



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:09 AM UTC

PDB ID : 2JA6 / pdb_00002ja6
Title : CPD lesion containing RNA Polymerase II elongation complex B
Authors : Brueckner, F.; Hennecke, U.; Carell, T.; Cramer, P.
Deposited on : 2006-11-23
Resolution : 4.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

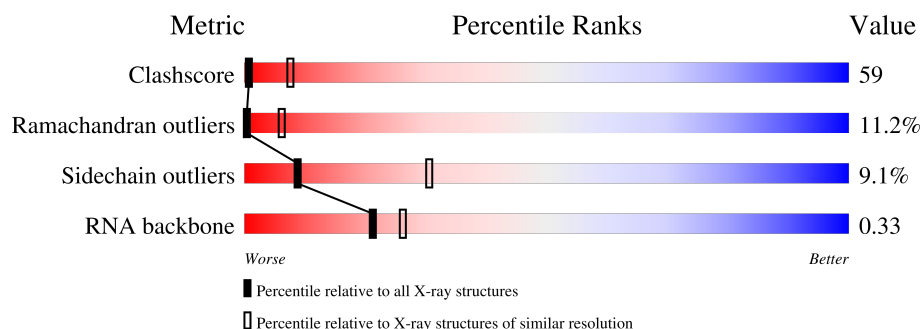
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RNA backbone	3983	1017 (4.84-3.10)

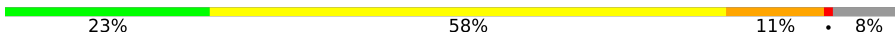
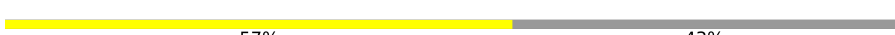
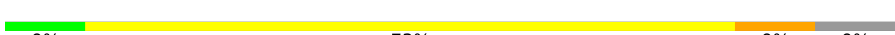
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1733	22% 44% 14% • 18%
2	B	1224	22% 54% 14% • 9%
3	C	318	22% 49% 11% • 16%
4	D	221	20% 42% 15% • 20%
5	E	215	36% 54% 9%
6	F	155	17% 30% 9% 44%

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Mol	Chain	Length	Quality of chain
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	N	14	
14	P	11	
15	T	25	

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
15	TT	T	17	-	-	X	-

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 32010 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-DIRECTED RNA POLYMERASE II LARGEST SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1421	Total	C	N	O	S	0	0	0
			11186	7048	1958	2118	62			

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II 140 KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1115	Total	C	N	O	S	0	0	0
			8866	5614	1553	1644	55			

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II 45KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	267	Total	C	N	O	S	0	0	0
			2101	1320	349	419	13			

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II 32KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	177	Total	C	N	O	S	0	0	0
			1427	882	256	287	2			

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III 27 KDA POLYPEPTIDE.

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

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III 23

KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	87	Total	C	N	O	S	0	0	0
			705	451	119	132	3			

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II 19KDA POLYPEPTIDE.

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

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III 14.5 KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	135	Total	C	N	O	S	0	0	0
			1084	683	183	214	4			

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT 9.

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

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I/II/III SUBUNIT 10.

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

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE II 13.6 KDA POLYPEPTIDE.

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

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III 7.7 KDA POLYPEPTIDE.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	8	Total	C	N	O	P	0	0	0
			165	79	29	49	8			

- Molecule 14 is a RNA chain called 5'-R(*UP*UP*CP*GP*AP*CP*CP*AP*GP*GP*AP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	P	10	Total	C	N	O	P	0	0	0
			213	95	38	70	10			

- Molecule 15 is a DNA chain called 5'-D(*AP*GP*CP*TP*CP*AP*AP*GP*TP*AP*CP*TP*TP*TP*TP*CP*CP*BRUP*GP*GP*TP*CP*AP*TP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	T	19	Total	Br	C	N	O	P	0	0
			403	1	196	62	125	19		

- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn).

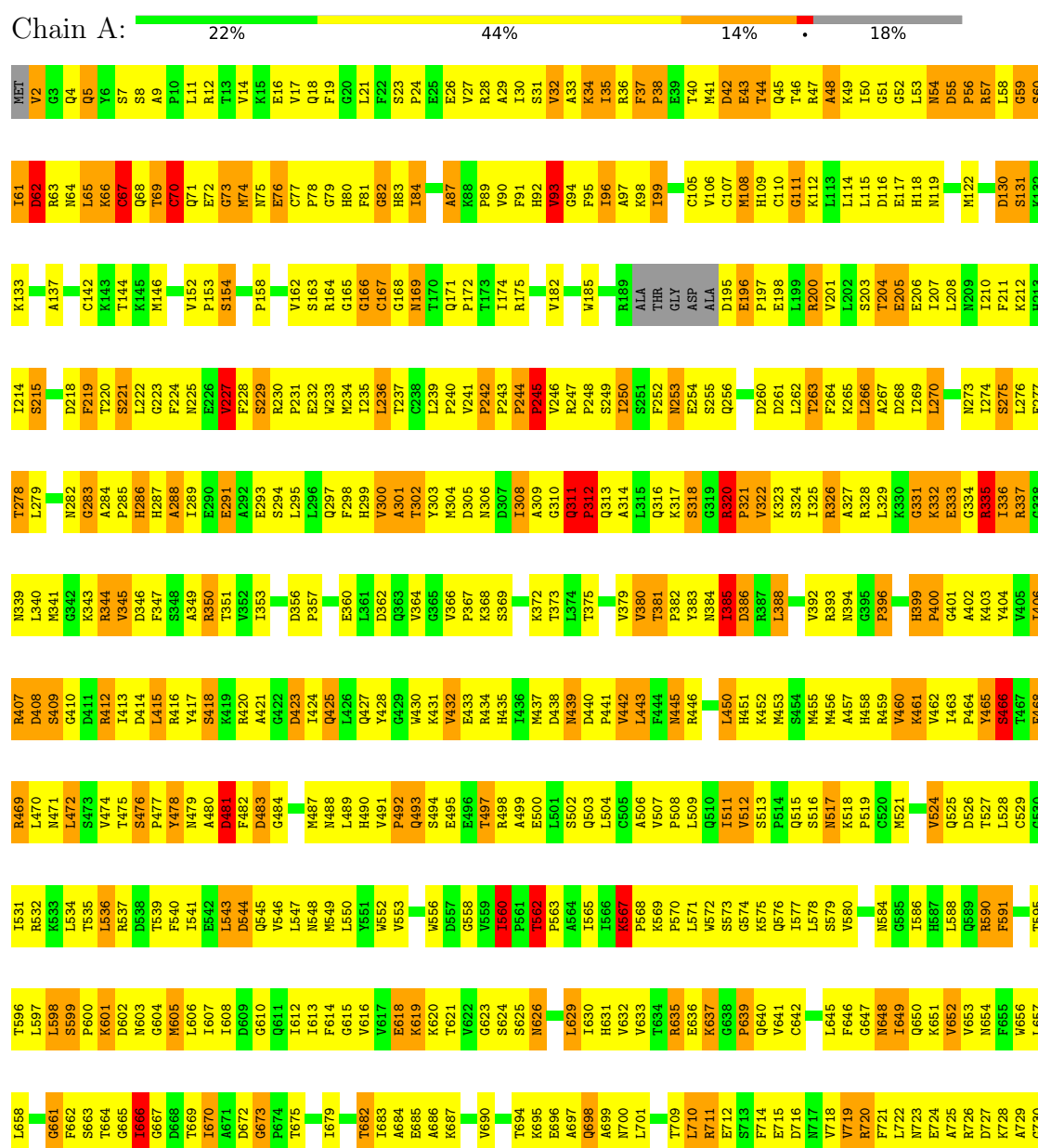
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	8	Total	Zn	0	0
			8	8		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

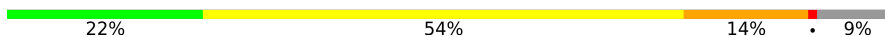
• Molecule 1: DNA-DIRECTED RNA POLYMERASE II LARGEST SUBUNIT



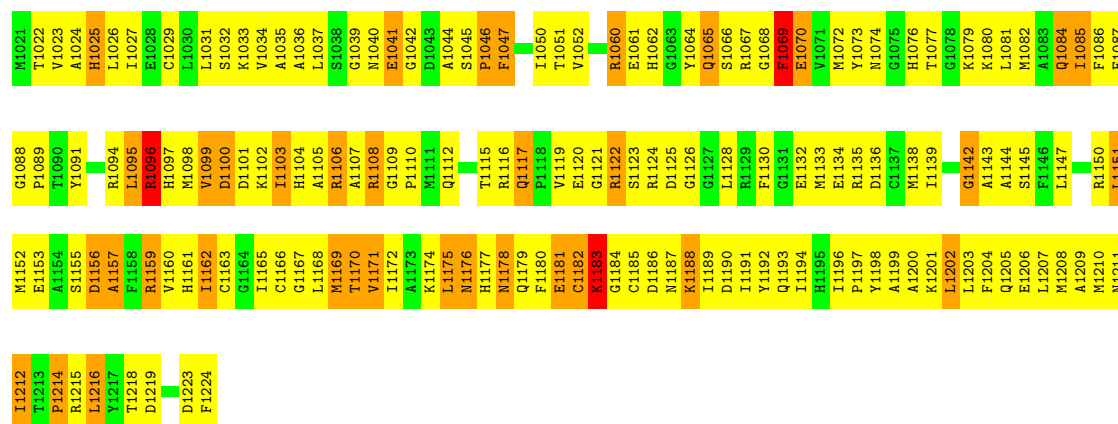
SER	PRO	THR	SER	PRO	ASN	TYR	ALA	S1449	H1387	D1323	E1256	S1189	H1124	M1063	R1001	G932	V863	F799	R731
PRO	THR	SER	GLY	F1388	G1388	P1324	TYR	L1450	G1388	P1324	E1256	P1190	A1126	V1064	G1002	Y933	I864	V800	L732
SER	PRO	THR	GLY	F1389	F1389	T1325	GLY	V1451	M1259	T1325	M1259	V1191	D1127	G1085	K1003	K934	K866	N802	E801
PRO	SER	PRO	ALA	S1392	S1392	R1326	ALA	M1454	K1260	L1192	K1261	L1192	Q1128	V1066	E1005	L936	S803	N804	V735
ASN	PRO	THR	ASP	P1455	P1455	I1327	ASP	P1455	K1262	R1194	L1263	L1195	E1129	L1068	I1006	V937	Y868	Y804	L737
TYR	THR	SER	TYR	T1394	T1394	T1329	TYR	T1455	L1263	L1195	L1263	L1195	Q1130	A1069	I1007	K938	K738	L805	K738
SER	THR	SER	GLY	G1395	G1395	N1330	GLY	P1455	E1284	L1196	L1263	L1196	Q1130	Q1070	Q1008	D939	R806	R806	D739
PRO	PRO	PRO	GLY	A1396	A1396	S1331	GLY	P1455	M1265	L1197	L1266	L1197	K1132	S1071	M1009	R940	D871	L740	L740
THR	SER	THR	ALA	L1397	L1397	I1332	ALA	L1455	M1265	L1197	L1266	L1197	K1132	I1072	A1010	K941	M808	T809	N741
THR	THR	THR	THR	M1398	M1398	I1333	THR	L1455	M1267	D1198	L1266	D1198	L1133	G1073	Q1011	F942	M873	T809	N742
PRO	SER	PRO	SER	L1399	L1399	I1334	SER	L1455	L1268	M1202	L1268	M1202	R1135	E1074	R1012	L943	D874	Q811	Q811
PRO	PRO	PRO	PRO	G1400	G1400	I1335	PRO	L1455	L1268	M1202	L1268	M1202	R1135	P1075	D1013	L943	A875	K743	K743
SER	THR	THR	PHE	S1401	S1401	M1336	PHE	L1455	I1271	K1205	L1271	K1205	I1138	A1076	A1014	F947	A876	Q744	Q744
TYR	THR	THR	GLY	F1402	F1402	V1337	GLY	L1455	R1274	D1206	L1274	D1206	E1139	T1077	T1016	N953	H877	M746	M746
PRO	PRO	PRO	ALA	E1403	E1403	V1338	ALA	L1455	G1275	L1207	L1275	L1207	T1142	Q1078	T1016	N953	H816	V747	M748
THR	PRO	THR	TYR	L1404	L1404	G1339	TYR	L1455	G1275	T1208	L1275	T1208	T1142	M1079	F1018	P955	A817	A817	
SER	TYR	THR	GLY	T1405	T1405	G1340	GLY	L1455	V1276	M1209	L1276	M1209	L1143	T1080	L1017	P957	M818		S751
PRO	SER	PRO	GLY	V1406	V1406	I1341	GLY	L1455	E1277	G1210	L1277	G1210	K1144	L1081	C1019	L956	G819	G819	S751
ALA	PRO	ALA	ALA	E1407	E1407	E1342	ALA	L1455	M1278	Q1211	L1278	Q1211	S1145	ASN	G1020	P957	L883	G819	K752
TYR	THR	THR	VAL	I1408	I1408	A1343	VAL	L1455	L1279	D1212	L1279	D1212	V1146	THR	L1021	V958	D894	G820	K753
PRO	SER	PRO	THR	L1409	L1409	G1344	THR	L1455	E1280	G1213	L1280	G1213	T1147	PHE	L1022	N959	T885	S754	S754
PRO	PRO	PRO	PRO	F1410	F1410	R1345	PRO	L1455	L1281	E1214	L1281	E1214	I1148	HIS	L1022	I960	T886	F755	F755
GLY	SER	GLY	TYR	G1413	G1413	A1346	TYR	L1455	V1282	R1215	L1282	R1215	A1149	PHE	R1025	R961	I825	I756	I756
PRO	PRO	PRO	PHE	A1414	A1414	L1348	PHE	L1455	M1284	L1216	L1284	L1216	S1150	ALA	R1026	R962	D826	N757	N757
ALA	PRO	ALA	GLY	S1415	S1415	K1349	GLY	L1455	M1284	K1217	L1284	K1217	E1151	GLY	A1027	I963	T827	I758	I758
TYR	THR	TYR	VAL	A1416	A1416	K1350	VAL	L1455	R1289	Q1218	L1289	Q1218	T1152	ALA	T1028	I964	A828	A759	A759
SER	PRO	SER	SER	L1417	L1417	V1351	SER	L1455	L1219	V1153	L1219	V1153	T1152	ALA	R1029	I964	V829	G760	G760
PRO	PRO	PRO	SER	L1418	L1418	V1352	SER	L1455	K1290	V1154	L1290	V1154	T1154	SER	R1030	N966	K830	N966	K830
LYS	ALA	PRO	PRO	D1419	D1419	V1353	PRO	L1455	V1291	K1221	L1291	K1221	D1155	K1092	V1031	A967	T831	S762	S762
GLN	THR	THR	GLY	D1420	D1420	N1354	GLY	L1455	S1293	D1223	L1293	D1223	D1157	V1094	L1032	Q968	A832	A832	C763
ASP	PRO	THR	PHE	C1421	C1421	V1355	PHE	L1455	P1294	D1223	L1294	D1223	P1158	V1094	G1033	Q969	E833	C764	C764
GLU	PRO	GLU	ASP	G1422	G1422	I1356	ASP	L1455	P1295	F1225	L1295	F1225	P1159	S1096	Y1035	F971	G835	V765	V765
LYS	SER	LYS	THR	G1423	G1423	I1356	THR	L1455	G1296	V1226	L1296	V1226	S1160	G1097	R1036	H972	G836	Q767	Q767
ASN	PRO	ASN	VAL	S1425	S1425	D1359	VAL	L1455	E1297	I1227	L1297	I1227	T1161	V1098	L1037	I973	I837	Q768	Q768
GLU	THR	GLU	LYS	A1426	A1426	V1362	LYS	L1455	V1298	V1228	L1298	V1228	V1162	P1099	T1038	D974	Q838	K773	K773
ASN	THR	ASN	ASP	N1427	N1427	V1363	ASP	L1455	V1299	V1228	L1299	V1228	T1163	R1100	D905	H966	R839	R840	R840
GLU	GLU	GLU	GLU	V1428	V1428	N1364	GLU	L1455	E1300	D1283	L1428	D1283	P1164	L1101	K1039	H975	R840	L774	L774
GLU	PRO	GLU	TYR	T1429	T1429	V1365	TYR	L1455	E1301	L1236	L1429	L1236	E1165	K1102	Q1040	T976	L841	I775	I775
ASN	THR	ASN	PRO	L1430	L1430	R1366	PRO	L1455	P1302	L1237	L1430	L1237	D1166	E1103	F1042	P978	V842	A776	A776
SER	PRO	SER	THR	G1431	G1431	H1367	THR	L1455	E1303	L1238	L1431	L1238	T1170	I1104	D1043	S979	K843	G777	G777
PRO	PRO	PRO	SER	Q1432	Q1432	M1368	SER	L1455	V1304	R1239	L1432	R1239	Q1171	L1105	V1044	D980	A844	G778	G778
SER	PRO	SER	PRO	M1433	M1433	A1369	PRO	L1455	V1305	L1239	L1433	L1239	Q1171	M1106	V1045	L981	L845	F779	F779
TYR	THR	TYR	ALA	A1434	A1434	L1370	ALA	L1455	L1306	C1240	L1434	C1240	F1174	V1107	L1046	T982	E846	V780	V780
PRO	PRO	PRO	ASP	I1435	I1435	L1371	ASP	L1455	E1307	R1241	L1435	R1241	S1175	M1110	S1047	T983	D847	D781	D781
THR	THR	THR	VAL	P1436	P1436	V1372	VAL	L1455	D1309	V1242	L1436	V1242	L1176	M1111	N1048	S915	I848	K849	K849
SER	PRO	SER	SER	G1437	G1437	D1373	SER	L1455	G1310	R1244	L1437	R1244	LEU	K1112	I1919	D986	L784	L784	L784
TYR	THR	TYR	GLY	T1438	T1438	V1374	GLY	L1455	V1311	P1245	L1438	P1245	ASP	T1113	L920	V987	Y852	P785	P785
PRO	PRO	PRO	SER	A1439	A1439	M1376	SER	L1455	N1312	LYS	L1439	LYS	GLU	P1114	Q1052	V987	D853	H786	H786
SER	PRO	SER	ASN	L1440	L1440	T1376	ASN	L1455	L1313	SER	L1440	SER	GLU	P1114	F1053	Q921	D853	N854	N854
TYR	THR	TYR	ASP	F1441	F1441	T1377	ASP	L1455	S1314	LEU	L1441	LEU	ALA	P1115	L1054	D922	N854	T782	T782
SER	THR	SER	ALA	D1442	D1442	Q1378	ALA	L1455	E1315	ASP	L1442	ASP	GLU	T1116	R1055	D922	T855	T783	T783
PRO	PRO	PRO	MET	V1443	V1443	G1379	MET	L1455	V1316	ALA	L1443	ALA	GLN	T1117	S1056	L925	T856	K789	K789
ALA	THR	ALA	ALA	M1444	M1444	G1380	ALA	L1455	M1317	GLU	L1444	GLU	GLN	V1119	V1057	Q926	R857	R857	P794
SER	THR	SER	GLY	T1445	T1445	L1381	GLY	L1455	T1318	THR	L1445	THR	PHE	L1120	H1058	L928	N858	E795	E795
PRO	PRO	PRO	GLY	D1446	D1446	L1381	GLY	L1455	V1319	GLU	L1446	GLU	ASP	L1120	H1059	L928	S859	S796	S796
PRO	PRO	PRO	PHE	E1447	E1447	T1385	PHE	L1455	P1320	A1254	L1447	A1254	Q1187	E1121	G1061	L929	L860	K797	K797
THR	THR	THR	THR	E1448	E1448	R1386	THR	L1455	E1255	E1255	L1448	E1255	Q1188	G1123	E1062	E931	N862	G798	G798

● Molecule 2: DNA-DIRECTED RNA POLYMERASE II 140 KDA POLYPEPTIDE

Chain B:

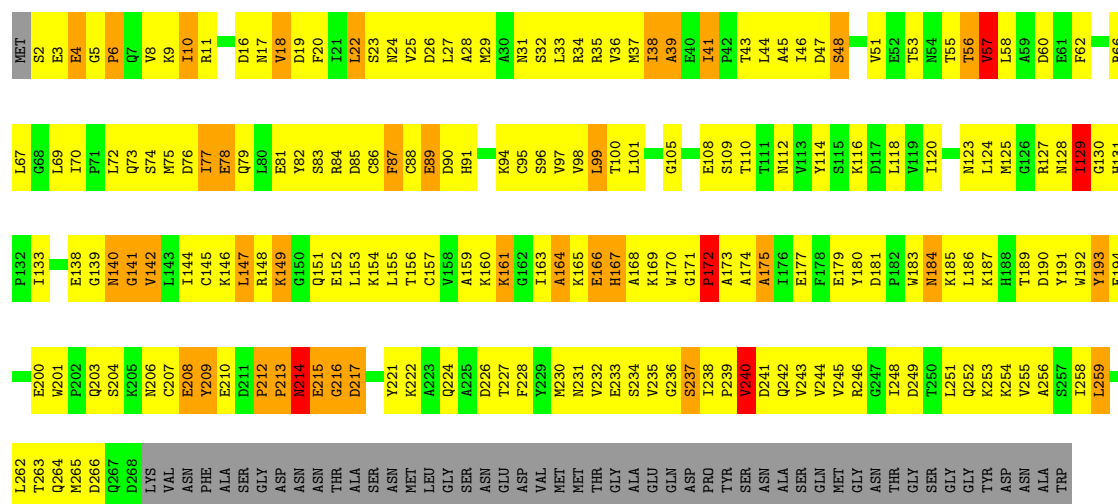


D959	G960	L961	G962	F963	G964	K965	V966																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
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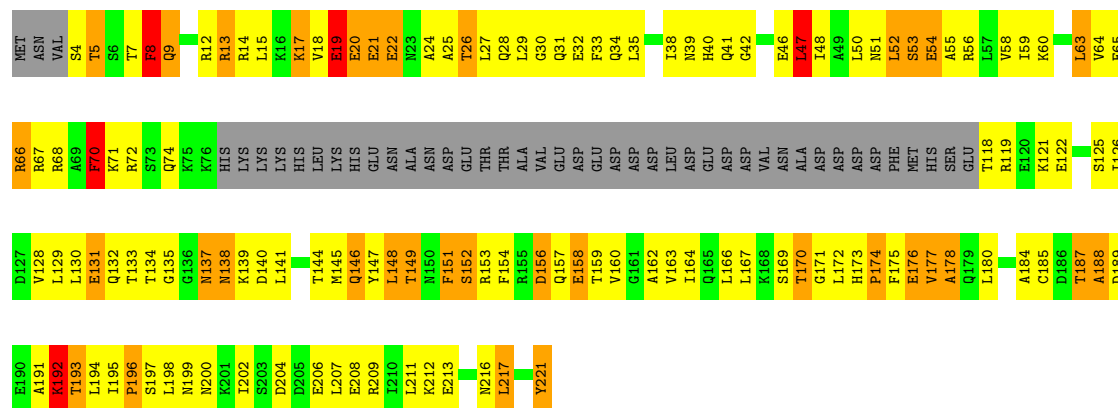
• Molecule 3: DNA-DIRECTED RNA POLYMERASE II 45KDA POLYPEPTIDE

Chain C: 22% 49% 11% 16%

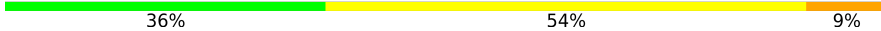


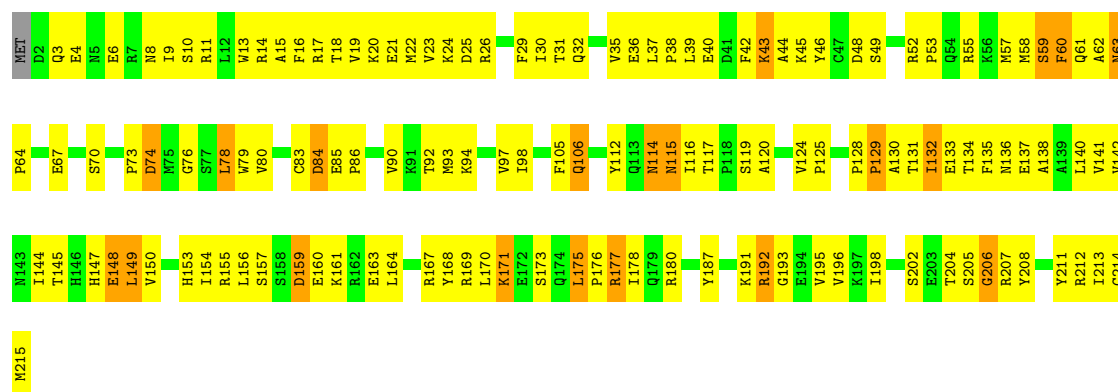
• Molecule 4: DNA-DIRECTED RNA POLYMERASE II 32KDA POLYPEPTIDE

Chain D: 20% 42% 15% 20%



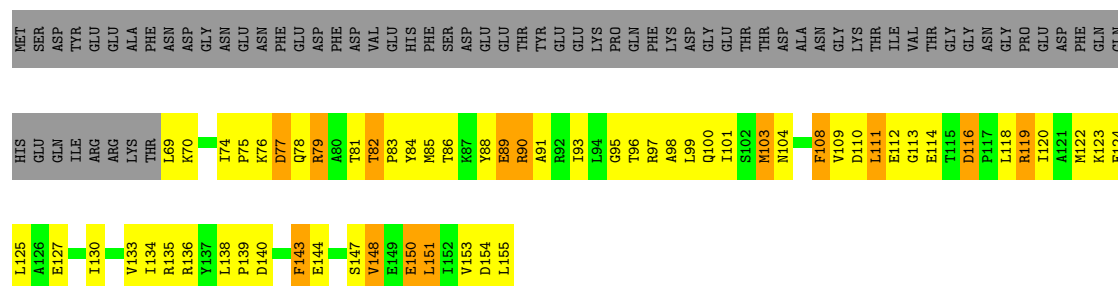
• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III 27 KDA POLYPEPTIDE

Chain E: 

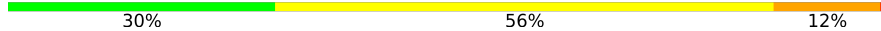


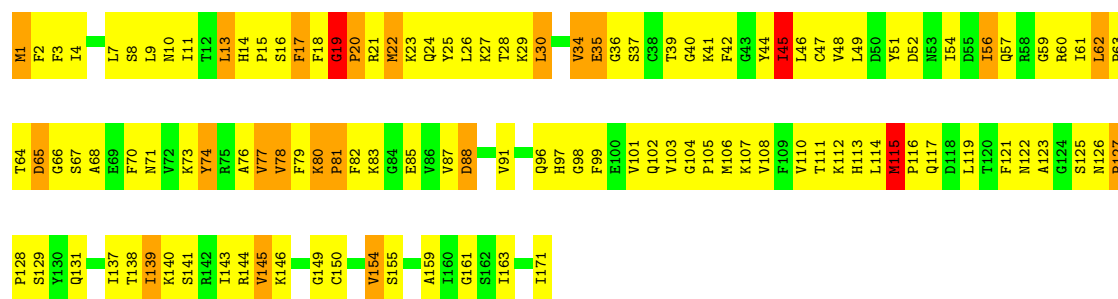
- Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III 23 KDA POLYPEPTIDE

Chain F: 

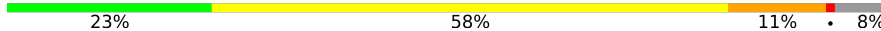


- Molecule 7: DNA-DIRECTED RNA POLYMERASE II 19KDA POLYPEPTIDE

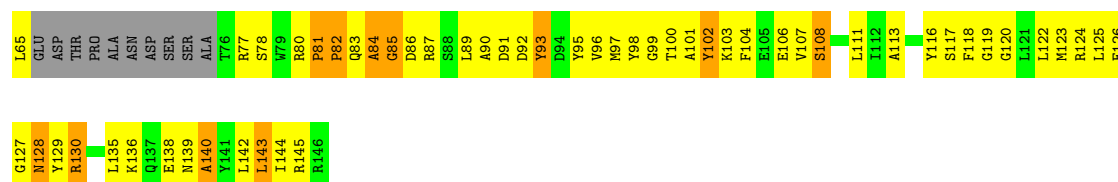
Chain G: 



- Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III 14.5 KDA POLYPEPTIDE

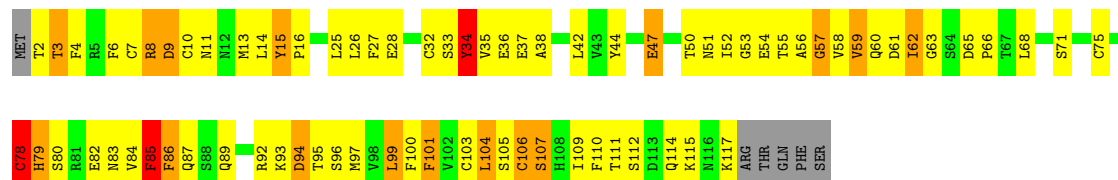
Chain H: 





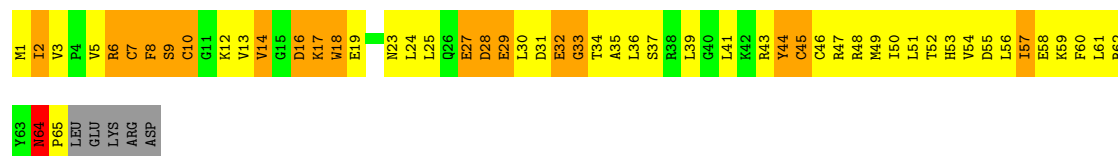
• Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT 9

Chain I: 32% 48% 13% • 5%



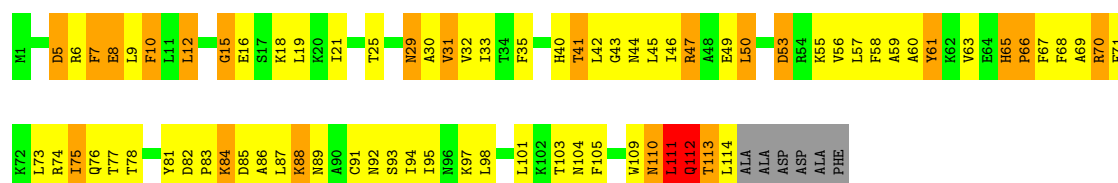
• Molecule 10: DNA-DIRECTED RNA POLYMERASES I/II/III SUBUNIT 10

Chain J: 16% 50% 26% • 7%



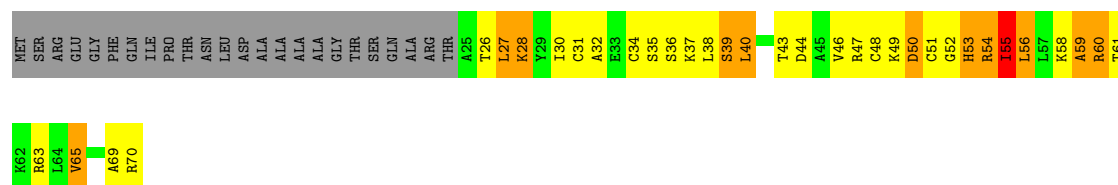
• Molecule 11: DNA-DIRECTED RNA POLYMERASE II 13.6 KDA POLYPEPTIDE

Chain K: 31% 45% 18% • 5%



• Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III 7.7 KDA POLYPEPTIDE

Chain L: 17% 31% 16% • 34%

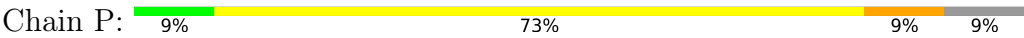


• Molecule 13: 5'-D(*TP*AP*AP*GP*TP*AP*CP*TP*TP*GP *AP*GP*CP*T)-3'

Chain N: 57% 43%

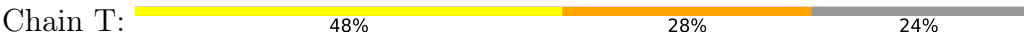
T0	A1	A2	G3	T4	A5	C6	T7	DT	DG	DA	DG	DC	DT
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● Molecule 14: 5'-R(*UP*UP*CP*GP*AP*CP*CP*AP*GP*GP*AP)-3'



U0	U1	C2	G3	A4	C5	C6	A7	G8	G9	A
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● Molecule 15: 5'-D(*AP*GP*CP*TP*CP*AP*AP*GP*TP*AP *CP*TP*TP*TTP*TP*CP*CP *BRUP*GP*GP*TP*CP*AP*TP*T)-3'



DA	DG	DC	DT	DC	DA	A10	G11	T12	A13	C14	T15	T16	M17	T19	C20	C21	U22	G23	G24	T25	C26	A27	T28	T29
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4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	223.58Å 393.49Å 283.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 4.00	Depositor
% Data completeness (in resolution range)	99.3 (50.00-4.00)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.292 , 0.301	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	32010	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.60	0/11385	1.11	93/15393 (0.6%)
2	B	0.56	0/9037	1.05	53/12181 (0.4%)
3	C	0.58	0/2138	1.10	13/2896 (0.4%)
4	D	0.50	0/1437	1.09	15/1925 (0.8%)
5	E	0.50	0/1788	1.01	15/2406 (0.6%)
6	F	0.67	0/716	1.15	6/964 (0.6%)
7	G	0.59	0/1368	1.14	17/1844 (0.9%)
8	H	0.48	0/1102	1.00	7/1492 (0.5%)
9	I	0.46	0/962	1.03	5/1295 (0.4%)
10	J	0.61	0/541	0.99	1/727 (0.1%)
11	K	0.66	1/937 (0.1%)	1.20	11/1265 (0.9%)
12	L	0.56	0/366	0.92	0/485
13	N	0.61	0/184	0.91	0/280
14	P	0.45	0/237	0.92	0/367
15	T	0.63	0/382	1.21	5/582 (0.9%)
All	All	0.57	1/32580 (0.0%)	1.08	241/44102 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	113	THR	CA-C	5.60	1.59	1.53

All (241) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	113	THR	N-CA-C	15.33	128.47	108.24
1	A	56	PRO	N-CA-C	-12.29	101.90	114.68
4	D	26	THR	N-CA-C	-11.82	96.65	112.26
2	B	1185	CYS	N-CA-C	-10.78	100.13	113.18
2	B	473	MET	N-CA-C	-10.72	99.86	113.16
7	G	22	MET	N-CA-C	-10.17	99.16	112.68
1	A	452	LYS	N-CA-C	-10.03	100.43	111.36
4	D	54	GLU	N-CA-C	-9.88	101.35	113.41
2	B	427	ASP	N-CA-C	-9.63	101.30	113.43
7	G	62	LEU	CA-C-N	-9.30	108.21	119.84
7	G	62	LEU	C-N-CA	-9.30	108.21	119.84
1	A	982	THR	N-CA-C	-8.99	98.93	110.53
4	D	72	ARG	N-CA-C	-8.96	101.43	111.82
1	A	288	ALA	N-CA-C	-8.82	100.50	112.94
1	A	1261	LYS	N-CA-C	-8.66	104.74	114.62
2	B	574	SER	CA-C-N	8.61	127.93	118.97
2	B	574	SER	C-N-CA	8.61	127.93	118.97
7	G	52	ASP	N-CA-C	8.40	120.21	111.14
1	A	242	PRO	CA-C-N	8.34	128.97	120.38
1	A	242	PRO	C-N-CA	8.34	128.97	120.38
1	A	1422	ARG	N-CA-C	-8.26	102.64	114.12
1	A	344	ARG	N-CA-C	-8.11	98.51	110.52
1	A	466	SER	N-CA-C	8.10	124.21	113.20
3	C	39	ALA	N-CA-C	7.82	123.50	113.88
1	A	266	LEU	N-CA-C	-7.76	102.77	111.07
2	B	66	ASP	N-CA-C	-7.70	103.20	112.59
1	A	425	GLN	N-CA-C	-7.66	96.42	108.90
3	C	38	ILE	N-CA-C	7.56	117.64	110.30
3	C	41	ILE	CA-C-N	7.55	128.01	119.93
3	C	41	ILE	C-N-CA	7.55	128.01	119.93
8	H	85	GLY	N-CA-C	-7.45	103.48	113.24
11	K	18	LYS	N-CA-C	-7.43	103.18	111.28
2	B	363	HIS	N-CA-C	-7.38	101.01	110.53
2	B	296	GLU	N-CA-C	-7.35	103.29	111.82
2	B	294	ASP	N-CA-C	-7.33	101.39	110.41
7	G	129	SER	N-CA-C	7.29	117.64	108.45
2	B	112	LEU	N-CA-C	7.20	121.13	110.48
1	A	468	PHE	N-CA-C	-7.17	99.06	109.59
5	E	171	LYS	N-CA-C	-7.17	99.31	110.42
1	A	567	LYS	CA-C-N	-7.16	110.89	119.84
1	A	567	LYS	C-N-CA	-7.16	110.89	119.84
1	A	1291	VAL	CA-C-N	7.16	128.79	119.84
1	A	1291	VAL	C-N-CA	7.16	128.79	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	539	THR	N-CA-C	7.12	120.28	108.96
3	C	57	VAL	N-CA-C	-7.10	105.69	113.43
1	A	60	SER	N-CA-C	7.07	117.61	108.34
1	A	938	LYS	N-CA-C	-7.07	103.50	111.07
15	T	19	DT	C5'-C4'-C3'	-7.05	104.33	114.90
7	G	19	GLY	CA-C-N	7.04	128.65	119.84
7	G	19	GLY	C-N-CA	7.04	128.65	119.84
5	E	173	SER	N-CA-C	7.04	118.95	111.28
1	A	560	ILE	CA-C-N	7.00	126.97	119.76
1	A	560	ILE	C-N-CA	7.00	126.97	119.76
1	A	1243	VAL	N-CA-C	6.98	117.56	108.35
1	A	1344	GLY	N-CA-C	-6.98	104.41	112.50
1	A	472	LEU	N-CA-C	6.93	118.63	111.14
4	D	38	ILE	N-CA-C	6.80	117.69	108.17
2	B	1096	ARG	NE-CZ-NH1	-6.78	114.72	121.50
6	F	127	GLU	N-CA-C	-6.78	104.58	112.92
2	B	395	GLN	N-CA-C	-6.78	101.58	110.53
11	K	65	HIS	CA-C-N	6.73	128.25	119.84
11	K	65	HIS	C-N-CA	6.73	128.25	119.84
1	A	82	GLY	N-CA-C	-6.68	101.38	111.14
1	A	511	ILE	N-CA-C	6.68	118.24	110.62
1	A	861	GLY	N-CA-C	-6.66	105.92	115.64
1	A	291	GLU	N-CA-C	-6.65	105.20	113.38
6	F	77	ASP	N-CA-C	-6.64	100.14	110.17
2	B	606	LYS	N-CA-C	-6.62	104.84	113.12
1	A	1064	VAL	N-CA-C	6.56	118.10	110.62
6	F	82	THR	CA-C-N	6.52	126.21	119.82
6	F	82	THR	C-N-CA	6.52	126.21	119.82
7	G	2	PHE	N-CA-C	-6.51	99.91	110.20
1	A	1275	GLY	N-CA-C	6.45	120.14	112.33
1	A	293	GLU	N-CA-C	-6.40	105.63	113.50
2	B	208	SER	N-CA-C	6.39	118.27	110.41
2	B	628	THR	N-CA-C	-6.39	105.24	114.12
4	D	176	GLU	N-CA-C	-6.38	104.25	111.14
1	A	598	LEU	N-CA-C	-6.38	104.28	113.21
1	A	553	VAL	CA-C-N	6.31	127.73	119.84
1	A	553	VAL	C-N-CA	6.31	127.73	119.84
11	K	111	LEU	N-CA-C	6.30	124.22	110.80
4	D	171	GLY	N-CA-C	-6.30	106.55	115.30
1	A	999	VAL	N-CA-C	-6.29	105.57	111.48
1	A	710	LEU	N-CA-C	-6.29	104.43	111.28
1	A	698	GLN	N-CA-C	-6.28	105.89	112.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	360	GLU	N-CA-C	-6.27	102.26	110.53
2	B	949	VAL	N-CA-C	-6.26	100.70	110.09
4	D	188	ALA	N-CA-C	-6.22	104.60	111.82
2	B	1009	ASP	N-CA-C	-6.21	103.81	112.45
1	A	1403	GLU	N-CA-C	6.21	123.03	113.28
1	A	432	VAL	CB-CA-C	-6.20	104.96	111.23
2	B	99	LYS	CA-C-N	6.19	127.58	119.84
2	B	99	LYS	C-N-CA	6.19	127.58	119.84
1	A	1262	LYS	N-CA-C	-6.15	104.68	111.82
1	A	513	SER	N-CA-C	6.15	118.53	109.62
2	B	748	ILE	N-CA-C	-6.13	104.73	113.07
1	A	137	ALA	N-CA-C	-6.11	105.85	113.55
1	A	513	SER	CA-C-N	6.11	125.73	119.56
1	A	513	SER	C-N-CA	6.11	125.73	119.56
5	E	4	GLU	N-CA-C	6.10	117.73	111.14
2	B	1025	HIS	N-CA-C	-6.09	104.55	111.07
2	B	472	ALA	N-CA-C	6.07	117.63	108.46
4	D	158	GLU	N-CA-C	-6.07	105.53	113.12
15	T	24	DG	C2'-C3'-O3'	-6.07	102.40	111.50
2	B	837	ASP	N-CA-C	6.06	120.22	111.56
1	A	1311	VAL	N-CA-C	6.03	117.61	107.18
1	A	491	VAL	N-CA-C	6.00	114.58	107.73
1	A	67	CYS	N-CA-C	-6.00	98.02	110.80
1	A	87	ALA	N-CA-C	-5.97	103.54	111.96
1	A	311	GLN	N-CA-C	5.95	122.96	109.81
3	C	96	SER	N-CA-C	5.93	118.30	108.99
2	B	292	ILE	N-CA-C	5.93	121.68	108.88
1	A	931	GLU	N-CA-C	-5.91	104.75	111.07
5	E	177	ARG	N-CA-C	5.89	119.15	109.85
15	T	10	DA	C2'-C3'-O3'	5.88	120.33	111.50
1	A	158	PRO	N-CA-C	-5.88	106.33	114.27
1	A	415	LEU	N-CA-C	5.87	119.97	112.34
1	A	320	ARG	CA-C-N	5.87	127.18	119.84
1	A	320	ARG	C-N-CA	5.87	127.18	119.84
3	C	5	GLY	CA-C-N	5.87	127.17	119.84
3	C	5	GLY	C-N-CA	5.87	127.17	119.84
1	A	440	ASP	N-CA-C	-5.86	100.14	109.04
1	A	524	VAL	N-CA-C	5.84	115.94	108.82
8	H	42	ILE	N-CA-C	5.83	116.04	108.35
7	G	45	ILE	N-CA-C	-5.82	99.32	108.23
1	A	294	SER	N-CA-C	-5.81	105.69	112.89
6	F	119	ARG	N-CA-C	-5.81	104.31	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	392	ARG	N-CA-C	-5.80	106.85	114.04
1	A	778	GLY	N-CA-C	-5.80	105.35	112.77
8	H	129	TYR	N-CA-C	5.79	120.34	112.88
8	H	16	ASP	N-CA-C	5.78	119.76	107.91
1	A	1104	ILE	N-CA-C	5.78	116.56	110.72
2	B	543	SER	N-CA-C	5.78	117.75	110.24
5	E	63	ASN	CA-C-N	5.77	125.95	119.90
5	E	63	ASN	C-N-CA	5.77	125.95	119.90
7	G	104	GLY	CA-C-N	5.75	125.45	119.82
7	G	104	GLY	C-N-CA	5.75	125.45	119.82
11	K	75	ILE	N-CA-C	5.74	116.39	108.12
15	T	28	DT	C2'-C3'-O3'	-5.74	102.89	111.50
1	A	690	VAL	N-CA-C	-5.73	106.63	111.56
1	A	927	VAL	N-CA-C	-5.73	106.12	111.45
7	G	65	ASP	N-CA-C	-5.73	100.00	108.99
2	B	1151	LEU	N-CA-C	5.69	117.56	111.36
9	I	104	LEU	N-CA-C	-5.68	106.31	113.18
1	A	682	THR	N-CA-C	-5.68	106.31	113.18
2	B	1142	GLY	N-CA-C	-5.67	107.41	115.30
5	E	159	ASP	N-CA-C	-5.65	105.17	112.68
8	H	80	ARG	CA-C-N	5.65	126.20	120.38
8	H	80	ARG	C-N-CA	5.65	126.20	120.38
4	D	66	ARG	N-CA-C	-5.62	103.94	112.04
5	E	149	LEU	N-CA-C	5.61	117.09	110.97
2	B	1008	PRO	N-CA-C	5.61	120.29	111.38
2	B	1104	HIS	N-CA-C	5.61	117.51	108.32
3	C	200	GLU	N-CA-C	5.59	118.31	111.82
11	K	8	GLU	N-CA-C	-5.57	106.15	113.17
5	E	84	ASP	N-CA-C	-5.56	106.34	113.02
2	B	937	ALA	N-CA-C	-5.54	105.46	113.21
2	B	213	ILE	N-CA-C	5.53	116.56	108.53
3	C	194	GLU	N-CA-C	-5.53	107.18	114.04
11	K	84	LYS	N-CA-C	-5.53	104.47	111.11
1	A	590	ARG	N-CA-C	5.52	116.89	108.12
2	B	1013	ASN	N-CA-C	5.49	117.58	109.50
1	A	229	SER	N-CA-C	5.49	116.38	107.32
10	J	64	ASN	N-CA-C	5.48	121.92	109.81
1	A	1445	ILE	CB-CA-C	-5.46	104.69	111.08
1	A	227	VAL	N-CA-C	5.46	116.50	111.81
1	A	413	ILE	CB-CA-C	-5.44	104.38	110.96
1	A	928	LEU	N-CA-C	-5.43	105.28	111.14
1	A	337	ARG	N-CA-C	5.42	118.11	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	VAL	CB-CA-C	-5.40	105.34	111.55
5	E	6	GLU	N-CA-C	-5.39	105.06	111.69
11	K	113	THR	CA-C-N	5.39	131.40	121.70
11	K	113	THR	C-N-CA	5.39	131.40	121.70
4	D	138	ASN	N-CA-C	-5.39	104.17	111.55
2	B	1117	GLN	N-CA-C	-5.38	103.85	110.31
1	A	776	ALA	N-CA-C	5.37	118.38	109.94
2	B	872	GLU	N-CA-C	-5.35	103.63	110.53
7	G	145	VAL	N-CA-C	5.35	117.49	109.20
7	G	30	LEU	N-CA-C	-5.35	104.50	111.02
2	B	964	VAL	N-CA-C	5.34	116.42	108.46
9	I	53	GLY	N-CA-C	-5.34	107.64	114.85
1	A	1102	LYS	N-CA-C	-5.34	105.36	111.07
2	B	111	ALA	N-CA-C	-5.33	98.60	107.99
2	B	782	LEU	N-CA-C	-5.33	100.03	108.14
8	H	12	VAL	N-CA-C	5.33	115.27	108.12
3	C	234	SER	N-CA-C	5.33	116.63	108.42
1	A	478	TYR	N-CA-C	-5.32	106.30	112.89
9	I	85	PHE	N-CA-C	5.31	118.19	110.17
2	B	640	VAL	N-CA-C	5.30	117.99	112.90
1	A	1444	MET	N-CA-C	5.28	117.41	109.23
4	D	169	SER	N-CA-C	-5.28	105.69	113.61
1	A	1343	ALA	N-CA-C	-5.26	105.61	112.23
2	B	366	GLN	N-CA-C	-5.21	106.32	113.30
1	A	481	ASP	N-CA-C	-5.20	102.47	109.95
11	K	31	VAL	N-CA-C	5.18	116.17	108.65
1	A	1299	VAL	N-CA-C	5.18	117.50	108.90
4	D	178	ALA	N-CA-C	-5.18	105.18	112.12
15	T	26	DC	C2'-C3'-O3'	-5.17	103.75	111.50
3	C	193	TYR	N-CA-C	5.14	116.11	108.86
1	A	236	LEU	N-CA-C	5.14	117.11	109.25
1	A	204	THR	N-CA-C	-5.13	104.77	111.02
1	A	637	LYS	N-CA-C	5.13	116.87	111.28
2	B	681	TRP	N-CA-C	-5.12	103.72	111.56
2	B	663	ALA	N-CA-C	-5.12	105.78	111.36
1	A	301	ALA	N-CA-C	-5.12	104.74	111.96
4	D	157	GLN	N-CA-C	-5.11	106.32	113.37
2	B	732	SER	N-CA-C	5.11	116.06	108.86
1	A	1155	ASP	CA-C-N	5.10	125.93	120.47
1	A	1155	ASP	C-N-CA	5.10	125.93	120.47
7	G	127	PRO	CA-C-N	5.10	125.11	119.90
7	G	127	PRO	C-N-CA	5.10	125.11	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1070	GLU	N-CA-C	-5.10	100.77	108.52
2	B	468	GLU	N-CA-C	5.09	115.54	108.00
7	G	56	ILE	CB-CA-C	-5.09	106.58	111.06
9	I	65	ASP	CA-C-N	5.09	124.40	118.85
9	I	65	ASP	C-N-CA	5.09	124.40	118.85
5	E	150	VAL	CA-C-N	5.09	125.30	120.31
5	E	150	VAL	C-N-CA	5.09	125.30	120.31
2	B	882	THR	N-CA-C	5.08	119.71	111.37
2	B	192	LEU	N-CA-C	-5.08	107.12	113.72
2	B	215	GLN	N-CA-C	5.08	115.69	108.54
5	E	52	ARG	CA-C-N	5.07	125.23	119.90
5	E	52	ARG	C-N-CA	5.07	125.23	119.90
2	B	934	LYS	N-CA-C	5.07	117.89	107.69
3	C	109	SER	N-CA-C	5.07	119.02	108.53
2	B	361	LEU	CA-C-N	5.06	126.16	119.84
2	B	361	LEU	C-N-CA	5.06	126.16	119.84
4	D	217	LEU	N-CA-C	-5.06	107.28	113.50
1	A	1009	ASN	N-CA-C	-5.05	105.43	112.45
4	D	70	PHE	N-CA-C	-5.05	106.81	113.17
2	B	858	SER	N-CA-C	5.05	117.82	107.37
1	A	562	THR	CA-C-N	5.04	125.04	119.90
1	A	562	THR	C-N-CA	5.04	125.04	119.90
2	B	1015	HIS	N-CA-C	5.04	118.19	111.75
1	A	476	SER	CA-C-N	-5.02	113.56	119.84
1	A	476	SER	C-N-CA	-5.02	113.56	119.84
1	A	983	ILE	N-CA-C	-5.02	104.71	111.44
5	E	32	GLN	N-CA-C	-5.01	106.42	112.54
6	F	108	PHE	N-CA-C	5.01	118.54	112.93
1	A	166	GLY	N-CA-C	5.01	118.43	110.96
1	A	865	GLN	N-CA-C	-5.01	100.11	108.32

