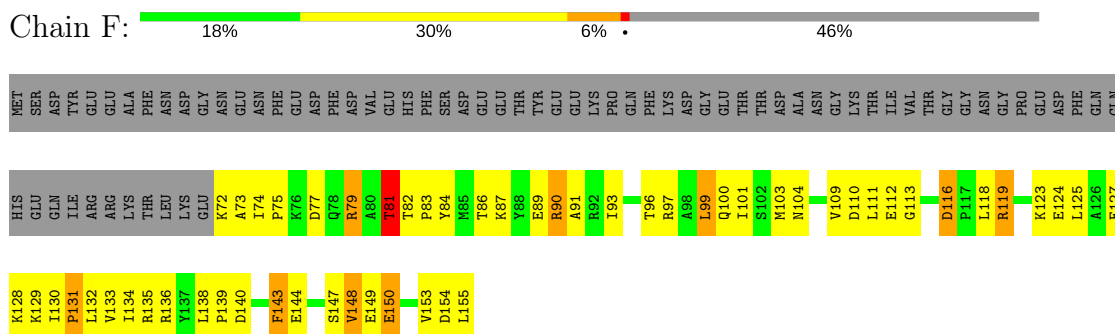
Chain D: 



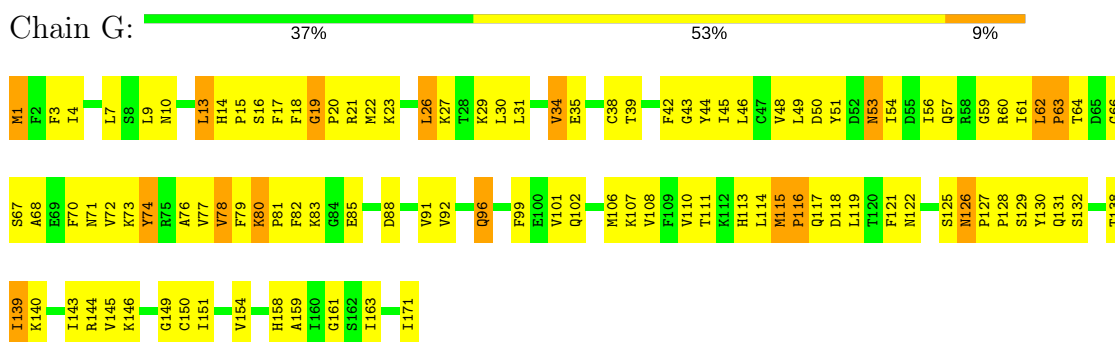
- Molecule 8: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide



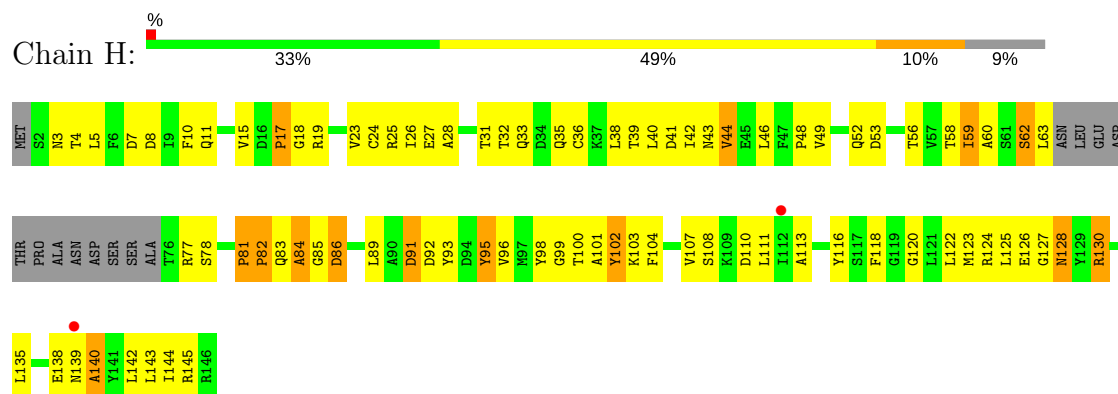
- Molecule 9: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide



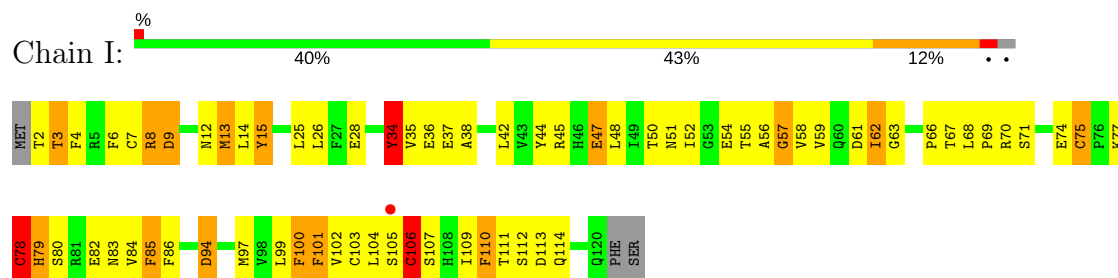
- Molecule 10: DNA-directed RNA polymerase II 19 kDa polypeptide



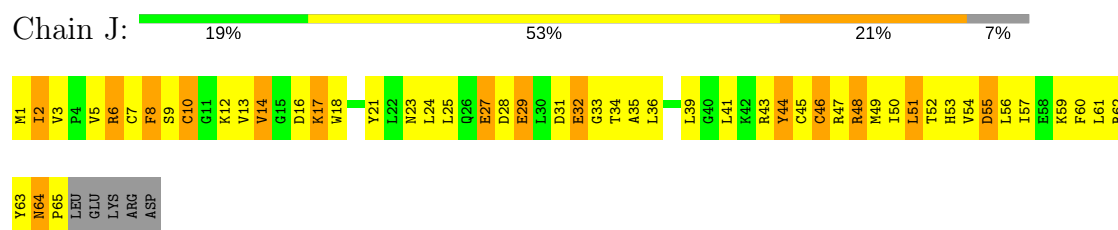
- Molecule 11: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide



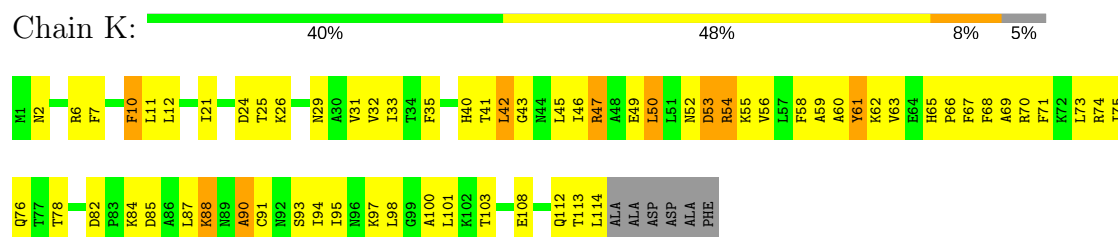
- Molecule 12: DNA-directed RNA polymerase II subunit 9



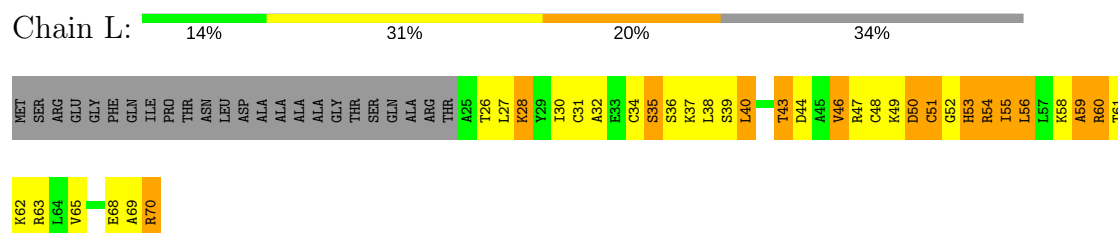
- Molecule 13: DNA-directed RNA polymerases I/II/III subunit 10



- Molecule 14: DNA-directed RNA polymerase II 13.6 kDa polypeptide



- Molecule 15: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	222.46Å 393.07Å 283.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 4.50 48.95 – 4.49	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-4.50) 78.3 (48.95-4.49)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.98 (at 4.45Å)	Xtriage
Refinement program	unknown	Depositor
R, $R_{free}$	0.297 , (Not available) 0.270 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	137.1	Xtriage
Anisotropy	0.467	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 54.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.019 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.030 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	31835	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, G2P

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	T	1.18	0/433	1.16	2/666 (0.3%)
2	N	1.35	0/158	0.85	0/242
3	P	1.14	0/240	2.32	6/373 (1.6%)
4	A	0.59	6/11339 (0.1%)	0.78	16/15334 (0.1%)
5	B	0.57	5/9008 (0.1%)	0.86	16/12146 (0.1%)
6	C	0.63	2/2133 (0.1%)	1.10	5/2891 (0.2%)
7	D	0.49	0/1365	0.73	2/1837 (0.1%)
8	E	0.44	0/1788	0.64	0/2406
9	F	0.54	0/691	0.78	0/933
10	G	0.54	0/1368	0.75	0/1844
11	H	0.40	0/1086	0.66	0/1470
12	I	0.44	0/989	0.75	0/1331
13	J	0.54	0/541	0.82	1/727 (0.1%)
14	K	0.48	0/937	0.68	0/1265
15	L	0.46	0/365	0.75	0/485
All	All	0.58	13/32441 (0.0%)	0.84	48/43950 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	T	0	3
4	A	0	3
5	B	1	7
6	C	0	4
All	All	1	17

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	119	ASN	C-N	27.87	1.98	1.34
4	A	150	THR	C-N	-17.84	0.93	1.34
5	B	503	GLY	C-N	14.88	1.68	1.34
6	C	89	GLU	C-N	-14.40	1.00	1.34
5	B	363	HIS	C-N	-13.51	1.02	1.34
5	B	506	GLY	C-N	9.87	1.56	1.34
5	B	511	PRO	C-N	-9.24	1.12	1.34
4	A	47	ARG	CB-CG	8.02	1.74	1.52
6	C	90	ASP	C-N	-8.01	1.15	1.34
5	B	502	ILE	C-N	-6.76	1.20	1.33
4	A	346	ASP	C-N	6.21	1.48	1.34
4	A	77	CYS	CB-SG	5.81	1.92	1.82
4	A	77	CYS	C-N	-5.44	1.24	1.34

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	503	GLY	O-C-N	-24.37	83.71	122.70
6	C	90	ASP	CB-CG-OD1	-24.17	96.54	118.30
5	B	469	GLN	O-C-N	-23.96	84.36	122.70
6	C	89	GLU	O-C-N	-23.94	84.40	122.70
3	P	3	G	O5'-P-OP2	23.57	138.99	110.70
3	P	2	A	OP2-P-O3'	-23.33	53.87	105.20
6	C	89	GLU	CA-C-N	17.29	155.23	117.20
6	C	89	GLU	C-N-CA	17.27	164.87	121.70
5	B	363	HIS	O-C-N	-17.24	95.12	122.70
3	P	3	G	O5'-P-OP1	-15.64	91.62	105.70
4	A	76	GLU	CB-CA-C	-15.14	80.11	110.40
5	B	363	HIS	C-N-CA	14.77	158.62	121.70
5	B	363	HIS	CA-C-N	12.37	144.41	117.20
3	P	2	A	OP1-P-O3'	11.89	131.37	105.20
5	B	502	ILE	CA-C-N	-11.65	92.89	116.20
5	B	499	ASN	O-C-N	11.43	140.99	122.70
4	A	119	ASN	O-C-N	-11.08	104.97	122.70
3	P	2	A	O3'-P-O5'	-9.93	85.13	104.00
6	C	90	ASP	O-C-N	-9.86	106.93	122.70
4	A	77	CYS	C-N-CD	-9.03	100.73	120.60
5	B	506	GLY	O-C-N	8.56	136.39	122.70
4	A	150	THR	C-N-CA	-8.53	100.36	121.70
1	T	18	DC	O4'-C1'-N1	8.29	113.80	108.00
5	B	499	ASN	CA-C-N	-8.10	99.39	117.20
4	A	150	THR	CA-C-N	-7.95	99.71	117.20
4	A	119	ASN	CA-C-N	7.72	134.18	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	506	GLY	C-N-CA	-7.18	103.74	121.70
5	B	479	VAL	O-C-N	7.03	133.95	122.70
5	B	506	GLY	CA-C-N	-6.74	102.38	117.20
5	B	499	ASN	C-N-CA	-6.11	106.42	121.70
5	B	473	MET	O-C-N	-6.09	112.96	122.70
1	T	18	DC	N1-C1'-C2'	-5.93	101.34	112.60
3	P	2	A	C2'-C3'-O3'	5.74	122.88	113.70
4	A	4	GLN	CB-CA-C	5.69	121.77	110.40
13	J	10	CYS	CA-CB-SG	5.69	124.24	114.00
4	A	150	THR	O-C-N	5.66	131.75	122.70
4	A	77	CYS	CA-CB-SG	-5.54	104.03	114.00
4	A	47	ARG	CA-CB-CG	-5.51	101.27	113.40
5	B	466	TRP	CA-C-N	-5.36	105.48	116.20
4	A	1403	GLU	N-CA-C	5.33	125.39	111.00
5	B	1185	CYS	N-CA-C	-5.32	96.63	111.00
4	A	119	ASN	C-N-CA	5.30	134.94	121.70
4	A	567	LYS	C-N-CD	5.29	139.52	128.40
7	D	8	PHE	N-CA-C	5.29	125.28	111.00
4	A	452	LYS	N-CA-C	-5.20	96.96	111.00
4	A	344	ARG	N-CA-C	-5.15	97.09	111.00
7	D	54	GLU	N-CA-C	-5.08	97.27	111.00
4	A	77	CYS	CA-C-N	5.06	131.27	117.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	364	ILE	CB

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	150	THR	Mainchain
4	A	303	TYR	Sidechain
4	A	77	CYS	Peptide
5	B	363	HIS	Mainchain,Peptide
5	B	466	TRP	Mainchain
5	B	469	GLN	Mainchain
5	B	473	MET	Mainchain,Peptide
5	B	502	ILE	Mainchain
6	C	82	TYR	Sidechain
6	C	90	ASP	Sidechain,Mainchain,Peptide
1	T	19	DG	Sidechain

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Mol	Chain	Res	Type	Group
1	T	20	DC	Sidechain
1	T	21	DC	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	T	388	0	216	51	0
2	N	141	0	81	8	0
3	P	214	0	111	20	0
4	A	11140	0	11218	1205	0
5	B	8836	0	8869	984	0
6	C	2095	0	2049	244	0
7	D	1356	0	1319	118	0
8	E	1752	0	1776	152	0
9	F	679	0	701	83	0
10	G	1340	0	1357	154	0
11	H	1068	0	1040	104	0
12	I	971	0	928	99	0
13	J	532	0	542	94	0
14	K	919	0	929	81	0
15	L	363	0	387	43	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	A	1	0	0	0	0
18	B	32	0	12	0	0
All	All	31835	0	31535	3108	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 49.