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	303	TYR	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	A	11186	0	11266	1469	0
2	B	8866	0	8898	1140	0
3	C	2101	0	2055	288	0
4	D	1427	0	1451	161	0
5	E	1752	0	1776	155	0
6	F	705	0	730	82	0
7	G	1340	0	1357	172	0
8	H	1084	0	1057	139	0
9	I	944	0	901	110	0
10	J	532	0	542	107	0
11	K	919	0	929	122	0
12	L	364	0	386	49	0
13	N	165	0	92	14	0
14	P	213	0	109	22	0
15	T	403	0	229	56	0
16	A	1	0	0	0	0
17	A	8	0	0	0	0
All	All	32010	0	31778	3778	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 59.

All (3778) 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)
8:H:100:THR:HG23	8:H:138:GLU:HA	1.33	1.11
2:B:343:ILE:HG23	2:B:347:LYS:HB2	1.13	1.11
1:A:34:LYS:HD3	1:A:57:ARG:HH22	1.07	1.10
1:A:541:ILE:HD13	1:A:549:MET:HE1	1.32	1.09
15:T:16:DT:C5	15:T:17:TT:H5A1	1.88	1.09
1:A:53:LEU:HD23	1:A:54:ASN:H	0.94	1.09
7:G:138:THR:HG22	7:G:139:ILE:H	1.19	1.08
2:B:336:ARG:HG2	2:B:348:ARG:HD3	1.36	1.08
1:A:855:THR:HG21	1:A:857:ARG:HE	1.13	1.08
11:K:47:ARG:HB3	11:K:47:ARG:HH11	1.15	1.08
2:B:806:THR:HG22	2:B:808:ALA:H	1.11	1.07
2:B:273:LEU:HB2	2:B:276:ILE:HD12	1.25	1.07
2:B:467:GLY:H	2:B:475:SER:HB3	1.17	1.07
10:J:3:VAL:HG21	10:J:18:TRP:HB2	1.37	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:LEU:HD23	1:A:54:ASN:N	1.68	1.06
2:B:189:LEU:HA	2:B:192:LEU:HD12	1.37	1.06
1:A:779:PHE:HE1	1:A:785:PRO:HD3	1.21	1.05
9:I:34:TYR:HD2	9:I:35:VAL:N	1.53	1.05
1:A:58:LEU:HD12	1:A:59:GLY:H	1.17	1.04
15:T:15:DT:C6	15:T:16:DT:H72	1.90	1.04
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.24	1.03
2:B:882:THR:HG22	2:B:884:ARG:H	1.20	1.03
2:B:65:GLU:HG3	2:B:66:ASP:H	1.21	1.02
2:B:515:HIS:H	2:B:518:HIS:HD2	1.07	1.02
1:A:963:ILE:HD11	1:A:1048:ASN:HB3	1.36	1.02
2:B:214:ALA:HB3	2:B:498:THR:HA	1.42	1.02
2:B:336:ARG:HH22	2:B:345:LYS:HE2	1.23	1.02
2:B:589:VAL:HG12	2:B:590:HIS:H	1.22	1.01
7:G:15:PRO:HA	7:G:18:PHE:CD1	1.94	1.01
1:A:356:ASP:HB2	1:A:469:ARG:NH1	1.76	1.01
7:G:14:HIS:CD2	7:G:16:SER:HB2	1.95	1.01
2:B:1002:THR:HG21	2:B:1006:ILE:HD12	1.44	1.00
3:C:101:LEU:HD13	3:C:118:LEU:HD23	1.41	1.00
1:A:524:VAL:HG12	1:A:525:GLN:H	1.25	1.00
9:I:8:ARG:HG3	9:I:34:TYR:HE1	1.25	0.99
10:J:1:MET:N	10:J:57:ILE:H	1.61	0.99
15:T:28:DT:H2''	15:T:29:DT:H5'	1.44	0.99
5:E:94:LYS:HE2	5:E:98:ILE:HD11	1.41	0.98
1:A:40:THR:HG22	1:A:41:MET:HG3	1.44	0.98
1:A:903:ASN:HD22	1:A:904:THR:N	1.62	0.98
4:D:144:THR:O	4:D:148:LEU:HB2	1.64	0.97
2:B:879:ARG:HH11	2:B:883:LEU:HD22	1.30	0.97
7:G:7:LEU:HB2	7:G:74:TYR:CE2	1.99	0.97
2:B:510:LYS:CG	2:B:511:PRO:HD3	1.94	0.97
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.42	0.97
1:A:1094:VAL:HG12	1:A:1095:THR:H	1.27	0.96
1:A:567:LYS:CG	1:A:568:PRO:HD2	1.95	0.96
1:A:567:LYS:HB3	8:H:96:VAL:H	1.30	0.96
3:C:47:ASP:HA	12:L:69:ALA:HB3	1.47	0.95
3:C:166:GLU:HG3	11:K:10:PHE:HZ	1.30	0.95
1:A:225:ASN:HD22	1:A:228:PHE:H	1.11	0.95
2:B:232:SER:HB3	2:B:261:ARG:HH21	1.28	0.95
4:D:40:HIS:HB3	7:G:73:LYS:NZ	1.80	0.95
1:A:353:ILE:HD13	1:A:487:MET:HE2	1.49	0.95
1:A:913:LEU:HD12	1:A:914:GLU:H	1.31	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:364:ILE:HG12	2:B:585:VAL:HG13	1.44	0.95
2:B:1159:ARG:HD3	2:B:1193:GLN:HG3	1.46	0.94
11:K:65:HIS:HD2	11:K:67:PHE:H	1.11	0.94
1:A:14:VAL:HG21	2:B:1216:LEU:HD13	1.49	0.94
11:K:12:LEU:H	11:K:12:LEU:HD12	1.32	0.94
1:A:254:GLU:HB2	2:B:935:ARG:HH12	1.33	0.94
1:A:535:THR:HG21	1:A:616:VAL:HA	1.49	0.94
3:C:43:THR:HG22	3:C:44:LEU:H	1.29	0.94
10:J:5:VAL:HG12	10:J:6:ARG:HG3	1.48	0.94
10:J:1:MET:H1	10:J:57:ILE:N	1.64	0.93
1:A:709:THR:HG22	1:A:711:ARG:H	1.30	0.93
2:B:1084:GLN:HE21	2:B:1084:GLN:H	1.11	0.93
1:A:67:CYS:O	1:A:70:CYS:HB3	1.68	0.93
1:A:382:PRO:HB3	1:A:428:TYR:HE2	1.33	0.93
9:I:34:TYR:CD2	9:I:35:VAL:N	2.37	0.93
1:A:53:LEU:CD2	1:A:54:ASN:H	1.81	0.93
7:G:34:VAL:HG12	7:G:45:ILE:HG21	1.51	0.92
2:B:343:ILE:CG2	2:B:348:ARG:HG3	2.00	0.92
2:B:1187:ASN:O	2:B:1188:LYS:HB2	1.66	0.92
2:B:821:GLN:HE22	2:B:851:PHE:HA	1.35	0.92
1:A:58:LEU:CD1	1:A:59:GLY:H	1.83	0.92
2:B:1201:LYS:HE2	2:B:1205:GLN:OE1	1.70	0.91
6:F:111:LEU:HD12	6:F:111:LEU:H	1.34	0.91
1:A:63:ARG:HA	1:A:74:MET:SD	2.09	0.91
1:A:754:SER:H	1:A:757:ASN:HD22	1.12	0.91
3:C:6:PRO:HB3	3:C:25:VAL:HG12	1.51	0.91
2:B:467:GLY:N	2:B:475:SER:HB3	1.84	0.91
1:A:1017:LEU:HB2	5:E:206:GLY:H	1.35	0.91
3:C:47:ASP:HA	12:L:69:ALA:CB	2.01	0.90
9:I:85:PHE:H	9:I:85:PHE:HD2	1.19	0.90
1:A:901:LEU:H	1:A:926:GLN:NE2	1.69	0.90
2:B:577:ALA:HB1	2:B:589:VAL:HG11	1.53	0.90
2:B:622:LYS:HE2	9:I:59:VAL:HG22	1.51	0.90
1:A:34:LYS:HE3	1:A:57:ARG:HH12	1.36	0.90
15:T:17:TT:H4R	15:T:19:DT:OP2	1.69	0.90
1:A:590:ARG:NH2	1:A:620:LYS:HB3	1.87	0.90
1:A:115:LEU:HB2	1:A:122:MET:HE2	1.53	0.89
8:H:4:THR:HA	8:H:60:ALA:HB2	1.53	0.89
2:B:1007:VAL:HG22	2:B:1008:PRO:HD2	1.52	0.89
1:A:779:PHE:CE1	1:A:785:PRO:HD3	2.08	0.89
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.07	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:549:THR:HG22	2:B:550:ASP:H	1.36	0.89
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.54	0.89
1:A:1409:LEU:HD13	2:B:1207:LEU:HD11	1.52	0.89
4:D:40:HIS:HB3	7:G:73:LYS:HZ3	1.35	0.89
2:B:510:LYS:HG3	2:B:511:PRO:HD3	1.55	0.88
3:C:66:ARG:NH1	10:J:2:ILE:HG21	1.87	0.88
3:C:57:VAL:HG11	10:J:60:PHE:HB3	1.52	0.88
8:H:36:CYS:HA	8:H:126:GLU:O	1.72	0.88
1:A:285:PRO:HG2	1:A:288:ALA:HB3	1.56	0.88
1:A:567:LYS:HG3	1:A:568:PRO:HD2	1.55	0.88
5:E:19:VAL:O	5:E:23:VAL:HG23	1.74	0.88
15:T:16:DT:C6	15:T:17:TT:H5A1	2.07	0.88
2:B:502:ILE:H	2:B:502:ILE:HD12	1.39	0.87
3:C:32:SER:O	3:C:36:VAL:HG23	1.74	0.87
3:C:6:PRO:HB3	3:C:25:VAL:CG1	2.05	0.87
14:P:5:C:H2'	14:P:6:C:O4'	1.74	0.87
2:B:899:ILE:HD11	2:B:911:ILE:HA	1.56	0.87
2:B:172:ILE:HD13	2:B:178:ASN:HB3	1.55	0.87
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.55	0.87
2:B:343:ILE:CG2	2:B:347:LYS:HB2	2.03	0.87
2:B:112:LEU:HD12	2:B:113:TYR:H	1.40	0.87
4:D:47:LEU:HD11	7:G:3:PHE:CD2	2.08	0.87
4:D:134:THR:HG22	4:D:135:GLY:H	1.40	0.86
1:A:321:PRO:O	1:A:322:VAL:HB	1.76	0.86
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.55	0.86
2:B:1084:GLN:H	2:B:1084:GLN:NE2	1.73	0.86
14:P:6:C:H2'	14:P:7:A:C8	2.10	0.86
2:B:911:ILE:HD11	2:B:941:LEU:HD13	1.56	0.86
1:A:855:THR:HG21	1:A:857:ARG:NE	1.90	0.86
1:A:828:ALA:CB	2:B:530:GLY:HA2	2.05	0.86
2:B:613:VAL:HG13	2:B:627:PHE:O	1.76	0.86
1:A:1291:VAL:HG13	1:A:1292:PRO:HD2	1.57	0.86
2:B:953:LEU:HD21	2:B:965:LYS:HB2	1.56	0.86
7:G:81:PRO:HG3	7:G:106:MET:SD	2.15	0.86
1:A:34:LYS:HD3	1:A:57:ARG:NH2	1.89	0.86
1:A:1332:PHE:H	1:A:1332:PHE:HD2	1.23	0.86
3:C:44:LEU:HB2	3:C:77:ILE:HD11	1.58	0.86
7:G:14:HIS:HD2	7:G:16:SER:HB2	1.41	0.86
1:A:913:LEU:HD12	1:A:914:GLU:N	1.91	0.85
1:A:58:LEU:HD12	1:A:59:GLY:N	1.91	0.85
7:G:18:PHE:HA	7:G:22:MET:HE3	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:56:THR:HG22	3:C:57:VAL:H	1.40	0.85
2:B:515:HIS:H	2:B:518:HIS:CD2	1.95	0.85
2:B:806:THR:HG22	2:B:808:ALA:N	1.91	0.85
11:K:65:HIS:CD2	11:K:67:PHE:H	1.95	0.85
2:B:737:THR:HG21	9:I:66:PRO:HA	1.59	0.85
4:D:47:LEU:HD13	4:D:48:ILE:H	1.39	0.85
2:B:1085:ILE:N	2:B:1085:ILE:HD12	1.92	0.85
1:A:427:GLN:HG3	1:A:430:TRP:CZ2	2.10	0.84
2:B:363:HIS:O	2:B:364:ILE:HB	1.76	0.84
1:A:563:PRO:HG3	1:A:572:TRP:CZ2	2.13	0.84
2:B:378:LEU:O	2:B:382:ILE:HG13	1.78	0.84
4:D:134:THR:HG22	4:D:135:GLY:N	1.92	0.84
15:T:28:DT:H2''	15:T:29:DT:C5'	2.08	0.84
2:B:549:THR:H	2:B:628:THR:HG23	1.40	0.84
2:B:654:ARG:H	2:B:657:HIS:HD2	1.22	0.84
1:A:70:CYS:O	1:A:72:GLU:HG2	1.76	0.84
1:A:1325:THR:O	5:E:148:GLU:HB2	1.78	0.84
5:E:180:ARG:HH21	5:E:192:ARG:HB2	1.41	0.84
2:B:770:GLN:OE1	2:B:983:ARG:HA	1.77	0.83
5:E:16:PHE:CZ	5:E:20:LYS:HE2	2.14	0.83
15:T:27:DA:H2''	15:T:28:DT:H5'	1.58	0.83
2:B:98:THR:O	2:B:126:SER:HB2	1.77	0.83
1:A:1116:LEU:N	1:A:1308:THR:HG22	1.93	0.83
2:B:308:TRP:HA	2:B:311:LEU:HD12	1.60	0.83
2:B:244:LEU:HD21	2:B:366:GLN:NE2	1.94	0.83
1:A:34:LYS:CD	1:A:57:ARG:HH22	1.90	0.82
1:A:1420:ASP:HB3	1:A:1422:ARG:HG3	1.61	0.82
7:G:13:LEU:HD21	7:G:17:PHE:HB2	1.59	0.82
2:B:879:ARG:NH1	2:B:883:LEU:HD22	1.94	0.82
1:A:335:ARG:NH1	2:B:1202:LEU:HD13	1.95	0.82
1:A:866:PHE:C	1:A:867:ILE:HD12	2.03	0.82
9:I:115:LYS:HD3	9:I:117:LYS:HE3	1.62	0.82
2:B:1224:PHE:HE2	5:E:171:LYS:HG3	1.43	0.82
3:C:238:ILE:CG2	3:C:242:GLN:HB2	2.10	0.82
6:F:82:THR:HG22	6:F:84:TYR:H	1.44	0.82
1:A:590:ARG:HH21	1:A:620:LYS:HB3	1.43	0.81
1:A:855:THR:CG2	1:A:857:ARG:HE	1.91	0.81
2:B:171:PRO:HD2	2:B:457:LEU:HD13	1.60	0.81
2:B:516:ASN:HD22	2:B:516:ASN:N	1.74	0.81
6:F:86:THR:OG1	6:F:89:GLU:HG3	1.80	0.81
11:K:6:ARG:O	11:K:9:LEU:HG	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:646:PHE:O	1:A:650:GLN:HG3	1.80	0.81
1:A:1348:LEU:HG	1:A:1372:VAL:CG2	2.11	0.81
2:B:46:GLN:HG3	2:B:47:GLN:H	1.45	0.81
9:I:50:THR:HG22	9:I:52:ILE:H	1.43	0.81
9:I:111:THR:HG22	9:I:112:SER:H	1.46	0.81
1:A:567:LYS:HB3	8:H:95:TYR:HA	1.63	0.81
1:A:1030:ARG:HG3	1:A:1034:GLU:OE2	1.79	0.81
2:B:824:ILE:HG22	2:B:1087:PHE:HE2	1.46	0.81
2:B:850:LEU:HD12	2:B:851:PHE:N	1.95	0.81
2:B:1072:MET:HE3	2:B:1085:ILE:HB	1.59	0.81
1:A:325:ILE:HG21	2:B:1210:MET:HG3	1.63	0.81
1:A:1445:ILE:H	1:A:1445:ILE:HD12	1.45	0.81
2:B:770:GLN:CD	2:B:983:ARG:HA	2.05	0.81
2:B:859:TYR:OH	2:B:941:LEU:HD12	1.81	0.81
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.61	0.81
9:I:8:ARG:HG3	9:I:34:TYR:CE1	2.13	0.81
1:A:356:ASP:HB2	1:A:469:ARG:HH12	1.44	0.81
2:B:1197:PRO:HG2	2:B:1200:ALA:HB2	1.63	0.81
2:B:1084:GLN:NE2	2:B:1084:GLN:N	2.29	0.81
9:I:26:LEU:HD23	9:I:37:GLU:HA	1.60	0.80
3:C:43:THR:HG22	3:C:44:LEU:N	1.96	0.80
11:K:47:ARG:HB3	11:K:47:ARG:NH1	1.95	0.80
15:T:14:DC:H1'	15:T:15:DT:H5'	1.62	0.80
1:A:534:LEU:O	1:A:574:GLY:HA3	1.80	0.80
1:A:567:LYS:CD	1:A:568:PRO:HD2	2.12	0.80
2:B:217:ARG:HE	2:B:405:ARG:HB2	1.47	0.80
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.62	0.80
2:B:175:ARG:HG2	2:B:175:ARG:HH11	1.47	0.80
2:B:955:THR:HG22	2:B:956:THR:N	1.97	0.80
9:I:105:SER:O	9:I:106:CYS:HB3	1.80	0.80
3:C:166:GLU:HG3	11:K:10:PHE:CZ	2.15	0.80
2:B:343:ILE:HG21	2:B:348:ARG:HG3	1.64	0.80
4:D:153:ARG:NH2	4:D:184:ALA:HA	1.97	0.80
2:B:824:ILE:HG22	2:B:1087:PHE:CE2	2.17	0.80
2:B:863:GLU:OE2	2:B:873:THR:HA	1.82	0.80
1:A:768:GLN:CG	1:A:816:HIS:HA	2.11	0.80
1:A:1387:HIS:CE1	13:N:4:DT:H4'	2.17	0.80
8:H:81:PRO:HB2	8:H:82:PRO:HD2	1.63	0.79
10:J:57:ILE:HA	10:J:60:PHE:HD2	1.48	0.79
1:A:335:ARG:HA	1:A:339:ASN:HB2	1.63	0.79
6:F:69:LEU:HA	6:F:70:LYS:N	1.96	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:110:ASN:O	11:K:111:LEU:HD23	1.82	0.79
2:B:254:LEU:HD23	2:B:381:MET:HE1	1.63	0.79
2:B:361:LEU:HD21	2:B:377:PHE:CD2	2.16	0.79
2:B:486:TYR:HE2	2:B:1096:ARG:HH12	1.31	0.79
2:B:1077:THR:HG22	11:K:44:ASN:HD21	1.46	0.79
12:L:32:ALA:HB3	12:L:55:ILE:HD12	1.65	0.79
2:B:1084:GLN:HE21	2:B:1084:GLN:N	1.81	0.79
3:C:147:LEU:HB2	3:C:151:GLN:HB2	1.64	0.79
1:A:1424:VAL:HG13	1:A:1436:ILE:HD11	1.65	0.79
2:B:393:LYS:HA	2:B:393:LYS:HE3	1.63	0.79
4:D:71:LYS:HA	4:D:74:GLN:HB2	1.63	0.79
1:A:858:ASN:C	1:A:858:ASN:HD22	1.87	0.79
2:B:642:ASP:HA	2:B:649:LYS:HA	1.62	0.79
3:C:174:ALA:HB2	3:C:235:VAL:HG22	1.63	0.79
4:D:47:LEU:HD11	7:G:3:PHE:HD2	1.47	0.79
11:K:21:ILE:HG12	11:K:33:ILE:HG12	1.65	0.79
1:A:58:LEU:HD21	1:A:243:PRO:HA	1.65	0.79
1:A:524:VAL:HG12	1:A:525:GLN:N	1.98	0.79
1:A:21:LEU:HD11	1:A:1414:ALA:HA	1.63	0.79
1:A:34:LYS:CE	1:A:57:ARG:HH12	1.95	0.79
1:A:269:ILE:HD13	1:A:300:VAL:HG22	1.64	0.79
3:C:232:VAL:HG21	3:C:244:VAL:HG22	1.65	0.79
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.64	0.78
2:B:365:THR:HG23	2:B:367:LEU:H	1.48	0.78
2:B:800:GLN:HB3	10:J:52:THR:HG21	1.63	0.78
2:B:121:ASN:HA	2:B:207:GLY:HA2	1.66	0.78
2:B:850:LEU:HD12	2:B:851:PHE:H	1.49	0.78
2:B:999:MET:HA	2:B:999:MET:HE3	1.65	0.78
1:A:450:LEU:HB3	1:A:838:GLN:NE2	1.99	0.78
8:H:100:THR:OG1	8:H:138:GLU:HG3	1.83	0.78
1:A:567:LYS:HD3	8:H:95:TYR:CG	2.19	0.78
1:A:58:LEU:HD11	1:A:243:PRO:HB3	1.64	0.78
2:B:65:GLU:HG3	2:B:66:ASP:N	1.99	0.78
1:A:438:ASP:O	1:A:439:ASN:HB2	1.83	0.77
1:A:1445:ILE:HG12	7:G:18:PHE:CE2	2.19	0.77
2:B:807:ARG:HG2	2:B:1045:SER:OG	1.84	0.77
5:E:198:ILE:HD11	5:E:212:ARG:HG3	1.66	0.77
11:K:47:ARG:HH11	11:K:47:ARG:CB	1.96	0.77
2:B:114:PRO:HG2	2:B:115:GLN:H	1.50	0.77
1:A:353:ILE:CD1	1:A:487:MET:HE2	2.13	0.77
1:A:567:LYS:HB3	8:H:96:VAL:N	1.98	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1226:VAL:HG22	1:A:1240:CYS:HB3	1.64	0.77
3:C:172:PRO:O	3:C:235:VAL:HG23	1.84	0.77
5:E:213:ILE:HG12	5:E:214:CYS:H	1.47	0.77
15:T:27:DA:H2''	15:T:28:DT:C5'	2.13	0.77
1:A:68:GLN:C	1:A:70:CYS:H	1.92	0.77
1:A:903:ASN:ND2	1:A:905:ASP:H	1.81	0.77
2:B:563:MET:HE3	2:B:580:VAL:HB	1.67	0.77
3:C:33:LEU:HG	3:C:37:MET:HE2	1.65	0.77
3:C:70:ILE:HG12	3:C:142:VAL:HG11	1.67	0.77
2:B:467:GLY:H	2:B:475:SER:CB	1.96	0.77
2:B:1106:ARG:NH1	2:B:1110:PRO:HG2	2.00	0.77
6:F:111:LEU:C	6:F:113:GLY:H	1.92	0.77
8:H:59:ILE:HG22	8:H:60:ALA:N	1.98	0.77
1:A:886:ILE:HD11	1:A:943:LEU:HB3	1.65	0.77
1:A:1341:ILE:HG23	1:A:1342:GLU:N	1.99	0.77
1:A:1341:ILE:HD12	1:A:1379:GLY:O	1.85	0.77
2:B:189:LEU:O	2:B:192:LEU:N	2.16	0.77
3:C:239:PRO:HB2	3:C:241:ASP:OD1	1.85	0.77
15:T:22:BRU:H2'	15:T:23:DG:C8	2.20	0.77
1:A:254:GLU:HB2	2:B:935:ARG:NH1	1.99	0.76
1:A:450:LEU:H	1:A:450:LEU:HD12	1.50	0.76
3:C:73:GLN:NE2	3:C:74:SER:H	1.82	0.76
1:A:858:ASN:ND2	1:A:860:LEU:H	1.82	0.76
1:A:1076:ALA:HA	1:A:1079:MET:HE2	1.67	0.76
2:B:36:ALA:HA	2:B:39:ARG:HD2	1.68	0.76
7:G:138:THR:HG22	7:G:139:ILE:N	1.98	0.76
1:A:821:ARG:HB2	1:A:821:ARG:HH11	1.49	0.76
2:B:359:GLU:O	2:B:362:PRO:HD3	1.85	0.76
8:H:40:LEU:HD13	8:H:123:MET:HB2	1.66	0.76
15:T:16:DT:H1'	15:T:17:TT:H5'1	1.66	0.76
2:B:486:TYR:CE2	2:B:1096:ARG:NH1	2.52	0.76
5:E:78:LEU:HD21	5:E:80:VAL:HG23	1.66	0.76
2:B:840:ILE:HB	2:B:1011:ILE:HB	1.65	0.76
13:N:0:DT:H1'	13:N:1:DA:H5'	1.67	0.76
1:A:366:VAL:HG21	1:A:460:VAL:HG22	1.68	0.76
1:A:244:PRO:HB2	1:A:245:PRO:HD3	1.68	0.76
1:A:351:THR:HB	2:B:1103:ILE:HD12	1.68	0.76
2:B:1069:PHE:H	2:B:1069:PHE:HD1	1.34	0.76
3:C:253:LYS:O	3:C:256:ALA:HB3	1.86	0.76
4:D:7:THR:HG21	4:D:32:GLU:CD	2.10	0.76
7:G:1:MET:SD	7:G:79:PHE:CD1	2.79	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ILE:HG22	1:A:62:ASP:H	1.50	0.76
1:A:1332:PHE:HD2	1:A:1332:PHE:N	1.84	0.76
4:D:56:ARG:HB2	4:D:148:LEU:HD22	1.67	0.76
1:A:382:PRO:HB3	1:A:428:TYR:CE2	2.20	0.76
1:A:414:ASP:OD1	1:A:416:ARG:HG2	1.85	0.76
1:A:588:LEU:O	1:A:606:LEU:HA	1.86	0.76
1:A:269:ILE:HD11	1:A:300:VAL:HA	1.67	0.75
1:A:1444:MET:HG2	7:G:60:ARG:HA	1.67	0.75
7:G:1:MET:SD	7:G:79:PHE:HD1	2.09	0.75
8:H:17:PRO:HB3	8:H:24:CYS:SG	2.26	0.75
1:A:225:ASN:ND2	1:A:228:PHE:H	1.84	0.75
2:B:521:LEU:HB3	2:B:633:VAL:HG11	1.66	0.75
1:A:1438:THR:HB	2:B:1144:ALA:HB3	1.68	0.75
8:H:84:ALA:HA	8:H:87:ARG:HB2	1.67	0.75
10:J:64:ASN:HB3	10:J:65:PRO:CD	2.16	0.75
1:A:528:LEU:O	1:A:531:ILE:HG22	1.85	0.75
1:A:763:ALA:O	1:A:803:SER:HB3	1.87	0.75
2:B:589:VAL:HG12	2:B:590:HIS:N	1.97	0.75
2:B:1065:GLN:HE21	2:B:1067:ARG:H	1.34	0.75
14:P:6:C:H2'	14:P:7:A:H8	1.48	0.75
1:A:783:THR:HG21	1:A:815:PHE:CZ	2.21	0.75
1:A:794:PRO:HG2	1:A:795:GLU:OE2	1.86	0.75
2:B:411:PRO:O	2:B:414:ALA:HB3	1.86	0.75
3:C:36:VAL:HG21	3:C:251:LEU:HB2	1.68	0.75
1:A:567:LYS:HE3	8:H:46:LEU:HB2	1.67	0.75
1:A:1028:THR:O	1:A:1032:LEU:HD12	1.85	0.75
2:B:579:ARG:HB2	2:B:586:TRP:NE1	2.02	0.75
2:B:615:MET:C	2:B:616:ILE:HD12	2.12	0.75
2:B:821:GLN:NE2	2:B:851:PHE:HA	2.01	0.75
2:B:862:GLN:HG2	2:B:963:PHE:HD1	1.50	0.75
2:B:1077:THR:HG22	11:K:44:ASN:ND2	2.02	0.75
2:B:1159:ARG:HB3	2:B:1159:ARG:NH1	2.02	0.75
2:B:510:LYS:HG2	2:B:511:PRO:HD3	1.69	0.74
2:B:953:LEU:CD2	2:B:965:LYS:HB2	2.16	0.74
7:G:14:HIS:ND1	7:G:15:PRO:HD2	2.02	0.74
12:L:38:LEU:O	12:L:39:SER:HB3	1.84	0.74
2:B:782:LEU:HD12	2:B:788:ARG:HH11	1.52	0.74
1:A:239:LEU:HD12	1:A:240:PRO:HD2	1.70	0.74
1:A:843:LYS:HD3	1:A:846:GLU:OE2	1.87	0.74
1:A:1402:PHE:CE1	1:A:1403:GLU:HG3	2.21	0.74
2:B:1163:CYS:SG	2:B:1165:ILE:HB	2.27	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:133:ILE:HD11	3:C:237:SER:HA	1.68	0.74
1:A:1372:VAL:O	1:A:1376:THR:HG22	1.87	0.74
2:B:336:ARG:NH2	2:B:345:LYS:HE2	1.99	0.74
2:B:847:ASP:HB3	3:C:167:HIS:NE2	2.02	0.74
1:A:254:GLU:CB	2:B:935:ARG:HH12	2.01	0.74
1:A:265:LYS:HD2	1:A:265:LYS:H	1.52	0.74
1:A:442:VAL:HB	1:A:489:LEU:HD11	1.70	0.74
2:B:1065:GLN:HE21	2:B:1067:ARG:N	1.85	0.74
15:T:16:DT:H2''	15:T:17:TT:O2P	1.86	0.74
1:A:1189:SER:O	1:A:1241:ARG:HD3	1.87	0.74
2:B:1096:ARG:O	2:B:1097:HIS:HB2	1.88	0.74
2:B:1165:ILE:HG22	2:B:1166:CYS:N	2.01	0.74
1:A:353:ILE:HG21	1:A:487:MET:HE3	1.68	0.74
1:A:567:LYS:CB	8:H:95:TYR:HA	2.17	0.74
4:D:66:ARG:HD2	4:D:133:THR:HB	1.69	0.74
4:D:144:THR:HG21	7:G:46:LEU:HD13	1.69	0.74
5:E:198:ILE:CD1	5:E:212:ARG:HG3	2.18	0.74
6:F:111:LEU:HD12	6:F:111:LEU:N	2.03	0.74
1:A:58:LEU:HD13	1:A:80:HIS:O	1.86	0.74
2:B:824:ILE:CG2	2:B:1087:PHE:HE2	2.00	0.74
2:B:906:SER:O	2:B:941:LEU:HD23	1.88	0.74
4:D:48:ILE:HG21	7:G:4:ILE:HB	1.68	0.74
1:A:385:ILE:HG22	1:A:386:ASP:N	2.02	0.73
1:A:1206:ASP:HB3	1:A:1274:ARG:HH12	1.50	0.73
2:B:776:GLN:HE22	14:P:8:G:H5'	1.51	0.73
4:D:176:GLU:C	4:D:178:ALA:H	1.95	0.73
1:A:446:ARG:CD	1:A:480:ALA:HB2	2.19	0.73
2:B:343:ILE:HG21	2:B:348:ARG:N	2.04	0.73
2:B:863:GLU:O	2:B:961:LEU:HD22	1.87	0.73
4:D:153:ARG:HB3	4:D:154:PHE:CE1	2.23	0.73
1:A:868:TYR:HD2	1:A:1058:VAL:HG21	1.52	0.73
1:A:901:LEU:HB2	1:A:926:GLN:HG2	1.70	0.73
1:A:34:LYS:HB3	1:A:36:ARG:HE	1.53	0.73
1:A:35:ILE:HA	1:A:52:GLY:O	1.89	0.73
1:A:537:ARG:HD2	8:H:20:TYR:HE1	1.52	0.73
1:A:886:ILE:HG22	1:A:887:GLY:N	2.04	0.73
2:B:847:ASP:HB3	3:C:167:HIS:HE2	1.53	0.73
4:D:40:HIS:CE1	4:D:41:GLN:HG3	2.24	0.73
1:A:215:SER:HB3	1:A:218:ASP:OD2	1.88	0.73
1:A:853:ASP:O	1:A:854:ASN:HB2	1.89	0.73
2:B:309:GLN:OE1	9:I:52:ILE:HD11	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:ILE:HB	1:A:470:LEU:CD2	2.18	0.73
1:A:842:VAL:HG11	2:B:1136:ASP:OD2	1.89	0.73
1:A:49:LYS:HE2	1:A:61:ILE:HD12	1.68	0.73
5:E:94:LYS:CE	5:E:98:ILE:HD11	2.19	0.73
1:A:885:THR:O	1:A:940:ARG:HD2	1.88	0.73
3:C:73:GLN:HE21	3:C:74:SER:H	1.37	0.73
12:L:30:ILE:O	12:L:56:LEU:HA	1.88	0.73
1:A:1121:GLU:HG2	1:A:1122:PRO:HD2	1.71	0.73
1:A:1329:THR:HG22	1:A:1331:SER:N	2.04	0.73
1:A:901:LEU:HG	1:A:926:GLN:HE21	1.53	0.72
3:C:147:LEU:HD12	3:C:151:GLN:O	1.89	0.72
7:G:15:PRO:HA	7:G:18:PHE:CE1	2.24	0.72
1:A:49:LYS:NZ	1:A:61:ILE:HG13	2.03	0.72
1:A:472:LEU:O	1:A:475:THR:HB	1.90	0.72
1:A:1333:ILE:O	1:A:1337:GLU:HG3	1.89	0.72
7:G:79:PHE:HZ	7:G:106:MET:HE2	1.52	0.72
9:I:25:LEU:HB3	9:I:38:ALA:HB2	1.71	0.72
1:A:19:PHE:O	1:A:1416:ALA:HA	1.89	0.72
1:A:1394:THR:HG21	1:A:1398:MET:SD	2.29	0.72
2:B:825:VAL:CG1	2:B:826:ALA:N	2.51	0.72
3:C:147:LEU:N	3:C:147:LEU:HD23	2.03	0.72
15:T:17:TT:C3R	15:T:19:DT:H5''	2.20	0.72
2:B:810:GLU:HB2	2:B:815:ARG:HH22	1.52	0.72
3:C:99:LEU:HD12	3:C:118:LEU:HB3	1.71	0.72
9:I:111:THR:HG22	9:I:112:SER:N	2.04	0.72
1:A:1291:VAL:HG13	1:A:1292:PRO:CD	2.18	0.72
10:J:23:ASN:C	10:J:25:LEU:H	1.97	0.72
2:B:1007:VAL:CG2	2:B:1008:PRO:HD2	2.19	0.72
3:C:212:PRO:HB3	3:C:213:PRO:HD2	1.69	0.72
4:D:13:ARG:HB2	4:D:17:LYS:HZ2	1.55	0.72
1:A:58:LEU:HD11	1:A:243:PRO:CB	2.20	0.72
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.72	0.72
8:H:102:TYR:OH	8:H:122:LEU:HD22	1.90	0.72
4:D:47:LEU:HD13	4:D:48:ILE:N	2.04	0.72
6:F:103:MET:HE1	7:G:65:ASP:HB2	1.71	0.72
1:A:598:LEU:HA	8:H:122:LEU:HD13	1.72	0.72
3:C:36:VAL:HG21	3:C:251:LEU:HD22	1.72	0.72
1:A:50:ILE:C	1:A:52:GLY:H	1.99	0.71
2:B:100:PRO:HD2	2:B:180:TYR:HE1	1.54	0.71
8:H:15:VAL:HG22	8:H:26:ILE:HG12	1.71	0.71
15:T:26:DC:H2''	15:T:27:DA:H5'	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:963:ILE:HD11	1:A:1048:ASN:CB	2.16	0.71
2:B:1072:MET:CE	2:B:1085:ILE:HB	2.20	0.71
2:B:1087:PHE:HD2	2:B:1088:GLY:N	1.88	0.71
3:C:186:LEU:HD21	3:C:224:GLN:O	1.90	0.71
15:T:16:DT:C7	15:T:17:TT:H5A1	2.20	0.71
1:A:547:LEU:HD22	11:K:58:PHE:CD1	2.25	0.71
2:B:1159:ARG:HB3	2:B:1159:ARG:HH11	1.54	0.71
10:J:14:VAL:O	10:J:14:VAL:HG12	1.88	0.71
2:B:918:ILE:HB	2:B:935:ARG:HD2	1.72	0.71
6:F:111:LEU:O	6:F:113:GLY:N	2.22	0.71
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.71	0.71
1:A:1329:THR:HG22	1:A:1331:SER:H	1.54	0.71
2:B:708:GLU:O	2:B:710:LEU:N	2.24	0.71
3:C:213:PRO:O	3:C:214:ASN:HB2	1.91	0.71
11:K:31:VAL:HG12	11:K:32:VAL:N	2.06	0.71
1:A:351:THR:HB	2:B:1103:ILE:CD1	2.21	0.71
2:B:601:ARG:O	2:B:605:ARG:HG3	1.91	0.71
3:C:46:ILE:HG23	3:C:157:CYS:HB3	1.73	0.71
5:E:117:THR:HG22	5:E:119:SER:H	1.55	0.71
8:H:4:THR:HA	8:H:60:ALA:CB	2.20	0.71
8:H:64:ASN:O	8:H:65:LEU:HB2	1.89	0.71
1:A:743:VAL:O	1:A:747:VAL:HG23	1.91	0.71
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.73	0.71
1:A:1336:MET:HE3	1:A:1381:LEU:HG	1.73	0.71
3:C:208:GLU:O	3:C:210:GLU:N	2.24	0.71
1:A:106:VAL:HG13	1:A:112:LYS:O	1.90	0.70
1:A:230:ARG:H	1:A:233:TRP:HE3	1.38	0.70
1:A:1444:MET:HE1	6:F:135:ARG:HB2	1.71	0.70
1:A:1332:PHE:N	1:A:1332:PHE:CD2	2.56	0.70
2:B:955:THR:HG22	2:B:956:THR:H	1.53	0.70
11:K:53:ASP:OD1	11:K:55:LYS:HB2	1.91	0.70
1:A:92:HIS:O	1:A:94:GLY:N	2.24	0.70
1:A:1127:ASP:HB3	1:A:1130:GLN:HB3	1.72	0.70
1:A:1410:PHE:HA	2:B:1212:ILE:HD11	1.73	0.70
2:B:34:ILE:HD13	2:B:747:MET:HE2	1.72	0.70
2:B:756:ILE:O	2:B:759:PRO:HD3	1.92	0.70
1:A:341:MET:HE2	1:A:843:LYS:NZ	2.07	0.70
2:B:1020:ARG:HB2	2:B:1022:THR:HG22	1.73	0.70
3:C:60:ASP:OD2	12:L:60:ARG:NH2	2.22	0.70
3:C:179:GLU:HG2	3:C:180:TYR:N	2.06	0.70
4:D:189:ASP:O	4:D:193:THR:HB	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:CYS:SG	1:A:171:GLN:HG2	2.32	0.70
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.74	0.70
2:B:280:ILE:HD13	2:B:334:ILE:HG12	1.72	0.70
2:B:557:PHE:C	2:B:557:PHE:CD2	2.69	0.70
9:I:75:CYS:SG	9:I:79:HIS:N	2.63	0.70
1:A:714:PHE:CB	9:I:97:MET:HE1	2.22	0.70
1:A:1397:LEU:HB2	1:A:1426:GLU:OE1	1.91	0.70
6:F:90:ARG:HD3	6:F:155:LEU:CD1	2.20	0.70