All (3108) 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)
4:A:825:ILE:CG2	5:B:508:LEU:HD11	1.45	1.45
5:B:503:GLY:C	5:B:504:ARG:N	1.68	1.44
1:T:16:DT:C4'	4:A:1403:GLU:OE2	1.77	1.30
1:T:20:DC:H4'	4:A:447:GLN:NE2	1.44	1.29
4:A:56:PRO:O	4:A:57:ARG:HG3	1.28	1.28
5:B:466:TRP:O	5:B:468:GLU:N	1.75	1.19
1:T:15:DT:H1'	4:A:1386:ARG:NH1	1.55	1.19
4:A:119:ASN:C	4:A:120:GLU:N	1.98	1.16
4:A:829:VAL:HG21	5:B:508:LEU:HD13	1.29	1.15
13:J:5:VAL:HG12	13:J:6:ARG:HG3	1.29	1.13
3:P:9:G:H5''	5:B:776:GLN:HE22	1.10	1.12
5:B:502:ILE:HG22	5:B:503:GLY:H	1.06	1.12
4:A:76:GLU:O	4:A:76:GLU:CG	1.84	1.11
10:G:138:THR:HG22	10:G:139:ILE:H	1.14	1.10
1:T:16:DT:H4'	4:A:1403:GLU:OE2	0.94	1.09
4:A:825:ILE:CG2	5:B:508:LEU:CD1	2.31	1.07
4:A:77:CYS:SG	4:A:77:CYS:O	2.13	1.07
7:D:40:HIS:HB3	10:G:73:LYS:NZ	1.69	1.07
5:B:503:GLY:HA3	5:B:507:LYS:HE3	1.10	1.07
5:B:503:GLY:HA3	5:B:507:LYS:CE	1.86	1.06
4:A:53:LEU:HD23	4:A:54:ASN:N	1.70	1.05
5:B:273:LEU:HB2	5:B:276:ILE:HD12	1.36	1.04
1:T:16:DT:H5'	4:A:1386:ARG:NH1	1.73	1.04
7:D:48:ILE:HG21	10:G:4:ILE:HB	1.39	1.04
11:H:100:THR:HG23	11:H:138:GLU:HA	1.37	1.03
5:B:217:ARG:HE	5:B:405:ARG:HB2	1.21	1.03
4:A:855:THR:HG21	4:A:857:ARG:HE	1.22	1.02
3:P:9:G:H5''	5:B:776:GLN:NE2	1.74	1.02
5:B:502:ILE:HG12	5:B:535:LEU:CD1	1.90	1.02
4:A:1161:THR:HG22	4:A:1163:ILE:H	1.23	1.01
5:B:502:ILE:CG2	5:B:503:GLY:H	1.63	1.01
10:G:15:PRO:HA	10:G:18:PHE:CD1	1.96	1.00
4:A:1017:LEU:HB2	8:E:206:GLY:H	1.25	0.99
5:B:806:THR:HG22	5:B:808:ALA:H	1.26	0.99
5:B:549:THR:HG22	5:B:550:ASP:H	1.26	0.98
1:T:15:DT:H1'	4:A:1386:ARG:HH12	1.14	0.98
12:I:85:PHE:HD2	12:I:85:PHE:H	1.05	0.98
5:B:65:GLU:HG3	5:B:66:ASP:H	1.27	0.97
9:F:93:ILE:HD11	9:F:134:ILE:HD11	1.43	0.97
5:B:502:ILE:CG1	5:B:535:LEU:HD13	1.94	0.97
4:A:1329:THR:HG22	4:A:1331:SER:H	1.29	0.97
4:A:563:PRO:HG3	4:A:572:TRP:CZ2	2.00	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:779:PHE:HE1	4:A:785:PRO:HD3	1.28	0.97
10:G:7:LEU:HB2	10:G:74:TYR:CE2	2.00	0.97
4:A:825:ILE:HG22	5:B:508:LEU:HD11	1.00	0.96
5:B:23:ALA:HB1	5:B:24:PRO:HD2	1.46	0.96
5:B:800:GLN:HB3	13:J:52:THR:HG21	1.47	0.96
7:D:47:LEU:HD13	7:D:48:ILE:H	1.30	0.96
5:B:189:LEU:HA	5:B:192:LEU:HD12	1.46	0.95
5:B:806:THR:N	5:B:809:MET:HE3	1.81	0.95
4:A:754:SER:H	4:A:757:ASN:HD22	1.11	0.95
5:B:503:GLY:O	5:B:504:ARG:N	1.99	0.95
5:B:466:TRP:C	5:B:468:GLU:H	1.68	0.95
5:B:46:GLN:HG3	5:B:47:GLN:H	1.28	0.95
6:C:166:GLU:HG3	14:K:10:PHE:HZ	1.31	0.95
14:K:47:ARG:HH11	14:K:47:ARG:HB3	1.32	0.94
4:A:84:ILE:HD11	4:A:270:LEU:HD13	1.50	0.94
1:T:19:DG:H4'	5:B:1133:MET:SD	2.08	0.94
5:B:1072:MET:HE3	5:B:1085:ILE:HB	1.48	0.93
5:B:507:LYS:CA	5:B:512:ARG:HH21	1.82	0.93
6:C:39:ALA:HA	6:C:164:ALA:HB3	1.48	0.93
4:A:709:THR:HG22	4:A:711:ARG:H	1.32	0.93
5:B:1224:PHE:HE2	8:E:171:LYS:HG3	1.31	0.93
11:H:4:THR:HA	11:H:60:ALA:HB2	1.51	0.93
5:B:1201:LYS:HE2	5:B:1205:GLN:OE1	1.69	0.93
6:C:47:ASP:HA	15:L:69:ALA:HB3	1.49	0.92
4:A:55:ASP:C	4:A:57:ARG:H	1.70	0.92
4:A:825:ILE:HG22	5:B:508:LEU:CD1	1.94	0.92
4:A:768:GLN:HG2	4:A:816:HIS:HA	1.51	0.92
4:A:399:HIS:HB3	4:A:400:PRO:HD3	1.51	0.92
5:B:502:ILE:CD1	5:B:535:LEU:HD13	1.98	0.92
6:C:142:VAL:H	13:J:16:ASP:HB3	1.33	0.92
4:A:963:ILE:HD11	4:A:1048:ASN:HB3	1.50	0.92
9:F:81:THR:HG21	9:F:136:ARG:HD3	1.52	0.92
4:A:40:THR:HG22	4:A:41:MET:HG3	1.52	0.92
4:A:2:VAL:HG21	5:B:1158:PHE:N	1.85	0.91
7:D:134:THR:HG22	7:D:136:GLY:H	1.35	0.91
5:B:502:ILE:HG22	5:B:503:GLY:N	1.86	0.91
12:I:34:TYR:HD2	12:I:35:VAL:N	1.68	0.91
1:T:20:DC:H4'	4:A:447:GLN:HE22	1.01	0.91
5:B:824:ILE:HG22	5:B:1087:PHE:HE2	1.33	0.91
4:A:901:LEU:H	4:A:926:GLN:NE2	1.69	0.91
1:T:15:DT:C1'	4:A:1386:ARG:NH1	2.34	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:2:A:H2'	3:P:3:G:C8	2.07	0.90
4:A:53:LEU:HD23	4:A:54:ASN:H	1.29	0.90
4:A:353:ILE:HG21	4:A:487:MET:HE3	1.53	0.89
4:A:56:PRO:O	4:A:57:ARG:CG	2.18	0.89
5:B:1072:MET:CE	5:B:1085:ILE:HB	2.02	0.89
8:E:180:ARG:HH21	8:E:192:ARG:HB2	1.37	0.89
4:A:524:VAL:HG12	4:A:525:GLN:H	1.36	0.89
11:H:81:PRO:HB2	11:H:82:PRO:HD2	1.54	0.89
1:T:20:DC:C4'	4:A:447:GLN:NE2	2.34	0.89
4:A:76:GLU:O	4:A:76:GLU:HG3	1.07	0.88
13:J:3:VAL:HG21	13:J:18:TRP:HB2	1.54	0.88
5:B:364:ILE:HG12	5:B:585:VAL:HG13	1.56	0.88
4:A:903:ASN:HD22	4:A:904:THR:N	1.72	0.88
6:C:44:LEU:HB2	6:C:77:ILE:HD11	1.53	0.88
5:B:98:THR:O	5:B:126:SER:HB2	1.74	0.88
5:B:800:GLN:HB3	13:J:52:THR:CG2	2.04	0.87
12:I:7:CYS:HB3	12:I:14:LEU:HD21	1.55	0.87
7:D:144:THR:O	7:D:148:LEU:HB2	1.73	0.87
14:K:65:HIS:HD2	14:K:67:PHE:H	1.23	0.87
5:B:212:LEU:HD23	5:B:480:SER:HB2	1.56	0.87
3:P:1:A:H2'	3:P:2:A:C8	2.10	0.87
4:A:567:LYS:CG	4:A:568:PRO:HD2	2.04	0.87
4:A:829:VAL:CG2	5:B:508:LEU:HD13	2.05	0.87
13:J:16:ASP:OD1	13:J:17:LYS:HD2	1.75	0.87
8:E:94:LYS:HE2	8:E:98:ILE:HD11	1.57	0.86
8:E:22:MET:HE3	8:E:26:ARG:HE	1.40	0.86
12:I:34:TYR:CD2	12:I:35:VAL:N	2.42	0.86
5:B:502:ILE:HD11	5:B:535:LEU:HD13	1.55	0.86
6:C:164:ALA:HA	6:C:167:HIS:O	1.76	0.86
6:C:20:PHE:HE1	6:C:22:LEU:HD12	1.41	0.86
4:A:1242:VAL:HG12	4:A:1243:VAL:H	1.38	0.86
4:A:1445:ILE:H	4:A:1445:ILE:HD12	1.39	0.86
6:C:232:VAL:HG21	6:C:244:VAL:HG22	1.58	0.86
4:A:1189:SER:O	4:A:1241:ARG:HD3	1.75	0.85
6:C:47:ASP:HA	15:L:69:ALA:CB	2.06	0.85
5:B:507:LYS:CB	5:B:512:ARG:HH21	1.89	0.85
10:G:1:MET:SD	10:G:79:PHE:CD1	2.69	0.85
13:J:57:ILE:HA	13:J:60:PHE:HD2	1.41	0.85
5:B:515:HIS:H	5:B:518:HIS:HD2	1.19	0.85
5:B:282:ILE:HD12	5:B:382:ILE:HD13	1.58	0.85
5:B:705:MET:H	5:B:710:LEU:HD12	1.42	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:168:GLY:H	5:B:450:ALA:HB1	1.40	0.85
5:B:806:THR:H	5:B:809:MET:HE3	1.40	0.85
1:T:16:DT:H4'	4:A:1403:GLU:CD	1.97	0.85
5:B:233:PRO:HG2	5:B:234:ILE:HD12	1.57	0.85
6:C:57:VAL:HG11	13:J:60:PHE:HB3	1.57	0.85
5:B:589:VAL:HG12	5:B:590:HIS:H	1.41	0.84
5:B:507:LYS:HB2	5:B:512:ARG:HH21	1.42	0.84
5:B:955:THR:HG23	15:L:54:ARG:O	1.77	0.84
8:E:19:VAL:O	8:E:23:VAL:HG23	1.77	0.84
10:G:1:MET:SD	10:G:79:PHE:HD1	2.00	0.84
5:B:37:PHE:CE1	5:B:41:LYS:HG3	2.12	0.84
7:D:40:HIS:HB3	10:G:73:LYS:HZ1	1.39	0.84
4:A:1094:VAL:HG13	4:A:1113:THR:HG21	1.58	0.84
5:B:483:LEU:HD11	5:B:491:THR:HG23	1.57	0.84
5:B:467:GLY:N	5:B:475:SER:HB3	1.92	0.84
6:C:90:ASP:OD1	6:C:90:ASP:O	1.96	0.84
5:B:882:THR:HG22	5:B:884:ARG:H	1.44	0.83
5:B:507:LYS:HB2	5:B:512:ARG:NH2	1.91	0.83
4:A:598:LEU:HA	11:H:122:LEU:HD13	1.61	0.83
4:A:70:CYS:O	4:A:72:GLU:HG2	1.76	0.83
5:B:847:ASP:HB3	6:C:167:HIS:HE2	1.43	0.83
4:A:1329:THR:HG22	4:A:1331:SER:N	1.93	0.83
4:A:351:THR:HB	5:B:1103:ILE:HD12	1.61	0.83
5:B:778:MET:HE1	5:B:1094:ARG:HD3	1.58	0.83
11:H:23:VAL:HG22	11:H:43:ASN:HA	1.61	0.83
10:G:128:PRO:O	10:G:138:THR:HG23	1.77	0.83
13:J:64:ASN:HB3	13:J:65:PRO:CD	2.08	0.83
3:P:8:G:O2'	3:P:9:G:H5'	1.78	0.83
6:C:213:PRO:O	6:C:214:ASN:HB2	1.77	0.83
10:G:138:THR:HG22	10:G:139:ILE:N	1.93	0.83
5:B:502:ILE:HG12	5:B:535:LEU:HD13	1.53	0.82
10:G:34:VAL:HG12	10:G:45:ILE:HG21	1.61	0.82
5:B:1163:CYS:SG	5:B:1165:ILE:HB	2.19	0.82
5:B:842:ASN:ND2	5:B:845:SER:H	1.78	0.82
5:B:918:ILE:HB	5:B:935:ARG:HD2	1.59	0.82
4:A:335:ARG:NH1	5:B:1202:LEU:HD13	1.93	0.82
5:B:847:ASP:HB3	6:C:167:HIS:NE2	1.94	0.82
4:A:438:ASP:O	4:A:439:ASN:HB2	1.77	0.82
4:A:868:TYR:CE1	4:A:1064:VAL:HG11	2.15	0.82
6:C:43:THR:HG22	6:C:44:LEU:N	1.95	0.82
7:D:170:THR:CG2	7:D:172:LEU:HG	2.09	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:35:SER:HA	5:B:811:TYR:HE2	1.45	0.82
4:A:567:LYS:NZ	11:H:46:LEU:HB2	1.95	0.82
5:B:1096:ARG:O	5:B:1097:HIS:HB2	1.79	0.82
8:E:135:PHE:HD2	8:E:140:LEU:HD21	1.45	0.82
4:A:567:LYS:HG3	4:A:568:PRO:HD2	1.60	0.81
6:C:56:THR:HG22	6:C:57:VAL:H	1.45	0.81
5:B:1007:VAL:HG22	5:B:1008:PRO:HD2	1.62	0.81
6:C:66:ARG:NH2	13:J:5:VAL:HG23	1.95	0.81
4:A:1118:VAL:HG12	4:A:1327:ILE:HG13	1.63	0.81
4:A:1332:PHE:H	4:A:1332:PHE:HD2	1.26	0.81
11:H:40:LEU:HD13	11:H:123:MET:HB2	1.61	0.81
4:A:265:LYS:HZ3	4:A:322:VAL:HG13	1.45	0.81
4:A:534:LEU:O	4:A:574:GLY:HA3	1.80	0.81
10:G:13:LEU:HD21	10:G:17:PHE:HB2	1.60	0.81
4:A:249:SER:O	4:A:250:ILE:HG13	1.80	0.81
4:A:779:PHE:CE1	4:A:785:PRO:HD3	2.13	0.81
7:D:5:THR:O	7:D:6:SER:O	1.99	0.81
5:B:1065:GLN:HE21	5:B:1067:ARG:H	1.27	0.81
5:B:401:PHE:HA	5:B:404:LYS:HG3	1.60	0.81
6:C:262:LEU:HD11	14:K:87:LEU:HD23	1.60	0.81
10:G:23:LYS:HG3	10:G:56:ILE:HD11	1.63	0.80
4:A:670:ILE:HG23	4:A:805:LEU:HD21	1.63	0.80
5:B:577:ALA:HB1	5:B:589:VAL:HG11	1.62	0.80
4:A:503:GLN:HE21	9:F:90:ARG:HH21	1.27	0.80
4:A:741:ASN:HD22	4:A:744:LYS:H	1.26	0.80
4:A:709:THR:HG23	12:I:94:ASP:HA	1.64	0.80
6:C:212:PRO:HB3	6:C:213:PRO:HD2	1.62	0.80
5:B:102:VAL:HG23	5:B:112:LEU:HB2	1.61	0.80
7:D:40:HIS:HB3	10:G:73:LYS:HZ3	1.46	0.80
4:A:340:LEU:HD13	4:A:1429:ILE:HG23	1.62	0.80
5:B:25:ILE:HD11	5:B:653:VAL:O	1.81	0.80
6:C:32:SER:O	6:C:36:VAL:HG23	1.82	0.80
4:A:67:CYS:O	4:A:70:CYS:HB3	1.82	0.80
5:B:200:GLY:HA2	5:B:202:TYR:CE2	2.17	0.79
5:B:476:ARG:NH1	5:B:501:PRO:HB3	1.97	0.79
8:E:29:PHE:O	8:E:30:ILE:HG13	1.82	0.79
4:A:1155:ASP:OD2	4:A:1161:THR:HG23	1.81	0.79
4:A:335:ARG:HA	4:A:339:ASN:HB2	1.64	0.79
4:A:1422:ARG:HH22	5:B:1224:PHE:C	1.86	0.79
13:J:14:VAL:CG1	13:J:50:ILE:HD11	2.13	0.79
14:K:113:THR:O	14:K:114:LEU:HB2	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:93:VAL:HG13	4:A:301:ALA:HB1	1.62	0.79
5:B:515:HIS:HD2	5:B:517:THR:H	1.27	0.79
5:B:611:PRO:HB3	5:B:685:LEU:HD11	1.64	0.79
5:B:1162:ILE:HG22	5:B:1163:CYS:H	1.48	0.79
4:A:886:ILE:HD11	4:A:943:LEU:HB3	1.63	0.78
4:A:4:GLN:O	4:A:5:GLN:O	2.00	0.78
4:A:855:THR:HG21	4:A:857:ARG:NE	1.97	0.78
5:B:502:ILE:HG12	5:B:535:LEU:HD11	1.65	0.78
5:B:465:ASN:HD22	5:B:465:ASN:N	1.78	0.78
5:B:1034:VAL:HG12	5:B:1035:ALA:N	1.98	0.78
5:B:361:LEU:HD21	5:B:377:PHE:CD2	2.18	0.78
10:G:81:PRO:HG3	10:G:106:MET:SD	2.24	0.78
11:H:102:TYR:OH	11:H:122:LEU:HD22	1.82	0.78
13:J:64:ASN:HB3	13:J:65:PRO:HD3	1.64	0.78
4:A:340:LEU:HD21	5:B:1200:ALA:N	1.99	0.77
5:B:955:THR:HG22	5:B:956:THR:N	1.99	0.77
4:A:1341:ILE:HG23	4:A:1342:GLU:N	1.98	0.77
4:A:285:PRO:HG2	4:A:288:ALA:HB3	1.64	0.77
5:B:53:GLN:HG2	5:B:547:VAL:HG22	1.67	0.77
1:T:19:DG:OP2	4:A:332:LYS:NZ	2.17	0.77
4:A:356:ASP:HB2	4:A:469:ARG:NH1	1.99	0.77
6:C:77:ILE:HG23	6:C:161:LYS:HE3	1.67	0.77
8:E:175:LEU:HD23	8:E:176:PRO:HD2	1.66	0.77
4:A:1394:THR:HG21	4:A:1398:MET:SD	2.24	0.77
5:B:1159:ARG:HD3	5:B:1193:GLN:HG3	1.66	0.77
5:B:763:GLN:HG2	5:B:765:PRO:HD2	1.65	0.77
6:C:98:VAL:C	6:C:99:LEU:HD23	2.04	0.77
14:K:21:ILE:HG12	14:K:33:ILE:HG12	1.66	0.77
4:A:567:LYS:HB3	11:H:95:TYR:HA	1.65	0.77
4:A:855:THR:HG23	4:A:857:ARG:HG3	1.67	0.77
5:B:120:ARG:HG2	5:B:955:THR:HG21	1.66	0.77
5:B:613:VAL:HG13	5:B:627:PHE:O	1.85	0.77
4:A:1116:LEU:N	4:A:1308:THR:HG22	2.00	0.77
5:B:999:MET:HG3	5:B:1000:PRO:HD2	1.66	0.77
7:D:130:LEU:C	7:D:132:GLN:H	1.86	0.77
4:A:2:VAL:HG21	5:B:1157:ALA:C	2.06	0.77
11:H:42:ILE:HG23	11:H:95:TYR:HE1	1.47	0.77
4:A:1329:THR:H	4:A:1335:ILE:HD11	1.50	0.77
4:A:1063:MET:HG3	4:A:1436:ILE:HG23	1.67	0.77
5:B:1065:GLN:HE21	5:B:1066:SER:N	1.83	0.77
5:B:1069:PHE:HD1	5:B:1069:PHE:H	1.33	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1224:PHE:CE2	8:E:171:LYS:HG3	2.17	0.76
4:A:388:LEU:O	4:A:392:VAL:HG23	1.85	0.76
5:B:978:ASP:OD2	5:B:1098:MET:HG2	1.86	0.76
7:D:153:ARG:NH2	7:D:184:ALA:HA	2.00	0.76
5:B:863:GLU:OE2	5:B:873:THR:HA	1.85	0.76
1:T:15:DT:H5"	4:A:1407:GLU:OE2	1.84	0.76
8:E:90:VAL:HG23	8:E:120:ALA:HA	1.67	0.76
4:A:598:LEU:HD22	11:H:25:ARG:NH1	2.01	0.76
5:B:1065:GLN:NE2	5:B:1067:ARG:H	1.83	0.76
5:B:37:PHE:CD1	5:B:41:LYS:HG3	2.20	0.76
4:A:560:ILE:HG13	11:H:78:SER:HB2	1.67	0.76
8:E:117:THR:HG22	8:E:119:SER:H	1.50	0.76
4:A:87:ALA:HB3	4:A:276:LEU:HD23	1.67	0.76
4:A:528:LEU:O	4:A:531:ILE:HG22	1.86	0.76
14:K:46:ILE:O	14:K:50:LEU:HB2	1.84	0.76
4:A:1424:VAL:HG11	5:B:1139:ILE:HD13	1.65	0.76
5:B:879:ARG:HH11	5:B:883:LEU:HD22	1.49	0.76
14:K:45:LEU:HG	14:K:94:ILE:HD13	1.66	0.76
4:A:1341:ILE:HD12	4:A:1379:GLY:O	1.85	0.76
4:A:23:SER:HB3	4:A:233:TRP:CZ2	2.21	0.76
4:A:588:LEU:O	4:A:606:LEU:HA	1.85	0.75
4:A:1409:LEU:HD13	5:B:1207:LEU:HD21	1.68	0.75
5:B:172:ILE:HD13	5:B:178:ASN:HB3	1.69	0.75
6:C:43:THR:HG22	6:C:44:LEU:H	1.52	0.75
4:A:356:ASP:HB2	4:A:469:ARG:HH11	1.51	0.75
4:A:23:SER:HB3	4:A:233:TRP:CE2	2.21	0.75
4:A:836:TYR:CE2	4:A:840:ARG:HD2	2.21	0.75
5:B:899:ILE:HD11	5:B:911:ILE:HA	1.67	0.75
10:G:115:MET:HB3	10:G:116:PRO:HD2	1.67	0.75
5:B:579:ARG:HB2	5:B:586:TRP:NE1	2.01	0.75
4:A:858:ASN:ND2	4:A:860:LEU:H	1.84	0.75
8:E:198:ILE:HD11	8:E:212:ARG:HG3	1.69	0.75
4:A:253:ASN:HB3	5:B:935:ARG:NH2	2.02	0.75
5:B:521:LEU:HD22	5:B:633:VAL:HG12	1.68	0.75
4:A:1323:ASP:OD1	4:A:1325:THR:HB	1.87	0.74
5:B:806:THR:HG22	5:B:808:ALA:N	2.02	0.74
7:D:66:ARG:HD2	7:D:133:THR:HB	1.67	0.74
5:B:37:PHE:HE2	5:B:542:MET:HA	1.52	0.74
5:B:580:VAL:HG22	5:B:624:LEU:HB3	1.69	0.74
5:B:642:ASP:HB3	5:B:649:LYS:CD	2.17	0.74
4:A:445:ASN:HB2	4:A:455:MET:HG2	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:15:DT:H1'	1:T:16:DT:H5'	1.70	0.74
4:A:87:ALA:CB	4:A:276:LEU:HD23	2.18	0.74
4:A:1332:PHE:HD2	4:A:1332:PHE:N	1.85	0.74
4:A:91:PHE:HB2	4:A:297:GLN:NE2	2.03	0.74
8:E:2:ASP:O	8:E:3:GLN:HG2	1.87	0.74
12:I:34:TYR:HE2	12:I:36:GLU:HB3	1.51	0.74
14:K:65:HIS:CD2	14:K:67:PHE:H	2.06	0.74
4:A:1312:ASN:O	4:A:1316:VAL:HG23	1.88	0.74
4:A:590:ARG:NH1	4:A:590:ARG:HG3	2.01	0.74
5:B:408:LEU:HG	5:B:409:ALA:H	1.51	0.74
5:B:871:THR:HG22	5:B:872:GLU:O	1.87	0.74
5:B:859:TYR:OH	5:B:941:LEU:HD12	1.86	0.74
9:F:111:LEU:C	9:F:113:GLY:H	1.91	0.74
10:G:15:PRO:HA	10:G:18:PHE:CE1	2.22	0.74
1:T:16:DT:C5'	4:A:1386:ARG:NH1	2.51	0.74
4:A:230:ARG:H	4:A:233:TRP:HE3	1.35	0.74
4:A:535:THR:HG21	4:A:616:VAL:HA	1.70	0.74
5:B:801:LYS:O	13:J:52:THR:HG23	1.86	0.74
5:B:847:ASP:HB3	6:C:167:HIS:CD2	2.23	0.74
4:A:1450:LEU:HG	4:A:1450:LEU:O	1.88	0.73
4:A:567:LYS:HD3	11:H:95:TYR:CD2	2.23	0.73
5:B:510:LYS:N	5:B:511:PRO:HD3	2.03	0.73
8:E:16:PHE:CZ	8:E:20:LYS:HE2	2.23	0.73
4:A:335:ARG:HH12	5:B:1202:LEU:HD13	1.53	0.73
4:A:590:ARG:NH2	4:A:620:LYS:HB3	2.02	0.73
4:A:853:ASP:OD1	4:A:855:THR:HB	1.89	0.73
5:B:1183:LYS:HE3	5:B:1183:LYS:N	2.03	0.73
13:J:36:LEU:HD12	13:J:47:ARG:NH1	2.03	0.73
4:A:164:ARG:HG3	4:A:165:GLY:H	1.52	0.73
8:E:213:ILE:HG12	8:E:214:CYS:H	1.54	0.73
4:A:1402:PHE:CE1	4:A:1403:GLU:HG3	2.24	0.73
4:A:590:ARG:HH11	4:A:590:ARG:HG3	1.53	0.73
5:B:411:PRO:O	5:B:414:ALA:HB3	1.88	0.73
5:B:953:LEU:HD21	5:B:965:LYS:HB2	1.69	0.73
8:E:202:SER:OG	8:E:204:THR:HG22	1.89	0.73
11:H:36:CYS:HA	11:H:126:GLU:O	1.89	0.73
10:G:43:GLY:HA3	10:G:80:LYS:HB3	1.70	0.73
4:A:768:GLN:CG	4:A:816:HIS:HA	2.19	0.73
5:B:616:ILE:HG13	5:B:697:GLU:HG3	1.70	0.73
8:E:22:MET:HE3	8:E:26:ARG:NE	2.04	0.73
1:T:16:DT:H5'	4:A:1386:ARG:HH12	1.54	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:754:SER:H	4:A:757:ASN:ND2	1.87	0.73
5:B:472:ALA:HB1	5:B:474:SER:HB3	1.71	0.73
4:A:244:PRO:HB2	4:A:245:PRO:HD3	1.71	0.72
5:B:1182:CYS:SG	5:B:1182:CYS:O	2.47	0.72
12:I:75:CYS:SG	12:I:79:HIS:N	2.62	0.72
13:J:5:VAL:HG12	13:J:6:ARG:CG	2.15	0.72
5:B:502:ILE:HG22	5:B:507:LYS:HD2	1.70	0.72
5:B:603:LEU:HD13	5:B:608:ASP:HB2	1.71	0.72
8:E:192:ARG:HH11	8:E:192:ARG:HG3	1.53	0.72
10:G:80:LYS:HD3	10:G:80:LYS:N	2.04	0.72
11:H:59:ILE:HG22	11:H:60:ALA:N	2.03	0.72
4:A:319:GLY:HA3	5:B:471:LYS:HA	1.70	0.72
5:B:507:LYS:N	5:B:512:ARG:HH21	1.88	0.72
4:A:567:LYS:CD	4:A:568:PRO:HD2	2.20	0.72
5:B:516:ASN:N	5:B:516:ASN:HD22	1.88	0.72
5:B:642:ASP:O	5:B:644:GLU:N	2.22	0.72
11:H:81:PRO:CB	11:H:82:PRO:HD2	2.19	0.72
4:A:1114:PRO:O	4:A:1115:SER:O	2.05	0.72
5:B:594:ALA:HA	5:B:617:ARG:NH1	2.05	0.72
5:B:39:ARG:NH2	5:B:665:GLU:HG2	2.05	0.72
9:F:138:LEU:HB3	9:F:139:PRO:HD2	1.71	0.72
4:A:1445:ILE:N	4:A:1445:ILE:HD12	2.04	0.72
4:A:321:PRO:O	4:A:322:VAL:HB	1.90	0.72
4:A:783:THR:HG21	4:A:815:PHE:CZ	2.24	0.72
5:B:1065:GLN:HE21	5:B:1067:ARG:N	1.88	0.72
6:C:175:ALA:O	6:C:176:ILE:HG13	1.90	0.72
1:T:19:DG:C4'	5:B:1133:MET:SD	2.78	0.71
5:B:778:MET:CE	5:B:1094:ARG:HD3	2.19	0.71
6:C:73:GLN:HB3	6:C:131:HIS:H	1.55	0.71
4:A:1121:GLU:HG2	4:A:1122:PRO:HD2	1.71	0.71
6:C:167:HIS:CE1	15:L:70:ARG:HB3	2.25	0.71
5:B:378:LEU:HD12	5:B:378:LEU:O	1.89	0.71
5:B:509:ALA:C	5:B:511:PRO:HD3	2.09	0.71
4:A:1239:ARG:HH22	4:A:1241:ARG:NH2	1.88	0.71
4:A:741:ASN:HD21	4:A:743:VAL:HB	1.54	0.71
4:A:808:LEU:HD23	4:A:813:PHE:HA	1.71	0.71
7:D:47:LEU:HD13	7:D:48:ILE:N	2.03	0.71
4:A:164:ARG:HG3	4:A:165:GLY:N	2.04	0.71
4:A:475:THR:HG23	4:A:476:SER:N	2.06	0.71
15:L:32:ALA:HB3	15:L:55:ILE:HD12	1.73	0.71
5:B:508:LEU:O	5:B:509:ALA:HB2	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:351:THR:HB	5:B:1103:ILE:CD1	2.20	0.71
5:B:593:PRO:HG2	5:B:617:ARG:NH2	2.06	0.71
8:E:179:GLN:HB2	8:E:182:ASP:HB2	1.73	0.71
4:A:441:PRO:HD2	4:A:498:ARG:NH2	2.05	0.71
4:A:816:HIS:CD2	5:B:764:SER:HB2	2.26	0.71
5:B:766:ARG:HH22	5:B:1020:ARG:HH11	1.38	0.71
5:B:1169:MET:HE1	5:B:1201:LYS:HA	1.70	0.71
4:A:14:VAL:HG21	5:B:1216:LEU:HD13	1.73	0.71
5:B:745:PRO:O	5:B:748:ILE:HG12	1.90	0.71
10:G:138:THR:CG2	10:G:139:ILE:H	1.97	0.71
15:L:30:ILE:O	15:L:56:LEU:HA	1.91	0.71
4:A:1420:ASP:HB3	4:A:1422:ARG:HG3	1.72	0.71
5:B:1115:THR:HG22	5:B:1117:GLN:HG3	1.72	0.71
4:A:1445:ILE:HG12	10:G:18:PHE:CE2	2.25	0.71
4:A:1152:ILE:HG13	12:I:44:TYR:HB3	1.72	0.70
4:A:1437:GLY:O	4:A:1439:GLY:N	2.23	0.70
5:B:1197:PRO:HG2	5:B:1200:ALA:CB	2.21	0.70
4:A:2:VAL:HG21	5:B:1158:PHE:CA	2.20	0.70
10:G:14:HIS:CD2	10:G:16:SER:HB2	2.26	0.70
4:A:899:VAL:HB	4:A:929:LEU:CD1	2.21	0.70
7:D:170:THR:HG21	7:D:172:LEU:HG	1.72	0.70
11:H:113:ALA:HB2	11:H:126:GLU:HG3	1.72	0.70
4:A:901:LEU:HD22	4:A:919:ILE:CG2	2.21	0.70
5:B:701:ILE:HD11	5:B:703:ILE:HD11	1.73	0.70
4:A:91:PHE:HB2	4:A:297:GLN:HE22	1.54	0.70
7:D:130:LEU:O	7:D:132:GLN:N	2.23	0.70
4:A:68:GLN:C	4:A:70:CYS:H	1.95	0.70
5:B:1099:VAL:O	5:B:1101:ASP:N	2.25	0.70
5:B:708:GLU:O	5:B:710:LEU:N	2.25	0.70
5:B:975:GLN:HG2	5:B:976:ILE:H	1.56	0.70
5:B:351:TYR:CE1	5:B:355:ILE:HD11	2.27	0.70
5:B:227:LYS:HB2	5:B:395:GLN:OE1	1.90	0.70
5:B:953:LEU:O	5:B:953:LEU:HD23	1.91	0.70
14:K:47:ARG:NH1	14:K:47:ARG:HB3	2.05	0.70
4:A:1438:THR:HB	5:B:1144:ALA:HB3	1.74	0.70
5:B:955:THR:HG22	5:B:956:THR:H	1.53	0.70
4:A:1308:THR:HG23	4:A:1309:ASP:N	2.06	0.70
4:A:92:HIS:O	4:A:94:GLY:N	2.24	0.70
5:B:333:PHE:O	5:B:334:ILE:HG13	1.90	0.70
5:B:737:THR:HG21	12:I:66:PRO:HA	1.74	0.70
10:G:18:PHE:HA	10:G:22:MET:HE3	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:384:ASN:OD1	4:A:388:LEU:HD12	1.92	0.70
4:A:466:SER:O	5:B:1103:ILE:HD11	1.92	0.70
5:B:999:MET:HE3	5:B:999:MET:HA	1.72	0.70
11:H:4:THR:HA	11:H:60:ALA:CB	2.22	0.70
4:A:1329:THR:CG2	4:A:1331:SER:H	2.02	0.69
5:B:770:GLN:OE1	5:B:983:ARG:HA	1.91	0.69
6:C:20:PHE:CE1	6:C:22:LEU:HD12	2.24	0.69
8:E:124:VAL:HG13	8:E:132:ILE:HB	1.73	0.69
4:A:913:LEU:HD12	4:A:914:GLU:N	2.05	0.69
7:D:48:ILE:CG2	10:G:4:ILE:HB	2.19	0.69
11:H:59:ILE:HG22	11:H:60:ALA:H	1.56	0.69
1:T:15:DT:O2	4:A:1386:ARG:NH2	2.24	0.69
4:A:675:THR:O	4:A:679:ILE:HG13	1.91	0.69
7:D:33:PHE:CE1	10:G:80:LYS:HE3	2.27	0.69
6:C:184:ASN:ND2	6:C:187:LYS:HA	2.06	0.69
4:A:541:ILE:HD13	4:A:549:MET:HE1	1.74	0.69
4:A:794:PRO:HG2	4:A:795:GLU:OE2	1.92	0.69
5:B:830:TYR:CE2	5:B:1000:PRO:HD3	2.28	0.69
5:B:579:ARG:HB2	5:B:586:TRP:HE1	1.58	0.69
4:A:1239:ARG:HH22	4:A:1241:ARG:HH22	1.39	0.69
4:A:901:LEU:HG	4:A:926:GLN:HE21	1.57	0.69
5:B:46:GLN:HG3	5:B:47:GLN:N	2.07	0.69
5:B:642:ASP:HB3	5:B:649:LYS:CG	2.22	0.69
12:I:101:PHE:N	12:I:101:PHE:CD1	2.59	0.69
7:D:40:HIS:CB	10:G:73:LYS:HZ3	2.06	0.69
4:A:311:GLN:HB3	4:A:312:PRO:HD3	1.73	0.69
5:B:211:VAL:O	5:B:480:SER:HA	1.93	0.69
7:D:53:SER:HB3	7:D:152:SER:CB	2.23	0.69
10:G:18:PHE:HA	10:G:22:MET:CE	2.23	0.69
5:B:654:ARG:H	5:B:657:HIS:HD2	1.38	0.69
4:A:1291:VAL:HG13	4:A:1292:PRO:HD2	1.74	0.69
5:B:728:ARG:HH12	5:B:1047:PHE:HB3	1.57	0.69
4:A:825:ILE:HG23	5:B:508:LEU:CD1	2.19	0.69
6:C:166:GLU:HG3	14:K:10:PHE:CZ	2.21	0.69
1:T:18:DC:H5'	4:A:832:ALA:O	1.93	0.69
4:A:152:VAL:CG1	4:A:153:PRO:HD2	2.23	0.68
5:B:217:ARG:NE	5:B:405:ARG:HB2	2.03	0.68
5:B:39:ARG:HH21	5:B:665:GLU:HG2	1.58	0.68
5:B:95:ILE:HG13	5:B:130:VAL:HG22	1.75	0.68
9:F:97:ARG:O	9:F:101:ILE:HG13	1.93	0.68
4:A:1209:MET:HE1	4:A:1236:LEU:HB3	1.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:766:ARG:NH2	5:B:1020:ARG:HH11	1.91	0.68
5:B:365:THR:HG23	5:B:367:LEU:H	1.57	0.68
5:B:393:LYS:HE3	5:B:393:LYS:HA	1.75	0.68
5:B:1006:ILE:HD13	13:J:44:TYR:CE2	2.28	0.68
4:A:302:THR:HA	4:A:305:ASP:O	1.93	0.68
4:A:35:ILE:O	4:A:35:ILE:HG22	1.93	0.68
6:C:179:GLU:HG2	6:C:180:TYR:N	2.08	0.68
6:C:67:LEU:HD11	6:C:155:LEU:CD1	2.24	0.68
12:I:111:THR:HG22	12:I:112:SER:N	2.09	0.68
4:A:1120:LEU:O	4:A:1323:ASP:HB2	1.94	0.68
4:A:856:THR:HB	4:A:865:GLN:HB2	1.74	0.68
5:B:467:GLY:O	5:B:468:GLU:HB2	1.93	0.68
4:A:1063:MET:CG	4:A:1436:ILE:HG23	2.22	0.68
4:A:23:SER:HA	4:A:233:TRP:CD1	2.28	0.68
4:A:388:LEU:HD22	4:A:432:VAL:HG21	1.75	0.68
5:B:65:GLU:HG3	5:B:66:ASP:N	2.05	0.68
5:B:707:PRO:O	5:B:711:GLU:HG3	1.93	0.68
4:A:106:VAL:HG13	4:A:112:LYS:O	1.93	0.68
4:A:107:CYS:H	4:A:114:LEU:HD21	1.58	0.68
4:A:107:CYS:N	4:A:114:LEU:HD21	2.08	0.68
5:B:1001:PHE:CE1	5:B:1073:TYR:HB2	2.28	0.68
5:B:1017:ILE:HB	5:B:1018:PRO:HD3	1.74	0.68
5:B:1087:PHE:HD2	5:B:1088:GLY:N	1.91	0.68
5:B:112:LEU:HD12	5:B:113:TYR:H	1.58	0.68
4:A:567:LYS:CE	11:H:46:LEU:HB2	2.23	0.68
12:I:50:THR:HG22	12:I:52:ILE:H	1.59	0.68
14:K:31:VAL:HG12	14:K:32:VAL:N	2.08	0.68
4:A:1424:VAL:HG13	4:A:1436:ILE:HD11	1.75	0.68
4:A:79:GLY:HA3	4:A:243:PRO:CG	2.24	0.68
4:A:903:ASN:C	4:A:903:ASN:HD22	1.96	0.68
5:B:824:ILE:CG2	5:B:1087:PHE:HE2	2.07	0.68
9:F:82:THR:HG22	9:F:84:TYR:H	1.59	0.68
5:B:357:GLN:O	5:B:366:GLN:HA	1.94	0.68
5:B:563:MET:HE3	5:B:580:VAL:HB	1.75	0.68
5:B:642:ASP:HB3	5:B:649:LYS:HG3	1.74	0.68
4:A:666:ILE:HD12	4:A:667:GLY:H	1.58	0.68
5:B:1197:PRO:HG2	5:B:1200:ALA:HB2	1.75	0.68
6:C:186:LEU:HD21	6:C:224:GLN:O	1.94	0.68
11:H:93:TYR:HB3	11:H:144:ILE:O	1.93	0.68
13:J:47:ARG:HH11	13:J:47:ARG:HG2	1.59	0.68
4:A:19:PHE:O	4:A:1416:ALA:HA	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:172:PRO:O	6:C:235:VAL:HG23	1.93	0.68
6:C:263:THR:C	6:C:265:MET:H	1.97	0.68
12:I:71:SER:OG	12:I:83:ASN:HB2	1.93	0.68
15:L:40:LEU:HD13	15:L:44:ASP:HB3	1.75	0.68
4:A:450:LEU:N	4:A:450:LEU:HD12	2.09	0.67
5:B:839:MET:HG3	5:B:1010:LEU:HD11	1.76	0.67
6:C:45:ALA:HA	6:C:72:LEU:HD12	1.76	0.67
8:E:135:PHE:HB3	8:E:140:LEU:HD11	1.76	0.67
10:G:30:LEU:HD13	10:G:72:VAL:HG11	1.75	0.67
15:L:38:LEU:O	15:L:39:SER:HB3	1.93	0.67
4:A:55:ASP:C	4:A:57:ARG:N	2.39	0.67
5:B:378:LEU:O	5:B:382:ILE:HG13	1.94	0.67
5:B:521:LEU:HB3	5:B:633:VAL:HG11	1.76	0.67
5:B:615:MET:HB3	5:B:626:ILE:HG12	1.75	0.67
6:C:90:ASP:CG	6:C:90:ASP:O	2.32	0.67
4:A:567:LYS:HE3	11:H:46:LEU:HB2	1.77	0.67
4:A:225:ASN:HD22	4:A:228:PHE:H	1.41	0.67
4:A:54:ASN:HB3	4:A:247:ARG:HH12	1.59	0.67
5:B:192:LEU:O	5:B:193:LYS:HB2	1.93	0.67
6:C:114:TYR:HB3	6:C:140:ASN:O	1.93	0.67
5:B:996:ARG:NH1	6:C:38:ILE:HG23	2.09	0.67
4:A:1343:ALA:HB2	8:E:150:VAL:HG22	1.76	0.67
4:A:1004:ASN:ND2	8:E:167:ARG:HD2	2.09	0.67
10:G:14:HIS:ND1	10:G:15:PRO:HD2	2.09	0.67
11:H:81:PRO:CB	11:H:82:PRO:CD	2.72	0.67
14:K:50:LEU:HD11	14:K:75:ILE:HD13	1.74	0.67
5:B:1162:ILE:HG22	5:B:1163:CYS:N	2.09	0.67
6:C:179:GLU:HG2	6:C:180:TYR:H	1.60	0.67
9:F:86:THR:OG1	9:F:89:GLU:HG3	1.95	0.67
4:A:798:GLY:HA2	4:A:815:PHE:CD1	2.29	0.67
4:A:866:PHE:O	4:A:867:ILE:HG13	1.94	0.67
7:D:34:GLN:O	7:D:47:LEU:HD23	1.94	0.67
9:F:125:LEU:O	9:F:125:LEU:HG	1.93	0.67
4:A:1424:VAL:HG13	4:A:1436:ILE:CD1	2.25	0.67
4:A:63:ARG:HA	4:A:74:MET:SD	2.35	0.67
5:B:999:MET:HA	5:B:999:MET:CE	2.25	0.67
4:A:567:LYS:HB3	11:H:96:VAL:H	1.59	0.67
12:I:52:ILE:HG13	12:I:52:ILE:O	1.95	0.67
4:A:3:GLY:O	4:A:4:GLN:HB2	1.93	0.67
5:B:1073:TYR:CE2	5:B:1080:LYS:HG2	2.30	0.67
4:A:248:PRO:O	4:A:260:ASP:HB2	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:463:ILE:HD12	4:A:469:ARG:HD2	1.75	0.67
4:A:858:ASN:HD22	4:A:858:ASN:C	1.96	0.67
5:B:1099:VAL:CG1	5:B:1100:ASP:N	2.57	0.67
5:B:515:HIS:CD2	5:B:517:THR:H	2.12	0.67
5:B:569:TYR:CE1	5:B:589:VAL:HG21	2.30	0.67
6:C:123:ASN:HD22	6:C:125:MET:HG2	1.59	0.67
4:A:541:ILE:HD13	4:A:549:MET:CE	2.25	0.67
5:B:36:ALA:HA	5:B:39:ARG:HD2	1.76	0.67
10:G:143:ILE:HG22	10:G:144:ARG:N	2.08	0.67
4:A:809:THR:OG1	4:A:812:GLU:HG3	1.95	0.67
4:A:843:LYS:HD3	4:A:846:GLU:OE2	1.94	0.67
5:B:980:PHE:CE2	5:B:1094:ARG:HG3	2.30	0.67
5:B:831:SER:HB3	5:B:994:TYR:OH	1.95	0.67
7:D:176:GLU:O	7:D:178:ALA:N	2.25	0.67
8:E:15:ALA:O	8:E:19:VAL:HG23	1.95	0.67
9:F:90:ARG:HD3	9:F:155:LEU:CD1	2.24	0.67
12:I:13:MET:HG3	12:I:14:LEU:N	2.10	0.67
4:A:1332:PHE:N	4:A:1332:PHE:CD2	2.58	0.66
6:C:18:VAL:O	6:C:18:VAL:HG12	1.94	0.66
7:D:29:LEU:HD22	10:G:82:PHE:CE2	2.29	0.66
4:A:1002:GLY:HA3	4:A:1007:ILE:HG21	1.77	0.66
4:A:69:THR:C	4:A:71:GLN:H	1.98	0.66
4:A:979:SER:OG	4:A:981:LEU:HG	1.94	0.66
5:B:549:THR:HG22	5:B:550:ASP:N	2.06	0.66
7:D:50:LEU:HD11	10:G:4:ILE:HD11	1.78	0.66
12:I:51:ASN:O	12:I:54:GLU:HG3	1.95	0.66
4:A:399:HIS:O	4:A:401:GLY:N	2.28	0.66
5:B:798:TYR:HE2	6:C:62:PHE:CE2	2.14	0.66
10:G:91:VAL:HB	10:G:139:ILE:O	1.95	0.66
4:A:18:GLN:HB2	5:B:1215:ARG:HB2	1.77	0.66
9:F:97:ARG:HD3	9:F:130:ILE:HG23	1.78	0.66
12:I:78:CYS:HB3	12:I:106:CYS:SG	2.36	0.66
4:A:1107:VAL:HG12	4:A:1107:VAL:O	1.96	0.66
4:A:427:GLN:HG3	4:A:430:TRP:CZ2	2.29	0.66
4:A:902:LEU:HG	4:A:926:GLN:HG3	1.76	0.66
5:B:557:PHE:CD2	5:B:557:PHE:C	2.68	0.66
4:A:332:LYS:HG3	4:A:333:GLU:HG2	1.78	0.66
8:E:48:ASP:CG	8:E:49:SER:H	1.99	0.66
9:F:86:THR:HG23	9:F:89:GLU:OE1	1.95	0.66
10:G:7:LEU:HD11	10:G:45:ILE:HD11	1.77	0.66
5:B:1051:THR:HB	5:B:1054:GLY:H	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:46:TYR:CD2	8:E:58:MET:HG2	2.30	0.66
4:A:1017:LEU:HB2	8:E:206:GLY:N	2.06	0.66
4:A:986:ILE:HG22	4:A:987:VAL:N	2.10	0.66
5:B:1202:LEU:O	5:B:1206:GLU:HG3	1.96	0.66
5:B:710:LEU:HA	5:B:733:HIS:HB3	1.78	0.66
14:K:53:ASP:HB3	14:K:56:VAL:HG23	1.78	0.66
5:B:902:GLY:O	15:L:65:VAL:HG11	1.96	0.66
4:A:385:ILE:HG22	4:A:386:ASP:N	2.10	0.66
5:B:370:PHE:HE2	5:B:373:ARG:HH11	1.43	0.66
5:B:635:ARG:NH2	5:B:742:GLU:OE2	2.27	0.66
5:B:995:ARG:HH12	6:C:165:LYS:HG2	1.60	0.66
6:C:147:LEU:HB2	6:C:151:GLN:HB2	1.78	0.66
6:C:238:ILE:CG2	6:C:242:GLN:HB2	2.26	0.66
4:A:50:ILE:O	4:A:52:GLY:N	2.27	0.65
4:A:2:VAL:CG2	5:B:1158:PHE:HA	2.26	0.65
4:A:1017:LEU:HB3	8:E:205:SER:HA	1.78	0.65
11:H:56:THR:HB	11:H:145:ARG:HG2	1.78	0.65
12:I:34:TYR:CE2	12:I:36:GLU:HB3	2.31	0.65
4:A:1227:ILE:HG22	4:A:1228:TRP:N	2.10	0.65
4:A:842:VAL:HG11	5:B:1136:ASP:OD2	1.96	0.65
5:B:473:MET:O	5:B:475:SER:N	2.28	0.65
6:C:168:ALA:O	6:C:170:TRP:N	2.30	0.65
4:A:1161:THR:HG22	4:A:1163:ILE:N	2.04	0.65
4:A:55:ASP:CG	4:A:55:ASP:O	2.33	0.65
4:A:84:ILE:HG23	4:A:84:ILE:O	1.95	0.65
5:B:798:TYR:HE2	6:C:62:PHE:CZ	2.13	0.65
6:C:165:LYS:O	14:K:6:ARG:NH1	2.29	0.65
4:A:23:SER:HA	4:A:233:TRP:NE1	2.11	0.65
4:A:541:ILE:HG22	4:A:546:VAL:HG23	1.78	0.65
4:A:547:LEU:HD22	14:K:58:PHE:CD1	2.31	0.65
4:A:500:GLU:OE2	5:B:1145:SER:HB2	1.97	0.65
4:A:504:LEU:HD11	9:F:91:ALA:HB1	1.77	0.65
9:F:90:ARG:HG3	9:F:91:ALA:N	2.11	0.65
13:J:12:LYS:O	13:J:14:VAL:HG23	1.97	0.65
15:L:39:SER:O	15:L:40:LEU:HG	1.96	0.65
5:B:952:VAL:HG12	5:B:953:LEU:H	1.61	0.65
5:B:1056:SER:HB3	5:B:1066:SER:HB2	1.79	0.65
5:B:642:ASP:HA	5:B:649:LYS:HA	1.77	0.65
5:B:758:PHE:CE2	5:B:1044:ALA:HA	2.32	0.65
7:D:176:GLU:C	7:D:178:ALA:H	1.98	0.65
11:H:38:LEU:HD12	11:H:124:ARG:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:372:LYS:HA	4:A:435:HIS:ND1	2.11	0.65
4:A:351:THR:HG22	5:B:1103:ILE:HA	1.77	0.65
5:B:1182:CYS:C	5:B:1183:LYS:HE3	2.16	0.65
5:B:604:ARG:NH2	5:B:613:VAL:O	2.30	0.65
5:B:857:ARG:HD2	5:B:945:GLU:OE1	1.95	0.65
8:E:176:PRO:O	8:E:212:ARG:HA	1.97	0.65
12:I:101:PHE:HD1	12:I:101:PHE:H	1.44	0.65
5:B:1085:ILE:HD12	5:B:1085:ILE:N	2.11	0.65
5:B:653:VAL:CG2	5:B:689:LEU:HB3	2.27	0.65
6:C:99:LEU:HA	6:C:119:VAL:O	1.97	0.65
4:A:1445:ILE:HG12	10:G:18:PHE:HE2	1.60	0.65
5:B:229:ALA:HB1	5:B:231:PRO:HD2	1.79	0.65
5:B:899:ILE:CD1	5:B:911:ILE:HA	2.27	0.65
5:B:975:GLN:O	5:B:990:ILE:HD12	1.97	0.65
6:C:189:THR:HG22	6:C:190:ASP:H	1.60	0.65
7:D:122:GLU:HA	7:D:125:SER:OG	1.96	0.65
15:L:32:ALA:HB3	15:L:55:ILE:CD1	2.27	0.65
4:A:535:THR:HG23	4:A:575:LYS:HE2	1.79	0.65
5:B:197:PHE:CZ	5:B:816:GLU:HG2	2.32	0.65
9:F:119:ARG:HG3	9:F:119:ARG:HH11	1.62	0.65
10:G:34:VAL:CG1	10:G:45:ILE:HG21	2.26	0.65
12:I:6:PHE:HB3	12:I:12:ASN:O	1.96	0.65
4:A:670:ILE:HG23	4:A:805:LEU:CD2	2.27	0.64
4:A:979:SER:OG	4:A:980:ASP:N	2.28	0.64
5:B:1002:THR:HG23	5:B:1006:ILE:HG13	1.80	0.64
5:B:601:ARG:O	5:B:605:ARG:HG3	1.97	0.64
8:E:84:ASP:O	8:E:86:PRO:HD3	1.97	0.64
10:G:59:GLY:HA3	10:G:70:PHE:CD2	2.32	0.64
15:L:58:LYS:O	15:L:58:LYS:HG2	1.97	0.64
4:A:672:ASP:HB2	4:A:736:ASN:OD1	1.98	0.64
4:A:743:VAL:O	4:A:747:VAL:HG23	1.96	0.64
4:A:818:MET:HA	5:B:514:LEU:HB3	1.79	0.64
6:C:189:THR:HG22	6:C:190:ASP:N	2.12	0.64
6:C:183:TRP:CZ2	6:C:207:CYS:HB3	2.32	0.64
4:A:867:ILE:HD12	8:E:208:TYR:HE1	1.62	0.64
4:A:1191:TRP:CD1	4:A:1256:GLU:HB2	2.33	0.64
5:B:1223:ASP:O	5:B:1224:PHE:HB2	1.96	0.64
5:B:770:GLN:CD	5:B:983:ARG:HA	2.16	0.64
8:E:22:MET:CE	8:E:26:ARG:HH21	2.10	0.64
4:A:844:ALA:C	4:A:845:LEU:HD23	2.18	0.64
4:A:869:GLY:O	8:E:204:THR:HG21	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1045:SER:O	5:B:1046:PRO:O	2.15	0.64
5:B:847:ASP:C	5:B:849:GLY:H	1.99	0.64
5:B:880:THR:O	5:B:881:ASN:HB2	1.96	0.64
7:D:54:GLU:O	7:D:58:VAL:HG23	1.98	0.64
9:F:111:LEU:N	9:F:111:LEU:HD12	2.13	0.64
4:A:88:LYS:HE3	4:A:280:GLU:OE2	1.97	0.64
4:A:384:ASN:CG	4:A:388:LEU:HD12	2.18	0.64
8:E:157:SER:OG	8:E:160:GLU:HG3	1.97	0.64
4:A:1115:SER:O	4:A:1116:LEU:HB3	1.97	0.64
4:A:1293:SER:OG	4:A:1294:PRO:HD2	1.97	0.64
5:B:850:LEU:HD12	5:B:851:PHE:H	1.63	0.64
4:A:1039:LYS:HG3	4:A:1043:ASP:OD2	1.98	0.64
4:A:1341:ILE:HG23	4:A:1342:GLU:H	1.61	0.64
4:A:1348:LEU:HG	4:A:1372:VAL:HG23	1.79	0.64
4:A:69:THR:O	4:A:71:GLN:N	2.30	0.64
5:B:704:ALA:HB3	5:B:741:CYS:SG	2.38	0.64
4:A:590:ARG:HH21	4:A:620:LYS:HB3	1.62	0.64
4:A:897:TYR:HD2	4:A:936:LEU:HD13	1.62	0.64
4:A:665:GLY:HA2	5:B:1026:LEU:HD21	1.78	0.64
5:B:604:ARG:NH1	5:B:691:GLU:OE2	2.30	0.64
10:G:74:TYR:HD2	10:G:74:TYR:H	1.46	0.64
5:B:23:ALA:HB1	5:B:24:PRO:CD	2.27	0.64
5:B:511:PRO:CD	5:B:512:ARG:N	2.61	0.64
5:B:879:ARG:NH1	5:B:883:LEU:HD22	2.12	0.64
6:C:152:GLU:OE2	6:C:154:LYS:HE3	1.98	0.64
11:H:89:LEU:C	11:H:91:ASP:H	2.01	0.64
4:A:720:ARG:O	4:A:724:GLU:HB2	1.98	0.64
14:K:49:GLU:HG3	14:K:94:ILE:HG12	1.80	0.64
5:B:1172:ILE:O	5:B:1172:ILE:HG22	1.98	0.63
5:B:580:VAL:HG22	5:B:624:LEU:CB	2.28	0.63
5:B:842:ASN:HD22	5:B:845:SER:CB	2.11	0.63
6:C:43:THR:CG2	6:C:44:LEU:N	2.60	0.63
7:D:56:ARG:HB2	7:D:148:LEU:HD22	1.80	0.63
8:E:213:ILE:HG12	8:E:214:CYS:N	2.12	0.63
4:A:407:ARG:HG2	4:A:430:TRP:CH2	2.33	0.63
6:C:212:PRO:CB	6:C:213:PRO:HD2	2.29	0.63
4:A:1206:ASP:HB3	4:A:1274:ARG:HH12	1.63	0.63
4:A:404:TYR:HB2	4:A:433:GLU:HB2	1.80	0.63
5:B:862:GLN:HG2	5:B:963:PHE:HD1	1.63	0.63
7:D:40:HIS:CB	10:G:73:LYS:NZ	2.55	0.63
6:C:66:ARG:HH21	13:J:5:VAL:HG23	1.60	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1224:LEU:HD12	4:A:1241:ARG:O	1.98	0.63
4:A:295:LEU:O	4:A:298:PHE:HB3	1.97	0.63
5:B:731:VAL:HG12	5:B:732:SER:H	1.63	0.63
9:F:89:GLU:OE2	9:F:134:ILE:HG21	1.98	0.63
4:A:254:GLU:HB2	5:B:935:ARG:HH12	1.62	0.63
4:A:47:ARG:HH12	4:A:254:GLU:HG2	1.64	0.63
5:B:121:ASN:HA	5:B:207:GLY:HA2	1.81	0.63
5:B:549:THR:H	5:B:628:THR:HG23	1.64	0.63
6:C:177:GLU:HB2	6:C:231:ASN:HB3	1.80	0.63
11:H:99:GLY:N	11:H:118:PHE:HD2	1.96	0.63
4:A:1341:ILE:CG2	4:A:1342:GLU:N	2.62	0.63
5:B:906:SER:O	5:B:941:LEU:HD23	1.99	0.63
6:C:43:THR:CG2	6:C:44:LEU:H	2.10	0.63
1:T:23:DG:H2'	1:T:24:DG:C8	2.33	0.63
4:A:886:ILE:HG22	4:A:887:GLY:N	2.13	0.63
10:G:122:ASN:ND2	10:G:125:SER:HB3	2.14	0.63
4:A:1193:LEU:HD12	4:A:1194:ARG:N	2.14	0.63
5:B:309:GLN:HG3	12:I:52:ILE:CD1	2.29	0.63
5:B:63:ILE:O	5:B:67:SER:HB3	1.98	0.63
7:D:191:ALA:O	7:D:193:THR:N	2.32	0.63
10:G:1:MET:C	10:G:1:MET:SD	2.78	0.63
12:I:8:ARG:CG	12:I:34:TYR:HE1	2.11	0.63
4:A:1348:LEU:HG	4:A:1372:VAL:CG2	2.28	0.63
4:A:591:PHE:HA	4:A:595:THR:HG21	1.80	0.63
5:B:1007:VAL:CG2	5:B:1008:PRO:HD2	2.27	0.63
5:B:852:ARG:HH22	15:L:70:ARG:C	2.02	0.63
8:E:23:VAL:HG13	8:E:78:LEU:HD13	1.80	0.63
4:A:1261:LYS:O	4:A:1264:GLU:HB3	1.99	0.62
4:A:442:VAL:HB	4:A:489:LEU:HD11	1.78	0.62
4:A:899:VAL:HB	4:A:929:LEU:HD11	1.81	0.62
5:B:365:THR:HG23	5:B:367:LEU:HG	1.81	0.62
7:D:56:ARG:HA	7:D:148:LEU:HD13	1.80	0.62
14:K:49:GLU:HG3	14:K:94:ILE:CG1	2.28	0.62
4:A:114:LEU:HD13	4:A:171:GLN:OE1	1.99	0.62
4:A:481:ASP:OD1	4:A:485:ASP:OD2	2.17	0.62
4:A:49:LYS:HE2	4:A:61:ILE:HD12	1.80	0.62
5:B:205:ILE:O	5:B:207:GLY:N	2.32	0.62
4:A:1121:GLU:CG	4:A:1122:PRO:HD2	2.28	0.62
4:A:567:LYS:CB	11:H:95:TYR:HA	2.28	0.62
5:B:217:ARG:C	5:B:217:ARG:HD2	2.19	0.62
7:D:202:ILE:HG21	7:D:207:LEU:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1021:LEU:O	4:A:1024:SER:HB3	1.99	0.62
5:B:1001:PHE:CE2	6:C:34:ARG:CZ	2.82	0.62
4:A:412:ARG:NH2	5:B:1108:ARG:NH1	2.47	0.62
5:B:97:VAL:HG12	5:B:178:ASN:HD21	1.63	0.62
10:G:110:VAL:HG22	10:G:161:GLY:O	2.00	0.62
4:A:1444:MET:HG2	10:G:60:ARG:HA	1.81	0.62
4:A:981:LEU:HD21	4:A:1038:THR:C	2.20	0.62
5:B:509:ALA:C	5:B:511:PRO:CD	2.68	0.62
8:E:124:VAL:HG13	8:E:132:ILE:HD12	1.80	0.62
4:A:1418:LEU:HD23	5:B:1222:ARG:HD2	1.81	0.62
4:A:252:PHE:O	4:A:256:GLN:NE2	2.33	0.62
5:B:1180:PHE:HB3	5:B:1191:ILE:HD12	1.82	0.62
5:B:121:ASN:HA	5:B:207:GLY:CA	2.29	0.62
5:B:507:LYS:N	5:B:512:ARG:NH2	2.47	0.62
10:G:1:MET:HE3	10:G:80:LYS:C	2.19	0.62
12:I:85:PHE:N	12:I:85:PHE:HD2	1.88	0.62
4:A:1120:LEU:HD12	4:A:1120:LEU:N	2.14	0.62
4:A:154:SER:HB3	4:A:162:VAL:HG21	1.81	0.62
4:A:108:MET:SD	4:A:210:ILE:HD13	2.39	0.62
4:A:646:PHE:O	4:A:650:GLN:HG3	1.99	0.62
4:A:866:PHE:C	4:A:867:ILE:HG13	2.19	0.62
5:B:43:LEU:HD11	5:B:811:TYR:O	1.99	0.62
11:H:100:THR:OG1	11:H:138:GLU:HG3	1.99	0.62
4:A:722:LEU:O	4:A:725:ALA:HB3	1.99	0.62
4:A:2:VAL:CG2	5:B:1158:PHE:CA	2.78	0.62
5:B:1165:ILE:HG22	5:B:1166:CYS:N	2.14	0.62
5:B:171:PRO:HD2	5:B:457:LEU:HD13	1.82	0.62
9:F:111:LEU:H	9:F:111:LEU:HD12	1.65	0.62
9:F:135:ARG:HD3	9:F:143:PHE:CD2	2.35	0.62
4:A:1057:VAL:HG12	4:A:1058:VAL:H	1.64	0.62
4:A:366:VAL:HG21	4:A:460:VAL:HG22	1.81	0.62
5:B:824:ILE:HG22	5:B:1087:PHE:CE2	2.23	0.62