8:H:61:SER:O	8:H:62:SER:HB3	1.91	0.70
8:H:142:LEU:C	8:H:143:LEU:HD12	2.17	0.70
1:A:341:MET:HE1	2:B:1135:ARG:NH1	2.07	0.70
2:B:365:THR:HG23	2:B:367:LEU:HG	1.71	0.70
6:F:125:LEU:HG	6:F:125:LEU:O	1.92	0.70
10:J:3:VAL:HG21	10:J:18:TRP:CB	2.18	0.70
1:A:249:SER:O	1:A:250:ILE:HG13	1.92	0.70
1:A:665:GLY:O	1:A:667:GLY:N	2.25	0.70
1:A:896:ARG:HD3	1:A:897:TYR:HE1	1.57	0.70
2:B:29:ASP:HB3	2:B:658:ILE:CD1	2.22	0.70
2:B:53:GLN:HG2	2:B:547:VAL:HG22	1.74	0.70
2:B:313:MET:HE3	2:B:386:LEU:HD22	1.74	0.70
2:B:778:MET:CE	2:B:1094:ARG:HD3	2.22	0.70
2:B:1177:HIS:HB2	2:B:1179:GLN:HE21	1.56	0.70
1:A:1094:VAL:HG12	1:A:1095:THR:N	2.04	0.70
1:A:1299:VAL:HG12	1:A:1300:LYS:N	2.05	0.70
1:A:896:ARG:NH2	1:A:1030:ARG:HH21	1.90	0.69
1:A:1161:THR:HG22	1:A:1163:ILE:N	2.03	0.69
2:B:1099:VAL:CG1	2:B:1100:ASP:N	2.55	0.69
6:F:103:MET:O	6:F:104:ASN:HB2	1.91	0.69
7:G:111:THR:HG22	7:G:113:HIS:H	1.56	0.69
8:H:89:LEU:HB3	8:H:91:ASP:OD1	1.92	0.69
1:A:1447:GLU:OE2	7:G:23:LYS:HB2	1.92	0.69
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.73	0.69
4:D:22:GLU:H	4:D:22:GLU:CD	1.99	0.69
7:G:7:LEU:HB2	7:G:74:TYR:HE2	1.54	0.69
7:G:128:PRO:O	7:G:138:THR:HG23	1.91	0.69
8:H:42:ILE:HG23	8:H:95:TYR:HE1	1.57	0.69
2:B:847:ASP:HB3	3:C:167:HIS:CD2	2.27	0.69
2:B:1115:THR:O	2:B:1116:ARG:HB2	1.89	0.69
1:A:590:ARG:HG3	1:A:590:ARG:NH1	2.07	0.69
1:A:35:ILE:HG22	1:A:35:ILE:O	1.91	0.69
4:D:185:CYS:HB2	4:D:211:LEU:HD22	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:1:MET:H1	10:J:57:ILE:H	0.79	0.69
10:J:48:ARG:HD2	10:J:49:MET:N	2.06	0.69
15:T:19:DT:H2''	15:T:20:DC:C5'	2.22	0.69
1:A:55:ASP:N	1:A:56:PRO:HD3	2.07	0.69
2:B:874:PHE:HA	2:B:913:GLY:O	1.91	0.69
2:B:882:THR:CG2	2:B:884:ARG:HB2	2.23	0.69
1:A:903:ASN:HD22	1:A:903:ASN:C	2.00	0.69
1:A:1424:VAL:HG13	1:A:1436:ILE:CD1	2.23	0.69
2:B:340:ALA:HB2	2:B:343:ILE:HD12	1.72	0.69
5:E:202:SER:OG	5:E:204:THR:HG22	1.93	0.69
11:K:45:LEU:HG	11:K:94:ILE:HD13	1.74	0.69
1:A:69:THR:C	1:A:71:GLN:H	1.97	0.69
1:A:265:LYS:HD2	1:A:265:LYS:N	2.08	0.69
1:A:714:PHE:O	1:A:718:VAL:HG23	1.93	0.69
2:B:515:HIS:HD2	2:B:517:THR:H	1.39	0.69
7:G:59:GLY:HA3	7:G:70:PHE:CD2	2.28	0.69
1:A:1290:LYS:O	1:A:1291:VAL:HG23	1.92	0.69
2:B:168:GLY:H	2:B:450:ALA:HB1	1.57	0.69
3:C:2:SER:N	3:C:3:GLU:N	2.40	0.69
1:A:798:GLY:HA2	1:A:815:PHE:CD1	2.28	0.68
2:B:798:TYR:HE2	3:C:62:PHE:CZ	2.11	0.68
5:E:22:MET:HE3	5:E:26:ARG:HH21	1.58	0.68
8:H:89:LEU:C	8:H:91:ASP:H	2.01	0.68
1:A:253:ASN:HB3	2:B:935:ARG:CZ	2.23	0.68
1:A:335:ARG:HH11	2:B:1202:LEU:HD13	1.57	0.68
2:B:361:LEU:HD21	2:B:377:PHE:HD2	1.56	0.68
2:B:1197:PRO:HG2	2:B:1200:ALA:CB	2.22	0.68
10:J:44:TYR:HA	10:J:47:ARG:CB	2.23	0.68
1:A:69:THR:C	1:A:71:GLN:N	2.48	0.68
1:A:979:SER:OG	1:A:980:ASP:N	2.25	0.68
1:A:401:GLY:C	1:A:435:HIS:HD2	2.02	0.68
2:B:23:ALA:HB1	2:B:24:PRO:HD2	1.76	0.68
2:B:217:ARG:HD2	2:B:217:ARG:C	2.19	0.68
2:B:579:ARG:HB2	2:B:586:TRP:HE1	1.57	0.68
2:B:642:ASP:O	2:B:644:GLU:N	2.26	0.68
1:A:463:ILE:HB	1:A:464:PRO:HD2	1.75	0.68
4:D:40:HIS:CB	7:G:73:LYS:HZ3	2.05	0.68
5:E:177:ARG:C	5:E:212:ARG:HD3	2.18	0.68
1:A:55:ASP:C	1:A:57:ARG:H	2.01	0.68
2:B:603:LEU:HD13	2:B:608:ASP:HB2	1.75	0.68
4:D:33:PHE:CE1	7:G:80:LYS:HE3	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1116:LEU:HB3	1:A:1308:THR:HG21	1.76	0.68
1:A:1336:MET:CE	1:A:1381:LEU:HG	2.23	0.68
2:B:232:SER:HB3	2:B:261:ARG:NH2	2.07	0.68
2:B:401:PHE:HD2	2:B:521:LEU:HD12	1.59	0.68
2:B:611:PRO:HB3	2:B:685:LEU:HD11	1.74	0.68
2:B:953:LEU:HD23	2:B:953:LEU:O	1.93	0.68
5:E:157:SER:OG	5:E:160:GLU:HG3	1.94	0.68
7:G:119:LEU:HD12	7:G:131:GLN:O	1.94	0.68
2:B:582:VAL:HG23	2:B:626:ILE:HB	1.75	0.68
2:B:882:THR:HG22	2:B:884:ARG:N	2.02	0.68
2:B:980:PHE:HE1	2:B:990:ILE:HD11	1.57	0.68
13:N:1:DA:H2"	13:N:2:DA:OP2	1.93	0.68
1:A:55:ASP:CG	1:A:55:ASP:O	2.33	0.68
2:B:1001:PHE:CE1	2:B:1073:TYR:HB2	2.28	0.68
4:D:138:ASN:OD1	4:D:141:LEU:HB2	1.94	0.68
5:E:153:HIS:HB3	5:E:196:VAL:CG1	2.24	0.68
6:F:135:ARG:HD3	6:F:143:PHE:CD2	2.29	0.68
1:A:152:VAL:CG1	1:A:153:PRO:HD2	2.23	0.68
1:A:856:THR:HB	1:A:865:GLN:HB2	1.75	0.68
2:B:336:ARG:HH21	2:B:345:LYS:HG2	1.59	0.68
2:B:516:ASN:N	2:B:516:ASN:ND2	2.41	0.68
2:B:1095:LEU:H	2:B:1095:LEU:HD12	1.59	0.68
5:E:114:ASN:O	5:E:115:ASN:HB3	1.92	0.68
1:A:658:LEU:HD13	2:B:831:SER:N	2.08	0.67
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	2.29	0.67
2:B:800:GLN:HB3	10:J:52:THR:CG2	2.23	0.67
11:K:61:TYR:C	11:K:61:TYR:CD2	2.71	0.67
1:A:302:THR:HA	1:A:305:ASP:O	1.93	0.67
2:B:37:PHE:CD1	2:B:41:LYS:HG3	2.30	0.67
2:B:616:ILE:CG1	2:B:697:GLU:HA	2.25	0.67
2:B:705:MET:HE2	2:B:745:PRO:HB3	1.75	0.67
4:D:4:SER:OG	4:D:5:THR:N	2.27	0.67
9:I:13:MET:O	9:I:14:LEU:HD23	1.94	0.67
1:A:828:ALA:HB2	2:B:530:GLY:HA2	1.75	0.67
4:D:134:THR:CG2	4:D:135:GLY:H	2.06	0.67
6:F:76:LYS:O	6:F:79:ARG:HD3	1.95	0.67
8:H:40:LEU:HD22	8:H:123:MET:HE3	1.76	0.67
12:L:32:ALA:HB3	12:L:55:ILE:CD1	2.24	0.67
1:A:14:VAL:CG2	2:B:1216:LEU:HD13	2.22	0.67
1:A:1348:LEU:HG	1:A:1372:VAL:HG23	1.76	0.67
2:B:295:GLY:H	2:B:298:LEU:HD23	1.57	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:238:ILE:HG23	3:C:242:GLN:HB2	1.75	0.67
5:E:48:ASP:CG	5:E:49:SER:H	2.03	0.67
1:A:384:ASN:O	1:A:385:ILE:C	2.37	0.67
1:A:869:GLY:O	5:E:204:THR:HG21	1.94	0.67
1:A:881:GLN:NE2	1:A:958:VAL:O	2.27	0.67
2:B:542:MET:HG2	2:B:747:MET:HB3	1.76	0.67
2:B:710:LEU:HA	2:B:733:HIS:HB3	1.74	0.67
1:A:16:GLU:HB3	1:A:1418:LEU:HD11	1.76	0.67
1:A:853:ASP:OD1	1:A:855:THR:N	2.28	0.67
2:B:39:ARG:NH2	2:B:665:GLU:HG2	2.10	0.67
2:B:199:MET:HE2	2:B:492:LEU:HD23	1.76	0.67
2:B:314:LEU:O	2:B:317:CYS:HB3	1.95	0.67
1:A:340:LEU:HD21	2:B:1200:ALA:N	2.09	0.67
1:A:1409:LEU:CD1	2:B:1207:LEU:HD11	2.23	0.67
2:B:351:TYR:O	2:B:355:ILE:HG13	1.95	0.67
8:H:59:ILE:HG22	8:H:60:ALA:H	1.60	0.67
1:A:709:THR:HG23	9:I:94:ASP:HA	1.77	0.67
2:B:580:VAL:HG22	2:B:624:LEU:HB3	1.76	0.67
2:B:859:TYR:CZ	2:B:941:LEU:HD12	2.29	0.67
1:A:254:GLU:O	1:A:256:GLN:N	2.27	0.66
1:A:548:ASN:OD1	11:K:60:ALA:HB1	1.95	0.66
1:A:844:ALA:C	1:A:845:LEU:HD23	2.20	0.66
2:B:293:PRO:HG2	2:B:296:GLU:CB	2.25	0.66
3:C:179:GLU:HG2	3:C:180:TYR:H	1.60	0.66
8:H:62:SER:C	8:H:64:ASN:H	2.03	0.66
11:K:7:PHE:HA	11:K:10:PHE:CE2	2.30	0.66
15:T:17:TT:C4R	15:T:19:DT:OP2	2.43	0.66
1:A:12:ARG:HD2	2:B:1218:THR:HB	1.78	0.66
1:A:1428:VAL:HG13	2:B:1151:LEU:HD21	1.77	0.66
2:B:336:ARG:NH2	2:B:345:LYS:HG2	2.10	0.66
5:E:157:SER:C	5:E:159:ASP:H	2.02	0.66
10:J:44:TYR:HD2	10:J:44:TYR:N	1.94	0.66
1:A:382:PRO:HD3	1:A:428:TYR:CD2	2.30	0.66
1:A:537:ARG:HD2	8:H:20:TYR:CE1	2.30	0.66
1:A:709:THR:HG22	1:A:711:ARG:N	2.09	0.66
1:A:899:VAL:HB	1:A:929:LEU:HD12	1.75	0.66
1:A:996:ASN:O	1:A:998:LEU:HD12	1.94	0.66
2:B:211:VAL:O	2:B:480:SER:HA	1.96	0.66
2:B:233:PRO:HG2	2:B:234:ILE:HD12	1.76	0.66
3:C:66:ARG:NH2	10:J:5:VAL:HG23	2.10	0.66
1:A:105:CYS:O	1:A:114:LEU:HG	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:683:ILE:HD13	1:A:801:GLU:HG3	1.77	0.66
1:A:899:VAL:HB	1:A:929:LEU:CD1	2.25	0.66
3:C:244:VAL:O	3:C:248:ILE:HG13	1.95	0.66
9:I:50:THR:CG2	9:I:52:ILE:HG12	2.25	0.66
10:J:32:GLU:CD	10:J:32:GLU:H	2.03	0.66
13:N:3:DG:H1'	13:N:4:DT:H5'	1.77	0.66
1:A:1348:LEU:O	1:A:1352:VAL:HG23	1.95	0.66
2:B:100:PRO:HD2	2:B:180:TYR:CE1	2.30	0.66
4:D:191:ALA:C	4:D:193:THR:H	2.03	0.66
1:A:54:ASN:HB3	1:A:247:ARG:HH12	1.59	0.66
2:B:37:PHE:HE2	2:B:542:MET:HA	1.60	0.66
2:B:616:ILE:HG13	2:B:697:GLU:HA	1.78	0.66
2:B:880:THR:O	2:B:881:ASN:HB2	1.95	0.66
2:B:1180:PHE:HB3	2:B:1191:ILE:HD12	1.77	0.66
4:D:47:LEU:HD11	7:G:3:PHE:CE2	2.31	0.66
9:I:103:CYS:HB3	9:I:106:CYS:SG	2.36	0.66
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.77	0.66
1:A:1293:SER:OG	1:A:1294:PRO:HD2	1.96	0.66
1:A:1348:LEU:HG	1:A:1372:VAL:HG22	1.78	0.66
2:B:745:PRO:O	2:B:748:ILE:HG12	1.95	0.66
3:C:18:VAL:HG12	3:C:18:VAL:O	1.94	0.66
1:A:666:ILE:HD12	1:A:667:GLY:H	1.61	0.66
1:A:1424:VAL:HG11	2:B:1139:ILE:HD13	1.78	0.66
11:K:49:GLU:HG3	11:K:94:ILE:HG12	1.77	0.66
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.77	0.66
1:A:384:ASN:O	1:A:386:ASP:N	2.28	0.66
2:B:180:TYR:HD1	2:B:180:TYR:H	1.44	0.66
3:C:226:ASP:O	3:C:227:THR:HB	1.96	0.66
8:H:38:LEU:HD12	8:H:124:ARG:O	1.96	0.66
9:I:34:TYR:HE2	9:I:36:GLU:HB3	1.61	0.66
15:T:17:TT:H5R1	15:T:17:TT:H1'	1.77	0.66
1:A:347:PHE:H	2:B:1107:ALA:HA	1.61	0.66
1:A:512:VAL:HA	1:A:519:PRO:HA	1.77	0.66
1:A:768:GLN:HG2	1:A:816:HIS:CA	2.26	0.66
1:A:1057:VAL:HG12	1:A:1058:VAL:N	2.11	0.66
9:I:55:THR:HG22	9:I:58:VAL:HG21	1.77	0.66
1:A:605:MET:HE2	1:A:607:ILE:CG1	2.26	0.65
1:A:728:LYS:O	1:A:732:LEU:HG	1.96	0.65
1:A:1436:ILE:O	1:A:1437:GLY:C	2.39	0.65
3:C:45:ALA:HA	3:C:72:LEU:HD12	1.78	0.65
10:J:2:ILE:HG22	10:J:3:VAL:O	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:GLN:HG3	1:A:430:TRP:CE2	2.30	0.65
1:A:1004:ASN:ND2	5:E:167:ARG:HD2	2.10	0.65
2:B:526:GLU:HG2	2:B:538:ASN:HD22	1.62	0.65
2:B:975:GLN:HG2	2:B:976:ILE:H	1.62	0.65
1:A:84:ILE:O	1:A:84:ILE:HG23	1.96	0.65
1:A:332:LYS:HG3	1:A:333:GLU:HG2	1.78	0.65
1:A:353:ILE:HG21	1:A:487:MET:CE	2.25	0.65
1:A:1362:TYR:CD1	1:A:1363:VAL:N	2.64	0.65
2:B:1039:GLY:HA2	10:J:51:LEU:HD22	1.77	0.65
6:F:118:LEU:HD12	6:F:118:LEU:O	1.97	0.65
1:A:1102:LYS:HG2	1:A:1106:ASN:HD21	1.61	0.65
2:B:778:MET:HE3	2:B:1094:ARG:HD3	1.79	0.65
3:C:69:LEU:N	3:C:69:LEU:HD12	2.11	0.65
4:D:130:LEU:C	4:D:132:GLN:H	2.04	0.65
2:B:1023:VAL:O	2:B:1026:LEU:N	2.29	0.65
10:J:8:PHE:H	10:J:49:MET:HE3	1.61	0.65
15:T:15:DT:C5	15:T:16:DT:H72	2.31	0.65
15:T:17:TT:C3R	15:T:19:DT:C5'	2.74	0.65
1:A:311:GLN:O	1:A:312:PRO:C	2.39	0.65
1:A:372:LYS:HA	1:A:435:HIS:ND1	2.11	0.65
1:A:897:TYR:CD2	1:A:936:LEU:HD13	2.31	0.65
2:B:37:PHE:CE1	2:B:41:LYS:HG3	2.32	0.65
2:B:102:VAL:CG2	2:B:112:LEU:HD22	2.27	0.65
2:B:582:VAL:HA	2:B:626:ILE:O	1.97	0.65
2:B:653:VAL:CG2	2:B:689:LEU:HB3	2.26	0.65
3:C:66:ARG:NH2	10:J:3:VAL:O	2.29	0.65
4:D:118:THR:HB	4:D:121:LYS:HB2	1.79	0.65
6:F:103:MET:HE2	7:G:66:GLY:H	1.62	0.65
15:T:24:DG:H2''	15:T:25:DT:O5'	1.97	0.65
1:A:897:TYR:HD2	1:A:936:LEU:HD13	1.62	0.65
1:A:1341:ILE:CG2	1:A:1342:GLU:N	2.60	0.65
3:C:77:ILE:HG23	3:C:161:LYS:HE3	1.78	0.65
1:A:144:THR:O	1:A:146:MET:HG3	1.96	0.65
1:A:675:THR:O	1:A:679:ILE:HG13	1.97	0.65
1:A:741:ASN:HD22	1:A:744:LYS:H	1.45	0.65
1:A:1312:ASN:O	1:A:1316:VAL:HG23	1.96	0.65
2:B:871:THR:HG22	2:B:872:GLU:O	1.97	0.65
4:D:40:HIS:CB	7:G:73:LYS:NZ	2.58	0.65
6:F:89:GLU:OE2	6:F:134:ILE:HG21	1.97	0.65
1:A:590:ARG:O	1:A:591:PHE:HB2	1.97	0.65
1:A:852:TYR:CD2	1:A:1060:PRO:HB2	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:344:LYS:O	2:B:345:LYS:HB2	1.95	0.65
5:E:156:LEU:HD12	5:E:195:VAL:HB	1.79	0.65
11:K:47:ARG:C	11:K:47:ARG:HD2	2.22	0.65
15:T:19:DT:H2''	15:T:20:DC:H5'	1.77	0.65
1:A:490:HIS:HB3	2:B:1150:ARG:NH1	2.13	0.65
15:T:26:DC:H2''	15:T:27:DA:C5'	2.27	0.65
1:A:78:PRO:HA	2:B:1201:LYS:HZ2	1.61	0.64
2:B:336:ARG:CD	2:B:348:ARG:HH11	2.09	0.64
2:B:589:VAL:CG1	2:B:590:HIS:H	2.05	0.64
2:B:603:LEU:HD12	2:B:609:ILE:HG13	1.78	0.64
2:B:978:ASP:OD2	2:B:1098:MET:HG2	1.97	0.64
7:G:23:LYS:HG3	7:G:56:ILE:CD1	2.27	0.64
1:A:51:GLY:HA2	1:A:56:PRO:HA	1.79	0.64
10:J:1:MET:H3	10:J:56:LEU:N	1.95	0.64
11:K:15:GLY:O	11:K:16:GLU:HG3	1.97	0.64
1:A:711:ARG:HA	9:I:97:MET:HE2	1.79	0.64
1:A:714:PHE:HB2	9:I:97:MET:HE1	1.79	0.64
1:A:1226:VAL:HG22	1:A:1240:CYS:CB	2.28	0.64
5:E:153:HIS:HB3	5:E:196:VAL:HG11	1.80	0.64
7:G:79:PHE:CZ	7:G:106:MET:HE2	2.31	0.64
1:A:567:LYS:HD3	8:H:95:TYR:CD2	2.32	0.64
1:A:630:ILE:HD13	1:A:646:PHE:CZ	2.33	0.64
1:A:960:ILE:O	1:A:963:ILE:HG22	1.97	0.64
1:A:965:GLN:O	1:A:968:GLN:HB2	1.98	0.64
1:A:1006:ILE:CD1	5:E:163:GLU:HG3	2.28	0.64
1:A:1428:VAL:HG13	2:B:1151:LEU:CD2	2.28	0.64
2:B:57:TYR:N	2:B:57:TYR:HD1	1.95	0.64
2:B:843:GLN:N	2:B:994:TYR:O	2.26	0.64
1:A:114:LEU:HD13	1:A:171:GLN:HE22	1.62	0.64
2:B:57:TYR:N	2:B:57:TYR:CD1	2.65	0.64
2:B:616:ILE:HD12	2:B:616:ILE:N	2.13	0.64
2:B:997:GLU:CD	2:B:997:GLU:H	2.05	0.64
11:K:12:LEU:HD12	11:K:12:LEU:N	2.11	0.64
1:A:93:VAL:CG1	1:A:301:ALA:HB1	2.24	0.64
1:A:590:ARG:HG3	1:A:590:ARG:HH11	1.61	0.64
1:A:1153:TYR:CE1	9:I:42:LEU:HD13	2.33	0.64
4:D:53:SER:HB3	4:D:153:ARG:H	1.61	0.64
7:G:1:MET:HE1	7:G:80:LYS:H	1.63	0.64
8:H:40:LEU:CD1	8:H:123:MET:HB2	2.26	0.64
1:A:84:ILE:HD11	1:A:270:LEU:HD13	1.79	0.64
1:A:265:LYS:HZ3	1:A:322:VAL:HG13	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:809:THR:OG1	1:A:812:GLU:HG3	1.97	0.64
2:B:569:TYR:CE1	2:B:589:VAL:HG21	2.33	0.64
4:D:8:PHE:CE2	4:D:40:HIS:HA	2.32	0.64
5:E:22:MET:HE3	5:E:26:ARG:HE	1.61	0.64
5:E:180:ARG:NH2	5:E:192:ARG:HB2	2.12	0.64
6:F:90:ARG:HG3	6:F:91:ALA:N	2.11	0.64
1:A:320:ARG:NH2	14:P:1:U:O2'	2.31	0.64
1:A:1224:LEU:HD12	1:A:1241:ARG:O	1.96	0.64
1:A:1437:GLY:O	1:A:1439:GLY:N	2.31	0.64
2:B:821:GLN:HE22	2:B:851:PHE:CA	2.09	0.64
4:D:191:ALA:O	4:D:193:THR:N	2.31	0.64
13:N:6:DC:H2''	13:N:7:DT:OP2	1.97	0.64
1:A:41:MET:HB3	1:A:48:ALA:O	1.98	0.64
1:A:1166:ASP:OD2	1:A:1239:ARG:HD2	1.98	0.64
2:B:340:ALA:CB	2:B:343:ILE:HD12	2.26	0.64
8:H:44:VAL:O	8:H:44:VAL:HG12	1.98	0.64
1:A:69:THR:O	1:A:71:GLN:N	2.30	0.64
1:A:95:PHE:O	1:A:96:ILE:C	2.41	0.64
1:A:658:LEU:HD13	2:B:831:SER:H	1.62	0.64
1:A:701:LEU:HA	9:I:115:LYS:HE3	1.80	0.64
2:B:955:THR:HG23	12:L:54:ARG:O	1.97	0.64
2:B:1065:GLN:HG3	2:B:1067:ARG:H	1.62	0.64
2:B:1161:HIS:NE2	2:B:1175:LEU:HD21	2.13	0.64
10:J:44:TYR:HA	10:J:47:ARG:HB3	1.80	0.64
15:T:16:DT:H1'	15:T:17:TT:C5'	2.28	0.64
1:A:108:MET:N	1:A:108:MET:SD	2.71	0.63
1:A:482:PHE:C	1:A:484:GLY:H	2.05	0.63
1:A:877:HIS:O	1:A:878:ILE:HG12	1.99	0.63
2:B:520:GLY:H	2:B:748:ILE:HG22	1.62	0.63
2:B:770:GLN:HG2	2:B:983:ARG:O	1.97	0.63
2:B:950:ASP:O	2:B:951:GLN:HB2	1.98	0.63
10:J:8:PHE:H	10:J:49:MET:CE	2.10	0.63
10:J:44:TYR:N	10:J:44:TYR:CD2	2.65	0.63
1:A:18:GLN:HB2	2:B:1215:ARG:HB2	1.79	0.63
1:A:164:ARG:HG3	1:A:165:GLY:N	2.12	0.63
1:A:605:MET:HE1	1:A:612:ILE:HG23	1.79	0.63
1:A:774:ARG:O	1:A:775:ILE:C	2.41	0.63
2:B:542:MET:HE3	2:B:636:PRO:HG3	1.81	0.63
3:C:31:ASN:O	3:C:34:ARG:HB3	1.98	0.63
3:C:245:VAL:HA	3:C:248:ILE:HD12	1.80	0.63
6:F:90:ARG:HD3	6:F:155:LEU:HD11	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:103:MET:CE	7:G:66:GLY:H	2.11	0.63
1:A:471:ASN:OD1	1:A:472:LEU:N	2.31	0.63
1:A:979:SER:OG	1:A:981:LEU:HG	1.98	0.63
2:B:278:GLN:HG2	2:B:279:ASP:H	1.62	0.63
2:B:842:ASN:ND2	2:B:845:SER:H	1.96	0.63
1:A:343:LYS:NZ	2:B:1151:LEU:O	2.29	0.63
1:A:1418:LEU:HD12	1:A:1419:ASP:N	2.13	0.63
2:B:642:ASP:HB3	2:B:649:LYS:CD	2.28	0.63
2:B:815:ARG:HD3	2:B:1041:GLU:OE2	1.98	0.63
8:H:81:PRO:CB	8:H:82:PRO:CD	2.77	0.63
2:B:121:ASN:HA	2:B:207:GLY:CA	2.27	0.63
2:B:579:ARG:HG2	2:B:579:ARG:HH11	1.63	0.63
2:B:843:GLN:O	2:B:844:SER:C	2.42	0.63
2:B:879:ARG:HH11	2:B:883:LEU:CD2	2.09	0.63
1:A:605:MET:HE2	1:A:607:ILE:HG12	1.80	0.63
1:A:896:ARG:HD3	1:A:897:TYR:CE1	2.33	0.63
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.34	0.63
2:B:217:ARG:NE	2:B:405:ARG:HB2	2.13	0.63
2:B:955:THR:CG2	2:B:956:THR:H	2.12	0.63
2:B:1180:PHE:HB3	2:B:1191:ILE:CD1	2.28	0.63
4:D:176:GLU:O	4:D:178:ALA:N	2.32	0.63
8:H:81:PRO:HB2	8:H:82:PRO:CD	2.29	0.63
9:I:52:ILE:HG13	9:I:52:ILE:O	1.97	0.63
1:A:475:THR:HG23	1:A:476:SER:N	2.13	0.63
1:A:1283:VAL:HG12	1:A:1284:MET:N	2.14	0.63
1:A:7:SER:C	1:A:9:ALA:H	2.06	0.63
1:A:547:LEU:HD22	11:K:58:PHE:HD1	1.64	0.63
1:A:1373:ASP:HA	1:A:1376:THR:CG2	2.29	0.63
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.81	0.63
2:B:952:VAL:HG22	2:B:966:VAL:HG13	1.81	0.63
1:A:663:SER:OG	1:A:664:THR:N	2.24	0.63
1:A:682:THR:HG23	1:A:728:LYS:HE3	1.81	0.63
1:A:863:VAL:HG11	1:A:866:PHE:CD2	2.34	0.63
1:A:1197:LEU:HD12	1:A:1209:MET:HE1	1.80	0.63
2:B:822:ASN:O	10:J:48:ARG:NH1	2.32	0.63
3:C:263:THR:C	3:C:265:MET:H	2.07	0.63
1:A:42:ASP:HB3	1:A:45:GLN:HA	1.81	0.62
1:A:326:ARG:HH22	1:A:1407:GLU:HG3	1.62	0.62
2:B:31:TRP:CE3	2:B:34:ILE:HD12	2.33	0.62
2:B:830:TYR:CE2	2:B:1000:PRO:HD3	2.34	0.62
4:D:130:LEU:O	4:D:132:GLN:N	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:12:LEU:H	11:K:12:LEU:CD1	2.11	0.62
11:K:42:LEU:HD21	11:K:46:ILE:HD11	1.80	0.62
1:A:500:GLU:OE2	1:A:1438:THR:HG21	1.99	0.62
1:A:782:ARG:NH2	2:B:699:GLU:O	2.31	0.62
2:B:563:MET:CE	2:B:580:VAL:HB	2.28	0.62
6:F:143:PHE:C	6:F:143:PHE:CD1	2.77	0.62
7:G:83:LYS:HE2	7:G:150:CYS:H	1.64	0.62
1:A:90:VAL:HG13	1:A:297:GLN:HA	1.79	0.62
1:A:381:THR:CG2	1:A:383:TYR:H	2.12	0.62
1:A:534:LEU:HD13	1:A:656:TRP:CG	2.34	0.62
1:A:591:PHE:HA	1:A:595:THR:HG21	1.80	0.62
6:F:77:ASP:C	6:F:79:ARG:H	2.06	0.62
6:F:114:GLU:OE2	6:F:119:ARG:HG2	1.99	0.62
7:G:80:LYS:HD3	7:G:80:LYS:N	2.14	0.62
8:H:127:GLY:O	8:H:128:ASN:HB2	1.99	0.62
8:H:130:ARG:H	8:H:130:ARG:HD2	1.64	0.62
10:J:16:ASP:OD1	10:J:17:LYS:HD2	1.99	0.62
1:A:92:HIS:HD2	1:A:304:MET:HE1	1.64	0.62
7:G:143:ILE:HG22	7:G:144:ARG:N	2.13	0.62
1:A:37:PHE:N	1:A:37:PHE:CD1	2.67	0.62
1:A:341:MET:CE	1:A:843:LYS:HZ3	2.12	0.62
1:A:477:PRO:HG2	1:A:521:MET:HG2	1.82	0.62
2:B:336:ARG:HD3	2:B:348:ARG:HH11	1.63	0.62
3:C:152:GLU:OE2	3:C:154:LYS:HE3	2.00	0.62
3:C:164:ALA:HA	3:C:167:HIS:O	1.99	0.62
15:T:17:TT:H3R	15:T:19:DT:H5"	1.79	0.62
1:A:381:THR:HG22	1:A:383:TYR:H	1.64	0.62
1:A:541:ILE:HD13	1:A:549:MET:CE	2.19	0.62
2:B:29:ASP:HB3	2:B:658:ILE:HD13	1.82	0.62
2:B:273:LEU:CB	2:B:276:ILE:HD12	2.16	0.62
3:C:183:TRP:O	3:C:185:LYS:N	2.33	0.62
5:E:124:VAL:HG13	5:E:132:ILE:HB	1.81	0.62
1:A:450:LEU:HD12	1:A:450:LEU:N	2.14	0.62
2:B:1169:MET:HE1	2:B:1201:LYS:HA	1.81	0.62
5:E:13:TRP:CE3	5:E:39:LEU:HD13	2.34	0.62
9:I:16:PRO:HB3	9:I:27:PHE:CE2	2.35	0.62
11:K:46:ILE:O	11:K:50:LEU:HB2	1.98	0.62
11:K:111:LEU:O	11:K:112:GLN:NE2	2.30	0.62
1:A:446:ARG:HB2	1:A:487:MET:SD	2.40	0.62
1:A:475:THR:CG2	1:A:476:SER:N	2.63	0.62
1:A:1244:ARG:HB3	1:A:1245:PRO:HD2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1450:LEU:O	1:A:1450:LEU:HG	1.99	0.62
2:B:39:ARG:HH21	2:B:665:GLU:CD	2.07	0.62
2:B:1006:ILE:HD13	10:J:44:TYR:CE2	2.35	0.62
7:G:127:PRO:HG2	7:G:138:THR:HG21	1.80	0.62
1:A:825:ILE:HG22	1:A:826:ASP:N	2.14	0.62
4:D:64:VAL:C	4:D:66:ARG:H	2.07	0.62
1:A:1313:LEU:HD23	1:A:1338:VAL:HG21	1.80	0.61
2:B:496:ARG:NH1	2:B:539:LEU:HB2	2.15	0.61
2:B:737:THR:CG2	9:I:66:PRO:HA	2.29	0.61
4:D:5:THR:O	4:D:5:THR:HG23	2.00	0.61
10:J:44:TYR:HD2	10:J:44:TYR:H	1.48	0.61
10:J:57:ILE:HA	10:J:60:PHE:CD2	2.34	0.61
15:T:16:DT:C1'	15:T:17:TT:H5'1	2.29	0.61
1:A:466:SER:O	2:B:1103:ILE:HD11	2.00	0.61
1:A:546:VAL:O	1:A:550:LEU:HG	2.01	0.61
1:A:852:TYR:CE2	1:A:1060:PRO:HB2	2.35	0.61
1:A:1341:ILE:HG23	1:A:1342:GLU:H	1.64	0.61
1:A:1341:ILE:CG2	1:A:1342:GLU:H	2.13	0.61
2:B:31:TRP:CZ3	2:B:34:ILE:HD12	2.35	0.61
2:B:305:VAL:O	2:B:305:VAL:HG12	1.98	0.61
2:B:847:ASP:C	2:B:849:GLY:H	2.06	0.61
10:J:48:ARG:HE	10:J:49:MET:CE	2.13	0.61
1:A:1323:ASP:OD1	1:A:1325:THR:HB	2.00	0.61
2:B:557:PHE:C	2:B:557:PHE:HD2	2.08	0.61
2:B:1073:TYR:CE2	2:B:1080:LYS:HG2	2.35	0.61
2:B:1176:ASN:C	2:B:1178:ASN:H	2.08	0.61
1:A:164:ARG:HG3	1:A:165:GLY:H	1.65	0.61
1:A:1013:ASP:O	1:A:1015:VAL:N	2.33	0.61
1:A:1121:GLU:CG	1:A:1122:PRO:HD2	2.30	0.61
2:B:44:VAL:O	2:B:45:SER:C	2.44	0.61
8:H:41:ASP:O	8:H:42:ILE:HG13	2.00	0.61
1:A:698:GLN:HA	9:I:97:MET:O	2.00	0.61
1:A:901:LEU:O	1:A:921:GLY:N	2.29	0.61
3:C:43:THR:CG2	3:C:44:LEU:H	2.08	0.61
5:E:175:LEU:HD23	5:E:176:PRO:HD2	1.81	0.61
1:A:567:LYS:CE	8:H:46:LEU:HB2	2.29	0.61
1:A:821:ARG:HB2	1:A:821:ARG:NH1	2.15	0.61
1:A:1134:ILE:O	1:A:1138:ILE:HG13	2.00	0.61
2:B:35:SER:HA	2:B:811:TYR:HE2	1.65	0.61
2:B:291:ILE:HD13	2:B:300:HIS:NE2	2.16	0.61
2:B:637:LEU:HD12	2:B:693:ILE:HD12	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1022:THR:HG23	2:B:1022:THR:O	1.99	0.61
2:B:1159:ARG:HE	2:B:1193:GLN:HE21	1.47	0.61
2:B:1174:LYS:O	2:B:1176:ASN:N	2.34	0.61
4:D:128:VAL:O	4:D:132:GLN:HG3	2.01	0.61
4:D:195:ILE:O	4:D:197:SER:N	2.34	0.61
1:A:12:ARG:NE	2:B:1192:TYR:HE2	1.98	0.61
1:A:1120:LEU:HD12	1:A:1120:LEU:N	2.16	0.61
2:B:549:THR:N	2:B:628:THR:HG23	2.14	0.61
3:C:70:ILE:HD11	3:C:144:ILE:CG1	2.31	0.61
3:C:73:GLN:HE21	3:C:74:SER:N	1.98	0.61
9:I:13:MET:HG3	9:I:14:LEU:N	2.15	0.61
11:K:21:ILE:HG23	11:K:31:VAL:HG11	1.81	0.61
15:T:16:DT:H2''	15:T:17:TT:H5'1	1.83	0.61
2:B:221:ASN:N	2:B:241:ARG:O	2.28	0.61
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.83	0.61
2:B:857:ARG:HD2	2:B:945:GLU:OE1	2.00	0.61
2:B:955:THR:CG2	2:B:956:THR:N	2.63	0.61
3:C:100:THR:HG22	3:C:101:LEU:N	2.15	0.61
12:L:39:SER:O	12:L:40:LEU:HG	2.00	0.61
1:A:252:PHE:O	1:A:253:ASN:HB2	2.01	0.61
1:A:337:ARG:HD3	2:B:1132:GLU:OE1	2.01	0.61
1:A:381:THR:HG23	1:A:382:PRO:HD2	1.83	0.61
1:A:694:THR:O	1:A:698:GLN:HG3	2.01	0.61
1:A:866:PHE:O	1:A:867:ILE:HD12	2.00	0.61
2:B:750:GLY:O	2:B:751:VAL:C	2.44	0.61
2:B:852:ARG:NH2	12:L:70:ARG:OXT	2.30	0.61
4:D:119:ARG:HD3	4:D:221:TYR:CE2	2.35	0.61
5:E:135:PHE:HD2	5:E:140:LEU:HD21	1.66	0.61
6:F:69:LEU:N	6:F:70:LYS:CA	2.64	0.61
8:H:91:ASP:C	8:H:93:TYR:H	2.09	0.61
9:I:10:CYS:SG	9:I:32:CYS:HB3	2.41	0.61
1:A:264:PHE:O	1:A:267:ALA:HB3	2.01	0.61
3:C:66:ARG:CZ	10:J:2:ILE:HG21	2.30	0.61
7:G:145:VAL:HG12	7:G:146:LYS:N	2.14	0.61
11:K:10:PHE:N	11:K:10:PHE:CD2	2.69	0.61
12:L:31:CYS:SG	12:L:34:CYS:N	2.72	0.61
1:A:4:GLN:O	1:A:5:GLN:HB2	2.01	0.60
1:A:68:GLN:O	1:A:70:CYS:N	2.33	0.60
1:A:456:MET:HB2	1:A:478:TYR:OH	2.01	0.60
1:A:1118:VAL:CG2	1:A:1306:LEU:HB2	2.30	0.60
2:B:357:GLN:O	2:B:366:GLN:HA	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:653:VAL:HG22	2:B:689:LEU:HD13	1.83	0.60
2:B:830:TYR:O	2:B:832:GLY:N	2.34	0.60
14:P:4:A:O2'	14:P:5:C:H5'	2.01	0.60
1:A:49:LYS:HZ1	1:A:61:ILE:HG13	1.65	0.60
1:A:524:VAL:HG12	1:A:525:GLN:HE21	1.67	0.60
1:A:1189:SER:OG	1:A:1190:PRO:HD2	2.01	0.60
1:A:1369:ALA:O	1:A:1370:LEU:C	2.44	0.60
9:I:2:THR:O	9:I:3:THR:C	2.43	0.60
1:A:18:GLN:HB3	2:B:1215:ARG:HG3	1.83	0.60
1:A:265:LYS:NZ	1:A:322:VAL:HG22	2.16	0.60
1:A:720:ARG:O	1:A:724:GLU:HB2	2.01	0.60