5:B:622:LYS:HE2	12:I:59:VAL:HG22	1.80	0.62
1:T:20:DC:H2''	1:T:21:DC:H5'	1.81	0.62
4:A:472:LEU:HD11	5:B:835:GLN:NE2	2.15	0.62
6:C:244:VAL:O	6:C:248:ILE:HG13	2.00	0.62
11:H:81:PRO:HB2	11:H:82:PRO:CD	2.27	0.62
15:L:48:CYS:HB3	15:L:51:CYS:O	2.00	0.62
4:A:475:THR:CG2	4:A:476:SER:N	2.63	0.61
5:B:314:LEU:O	5:B:317:CYS:HB3	1.99	0.61
4:A:1015:VAL:HG12	4:A:1019:CYS:SG	2.40	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:503:GLN:HE21	9:F:90:ARG:NH2	1.98	0.61
5:B:469:GLN:C	5:B:470:LYS:HG3	2.21	0.61
11:H:126:GLU:C	11:H:130:ARG:HH22	2.03	0.61
4:A:265:LYS:NZ	4:A:322:VAL:HG13	2.13	0.61
4:A:90:VAL:HG13	4:A:297:GLN:HA	1.82	0.61
5:B:953:LEU:CD2	5:B:965:LYS:HB2	2.29	0.61
6:C:66:ARG:NH1	13:J:2:ILE:HG21	2.15	0.61
5:B:1159:ARG:NH1	5:B:1159:ARG:HB3	2.15	0.61
7:D:198:LEU:O	7:D:200:ASN:N	2.32	0.61
1:T:16:DT:H5'	4:A:1386:ARG:HH11	1.63	0.61
4:A:590:ARG:HD2	4:A:605:MET:HB3	1.82	0.61
5:B:1065:GLN:NE2	5:B:1066:SER:N	2.47	0.61
5:B:465:ASN:ND2	5:B:465:ASN:N	2.49	0.61
5:B:731:VAL:HG12	5:B:732:SER:N	2.16	0.61
5:B:882:THR:HG22	5:B:884:ARG:N	2.13	0.61
10:G:9:LEU:HD12	10:G:10:ASN:H	1.65	0.61
4:A:613:ILE:O	4:A:614:PHE:HB3	1.99	0.61
10:G:23:LYS:HG3	10:G:56:ILE:CD1	2.29	0.61
12:I:103:CYS:CB	12:I:106:CYS:SG	2.89	0.61
4:A:1097:GLY:O	4:A:1100:ARG:HB3	2.00	0.61
4:A:1444:MET:CE	9:F:135:ARG:HB2	2.31	0.61
4:A:344:ARG:HD2	5:B:1118:PRO:O	2.00	0.61
4:A:382:PRO:HB3	4:A:428:TYR:HE2	1.65	0.61
4:A:590:ARG:HB3	4:A:605:MET:N	2.15	0.61
4:A:907:THR:CG2	4:A:908:LEU:N	2.63	0.61
5:B:287:ARG:NH1	5:B:324:ILE:O	2.34	0.61
5:B:778:MET:HE1	5:B:1094:ARG:CD	2.30	0.61
5:B:860:MET:HG2	5:B:861:ASP:N	2.14	0.61
6:C:66:ARG:NH1	6:C:144:ILE:O	2.34	0.61
6:C:238:ILE:HG23	6:C:242:GLN:HB2	1.82	0.61
8:E:131:THR:HG21	8:E:191:LYS:NZ	2.15	0.61
13:J:1:MET:H2	13:J:56:LEU:N	1.97	0.61
4:A:728:LYS:O	4:A:732:LEU:HG	2.00	0.61
7:D:20:GLU:O	7:D:21:GLU:O	2.19	0.61
12:I:111:THR:HG22	12:I:112:SER:H	1.65	0.61
4:A:1007:ILE:C	4:A:1009:ASN:H	2.02	0.61
4:A:1454:MET:O	4:A:1454:MET:HG3	1.99	0.61
4:A:152:VAL:HG12	4:A:153:PRO:HD2	1.82	0.61
4:A:524:VAL:HG12	4:A:525:GLN:N	2.11	0.61
8:E:157:SER:C	8:E:159:ASP:H	2.04	0.61
13:J:53:HIS:C	13:J:53:HIS:CD2	2.73	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1299:VAL:HG12	4:A:1300:LYS:N	2.16	0.61
4:A:224:PHE:CE2	4:A:231:PRO:HG3	2.35	0.61
5:B:1152:MET:CE	5:B:1157:ALA:HA	2.31	0.61
5:B:212:LEU:CD2	5:B:480:SER:HB2	2.31	0.61
4:A:1116:LEU:HG	4:A:1308:THR:HB	1.83	0.60
4:A:467:THR:O	4:A:469:ARG:HG3	2.00	0.60
5:B:310:MET:O	5:B:313:MET:HB2	2.01	0.60
5:B:606:LYS:HD2	5:B:608:ASP:OD2	2.01	0.60
10:G:51:TYR:C	10:G:51:TYR:CD2	2.74	0.60
4:A:1063:MET:SD	4:A:1436:ILE:HG12	2.41	0.60
8:E:78:LEU:HD23	8:E:79:TRP:N	2.16	0.60
5:B:502:ILE:CG2	5:B:507:LYS:HD2	2.30	0.60
5:B:834:ASN:HB3	5:B:840:ILE:HG13	1.83	0.60
4:A:1343:ALA:HB2	8:E:150:VAL:CG2	2.32	0.60
5:B:980:PHE:HE2	5:B:1094:ARG:CG	2.14	0.60
5:B:197:PHE:HZ	5:B:816:GLU:HG2	1.66	0.60
5:B:642:ASP:HB3	5:B:649:LYS:HD2	1.82	0.60
5:B:859:TYR:CZ	5:B:941:LEU:HD12	2.37	0.60
6:C:208:GLU:O	6:C:210:GLU:N	2.34	0.60
4:A:399:HIS:CB	4:A:400:PRO:HD3	2.28	0.60
4:A:590:ARG:O	4:A:591:PHE:HB2	2.02	0.60
4:A:854:ASN:HB3	4:A:1000:LEU:HD21	1.82	0.60
12:I:2:THR:O	12:I:3:THR:C	2.39	0.60
4:A:518:LYS:HE2	4:A:624:SER:O	2.02	0.60
4:A:81:PHE:CZ	5:B:1208:MET:HE2	2.36	0.60
5:B:446:LEU:O	5:B:447:ALA:HB3	2.02	0.60
5:B:511:PRO:HD2	5:B:512:ARG:N	2.16	0.60
5:B:822:ASN:O	13:J:48:ARG:NH1	2.34	0.60
4:A:1151:GLU:OE2	12:I:45:ARG:HD2	2.01	0.60
14:K:10:PHE:CD2	14:K:10:PHE:N	2.70	0.60
3:P:2:A:H2'	3:P:3:G:H8	1.63	0.60
4:A:1027:ALA:O	4:A:1031:VAL:HG23	2.01	0.60
4:A:1074:GLU:HB3	4:A:1075:PRO:CD	2.30	0.60
5:B:955:THR:CG2	5:B:956:THR:H	2.15	0.60
6:C:254:LYS:O	6:C:256:ALA:N	2.35	0.60
7:D:56:ARG:HD3	7:D:149:THR:HA	1.82	0.60
12:I:62:ILE:O	12:I:62:ILE:HG12	2.02	0.60
4:A:1291:VAL:HG13	4:A:1292:PRO:CD	2.31	0.60
4:A:150:THR:O	4:A:151:ASP:OD1	2.20	0.60
5:B:787:VAL:O	5:B:787:VAL:HG12	2.00	0.60
6:C:56:THR:HG22	6:C:57:VAL:N	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:128:VAL:O	7:D:132:GLN:HG3	2.02	0.60
5:B:758:PHE:CE1	5:B:1027:ILE:HG22	2.37	0.60
5:B:949:VAL:HG12	5:B:950:ASP:N	2.16	0.60
3:P:10:C:H4'	4:A:485:ASP:OD1	2.02	0.60
4:A:472:LEU:O	4:A:475:THR:HB	2.02	0.60
4:A:738:LYS:HB2	4:A:740:LEU:HG	1.83	0.60
4:A:666:ILE:HD11	5:B:1067:ARG:O	2.02	0.60
13:J:14:VAL:HG12	13:J:14:VAL:O	2.02	0.60
14:K:21:ILE:HG23	14:K:31:VAL:HG11	1.82	0.60
14:K:65:HIS:CD2	14:K:67:PHE:HB2	2.36	0.60
4:A:1436:ILE:O	4:A:1437:GLY:C	2.38	0.59
4:A:567:LYS:CG	4:A:568:PRO:CD	2.79	0.59
7:D:130:LEU:HD22	7:D:134:THR:OG1	2.02	0.59
14:K:63:VAL:HG23	14:K:63:VAL:O	2.02	0.59
5:B:189:LEU:O	5:B:192:LEU:N	2.29	0.59
4:A:825:ILE:HG21	5:B:508:LEU:HD11	1.71	0.59
5:B:616:ILE:CG1	5:B:697:GLU:HA	2.32	0.59
6:C:174:ALA:O	6:C:175:ALA:HB2	2.00	0.59
6:C:22:LEU:HD13	6:C:230:MET:CE	2.33	0.59
6:C:241:ASP:O	6:C:245:VAL:HG23	2.02	0.59
9:F:93:ILE:HD11	9:F:134:ILE:CD1	2.26	0.59
4:A:12:ARG:HD2	5:B:1218:THR:HB	1.83	0.59
4:A:384:ASN:O	4:A:386:ASP:N	2.34	0.59
10:G:119:LEU:HD12	10:G:131:GLN:O	2.03	0.59
4:A:1345:ARG:HG3	4:A:1376:THR:HG21	1.83	0.59
4:A:469:ARG:NH2	5:B:991:GLY:O	2.36	0.59
4:A:774:ARG:NH2	4:A:797:LYS:HB2	2.17	0.59
4:A:855:THR:CG2	4:A:857:ARG:HE	2.06	0.59
5:B:118:ARG:HH22	5:B:194:GLU:CD	2.05	0.59
5:B:118:ARG:HH11	5:B:204:ILE:HD11	1.68	0.59
5:B:515:HIS:H	5:B:518:HIS:CD2	2.10	0.59
5:B:705:MET:N	5:B:710:LEU:HD12	2.16	0.59
5:B:840:ILE:HB	5:B:1011:ILE:HB	1.84	0.59
7:D:220:LEU:O	7:D:221:TYR:HD1	1.85	0.59
4:A:1017:LEU:CB	8:E:205:SER:HA	2.32	0.59
4:A:1059:HIS:ND1	9:F:86:THR:HA	2.17	0.59
11:H:91:ASP:C	11:H:93:TYR:H	2.06	0.59
12:I:85:PHE:HD1	12:I:99:LEU:HD13	1.67	0.59
4:A:185:TRP:CZ3	4:A:200:ARG:HG2	2.38	0.59
4:A:384:ASN:O	4:A:385:ILE:C	2.41	0.59
5:B:744:HIS:CG	5:B:745:PRO:HD2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:999:MET:HE2	5:B:1000:PRO:HD2	1.82	0.59
8:E:207:ARG:HH11	8:E:207:ARG:CB	2.14	0.59
4:A:1166:ASP:OD2	4:A:1239:ARG:HD2	2.02	0.59
4:A:69:THR:C	4:A:71:GLN:N	2.55	0.59
4:A:490:HIS:HB3	5:B:1150:ARG:NH1	2.17	0.59
5:B:745:PRO:O	5:B:747:MET:N	2.34	0.59
11:H:18:GLY:O	11:H:19:ARG:HB2	2.03	0.59
11:H:44:VAL:O	11:H:44:VAL:HG12	2.03	0.59
4:A:311:GLN:HB3	4:A:312:PRO:CD	2.30	0.59
4:A:407:ARG:HB3	4:A:430:TRP:CE2	2.38	0.59
5:B:205:ILE:N	5:B:205:ILE:HD12	2.17	0.59
5:B:980:PHE:HD2	5:B:1094:ARG:HA	1.67	0.59
6:C:238:ILE:HG22	6:C:243:VAL:HG23	1.85	0.59
7:D:51:ASN:O	7:D:54:GLU:HB3	2.03	0.59
15:L:60:ARG:HG2	15:L:61:THR:H	1.68	0.59
5:B:172:ILE:HD13	5:B:178:ASN:CB	2.32	0.59
7:D:156:ASP:C	7:D:158:GLU:H	2.04	0.59
4:A:1341:ILE:CG2	4:A:1342:GLU:H	2.15	0.59
4:A:195:ASP:O	4:A:196:GLU:HB3	2.03	0.59
4:A:67:CYS:O	4:A:68:GLN:HB2	2.03	0.59
4:A:913:LEU:HD12	4:A:914:GLU:H	1.66	0.59
5:B:180:TYR:HD1	5:B:180:TYR:H	1.51	0.59
5:B:29:ASP:HB3	5:B:658:ILE:HD13	1.83	0.59
5:B:616:ILE:N	5:B:616:ILE:HD12	2.17	0.59
10:G:3:PHE:CD1	10:G:80:LYS:NZ	2.68	0.59
12:I:105:SER:O	12:I:106:CYS:HB3	2.03	0.59
6:C:35:ARG:NH1	14:K:41:THR:OG1	2.36	0.59
14:K:58:PHE:HB3	14:K:76:GLN:HB3	1.85	0.59
1:T:20:DC:H4'	4:A:447:GLN:CD	2.17	0.59
4:A:21:LEU:HG	4:A:1413:GLY:O	2.03	0.59
4:A:663:SER:OG	4:A:664:THR:N	2.36	0.59
4:A:75:ASN:O	4:A:76:GLU:CB	2.51	0.59
4:A:800:VAL:HG22	4:A:812:GLU:HB3	1.84	0.59
5:B:265:SER:O	5:B:266:ALA:HB3	2.02	0.59
6:C:124:LEU:O	6:C:125:MET:HB2	2.02	0.59
14:K:60:ALA:O	14:K:73:LEU:HD12	2.02	0.59
5:B:622:LYS:CE	12:I:59:VAL:HG22	2.33	0.58
7:D:144:THR:HG21	10:G:46:LEU:HD13	1.85	0.58
4:A:1444:MET:HE2	9:F:135:ARG:HB2	1.85	0.58
10:G:3:PHE:CE1	10:G:80:LYS:HE2	2.38	0.58
13:J:23:ASN:C	13:J:25:LEU:H	2.05	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1385:THR:HG22	4:A:1386:ARG:N	2.18	0.58
5:B:1180:PHE:O	5:B:1181:GLU:O	2.21	0.58
5:B:1196:ILE:HB	5:B:1197:PRO:HD2	1.84	0.58
5:B:811:TYR:N	5:B:811:TYR:CD1	2.71	0.58
5:B:838:SER:HB2	5:B:989:THR:O	2.02	0.58
12:I:26:LEU:HD23	12:I:37:GLU:HA	1.84	0.58
4:A:1105:LEU:HD22	4:A:1384:VAL:HG21	1.83	0.58
4:A:401:GLY:C	4:A:435:HIS:HD2	2.07	0.58
5:B:1031:LEU:HD23	5:B:1044:ALA:HB2	1.84	0.58
5:B:65:GLU:CG	5:B:66:ASP:H	2.11	0.58
4:A:503:GLN:NE2	9:F:90:ARG:HH21	1.99	0.58
5:B:737:THR:CG2	12:I:66:PRO:HA	2.32	0.58
5:B:1001:PHE:HE2	6:C:34:ARG:CZ	2.16	0.58
6:C:45:ALA:HA	6:C:72:LEU:CD1	2.33	0.58
8:E:114:ASN:O	8:E:115:ASN:HB3	2.03	0.58
8:E:90:VAL:HA	8:E:120:ALA:HB2	1.85	0.58
4:A:1030:ARG:NH1	4:A:1035:TYR:OH	2.36	0.58
4:A:262:LEU:O	4:A:264:PHE:N	2.36	0.58
4:A:265:LYS:NZ	4:A:322:VAL:HG22	2.18	0.58
11:H:143:LEU:N	11:H:143:LEU:HD12	2.19	0.58
11:H:17:PRO:HB3	11:H:24:CYS:SG	2.42	0.58
13:J:1:MET:N	13:J:56:LEU:N	2.52	0.58
13:J:44:TYR:HA	13:J:47:ARG:HB2	1.84	0.58
13:J:57:ILE:HA	13:J:60:PHE:CD2	2.30	0.58
15:L:53:HIS:O	15:L:55:ILE:HG12	2.04	0.58
4:A:1313:LEU:O	4:A:1315:GLU:N	2.36	0.58
4:A:768:GLN:HG2	4:A:816:HIS:CA	2.31	0.58
4:A:853:ASP:O	4:A:854:ASN:HB2	2.04	0.58
5:B:955:THR:CG2	5:B:956:THR:N	2.66	0.58
6:C:254:LYS:O	6:C:258:ILE:HD13	2.04	0.58
8:E:39:LEU:O	8:E:42:PHE:HB3	2.02	0.58
12:I:8:ARG:HG2	12:I:34:TYR:HE1	1.69	0.58
14:K:47:ARG:CB	14:K:47:ARG:HH11	2.11	0.58
4:A:868:TYR:HD2	4:A:1058:VAL:HG21	1.67	0.58
4:A:49:LYS:HZ1	4:A:61:ILE:N	2.02	0.58
4:A:658:LEU:HD13	5:B:831:SER:HA	1.85	0.58
4:A:836:TYR:CD2	4:A:840:ARG:HD2	2.38	0.58
5:B:705:MET:H	5:B:710:LEU:CD1	2.14	0.58
7:D:33:PHE:CZ	10:G:80:LYS:HE3	2.38	0.58
4:A:1198:ASP:O	4:A:1202:MET:HG2	2.04	0.58
4:A:658:LEU:HD23	4:A:659:HIS:CE1	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:875:ALA:HA	4:A:878:ILE:HD12	1.86	0.58
7:D:59:ILE:HG21	7:D:145:MET:SD	2.44	0.58
10:G:14:HIS:HD2	10:G:16:SER:HB2	1.67	0.58
10:G:7:LEU:CD1	10:G:45:ILE:HD11	2.33	0.58
12:I:55:THR:CG2	12:I:58:VAL:HG21	2.34	0.58
4:A:278:THR:O	4:A:282:ASN:HB2	2.04	0.58
4:A:853:ASP:OD1	4:A:855:THR:CB	2.51	0.58
5:B:1115:THR:O	5:B:1116:ARG:HB2	2.03	0.58
6:C:31:ASN:OD1	6:C:34:ARG:NH1	2.37	0.58
7:D:153:ARG:HH22	7:D:184:ALA:HA	1.67	0.58
8:E:198:ILE:CD1	8:E:212:ARG:HG3	2.31	0.58
4:A:971:PHE:CE2	4:A:1040:GLN:HG2	2.38	0.58
4:A:265:LYS:HE2	4:A:322:VAL:CG1	2.33	0.58
4:A:427:GLN:HB2	4:A:430:TRP:CD1	2.39	0.58
4:A:50:ILE:C	4:A:52:GLY:H	2.06	0.58
4:A:828:ALA:CB	5:B:530:GLY:HA2	2.33	0.58
5:B:1001:PHE:CE2	6:C:34:ARG:NE	2.72	0.58
5:B:1099:VAL:HG12	5:B:1100:ASP:H	1.69	0.58
5:B:1152:MET:HE3	5:B:1157:ALA:HA	1.86	0.58
5:B:196:PRO:HG2	5:B:197:PHE:H	1.69	0.58
10:G:35:GLU:OE2	10:G:48:VAL:HG23	2.04	0.58
15:L:27:LEU:O	15:L:28:LYS:HG2	2.03	0.58
4:A:78:PRO:HA	5:B:1201:LYS:NZ	2.18	0.57
5:B:579:ARG:HG2	5:B:579:ARG:HH11	1.69	0.57
5:B:957:ASN:O	5:B:959:ASP:N	2.37	0.57
7:D:134:THR:CG2	7:D:135:GLY:N	2.67	0.57
8:E:14:ARG:HH21	8:E:141:VAL:CG1	2.17	0.57
9:F:103:MET:O	9:F:104:ASN:HB2	2.04	0.57
10:G:99:PHE:HZ	10:G:163:ILE:HD13	1.69	0.57
10:G:1:MET:O	10:G:1:MET:SD	2.62	0.57
4:A:1155:ASP:OD1	4:A:1161:THR:HA	2.03	0.57
4:A:341:MET:HE1	4:A:843:LYS:HZ3	1.69	0.57
4:A:471:ASN:OD1	4:A:472:LEU:N	2.36	0.57
5:B:1099:VAL:HG12	5:B:1100:ASP:N	2.19	0.57
5:B:1103:ILE:O	5:B:1122:ARG:NH1	2.38	0.57
3:P:1:A:H2'	3:P:2:A:H8	1.66	0.57
4:A:1057:VAL:HG12	4:A:1058:VAL:N	2.18	0.57
4:A:666:ILE:CD1	4:A:667:GLY:H	2.18	0.57
4:A:965:GLN:O	4:A:968:GLN:HB2	2.04	0.57
4:A:325:ILE:HG21	5:B:1210:MET:HG3	1.84	0.57
7:D:189:ASP:O	7:D:193:THR:HB	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:109:VAL:HG12	9:F:110:ASP:N	2.19	0.57
9:F:99:LEU:HD12	9:F:99:LEU:O	2.05	0.57
4:A:1051:ALA:O	4:A:1055:ARG:HG3	2.04	0.57
4:A:1164:PRO:HG2	4:A:1165:GLU:H	1.69	0.57
4:A:1396:ALA:O	4:A:1398:MET:N	2.38	0.57
4:A:35:ILE:HA	4:A:52:GLY:O	2.04	0.57
4:A:532:ARG:HH22	4:A:745:GLN:HG2	1.69	0.57
4:A:63:ARG:HA	4:A:74:MET:CE	2.34	0.57
4:A:897:TYR:CD2	4:A:936:LEU:HD13	2.39	0.57
5:B:117:ALA:HA	5:B:122:LEU:HD12	1.85	0.57
5:B:899:ILE:HD11	5:B:910:VAL:O	2.03	0.57
7:D:192:LYS:HB3	7:D:192:LYS:HZ3	1.68	0.57
4:A:1116:LEU:HD11	4:A:1118:VAL:HG13	1.86	0.57
4:A:289:ILE:C	4:A:291:GLU:H	2.07	0.57
4:A:61:ILE:O	4:A:63:ARG:N	2.38	0.57
4:A:844:ALA:O	4:A:845:LEU:HD23	2.05	0.57
5:B:102:VAL:CG2	5:B:112:LEU:HD22	2.34	0.57
5:B:283:VAL:O	5:B:286:PHE:N	2.37	0.57
5:B:460:ALA:HB1	5:B:466:TRP:CZ3	2.38	0.57
5:B:825:VAL:CG1	5:B:826:ALA:N	2.68	0.57
11:H:83:GLN:C	11:H:85:GLY:H	2.08	0.57
15:L:43:THR:O	15:L:43:THR:HG22	2.03	0.57
4:A:11:LEU:HB2	5:B:1193:GLN:OE1	2.04	0.57
4:A:1430:LEU:HB2	4:A:1432:GLN:HG3	1.86	0.57
4:A:341:MET:HE1	4:A:843:LYS:NZ	2.19	0.57
5:B:1162:ILE:HD11	5:B:1194:ILE:HD13	1.86	0.57
5:B:472:ALA:CB	5:B:474:SER:HB3	2.32	0.57
5:B:615:MET:C	5:B:616:ILE:HD12	2.24	0.57
4:A:782:ARG:NH2	5:B:699:GLU:O	2.35	0.57
6:C:235:VAL:HG13	13:J:13:VAL:CG2	2.34	0.57
4:A:940:ARG:HG2	4:A:940:ARG:HH11	1.70	0.57
7:D:52:LEU:HD21	7:D:147:TYR:HE2	1.70	0.57
9:F:90:ARG:HD3	9:F:155:LEU:HD11	1.87	0.57
12:I:14:LEU:HA	12:I:28:GLU:O	2.05	0.57
12:I:25:LEU:HB3	12:I:38:ALA:HB2	1.87	0.57
4:A:547:LEU:HD22	14:K:58:PHE:CE1	2.40	0.57
4:A:119:ASN:O	4:A:122:MET:HB3	2.05	0.57
4:A:107:CYS:SG	4:A:171:GLN:HG2	2.44	0.57
4:A:382:PRO:HD3	4:A:428:TYR:CD2	2.39	0.57
5:B:604:ARG:HH22	5:B:614:SER:HA	1.70	0.57
12:I:55:THR:HG21	12:I:109:ILE:HD13	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:J:7:CYS:SG	13:J:49:MET:HE3	2.45	0.57
14:K:12:LEU:HD12	14:K:12:LEU:H	1.69	0.57
4:A:1364:ASN:HD22	4:A:1365:TYR:N	2.02	0.57
4:A:665:GLY:O	4:A:667:GLY:N	2.38	0.57
4:A:907:THR:HG22	4:A:908:LEU:N	2.20	0.57
5:B:224:GLN:O	5:B:238:ALA:HA	2.04	0.57
5:B:361:LEU:HD21	5:B:377:PHE:HD2	1.64	0.57
5:B:637:LEU:HD12	5:B:693:ILE:HD12	1.87	0.57
9:F:109:VAL:HG11	9:F:123:LYS:HG2	1.85	0.57
4:A:698:GLN:HA	12:I:97:MET:O	2.03	0.57
4:A:1400:CYS:SG	4:A:1409:LEU:HG	2.45	0.57
5:B:295:GLY:H	5:B:298:LEU:HD23	1.69	0.57
5:B:589:VAL:HG12	5:B:590:HIS:N	2.18	0.57
5:B:949:VAL:HG12	5:B:950:ASP:H	1.70	0.57
5:B:980:PHE:CD2	5:B:1094:ARG:HA	2.40	0.57
6:C:51:VAL:HG22	6:C:155:LEU:HD22	1.87	0.57
10:G:7:LEU:O	10:G:73:LYS:HD2	2.05	0.57
11:H:99:GLY:N	11:H:118:PHE:CD2	2.72	0.57
11:H:116:TYR:HB2	11:H:123:MET:HB3	1.86	0.57
14:K:61:TYR:C	14:K:61:TYR:CD2	2.78	0.57
4:A:549:MET:SD	4:A:577:ILE:HD11	2.45	0.56
5:B:1034:VAL:CG1	5:B:1035:ALA:N	2.67	0.56
5:B:244:LEU:HD21	5:B:366:GLN:NE2	2.20	0.56
5:B:465:ASN:H	5:B:465:ASN:HD22	1.52	0.56
6:C:60:ASP:OD2	15:L:60:ARG:NH2	2.38	0.56
8:E:180:ARG:HH21	8:E:192:ARG:CB	2.14	0.56
4:A:1283:VAL:HG12	4:A:1284:MET:N	2.20	0.56
4:A:1349:TYR:CE1	4:A:1368:MET:HE3	2.40	0.56
4:A:310:GLY:O	4:A:312:PRO:HD2	2.05	0.56
6:C:5:GLY:O	6:C:7:GLN:HG3	2.05	0.56
8:E:93:MET:SD	8:E:97:VAL:HG23	2.45	0.56
4:A:1362:TYR:CD1	4:A:1363:VAL:N	2.73	0.56
4:A:446:ARG:HD3	4:A:480:ALA:HB2	1.87	0.56
4:A:998:LEU:HD12	4:A:998:LEU:H	1.69	0.56
5:B:114:PRO:O	5:B:116:GLU:N	2.38	0.56
5:B:952:VAL:HG12	5:B:953:LEU:N	2.21	0.56
6:C:252:GLN:HG3	14:K:95:ILE:HG23	1.87	0.56
4:A:774:ARG:O	4:A:775:ILE:C	2.43	0.56
5:B:359:GLU:O	5:B:362:PRO:HD3	2.05	0.56
10:G:145:VAL:HG12	10:G:146:LYS:N	2.20	0.56
14:K:82:ASP:OD1	14:K:84:LYS:N	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1029:ARG:HG3	4:A:1029:ARG:HH11	1.71	0.56
4:A:265:LYS:CE	4:A:322:VAL:HG13	2.35	0.56
4:A:337:ARG:CZ	4:A:839:ARG:HH12	2.19	0.56
4:A:857:ARG:HD3	4:A:861:GLY:O	2.05	0.56
4:A:899:VAL:HB	4:A:929:LEU:HD12	1.87	0.56
4:A:1409:LEU:HD13	5:B:1207:LEU:CD2	2.35	0.56
5:B:376:PHE:CE2	5:B:569:TYR:HD2	2.23	0.56
5:B:467:GLY:CA	5:B:475:SER:HB3	2.35	0.56
10:G:111:THR:HB	10:G:114:LEU:HB2	1.88	0.56
10:G:125:SER:OG	10:G:128:PRO:HA	2.05	0.56
11:H:98:TYR:C	11:H:118:PHE:HD2	2.08	0.56
14:K:21:ILE:HG23	14:K:31:VAL:CG1	2.36	0.56
4:A:852:TYR:CE2	4:A:1060:PRO:HB2	2.40	0.56
4:A:231:PRO:HA	4:A:234:MET:HE2	1.87	0.56
4:A:492:PRO:O	4:A:493:GLN:NE2	2.38	0.56
5:B:1099:VAL:C	5:B:1101:ASP:H	2.07	0.56
13:J:14:VAL:HG12	13:J:50:ILE:HD11	1.87	0.56
4:A:244:PRO:CB	4:A:245:PRO:HD3	2.35	0.56
4:A:265:LYS:HD2	4:A:265:LYS:N	2.20	0.56
4:A:268:ASP:HB3	4:A:299:HIS:CE1	2.40	0.56
4:A:666:ILE:N	4:A:666:ILE:HD12	2.20	0.56
4:A:98:LYS:O	4:A:99:ILE:C	2.44	0.56
5:B:53:GLN:HG2	5:B:547:VAL:CG2	2.35	0.56
6:C:31:ASN:O	6:C:32:SER:C	2.42	0.56
8:E:78:LEU:C	8:E:78:LEU:HD23	2.25	0.56
10:G:106:MET:CG	10:G:107:LYS:N	2.68	0.56
14:K:90:ALA:O	14:K:94:ILE:HG13	2.04	0.56
5:B:351:TYR:O	5:B:355:ILE:HG13	2.05	0.56
5:B:54:PHE:HA	5:B:58:THR:HB	1.87	0.56
6:C:146:LYS:C	6:C:147:LEU:HD23	2.26	0.56
7:D:68:ARG:C	7:D:70:PHE:H	2.09	0.56
13:J:3:VAL:HA	13:J:53:HIS:CE1	2.40	0.56
13:J:53:HIS:CD2	13:J:54:VAL:N	2.74	0.56
4:A:321:PRO:O	4:A:322:VAL:CB	2.54	0.56
4:A:939:ASP:O	4:A:943:LEU:HG	2.06	0.56
4:A:958:VAL:O	4:A:958:VAL:HG12	2.05	0.56
4:A:1035:TYR:O	4:A:1037:LEU:N	2.38	0.56
4:A:35:ILE:HG22	4:A:84:ILE:HD12	1.88	0.56
4:A:353:ILE:HD13	4:A:487:MET:HE2	1.88	0.56
5:B:39:ARG:HG2	5:B:39:ARG:HH11	1.71	0.56
5:B:710:LEU:O	5:B:711:GLU:HG2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:309:GLN:HG3	12:I:52:ILE:HD11	1.88	0.56
4:A:863:VAL:HG11	4:A:866:PHE:CD2	2.41	0.56
5:B:190:TYR:CE2	13:J:62:ARG:HB3	2.40	0.56
5:B:29:ASP:HB3	5:B:658:ILE:CD1	2.36	0.56
5:B:911:ILE:HD11	5:B:941:LEU:HD13	1.87	0.56
6:C:239:PRO:HB2	6:C:241:ASP:OD1	2.06	0.56
8:E:23:VAL:O	8:E:28:TYR:HB2	2.06	0.56
12:I:68:LEU:HB3	12:I:84:VAL:HG23	1.87	0.56
3:P:5:C:H2'	3:P:6:C:C6	2.40	0.56
4:A:350:ARG:HB2	4:A:488:ASN:OD1	2.06	0.55
4:A:845:LEU:HB3	4:A:848:ILE:HD12	1.87	0.55
5:B:696:GLU:O	5:B:699:GLU:HB2	2.06	0.55
7:D:156:ASP:C	7:D:158:GLU:N	2.60	0.55
8:E:35:VAL:C	8:E:37:LEU:H	2.10	0.55
9:F:75:PRO:O	9:F:77:ASP:O	2.23	0.55
11:H:40:LEU:CD1	11:H:123:MET:HB2	2.35	0.55
1:T:18:DC:O4'	4:A:835:GLY:HA3	2.05	0.55
4:A:1214:GLU:O	4:A:1218:GLN:HG2	2.06	0.55
4:A:47:ARG:HH12	4:A:254:GLU:CG	2.19	0.55
4:A:548:ASN:HA	14:K:60:ALA:HB1	1.88	0.55
5:B:258:LEU:O	5:B:258:LEU:HG	2.05	0.55
5:B:527:THR:OG1	5:B:528:PRO:HD2	2.07	0.55
5:B:376:PHE:HB3	5:B:586:TRP:CZ3	2.42	0.55
5:B:833:TYR:N	5:B:833:TYR:CD1	2.73	0.55
8:E:94:LYS:CE	8:E:98:ILE:HD11	2.31	0.55
10:G:88:ASP:HB3	10:G:144:ARG:HA	1.88	0.55
10:G:17:PHE:C	10:G:19:GLY:H	2.10	0.55
10:G:51:TYR:O	10:G:54:ILE:HG13	2.05	0.55
4:A:356:ASP:OD2	14:K:65:HIS:HE1	1.89	0.55
4:A:185:TRP:HZ3	4:A:200:ARG:HG2	1.72	0.55
4:A:299:HIS:C	4:A:301:ALA:H	2.10	0.55
4:A:306:ASN:HD21	4:A:322:VAL:HB	1.71	0.55
4:A:416:ARG:C	4:A:417:TYR:HD2	2.10	0.55
5:B:604:ARG:NH2	5:B:614:SER:HA	2.21	0.55
5:B:893:LEU:HD11	5:B:910:VAL:HG11	1.88	0.55
5:B:984:HIS:CG	5:B:1025:HIS:HB2	2.42	0.55
12:I:8:ARG:HG3	12:I:34:TYR:CE1	2.41	0.55
1:T:15:DT:O2	4:A:1386:ARG:CZ	2.54	0.55
4:A:166:GLY:O	4:A:167:CYS:SG	2.64	0.55
4:A:475:THR:CG2	4:A:476:SER:H	2.20	0.55
4:A:504:LEU:HD12	4:A:504:LEU:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:467:GLY:N	5:B:475:SER:CB	2.68	0.55
5:B:483:LEU:HD11	5:B:491:THR:CG2	2.32	0.55
5:B:507:LYS:H	5:B:512:ARG:NH2	2.03	0.55
8:E:29:PHE:C	8:E:30:ILE:HG13	2.26	0.55
9:F:118:LEU:O	9:F:118:LEU:HD12	2.05	0.55
9:F:77:ASP:C	9:F:79:ARG:H	2.09	0.55
4:A:1127:ASP:HB3	4:A:1130:GLN:CB	2.36	0.55
4:A:265:LYS:HD2	4:A:265:LYS:H	1.72	0.55
4:A:268:ASP:HB3	4:A:299:HIS:ND1	2.21	0.55
4:A:586:ILE:HG22	4:A:587:HIS:N	2.22	0.55
4:A:714:PHE:O	4:A:718:VAL:HG23	2.06	0.55
5:B:199:MET:N	5:B:199:MET:SD	2.80	0.55
5:B:579:ARG:N	5:B:589:VAL:HG13	2.22	0.55
6:C:36:VAL:HG21	6:C:251:LEU:HD22	1.88	0.55
8:E:22:MET:HE1	8:E:26:ARG:HH21	1.72	0.55
8:E:3:GLN:HG3	8:E:4:GLU:N	2.21	0.55
10:G:1:MET:O	10:G:3:PHE:CE1	2.60	0.55
4:A:458:HIS:CE1	4:A:507:VAL:HG21	2.41	0.55
4:A:730:GLY:O	4:A:732:LEU:N	2.40	0.55
4:A:90:VAL:HG12	4:A:91:PHE:N	2.22	0.55
5:B:205:ILE:CD1	5:B:205:ILE:N	2.68	0.55
5:B:38:PHE:HD1	5:B:811:TYR:CD2	2.24	0.55
5:B:473:MET:C	5:B:475:SER:H	2.10	0.55
5:B:476:ARG:HH12	5:B:501:PRO:HB3	1.70	0.55
5:B:850:LEU:HD12	5:B:851:PHE:N	2.21	0.55
5:B:97:VAL:HG12	5:B:178:ASN:ND2	2.22	0.55
13:J:3:VAL:HG21	13:J:18:TRP:CB	2.31	0.55
4:A:1279:ILE:HD11	4:A:1316:VAL:HG21	1.89	0.55
4:A:1342:GLU:CG	8:E:198:ILE:HD13	2.37	0.55
4:A:269:ILE:HG12	4:A:299:HIS:HB3	1.88	0.55
4:A:798:GLY:HA2	4:A:815:PHE:HD1	1.68	0.55
4:A:814:PHE:O	4:A:817:ALA:HB3	2.07	0.55
4:A:867:ILE:HD12	8:E:208:TYR:CE1	2.42	0.55
5:B:1034:VAL:C	5:B:1036:ALA:H	2.10	0.55
5:B:1159:ARG:HD3	5:B:1193:GLN:CG	2.37	0.55
5:B:324:ILE:HD13	5:B:330:ALA:HA	1.88	0.55
4:A:567:LYS:HD3	11:H:95:TYR:CG	2.42	0.55
5:B:1082:MET:O	6:C:189:THR:HG23	2.07	0.55
5:B:114:PRO:HG2	5:B:115:GLN:H	1.72	0.55
5:B:654:ARG:H	5:B:657:HIS:CD2	2.23	0.55
5:B:872:GLU:HA	5:B:915:THR:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:76:ASP:O	6:C:79:GLN:HG2	2.06	0.55
12:I:50:THR:CG2	12:I:52:ILE:HG12	2.37	0.55
4:A:34:LYS:HB3	4:A:36:ARG:HE	1.72	0.55
5:B:1068:GLY:O	5:B:1069:PHE:O	2.25	0.55
5:B:1074:ASN:HB2	5:B:1081:LEU:HD21	1.89	0.55
5:B:603:LEU:HB3	5:B:609:ILE:CD1	2.37	0.55
4:A:567:LYS:HE3	11:H:46:LEU:HD12	1.89	0.55
4:A:896:ARG:NH2	4:A:1030:ARG:NH2	2.55	0.55
4:A:963:ILE:HD13	4:A:1049:ILE:HG12	1.89	0.55
5:B:526:GLU:OE2	5:B:752:ALA:HB2	2.07	0.55
6:C:226:ASP:O	6:C:227:THR:HB	2.07	0.55
11:H:89:LEU:HB3	11:H:91:ASP:OD1	2.06	0.55
15:L:36:SER:O	15:L:37:LYS:C	2.45	0.55
4:A:1010:ALA:HA	4:A:1013:ASP:OD2	2.06	0.54
4:A:1242:VAL:O	4:A:1243:VAL:HB	2.07	0.54
4:A:816:HIS:HE2	5:B:764:SER:H	1.55	0.54
7:D:51:ASN:O	7:D:52:LEU:O	2.25	0.54
12:I:103:CYS:CB	12:I:106:CYS:HG	2.20	0.54
2:N:1:DA:H1'	2:N:2:DA:O5'	2.07	0.54
1:T:15:DT:H1'	4:A:1386:ARG:HH11	1.64	0.54
4:A:1074:GLU:HB3	4:A:1075:PRO:HD3	1.88	0.54
4:A:1227:ILE:HG22	4:A:1228:TRP:H	1.71	0.54
5:B:95:ILE:CG1	5:B:130:VAL:HG22	2.37	0.54
5:B:129:PHE:HA	5:B:165:VAL:O	2.07	0.54
5:B:557:PHE:C	5:B:557:PHE:HD2	2.09	0.54
5:B:745:PRO:C	5:B:747:MET:H	2.10	0.54
5:B:980:PHE:HE1	5:B:990:ILE:HD11	1.73	0.54
9:F:130:ILE:O	9:F:148:VAL:HG21	2.08	0.54
4:A:817:ALA:O	4:A:819:GLY:N	2.41	0.54
4:A:858:ASN:ND2	4:A:858:ASN:C	2.61	0.54
5:B:39:ARG:HG2	5:B:39:ARG:NH1	2.22	0.54
5:B:843:GLN:O	5:B:846:ILE:HB	2.07	0.54
5:B:865:LYS:NZ	5:B:869:SER:HA	2.21	0.54
5:B:880:THR:HB	5:B:934:LYS:HD2	1.88	0.54
5:B:882:THR:HB	5:B:934:LYS:O	2.07	0.54
6:C:98:VAL:O	6:C:99:LEU:HD23	2.08	0.54
8:E:46:TYR:CE2	8:E:58:MET:HA	2.42	0.54
10:G:27:LYS:O	10:G:30:LEU:HB3	2.08	0.54
12:I:13:MET:O	12:I:14:LEU:HD23	2.07	0.54
4:A:114:LEU:O	4:A:115:LEU:HG	2.08	0.54
4:A:1322:ILE:O	4:A:1324:PRO:HD3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:763:GLN:HG2	5:B:765:PRO:CD	2.34	0.54
6:C:258:ILE:N	6:C:258:ILE:HD12	2.23	0.54
10:G:80:LYS:HG2	10:G:80:LYS:O	2.07	0.54
11:H:100:THR:HG22	11:H:101:ALA:N	2.21	0.54
5:B:1107:ALA:O	5:B:1108:ARG:O	2.26	0.54
5:B:235:SER:OG	5:B:236:HIS:CD2	2.60	0.54
5:B:315:LYS:N	5:B:316:PRO:HD2	2.23	0.54
6:C:263:THR:C	6:C:265:MET:N	2.61	0.54
7:D:202:ILE:CG2	7:D:207:LEU:HB2	2.37	0.54
7:D:19:GLU:O	7:D:21:GLU:N	2.40	0.54
9:F:111:LEU:C	9:F:113:GLY:N	2.56	0.54
11:H:95:TYR:HB3	11:H:144:ILE:HB	1.89	0.54
14:K:50:LEU:HD11	14:K:75:ILE:CD1	2.37	0.54
4:A:1279:ILE:HD11	4:A:1316:VAL:CG2	2.37	0.54
4:A:1336:MET:HE3	4:A:1381:LEU:HG	1.90	0.54
4:A:767:GLN:NE2	4:A:774:ARG:HB3	2.23	0.54
5:B:582:VAL:HG23	5:B:626:ILE:HB	1.89	0.54
6:C:235:VAL:HG13	13:J:13:VAL:HG23	1.89	0.54
13:J:44:TYR:HA	13:J:47:ARG:CB	2.37	0.54
4:A:1032:LEU:O	4:A:1036:ARG:HD3	2.07	0.54
4:A:1118:VAL:O	4:A:1305:VAL:HG13	2.08	0.54
4:A:1115:SER:C	4:A:1308:THR:HG22	2.28	0.54
4:A:1373:ASP:HA	4:A:1376:THR:HG22	1.89	0.54
4:A:1435:PRO:HA	4:A:1439:GLY:O	2.08	0.54
4:A:262:LEU:C	4:A:264:PHE:H	2.11	0.54
4:A:545:GLN:O	4:A:546:VAL:C	2.46	0.54
4:A:666:ILE:H	5:B:1026:LEU:HD22	1.72	0.54
4:A:71:GLN:C	4:A:73:GLY:H	2.11	0.54
6:C:18:VAL:CG2	6:C:240:VAL:HB	2.38	0.54
7:D:56:ARG:HD2	7:D:149:THR:OG1	2.07	0.54
8:E:197:LYS:HE2	8:E:199:ILE:HD11	1.89	0.54
10:G:1:MET:HG3	10:G:85:GLU:OE2	2.08	0.54
2:N:5:DA:H2"	2:N:6:DC:OP2	2.08	0.54
4:A:108:MET:N	4:A:108:MET:SD	2.78	0.54
4:A:306:ASN:ND2	4:A:322:VAL:HB	2.23	0.54
4:A:877:HIS:C	4:A:878:ILE:HG13	2.28	0.54
8:E:78:LEU:HD21	8:E:80:VAL:HG23	1.89	0.54
10:G:62:LEU:HB3	10:G:63:PRO:CD	2.38	0.54
11:H:139:ASN:O	11:H:140:ALA:HB2	2.08	0.54
12:I:103:CYS:HB3	12:I:106:CYS:SG	2.48	0.54
14:K:12:LEU:N	14:K:12:LEU:HD12	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:134:ARG:O	4:A:138:ILE:HG13	2.08	0.54
5:B:806:THR:HA	5:B:1045:SER:OG	2.07	0.54
5:B:1110:PRO:O	5:B:1119:VAL:HG13	2.08	0.54
5:B:1159:ARG:HB3	5:B:1159:ARG:HH11	1.72	0.54
5:B:803:LEU:CD1	5:B:1032:SER:HB3	2.38	0.54
6:C:8:VAL:HG12	6:C:9:LYS:N	2.23	0.54
8:E:55:ARG:HD2	8:E:83:CYS:O	2.08	0.54
14:K:47:ARG:HD2	14:K:47:ARG:O	2.08	0.54
4:A:1220:PHE:O	4:A:1221:LYS:HB2	2.08	0.54
4:A:464:PRO:HG2	4:A:465:TYR:HD1	1.72	0.54
4:A:534:LEU:HG	4:A:534:LEU:O	2.07	0.54
5:B:1050:ILE:HG22	5:B:1051:THR:N	2.23	0.54
5:B:234:ILE:N	5:B:234:ILE:HD12	2.23	0.54
5:B:516:ASN:ND2	5:B:516:ASN:N	2.52	0.54
5:B:833:TYR:N	5:B:833:TYR:HD1	2.06	0.54
8:E:157:SER:C	8:E:159:ASP:N	2.61	0.54
8:E:207:ARG:HH11	8:E:207:ARG:HB3	1.73	0.54
4:A:1004:ASN:OD1	4:A:1005:GLU:N	2.41	0.53
4:A:1336:MET:CE	4:A:1381:LEU:HG	2.37	0.53
4:A:1441:PHE:CZ	9:F:89:GLU:HA	2.43	0.53
4:A:47:ARG:O	4:A:48:ALA:HB2	2.08	0.53
4:A:503:GLN:C	4:A:504:LEU:HD12	2.28	0.53
4:A:567:LYS:HB3	11:H:95:TYR:CA	2.37	0.53
4:A:901:LEU:HD22	4:A:919:ILE:HG22	1.90	0.53
5:B:57:TYR:CD1	5:B:57:TYR:N	2.73	0.53
5:B:777:ALA:HA	5:B:1095:LEU:HA	1.89	0.53
9:F:90:ARG:HD3	9:F:155:LEU:HD12	1.88	0.53
11:H:41:ASP:OD2	11:H:122:LEU:N	2.40	0.53
12:I:61:ASP:C	12:I:63:GLY:H	2.11	0.53
4:A:567:LYS:CB	4:A:568:PRO:CD	2.85	0.53
4:A:528:LEU:HD23	4:A:751:SER:HA	1.90	0.53
5:B:746:SER:HB2	5:B:1046:PRO:HG2	1.89	0.53
5:B:1115:THR:CG2	5:B:1117:GLN:HG3	2.37	0.53
5:B:125:SER:HA	5:B:171:PRO:HA	1.90	0.53
4:A:1377:THR:O	4:A:1379:GLY:N	2.41	0.53
4:A:366:VAL:CG2	4:A:460:VAL:HG22	2.38	0.53
4:A:546:VAL:O	4:A:550:LEU:HG	2.08	0.53
4:A:847:ASP:OD1	4:A:848:ILE:HG13	2.08	0.53
5:B:195:CYS:SG	5:B:197:PHE:HB2	2.48	0.53
5:B:35:SER:O	5:B:39:ARG:HG3	2.06	0.53
7:D:192:LYS:HZ3	7:D:199:ASN:HA	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:9:ILE:HD11	8:E:53:PRO:HD3	1.90	0.53
10:G:56:ILE:O	10:G:57:GLN:HB2	2.06	0.53
4:A:1149:ALA:HB2	12:I:47:GLU:HA	1.90	0.53
4:A:1299:VAL:HG12	4:A:1300:LYS:H	1.73	0.53
4:A:382:PRO:HD3	4:A:428:TYR:CE2	2.44	0.53
4:A:618:GLU:O	4:A:620:LYS:N	2.41	0.53
4:A:746:MET:CE	5:B:1018:PRO:HG2	2.38	0.53
5:B:1107:ALA:O	5:B:1108:ARG:HG2	2.09	0.53
9:F:101:ILE:HD11	9:F:124:GLU:OE1	2.08	0.53
11:H:4:THR:CA	11:H:60:ALA:HB2	2.33	0.53
4:A:1164:PRO:O	4:A:1166:ASP:N	2.42	0.53
4:A:567:LYS:HB2	4:A:568:PRO:CD	2.39	0.53
5:B:847:ASP:C	5:B:849:GLY:N	2.62	0.53
6:C:6:PRO:HB3	6:C:25:VAL:HG12	1.90	0.53
6:C:73:GLN:NE2	6:C:74:SER:H	2.06	0.53
7:D:63:LEU:HD13	7:D:133:THR:OG1	2.08	0.53
1:T:24:DG:OP1	5:B:792:MET:CE	2.56	0.53
4:A:1372:VAL:O	4:A:1376:THR:HG22	2.08	0.53
4:A:207:ILE:O	4:A:208:LEU:C	2.47	0.53
4:A:244:PRO:O	4:A:247:ARG:N	2.41	0.53
4:A:356:ASP:O	4:A:358:ASN:N	2.42	0.53
4:A:567:LYS:HB3	11:H:96:VAL:N	2.22	0.53
4:A:722:LEU:HD22	4:A:799:PHE:CD1	2.44	0.53
5:B:466:TRP:C	5:B:468:GLU:N	2.37	0.53
6:C:181:ASP:OD2	6:C:185:LYS:N	2.42	0.53
5:B:798:TYR:CE2	6:C:62:PHE:CE2	2.95	0.53
9:F:73:ALA:HA	9:F:143:PHE:CE1	2.44	0.53
4:A:548:ASN:OD1	14:K:60:ALA:HB1	2.09	0.53
14:K:7:PHE:HA	14:K:10:PHE:CE2	2.44	0.53
4:A:1365:TYR:O	4:A:1367:HIS:N	2.41	0.53
4:A:311:GLN:O	4:A:312:PRO:C	2.46	0.53
4:A:427:GLN:HG3	4:A:430:TRP:CE2	2.44	0.53
4:A:567:LYS:HZ1	11:H:46:LEU:HB2	1.69	0.53
4:A:694:THR:O	4:A:698:GLN:HG3	2.09	0.53
5:B:181:LEU:HD22	5:B:189:LEU:HD22	1.91	0.53
5:B:213:ILE:HD12	5:B:497:ARG:HB3	1.90	0.53
5:B:971:THR:OG1	6:C:61:GLU:HG3	2.08	0.53
4:A:1094:VAL:HG12	4:A:1095:THR:N	2.24	0.53
5:B:399:ASP:CG	5:B:510:LYS:O	2.47	0.53
5:B:640:VAL:O	5:B:641:GLU:C	2.46	0.53
6:C:18:VAL:HG23	6:C:240:VAL:HB	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:3:GLU:HG2	6:C:4:GLU:N	2.24	0.53
9:F:79:ARG:HG3	9:F:144:GLU:OE1	2.09	0.53
9:F:96:THR:O	9:F:100:GLN:HG3	2.08	0.53
13:J:43:ARG:HG3	13:J:45:CYS:SG	2.48	0.53
5:B:1039:GLY:HA2	13:J:51:LEU:HD21	1.89	0.53
15:L:52:GLY:O	15:L:53:HIS:C	2.47	0.53
3:P:5:C:H2'	3:P:6:C:H6	1.74	0.53
4:A:1007:ILE:C	4:A:1009:ASN:N	2.62	0.53
4:A:1120:LEU:HD13	4:A:1304:TRP:O	2.09	0.53
4:A:852:TYR:CD2	4:A:1060:PRO:HB2	2.44	0.53
4:A:92:HIS:HB3	4:A:95:PHE:HB2	1.91	0.53
4:A:996:ASN:O	4:A:998:LEU:HD12	2.09	0.53
5:B:1002:THR:HG21	5:B:1006:ILE:HD12	1.89	0.53
5:B:281:PRO:O	5:B:283:VAL:N	2.42	0.53
5:B:615:MET:CB	5:B:626:ILE:HG12	2.38	0.53
8:E:116:ILE:HG22	8:E:117:THR:N	2.24	0.53
13:J:1:MET:HE2	13:J:60:PHE:CE2	2.44	0.53
1:T:21:DC:H2''	1:T:22:DT:H5'	1.91	0.53
4:A:1007:ILE:O	4:A:1009:ASN:N	2.41	0.53
4:A:1208:THR:HG22	4:A:1210:GLY:H	1.74	0.53
4:A:746:MET:HE3	5:B:1018:PRO:HG2	1.91	0.53
3:P:9:G:C5'	5:B:776:GLN:NE2	2.63	0.53
5:B:948:ILE:HG22	5:B:949:VAL:O	2.08	0.53
6:C:166:GLU:O	6:C:167:HIS:HB2	2.08	0.53
4:A:417:TYR:CD2	4:A:417:TYR:N	2.76	0.52
5:B:240:ILE:HG23	5:B:240:ILE:O	2.09	0.52
5:B:223:VAL:HG11	5:B:381:MET:HG2	1.90	0.52
5:B:496:ARG:HB3	5:B:496:ARG:HH11	1.73	0.52
6:C:27:LEU:O	6:C:28:ALA:C	2.48	0.52
7:D:191:ALA:C	7:D:193:THR:H	2.12	0.52
8:E:192:ARG:NH1	8:E:192:ARG:HG3	2.22	0.52
9:F:109:VAL:HG13	9:F:127:GLU:OE1	2.09	0.52
13:J:3:VAL:HA	13:J:53:HIS:ND1	2.24	0.52
4:A:1305:VAL:HG12	4:A:1306:LEU:N	2.24	0.52
4:A:263:THR:HG22	4:A:263:THR:O	2.07	0.52
4:A:43:GLU:O	4:A:44:THR:HB	2.09	0.52
4:A:577:ILE:HA	4:A:580:VAL:HG23	1.91	0.52
4:A:578:LEU:HD23	4:A:612:ILE:CD1	2.39	0.52
4:A:673:GLY:O	4:A:676:MET:HB2	2.09	0.52
4:A:71:GLN:O	4:A:73:GLY:N	2.39	0.52
5:B:1065:GLN:NE2	5:B:1067:ARG:N	2.52	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:818:MET:N	5:B:514:LEU:HD23	2.24	0.52
5:B:526:GLU:HG2	5:B:538:ASN:HD22	1.74	0.52
5:B:785:TYR:CD1	5:B:785:TYR:C	2.82	0.52
8:E:161:LYS:HD2	8:E:195:VAL:HG23	1.91	0.52
14:K:65:HIS:HD2	14:K:67:PHE:N	1.99	0.52
1:T:17:DA:H2	2:N:1:DA:N1	2.08	0.52
4:A:1116:LEU:HB2	4:A:1329:THR:OG1	2.09	0.52
4:A:1323:ASP:C	4:A:1325:THR:H	2.12	0.52
4:A:399:HIS:HB3	4:A:400:PRO:CD	2.30	0.52
4:A:42:ASP:HB3	4:A:45:GLN:H	1.73	0.52
4:A:463:ILE:HB	4:A:464:PRO:HD2	1.91	0.52
4:A:598:LEU:O	4:A:599:SER:C	2.47	0.52
4:A:590:ARG:HB2	4:A:605:MET:HB3	1.91	0.52
5:B:555:ILE:HD11	5:B:587:HIS:CE1	2.45	0.52
5:B:616:ILE:HG13	5:B:697:GLU:HA	1.92	0.52
5:B:879:ARG:HH11	5:B:883:LEU:CD2	2.19	0.52
7:D:130:LEU:C	7:D:132:GLN:N	2.54	0.52
8:E:14:ARG:HH21	8:E:141:VAL:HG12	1.74	0.52
11:H:113:ALA:HB1	11:H:125:LEU:O	2.10	0.52
4:A:1438:THR:HB	5:B:1144:ALA:CB	2.37	0.52
4:A:868:TYR:CE1	4:A:1064:VAL:CG1	2.91	0.52
4:A:90:VAL:CG1	4:A:297:GLN:HA	2.39	0.52
6:C:39:ALA:CA	6:C:164:ALA:HB3	2.29	0.52
7:D:53:SER:HB3	7:D:152:SER:CA	2.39	0.52
8:E:90:VAL:HG22	8:E:90:VAL:O	2.09	0.52
10:G:9:LEU:HG	10:G:10:ASN:N	2.23	0.52
11:H:31:THR:O	11:H:31:THR:HG22	2.10	0.52
13:J:27:GLU:C	13:J:29:GLU:H	2.13	0.52
14:K:47:ARG:HD3	14:K:59:ALA:O	2.09	0.52
4:A:1342:GLU:OE2	8:E:212:ARG:NH1	2.42	0.52
4:A:381:THR:HG23	4:A:383:TYR:H	1.75	0.52
4:A:55:ASP:N	4:A:56:PRO:HD3	2.25	0.52
4:A:608:ILE:HB	4:A:613:ILE:HD11	1.91	0.52
4:A:18:GLN:CB	5:B:1215:ARG:HB2	2.39	0.52
5:B:877:PRO:C	5:B:878:GLN:HG3	2.30	0.52
11:H:59:ILE:O	11:H:60:ALA:HB3	2.09	0.52
15:L:27:LEU:HD13	15:L:37:LYS:HE2	1.91	0.52
3:P:7:A:H2'	3:P:8:G:O4'	2.08	0.52
4:A:418:SER:O	4:A:420:ARG:N	2.42	0.52
4:A:49:LYS:NZ	4:A:61:ILE:HG13	2.24	0.52
5:B:1180:PHE:HB3	5:B:1191:ILE:CD1	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:315:LEU:HD13	5:B:471:LYS:HB3	1.91	0.52
5:B:862:GLN:HG2	5:B:963:PHE:CD1	2.44	0.52
6:C:147:LEU:HD12	6:C:151:GLN:O	2.09	0.52
10:G:79:PHE:CZ	10:G:106:MET:HE2	2.44	0.52
14:K:31:VAL:CG1	14:K:32:VAL:N	2.72	0.52
14:K:85:ASP:O	14:K:88:LYS:HB2	2.10	0.52
4:A:1141:THR:OG1	4:A:1205:LYS:HD3	2.10	0.52
4:A:1394:THR:O	4:A:1395:GLY:O	2.28	0.52
5:B:300:HIS:CE1	5:B:376:PHE:CE1	2.97	0.52
5:B:282:ILE:CD1	5:B:382:ILE:HD13	2.35	0.52
5:B:810:GLU:HB2	5:B:815:ARG:HH22	1.75	0.52
4:A:483:ASP:O	5:B:979:LYS:HE3	2.10	0.52
7:D:167:LEU:O	7:D:170:THR:OG1	2.24	0.52
7:D:29:LEU:HD22	10:G:82:PHE:CD2	2.45	0.52
7:D:33:PHE:CZ	10:G:80:LYS:CE	2.93	0.52
11:H:127:GLY:O	11:H:128:ASN:HB2	2.10	0.52
13:J:45:CYS:O	13:J:48:ARG:HG3	2.09	0.52
14:K:69:ALA:O	14:K:70:ARG:HB3	2.10	0.52
4:A:364:VAL:O	4:A:364:VAL:HG13	2.09	0.52
5:B:35:SER:HA	5:B:811:TYR:CE2	2.35	0.52
9:F:81:THR:HG21	9:F:136:ARG:CD	2.32	0.52
10:G:26:LEU:O	10:G:27:LYS:C	2.47	0.52
11:H:27:GLU:HA	11:H:38:LEU:O	2.10	0.52
12:I:77:LYS:O	12:I:79:HIS:N	2.43	0.52
4:A:18:GLN:O	5:B:1215:ARG:HG2	2.09	0.52
4:A:93:VAL:HG22	4:A:301:ALA:HA	1.92	0.52
4:A:388:LEU:HD22	4:A:432:VAL:CG2	2.40	0.52
4:A:353:ILE:HG21	4:A:487:MET:HG3	1.92	0.52
4:A:60:SER:C	4:A:61:ILE:HG13	2.30	0.52
5:B:370:PHE:HE2	5:B:373:ARG:NH1	2.08	0.52
5:B:377:PHE:C	5:B:379:GLY:N	2.62	0.52
6:C:191:TYR:HD2	6:C:201:TRP:CD1	2.27	0.52
4:A:1325:THR:O	8:E:148:GLU:HB2	2.10	0.52
8:E:92:THR:O	8:E:95:THR:HB	2.10	0.52
10:G:17:PHE:CD2	10:G:17:PHE:N	2.77	0.52
10:G:1:MET:SD	10:G:79:PHE:CE1	3.03	0.52
1:T:20:DC:H2''	1:T:21:DC:C5'	2.38	0.52
4:A:1030:ARG:HG3	4:A:1034:GLU:OE2	2.10	0.52
4:A:265:LYS:HE2	4:A:322:VAL:HG13	1.92	0.52
4:A:399:HIS:CG	4:A:400:PRO:N	2.77	0.52
4:A:632:VAL:O	4:A:633:VAL:C	2.47	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:901:LEU:HD22	4:A:919:ILE:HG21	1.92	0.52
5:B:57:TYR:N	5:B:57:TYR:HD1	2.08	0.52
5:B:999:MET:HE2	5:B:1000:PRO:CD	2.39	0.52
12:I:50:THR:HG22	12:I:51:ASN:N	2.25	0.52
4:A:1161:THR:OG1	4:A:1239:ARG:NH2	2.43	0.51
4:A:1289:ARG:HD2	4:A:1303:GLU:OE2	2.10	0.51
4:A:1364:ASN:O	4:A:1365:TYR:C	2.49	0.51
4:A:414:ASP:OD1	4:A:416:ARG:HG3	2.09	0.51
5:B:1174:LYS:O	5:B:1176:ASN:N	2.43	0.51
5:B:521:LEU:HD13	5:B:633:VAL:HB	1.92	0.51
6:C:215:GLU:O	6:C:217:ASP:N	2.43	0.51
12:I:100:PHE:N	12:I:100:PHE:CD1	2.79	0.51
13:J:44:TYR:N	13:J:44:TYR:CD2	2.78	0.51
5:B:1132:GLU:O	5:B:1135:ARG:HB3	2.09	0.51
5:B:460:ALA:HB1	5:B:466:TRP:CE3	2.45	0.51
5:B:492:LEU:O	5:B:495:LEU:N	2.39	0.51
6:C:168:ALA:C	6:C:170:TRP:N	2.64	0.51
10:G:26:LEU:O	10:G:29:LYS:N	2.42	0.51
4:A:1334:ASP:O	4:A:1336:MET:N	2.43	0.51
4:A:241:VAL:HG13	4:A:266:LEU:HD13	1.91	0.51
4:A:50:ILE:C	4:A:52:GLY:N	2.64	0.51
4:A:628:GLY:O	4:A:632:VAL:HG23	2.11	0.51
5:B:1102:LYS:O	5:B:1103:ILE:C	2.47	0.51
5:B:999:MET:HB3	5:B:1007:VAL:HG21	1.91	0.51
6:C:263:THR:O	6:C:265:MET:N	2.43	0.51
8:E:168:TYR:HB2	8:E:170:LEU:HG	1.91	0.51
15:L:40:LEU:HD22	15:L:44:ASP:CG	2.30	0.51
4:A:75:ASN:O	4:A:76:GLU:HB2	2.11	0.51
4:A:79:GLY:HA3	4:A:243:PRO:HG2	1.92	0.51
5:B:493:SER:HA	5:B:751:VAL:HG21	1.91	0.51
5:B:1084:GLN:OE1	6:C:189:THR:CG2	2.59	0.51
6:C:76:ASP:O	6:C:77:ILE:C	2.48	0.51
4:A:504:LEU:HD11	9:F:91:ALA:CB	2.40	0.51
10:G:80:LYS:HD3	10:G:80:LYS:H	1.75	0.51