1:A:1193:LEU:HD22	1:A:1260:LEU:HD11	1.82	0.60
2:B:123:THR:O	2:B:125:SER:N	2.33	0.60
2:B:434:ARG:O	2:B:437:GLU:HB2	2.02	0.60
2:B:1085:ILE:N	2:B:1085:ILE:CD1	2.60	0.60
15:T:13:DA:H1'	15:T:14:DC:H5'	1.83	0.60
1:A:244:PRO:O	1:A:246:VAL:N	2.34	0.60
1:A:896:ARG:NH2	1:A:1030:ARG:NH2	2.49	0.60
1:A:1057:VAL:HG12	1:A:1058:VAL:H	1.67	0.60
5:E:29:PHE:O	5:E:30:ILE:HG13	2.00	0.60
5:E:30:ILE:HG22	5:E:31:THR:N	2.16	0.60
12:L:53:HIS:HB3	12:L:55:ILE:CD1	2.30	0.60
1:A:567:LYS:CG	1:A:568:PRO:CD	2.77	0.60
1:A:1329:THR:CG2	1:A:1331:SER:H	2.15	0.60
2:B:826:ALA:HB2	2:B:1008:PRO:HB3	1.83	0.60
4:D:53:SER:CB	4:D:153:ARG:H	2.14	0.60
5:E:135:PHE:HB3	5:E:140:LEU:HD11	1.83	0.60
6:F:143:PHE:C	6:F:143:PHE:HD1	2.09	0.60
9:I:13:MET:HG3	9:I:14:LEU:H	1.64	0.60
1:A:321:PRO:O	1:A:322:VAL:CB	2.48	0.60
2:B:833:TYR:N	2:B:833:TYR:CD1	2.67	0.60
4:D:29:LEU:HD22	7:G:82:PHE:CE2	2.37	0.60
7:G:115:MET:HB3	7:G:163:ILE:HD11	1.83	0.60
8:H:56:THR:HB	8:H:145:ARG:HG2	1.83	0.60
15:T:15:DT:H1'	15:T:16:DT:H5'	1.84	0.60
1:A:305:ASP:CG	1:A:326:ARG:HD2	2.26	0.60
1:A:821:ARG:HD2	1:A:825:ILE:HD11	1.83	0.60
1:A:1261:LYS:O	1:A:1264:GLU:HB3	2.01	0.60
2:B:190:TYR:CE2	10:J:62:ARG:HB3	2.36	0.60
2:B:769:TYR:O	2:B:772:ALA:N	2.34	0.60
4:D:170:THR:CG2	4:D:172:LEU:HG	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:801:LYS:O	10:J:52:THR:HG23	2.01	0.60
8:H:40:LEU:HD13	8:H:123:MET:HE3	1.84	0.60
8:H:93:TYR:HB3	8:H:144:ILE:O	2.01	0.60
9:I:7:CYS:HB3	9:I:14:LEU:HD21	1.83	0.60
1:A:98:LYS:O	1:A:99:ILE:C	2.44	0.60
1:A:507:VAL:HG13	1:A:521:MET:HE1	1.84	0.60
1:A:1102:LYS:HG2	1:A:1106:ASN:ND2	2.17	0.60
1:A:1385:THR:HG22	1:A:1386:ARG:H	1.67	0.60
2:B:616:ILE:HG13	2:B:697:GLU:HG3	1.84	0.60
2:B:1069:PHE:HA	2:B:1085:ILE:O	2.02	0.60
7:G:49:LEU:HG	7:G:76:ALA:HA	1.81	0.60
1:A:42:ASP:HB3	1:A:45:GLN:CA	2.32	0.60
1:A:265:LYS:HE2	1:A:322:VAL:CG1	2.32	0.60
1:A:401:GLY:C	1:A:435:HIS:CD2	2.79	0.60
1:A:968:GLN:O	1:A:970:THR:N	2.35	0.60
1:A:981:LEU:CD2	1:A:1039:LYS:HA	2.32	0.60
2:B:497:ARG:NH2	2:B:775:LYS:NZ	2.49	0.60
2:B:1180:PHE:O	2:B:1181:GLU:O	2.20	0.60
5:E:22:MET:CE	5:E:26:ARG:HH21	2.15	0.60
9:I:34:TYR:CD2	9:I:34:TYR:C	2.80	0.60
9:I:61:ASP:C	9:I:63:GLY:H	2.09	0.60
1:A:90:VAL:CG1	1:A:297:GLN:HA	2.32	0.59
1:A:289:ILE:C	1:A:291:GLU:H	2.08	0.59
1:A:345:VAL:HG23	1:A:346:ASP:O	2.02	0.59
1:A:908:LEU:HD11	1:A:983:ILE:HD11	1.84	0.59
1:A:1030:ARG:NH1	1:A:1035:TYR:OH	2.35	0.59
1:A:1445:ILE:HG12	7:G:18:PHE:HE2	1.62	0.59
2:B:654:ARG:N	2:B:657:HIS:HD2	1.97	0.59
2:B:1001:PHE:CD2	3:C:34:ARG:NH2	2.70	0.59
2:B:1039:GLY:HA2	10:J:51:LEU:CD2	2.30	0.59
2:B:1107:ALA:O	2:B:1108:ARG:HG2	2.02	0.59
1:A:356:ASP:HB2	1:A:469:ARG:HH11	1.62	0.59
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.83	0.59
2:B:654:ARG:H	2:B:657:HIS:CD2	2.11	0.59
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.84	0.59
2:B:745:PRO:C	2:B:747:MET:H	2.10	0.59
2:B:792:MET:HG3	2:B:855:PHE:HE1	1.67	0.59
2:B:825:VAL:HG13	2:B:826:ALA:H	1.66	0.59
7:G:7:LEU:HD11	7:G:45:ILE:HD11	1.84	0.59
4:D:50:LEU:HD13	4:D:55:ALA:HA	1.85	0.59
10:J:14:VAL:HG12	10:J:50:ILE:HD11	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:VAL:CG1	1:A:525:GLN:HE21	2.15	0.59
1:A:915:SER:O	1:A:919:ILE:HG13	2.02	0.59
1:A:1002:GLY:HA3	1:A:1007:ILE:HG21	1.84	0.59
1:A:1362:TYR:HD1	1:A:1363:VAL:N	2.00	0.59
2:B:213:ILE:HD12	2:B:497:ARG:HB3	1.85	0.59
2:B:496:ARG:HH12	2:B:539:LEU:HB2	1.67	0.59
3:C:11:ARG:HD3	3:C:209:TYR:CE2	2.36	0.59
4:D:24:ALA:C	4:D:26:THR:H	2.10	0.59
5:E:23:VAL:HG13	5:E:78:LEU:HD13	1.83	0.59
6:F:69:LEU:CA	6:F:70:LYS:N	2.64	0.59
8:H:95:TYR:CE2	8:H:97:MET:HG3	2.38	0.59
1:A:2:VAL:HG21	2:B:1157:ALA:C	2.27	0.59
1:A:172:PRO:HD3	1:A:185:TRP:NE1	2.17	0.59
1:A:392:VAL:HG13	1:A:415:LEU:HD11	1.84	0.59
1:A:601:LYS:HB2	1:A:603:ASN:ND2	2.18	0.59
2:B:1087:PHE:CD2	2:B:1088:GLY:N	2.71	0.59
5:E:22:MET:HE3	5:E:26:ARG:NH2	2.18	0.59
8:H:82:PRO:C	8:H:84:ALA:H	2.10	0.59
12:L:53:HIS:HB3	12:L:55:ILE:HD11	1.85	0.59
1:A:800:VAL:HG22	1:A:812:GLU:HB3	1.83	0.59
1:A:1299:VAL:HG12	1:A:1300:LYS:H	1.67	0.59
3:C:167:HIS:HD2	3:C:168:ALA:H	1.51	0.59
6:F:111:LEU:H	6:F:111:LEU:CD1	2.10	0.59
1:A:63:ARG:HA	1:A:74:MET:CE	2.33	0.59
1:A:849:MET:CE	1:A:1061:GLY:HA2	2.33	0.59
1:A:907:THR:CG2	1:A:908:LEU:N	2.65	0.59
1:A:940:ARG:HG2	1:A:940:ARG:HH11	1.67	0.59
1:A:1214:GLU:O	1:A:1218:GLN:HG2	2.01	0.59
2:B:23:ALA:H	2:B:654:ARG:HB3	1.67	0.59
8:H:99:GLY:HA3	8:H:118:PHE:HA	1.83	0.59
1:A:806:ARG:HH12	2:B:729:ILE:CD1	2.15	0.59
2:B:125:SER:HA	2:B:171:PRO:HA	1.84	0.59
2:B:657:HIS:CE1	2:B:689:LEU:HD11	2.37	0.59
3:C:133:ILE:CD1	3:C:237:SER:HA	2.31	0.59
6:F:138:LEU:HB3	6:F:139:PRO:HD2	1.84	0.59
10:J:23:ASN:C	10:J:25:LEU:N	2.61	0.59
1:A:596:THR:C	1:A:598:LEU:H	2.10	0.59
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.42	0.59
1:A:1076:ALA:HA	1:A:1079:MET:CE	2.32	0.59
1:A:1164:PRO:HG2	1:A:1165:GLU:H	1.66	0.59
2:B:192:LEU:O	2:B:193:LYS:HB2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:745:PRO:O	2:B:747:MET:N	2.35	0.59
7:G:10:ASN:OD1	7:G:71:ASN:HA	2.02	0.59
1:A:268:ASP:HB3	1:A:299:HIS:CE1	2.37	0.59
1:A:381:THR:HG21	1:A:383:TYR:CD1	2.38	0.59
1:A:534:LEU:O	1:A:534:LEU:HG	2.01	0.59
1:A:1074:GLU:C	1:A:1076:ALA:H	2.10	0.59
2:B:193:LYS:NZ	12:L:32:ALA:HB1	2.17	0.59
5:E:78:LEU:HD23	5:E:79:TRP:N	2.18	0.59
7:G:80:LYS:O	7:G:80:LYS:HG2	2.01	0.59
1:A:317:LYS:O	1:A:318:SER:HB3	2.03	0.58
1:A:500:GLU:OE1	2:B:1143:ALA:C	2.46	0.58
1:A:541:ILE:HG22	1:A:546:VAL:HG23	1.85	0.58
1:A:929:LEU:HD21	1:A:983:ILE:HD13	1.85	0.58
2:B:336:ARG:CG	2:B:348:ARG:HD3	2.22	0.58
2:B:816:GLU:O	2:B:817:LEU:HD23	2.03	0.58
2:B:1001:PHE:CE2	3:C:34:ARG:CZ	2.86	0.58
2:B:1065:GLN:HB2	3:C:201:TRP:CZ3	2.37	0.58
8:H:89:LEU:O	8:H:91:ASP:N	2.36	0.58
1:A:42:ASP:HB3	1:A:45:GLN:H	1.68	0.58
1:A:62:ASP:HB3	1:A:64:ASN:ND2	2.17	0.58
1:A:382:PRO:CB	1:A:428:TYR:HE2	2.12	0.58
1:A:1127:ASP:HB3	1:A:1130:GLN:CB	2.33	0.58
7:G:35:GLU:OE2	7:G:48:VAL:HG23	2.03	0.58
7:G:149:GLY:O	7:G:159:ALA:HB1	2.03	0.58
9:I:34:TYR:HD2	9:I:34:TYR:C	2.10	0.58
1:A:23:SER:HB3	1:A:233:TRP:CE2	2.38	0.58
2:B:510:LYS:HG3	2:B:511:PRO:CD	2.31	0.58
2:B:1034:VAL:HG12	2:B:1035:ALA:N	2.18	0.58
2:B:1045:SER:O	2:B:1046:PRO:O	2.21	0.58
1:A:89:PRO:HB2	1:A:204:THR:CG2	2.34	0.58
1:A:474:VAL:C	1:A:477:PRO:HD2	2.29	0.58
1:A:535:THR:CG2	1:A:616:VAL:HA	2.30	0.58
1:A:1305:VAL:HG12	1:A:1306:LEU:N	2.18	0.58
1:A:1410:PHE:HA	2:B:1212:ILE:CD1	2.33	0.58
2:B:95:ILE:CG1	2:B:130:VAL:HG22	2.34	0.58
2:B:247:GLY:C	2:B:249:ARG:H	2.11	0.58
2:B:899:ILE:HG21	2:B:949:VAL:HG21	1.83	0.58
4:D:7:THR:HB	7:G:42:PHE:CE2	2.39	0.58
4:D:52:LEU:HD21	4:D:147:TYR:HE2	1.67	0.58
4:D:56:ARG:HA	4:D:148:LEU:HD13	1.86	0.58
11:K:67:PHE:C	11:K:68:PHE:HD2	2.10	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ALA:CB	1:A:276:LEU:HD23	2.34	0.58
1:A:767:GLN:NE2	1:A:774:ARG:HB3	2.18	0.58
2:B:112:LEU:HD12	2:B:113:TYR:N	2.15	0.58
2:B:1008:PRO:HB2	2:B:1010:LEU:O	2.03	0.58
3:C:262:LEU:HD11	11:K:87:LEU:HD23	1.85	0.58
7:G:51:TYR:C	7:G:51:TYR:CD2	2.81	0.58
9:I:92:ARG:HB3	9:I:95:THR:OG1	2.03	0.58
1:A:23:SER:HA	1:A:233:TRP:CD1	2.39	0.58
1:A:1227:ILE:HG22	1:A:1228:TRP:N	2.18	0.58
1:A:1376:THR:O	1:A:1377:THR:C	2.46	0.58
2:B:185:THR:H	2:B:188:ASP:HB2	1.69	0.58
2:B:522:VAL:HG11	2:B:537:LYS:HB3	1.86	0.58
8:H:116:TYR:HE2	8:H:140:ALA:CB	2.16	0.58
11:K:93:SER:O	11:K:97:LYS:HG3	2.04	0.58
1:A:407:ARG:HB3	1:A:430:TRP:CE2	2.39	0.58
1:A:901:LEU:HD22	1:A:919:ILE:CG2	2.34	0.58
1:A:1120:LEU:N	1:A:1120:LEU:CD1	2.66	0.58
2:B:1095:LEU:HD12	2:B:1095:LEU:N	2.19	0.58
3:C:167:HIS:HA	11:K:6:ARG:HH12	1.68	0.58
7:G:1:MET:SD	7:G:1:MET:O	2.62	0.58
7:G:1:MET:HE1	7:G:80:LYS:N	2.18	0.58
10:J:7:CYS:SG	10:J:8:PHE:N	2.76	0.58
1:A:1409:LEU:HD13	2:B:1207:LEU:CD1	2.30	0.58
2:B:680:THR:O	2:B:684:LEU:HD12	2.02	0.58
2:B:731:VAL:HG12	2:B:732:SER:N	2.18	0.58
3:C:39:ALA:CA	3:C:164:ALA:HB3	2.33	0.58
4:D:52:LEU:C	4:D:54:GLU:H	2.11	0.58
4:D:160:VAL:O	4:D:164:ILE:HG13	2.04	0.58
7:G:39:THR:HG22	7:G:40:GLY:N	2.18	0.58
1:A:58:LEU:HD21	1:A:243:PRO:CA	2.33	0.58
1:A:886:ILE:HD11	1:A:943:LEU:CB	2.32	0.58
1:A:1289:ARG:NH1	1:A:1326:ARG:NH1	2.52	0.58
1:A:1332:PHE:O	1:A:1333:ILE:C	2.47	0.58
2:B:25:ILE:HD11	2:B:653:VAL:O	2.03	0.58
2:B:705:MET:H	2:B:710:LEU:HD12	1.69	0.58
2:B:792:MET:HA	2:B:856:PHE:O	2.04	0.58
3:C:73:GLN:HB3	3:C:131:HIS:H	1.69	0.58
4:D:34:GLN:O	4:D:47:LEU:HD23	2.04	0.58
4:D:48:ILE:CG2	7:G:4:ILE:HB	2.33	0.58
5:E:192:ARG:HH11	5:E:192:ARG:HG3	1.69	0.58
5:E:213:ILE:HG12	5:E:214:CYS:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:LEU:HD22	1:A:54:ASN:HD22	1.69	0.58
2:B:687:GLU:O	2:B:689:LEU:HG	2.04	0.58
2:B:1201:LYS:HE2	2:B:1205:GLN:CD	2.27	0.58
5:E:55:ARG:C	5:E:57:MET:H	2.10	0.58
8:H:81:PRO:CB	8:H:82:PRO:HD2	2.33	0.58
1:A:567:LYS:HD2	1:A:568:PRO:HD2	1.83	0.57
2:B:265:SER:O	2:B:266:ALA:HB3	2.03	0.57
2:B:758:PHE:HB3	2:B:761:HIS:CD2	2.39	0.57
2:B:810:GLU:CB	2:B:815:ARG:HH22	2.17	0.57
3:C:168:ALA:C	3:C:170:TRP:N	2.60	0.57
4:D:56:ARG:HD3	4:D:149:THR:HA	1.87	0.57
7:G:15:PRO:O	7:G:16:SER:C	2.46	0.57
10:J:36:LEU:HD12	10:J:47:ARG:NH1	2.19	0.57
10:J:64:ASN:CB	10:J:65:PRO:HD3	2.32	0.57
11:K:50:LEU:HD11	11:K:75:ILE:HD13	1.85	0.57
12:L:32:ALA:CB	12:L:55:ILE:HD12	2.34	0.57
1:A:23:SER:HB3	1:A:233:TRP:CZ2	2.40	0.57
1:A:79:GLY:HA3	1:A:243:PRO:CG	2.34	0.57
1:A:1064:VAL:O	1:A:1067:LEU:HB3	2.04	0.57
2:B:797:TYR:HB2	2:B:852:ARG:O	2.04	0.57
2:B:882:THR:HB	2:B:934:LYS:O	2.04	0.57
7:G:1:MET:SD	7:G:1:MET:C	2.87	0.57
8:H:95:TYR:HE2	8:H:97:MET:CG	2.18	0.57
1:A:1036:ARG:HG2	1:A:1036:ARG:HH11	1.68	0.57
1:A:1063:MET:CG	1:A:1436:ILE:HG23	2.34	0.57
1:A:1209:MET:CE	1:A:1236:LEU:HB3	2.34	0.57
1:A:1423:GLY:HA3	1:A:1426:GLU:HG2	1.86	0.57
2:B:53:GLN:HG2	2:B:547:VAL:CG2	2.33	0.57
2:B:1070:GLU:OE1	10:J:44:TYR:OH	2.23	0.57
8:H:15:VAL:HG22	8:H:26:ILE:CG1	2.33	0.57
2:B:240:ILE:CG2	2:B:254:LEU:HB3	2.34	0.57
2:B:412:LEU:HB3	2:B:466:TRP:CZ2	2.39	0.57
2:B:1095:LEU:H	2:B:1095:LEU:CD1	2.15	0.57
3:C:18:VAL:O	3:C:20:PHE:HD2	1.87	0.57
5:E:134:THR:C	5:E:135:PHE:HD1	2.12	0.57
11:K:114:LEU:HD13	11:K:114:LEU:C	2.29	0.57
1:A:42:ASP:HA	1:A:46:THR:O	2.05	0.57
1:A:406:ILE:HG22	1:A:412:ARG:HA	1.85	0.57
2:B:1099:VAL:HG12	2:B:1100:ASP:N	2.20	0.57
3:C:27:LEU:O	3:C:28:ALA:C	2.47	0.57
4:D:27:LEU:HD22	4:D:173:HIS:CD2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:78:LEU:HD23	5:E:78:LEU:C	2.28	0.57
7:G:39:THR:HG22	7:G:40:GLY:H	1.68	0.57
1:A:24:PRO:HD2	1:A:233:TRP:CD1	2.40	0.57
1:A:325:ILE:O	1:A:326:ARG:C	2.45	0.57
1:A:332:LYS:C	1:A:334:GLY:H	2.11	0.57
1:A:500:GLU:OE2	2:B:1145:SER:HB2	2.04	0.57
1:A:836:TYR:CD2	1:A:840:ARG:HD2	2.38	0.57
1:A:1438:THR:HB	2:B:1144:ALA:CB	2.35	0.57
2:B:635:ARG:NH2	2:B:742:GLU:OE2	2.37	0.57
5:E:163:GLU:O	5:E:164:LEU:C	2.47	0.57
10:J:1:MET:N	10:J:56:LEU:N	2.52	0.57
1:A:282:ASN:O	1:A:284:ALA:N	2.38	0.57
1:A:442:VAL:O	1:A:457:ALA:HA	2.05	0.57
1:A:469:ARG:HH11	1:A:469:ARG:HB3	1.69	0.57