7:D:175:PHE:HZ	10:G:85:GLU:HG3	1.74	0.51
12:I:4:PHE:HE1	12:I:6:PHE:HE2	1.58	0.51
5:B:309:GLN:OE1	12:I:52:ILE:HD11	2.10	0.51
13:J:53:HIS:HD2	13:J:54:VAL:N	2.09	0.51
1:T:14:DC:C6	1:T:15:DT:H73	2.45	0.51
4:A:874:ASP:N	4:A:1058:VAL:HG22	2.25	0.51
4:A:535:THR:CG2	4:A:616:VAL:HA	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:658:LEU:HD23	4:A:659:HIS:HE1	1.75	0.51
5:B:503:GLY:CA	5:B:507:LYS:CE	2.76	0.51
5:B:603:LEU:HB3	5:B:609:ILE:HG13	1.91	0.51
5:B:843:GLN:HB2	5:B:993:THR:HB	1.92	0.51
4:A:1242:VAL:HG12	4:A:1243:VAL:N	2.17	0.51
4:A:24:PRO:HD2	4:A:233:TRP:CD1	2.45	0.51
4:A:401:GLY:C	4:A:435:HIS:CD2	2.84	0.51
4:A:58:LEU:HD22	4:A:80:HIS:O	2.11	0.51
4:A:630:ILE:HD13	4:A:646:PHE:CZ	2.46	0.51
4:A:853:ASP:OD1	4:A:855:THR:N	2.44	0.51
4:A:89:PRO:HB2	4:A:204:THR:HG22	1.91	0.51
4:A:903:ASN:ND2	4:A:905:ASP:H	2.07	0.51
5:B:1034:VAL:HG12	5:B:1035:ALA:H	1.74	0.51
5:B:1166:CYS:O	5:B:1166:CYS:SG	2.69	0.51
5:B:179:CYS:SG	5:B:181:LEU:HB2	2.51	0.51
5:B:235:SER:C	5:B:236:HIS:HD2	2.14	0.51
5:B:240:ILE:CG2	5:B:254:LEU:HB3	2.40	0.51
5:B:841:MET:SD	5:B:846:ILE:HD11	2.50	0.51
15:L:49:LYS:O	15:L:50:ASP:CB	2.58	0.51
4:A:18:GLN:HB3	5:B:1215:ARG:HG3	1.91	0.51
4:A:215:SER:HB3	4:A:218:ASP:OD2	2.11	0.51
4:A:21:LEU:HD11	4:A:1414:ALA:HA	1.93	0.51
5:B:102:VAL:HG22	5:B:112:LEU:HD22	1.93	0.51
5:B:311:LEU:O	5:B:312:GLU:C	2.48	0.51
5:B:918:ILE:HD12	5:B:935:ARG:HD3	1.93	0.51
5:B:953:LEU:HD23	5:B:965:LYS:H	1.76	0.51
7:D:66:ARG:O	7:D:70:PHE:HB2	2.10	0.51
5:B:1039:GLY:HA2	13:J:51:LEU:CD2	2.41	0.51
6:C:47:ASP:CA	15:L:69:ALA:CB	2.86	0.51
4:A:37:PHE:N	4:A:37:PHE:CD1	2.79	0.51
4:A:64:ASN:O	4:A:65:LEU:C	2.48	0.51
4:A:840:ARG:O	4:A:841:LEU:C	2.48	0.51
4:A:901:LEU:CG	4:A:926:GLN:HE21	2.23	0.51
4:A:757:ASN:HA	5:B:1021:MET:SD	2.51	0.51
5:B:1022:THR:HG23	5:B:1022:THR:O	2.10	0.51
5:B:1197:PRO:HG2	5:B:1200:ALA:HB3	1.91	0.51
5:B:327:ARG:O	5:B:331:LEU:HD13	2.11	0.51
5:B:997:GLU:H	5:B:997:GLU:CD	2.13	0.51
7:D:210:ILE:O	7:D:214:LEU:HG	2.11	0.51
1:T:16:DT:OP1	4:A:1403:GLU:O	2.28	0.51
4:A:365:GLY:O	4:A:468:PHE:HA	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:482:PHE:C	4:A:484:GLY:H	2.14	0.51
4:A:809:THR:H	4:A:812:GLU:HB2	1.76	0.51
4:A:783:THR:HG21	4:A:815:PHE:CE2	2.46	0.51
4:A:829:VAL:C	4:A:831:THR:H	2.14	0.51
4:A:341:MET:CE	4:A:843:LYS:NZ	2.73	0.51
7:D:176:GLU:C	7:D:178:ALA:N	2.63	0.51
4:A:1342:GLU:HG3	8:E:198:ILE:HD13	1.93	0.51
10:G:117:GLN:O	10:G:119:LEU:N	2.44	0.51
10:G:150:CYS:C	10:G:151:ILE:HG13	2.31	0.51
4:A:1153:TYR:CE1	12:I:42:LEU:HD13	2.46	0.51
13:J:44:TYR:HD2	13:J:44:TYR:N	2.09	0.51
5:B:900:ALA:HB3	15:L:61:THR:OG1	2.10	0.51
4:A:283:GLY:O	4:A:285:PRO:HD3	2.10	0.51
4:A:881:GLN:NE2	4:A:958:VAL:O	2.38	0.51
4:A:466:SER:HB3	5:B:1103:ILE:HG12	1.92	0.51
5:B:1183:LYS:N	5:B:1183:LYS:CE	2.71	0.51
4:A:14:VAL:CG2	5:B:1216:LEU:HD13	2.40	0.51
5:B:230:ALA:N	5:B:231:PRO:HD2	2.26	0.51
6:C:46:ILE:HG13	6:C:72:LEU:HD11	1.92	0.51
12:I:69:PRO:HG2	12:I:85:PHE:CD2	2.46	0.51
13:J:23:ASN:C	13:J:25:LEU:N	2.63	0.51
13:J:47:ARG:HG2	13:J:47:ARG:NH1	2.26	0.51
4:A:1157:ASP:C	4:A:1159:ARG:H	2.14	0.50
4:A:1280:GLU:O	4:A:1281:ARG:O	2.29	0.50
4:A:61:ILE:HG22	4:A:62:ASP:H	1.76	0.50
5:B:108:VAL:HG12	5:B:109:THR:H	1.74	0.50
4:A:346:ASP:HB3	5:B:1108:ARG:H	1.76	0.50
5:B:284:ILE:HG12	5:B:324:ILE:HD12	1.91	0.50
5:B:594:ALA:HA	5:B:617:ARG:HH12	1.76	0.50
5:B:765:PRO:O	5:B:768:THR:N	2.43	0.50
5:B:882:THR:O	5:B:883:LEU:HB2	2.11	0.50
12:I:8:ARG:CG	12:I:34:TYR:CE1	2.93	0.50
4:A:23:SER:O	4:A:24:PRO:C	2.48	0.50
4:A:399:HIS:CB	4:A:400:PRO:CD	2.88	0.50
4:A:763:ALA:O	4:A:803:SER:HB3	2.11	0.50
4:A:901:LEU:H	4:A:926:GLN:HE21	1.57	0.50
4:A:903:ASN:C	4:A:903:ASN:ND2	2.63	0.50
5:B:1087:PHE:HD2	5:B:1088:GLY:H	1.59	0.50
6:C:243:VAL:HG12	6:C:243:VAL:O	2.10	0.50
6:C:99:LEU:HD23	6:C:99:LEU:N	2.25	0.50
4:A:871:ASP:HB3	8:E:204:THR:HG23	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:82:PRO:O	11:H:84:ALA:N	2.35	0.50
5:B:984:HIS:CD2	5:B:1025:HIS:HB2	2.47	0.50
5:B:773:MET:C	5:B:775:LYS:H	2.13	0.50
6:C:98:VAL:HG23	6:C:122:SER:HB3	1.93	0.50
6:C:258:ILE:CD1	6:C:258:ILE:N	2.74	0.50
10:G:53:ASN:HD22	10:G:53:ASN:N	2.08	0.50
11:H:84:ALA:C	11:H:86:ASP:H	2.14	0.50
4:A:1053:PHE:C	4:A:1055:ARG:H	2.14	0.50
4:A:269:ILE:CG1	4:A:299:HIS:HB3	2.42	0.50
4:A:311:GLN:CB	4:A:312:PRO:CD	2.90	0.50
4:A:442:VAL:O	4:A:457:ALA:HA	2.12	0.50
4:A:877:HIS:O	4:A:878:ILE:CG1	2.59	0.50
4:A:909:ASP:O	4:A:911:SER:N	2.45	0.50
4:A:78:PRO:HA	5:B:1201:LYS:HZ2	1.76	0.50
5:B:299:GLU:HB3	5:B:571:PRO:HG3	1.94	0.50
5:B:637:LEU:O	5:B:690:VAL:HG13	2.12	0.50
5:B:642:ASP:CB	5:B:649:LYS:HA	2.41	0.50
6:C:54:ASN:HB2	6:C:153:LEU:HD12	1.94	0.50
8:E:96:PHE:CZ	8:E:100:ILE:HD11	2.46	0.50
9:F:81:THR:HB	9:F:136:ARG:HH11	1.76	0.50
10:G:80:LYS:O	10:G:82:PHE:CE1	2.64	0.50
10:G:81:PRO:HA	10:G:85:GLU:OE1	2.12	0.50
12:I:55:THR:HG22	12:I:58:VAL:HG21	1.91	0.50
4:A:1319:VAL:HG13	4:A:1320:PRO:HD2	1.94	0.50
4:A:130:ASP:HB2	4:A:133:LYS:HB2	1.94	0.50
4:A:416:ARG:C	4:A:417:TYR:CD2	2.85	0.50
5:B:1007:VAL:HG22	5:B:1008:PRO:CD	2.39	0.50
5:B:806:THR:CG2	5:B:808:ALA:HB3	2.41	0.50
6:C:215:GLU:O	6:C:216:GLY:C	2.50	0.50
8:E:168:TYR:CB	8:E:170:LEU:HG	2.40	0.50
12:I:82:GLU:HB3	12:I:104:LEU:HD12	1.94	0.50
15:L:47:ARG:HG3	15:L:47:ARG:HH11	1.76	0.50
3:P:4:A:O2'	3:P:5:C:H5'	2.11	0.50
4:A:1420:ASP:O	4:A:1421:CYS:HB2	2.12	0.50
4:A:1447:GLU:OE2	10:G:23:LYS:HB2	2.12	0.50
4:A:823:GLY:O	4:A:825:ILE:N	2.44	0.50
4:A:1431:GLY:HA3	5:B:1152:MET:SD	2.52	0.50
5:B:360:PHE:CD2	5:B:360:PHE:C	2.85	0.50
5:B:558:LEU:C	5:B:560:GLU:H	2.15	0.50
5:B:642:ASP:CA	5:B:649:LYS:HA	2.41	0.50
6:C:239:PRO:O	6:C:241:ASP:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:111:THR:HG22	10:G:113:HIS:H	1.77	0.50
4:A:1349:TYR:HB2	4:A:1372:VAL:HG21	1.94	0.50
4:A:58:LEU:O	4:A:59:GLY:O	2.29	0.50
4:A:738:LYS:C	4:A:740:LEU:H	2.15	0.50
4:A:854:ASN:CB	4:A:1000:LEU:HD21	2.42	0.50
5:B:44:VAL:O	5:B:45:SER:C	2.49	0.50
8:E:22:MET:CE	8:E:26:ARG:NH2	2.73	0.50
9:F:130:ILE:O	9:F:148:VAL:CG2	2.60	0.50
10:G:117:GLN:C	10:G:119:LEU:H	2.15	0.50
13:J:44:TYR:HD2	13:J:44:TYR:H	1.57	0.50
15:L:46:VAL:HG12	15:L:46:VAL:O	2.12	0.50
4:A:116:ASP:O	4:A:118:HIS:N	2.44	0.50
4:A:244:PRO:O	4:A:246:VAL:N	2.44	0.50
4:A:299:HIS:O	4:A:301:ALA:N	2.45	0.50
4:A:347:PHE:H	5:B:1107:ALA:HA	1.77	0.50
4:A:794:PRO:C	4:A:796:SER:H	2.15	0.50
6:C:168:ALA:C	6:C:170:TRP:H	2.15	0.50
6:C:18:VAL:O	6:C:20:PHE:HD2	1.94	0.50
6:C:22:LEU:HD13	6:C:230:MET:HE3	1.93	0.50
8:E:94:LYS:HE2	8:E:98:ILE:CD1	2.38	0.50
4:A:1094:VAL:HG13	4:A:1113:THR:CG2	2.37	0.50
4:A:1120:LEU:CD1	4:A:1120:LEU:H	2.24	0.50
4:A:885:THR:O	4:A:940:ARG:HD2	2.11	0.50
4:A:982:THR:HB	4:A:985:ASP:H	1.76	0.50
5:B:234:ILE:H	5:B:234:ILE:HD12	1.77	0.50
6:C:22:LEU:HD13	6:C:230:MET:HE1	1.94	0.50
9:F:119:ARG:NH1	9:F:119:ARG:HG3	2.27	0.50
12:I:99:LEU:C	12:I:100:PHE:HD1	2.15	0.50
4:A:244:PRO:CB	4:A:245:PRO:CD	2.90	0.49
4:A:512:VAL:HA	4:A:519:PRO:HA	1.93	0.49
4:A:845:LEU:O	4:A:846:GLU:C	2.49	0.49
4:A:886:ILE:HD11	4:A:943:LEU:CB	2.36	0.49
5:B:758:PHE:CE1	5:B:1027:ILE:CG2	2.95	0.49
5:B:1040:ASN:O	5:B:1041:GLU:C	2.49	0.49
5:B:1208:MET:O	5:B:1211:ASN:N	2.42	0.49
5:B:552:MET:C	5:B:554:ILE:H	2.15	0.49
5:B:806:THR:HG22	5:B:808:ALA:HB3	1.94	0.49
5:B:950:ASP:O	5:B:951:GLN:HB2	2.12	0.49
6:C:145:CYS:HA	13:J:2:ILE:HD11	1.93	0.49
7:D:153:ARG:C	7:D:154:PHE:CD1	2.85	0.49
13:J:32:GLU:O	13:J:34:THR:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1130:GLN:O	4:A:1134:ILE:HG13	2.12	0.49
4:A:1195:LEU:HD11	4:A:1267:MET:HE3	1.94	0.49
4:A:218:ASP:HA	4:A:221:SER:OG	2.12	0.49
4:A:443:LEU:O	4:A:489:LEU:HD12	2.12	0.49
4:A:784:LEU:HB3	4:A:785:PRO:HD2	1.94	0.49
6:C:163:ILE:O	6:C:165:LYS:N	2.44	0.49
7:D:134:THR:HG22	7:D:135:GLY:N	2.28	0.49
7:D:56:ARG:NH2	7:D:57:LEU:HD21	2.27	0.49
10:G:49:LEU:HG	10:G:76:ALA:HA	1.94	0.49
11:H:102:TYR:N	11:H:102:TYR:CD2	2.80	0.49
4:A:1005:GLU:O	4:A:1009:ASN:HB2	2.12	0.49
4:A:367:PRO:HA	4:A:463:ILE:O	2.11	0.49
4:A:68:GLN:O	4:A:70:CYS:N	2.44	0.49
4:A:817:ALA:O	4:A:818:MET:C	2.50	0.49
5:B:435:THR:CG2	5:B:437:GLU:HB2	2.42	0.49
5:B:63:ILE:HD12	5:B:421:PHE:CE2	2.47	0.49
1:T:24:DG:OP1	5:B:857:ARG:NH2	2.46	0.49
6:C:39:ALA:HA	6:C:164:ALA:CB	2.32	0.49
7:D:24:ALA:HA	10:G:83:LYS:O	2.12	0.49
13:J:45:CYS:SG	13:J:46:CYS:N	2.85	0.49
4:A:1209:MET:CE	4:A:1236:LEU:HB3	2.42	0.49
4:A:38:PRO:HA	4:A:270:LEU:HD23	1.94	0.49
4:A:402:ALA:CB	4:A:434:ARG:HA	2.43	0.49
4:A:783:THR:HG22	4:A:784:LEU:HG	1.93	0.49
4:A:981:LEU:CD2	4:A:1039:LYS:HA	2.42	0.49
4:A:343:LYS:NZ	5:B:1151:LEU:O	2.45	0.49
4:A:1410:PHE:HA	5:B:1212:ILE:CD1	2.41	0.49
5:B:890:TYR:O	5:B:892:LYS:N	2.46	0.49
6:C:140:ASN:O	6:C:141:GLY:O	2.30	0.49
7:D:64:VAL:C	7:D:66:ARG:H	2.15	0.49
8:E:128:PRO:HA	8:E:129:PRO:C	2.33	0.49
4:A:857:ARG:NH1	9:F:139:PRO:HB2	2.28	0.49
11:H:27:GLU:HG2	11:H:39:THR:HG23	1.93	0.49
1:T:17:DA:C2	2:N:1:DA:N1	2.81	0.49
4:A:1327:ILE:HG22	8:E:147:HIS:CE1	2.47	0.49
4:A:300:VAL:O	4:A:300:VAL:HG12	2.11	0.49
4:A:353:ILE:HG21	4:A:487:MET:CE	2.36	0.49
4:A:765:VAL:HG12	4:A:766:GLY:N	2.26	0.49
4:A:84:ILE:HD11	4:A:270:LEU:CD1	2.34	0.49
4:A:873:MET:HG2	4:A:957:PRO:HB3	1.95	0.49
5:B:728:ARG:NH1	5:B:1047:PHE:HB3	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:550:ASP:OD1	5:B:551:PRO:HD2	2.13	0.49
5:B:563:MET:HA	5:B:589:VAL:O	2.12	0.49
5:B:831:SER:CB	5:B:994:TYR:OH	2.60	0.49
12:I:100:PHE:N	12:I:100:PHE:HD1	2.10	0.49
12:I:111:THR:HG22	12:I:113:ASP:N	2.27	0.49
14:K:108:GLU:O	14:K:112:GLN:HG2	2.12	0.49
1:T:12:DT:H2"	1:T:13:DA:OP2	2.11	0.49
4:A:1120:LEU:CD1	4:A:1120:LEU:N	2.76	0.49
4:A:174:ILE:HG23	4:A:182:VAL:O	2.12	0.49
4:A:92:HIS:HB2	4:A:236:LEU:HD21	1.95	0.49
4:A:311:GLN:CB	4:A:312:PRO:HD3	2.41	0.49
4:A:626:ASN:O	4:A:628:GLY:N	2.43	0.49
5:B:980:PHE:HE2	5:B:1094:ARG:CB	2.24	0.49
5:B:38:PHE:CD1	5:B:811:TYR:CD2	3.00	0.49
5:B:773:MET:C	5:B:775:LYS:N	2.65	0.49
6:C:254:LYS:C	6:C:256:ALA:H	2.15	0.49
7:D:47:LEU:HD11	10:G:3:PHE:CD2	2.48	0.49
4:A:1435:PRO:O	4:A:1436:ILE:HG13	2.12	0.49
4:A:316:GLN:O	4:A:317:LYS:C	2.50	0.49
4:A:82:GLY:O	4:A:241:VAL:N	2.42	0.49
5:B:515:HIS:CD2	5:B:517:THR:HG23	2.47	0.49
5:B:1006:ILE:HD13	13:J:44:TYR:HE2	1.74	0.49
4:A:277:GLU:C	4:A:279:LEU:H	2.16	0.49
4:A:852:TYR:HA	4:A:1060:PRO:HB3	1.95	0.49
4:A:977:LYS:HB3	4:A:978:PRO:HD2	1.94	0.49
5:B:251:ILE:HG22	5:B:251:ILE:O	2.13	0.49
5:B:333:PHE:C	5:B:334:ILE:HG13	2.33	0.49
5:B:210:LYS:HG3	5:B:461:LEU:O	2.13	0.49
5:B:523:CYS:SG	5:B:524:PRO:HD2	2.53	0.49
5:B:653:VAL:HG23	5:B:689:LEU:HB3	1.93	0.49
5:B:734:HIS:O	5:B:735:ALA:HB2	2.12	0.49
6:C:30:ALA:O	6:C:33:LEU:HB3	2.12	0.49
8:E:13:TRP:O	8:E:16:PHE:HB3	2.13	0.49
11:H:99:GLY:HA3	11:H:118:PHE:HA	1.95	0.49
4:A:551:TYR:CE2	14:K:62:LYS:HE2	2.48	0.49
14:K:93:SER:O	14:K:97:LYS:HG3	2.13	0.49
4:A:1120:LEU:HD12	4:A:1120:LEU:H	1.78	0.49
4:A:1369:ALA:O	4:A:1373:ASP:OD2	2.31	0.49
4:A:262:LEU:C	4:A:264:PHE:N	2.66	0.49
5:B:803:LEU:HD12	5:B:1032:SER:HB3	1.95	0.49
5:B:361:LEU:N	5:B:362:PRO:CD	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:579:ARG:CB	5:B:586:TRP:HE1	2.25	0.49
6:C:147:LEU:HD23	6:C:147:LEU:N	2.28	0.49
5:B:995:ARG:NH1	6:C:165:LYS:HG2	2.28	0.49
7:D:138:ASN:OD1	7:D:141:LEU:HB2	2.12	0.49
7:D:54:GLU:OE1	7:D:164:ILE:HD11	2.12	0.49
10:G:1:MET:O	10:G:3:PHE:CD1	2.66	0.49
12:I:70:ARG:NH1	12:I:104:LEU:HD11	2.28	0.49
13:J:16:ASP:O	13:J:18:TRP:N	2.46	0.49
4:A:1004:ASN:O	4:A:1008:GLN:HB2	2.13	0.48
4:A:873:MET:C	4:A:1058:VAL:CG2	2.80	0.48
4:A:236:LEU:HD23	4:A:236:LEU:N	2.28	0.48
4:A:340:LEU:HD21	5:B:1200:ALA:CA	2.43	0.48
5:B:1034:VAL:O	5:B:1036:ALA:N	2.46	0.48
7:D:192:LYS:NZ	7:D:192:LYS:HB3	2.27	0.48
8:E:135:PHE:CD2	8:E:140:LEU:HD21	2.37	0.48
14:K:24:ASP:OD1	14:K:26:LYS:HB2	2.13	0.48
4:A:874:ASP:CA	4:A:1058:VAL:HG22	2.43	0.48
4:A:16:GLU:HB3	4:A:1418:LEU:HD11	1.95	0.48
4:A:326:ARG:HH22	4:A:1407:GLU:HG3	1.76	0.48
4:A:68:GLN:C	4:A:70:CYS:N	2.65	0.48
5:B:205:ILE:O	5:B:206:ASN:C	2.52	0.48
5:B:459:TYR:CD2	5:B:459:TYR:C	2.86	0.48
5:B:496:ARG:NH1	5:B:539:LEU:HB2	2.28	0.48
5:B:593:PRO:HG2	5:B:617:ARG:CZ	2.42	0.48
6:C:254:LYS:C	6:C:256:ALA:N	2.67	0.48
8:E:124:VAL:HA	8:E:132:ILE:HD12	1.94	0.48
8:E:202:SER:HB3	8:E:205:SER:O	2.12	0.48
13:J:27:GLU:O	13:J:29:GLU:N	2.45	0.48
3:P:2:A:O5'	3:P:2:A:H8	1.95	0.48
4:A:1001:ARG:O	4:A:1002:GLY:O	2.31	0.48
4:A:1045:VAL:O	4:A:1049:ILE:HG13	2.12	0.48
4:A:1340:GLY:O	4:A:1343:ALA:N	2.44	0.48
4:A:1451:VAL:C	4:A:1453:TYR:H	2.15	0.48
4:A:244:PRO:HB2	4:A:245:PRO:CD	2.42	0.48
4:A:540:PHE:HB3	4:A:571:LEU:HD23	1.95	0.48
5:B:520:GLY:HA2	5:B:748:ILE:HG22	1.95	0.48
6:C:11:ARG:HD3	6:C:209:TYR:CE2	2.48	0.48
4:A:1127:ASP:HB3	4:A:1130:GLN:HB3	1.93	0.48
4:A:1220:PHE:CD1	4:A:1224:LEU:HD23	2.49	0.48
4:A:406:ILE:HG13	4:A:431:LYS:HB2	1.95	0.48
4:A:573:SER:O	4:A:576:GLN:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:622:VAL:O	4:A:622:VAL:HG22	2.14	0.48
5:B:189:LEU:O	5:B:192:LEU:HB2	2.14	0.48
6:C:107:SER:C	6:C:109:SER:H	2.16	0.48
6:C:174:ALA:O	6:C:175:ALA:CB	2.61	0.48
10:G:44:TYR:O	10:G:78:VAL:HA	2.14	0.48
6:C:142:VAL:N	13:J:16:ASP:HB3	2.15	0.48
4:A:1101:LEU:O	4:A:1101:LEU:HD12	2.13	0.48
4:A:40:THR:HG22	4:A:41:MET:CG	2.32	0.48
6:C:6:PRO:HB3	6:C:25:VAL:CG1	2.44	0.48
9:F:128:LYS:HD3	9:F:149:GLU:O	2.14	0.48
9:F:77:ASP:C	9:F:79:ARG:N	2.67	0.48
10:G:1:MET:CE	10:G:1:MET:O	2.61	0.48
13:J:48:ARG:HD2	13:J:49:MET:N	2.28	0.48
4:A:1028:THR:O	4:A:1032:LEU:HD12	2.14	0.48
4:A:1388:GLY:O	4:A:1390:ASN:N	2.46	0.48
4:A:629:LEU:O	4:A:633:VAL:HG23	2.13	0.48
5:B:333:PHE:O	5:B:334:ILE:CG1	2.60	0.48
5:B:616:ILE:HG12	5:B:697:GLU:HA	1.94	0.48
5:B:882:THR:HG21	5:B:935:ARG:HA	1.95	0.48
10:G:26:LEU:HD12	10:G:56:ILE:HD13	1.95	0.48
12:I:85:PHE:CD1	12:I:99:LEU:HD13	2.46	0.48
6:C:66:ARG:NH2	13:J:3:VAL:O	2.46	0.48
4:A:166:GLY:O	4:A:167:CYS:CB	2.62	0.48
4:A:299:HIS:C	4:A:301:ALA:N	2.66	0.48
4:A:683:ILE:HD13	4:A:801:GLU:HG3	1.95	0.48
4:A:785:PRO:HG2	4:A:786:HIS:HD2	1.78	0.48
4:A:929:LEU:HD23	4:A:983:ILE:HG21	1.96	0.48
5:B:1174:LYS:O	5:B:1176:ASN:HB2	2.12	0.48
5:B:125:SER:HA	5:B:172:ILE:H	1.78	0.48
5:B:360:PHE:O	5:B:361:LEU:C	2.52	0.48
5:B:373:ARG:CG	5:B:566:LEU:HD23	2.44	0.48
5:B:642:ASP:CB	5:B:649:LYS:HG3	2.43	0.48
5:B:750:GLY:O	5:B:751:VAL:C	2.52	0.48
4:A:1327:ILE:HG22	8:E:147:HIS:HE1	1.77	0.48
11:H:84:ALA:C	11:H:86:ASP:N	2.66	0.48
2:N:3:DG:H2"	2:N:4:DT:OP2	2.14	0.48
4:A:93:VAL:CG1	4:A:301:ALA:HB1	2.37	0.48
4:A:577:ILE:O	4:A:580:VAL:HG23	2.13	0.48
5:B:1197:PRO:O	5:B:1200:ALA:N	2.46	0.48
7:D:137:ASN:C	7:D:137:ASN:HD22	2.17	0.48
7:D:35:LEU:N	7:D:35:LEU:HD12	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:124:GLU:HB3	9:F:130:ILE:HG12	1.95	0.48
13:J:32:GLU:O	13:J:35:ALA:N	2.47	0.48
15:L:46:VAL:CG1	15:L:56:LEU:HD12	2.44	0.48
1:T:15:DT:C1'	4:A:1386:ARG:HH11	2.23	0.48
4:A:545:GLN:O	4:A:548:ASN:N	2.47	0.48
5:B:502:ILE:HG22	5:B:507:LYS:CD	2.43	0.48
5:B:872:GLU:CD	5:B:914:LYS:HE2	2.34	0.48
6:C:105:GLY:O	6:C:149:LYS:O	2.32	0.48
8:E:153:HIS:HB3	8:E:196:VAL:HG11	1.95	0.48
10:G:77:VAL:O	10:G:77:VAL:HG12	2.14	0.48
10:G:43:GLY:CA	10:G:80:LYS:HB3	2.42	0.48
11:H:41:ASP:O	11:H:42:ILE:HG13	2.14	0.48
12:I:13:MET:HG3	12:I:14:LEU:H	1.75	0.48
12:I:75:CYS:SG	12:I:78:CYS:C	2.92	0.48
4:A:1333:ILE:HG22	4:A:1334:ASP:N	2.29	0.48
4:A:244:PRO:HG2	4:A:245:PRO:CD	2.44	0.48
4:A:317:LYS:O	4:A:318:SER:CB	2.61	0.48
4:A:335:ARG:CA	4:A:339:ASN:HB2	2.40	0.48
4:A:369:SER:CB	14:K:2:ASN:OD1	2.61	0.48
4:A:62:ASP:HB3	4:A:64:ASN:ND2	2.28	0.48
5:B:778:MET:HE2	5:B:1094:ARG:HG2	1.96	0.48
5:B:461:LEU:HD12	5:B:461:LEU:N	2.29	0.48
5:B:542:MET:HG2	5:B:747:MET:HB3	1.96	0.48
5:B:780:VAL:HG12	5:B:782:LEU:O	2.13	0.48
5:B:806:THR:HG22	5:B:808:ALA:CB	2.44	0.48
6:C:167:HIS:CD2	6:C:168:ALA:H	2.32	0.48
7:D:40:HIS:CE1	7:D:41:GLN:HG3	2.49	0.48
4:A:553:VAL:HG13	4:A:648:ASN:HB3	1.95	0.47
4:A:921:GLY:O	4:A:922:ASP:C	2.53	0.47
5:B:225:VAL:HA	5:B:237:VAL:O	2.14	0.47
5:B:287:ARG:HG2	5:B:292:ILE:HA	1.94	0.47
5:B:893:LEU:HD11	5:B:910:VAL:CG1	2.44	0.47
6:C:90:ASP:O	6:C:91:HIS:CB	2.62	0.47
4:A:1446:ASP:HB2	9:F:133:VAL:CG2	2.44	0.47
5:B:954:VAL:O	15:L:55:ILE:O	2.31	0.47
4:A:1291:VAL:HG13	4:A:1292:PRO:N	2.29	0.47
4:A:332:LYS:O	4:A:334:GLY:N	2.46	0.47
4:A:553:VAL:HG22	4:A:652:VAL:CG2	2.44	0.47
4:A:552:TRP:O	4:A:554:PRO:HD3	2.14	0.47
4:A:898:ARG:HB2	4:A:933:TYR:CE1	2.49	0.47
4:A:1409:LEU:CD1	5:B:1207:LEU:HD21	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:552:MET:HA	5:B:555:ILE:HB	1.95	0.47
5:B:916:THR:O	5:B:935:ARG:HG3	2.14	0.47
6:C:77:ILE:CG2	6:C:161:LYS:HE3	2.39	0.47
6:C:179:GLU:O	6:C:180:TYR:HB3	2.13	0.47
6:C:255:VAL:HG12	6:C:255:VAL:O	2.15	0.47
8:E:124:VAL:CG1	8:E:132:ILE:HB	2.42	0.47
8:E:161:LYS:C	8:E:163:GLU:N	2.68	0.47
8:E:169:ARG:HH12	9:F:74:ILE:HD11	1.80	0.47
8:E:22:MET:HE3	8:E:26:ARG:HH21	1.78	0.47
10:G:143:ILE:HG22	10:G:144:ARG:H	1.75	0.47
10:G:13:LEU:CD2	10:G:17:PHE:HB2	2.38	0.47
13:J:1:MET:HE2	13:J:60:PHE:HE2	1.79	0.47
4:A:1006:ILE:HD12	8:E:163:GLU:HG3	1.95	0.47
4:A:872:GLY:O	4:A:1058:VAL:HG23	2.13	0.47
4:A:1076:ALA:HA	4:A:1079:MET:CE	2.43	0.47
4:A:1227:ILE:CG2	4:A:1228:TRP:N	2.78	0.47
4:A:1261:LYS:HA	4:A:1264:GLU:HB3	1.96	0.47
5:B:27:ALA:O	5:B:29:ASP:N	2.47	0.47
5:B:455:SER:O	5:B:456:GLY:C	2.51	0.47
5:B:464:GLY:HA3	5:B:479:VAL:O	2.14	0.47
5:B:638:PHE:HB2	5:B:741:CYS:O	2.15	0.47
5:B:865:LYS:HZ2	5:B:869:SER:HA	1.79	0.47
6:C:181:ASP:OD1	6:C:186:LEU:HD13	2.14	0.47
9:F:131:PRO:C	9:F:132:LEU:HD23	2.34	0.47
9:F:132:LEU:HD23	9:F:132:LEU:N	2.28	0.47
9:F:140:ASP:C	9:F:140:ASP:OD1	2.52	0.47
9:F:89:GLU:HB3	9:F:134:ILE:HD13	1.95	0.47
12:I:101:PHE:O	12:I:102:VAL:HG23	2.13	0.47
4:A:1162:VAL:HG12	4:A:1162:VAL:O	2.14	0.47
5:B:1050:ILE:CG2	5:B:1051:THR:N	2.78	0.47
5:B:1084:GLN:C	5:B:1085:ILE:HD12	2.34	0.47
5:B:1187:ASN:HD21	5:B:1190:ASP:HB3	1.79	0.47
5:B:865:LYS:HE2	5:B:871:THR:OG1	2.15	0.47
6:C:209:TYR:H	6:C:209:TYR:HD1	1.60	0.47
7:D:195:ILE:HG22	7:D:198:LEU:HG	1.95	0.47
8:E:161:LYS:C	8:E:163:GLU:H	2.17	0.47
10:G:91:VAL:HG12	10:G:92:VAL:N	2.29	0.47
4:A:420:ARG:O	4:A:421:ALA:C	2.51	0.47
4:A:450:LEU:H	4:A:450:LEU:HD12	1.79	0.47
4:A:563:PRO:HG3	4:A:572:TRP:CE2	2.49	0.47
5:B:1174:LYS:O	5:B:1175:LEU:C	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1214:PRO:HG2	5:B:1214:PRO:O	2.14	0.47
6:C:25:VAL:HG23	6:C:228:PHE:CE1	2.49	0.47
11:H:58:THR:HB	11:H:143:LEU:HD13	1.97	0.47
11:H:89:LEU:C	11:H:91:ASP:N	2.68	0.47
13:J:8:PHE:H	13:J:49:MET:CE	2.27	0.47
13:J:64:ASN:CB	13:J:65:PRO:CD	2.88	0.47
1:T:11:DG:H2"	1:T:12:DT:OP2	2.15	0.47
4:A:1127:ASP:HB3	4:A:1130:GLN:HB2	1.96	0.47
5:B:387:LEU:O	5:B:392:ARG:HB2	2.14	0.47
5:B:582:VAL:HG12	5:B:587:HIS:NE2	2.30	0.47
5:B:603:LEU:HD13	5:B:608:ASP:CB	2.42	0.47
5:B:681:TRP:O	5:B:683:SER:N	2.48	0.47
6:C:183:TRP:O	6:C:185:LYS:N	2.48	0.47
11:H:33:GLN:C	11:H:35:GLN:H	2.18	0.47
4:A:510:GLN:HA	4:A:510:GLN:OE1	2.14	0.47
4:A:960:ILE:O	4:A:961:ARG:C	2.51	0.47
5:B:284:ILE:HG23	5:B:324:ILE:CD1	2.44	0.47
5:B:744:HIS:HD2	5:B:746:SER:OG	1.96	0.47
6:C:70:ILE:HD11	6:C:144:ILE:HG12	1.97	0.47
6:C:77:ILE:O	6:C:79:GLN:N	2.45	0.47
7:D:154:PHE:HB2	7:D:160:VAL:HG22	1.96	0.47
10:G:121:PHE:HB2	10:G:130:TYR:CE2	2.50	0.47
13:J:23:ASN:O	13:J:25:LEU:N	2.47	0.47
15:L:30:ILE:HG22	15:L:31:CYS:N	2.30	0.47
1:T:14:DC:C2	1:T:15:DT:C4	3.03	0.47
4:A:250:ILE:O	4:A:258:GLY:HA3	2.15	0.47
4:A:340:LEU:HD13	4:A:1429:ILE:CG2	2.39	0.47
4:A:567:LYS:HD2	4:A:568:PRO:HD2	1.93	0.47
4:A:730:GLY:C	4:A:732:LEU:H	2.18	0.47
4:A:95:PHE:O	4:A:96:ILE:C	2.53	0.47
5:B:223:VAL:CG1	5:B:381:MET:HG2	2.44	0.47
5:B:383:ASN:O	5:B:384:ARG:C	2.53	0.47
5:B:563:MET:CE	5:B:580:VAL:HB	2.42	0.47
5:B:711:GLU:H	5:B:712:PRO:HD2	1.79	0.47
5:B:726:ALA:HB1	5:B:1051:THR:HG21	1.96	0.47
5:B:903:VAL:HG12	5:B:904:ARG:N	2.28	0.47
6:C:46:ILE:HG23	6:C:157:CYS:HB3	1.97	0.47
6:C:214:ASN:HB3	6:C:217:ASP:OD2	2.15	0.47
6:C:242:GLN:C	6:C:244:VAL:N	2.68	0.47
12:I:61:ASP:O	12:I:63:GLY:N	2.47	0.47
4:A:1451:VAL:O	4:A:1454:MET:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:167:CYS:SG	4:A:167:CYS:O	2.73	0.47
4:A:444:PHE:HB2	4:A:458:HIS:HD2	1.80	0.47
4:A:863:VAL:HG11	4:A:866:PHE:CE2	2.50	0.47
5:B:469:GLN:O	5:B:470:LYS:CB	2.62	0.47
5:B:654:ARG:O	5:B:656:GLY:N	2.48	0.47
8:E:157:SER:HG	8:E:160:GLU:HG3	1.79	0.47
4:A:1441:PHE:HB2	9:F:135:ARG:O	2.15	0.47
9:F:147:SER:OG	9:F:150:GLU:HG3	2.14	0.47
13:J:56:LEU:O	13:J:59:LYS:N	2.46	0.47
4:A:1369:ALA:O	4:A:1370:LEU:C	2.51	0.47
4:A:500:GLU:OE2	5:B:1145:SER:CB	2.63	0.47
4:A:524:VAL:HG12	4:A:525:GLN:HE21	1.80	0.47
4:A:730:GLY:C	4:A:732:LEU:N	2.67	0.47
4:A:761:MET:HA	4:A:804:TYR:HB2	1.97	0.47
4:A:768:GLN:NE2	4:A:816:HIS:ND1	2.63	0.47
5:B:104:GLU:OE1	15:L:54:ARG:NH2	2.48	0.47
5:B:1187:ASN:OD1	5:B:1188:LYS:N	2.40	0.47
5:B:558:LEU:O	5:B:560:GLU:N	2.47	0.47
6:C:253:LYS:O	6:C:256:ALA:HB3	2.15	0.47
7:D:206:GLU:C	7:D:208:GLU:N	2.68	0.47
7:D:64:VAL:C	7:D:66:ARG:N	2.67	0.47
8:E:145:THR:HG21	8:E:187:TYR:CE2	2.50	0.47
10:G:96:GLN:HA	10:G:121:PHE:CE2	2.50	0.47
11:H:138:GLU:O	11:H:139:ASN:C	2.52	0.47
11:H:15:VAL:HG22	11:H:26:ILE:HD11	1.96	0.47
11:H:91:ASP:O	11:H:93:TYR:N	2.47	0.47
12:I:111:THR:CG2	12:I:112:SER:N	2.77	0.47
13:J:16:ASP:OD1	13:J:17:LYS:N	2.43	0.47
14:K:31:VAL:HG12	14:K:32:VAL:H	1.78	0.47
4:A:547:LEU:HD22	14:K:58:PHE:HD1	1.78	0.47
14:K:59:ALA:HA	14:K:74:ARG:O	2.15	0.47
1:T:14:DC:H2"	1:T:15:DT:OP2	2.15	0.47
1:T:16:DT:H2"	1:T:17:DA:C8	2.49	0.47
4:A:1150:SER:O	4:A:1151:GLU:HG3	2.15	0.47
4:A:353:ILE:CG2	4:A:487:MET:HE3	2.37	0.47
4:A:741:ASN:ND2	4:A:743:VAL:HB	2.25	0.47
4:A:853:ASP:O	4:A:854:ASN:CB	2.63	0.47
4:A:979:SER:HG	4:A:981:LEU:HG	1.79	0.47
5:B:365:THR:HG23	5:B:367:LEU:N	2.28	0.47
5:B:465:ASN:ND2	5:B:465:ASN:H	2.11	0.47
5:B:653:VAL:HG22	5:B:689:LEU:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:357:PRO:HD2	5:B:833:TYR:CE1	2.49	0.47
6:C:133:ILE:HD12	6:C:237:SER:HA	1.96	0.47
6:C:67:LEU:HD11	6:C:155:LEU:HD12	1.96	0.47
6:C:238:ILE:HD11	6:C:246:ARG:NH1	2.30	0.47
7:D:38:ILE:HG22	7:D:39:ASN:O	2.14	0.47
7:D:47:LEU:CD1	7:D:48:ILE:N	2.76	0.47
10:G:115:MET:HB3	10:G:116:PRO:CD	2.40	0.47
10:G:115:MET:CB	10:G:116:PRO:HD2	2.41	0.47
9:F:99:LEU:HD21	10:G:64:THR:O	2.15	0.47
13:J:2:ILE:HG12	13:J:57:ILE:HD12	1.96	0.47
4:A:1073:GLY:O	4:A:1076:ALA:HB3	2.15	0.46
4:A:279:LEU:O	4:A:284:ALA:HB2	2.15	0.46
4:A:326:ARG:HG2	4:A:327:ALA:N	2.29	0.46
4:A:608:ILE:HG13	4:A:613:ILE:HD12	1.95	0.46
4:A:901:LEU:HG	4:A:926:GLN:NE2	2.26	0.46
5:B:39:ARG:HH21	5:B:665:GLU:CG	2.26	0.46
5:B:729:ILE:O	5:B:729:ILE:HG22	2.14	0.46
5:B:844:SER:O	5:B:847:ASP:HB2	2.15	0.46
6:C:133:ILE:CD1	6:C:237:SER:HA	2.45	0.46
9:F:127:GLU:O	9:F:129:LYS:HG3	2.15	0.46
11:H:58:THR:HG22	11:H:59:ILE:H	1.80	0.46
4:A:1053:PHE:C	4:A:1055:ARG:N	2.69	0.46
4:A:524:VAL:CG1	4:A:525:GLN:H	2.17	0.46
4:A:614:PHE:C	4:A:614:PHE:CD1	2.89	0.46
4:A:699:ALA:HB3	4:A:701:LEU:HG	1.96	0.46
5:B:1001:PHE:C	5:B:1001:PHE:CD1	2.89	0.46
5:B:305:VAL:O	5:B:305:VAL:HG12	2.16	0.46
5:B:613:VAL:HG22	5:B:628:THR:HA	1.96	0.46
6:C:194:GLU:O	6:C:195:GLN:HG3	2.16	0.46
8:E:55:ARG:C	8:E:57:MET:N	2.69	0.46
8:E:55:ARG:C	8:E:57:MET:H	2.17	0.46
9:F:109:VAL:HG21	9:F:124:GLU:HA	1.97	0.46
10:G:14:HIS:CD2	10:G:16:SER:CB	2.97	0.46
11:H:128:ASN:CG	11:H:128:ASN:O	2.53	0.46
6:C:146:LYS:HB2	13:J:61:LEU:HD11	1.96	0.46
1:T:27:DT:H3	3:P:3:G:H22	1.61	0.46
4:A:1053:PHE:O	4:A:1055:ARG:N	2.49	0.46
4:A:105:CYS:O	4:A:114:LEU:HG	2.15	0.46
4:A:1222:ASN:O	4:A:1223:ASP:HB3	2.14	0.46
4:A:1283:VAL:HG12	4:A:1284:MET:H	1.80	0.46
4:A:402:ALA:HB1	4:A:433:GLU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:648:ASN:O	4:A:649:ILE:C	2.54	0.46
4:A:655:PHE:O	4:A:658:LEU:HB3	2.15	0.46
5:B:118:ARG:HG2	5:B:204:ILE:HD13	1.97	0.46
5:B:560:GLU:O	5:B:561:TRP:CD1	2.69	0.46
5:B:847:ASP:O	5:B:849:GLY:N	2.48	0.46
5:B:864:LYS:N	5:B:872:GLU:OE1	2.47	0.46
5:B:893:LEU:HD22	5:B:897:GLY:C	2.35	0.46
6:C:100:THR:HG22	6:C:101:LEU:N	2.30	0.46
4:A:1147:THR:HG22	12:I:48:LEU:HD12	1.98	0.46
4:A:567:LYS:HD2	4:A:568:PRO:CD	2.45	0.46
4:A:72:GLU:HB3	4:A:76:GLU:HG2	1.96	0.46
4:A:779:PHE:CE1	4:A:785:PRO:CD	2.93	0.46
5:B:1152:MET:O	5:B:1154:ALA:N	2.49	0.46
5:B:1160:VAL:HG11	5:B:1169:MET:SD	2.56	0.46
5:B:376:PHE:HE2	5:B:569:TYR:HD2	1.62	0.46
5:B:745:PRO:C	5:B:747:MET:N	2.69	0.46
5:B:785:TYR:C	5:B:787:VAL:H	2.19	0.46
5:B:973:ILE:HG23	5:B:974:PRO:HD2	1.97	0.46
6:C:35:ARG:NH1	14:K:41:THR:H	2.13	0.46
8:E:157:SER:O	8:E:159:ASP:N	2.49	0.46
4:A:1445:ILE:HD11	10:G:61:ILE:HG12	1.98	0.46
14:K:52:ASN:O	14:K:54:ARG:N	2.48	0.46
4:A:1237:ILE:HG22	4:A:1238:ILE:N	2.29	0.46
4:A:984:LYS:O	4:A:985:ASP:C	2.54	0.46
5:B:114:PRO:O	5:B:117:ALA:N	2.47	0.46
4:A:7:SER:CB	5:B:1175:LEU:HD22	2.45	0.46
5:B:230:ALA:N	5:B:231:PRO:CD	2.78	0.46
5:B:510:LYS:N	5:B:511:PRO:CD	2.76	0.46
5:B:862:GLN:O	5:B:914:LYS:HE3	2.16	0.46
5:B:900:ALA:O	5:B:903:VAL:HG23	2.16	0.46
5:B:990:ILE:HG22	5:B:991:GLY:N	2.31	0.46
8:E:22:MET:HE3	8:E:26:ARG:NH2	2.30	0.46
9:F:143:PHE:C	9:F:143:PHE:CD1	2.88	0.46
11:H:142:LEU:C	11:H:143:LEU:HD12	2.36	0.46
3:P:2:A:C2'	3:P:3:G:C8	2.92	0.46
4:A:1265:ASN:C	4:A:1267:MET:N	2.67	0.46
4:A:1265:ASN:O	4:A:1268:LEU:N	2.41	0.46
4:A:1369:ALA:O	4:A:1372:VAL:HG12	2.14	0.46
4:A:28:ARG:O	4:A:29:ALA:C	2.54	0.46
4:A:335:ARG:O	4:A:336:ILE:C	2.53	0.46
4:A:492:PRO:HB2	4:A:497:THR:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:608:ILE:HD12	4:A:613:ILE:CD1	2.46	0.46
4:A:767:GLN:HB2	4:A:799:PHE:HD1	1.81	0.46
4:A:89:PRO:C	4:A:204:THR:HG21	2.36	0.46
5:B:1017:ILE:CB	5:B:1018:PRO:HD3	2.45	0.46
5:B:1189:ILE:HG22	5:B:1190:ASP:N	2.31	0.46
5:B:205:ILE:HG22	5:B:206:ASN:N	2.31	0.46
5:B:508:LEU:O	5:B:509:ALA:CB	2.58	0.46
5:B:570:VAL:HA	5:B:571:PRO:HD2	1.74	0.46
6:C:63:ILE:O	6:C:64:ALA:C	2.54	0.46
6:C:75:MET:O	6:C:246:ARG:NH2	2.48	0.46
11:H:123:MET:HG2	11:H:124:ARG:N	2.31	0.46
4:A:577:ILE:C	4:A:579:SER:N	2.66	0.46
4:A:673:GLY:N	4:A:674:PRO:HD2	2.30	0.46
5:B:999:MET:HG2	5:B:1007:VAL:HG22	1.97	0.46
5:B:1186:ASP:C	5:B:1186:ASP:OD1	2.53	0.46
6:C:112:ASN:HD22	6:C:112:ASN:N	2.11	0.46
6:C:256:ALA:C	6:C:258:ILE:H	2.19	0.46
11:H:111:LEU:HD23	11:H:127:GLY:O	2.16	0.46
11:H:7:ASP:O	11:H:8:ASP:HB2	2.15	0.46
15:L:27:LEU:HD23	15:L:27:LEU:N	2.30	0.46
4:A:1019:CYS:O	4:A:1022:LEU:N	2.49	0.46
4:A:47:ARG:HH22	4:A:254:GLU:HA	1.81	0.46
4:A:33:ALA:HB1	4:A:35:ILE:HG13	1.98	0.46
4:A:929:LEU:CD2	4:A:983:ILE:HG21	2.46	0.46
5:B:204:ILE:C	5:B:205:ILE:HD12	2.35	0.46
5:B:400:HIS:ND1	5:B:517:THR:HG21	2.31	0.46
6:C:33:LEU:O	6:C:34:ARG:C	2.53	0.46
6:C:90:ASP:O	6:C:91:HIS:CG	2.69	0.46
6:C:99:LEU:HD12	6:C:118:LEU:HD13	1.97	0.46
8:E:161:LYS:O	8:E:163:GLU:N	2.49	0.46
11:H:25:ARG:HA	11:H:41:ASP:HA	1.98	0.46
14:K:46:ILE:O	14:K:46:ILE:HG22	2.15	0.46
4:A:1132:LYS:O	4:A:1134:ILE:N	2.49	0.46
4:A:231:PRO:C	4:A:233:TRP:H	2.17	0.46
4:A:407:ARG:HG2	4:A:430:TRP:CZ3	2.50	0.46
5:B:758:PHE:HE1	5:B:1027:ILE:HG22	1.78	0.46
5:B:1169:MET:HE1	5:B:1201:LYS:CA	2.45	0.46
5:B:180:TYR:CD1	5:B:180:TYR:N	2.82	0.46
5:B:401:PHE:HD2	5:B:521:LEU:HD12	1.79	0.46
5:B:800:GLN:HB3	13:J:52:THR:HG22	1.92	0.46
5:B:979:LYS:HG3	5:B:989:THR:HG22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:139:ILE:HG22	10:G:140:LYS:N	2.31	0.46
10:G:14:His:HD2	10:G:16:SER:CB	2.29	0.46
10:G:9:LEU:CG	10:G:10:ASN:N	2.79	0.46
12:I:56:ALA:O	12:I:57:GLY:O	2.34	0.46
12:I:85:PHE:N	12:I:85:PHE:CD2	2.60	0.46
4:A:35:ILE:CG2	4:A:84:ILE:HD12	2.46	0.46
4:A:496:GLU:O	4:A:499:ALA:HB3	2.16	0.46
4:A:498:ARG:O	4:A:501:LEU:N	2.47	0.46
4:A:499:ALA:O	4:A:503:GLN:HB2	2.16	0.46
4:A:73:GLY:O	4:A:75:ASN:N	2.49	0.46
5:B:1182:CYS:O	5:B:1183:LYS:C	2.54	0.46
5:B:284:ILE:HD13	5:B:333:PHE:HD2	1.81	0.46
6:C:259:LEU:CD1	14:K:91:CYS:HB2	2.46	0.46
6:C:82:TYR:O	6:C:83:SER:C	2.54	0.46
8:E:35:VAL:O	8:E:37:LEU:N	2.48	0.46
9:F:99:LEU:C	9:F:99:LEU:HD12	2.37	0.46
4:A:369:SER:HB3	14:K:2:ASN:HD21	1.81	0.46
4:A:896:ARG:NH2	4:A:1030:ARG:HH21	2.14	0.45
4:A:1098:VAL:N	4:A:1099:PRO:HD2	2.30	0.45
4:A:1195:LEU:HD11	4:A:1267:MET:CE	2.45	0.45
4:A:253:ASN:HB3	5:B:935:ARG:CZ	2.46	0.45
4:A:289:ILE:O	4:A:291:GLU:N	2.49	0.45
4:A:408:ASP:C	4:A:410:GLY:H	2.18	0.45
4:A:41:MET:HB3	4:A:48:ALA:O	2.15	0.45
4:A:701:LEU:HD21	12:I:114:GLN:HB2	1.98	0.45
5:B:1001:PHE:CD2	6:C:34:ARG:NH2	2.84	0.45
5:B:298:LEU:HD13	5:B:314:LEU:HD13	1.98	0.45
5:B:546:SER:OG	5:B:631:GLY:N	2.38	0.45
5:B:653:VAL:HG22	5:B:689:LEU:HB3	1.95	0.45
5:B:882:THR:CG2	5:B:884:ARG:HB2	2.46	0.45
6:C:104:PHE:HD2	6:C:105:GLY:N	2.15	0.45
6:C:242:GLN:C	6:C:244:VAL:H	2.18	0.45
11:H:58:THR:HG22	11:H:59:ILE:N	2.32	0.45
4:A:1018:PHE:O	4:A:1021:LEU:HB3	2.17	0.45
4:A:1348:LEU:O	4:A:1352:VAL:HG23	2.16	0.45
5:B:1034:VAL:HG23	5:B:1059:LEU:HD13	1.98	0.45
5:B:130:VAL:HG23	5:B:167:ILE:HD12	1.98	0.45
5:B:312:GLU:O	5:B:315:LYS:N	2.49	0.45
5:B:873:THR:O	5:B:914:LYS:HA	2.16	0.45
11:H:93:TYR:CD1	11:H:93:TYR:N	2.84	0.45
4:A:1001:ARG:HH11	4:A:1001:ARG:HG2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1197:LEU:HD12	4:A:1209:MET:HE1	1.98	0.45
5:B:1008:PRO:HB2	5:B:1010:LEU:O	2.16	0.45
5:B:981:ALA:HB3	5:B:1095:LEU:HD21	1.98	0.45
5:B:115:GLN:HG2	5:B:193:LYS:HB2	1.98	0.45
5:B:115:GLN:HG2	5:B:193:LYS:CB	2.46	0.45
5:B:840:ILE:CG2	5:B:994:TYR:HD1	2.29	0.45
5:B:843:GLN:O	5:B:844:SER:C	2.54	0.45
6:C:27:LEU:O	6:C:30:ALA:N	2.49	0.45
9:F:111:LEU:O	9:F:113:GLY:N	2.49	0.45
4:A:1444:MET:HE1	9:F:135:ARG:HB2	1.98	0.45
12:I:4:PHE:HE1	12:I:6:PHE:CE2	2.34	0.45
1:T:15:DT:O2	4:A:1386:ARG:NH1	2.49	0.45
4:A:215:SER:O	4:A:218:ASP:HB2	2.16	0.45
4:A:298:PHE:O	4:A:301:ALA:HB3	2.15	0.45
5:B:826:ALA:HB2	5:B:1008:PRO:HB3	1.98	0.45
5:B:345:LYS:O	5:B:347:LYS:HG2	2.17	0.45
5:B:758:PHE:N	5:B:759:PRO:CD	2.80	0.45
5:B:854:LEU:HB3	5:B:856:PHE:HE1	1.81	0.45
6:C:73:GLN:HE21	6:C:74:SER:H	1.63	0.45
8:E:153:HIS:HB3	8:E:196:VAL:CG1	2.45	0.45
8:E:22:MET:HE3	8:E:26:ARG:CZ	2.46	0.45
9:F:132:LEU:O	9:F:148:VAL:HG22	2.17	0.45
10:G:13:LEU:O	10:G:67:SER:HA	2.17	0.45
4:A:1156:PRO:HA	4:A:1190:PRO:CB	2.46	0.45
4:A:1297:GLU:H	4:A:1297:GLU:HG3	1.51	0.45
4:A:1377:THR:O	4:A:1378:GLN:C	2.54	0.45
4:A:254:GLU:HB2	5:B:935:ARG:NH1	2.31	0.45
4:A:508:PRO:O	4:A:511:ILE:HG13	2.16	0.45
5:B:113:TYR:CD2	5:B:192:LEU:HD22	2.51	0.45
5:B:1178:ASN:O	5:B:1179:GLN:C	2.55	0.45
5:B:1177:HIS:O	5:B:1179:GLN:N	2.50	0.45
5:B:168:GLY:HA2	5:B:454:THR:OG1	2.15	0.45
5:B:570:VAL:HG23	5:B:573:GLN:HB3	1.99	0.45
4:A:525:GLN:CD	5:B:836:GLU:HG2	2.36	0.45
5:B:899:ILE:O	5:B:952:VAL:HG21	2.16	0.45
7:D:51:ASN:ND2	7:D:54:GLU:OE2	2.50	0.45
10:G:15:PRO:O	10:G:16:SER:C	2.55	0.45
12:I:78:CYS:HB3	12:I:106:CYS:HG	1.81	0.45
4:A:1116:LEU:HD12	4:A:1116:LEU:C	2.37	0.45
1:T:16:DT:O4'	4:A:1403:GLU:OE2	2.32	0.45
4:A:325:ILE:O	4:A:326:ARG:C	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:947:PHE:CD2	4:A:954:TRP:CZ2	3.04	0.45
5:B:1001:PHE:HD2	6:C:34:ARG:HH21	1.65	0.45
5:B:1065:GLN:HE21	5:B:1066:SER:CA	2.30	0.45
4:A:17:VAL:HA	5:B:1215:ARG:O	2.16	0.45
5:B:185:THR:H	5:B:188:ASP:HB2	1.80	0.45
5:B:307:ASP:O	5:B:309:GLN:N	2.49	0.45
5:B:562:GLY:HA3	5:B:590:HIS:CE1	2.52	0.45
5:B:640:VAL:HG12	5:B:640:VAL:O	2.16	0.45
5:B:784:ASN:O	5:B:788:ARG:HG3	2.17	0.45
5:B:936:ASP:OD1	5:B:938:SER:N	2.42	0.45
6:C:112:ASN:HB2	6:C:114:TYR:CE1	2.51	0.45
6:C:123:ASN:ND2	6:C:125:MET:SD	2.89	0.45
7:D:170:THR:HB	7:D:172:LEU:H	1.82	0.45
8:E:136:ASN:OD1	8:E:137:GLU:N	2.50	0.45
10:G:73:LYS:HE3	10:G:74:TYR:O	2.16	0.45
13:J:13:VAL:C	13:J:14:VAL:HG23	2.36	0.45
4:A:1161:THR:CG2	4:A:1163:ILE:HG13	2.46	0.45
4:A:1401:SER:O	4:A:1402:PHE:HB2	2.17	0.45
4:A:1426:GLU:H	4:A:1426:GLU:HG2	1.56	0.45
4:A:278:THR:HG22	4:A:278:THR:O	2.17	0.45
4:A:474:VAL:HG22	4:A:474:VAL:O	2.16	0.45
4:A:590:ARG:HH11	4:A:590:ARG:CG	2.19	0.45
4:A:600:PRO:C	4:A:602:ASP:H	2.19	0.45
4:A:666:ILE:CD1	4:A:667:GLY:N	2.80	0.45
4:A:668:ASP:HA	4:A:741:ASN:OD1	2.17	0.45
4:A:71:GLN:C	4:A:73:GLY:N	2.70	0.45
5:B:405:ARG:HA	5:B:631:GLY:O	2.17	0.45
8:E:131:THR:HG21	8:E:191:LYS:HZ1	1.82	0.45
9:F:89:GLU:HB3	9:F:134:ILE:CD1	2.47	0.45
11:H:4:THR:O	11:H:5:LEU:HD23	2.17	0.45
12:I:78:CYS:CB	12:I:106:CYS:SG	3.03	0.45
6:C:66:ARG:CZ	13:J:2:ILE:HG21	2.47	0.45
5:B:1006:ILE:HG22	13:J:45:CYS:HB3	1.99	0.45
13:J:53:HIS:NE2	13:J:55:ASP:HA	2.32	0.45
14:K:47:ARG:HD2	14:K:47:ARG:C	2.37	0.45
4:A:1215:ARG:HA	4:A:1215:ARG:HD2	1.72	0.45
4:A:1226:VAL:HG22	4:A:1240:CYS:HB3	1.99	0.45
4:A:1265:ASN:O	4:A:1267:MET:N	2.50	0.45
4:A:146:MET:HA	4:A:171:GLN:HB2	1.98	0.45
4:A:95:PHE:CD1	4:A:234:MET:HG2	2.52	0.45
4:A:353:ILE:HB	4:A:470:LEU:CD2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:381:THR:CG2	4:A:383:TYR:H	2.30	0.45
4:A:559:VAL:HG12	4:A:559:VAL:O	2.16	0.45
4:A:709:THR:HB	4:A:712:GLU:HG3	1.99	0.45
4:A:971:PHE:HE2	4:A:1040:GLN:HG2	1.80	0.45
5:B:1162:ILE:CG2	5:B:1163:CYS:H	2.26	0.45
5:B:294:ASP:N	5:B:294:ASP:OD2	2.50	0.45
5:B:730:ARG:O	5:B:731:VAL:O	2.35	0.45
6:C:144:ILE:O	6:C:145:CYS:HB3	2.17	0.45
6:C:77:ILE:C	6:C:79:GLN:H	2.20	0.45
14:K:35:PHE:CD1	14:K:71:PHE:CE1	3.05	0.45
14:K:58:PHE:HB3	14:K:76:GLN:HE21	1.82	0.45
4:A:1344:GLY:O	4:A:1345:ARG:C	2.55	0.45
4:A:1100:ARG:NH2	4:A:1351:GLU:HG2	2.32	0.45
4:A:1438:THR:HG22	4:A:1438:THR:O	2.16	0.45
4:A:1451:VAL:C	4:A:1453:TYR:N	2.70	0.45
4:A:427:GLN:HB2	4:A:430:TRP:NE1	2.31	0.45
4:A:43:GLU:O	4:A:44:THR:CB	2.65	0.45
4:A:353:ILE:CD1	4:A:487:MET:HE2	2.46	0.45
5:B:1031:LEU:CD2	5:B:1044:ALA:HB2	2.47	0.45
5:B:1081:LEU:O	5:B:1082:MET:C	2.55	0.45
4:A:341:MET:CE	5:B:1135:ARG:NH1	2.80	0.45
5:B:769:TYR:O	5:B:772:ALA:N	2.50	0.45
5:B:879:ARG:O	5:B:880:THR:HB	2.16	0.45
4:A:254:GLU:HG3	5:B:935:ARG:HH22	1.82	0.45
6:C:36:VAL:HG21	6:C:251:LEU:HB2	1.97	0.45
7:D:192:LYS:NZ	7:D:199:ASN:HA	2.32	0.45
10:G:117:GLN:C	10:G:119:LEU:N	2.69	0.45
10:G:127:PRO:HG2	10:G:138:THR:HG21	1.98	0.45
10:G:34:VAL:HG12	10:G:45:ILE:CG2	2.41	0.45
4:A:1444:MET:CG	10:G:60:ARG:HA	2.47	0.45
11:H:110:ASP:O	11:H:128:ASN:ND2	2.49	0.45
11:H:40:LEU:HD21	11:H:142:LEU:HD21	1.98	0.45
4:A:1280:GLU:O	4:A:1281:ARG:C	2.55	0.45
4:A:265:LYS:HZ1	4:A:322:VAL:HG22	1.80	0.45
4:A:44:THR:O	4:A:45:GLN:HB2	2.17	0.45
4:A:494:SER:H	4:A:497:THR:HB	1.82	0.45
4:A:57:ARG:HB3	4:A:68:GLN:HG2	1.99	0.45
4:A:709:THR:HG22	4:A:710:LEU:N	2.32	0.45
5:B:200:GLY:HA2	5:B:202:TYR:HE2	1.79	0.45
5:B:744:HIS:CD2	5:B:745:PRO:HD2	2.52	0.45
5:B:763:GLN:HG2	5:B:765:PRO:CG	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:794:ASN:O	5:B:795:ILE:HD12	2.16	0.45
7:D:51:ASN:OD1	7:D:52:LEU:O	2.35	0.45
8:E:129:PRO:O	8:E:130:ALA:O	2.34	0.45
11:H:11:GLN:HA	11:H:53:ASP:O	2.17	0.45
11:H:62:SER:O	11:H:63:LEU:C	2.54	0.45
13:J:51:LEU:O	13:J:51:LEU:HD12	2.17	0.45
14:K:24:ASP:OD2	14:K:74:ARG:NH1	2.49	0.45
4:A:332:LYS:HG3	4:A:333:GLU:N	2.31	0.44
4:A:552:TRP:HE3	4:A:651:LYS:HB3	1.82	0.44
4:A:883:LEU:CD2	4:A:1021:LEU:HB2	2.47	0.44
4:A:901:LEU:O	4:A:921:GLY:N	2.48	0.44
5:B:1084:GLN:HG2	6:C:201:TRP:CZ2	2.52	0.44
5:B:51:PHE:HB2	5:B:173:MET:CE	2.47	0.44
5:B:503:GLY:HA3	5:B:507:LYS:NZ	2.30	0.44
5:B:579:ARG:HA	5:B:589:VAL:HG13	1.98	0.44
10:G:3:PHE:CD1	10:G:80:LYS:HE2	2.52	0.44
11:H:82:PRO:C	11:H:84:ALA:H	2.17	0.44
12:I:106:CYS:O	12:I:107:SER:HB2	2.17	0.44
15:L:58:LYS:O	15:L:59:ALA:O	2.35	0.44
4:A:1015:VAL:O	4:A:1018:PHE:N	2.48	0.44
4:A:652:VAL:O	4:A:653:VAL:C	2.56	0.44
4:A:841:LEU:O	4:A:845:LEU:HG	2.16	0.44
4:A:92:HIS:O	4:A:95:PHE:N	2.35	0.44
4:A:982:THR:O	4:A:985:ASP:HB2	2.17	0.44
5:B:1181:GLU:O	5:B:1182:CYS:HB2	2.17	0.44
5:B:181:LEU:CD2	5:B:189:LEU:HD22	2.47	0.44
5:B:294:ASP:O	5:B:296:GLU:N	2.48	0.44
5:B:756:ILE:O	5:B:759:PRO:HD3	2.16	0.44
7:D:7:THR:CB	10:G:42:PHE:CZ	3.00	0.44
9:F:81:THR:HB	9:F:136:ARG:NH1	2.31	0.44
12:I:15:TYR:CD1	12:I:15:TYR:N	2.85	0.44
4:A:1153:TYR:CD2	4:A:1163:ILE:HD11	2.52	0.44
4:A:89:PRO:HB2	4:A:204:THR:CG2	2.47	0.44
4:A:249:SER:HB2	4:A:250:ILE:H	1.60	0.44
4:A:315:LEU:CD1	5:B:471:LYS:HB3	2.47	0.44
4:A:626:ASN:C	4:A:628:GLY:H	2.20	0.44
5:B:1177:HIS:C	5:B:1179:GLN:H	2.21	0.44
5:B:237:VAL:HG12	5:B:238:ALA:N	2.32	0.44
5:B:329:THR:O	5:B:332:ASP:HB3	2.17	0.44
1:T:24:DG:H5'	5:B:792:MET:HE3	1.99	0.44
6:C:248:ILE:HG23	14:K:98:LEU:HD22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:262:LEU:HD23	6:C:262:LEU:HA	1.76	0.44
8:E:17:ARG:O	8:E:20:LYS:HB2	2.17	0.44
10:G:143:ILE:CG2	10:G:144:ARG:N	2.75	0.44
11:H:143:LEU:C	11:H:144:ILE:HG13	2.38	0.44
12:I:78:CYS:CB	12:I:106:CYS:HG	2.30	0.44
4:A:755:PHE:O	4:A:756:ILE:C	2.56	0.44
4:A:341:MET:CE	4:A:843:LYS:HZ3	2.31	0.44
5:B:1106:ARG:NH2	5:B:1109:GLY:H	2.16	0.44
5:B:62:ILE:HG23	5:B:418:LYS:HG2	1.98	0.44
5:B:882:THR:O	5:B:883:LEU:CB	2.65	0.44
6:C:76:ASP:OD2	6:C:128:ASN:N	2.50	0.44
8:E:124:VAL:HB	8:E:125:PRO:HD3	2.00	0.44
10:G:18:PHE:HZ	10:G:68:ALA:HB2	1.83	0.44
4:A:1101:LEU:HB2	4:A:1355:VAL:HG11	1.99	0.44
4:A:108:MET:HB3	4:A:210:ILE:CD1	2.47	0.44
4:A:626:ASN:O	4:A:631:HIS:CD2	2.71	0.44
4:A:666:ILE:HD12	4:A:667:GLY:N	2.30	0.44
4:A:93:VAL:CG2	4:A:301:ALA:HA	2.48	0.44
4:A:351:THR:HG21	5:B:1103:ILE:HG13	1.99	0.44
5:B:1110:PRO:HG3	5:B:1124:ARG:O	2.17	0.44
5:B:172:ILE:CG2	5:B:173:MET:N	2.81	0.44
5:B:521:LEU:HB3	5:B:633:VAL:CG1	2.47	0.44
5:B:581:PHE:HA	5:B:585:VAL:O	2.17	0.44
5:B:661:LEU:C	5:B:663:ALA:H	2.20	0.44
5:B:834:ASN:HA	5:B:838:SER:O	2.17	0.44
5:B:969:ARG:NH1	6:C:61:GLU:OE1	2.50	0.44
8:E:114:ASN:O	8:E:115:ASN:CB	2.65	0.44
11:H:116:TYR:HE2	11:H:140:ALA:CB	2.30	0.44
4:A:1132:LYS:O	4:A:1135:ARG:N	2.51	0.44
4:A:352:VAL:HG12	4:A:353:ILE:N	2.32	0.44
4:A:84:ILE:O	4:A:84:ILE:CG2	2.64	0.44
4:A:93:VAL:HG23	4:A:304:MET:HE3	1.99	0.44
5:B:258:LEU:O	5:B:259:TYR:O	2.36	0.44
5:B:693:ILE:HD13	5:B:701:ILE:HD13	2.00	0.44
5:B:765:PRO:O	5:B:767:ASN:N	2.50	0.44
6:C:161:LYS:O	6:C:170:TRP:NE1	2.51	0.44
6:C:226:ASP:O	6:C:227:THR:CB	2.65	0.44
9:F:116:ASP:C	9:F:116:ASP:OD1	2.55	0.44
10:G:108:VAL:HG13	10:G:159:ALA:O	2.17	0.44
11:H:10:PHE:N	11:H:10:PHE:CD1	2.85	0.44
13:J:21:TYR:HB2	13:J:39:LEU:CD1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:K:53:ASP:O	14:K:55:LYS:N	2.51	0.44
4:A:1349:TYR:CA	4:A:1372:VAL:HG21	2.48	0.44
4:A:1453:TYR:O	4:A:1454:MET:HB3	2.18	0.44
4:A:282:ASN:O	4:A:284:ALA:N	2.51	0.44
4:A:34:LYS:HD3	4:A:34:LYS:N	2.33	0.44
4:A:41:MET:O	4:A:42:ASP:C	2.56	0.44
4:A:500:GLU:OE1	5:B:1143:ALA:C	2.56	0.44
4:A:500:GLU:OE2	4:A:1438:THR:HG21	2.17	0.44
4:A:575:LYS:NZ	4:A:615:GLY:H	2.16	0.44
4:A:966:ASN:O	4:A:967:ALA:C	2.56	0.44
5:B:906:SER:O	5:B:907:GLY:O	2.34	0.44
6:C:22:LEU:HD23	6:C:25:VAL:HG21	2.00	0.44
8:E:124:VAL:HG13	8:E:132:ILE:CB	2.44	0.44
8:E:212:ARG:HH11	8:E:212:ARG:HG3	1.83	0.44
8:E:48:ASP:CG	8:E:49:SER:N	2.69	0.44
10:G:9:LEU:CD1	10:G:10:ASN:H	2.30	0.44
12:I:111:THR:HG21	12:I:113:ASP:HB2	1.99	0.44
14:K:95:ILE:O	14:K:98:LEU:HB2	2.17	0.44
3:P:6:C:O2'	3:P:7:A:H5'	2.18	0.44
1:T:14:DC:H2''	1:T:15:DT:H71	2.00	0.44
4:A:1335:ILE:CG2	4:A:1335:ILE:O	2.65	0.44
4:A:526:ASP:OD1	5:B:1013:ASN:ND2	2.49	0.44
4:A:522:GLY:O	4:A:646:PHE:HE2	2.01	0.44
4:A:682:THR:HG23	4:A:728:LYS:HE3	1.99	0.44
5:B:1207:LEU:HB3	5:B:1212:ILE:HG22	1.99	0.44
5:B:26:THR:O	5:B:29:ASP:HB2	2.17	0.44
5:B:414:ALA:O	5:B:415:GLN:C	2.57	0.44
5:B:399:ASP:OD2	5:B:510:LYS:HB2	2.18	0.44
5:B:591:ARG:O	5:B:592:ASN:C	2.56	0.44
5:B:753:ALA:HA	5:B:756:ILE:HD12	2.00	0.44
6:C:170:TRP:O	6:C:171:GLY:C	2.56	0.44
7:D:138:ASN:C	7:D:140:ASP:N	2.70	0.44
8:E:22:MET:HE1	8:E:26:ARG:NH2	2.32	0.44
10:G:106:MET:HG2	10:G:107:LYS:N	2.32	0.44
10:G:48:VAL:HG13	10:G:74:TYR:HD1	1.83	0.44
13:J:1:MET:HE2	13:J:1:MET:HB2	1.87	0.44
14:K:31:VAL:CG1	14:K:32:VAL:H	2.31	0.44
4:A:103:CYS:O	4:A:106:VAL:O	2.35	0.44
4:A:40:THR:CG2	4:A:41:MET:HG3	2.36	0.44
4:A:382:PRO:CB	4:A:428:TYR:HE2	2.30	0.44
4:A:846:GLU:HB2	4:A:847:ASP:H	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:932:GLU:O	4:A:936:LEU:HG	2.18	0.44
5:B:265:SER:O	5:B:266:ALA:CB	2.65	0.44
5:B:324:ILE:CG2	5:B:325:GLN:N	2.80	0.44
5:B:424:LEU:O	5:B:428:ILE:HG13	2.18	0.44
5:B:503:GLY:CA	5:B:507:LYS:NZ	2.81	0.44
5:B:846:ILE:HG23	5:B:974:PRO:HG2	1.99	0.44
5:B:838:SER:CB	5:B:989:THR:O	2.64	0.44
10:G:88:ASP:OD2	10:G:88:ASP:N	2.49	0.44
13:J:53:HIS:CD2	13:J:54:VAL:C	2.92	0.44
4:A:1373:ASP:HA	4:A:1376:THR:CG2	2.47	0.43
4:A:247:ARG:HG3	4:A:247:ARG:O	2.18	0.43
4:A:269:ILE:HD11	4:A:300:VAL:HA	2.00	0.43
4:A:350:ARG:HH11	4:A:350:ARG:HG3	1.83	0.43
4:A:42:ASP:HB3	4:A:45:GLN:HA	2.00	0.43
4:A:679:ILE:O	4:A:682:THR:N	2.51	0.43
5:B:1072:MET:HE3	5:B:1085:ILE:HD13	2.00	0.43
5:B:203:PHE:N	5:B:203:PHE:CD1	2.86	0.43
5:B:762:ASN:OD1	5:B:1022:THR:HA	2.18	0.43
5:B:839:MET:HG3	5:B:1010:LEU:CD1	2.44	0.43
5:B:842:ASN:ND2	5:B:845:SER:OG	2.48	0.43
5:B:855:PHE:CD1	5:B:855:PHE:C	2.89	0.43
6:C:38:ILE:HA	6:C:173:ALA:HB2	1.99	0.43
6:C:246:ARG:HA	6:C:249:ASP:HB3	1.99	0.43
6:C:33:LEU:HG	6:C:37:MET:HE2	2.00	0.43
8:E:129:PRO:O	8:E:130:ALA:C	2.57	0.43
10:G:31:LEU:HD22	10:G:48:VAL:HG21	2.00	0.43
2:N:2:DA:H2''	2:N:3:DG:H8	1.82	0.43
3:P:9:G:O2'	3:P:10:C:H5'	2.18	0.43
4:A:23:SER:CB	4:A:233:TRP:NE1	2.81	0.43
4:A:58:LEU:HD13	4:A:243:PRO:HA	1.99	0.43
4:A:309:ALA:C	4:A:311:GLN:H	2.20	0.43
4:A:590:ARG:HH21	4:A:620:LYS:CB	2.29	0.43
4:A:578:LEU:HD23	4:A:612:ILE:HD11	1.99	0.43
5:B:1099:VAL:C	5:B:1101:ASP:N	2.71	0.43
5:B:167:ILE:HG22	5:B:453:ILE:HD12	1.99	0.43
5:B:286:PHE:CD1	5:B:297:ILE:HG23	2.53	0.43
5:B:351:TYR:CD1	5:B:355:ILE:HD11	2.52	0.43
5:B:436:VAL:HG12	5:B:436:VAL:O	2.19	0.43
5:B:603:LEU:HB3	5:B:609:ILE:HD11	2.00	0.43
6:C:105:GLY:HA3	6:C:149:LYS:O	2.18	0.43
8:E:101:GLN:NE2	8:E:127:ILE:HG21	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:40:LEU:HD22	11:H:123:MET:CE	2.48	0.43
11:H:91:ASP:C	11:H:93:TYR:N	2.72	0.43
12:I:77:LYS:C	12:I:79:HIS:H	2.22	0.43
12:I:84:VAL:HG13	12:I:84:VAL:O	2.18	0.43
4:A:218:ASP:O	4:A:219:PHE:C	2.57	0.43
4:A:344:ARG:HG2	4:A:344:ARG:HH11	1.82	0.43
4:A:456:MET:HB2	4:A:478:TYR:OH	2.18	0.43
4:A:817:ALA:HA	5:B:764:SER:OG	2.17	0.43
5:B:108:VAL:HG12	5:B:109:THR:N	2.34	0.43
4:A:18:GLN:H	5:B:1215:ARG:HB2	1.83	0.43
5:B:1219:ASP:O	5:B:1219:ASP:OD1	2.37	0.43
5:B:291:ILE:HD13	5:B:300:HIS:CD2	2.53	0.43
5:B:308:TRP:HA	5:B:311:LEU:HD12	2.00	0.43
5:B:500:THR:OG1	5:B:535:LEU:O	2.31	0.43
5:B:651:LEU:HD11	5:B:707:PRO:CB	2.48	0.43
5:B:661:LEU:C	5:B:663:ALA:N	2.71	0.43
5:B:796:LEU:HD12	5:B:852:ARG:O	2.18	0.43
6:C:70:ILE:HG12	6:C:142:VAL:HG11	2.00	0.43
7:D:138:ASN:O	7:D:140:ASP:N	2.52	0.43
12:I:110:PHE:CD2	12:I:110:PHE:N	2.86	0.43
14:K:49:GLU:HG3	14:K:94:ILE:HG13	1.99	0.43
4:A:1011:GLN:NE2	4:A:1015:VAL:HG21	2.32	0.43
4:A:1019:CYS:O	4:A:1023:ARG:N	2.43	0.43
4:A:1036:ARG:HH11	4:A:1036:ARG:HG2	1.82	0.43
4:A:320:ARG:HA	4:A:321:PRO:HD3	1.87	0.43
4:A:336:ILE:HG22	4:A:337:ARG:N	2.32	0.43
4:A:415:LEU:HD23	4:A:415:LEU:HA	1.75	0.43
4:A:871:ASP:OD1	4:A:1366:ARG:NH2	2.52	0.43
4:A:874:ASP:O	4:A:876:ALA:N	2.52	0.43
5:B:37:PHE:CE1	5:B:41:LYS:CG	2.96	0.43
5:B:58:THR:O	5:B:62:ILE:HG13	2.18	0.43
6:C:80:LEU:HD22	6:C:129:ILE:HD13	2.01	0.43
6:C:70:ILE:HD11	6:C:144:ILE:CG1	2.49	0.43
7:D:53:SER:HB3	7:D:152:SER:HA	2.00	0.43
8:E:205:SER:O	8:E:206:GLY:C	2.57	0.43
12:I:34:TYR:C	12:I:34:TYR:CD2	2.91	0.43
4:A:1116:LEU:CD1	4:A:1118:VAL:HG13	2.48	0.43
4:A:1279:ILE:HG23	4:A:1308:THR:OG1	2.19	0.43
4:A:1409:LEU:O	4:A:1412:ALA:HB3	2.19	0.43
4:A:224:PHE:CZ	4:A:231:PRO:HG3	2.53	0.43
4:A:243:PRO:O	4:A:244:PRO:C	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:541:ILE:HG21	4:A:549:MET:HE3	2.00	0.43
4:A:843:LYS:HA	4:A:843:LYS:HD3	1.81	0.43
5:B:1131:GLY:O	5:B:1132:GLU:C	2.57	0.43
5:B:1147:LEU:CD2	5:B:1151:LEU:HD22	2.48	0.43
5:B:237:VAL:HG22	5:B:257:LYS:HA	1.99	0.43
5:B:467:GLY:H	5:B:475:SER:HB3	1.76	0.43
5:B:766:ARG:HD3	5:B:766:ARG:HA	1.71	0.43
6:C:91:HIS:ND1	6:C:158:VAL:HG11	2.33	0.43
6:C:238:ILE:HD11	6:C:246:ARG:HH11	1.83	0.43
6:C:92:CYS:O	6:C:94:LYS:N	2.51	0.43
7:D:51:ASN:O	7:D:52:LEU:C	2.57	0.43
8:E:112:TYR:CZ	8:E:136:ASN:HB2	2.54	0.43
9:F:99:LEU:O	9:F:103:MET:CG	2.67	0.43
10:G:10:ASN:OD1	10:G:71:ASN:HA	2.19	0.43
10:G:115:MET:CB	10:G:116:PRO:CD	2.96	0.43
10:G:119:LEU:HD13	10:G:132:SER:HB2	1.99	0.43
15:L:61:THR:CG2	15:L:63:ARG:HG2	2.48	0.43
1:T:15:DT:H2"	1:T:16:DT:H71	1.99	0.43
4:A:152:VAL:HG12	4:A:153:PRO:CD	2.47	0.43
4:A:335:ARG:HB3	4:A:336:ILE:H	1.66	0.43
4:A:353:ILE:HD13	4:A:487:MET:CE	2.48	0.43
4:A:450:LEU:N	4:A:450:LEU:CD1	2.81	0.43
4:A:556:TRP:CZ2	4:A:558:GLY:HA2	2.54	0.43
5:B:1029:CYS:HA	5:B:1089:PRO:O	2.18	0.43
5:B:410:GLY:O	5:B:412:LEU:N	2.52	0.43
5:B:467:GLY:HA3	5:B:475:SER:HB3	2.00	0.43
5:B:519:TRP:CD1	5:B:519:TRP:C	2.91	0.43
5:B:794:ASN:C	5:B:795:ILE:HD12	2.38	0.43
5:B:918:ILE:HD12	5:B:935:ARG:CD	2.49	0.43
4:A:253:ASN:CB	5:B:935:ARG:CZ	2.97	0.43
5:B:859:TYR:CE1	5:B:941:LEU:HD12	2.53	0.43
6:C:123:ASN:HD22	6:C:125:MET:CG	2.29	0.43
6:C:208:GLU:C	6:C:210:GLU:H	2.22	0.43
6:C:31:ASN:O	6:C:35:ARG:HG3	2.19	0.43
6:C:44:LEU:HD23	6:C:45:ALA:N	2.34	0.43
10:G:66:GLY:O	10:G:67:SER:C	2.56	0.43
13:J:13:VAL:O	13:J:14:VAL:CG2	2.67	0.43
15:L:61:THR:HG22	15:L:63:ARG:HG2	2.01	0.43
4:A:1168:GLU:O	4:A:1172:LEU:HG	2.18	0.43
4:A:252:PHE:HB2	4:A:256:GLN:CD	2.39	0.43
5:B:192:LEU:O	5:B:193:LYS:CB	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:32:ALA:O	5:B:35:SER:HB2	2.19	0.43
5:B:366:GLN:O	5:B:367:LEU:O	2.37	0.43
5:B:702:LEU:HD12	5:B:703:ILE:H	1.83	0.43
7:D:52:LEU:CD2	7:D:147:TYR:HE2	2.31	0.43
7:D:68:ARG:C	7:D:70:PHE:N	2.71	0.43
8:E:117:THR:O	8:E:120:ALA:N	2.45	0.43
11:H:40:LEU:CD2	11:H:142:LEU:HD21	2.49	0.43
11:H:3:ASN:HB3	11:H:4:THR:H	1.63	0.43
13:J:48:ARG:HE	13:J:49:MET:HE2	1.83	0.43
13:J:41:LEU:HD11	13:J:50:ILE:HG13	2.01	0.43
4:A:1015:VAL:O	4:A:1016:THR:C	2.57	0.43
4:A:275:SER:O	4:A:279:LEU:HG	2.18	0.43
4:A:277:GLU:O	4:A:279:LEU:N	2.52	0.43
4:A:298:PHE:HD2	4:A:299:HIS:CD2	2.37	0.43
1:T:20:DC:C5'	4:A:447:GLN:NE2	2.82	0.43
4:A:56:PRO:C	4:A:57:ARG:HG3	2.22	0.43
4:A:807:GLY:HA2	5:B:760:ASP:O	2.18	0.43
5:B:1034:VAL:C	5:B:1036:ALA:N	2.72	0.43
5:B:1084:GLN:NE2	5:B:1084:GLN:N	2.67	0.43
5:B:466:TRP:CE3	5:B:466:TRP:HA	2.53	0.43
5:B:680:THR:O	5:B:684:LEU:HD12	2.19	0.43
5:B:694:ASP:O	5:B:698:GLU:HB2	2.18	0.43
10:G:145:VAL:CG1	10:G:146:LYS:N	2.81	0.43
13:J:3:VAL:HG21	13:J:18:TRP:CG	2.54	0.43
14:K:101:LEU:HD23	14:K:101:LEU:O	2.19	0.43
14:K:100:ALA:O	14:K:103:THR:HB	2.19	0.43
14:K:58:PHE:CB	14:K:76:GLN:HE21	2.31	0.43
14:K:43:GLY:HA3	14:K:61:TYR:CE1	2.53	0.43
4:A:1265:ASN:C	4:A:1267:MET:H	2.23	0.43
4:A:12:ARG:O	5:B:1194:ILE:HG22	2.19	0.43
4:A:1370:LEU:O	4:A:1374:VAL:HG23	2.18	0.43
4:A:65:LEU:O	4:A:66:LYS:C	2.58	0.43
4:A:660:ASN:O	4:A:661:GLY:O	2.36	0.43
4:A:685:GLU:HG3	4:A:686:ALA:N	2.33	0.43
5:B:1182:CYS:O	5:B:1183:LYS:O	2.36	0.43
6:C:41:ILE:HA	6:C:42:PRO:HD3	1.84	0.43
6:C:67:LEU:HD11	6:C:155:LEU:HD13	2.01	0.43
7:D:135:GLY:C	7:D:137:ASN:H	2.22	0.43
8:E:18:THR:O	8:E:19:VAL:C	2.56	0.43
11:H:11:GLN:O	11:H:28:ALA:HB1	2.18	0.43
2:N:2:DA:H2''	2:N:3:DG:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1147:THR:HA	4:A:1197:LEU:HD23	2.00	0.43
4:A:18:GLN:O	5:B:1215:ARG:CG	2.67	0.43
4:A:403:LYS:O	4:A:404:TYR:CG	2.72	0.43
4:A:825:ILE:HG23	5:B:508:LEU:HD12	2.00	0.43
5:B:834:ASN:ND2	5:B:1013:ASN:HB2	2.34	0.43
5:B:113:TYR:HB3	5:B:114:PRO:HD2	2.00	0.43
5:B:129:PHE:CD2	5:B:166:PHE:HA	2.53	0.43
5:B:235:SER:C	5:B:236:HIS:CD2	2.92	0.43
5:B:63:ILE:HA	5:B:421:PHE:CE2	2.54	0.43
5:B:503:GLY:O	5:B:504:ARG:HG3	2.18	0.43
5:B:60:GLN:O	5:B:63:ILE:HG22	2.19	0.43
6:C:91:HIS:HD2	6:C:91:HIS:O	2.02	0.43
7:D:146:GLN:O	7:D:147:TYR:C	2.57	0.43
8:E:135:PHE:CB	8:E:140:LEU:HD11	2.48	0.43
4:A:537:ARG:NH1	11:H:120:GLY:O	2.48	0.43
11:H:38:LEU:HD13	11:H:125:LEU:CD1	2.49	0.43
14:K:58:PHE:HE2	14:K:74:ARG:HE	1.58	0.43
4:A:26:GLU:O	4:A:27:VAL:C	2.55	0.42
1:T:19:DG:P	4:A:332:LYS:NZ	2.92	0.42
4:A:41:MET:O	4:A:50:ILE:HG13	2.19	0.42
4:A:444:PHE:CB	4:A:458:HIS:HD2	2.32	0.42
4:A:682:THR:HA	4:A:685:GLU:HG2	2.00	0.42
4:A:817:ALA:O	4:A:820:GLY:N	2.52	0.42
5:B:1069:PHE:CD1	5:B:1069:PHE:N	2.77	0.42
4:A:373:THR:HG21	5:B:1105:ALA:HB3	2.00	0.42
5:B:502:ILE:CD1	5:B:535:LEU:CD1	2.85	0.42
5:B:827:ILE:O	5:B:827:ILE:HG22	2.19	0.42
6:C:33:LEU:HG	6:C:37:MET:CE	2.49	0.42
6:C:80:LEU:HD11	6:C:95:CYS:CA	2.48	0.42
11:H:103:LYS:HG2	11:H:104:PHE:N	2.34	0.42
11:H:123:MET:HE3	11:H:142:LEU:CD2	2.49	0.42
11:H:15:VAL:HG22	11:H:26:ILE:CG1	2.49	0.42
3:P:8:G:HO2'	3:P:9:G:H5'	1.80	0.42
4:A:100:LYS:O	4:A:102:VAL:N	2.52	0.42
4:A:1206:ASP:HB3	4:A:1274:ARG:NH1	2.33	0.42
4:A:33:ALA:O	4:A:83:HIS:HD2	2.01	0.42
4:A:711:ARG:HA	12:I:97:MET:HE1	1.99	0.42
4:A:861:GLY:HA3	8:E:174:GLN:NE2	2.34	0.42
4:A:942:PHE:C	4:A:942:PHE:CD2	2.92	0.42
5:B:839:MET:HE3	5:B:1010:LEU:HD21	2.01	0.42
5:B:193:LYS:HD3	5:B:787:VAL:HG11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:552:MET:C	5:B:554:ILE:N	2.72	0.42
5:B:708:GLU:O	5:B:709:ASP:C	2.58	0.42
5:B:710:LEU:C	5:B:711:GLU:HG2	2.39	0.42
6:C:58:LEU:CD2	6:C:58:LEU:N	2.82	0.42
8:E:114:ASN:HA	8:E:114:ASN:HD22	1.62	0.42
11:H:83:GLN:C	11:H:85:GLY:N	2.73	0.42
12:I:101:PHE:HD1	12:I:110:PHE:O	2.02	0.42
4:A:1161:THR:HG22	4:A:1163:ILE:HG13	2.01	0.42
4:A:1173:HIS:C	4:A:1174:PHE:CD1	2.92	0.42
4:A:1148:ILE:HB	4:A:1196:GLU:O	2.19	0.42
4:A:1343:ALA:O	4:A:1346:ALA:HB3	2.19	0.42
4:A:1425:SER:O	4:A:1429:ILE:HG13	2.19	0.42
4:A:210:ILE:O	4:A:214:ILE:HG13	2.19	0.42
4:A:269:ILE:HD13	4:A:300:VAL:HG22	2.02	0.42
4:A:427:GLN:O	4:A:428:TYR:C	2.56	0.42
4:A:595:THR:O	4:A:596:THR:HG23	2.20	0.42
4:A:804:TYR:OH	4:A:816:HIS:NE2	2.52	0.42
4:A:825:ILE:HG22	4:A:826:ASP:N	2.33	0.42
4:A:877:HIS:C	4:A:878:ILE:CG1	2.87	0.42
4:A:886:ILE:CD1	4:A:943:LEU:HB3	2.41	0.42
5:B:1162:ILE:CG2	5:B:1163:CYS:N	2.79	0.42
5:B:293:PRO:HG2	5:B:296:GLU:CB	2.49	0.42
5:B:293:PRO:HG2	5:B:296:GLU:HB3	2.01	0.42
5:B:298:LEU:N	5:B:298:LEU:CD2	2.83	0.42
5:B:418:LYS:O	5:B:420:LEU:N	2.52	0.42
4:A:818:MET:H	5:B:514:LEU:HD23	1.82	0.42
5:B:593:PRO:O	5:B:596:LEU:N	2.52	0.42
5:B:654:ARG:N	5:B:657:HIS:HD2	2.13	0.42
5:B:792:MET:HA	5:B:856:PHE:O	2.20	0.42
5:B:911:ILE:HG22	5:B:912:ILE:HG13	2.00	0.42
6:C:116:LYS:HD3	6:C:140:ASN:HB3	2.02	0.42
6:C:183:TRP:CE2	6:C:207:CYS:HB3	2.55	0.42
6:C:259:LEU:HD11	14:K:91:CYS:HB2	2.00	0.42
7:D:66:ARG:CD	7:D:133:THR:HB	2.43	0.42
7:D:153:ARG:O	7:D:154:PHE:CG	2.72	0.42
8:E:31:THR:OG1	8:E:34:GLU:N	2.50	0.42
8:E:35:VAL:C	8:E:37:LEU:N	2.72	0.42
10:G:14:HIS:CE1	10:G:15:PRO:HD2	2.53	0.42
12:I:12:ASN:HB3	12:I:13:MET:H	1.57	0.42
14:K:42:LEU:O	14:K:46:ILE:HG13	2.19	0.42
4:A:1115:SER:O	4:A:1116:LEU:CB	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1115:SER:OG	4:A:1116:LEU:N	2.53	0.42
4:A:254:GLU:O	4:A:256:GLN:N	2.51	0.42
4:A:472:LEU:O	4:A:475:THR:CB	2.68	0.42
4:A:53:LEU:HD22	4:A:54:ASN:HD22	1.85	0.42
4:A:693:VAL:HA	4:A:696:GLU:HB3	2.01	0.42
4:A:752:LYS:HA	4:A:752:LYS:HD3	1.84	0.42
4:A:79:GLY:HA3	4:A:243:PRO:HG3	2.00	0.42
4:A:823:GLY:C	4:A:825:ILE:N	2.72	0.42
5:B:1060:ARG:HD2	5:B:1060:ARG:HA	1.53	0.42
5:B:1106:ARG:HD3	5:B:1127:GLY:CA	2.48	0.42
5:B:1198:TYR:CD2	5:B:1198:TYR:C	2.93	0.42
5:B:785:TYR:C	5:B:787:VAL:N	2.71	0.42
6:C:236:GLY:C	6:C:238:ILE:N	2.73	0.42
7:D:138:ASN:O	7:D:141:LEU:N	2.53	0.42
7:D:49:ALA:HB2	7:D:174:PRO:HB3	2.01	0.42
8:E:133:GLU:HB3	8:E:135:PHE:HE1	1.84	0.42
8:E:22:MET:O	8:E:26:ARG:HG3	2.18	0.42
8:E:29:PHE:O	8:E:30:ILE:CG1	2.59	0.42
10:G:126:ASN:HA	10:G:126:ASN:HD22	1.57	0.42
10:G:81:PRO:C	10:G:82:PHE:CD1	2.93	0.42
11:H:127:GLY:HA3	11:H:130:ARG:NH2	2.34	0.42
12:I:103:CYS:SG	12:I:106:CYS:SG	3.17	0.42
13:J:31:ASP:O	13:J:32:GLU:C	2.58	0.42
4:A:1209:MET:SD	4:A:1236:LEU:HD22	2.59	0.42
4:A:244:PRO:HG2	4:A:245:PRO:HD2	2.02	0.42
4:A:29:ALA:HB1	5:B:1184:GLY:HA2	2.01	0.42
4:A:626:ASN:HB3	4:A:627:GLY:H	1.70	0.42
4:A:890:ASP:H	4:A:1296:GLY:HA3	1.84	0.42
5:B:579:ARG:CA	5:B:589:VAL:HG13	2.49	0.42
5:B:654:ARG:C	5:B:656:GLY:H	2.23	0.42
5:B:798:TYR:CE2	6:C:62:PHE:HE2	2.37	0.42
6:C:15:LYS:O	6:C:240:VAL:HG22	2.20	0.42
8:E:177:ARG:O	8:E:212:ARG:CD	2.68	0.42
13:J:2:ILE:H	13:J:57:ILE:HG22	1.85	0.42
15:L:31:CYS:HB3	15:L:35:SER:N	2.35	0.42
4:A:150:THR:HG22	4:A:150:THR:O	2.20	0.42
4:A:19:PHE:HB3	4:A:1413:GLY:HA2	2.02	0.42
4:A:416:ARG:O	4:A:417:TYR:HD2	2.02	0.42
4:A:365:GLY:HA3	4:A:463:ILE:CD1	2.49	0.42
4:A:535:THR:O	4:A:575:LYS:HG3	2.19	0.42
4:A:853:ASP:OD1	4:A:855:THR:CG2	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:896:ARG:HD3	4:A:897:TYR:HE1	1.85	0.42
4:A:341:MET:HE3	5:B:1135:ARG:NH1	2.34	0.42
5:B:123:THR:O	5:B:125:SER:N	2.47	0.42
5:B:373:ARG:HG3	5:B:566:LEU:HD23	2.01	0.42
5:B:624:LEU:HA	5:B:624:LEU:HD12	1.85	0.42
5:B:948:ILE:C	5:B:949:VAL:O	2.56	0.42
6:C:99:LEU:HD22	6:C:120:ILE:HG12	2.02	0.42
4:A:1072:ILE:O	4:A:1075:PRO:HD2	2.19	0.42
4:A:1124:HIS:HB3	4:A:1130:GLN:HG2	2.01	0.42
4:A:231:PRO:O	4:A:233:TRP:N	2.52	0.42
4:A:23:SER:HB3	4:A:233:TRP:NE1	2.35	0.42
4:A:401:GLY:O	4:A:435:HIS:CD2	2.73	0.42
4:A:464:PRO:HG2	4:A:465:TYR:CD1	2.53	0.42
4:A:477:PRO:HG2	4:A:521:MET:HG2	2.01	0.42
4:A:570:PRO:C	4:A:571:LEU:HD12	2.40	0.42
4:A:599:SER:HB2	4:A:603:ASN:H	1.84	0.42
4:A:645:LEU:O	4:A:646:PHE:C	2.58	0.42
4:A:69:THR:O	4:A:71:GLN:HG2	2.19	0.42
5:B:476:ARG:HH12	5:B:501:PRO:CB	2.30	0.42
5:B:825:VAL:HG12	5:B:826:ALA:N	2.34	0.42
6:C:73:GLN:HE21	6:C:74:SER:N	2.18	0.42
6:C:83:SER:O	6:C:85:ASP:N	2.53	0.42
7:D:179:GLN:O	7:D:183:LEU:HB2	2.20	0.42
7:D:33:PHE:CE2	10:G:80:LYS:NZ	2.72	0.42
9:F:143:PHE:C	9:F:143:PHE:HD1	2.23	0.42
10:G:99:PHE:CD1	10:G:99:PHE:C	2.93	0.42
11:H:56:THR:O	11:H:144:ILE:HA	2.20	0.42
14:K:68:PHE:CD2	14:K:68:PHE:N	2.86	0.42
4:A:527:THR:O	4:A:531:ILE:HB	2.20	0.42
4:A:535:THR:CG2	4:A:575:LYS:HE2	2.49	0.42
4:A:765:VAL:HG23	4:A:802:ASN:O	2.20	0.42
5:B:1160:VAL:HG12	5:B:1161:HIS:H	1.85	0.42
5:B:854:LEU:HD23	5:B:854:LEU:HA	1.83	0.42
6:C:92:CYS:C	6:C:94:LYS:N	2.73	0.42
7:D:138:ASN:HD21	10:G:35:GLU:HB3	1.85	0.42
7:D:217:LEU:O	7:D:219:THR:N	2.53	0.42
12:I:8:ARG:HG3	12:I:34:TYR:CD1	2.55	0.42
2:N:4:DT:H2"	2:N:5:DA:OP2	2.20	0.42
4:A:116:ASP:O	4:A:117:GLU:C	2.57	0.42
4:A:1111:MET:CE	4:A:1330:ASN:OD1	2.68	0.42
4:A:1370:LEU:O	4:A:1373:ASP:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1434:ALA:HA	4:A:1435:PRO:HD3	1.77	0.42
4:A:150:THR:O	4:A:151:ASP:CG	2.57	0.42
4:A:427:GLN:HB2	4:A:430:TRP:CE2	2.55	0.42
4:A:51:GLY:HA2	4:A:56:PRO:HA	2.02	0.42
4:A:55:ASP:N	4:A:56:PRO:CD	2.83	0.42
4:A:7:SER:C	4:A:9:ALA:H	2.22	0.42
4:A:86:LEU:HD13	4:A:90:VAL:HG23	2.01	0.42
5:B:258:LEU:O	5:B:258:LEU:CG	2.67	0.42
5:B:307:ASP:O	5:B:308:TRP:C	2.58	0.42
6:C:131:HIS:HA	6:C:132:PRO:HD3	1.92	0.42
7:D:196:PRO:C	7:D:198:LEU:H	2.22	0.42
8:E:171:LYS:HA	8:E:171:LYS:HD3	1.88	0.42
8:E:198:ILE:HD11	8:E:212:ARG:CG	2.46	0.42
8:E:82:PHE:N	8:E:82:PHE:CD1	2.88	0.42
9:F:72:LYS:O	9:F:73:ALA:HB3	2.19	0.42
10:G:21:ARG:HD3	10:G:21:ARG:HA	1.85	0.42
6:C:252:GLN:CG	14:K:95:ILE:HG23	2.50	0.42
4:A:1031:VAL:HG12	4:A:1031:VAL:O	2.20	0.42
4:A:116:ASP:C	4:A:118:HIS:N	2.70	0.42
4:A:1339:LEU:HD13	8:E:147:HIS:CD2	2.55	0.42
4:A:1444:MET:O	9:F:132:LEU:HA	2.19	0.42
4:A:231:PRO:C	4:A:233:TRP:N	2.73	0.42
4:A:224:PHE:CD2	4:A:231:PRO:HG3	2.55	0.42
4:A:367:PRO:HB3	4:A:465:TYR:O	2.20	0.42
4:A:541:ILE:CG2	4:A:546:VAL:HG23	2.49	0.42
4:A:70:CYS:O	4:A:70:CYS:SG	2.77	0.42
4:A:822:GLU:O	4:A:825:ILE:HB	2.20	0.42
4:A:940:ARG:NH1	4:A:940:ARG:HG2	2.34	0.42
5:B:1002:THR:O	5:B:1003:ALA:C	2.58	0.42
5:B:102:VAL:CG2	5:B:112:LEU:HB2	2.40	0.42
5:B:610:ASN:O	5:B:612:GLU:N	2.53	0.42
5:B:753:ALA:HA	5:B:756:ILE:CD1	2.49	0.42
5:B:986:GLN:OE1	5:B:986:GLN:HA	2.20	0.42
6:C:8:VAL:HG12	6:C:9:LYS:H	1.83	0.42
7:D:153:ARG:HB3	7:D:154:PHE:CE1	2.55	0.42
7:D:170:THR:HG22	7:D:172:LEU:HG	1.97	0.42
7:D:180:LEU:HA	7:D:180:LEU:HD23	1.75	0.42
9:F:93:ILE:HD13	9:F:148:VAL:HG13	2.01	0.42
10:G:1:MET:HE1	10:G:80:LYS:H	1.84	0.42
12:I:74:GLU:HA	12:I:80:SER:O	2.19	0.42
15:L:34:CYS:SG	15:L:51:CYS:SG	3.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:24:DG:C5'	5:B:792:MET:HE3	2.50	0.42
4:A:1010:ALA:O	4:A:1013:ASP:HB2	2.20	0.41
4:A:1344:GLY:O	4:A:1347:ALA:N	2.51	0.41
4:A:1385:THR:HG22	4:A:1386:ARG:H	1.84	0.41
4:A:277:GLU:C	4:A:279:LEU:N	2.73	0.41
4:A:90:VAL:HG13	4:A:297:GLN:OE1	2.20	0.41
4:A:324:SER:O	4:A:325:ILE:C	2.56	0.41
4:A:414:ASP:OD1	4:A:416:ARG:CG	2.68	0.41
4:A:606:LEU:HB3	4:A:614:PHE:CE2	2.55	0.41
4:A:31:SER:OG	4:A:82:GLY:HA2	2.20	0.41
5:B:1115:THR:CG2	5:B:1117:GLN:CG	2.98	0.41
5:B:604:ARG:HG3	5:B:611:PRO:HA	2.02	0.41
5:B:841:MET:O	5:B:993:THR:HA	2.20	0.41
5:B:912:ILE:HD11	5:B:966:VAL:HG23	2.02	0.41
10:G:149:GLY:O	10:G:159:ALA:HB1	2.19	0.41
12:I:34:TYR:O	12:I:35:VAL:CG2	2.68	0.41
4:A:1149:ALA:CB	12:I:47:GLU:HA	2.50	0.41
5:B:822:ASN:HD22	13:J:52:THR:HG21	1.85	0.41
14:K:40:HIS:O	14:K:41:THR:C	2.59	0.41
4:A:1111:MET:H	4:A:1111:MET:HG2	1.57	0.41
4:A:1170:ILE:H	4:A:1170:ILE:HG13	1.62	0.41
4:A:1217:LYS:O	4:A:1221:LYS:N	2.52	0.41
4:A:1335:ILE:HG23	4:A:1339:LEU:HD12	2.01	0.41
4:A:1372:VAL:CG1	4:A:1373:ASP:N	2.82	0.41
4:A:276:LEU:O	4:A:279:LEU:N	2.47	0.41
4:A:337:ARG:HD3	5:B:1132:GLU:OE1	2.20	0.41
4:A:446:ARG:NH1	4:A:479:ASN:O	2.53	0.41
4:A:741:ASN:HD22	4:A:744:LYS:N	2.07	0.41
5:B:1164:GLY:HA3	5:B:1190:ASP:OD2	2.20	0.41
4:A:7:SER:HB2	5:B:1175:LEU:HD22	2.02	0.41
5:B:257:LYS:N	5:B:270:LYS:O	2.53	0.41
5:B:596:LEU:O	5:B:600:LEU:HG	2.20	0.41
5:B:582:VAL:HA	5:B:626:ILE:O	2.20	0.41
5:B:992:ILE:HD11	14:K:66:PRO:HB2	2.02	0.41
9:F:154:ASP:HB3	9:F:155:LEU:H	1.65	0.41
9:F:82:THR:HA	9:F:83:PRO:HD3	1.80	0.41
13:J:41:LEU:CD1	13:J:50:ILE:HG13	2.50	0.41
4:A:870:GLU:HB2	8:E:204:THR:HG21	2.02	0.41
4:A:901:LEU:N	4:A:926:GLN:NE2	2.51	0.41
5:B:1106:ARG:HG3	5:B:1107:ALA:N	2.34	0.41
5:B:1137:CYS:O	5:B:1140:ALA:HB3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:130:VAL:CG2	5:B:167:ILE:HD12	2.50	0.41
5:B:69:LEU:HD22	5:B:429:PHE:CE1	2.55	0.41
5:B:502:ILE:CG2	5:B:503:GLY:N	2.43	0.41
5:B:515:HIS:O	5:B:518:HIS:HB2	2.21	0.41
5:B:522:VAL:HG12	5:B:523:CYS:N	2.35	0.41
5:B:558:LEU:C	5:B:560:GLU:N	2.74	0.41
5:B:589:VAL:CG1	5:B:590:HIS:H	2.12	0.41
5:B:638:PHE:HD2	5:B:690:VAL:HG22	1.85	0.41
5:B:680:THR:HB	5:B:681:TRP:H	1.60	0.41
5:B:687:GLU:O	5:B:689:LEU:HG	2.20	0.41
7:D:206:GLU:O	7:D:208:GLU:N	2.53	0.41
8:E:61:GLN:HG2	8:E:62:ALA:N	2.35	0.41
9:F:97:ARG:NH1	9:F:100:GLN:OE1	2.53	0.41
12:I:111:THR:CG2	12:I:113:ASP:HB2	2.50	0.41
12:I:61:ASP:C	12:I:63:GLY:N	2.73	0.41
13:J:2:ILE:CG2	13:J:3:VAL:N	2.83	0.41
15:L:62:LYS:O	15:L:63:ARG:C	2.59	0.41
1:T:16:DT:C2'	1:T:17:DA:C8	3.03	0.41
4:A:497:THR:HG22	4:A:498:ARG:N	2.35	0.41
4:A:901:LEU:HA	4:A:907:THR:OG1	2.20	0.41
5:B:1032:SER:O	5:B:1036:ALA:HB2	2.20	0.41
5:B:1084:GLN:NE2	5:B:1084:GLN:H	2.18	0.41
5:B:20:ASP:O	5:B:22:SER:N	2.45	0.41
5:B:288:ALA:HA	5:B:331:LEU:HD12	2.01	0.41
5:B:496:ARG:HB3	5:B:496:ARG:NH1	2.35	0.41
5:B:593:PRO:O	5:B:595:ARG:N	2.53	0.41
6:C:229:TYR:CD1	6:C:229:TYR:N	2.88	0.41
6:C:257:SER:C	6:C:258:ILE:HD12	2.41	0.41
12:I:58:VAL:O	12:I:58:VAL:HG12	2.20	0.41
4:A:1157:ASP:O	4:A:1159:ARG:N	2.53	0.41
4:A:1206:ASP:O	4:A:1274:ARG:NH1	2.52	0.41
4:A:1334:ASP:C	4:A:1336:MET:N	2.74	0.41
4:A:152:VAL:HG13	4:A:153:PRO:HD2	1.98	0.41
4:A:264:PHE:O	4:A:267:ALA:HB3	2.21	0.41
4:A:306:ASN:ND2	4:A:322:VAL:CG1	2.83	0.41
4:A:399:HIS:O	4:A:400:PRO:C	2.57	0.41
4:A:444:PHE:CB	4:A:458:HIS:CD2	3.04	0.41
5:B:1029:CYS:HB3	5:B:1086:PHE:CZ	2.55	0.41
5:B:1187:ASN:OD1	5:B:1189:ILE:N	2.53	0.41
5:B:213:ILE:HD13	5:B:213:ILE:HA	1.88	0.41
5:B:758:PHE:HB3	5:B:761:HIS:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:166:GLU:HB3	6:C:170:TRP:HZ3	1.86	0.41
8:E:127:ILE:O	8:E:130:ALA:HB3	2.21	0.41
10:G:74:TYR:N	10:G:74:TYR:CD2	2.88	0.41
12:I:50:THR:HG22	12:I:52:ILE:N	2.32	0.41
14:K:113:THR:O	14:K:114:LEU:CB	2.62	0.41
4:A:1027:ALA:O	4:A:1028:THR:C	2.58	0.41
4:A:1041:ALA:O	4:A:1044:TRP:HB3	2.20	0.41
4:A:1044:TRP:O	4:A:1045:VAL:C	2.59	0.41
4:A:241:VAL:HA	4:A:242:PRO:HD2	1.88	0.41
4:A:24:PRO:O	4:A:28:ARG:HG3	2.20	0.41
4:A:452:LYS:HE2	4:A:452:LYS:HB3	1.74	0.41
4:A:829:VAL:C	4:A:831:THR:N	2.74	0.41
4:A:852:TYR:CD2	4:A:1060:PRO:CB	3.04	0.41
4:A:935:GLN:C	4:A:937:VAL:N	2.72	0.41
4:A:412:ARG:HH22	5:B:1108:ARG:NH1	2.19	0.41
5:B:211:VAL:HG23	5:B:483:LEU:HB2	2.02	0.41
5:B:469:GLN:O	5:B:470:LYS:HB2	2.21	0.41
5:B:54:PHE:CE2	5:B:59:LEU:HD13	2.55	0.41
5:B:820:GLY:C	5:B:1091:TYR:CE1	2.94	0.41
5:B:1080:LYS:HD2	6:C:188:HIS:HB2	2.03	0.41
10:G:101:VAL:HG12	10:G:102:GLN:N	2.35	0.41
14:K:10:PHE:CD1	14:K:11:LEU:CD2	3.04	0.41
4:A:106:VAL:HA	4:A:114:LEU:HD21	2.02	0.41
4:A:1127:ASP:O	4:A:1130:GLN:HB3	2.20	0.41
4:A:242:PRO:O	4:A:247:ARG:NE	2.52	0.41
4:A:93:VAL:CG2	4:A:304:MET:HE3	2.50	0.41
4:A:683:ILE:O	4:A:686:ALA:HB3	2.21	0.41
5:B:1068:GLY:O	5:B:1069:PHE:C	2.59	0.41
5:B:983:ARG:HD2	5:B:1091:TYR:HB3	2.01	0.41
5:B:128:LEU:HA	5:B:128:LEU:HD12	1.87	0.41
5:B:417:PHE:HE1	5:B:453:ILE:HD13	1.86	0.41
5:B:487:THR:CG2	5:B:488:TYR:N	2.83	0.41
5:B:552:MET:O	5:B:554:ILE:N	2.53	0.41
6:C:11:ARG:NH2	6:C:206:ASN:OD1	2.54	0.41
6:C:62:PHE:O	6:C:66:ARG:HG3	2.21	0.41
8:E:145:THR:HG21	8:E:187:TYR:CD2	2.56	0.41
4:A:870:GLU:HG2	8:E:208:TYR:CG	2.55	0.41
8:E:60:PHE:CE2	8:E:80:VAL:HB	2.56	0.41
4:A:1059:HIS:CE1	9:F:86:THR:HA	2.55	0.41
11:H:48:PRO:O	11:H:49:VAL:HG23	2.20	0.41
13:J:56:LEU:O	13:J:57:ILE:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1029:ARG:HG3	4:A:1029:ARG:NH1	2.34	0.41
4:A:1389:PHE:CD1	4:A:1389:PHE:C	2.93	0.41
4:A:356:ASP:C	4:A:358:ASN:H	2.24	0.41
4:A:466:SER:HB2	5:B:1099:VAL:HG11	2.03	0.41
5:B:446:LEU:O	5:B:447:ALA:CB	2.66	0.41
5:B:492:LEU:O	5:B:493:SER:C	2.59	0.41
5:B:637:LEU:HD23	5:B:742:GLU:HA	2.02	0.41
5:B:952:VAL:O	5:B:953:LEU:HB3	2.21	0.41
5:B:954:VAL:HA	5:B:964:VAL:HG22	2.02	0.41
6:C:146:LYS:HB2	13:J:57:ILE:HD11	2.02	0.41
6:C:181:ASP:CG	6:C:186:LEU:HD13	2.41	0.41
8:E:43:LYS:O	8:E:45:LYS:N	2.48	0.41
8:E:98:ILE:O	8:E:99:HIS:C	2.59	0.41
9:F:96:THR:O	9:F:99:LEU:HB3	2.21	0.41
10:G:18:PHE:HA	10:G:22:MET:HE2	1.99	0.41
15:L:30:ILE:HG22	15:L:31:CYS:O	2.21	0.41
4:A:1290:LYS:O	4:A:1291:VAL:HG23	2.21	0.41
4:A:1120:LEU:CD1	4:A:1304:TRP:O	2.69	0.41
4:A:1334:ASP:C	4:A:1336:MET:H	2.24	0.41
4:A:270:LEU:O	4:A:271:LYS:C	2.59	0.41
4:A:296:LEU:O	4:A:297:GLN:C	2.58	0.41
4:A:774:ARG:CZ	4:A:797:LYS:CB	2.98	0.41
4:A:963:ILE:HD13	4:A:1049:ILE:CG1	2.49	0.41
5:B:1099:VAL:HG13	5:B:1100:ASP:N	2.35	0.41
5:B:1216:LEU:HD23	5:B:1216:LEU:N	2.36	0.41
5:B:291:ILE:HD13	5:B:300:HIS:NE2	2.36	0.41
5:B:802:PRO:HB3	5:B:1091:TYR:CD2	2.55	0.41
5:B:821:GLN:NE2	5:B:851:PHE:HA	2.36	0.41
5:B:910:VAL:HG12	5:B:911:ILE:N	2.35	0.41
6:C:206:ASN:OD1	6:C:229:TYR:CD2	2.74	0.41
7:D:156:ASP:O	7:D:158:GLU:N	2.54	0.41
7:D:170:THR:HG21	7:D:172:LEU:CG	2.46	0.41
8:E:23:VAL:O	8:E:23:VAL:HG12	2.21	0.41
8:E:98:ILE:O	8:E:100:ILE:N	2.54	0.41
13:J:7:CYS:HA	13:J:49:MET:HE3	2.02	0.41
4:A:1039:LYS:HE3	4:A:1043:ASP:OD2	2.21	0.41
4:A:1213:GLY:O	4:A:1214:GLU:C	2.59	0.41
4:A:326:ARG:NH2	4:A:1407:GLU:HG3	2.35	0.41
4:A:1434:ALA:CB	4:A:1436:ILE:HD12	2.51	0.41
4:A:474:VAL:C	4:A:477:PRO:HD2	2.42	0.41
4:A:73:GLY:O	4:A:74:MET:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:809:THR:O	4:A:810:PRO:C	2.59	0.41
4:A:958:VAL:HG22	4:A:1052:GLN:HB3	2.03	0.41
5:B:1197:PRO:O	5:B:1200:ALA:HB3	2.21	0.41
5:B:205:ILE:CG2	5:B:206:ASN:N	2.84	0.41
5:B:593:PRO:CG	5:B:617:ARG:NH2	2.81	0.41
5:B:769:TYR:C	5:B:771:SER:N	2.74	0.41
5:B:838:SER:CA	5:B:989:THR:O	2.69	0.41
6:C:116:LYS:HD3	6:C:140:ASN:HA	2.03	0.41
6:C:80:LEU:CD1	6:C:95:CYS:HA	2.51	0.41
7:D:209:ARG:O	7:D:212:LYS:HB2	2.20	0.41
7:D:7:THR:CB	10:G:42:PHE:HZ	2.33	0.41
8:E:23:VAL:O	8:E:28:TYR:HD1	2.03	0.41
9:F:111:LEU:N	9:F:111:LEU:CD1	2.84	0.41
10:G:50:ASP:OD1	10:G:50:ASP:O	2.39	0.41
10:G:50:ASP:O	10:G:51:TYR:C	2.58	0.41
4:A:1332:PHE:HA	4:A:1335:ILE:HB	2.03	0.41
4:A:1444:MET:HB2	4:A:1444:MET:HE3	1.85	0.41
4:A:31:SER:OG	4:A:32:VAL:N	2.54	0.41
4:A:332:LYS:C	4:A:334:GLY:H	2.25	0.41
4:A:457:ALA:HB3	4:A:506:ALA:HA	2.02	0.41
4:A:1422:ARG:NH2	5:B:1224:PHE:C	2.65	0.41
4:A:1265:ASN:ND2	5:B:265:SER:HB3	2.35	0.41
5:B:361:LEU:O	5:B:363:HIS:O	2.39	0.41
5:B:839:MET:HE1	5:B:980:PHE:CB	2.51	0.41
6:C:123:ASN:HD21	6:C:125:MET:HA	1.86	0.41
8:E:116:ILE:CG2	8:E:117:THR:N	2.83	0.41
8:E:90:VAL:CA	8:E:120:ALA:HB2	2.49	0.41
4:A:1152:ILE:CG1	12:I:44:TYR:HB3	2.46	0.41
4:A:1289:ARG:NH1	4:A:1326:ARG:NH1	2.68	0.40
4:A:1409:LEU:HA	4:A:1409:LEU:HD23	1.94	0.40
4:A:1450:LEU:HD21	10:G:19:GLY:O	2.21	0.40
4:A:343:LYS:HE2	5:B:1156:ASP:OD2	2.21	0.40
4:A:446:ARG:HB2	4:A:487:MET:SD	2.61	0.40
4:A:567:LYS:HG3	4:A:568:PRO:CD	2.39	0.40
4:A:577:ILE:O	4:A:578:LEU:C	2.57	0.40
4:A:621:THR:O	4:A:629:LEU:HB2	2.22	0.40
4:A:744:LYS:O	4:A:747:VAL:N	2.54	0.40
4:A:877:HIS:O	4:A:878:ILE:HG12	2.21	0.40
5:B:1183:LYS:HE3	5:B:1183:LYS:O	2.21	0.40
5:B:390:LEU:O	5:B:391:ASP:C	2.58	0.40
5:B:758:PHE:O	5:B:760:ASP:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:801:LYS:N	13:J:52:THR:HG22	2.36	0.40
7:D:206:GLU:C	7:D:208:GLU:H	2.22	0.40
8:E:201:LYS:HA	8:E:206:GLY:O	2.21	0.40
9:F:123:LYS:O	9:F:124:GLU:C	2.57	0.40
4:A:598:LEU:CA	11:H:122:LEU:HD13	2.43	0.40
13:J:1:MET:N	13:J:56:LEU:H	2.19	0.40
15:L:38:LEU:O	15:L:39:SER:CB	2.64	0.40
15:L:55:ILE:H	15:L:55:ILE:HG12	1.53	0.40
1:T:11:DG:H1'	1:T:12:DT:O5'	2.21	0.40
4:A:23:SER:CA	4:A:233:TRP:NE1	2.84	0.40
4:A:331:GLY:O	4:A:332:LYS:HB3	2.21	0.40
4:A:382:PRO:HD3	4:A:428:TYR:HD2	1.84	0.40
4:A:441:PRO:HD2	4:A:498:ARG:CZ	2.50	0.40
4:A:452:LYS:HE3	5:B:1141:HIS:ND1	2.36	0.40
4:A:532:ARG:O	4:A:535:THR:HB	2.21	0.40
4:A:596:THR:C	4:A:598:LEU:N	2.74	0.40
4:A:853:ASP:C	4:A:853:ASP:OD1	2.60	0.40
5:B:112:LEU:HD12	5:B:113:TYR:N	2.30	0.40
5:B:468:GLU:HB3	5:B:469:GLN:H	1.47	0.40
5:B:48:LEU:O	5:B:49:ASP:C	2.60	0.40
5:B:839:MET:HE3	5:B:1010:LEU:HD11	2.02	0.40
5:B:980:PHE:HE2	5:B:1094:ARG:HB2	1.84	0.40
6:C:94:LYS:HE3	6:C:94:LYS:HB2	1.87	0.40
4:A:1059:HIS:CE1	9:F:87:LYS:H	2.40	0.40
10:G:158:HIS:O	10:G:159:ALA:HB2	2.21	0.40
10:G:49:LEU:HD23	10:G:49:LEU:N	2.35	0.40
13:J:7:CYS:CA	13:J:49:MET:HE3	2.52	0.40
15:L:38:LEU:HG	15:L:39:SER:N	2.35	0.40
4:A:1313:LEU:HD23	4:A:1338:VAL:HG21	2.04	0.40
4:A:206:GLU:O	4:A:207:ILE:C	2.59	0.40
4:A:339:ASN:O	4:A:343:LYS:HG2	2.21	0.40
4:A:482:PHE:O	4:A:484:GLY:N	2.52	0.40
4:A:742:ASN:O	4:A:745:GLN:HB2	2.21	0.40
4:A:789:LYS:HE3	12:I:67:THR:HB	2.04	0.40
5:B:235:SER:O	5:B:236:HIS:HD2	2.05	0.40
5:B:214:ALA:HB3	5:B:498:THR:HA	2.02	0.40
5:B:827:ILE:HD12	5:B:1086:PHE:HD2	1.85	0.40
7:D:204:ASP:O	7:D:208:GLU:HB2	2.21	0.40
7:D:51:ASN:C	7:D:52:LEU:O	2.59	0.40
10:G:129:SER:HB3	10:G:138:THR:OG1	2.21	0.40
10:G:44:TYR:O	10:G:78:VAL:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:K:63:VAL:O	14:K:63:VAL:CG2	2.67	0.40
4:A:838:GLN:HG2	4:A:1073:GLY:HA3	2.04	0.40
4:A:1205:LYS:O	4:A:1206:ASP:C	2.59	0.40
4:A:1227:ILE:CG2	4:A:1228:TRP:H	2.35	0.40
4:A:222:LEU:O	4:A:224:PHE:N	2.55	0.40
4:A:47:ARG:O	4:A:48:ALA:CB	2.69	0.40
5:B:1001:PHE:HD2	6:C:34:ARG:NH2	2.19	0.40
5:B:635:ARG:HB2	5:B:636:PRO:HD2	2.02	0.40
6:C:163:ILE:C	6:C:165:LYS:H	2.25	0.40
7:D:153:ARG:C	7:D:154:PHE:CG	2.95	0.40
7:D:53:SER:CB	7:D:153:ARG:H	2.33	0.40
8:E:16:PHE:O	8:E:17:ARG:C	2.59	0.40
10:G:82:PHE:N	10:G:82:PHE:CD1	2.90	0.40
5:B:309:GLN:CG	12:I:52:ILE:HD11	2.51	0.40
13:J:34:THR:O	13:J:35:ALA:C	2.59	0.40
3:P:8:G:C2	3:P:9:G:C8	3.10	0.40
4:A:1135:ARG:C	4:A:1137:ALA:H	2.25	0.40
4:A:1349:TYR:O	4:A:1350:LYS:C	2.59	0.40
4:A:1373:ASP:O	4:A:1376:THR:HG22	2.22	0.40
4:A:335:ARG:HE	4:A:335:ARG:HB2	1.47	0.40
4:A:649:ILE:O	4:A:653:VAL:HG23	2.22	0.40
5:B:100:PRO:HD2	5:B:180:TYR:CE1	2.56	0.40
5:B:278:GLN:HG2	5:B:279:ASP:H	1.86	0.40
5:B:579:ARG:HA	5:B:589:VAL:HA	2.02	0.40
5:B:65:GLU:HG3	5:B:66:ASP:OD1	2.21	0.40
5:B:701:ILE:HG13	5:B:702:LEU:N	2.35	0.40
5:B:756:ILE:HG13	5:B:756:ILE:H	1.75	0.40
5:B:822:ASN:ND2	13:J:52:THR:HG21	2.36	0.40
5:B:842:ASN:HD22	5:B:845:SER:HB3	1.84	0.40
6:C:160:LYS:O	6:C:161:LYS:O	2.40	0.40
8:E:124:VAL:N	8:E:125:PRO:HD2	2.36	0.40
8:E:127:ILE:O	8:E:127:ILE:HG13	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	1406/1733 (81%)	962 (68%)	280 (20%)	164 (12%)	0	8
5	B	1096/1224 (90%)	740 (68%)	225 (20%)	131 (12%)	0	8
6	C	264/318 (83%)	158 (60%)	67 (25%)	39 (15%)	0	5
7	D	173/221 (78%)	121 (70%)	34 (20%)	18 (10%)	0	11
8	E	212/215 (99%)	149 (70%)	48 (23%)	15 (7%)	1	20
9	F	82/155 (53%)	64 (78%)	14 (17%)	4 (5%)	2	29
10	G	169/171 (99%)	131 (78%)	26 (15%)	12 (7%)	1	20
11	H	129/146 (88%)	84 (65%)	30 (23%)	15 (12%)	0	8
12	I	117/122 (96%)	81 (69%)	27 (23%)	9 (8%)	1	18
13	J	63/70 (90%)	37 (59%)	11 (18%)	15 (24%)	0	1
14	K	112/120 (93%)	89 (80%)	18 (16%)	5 (4%)	3	30
15	L	44/70 (63%)	18 (41%)	13 (30%)	13 (30%)	0	0
All	All	3867/4565 (85%)	2634 (68%)	793 (20%)	440 (11%)	0	9

All (440) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	4	GLN
4	A	5	GLN
4	A	48	ALA
4	A	54	ASN
4	A	55	ASP
4	A	57	ARG
4	A	62	ASP
4	A	65	LEU
4	A	74	MET
4	A	78	PRO
4	A	93	VAL
4	A	154	SER
4	A	167	CYS
4	A	250	ILE
4	A	255	SER
4	A	286	HIS
4	A	311	GLN
4	A	322	VAL

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Mol	Chain	Res	Type
4	A	335	ARG
4	A	385	ILE
4	A	418	SER
4	A	423	ASP
4	A	424	ILE
4	A	536	LEU
4	A	567	LYS
4	A	619	LYS
4	A	626	ASN
4	A	666	ILE
4	A	775	ILE
4	A	968	GLN
4	A	1002	GLY
4	A	1036	ARG
4	A	1115	SER
4	A	1122	PRO
4	A	1223	ASP
4	A	1281	ARG
4	A	1314	SER
4	A	1341	ILE
4	A	1365	TYR
4	A	1366	ARG
4	A	1378	GLN
4	A	1397	LEU
4	A	1403	GLU
4	A	1405	THR
4	A	1438	THR
5	B	108	VAL
5	B	115	GLN
5	B	186	GLU
5	B	206	ASN
5	B	258	LEU
5	B	259	TYR
5	B	334	ILE
5	B	364	ILE
5	B	367	LEU
5	B	467	GLY
5	B	470	LYS
5	B	509	ALA
5	B	510	LYS
5	B	511	PRO
5	B	629	ASP

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Mol	Chain	Res	Type
5	B	643	ASP
5	B	709	ASP
5	B	727	LYS
5	B	731	VAL
5	B	746	SER
5	B	751	VAL
5	B	881	ASN
5	B	891	ASP
5	B	907	GLY
5	B	958	GLN
5	B	1006	ILE
5	B	1046	PRO
5	B	1069	PHE
5	B	1100	ASP
5	B	1108	ARG
5	B	1156	ASP
5	B	1171	VAL
5	B	1175	LEU
5	B	1181	GLU
5	B	1182	CYS
5	B	1183	LYS
5	B	1186	ASP
5	B	1188	LYS
6	C	56	THR
6	C	78	GLU
6	C	141	GLY
6	C	149	LYS
6	C	156	THR
6	C	161	LYS
6	C	184	ASN
6	C	202	PRO
6	C	209	TYR
6	C	213	PRO
6	C	214	ASN
6	C	215	GLU
6	C	231	ASN
6	C	240	VAL
7	D	6	SER
7	D	8	PHE
7	D	12	ARG
7	D	19	GLU
7	D	20	GLU

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Mol	Chain	Res	Type
7	D	21	GLU
7	D	52	LEU
7	D	131	GLU
7	D	177	VAL
7	D	192	LYS
7	D	199	ASN
8	E	106	GLN
8	E	130	ALA
10	G	62	LEU
10	G	63	PRO
10	G	139	ILE
11	H	81	PRO
11	H	128	ASN
11	H	140	ALA
12	I	3	THR
12	I	9	ASP
12	I	79	HIS
12	I	106	CYS
13	J	2	ILE
13	J	6	ARG
13	J	17	LYS
13	J	28	ASP
13	J	32	GLU
13	J	64	ASN
15	L	50	ASP
15	L	53	HIS
15	L	59	ALA
4	A	42	ASP
4	A	44	THR
4	A	59	GLY
4	A	61	ILE
4	A	66	LYS
4	A	70	CYS
4	A	76	GLU
4	A	101	LYS
4	A	111	GLY
4	A	113	LEU
4	A	244	PRO
4	A	263	THR
4	A	290	GLU
4	A	312	PRO
4	A	318	SER

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Mol	Chain	Res	Type
4	A	333	GLU
4	A	336	ILE
4	A	364	VAL
4	A	409	SER
4	A	421	ALA
4	A	483	ASP
4	A	661	GLY
4	A	753	GLY
4	A	765	VAL
4	A	780	VAL
4	A	789	LYS
4	A	818	MET
4	A	824	LEU
4	A	846	GLU
4	A	847	ASP
4	A	875	ALA
4	A	986	ILE
4	A	1008	GLN
4	A	1016	THR
4	A	1116	LEU
4	A	1120	LEU
4	A	1133	LEU
4	A	1165	GLU
4	A	1212	VAL
4	A	1221	LYS
4	A	1233	ASP
4	A	1335	ILE
4	A	1377	THR
4	A	1386	ARG
4	A	1389	PHE
4	A	1393	ASN
4	A	1395	GLY
5	B	21	GLU
5	B	28	GLU
5	B	45	SER
5	B	46	GLN
5	B	114	PRO
5	B	229	ALA
5	B	260	GLY
5	B	266	ALA
5	B	282	ILE
5	B	308	TRP

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Mol	Chain	Res	Type
5	B	466	TRP
5	B	474	SER
5	B	502	ILE
5	B	503	GLY
5	B	513	GLN
5	B	559	SER
5	B	641	GLU
5	B	655	LYS
5	B	682	SER
5	B	869	SER
5	B	888	GLY
5	B	1003	ALA
5	B	1035	ALA
5	B	1041	GLU
5	B	1126	GLY
5	B	1153	GLU
5	B	1155	SER
5	B	1157	ALA
5	B	1167	GLY
5	B	1176	ASN
5	B	1178	ASN
6	C	84	ARG
6	C	87	PHE
6	C	89	GLU
6	C	91	HIS
6	C	110	THR
6	C	142	VAL
6	C	164	ALA
6	C	169	LYS
6	C	175	ALA
6	C	216	GLY
6	C	255	VAL
6	C	264	GLN
7	D	218	GLU
8	E	36	GLU
8	E	44	ALA
8	E	59	SER
8	E	73	PRO
8	E	74	ASP
8	E	192	ARG
8	E	206	GLY
9	F	81	THR

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Mol	Chain	Res	Type
10	G	118	ASP
10	G	154	VAL
11	H	32	THR
11	H	59	ILE
11	H	82	PRO
11	H	84	ALA
11	H	92	ASP
11	H	107	VAL
12	I	57	GLY
12	I	62	ILE
12	I	78	CYS
13	J	8	PHE
13	J	14	VAL
13	J	29	GLU
13	J	33	GLY
14	K	53	ASP
15	L	35	SER
4	A	71	GLN
4	A	117	GLU
4	A	170	THR
4	A	219	PHE
4	A	223	GLY
4	A	232	GLU
4	A	253	ASN
4	A	278	THR
4	A	317	LYS
4	A	357	PRO
4	A	399	HIS
4	A	419	LYS
4	A	439	ASN
4	A	465	TYR
4	A	517	ASN
4	A	543	LEU
4	A	592	ASP
4	A	605	MET
4	A	731	ARG
4	A	817	ALA
4	A	940	ARG
4	A	1164	PRO
4	A	1309	ASP
4	A	1411	GLU
5	B	58	THR

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Mol	Chain	Res	Type
5	B	383	ASN
5	B	450	ALA
5	B	459	TYR
5	B	468	GLU
5	B	571	PRO
5	B	590	HIS
5	B	591	ARG
5	B	648	HIS
5	B	711	GLU
5	B	738	PHE
5	B	792	MET
5	B	797	TYR
5	B	848	ARG
5	B	878	GLN
5	B	884	ARG
5	B	943	SER
5	B	1017	ILE
5	B	1082	MET
6	C	60	ASP
6	C	93	ASP
6	C	167	HIS
7	D	15	LEU
8	E	115	ASN
10	G	53	ASN
11	H	17	PRO
11	H	77	ARG
11	H	108	SER
11	H	135	LEU
13	J	24	LEU
13	J	51	LEU
13	J	55	ASP
14	K	54	ARG
14	K	88	LYS
15	L	40	LEU
15	L	51	CYS
15	L	54	ARG
15	L	56	LEU
4	A	58	LEU
4	A	226	GLU
4	A	276	LEU
4	A	283	GLY
4	A	400	PRO

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Mol	Chain	Res	Type
4	A	756	ILE
4	A	795	GLU
4	A	910	PRO
4	A	958	VAL
4	A	1011	GLN
4	A	1028	THR
4	A	1054	LEU
4	A	1114	PRO
4	A	1240	CYS
4	A	1242	VAL
4	A	1297	GLU
5	B	67	SER
5	B	68	THR
5	B	100	PRO
5	B	124	TYR
5	B	197	PHE
5	B	257	LYS
5	B	369	GLY
5	B	419	THR
5	B	478	GLY
5	B	480	SER
5	B	594	ALA
5	B	605	ARG
5	B	620	ARG
5	B	735	ALA
5	B	867	GLY
5	B	883	LEU
5	B	951	GLN
5	B	1011	ILE
5	B	1097	HIS
5	B	1144	ALA
6	C	77	ILE
6	C	108	GLU
6	C	198	ALA
7	D	11	ARG
10	G	26	LEU
11	H	44	VAL
11	H	52	GLN
12	I	47	GLU
13	J	27	GLU
14	K	29	ASN
15	L	43	THR

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Mol	Chain	Res	Type
4	A	68	GLN
4	A	69	THR
4	A	525	GLN
4	A	598	LEU
4	A	599	SER
4	A	633	VAL
4	A	739	ASP
4	A	755	PHE
4	A	841	LEU
4	A	871	ASP
4	A	969	GLN
4	A	1266	THR
4	A	1396	ALA
5	B	27	ALA
5	B	48	LEU
5	B	65	GLU
5	B	309	GLN
5	B	414	ALA
5	B	418	LYS
5	B	636	PRO
5	B	758	PHE
5	B	766	ARG
5	B	1016	ALA
5	B	1096	ARG
6	C	176	ILE
6	C	230	MET
7	D	30	GLY
7	D	168	LYS
8	E	40	GLU
9	F	112	GLU
10	G	19	GLY
10	G	34	VAL
12	I	34	TYR
13	J	63	TYR
15	L	46	VAL
15	L	60	ARG
4	A	84	ILE
4	A	245	PRO
4	A	300	VAL
4	A	492	PRO
4	A	627	GLY
4	A	649	ILE

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Mol	Chain	Res	Type
4	A	1057	VAL
4	A	1158	PRO
5	B	313	MET
5	B	387	LEU
5	B	530	GLY
5	B	1214	PRO
6	C	18	VAL
7	D	69	ALA
7	D	139	LYS
8	E	45	LYS
8	E	158	SER
9	F	150	GLU
10	G	115	MET
14	K	90	ALA
15	L	26	THR
15	L	28	LYS
4	A	196	GLU
5	B	611	PRO
5	B	712	PRO
6	C	212	PRO
4	A	652	VAL
4	A	653	VAL
5	B	551	PRO
6	C	172	PRO
8	E	37	LEU
4	A	546	VAL
4	A	825	ILE
4	A	1379	GLY
4	A	1454	MET
5	B	818	PRO
5	B	1018	PRO
6	C	171	GLY
4	A	77	CYS
5	B	411	PRO
5	B	524	PRO
6	C	126	GLY
9	F	131	PRO
10	G	20	PRO
4	A	35	ILE
4	A	867	ILE
4	A	1292	PRO
5	B	592	ASN

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Mol	Chain	Res	Type
10	G	116	PRO
8	E	129	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	1239/1520 (82%)	1135 (92%)	104 (8%)	13	45
5	B	964/1061 (91%)	876 (91%)	88 (9%)	11	41
6	C	234/274 (85%)	211 (90%)	23 (10%)	9	37
7	D	140/200 (70%)	124 (89%)	16 (11%)	7	31
8	E	196/197 (100%)	187 (95%)	9 (5%)	31	64
9	F	74/137 (54%)	65 (88%)	9 (12%)	6	29
10	G	152/152 (100%)	142 (93%)	10 (7%)	19	53
11	H	117/128 (91%)	111 (95%)	6 (5%)	28	61
12	I	113/116 (97%)	99 (88%)	14 (12%)	5	28
13	J	60/65 (92%)	55 (92%)	5 (8%)	13	46
14	K	99/102 (97%)	92 (93%)	7 (7%)	17	51
15	L	40/57 (70%)	37 (92%)	3 (8%)	16	49
All	All	3428/4009 (86%)	3134 (91%)	294 (9%)	12	44

All (294) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	2	VAL
4	A	11	LEU
4	A	22	PHE
4	A	34	LYS
4	A	38	PRO
4	A	62	ASP
4	A	67	CYS
4	A	93	VAL

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Mol	Chain	Res	Type
4	A	105	CYS
4	A	108	MET
4	A	122	MET
4	A	208	LEU
4	A	209	ASN
4	A	215	SER
4	A	236	LEU
4	A	245	PRO
4	A	261	ASP
4	A	270	LEU
4	A	293	GLU
4	A	302	THR
4	A	312	PRO
4	A	320	ARG
4	A	335	ARG
4	A	345	VAL
4	A	354	SER
4	A	369	SER
4	A	381	THR
4	A	404	TYR
4	A	406	ILE
4	A	407	ARG
4	A	408	ASP
4	A	418	SER
4	A	425	GLN
4	A	443	LEU
4	A	445	ASN
4	A	450	LEU
4	A	451	HIS
4	A	454	SER
4	A	460	VAL
4	A	470	LEU
4	A	481	ASP
4	A	493	GLN
4	A	497	THR
4	A	503	GLN
4	A	515	GLN
4	A	560	ILE
4	A	562	THR
4	A	587	HIS
4	A	598	LEU
4	A	618	GLU

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Mol	Chain	Res	Type
4	A	626	ASN
4	A	629	LEU
4	A	666	ILE
4	A	670	ILE
4	A	711	ARG
4	A	739	ASP
4	A	774	ARG
4	A	779	PHE
4	A	821	ARG
4	A	831	THR
4	A	834	THR
4	A	845	LEU
4	A	854	ASN
4	A	858	ASN
4	A	890	ASP
4	A	903	ASN
4	A	929	LEU
4	A	940	ARG
4	A	949	ASP
4	A	969	GLN
4	A	1006	ILE
4	A	1016	THR
4	A	1029	ARG
4	A	1035	TYR
4	A	1052	GLN
4	A	1067	LEU
4	A	1110	ASN
4	A	1111	MET
4	A	1116	LEU
4	A	1122	PRO
4	A	1127	ASP
4	A	1152	ILE
4	A	1155	ASP
4	A	1170	ILE
4	A	1173	HIS
4	A	1264	GLU
4	A	1271	ILE
4	A	1291	VAL
4	A	1295	THR
4	A	1298	TYR
4	A	1309	ASP
4	A	1332	PHE

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Mol	Chain	Res	Type
4	A	1333	ILE
4	A	1359	ASP
4	A	1364	ASN
4	A	1366	ARG
4	A	1372	VAL
4	A	1400	CYS
4	A	1405	THR
4	A	1432	GLN
4	A	1442	ASP
4	A	1443	VAL
4	A	1445	ILE
4	A	1447	GLU
5	B	44	VAL
5	B	57	TYR
5	B	61	ASP
5	B	128	LEU
5	B	175	ARG
5	B	188	ASP
5	B	194	GLU
5	B	199	MET
5	B	217	ARG
5	B	223	VAL
5	B	225	VAL
5	B	261	ARG
5	B	268	THR
5	B	286	PHE
5	B	294	ASP
5	B	298	LEU
5	B	360	PHE
5	B	365	THR
5	B	371	GLU
5	B	378	LEU
5	B	393	LYS
5	B	396	ASP
5	B	401	PHE
5	B	427	ASP
5	B	429	PHE
5	B	463	THR
5	B	465	ASN
5	B	466	TRP
5	B	469	GLN
5	B	476	ARG

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Mol	Chain	Res	Type
5	B	485	ARG
5	B	496	ARG
5	B	498	THR
5	B	516	ASN
5	B	555	ILE
5	B	557	PHE
5	B	570	VAL
5	B	582	VAL
5	B	593	PRO
5	B	603	LEU
5	B	615	MET
5	B	628	THR
5	B	635	ARG
5	B	636	PRO
5	B	644	GLU
5	B	682	SER
5	B	701	ILE
5	B	724	ASP
5	B	737	THR
5	B	742	GLU
5	B	751	VAL
5	B	811	TYR
5	B	830	TYR
5	B	835	GLN
5	B	839	MET
5	B	878	GLN
5	B	894	ASP
5	B	901	PRO
5	B	909	ASP
5	B	939	THR
5	B	953	LEU
5	B	956	THR
5	B	978	ASP
5	B	986	GLN
5	B	999	MET
5	B	1002	THR
5	B	1006	ILE
5	B	1010	LEU
5	B	1022	THR
5	B	1034	VAL
5	B	1047	PHE
5	B	1051	THR

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Mol	Chain	Res	Type
5	B	1065	GLN
5	B	1069	PHE
5	B	1077	THR
5	B	1084	GLN
5	B	1087	PHE
5	B	1095	LEU
5	B	1099	VAL
5	B	1103	ILE
5	B	1122	ARG
5	B	1159	ARG
5	B	1169	MET
5	B	1170	THR
5	B	1183	LYS
5	B	1202	LEU
5	B	1212	ILE
5	B	1216	LEU
6	C	22	LEU
6	C	23	SER
6	C	29	MET
6	C	54	ASN
6	C	57	VAL
6	C	58	LEU
6	C	62	PHE
6	C	77	ILE
6	C	89	GLU
6	C	90	ASP
6	C	91	HIS
6	C	104	PHE
6	C	106	GLU
6	C	108	GLU
6	C	128	ASN
6	C	140	ASN
6	C	145	CYS
6	C	147	LEU
6	C	166	GLU
6	C	202	PRO
6	C	233	GLU
6	C	240	VAL
6	C	266	ASP
7	D	32	GLU
7	D	47	LEU
7	D	63	LEU

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Mol	Chain	Res	Type
7	D	70	PHE
7	D	137	ASN
7	D	139	LYS
7	D	148	LEU
7	D	149	THR
7	D	152	SER
7	D	156	ASP
7	D	170	THR
7	D	187	THR
7	D	192	LYS
7	D	193	THR
7	D	202	ILE
7	D	221	TYR
8	E	60	PHE
8	E	74	ASP
8	E	104	ASN
8	E	114	ASN
8	E	146	HIS
8	E	175	LEU
8	E	183	PRO
8	E	207	ARG
8	E	215	MET
9	F	79	ARG
9	F	81	THR
9	F	90	ARG
9	F	99	LEU
9	F	116	ASP
9	F	119	ARG
9	F	143	PHE
9	F	148	VAL
9	F	153	VAL
10	G	1	MET
10	G	13	LEU
10	G	38	CYS
10	G	39	THR
10	G	74	TYR
10	G	78	VAL
10	G	80	LYS
10	G	96	GLN
10	G	126	ASN
10	G	171	ILE
11	H	62	SER

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Mol	Chain	Res	Type
11	H	86	ASP
11	H	91	ASP
11	H	95	TYR
11	H	102	TYR
11	H	130	ARG
12	I	8	ARG
12	I	9	ASP
12	I	13	MET
12	I	15	TYR
12	I	34	TYR
12	I	75	CYS
12	I	78	CYS
12	I	85	PHE
12	I	86	PHE
12	I	94	ASP
12	I	100	PHE
12	I	101	PHE
12	I	106	CYS
12	I	110	PHE
13	J	9	SER
13	J	10	CYS
13	J	44	TYR
13	J	46	CYS
13	J	48	ARG
14	K	10	PHE
14	K	25	THR
14	K	42	LEU
14	K	47	ARG
14	K	50	LEU
14	K	61	TYR
14	K	78	THR
15	L	55	ILE
15	L	68	GLU
15	L	70	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	54	ASN
4	A	64	ASN
4	A	68	GLN
4	A	225	ASN

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Mol	Chain	Res	Type
4	A	256	GLN
4	A	282	ASN
4	A	299	HIS
4	A	306	ASN
4	A	339	ASN
4	A	358	ASN
4	A	435	HIS
4	A	445	ASN
4	A	447	GLN
4	A	479	ASN
4	A	493	GLN
4	A	503	GLN
4	A	517	ASN
4	A	525	GLN
4	A	603	ASN
4	A	611	GLN
4	A	631	HIS
4	A	654	ASN
4	A	741	ASN
4	A	757	ASN
4	A	768	GLN
4	A	786	HIS
4	A	858	ASN
4	A	877	HIS
4	A	903	ASN
4	A	926	GLN
4	A	1106	ASN
4	A	1265	ASN
4	A	1364	ASN
5	B	60	GLN
5	B	178	ASN
5	B	215	GLN
5	B	236	HIS
5	B	363	HIS
5	B	366	GLN
5	B	465	ASN
5	B	484	ASN
5	B	515	HIS
5	B	518	HIS
5	B	538	ASN
5	B	734	HIS
5	B	744	HIS

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Mol	Chain	Res	Type
5	B	776	GLN
5	B	821	GLN
5	B	842	ASN
5	B	975	GLN
5	B	1015	HIS
5	B	1062	HIS
5	B	1065	GLN
5	B	1076	HIS
5	B	1097	HIS
5	B	1117	GLN
6	C	73	GLN
6	C	112	ASN
6	C	123	ASN
6	C	167	HIS
6	C	231	ASN
6	C	252	GLN
7	D	40	HIS
7	D	137	ASN
7	D	179	GLN
8	E	8	ASN
8	E	101	GLN
8	E	104	ASN
8	E	114	ASN
8	E	147	HIS
10	G	14	HIS
10	G	53	ASN
10	G	97	HIS
10	G	126	ASN
12	I	12	ASN
12	I	60	GLN
12	I	89	GLN
13	J	53	HIS
14	K	65	HIS
14	K	76	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	P	9/10 (90%)	1 (11%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	P	3	G

There are no RNA pucker outliers to report.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 9 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z  > 2$
18	G2P	B	1308	-	26,34,34	3.18	12 (46%)	26,54,54	3.92	14 (53%)

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
18	G2P	B	1308	-	1/1/7/7	0/18/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1308	G2P	C4-N9	-5.96	1.39	1.47
18	B	1308	G2P	C5-C6	-5.95	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1308	G2P	C3'-C4'	-5.36	1.39	1.53
18	B	1308	G2P	O3'-C3'	-4.44	1.32	1.43
18	B	1308	G2P	PB-O1B	-4.26	1.46	1.56
18	B	1308	G2P	O4'-C4'	-4.18	1.35	1.45
18	B	1308	G2P	PA-O1A	-3.05	1.48	1.56
18	B	1308	G2P	PB-O2B	-2.86	1.44	1.51
18	B	1308	G2P	C8-N9	-2.58	1.39	1.46
18	B	1308	G2P	C6-N1	3.93	1.39	1.33
18	B	1308	G2P	C5'-C4'	5.17	1.67	1.51
18	B	1308	G2P	O2'-C2'	5.34	1.55	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	1308	G2P	C5'-C4'-C3'	-6.51	90.48	115.29
18	B	1308	G2P	C2'-C1'-N9	-5.98	97.87	113.34
18	B	1308	G2P	O3'-C3'-C2'	-4.62	97.04	111.83
18	B	1308	G2P	O2'-C2'-C1'	-2.76	100.64	109.96
18	B	1308	G2P	O2'-C2'-C3'	-2.13	105.02	111.83
18	B	1308	G2P	O6-C6-N1	-2.10	119.90	122.70
18	B	1308	G2P	C4'-O4'-C1'	-2.01	105.00	109.47
18	B	1308	G2P	O1B-PB-C3A	2.25	116.11	106.54
18	B	1308	G2P	O1B-PB-O2B	2.43	118.22	110.09
18	B	1308	G2P	O1A-PA-O2A	3.00	120.14	110.09
18	B	1308	G2P	O4'-C4'-C3'	4.29	113.70	105.17
18	B	1308	G2P	O6-C6-C5	4.66	128.61	119.69
18	B	1308	G2P	O5'-C5'-C4'	6.57	132.31	109.00
18	B	1308	G2P	O4'-C4'-C5'	12.76	152.48	109.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	B	1308	G2P	C4'

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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	T	18/19 (94%)	0.99	4 (22%) <b>1</b> <b>3</b>	63, 85, 96, 104	0
2	N	6/7 (85%)	1.41	0 <b>100</b> <b>100</b>	51, 51, 51, 51	0
3	P	10/10 (100%)	0.51	0 <b>100</b> <b>100</b>	71, 75, 93, 93	0
4	A	1416/1733 (81%)	-0.35	2 (0%) <b>95</b> <b>94</b>	45, 110, 184, 223	0
5	B	1112/1224 (90%)	-0.31	1 (0%) <b>95</b> <b>94</b>	45, 119, 188, 216	0
6	C	266/318 (83%)	-0.37	0 <b>100</b> <b>100</b>	60, 102, 161, 182	0
7	D	177/221 (80%)	-0.37	0 <b>100</b> <b>100</b>	75, 131, 170, 187	0
8	E	214/215 (99%)	-0.31	0 <b>100</b> <b>100</b>	79, 164, 209, 215	0
9	F	84/155 (54%)	-0.38	0 <b>100</b> <b>100</b>	50, 81, 128, 147	0
10	G	171/171 (100%)	-0.32	0 <b>100</b> <b>100</b>	79, 106, 137, 162	0
11	H	133/146 (91%)	0.06	2 (1%) <b>74</b> <b>66</b>	124, 161, 197, 206	0
12	I	119/122 (97%)	-0.09	1 (0%) <b>86</b> <b>80</b>	97, 151, 181, 222	0
13	J	65/70 (92%)	-0.55	0 <b>100</b> <b>100</b>	64, 102, 142, 149	0
14	K	114/120 (95%)	-0.32	0 <b>100</b> <b>100</b>	65, 106, 136, 143	0
15	L	46/70 (65%)	-0.01	0 <b>100</b> <b>100</b>	99, 158, 191, 199	0
All	All	3951/4601 (85%)	-0.30	10 (0%) <b>93</b> <b>91</b>	45, 116, 188, 223	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	B	471	LYS	3.8
1	T	28	DG	2.6
4	A	1455	PRO	2.6
11	H	139	ASN	2.4
1	T	15	DT	2.4
1	T	11	DG	2.3
4	A	149	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
11	H	112	ILE	2.1
12	I	105	SER	2.1
1	T	12	DT	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
16	ZN	B	1307	1/1	0.96	0.15	-0.80	67,67,67,67	0
16	ZN	J	101	1/1	0.96	0.19	-1.05	90,90,90,90	0
16	ZN	C	319	1/1	0.94	0.06	-1.17	63,63,63,63	0
16	ZN	I	203	1/1	0.96	0.09	-1.20	108,108,108,108	0
16	ZN	I	204	1/1	0.98	0.28	-1.21	186,186,186,186	0
16	ZN	L	105	1/1	0.97	0.06	-1.82	130,130,130,130	0
16	ZN	A	1735	1/1	0.95	0.06	-2.12	68,68,68,68	0
16	ZN	A	1734	1/1	0.91	0.07	-3.42	112,112,112,112	0
18	G2P	B	1308	32/32	-	-	-	0,0,0,0	32
17	MG	A	1736	1/1	0.97	0.20	-	77,77,77,77	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.