2:B:360:PHE:C	2:B:360:PHE:CD2	2.82	0.57
2:B:865:LYS:HE2	2:B:871:THR:OG1	2.04	0.57
2:B:996:ARG:NH2	3:C:175:ALA:HA	2.20	0.57
3:C:112:ASN:HB2	3:C:114:TYR:CE1	2.39	0.57
4:D:71:LYS:HA	4:D:74:GLN:CB	2.32	0.57
5:E:10:SER:O	5:E:14:ARG:HG3	2.04	0.57
8:H:128:ASN:CG	8:H:128:ASN:O	2.47	0.57
1:A:427:GLN:O	1:A:428:TYR:C	2.48	0.57
1:A:722:LEU:HD22	1:A:799:PHE:CD1	2.39	0.57
2:B:954:VAL:O	12:L:55:ILE:O	2.22	0.57
3:C:214:ASN:HB3	3:C:217:ASP:OD2	2.04	0.57
15:T:16:DT:C2'	15:T:17:TT:H5'1	2.34	0.57
1:A:458:HIS:CE1	1:A:507:VAL:HG21	2.40	0.57
1:A:1171:GLN:HA	1:A:1174:PHE:CD1	2.39	0.57
2:B:336:ARG:HD3	2:B:348:ARG:NH1	2.18	0.57
2:B:527:THR:OG1	2:B:528:PRO:HD2	2.04	0.57
2:B:758:PHE:CE2	2:B:1044:ALA:HA	2.38	0.57
3:C:35:ARG:NH1	11:K:41:THR:N	2.53	0.57
5:E:145:THR:HG21	5:E:187:TYR:CD2	2.40	0.57
6:F:85:MET:HE2	6:F:93:ILE:HD12	1.87	0.57
7:G:18:PHE:HA	7:G:22:MET:CE	2.32	0.57
14:P:1:U:H2'	14:P:2:C:C6	2.39	0.57
1:A:115:LEU:CB	1:A:122:MET:HE2	2.32	0.57
1:A:152:VAL:HG13	1:A:153:PRO:HD2	1.86	0.57
1:A:332:LYS:C	1:A:334:GLY:N	2.62	0.57
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.86	0.57
1:A:648:ASN:O	1:A:649:ILE:C	2.47	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:667:GLY:HA3	3:C:192:TRP:CH2	2.40	0.57
1:A:1364:ASN:O	1:A:1365:TYR:C	2.47	0.57
2:B:126:SER:O	2:B:169:ARG:HA	2.03	0.57
2:B:758:PHE:CE1	2:B:1027:ILE:CG2	2.88	0.57
2:B:797:TYR:HE1	2:B:854:LEU:HD23	1.69	0.57
2:B:873:THR:O	2:B:914:LYS:HA	2.04	0.57
2:B:916:THR:O	2:B:935:ARG:HG3	2.05	0.57
2:B:1181:GLU:HG3	2:B:1188:LYS:HE3	1.85	0.57
2:B:1196:ILE:HB	2:B:1197:PRO:HD2	1.86	0.57
4:D:4:SER:O	4:D:5:THR:HB	2.04	0.57
1:A:42:ASP:C	1:A:44:THR:H	2.11	0.56
1:A:399:HIS:O	1:A:401:GLY:N	2.37	0.56
1:A:399:HIS:CB	1:A:400:PRO:HD3	2.30	0.56
1:A:596:THR:O	1:A:598:LEU:N	2.37	0.56
1:A:761:MET:HA	1:A:804:TYR:HB2	1.87	0.56
1:A:986:ILE:HG22	1:A:987:VAL:N	2.18	0.56
1:A:1308:THR:HG23	1:A:1309:ASP:N	2.19	0.56
2:B:758:PHE:CE1	2:B:1027:ILE:HG22	2.39	0.56
2:B:1106:ARG:HD3	2:B:1126:GLY:C	2.30	0.56
2:B:1183:LYS:N	2:B:1183:LYS:HE3	2.20	0.56
8:H:4:THR:O	8:H:5:LEU:HD23	2.04	0.56
14:P:7:A:H2'	14:P:8:G:C8	2.40	0.56
15:T:19:DT:H2''	15:T:20:DC:O5'	2.05	0.56
1:A:17:VAL:HA	2:B:1215:ARG:O	2.05	0.56
1:A:34:LYS:HB2	1:A:36:ARG:HH21	1.70	0.56
1:A:1039:LYS:HE3	1:A:1043:ASP:OD2	2.05	0.56
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.86	0.56
2:B:378:LEU:O	2:B:378:LEU:HD12	2.03	0.56
2:B:999:MET:HG2	2:B:1007:VAL:HG22	1.86	0.56
3:C:47:ASP:CA	12:L:69:ALA:CB	2.79	0.56
3:C:73:GLN:HE21	3:C:75:MET:N	2.02	0.56
3:C:212:PRO:CB	3:C:213:PRO:HD2	2.35	0.56
7:G:23:LYS:HG3	7:G:56:ILE:HD11	1.85	0.56
1:A:92:HIS:HD2	1:A:304:MET:CE	2.18	0.56
1:A:382:PRO:HD3	1:A:428:TYR:HD2	1.71	0.56
1:A:402:ALA:CB	1:A:434:ARG:HA	2.35	0.56
1:A:527:THR:HG23	1:A:650:GLN:HA	1.88	0.56
1:A:577:ILE:C	1:A:579:SER:N	2.60	0.56
1:A:695:LYS:C	1:A:697:ALA:H	2.11	0.56
1:A:709:THR:HB	1:A:712:GLU:HG3	1.86	0.56
1:A:898:ARG:HB2	1:A:933:TYR:CE1	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1025:ARG:O	1:A:1026:LEU:HD23	2.05	0.56
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	1.87	0.56
1:A:1349:TYR:CE1	1:A:1368:MET:HE3	2.40	0.56
2:B:114:PRO:O	2:B:116:GLU:N	2.38	0.56
2:B:593:PRO:HG2	2:B:617:ARG:NH2	2.20	0.56
2:B:642:ASP:HB3	2:B:649:LYS:HG3	1.87	0.56
2:B:744:HIS:HD2	2:B:746:SER:OG	1.88	0.56
2:B:1166:CYS:SG	2:B:1166:CYS:O	2.63	0.56
2:B:1166:CYS:O	2:B:1168:LEU:N	2.37	0.56
3:C:46:ILE:HD12	3:C:67:LEU:O	2.04	0.56
3:C:99:LEU:HB2	3:C:157:CYS:HB2	1.87	0.56
3:C:254:LYS:O	3:C:258:ILE:HD13	2.05	0.56
5:E:35:VAL:C	5:E:37:LEU:H	2.13	0.56
5:E:39:LEU:O	5:E:42:PHE:HB3	2.05	0.56
10:J:7:CYS:SG	10:J:49:MET:HE3	2.45	0.56
10:J:12:LYS:O	10:J:14:VAL:HG23	2.05	0.56
11:K:57:LEU:HD12	11:K:77:THR:O	2.05	0.56
11:K:65:HIS:CD2	11:K:65:HIS:C	2.83	0.56
1:A:349:ALA:C	2:B:1128:LEU:HD11	2.30	0.56
1:A:901:LEU:HD22	1:A:919:ILE:HG22	1.86	0.56
2:B:483:LEU:HD11	2:B:491:THR:HG23	1.86	0.56
2:B:1202:LEU:HD22	2:B:1206:GLU:CD	2.31	0.56
3:C:146:LYS:C	3:C:147:LEU:HD23	2.31	0.56
3:C:168:ALA:O	3:C:170:TRP:N	2.38	0.56
7:G:17:PHE:N	7:G:17:PHE:CD2	2.73	0.56
8:H:100:THR:HG22	8:H:101:ALA:N	2.19	0.56
11:K:19:LEU:HD22	11:K:33:ILE:CG2	2.35	0.56
1:A:35:ILE:CD1	1:A:241:VAL:HG21	2.36	0.56
1:A:78:PRO:HA	2:B:1201:LYS:NZ	2.21	0.56
1:A:567:LYS:HB3	8:H:95:TYR:CA	2.33	0.56
1:A:1213:GLY:O	1:A:1214:GLU:C	2.49	0.56
2:B:755:ILE:HG23	2:B:809:MET:HE2	1.86	0.56
1:A:524:VAL:CG1	1:A:525:GLN:H	2.06	0.56
1:A:596:THR:C	1:A:598:LEU:N	2.63	0.56
1:A:751:SER:O	1:A:752:LYS:HG2	2.05	0.56
1:A:939:ASP:O	1:A:940:ARG:C	2.49	0.56
1:A:1035:TYR:O	1:A:1037:LEU:N	2.38	0.56
2:B:899:ILE:CD1	2:B:911:ILE:HA	2.32	0.56
3:C:67:LEU:HD11	3:C:155:LEU:CD1	2.35	0.56
8:H:43:ASN:OD1	8:H:46:LEU:HG	2.05	0.56
8:H:102:TYR:N	8:H:102:TYR:CD2	2.73	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:ASP:OD2	11:K:65:HIS:HE1	1.88	0.56
1:A:798:GLY:HA2	1:A:815:PHE:HD1	1.70	0.56
2:B:825:VAL:HG12	2:B:826:ALA:N	2.20	0.56
3:C:236:GLY:C	3:C:238:ILE:N	2.63	0.56
7:G:26:LEU:O	7:G:27:LYS:C	2.48	0.56
9:I:59:VAL:C	9:I:61:ASP:H	2.14	0.56
1:A:107:CYS:N	1:A:114:LEU:HD21	2.20	0.56
1:A:225:ASN:ND2	1:A:227:VAL:H	2.02	0.56
1:A:244:PRO:CB	1:A:245:PRO:HD3	2.34	0.56
1:A:639:PRO:HG2	1:A:640:GLN:H	1.70	0.56
1:A:971:PHE:CE2	1:A:1040:GLN:HG2	2.41	0.56
1:A:1017:LEU:HB2	5:E:206:GLY:N	2.13	0.56
7:G:88:ASP:OD2	7:G:88:ASP:N	2.39	0.56
7:G:138:THR:CG2	7:G:139:ILE:H	1.98	0.56
8:H:143:LEU:HD12	8:H:143:LEU:N	2.20	0.56
11:K:47:ARG:HD3	11:K:59:ALA:O	2.05	0.56
1:A:224:PHE:CZ	1:A:234:MET:HE2	2.40	0.56
1:A:244:PRO:O	1:A:247:ARG:N	2.39	0.56
1:A:300:VAL:O	1:A:300:VAL:HG12	2.06	0.56
1:A:1313:LEU:HD23	1:A:1338:VAL:CG2	2.36	0.56
2:B:315:LYS:N	2:B:316:PRO:HD2	2.21	0.56
2:B:900:ALA:HB3	12:L:61:THR:OG1	2.06	0.56
2:B:983:ARG:HD2	2:B:1091:TYR:HD2	1.71	0.56
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.38	0.56
4:D:47:LEU:CD1	4:D:48:ILE:N	2.68	0.56
7:G:66:GLY:O	7:G:67:SER:C	2.48	0.56
8:H:38:LEU:HD13	8:H:125:LEU:HD13	1.88	0.56
8:H:40:LEU:HD22	8:H:123:MET:CE	2.35	0.56
10:J:44:TYR:HA	10:J:47:ARG:HB2	1.88	0.56
11:K:63:VAL:HG23	11:K:63:VAL:O	2.06	0.56
1:A:565:ILE:O	1:A:570:PRO:HA	2.06	0.56
1:A:1001:ARG:O	1:A:1002:GLY:O	2.24	0.56
1:A:1095:THR:O	1:A:1096:SER:HB2	2.05	0.56
2:B:128:LEU:O	2:B:167:ILE:N	2.31	0.56
2:B:220:GLY:O	2:B:222:ILE:HG13	2.06	0.56
2:B:1138:MET:HA	2:B:1138:MET:HE3	1.87	0.56
3:C:124:LEU:O	3:C:127:ARG:HG2	2.06	0.56
6:F:93:ILE:HD13	6:F:148:VAL:CG1	2.36	0.56
10:J:27:GLU:C	10:J:29:GLU:H	2.12	0.56
1:A:265:LYS:HE2	1:A:322:VAL:HG11	1.87	0.55
1:A:299:HIS:O	1:A:301:ALA:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:ARG:NH2	2:B:1108:ARG:NH1	2.54	0.55
1:A:474:VAL:HG22	1:A:478:TYR:HE1	1.71	0.55
1:A:921:GLY:O	1:A:922:ASP:C	2.47	0.55
1:A:1195:LEU:HD11	1:A:1267:MET:HE1	1.87	0.55
2:B:25:ILE:HD11	2:B:653:VAL:C	2.31	0.55
2:B:464:GLY:HA2	2:B:479:VAL:O	2.05	0.55
3:C:90:ASP:O	3:C:91:HIS:HB3	2.05	0.55
8:H:103:LYS:HG2	8:H:104:PHE:N	2.22	0.55
1:A:61:ILE:HG22	1:A:62:ASP:N	2.18	0.55
1:A:308:ILE:HG22	1:A:309:ALA:H	1.70	0.55
1:A:971:PHE:HE2	1:A:1040:GLN:HG2	1.71	0.55
2:B:223:VAL:CG1	2:B:381:MET:HG2	2.35	0.55
2:B:288:ALA:HA	2:B:331:LEU:HD12	1.88	0.55
2:B:1017:ILE:HB	2:B:1018:PRO:HD3	1.88	0.55
2:B:1183:LYS:N	2:B:1183:LYS:CE	2.69	0.55
3:C:189:THR:HG22	3:C:190:ASP:N	2.20	0.55
7:G:34:VAL:HG12	7:G:45:ILE:CG2	2.31	0.55
9:I:111:THR:CG2	9:I:112:SER:H	2.18	0.55
11:K:42:LEU:O	11:K:46:ILE:HG13	2.06	0.55
1:A:58:LEU:CG	1:A:59:GLY:H	2.18	0.55
1:A:265:LYS:HZ3	1:A:322:VAL:HG22	1.71	0.55
1:A:316:GLN:O	1:A:317:LYS:C	2.49	0.55
1:A:726:ARG:O	1:A:729:ALA:HB3	2.05	0.55
1:A:852:TYR:HA	1:A:1060:PRO:HB3	1.88	0.55
1:A:877:HIS:C	1:A:878:ILE:CG1	2.80	0.55
1:A:974:ASP:C	1:A:976:THR:H	2.15	0.55
2:B:957:ASN:O	2:B:959:ASP:N	2.39	0.55
3:C:45:ALA:HA	3:C:72:LEU:CD1	2.35	0.55
3:C:82:TYR:O	3:C:83:SER:C	2.49	0.55
3:C:154:LYS:O	3:C:155:LEU:HD23	2.07	0.55
3:C:238:ILE:HG22	3:C:243:VAL:HG23	1.88	0.55
4:D:13:ARG:HB2	4:D:17:LYS:NZ	2.19	0.55
1:A:12:ARG:O	2:B:1194:ILE:HG22	2.06	0.55
1:A:130:ASP:O	1:A:133:LYS:N	2.35	0.55
1:A:252:PHE:HB2	1:A:256:GLN:NE2	2.22	0.55
1:A:526:ASP:OD1	2:B:1013:ASN:ND2	2.40	0.55
1:A:1444:MET:HG2	7:G:60:ARG:CA	2.36	0.55
2:B:63:ILE:O	2:B:67:SER:HB3	2.06	0.55
2:B:542:MET:HE2	2:B:743:ILE:HG13	1.87	0.55
2:B:1162:ILE:HG22	2:B:1163:CYS:H	1.72	0.55
2:B:1187:ASN:OD1	2:B:1190:ASP:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:22:MET:HE3	5:E:26:ARG:NE	2.22	0.55
5:E:46:TYR:CD2	5:E:58:MET:HG2	2.41	0.55
8:H:4:THR:CA	8:H:60:ALA:HB2	2.31	0.55
11:K:42:LEU:HD21	11:K:46:ILE:CD1	2.37	0.55
12:L:58:LYS:O	12:L:58:LYS:HG2	2.06	0.55
1:A:168:GLY:O	1:A:169:ASN:C	2.49	0.55
1:A:253:ASN:HB3	2:B:935:ARG:NH1	2.22	0.55
1:A:1385:THR:HG22	1:A:1386:ARG:N	2.21	0.55
2:B:640:VAL:O	2:B:641:GLU:C	2.50	0.55
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.89	0.55
2:B:729:ILE:O	2:B:729:ILE:HG22	2.04	0.55
5:E:55:ARG:C	5:E:57:MET:N	2.63	0.55
8:H:11:GLN:HA	8:H:53:ASP:O	2.06	0.55
8:H:84:ALA:CA	8:H:87:ARG:HB2	2.34	0.55
1:A:34:LYS:HE3	1:A:57:ARG:NH1	2.15	0.55
1:A:219:PHE:O	1:A:222:LEU:O	2.24	0.55
1:A:606:LEU:HB3	1:A:614:PHE:CE2	2.42	0.55
1:A:1198:ASP:O	1:A:1202:MET:HG2	2.07	0.55
1:A:1206:ASP:CB	1:A:1274:ARG:HH12	2.17	0.55
2:B:35:SER:O	2:B:39:ARG:HG3	2.07	0.55
2:B:388:CYS:C	2:B:390:LEU:H	2.13	0.55
2:B:498:THR:HB	2:B:537:LYS:O	2.07	0.55
2:B:899:ILE:CG2	2:B:949:VAL:HG21	2.37	0.55
2:B:1202:LEU:O	2:B:1203:LEU:C	2.48	0.55
3:C:174:ALA:O	3:C:175:ALA:HB2	2.04	0.55
5:E:192:ARG:HG2	5:E:192:ARG:O	2.06	0.55
7:G:80:LYS:H	7:G:80:LYS:HD3	1.72	0.55
8:H:83:GLN:C	8:H:85:GLY:H	2.13	0.55
1:A:34:LYS:CE	1:A:57:ARG:NH1	2.66	0.55
1:A:373:THR:HG21	2:B:1105:ALA:HB3	1.89	0.55
1:A:492:PRO:O	1:A:493:GLN:NE2	2.40	0.55
2:B:337:ARG:C	2:B:338:GLY:N	2.64	0.55
3:C:208:GLU:C	3:C:210:GLU:H	2.14	0.55
6:F:97:ARG:O	6:F:101:ILE:HG13	2.07	0.55
7:G:154:VAL:HG12	7:G:155:SER:N	2.20	0.55
1:A:49:LYS:HZ1	1:A:61:ILE:N	2.05	0.55
1:A:71:GLN:C	1:A:73:GLY:H	2.14	0.55
1:A:666:ILE:HD11	2:B:1067:ARG:O	2.07	0.55
1:A:873:MET:C	1:A:1058:VAL:HG23	2.32	0.55
1:A:1094:VAL:CG1	1:A:1095:THR:H	2.12	0.55
1:A:1120:LEU:O	1:A:1323:ASP:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:33:VAL:HG21	2:B:638:PHE:HZ	1.70	0.55
2:B:814:PHE:C	2:B:816:GLU:H	2.13	0.55
2:B:1159:ARG:HD3	2:B:1193:GLN:CG	2.26	0.55
5:E:15:ALA:O	5:E:19:VAL:HG23	2.07	0.55
5:E:94:LYS:HE2	5:E:98:ILE:CD1	2.25	0.55
5:E:157:SER:C	5:E:159:ASP:N	2.62	0.55
8:H:61:SER:O	8:H:62:SER:CB	2.54	0.55
8:H:95:TYR:HB3	8:H:144:ILE:HB	1.89	0.55
9:I:103:CYS:CB	9:I:106:CYS:HG	2.20	0.55
11:K:46:ILE:O	11:K:46:ILE:HG22	2.06	0.55
1:A:567:LYS:CB	1:A:568:PRO:CD	2.84	0.55
1:A:842:VAL:HG12	1:A:843:LYS:N	2.21	0.55
2:B:113:TYR:HB3	2:B:114:PRO:HD2	1.88	0.55
2:B:806:THR:O	2:B:809:MET:HG3	2.06	0.55
9:I:62:ILE:O	9:I:62:ILE:HG12	2.06	0.55
15:T:22:BRU:H2'	15:T:23:DG:O4'	2.07	0.55
1:A:903:ASN:HD22	1:A:904:THR:H	1.46	0.55
1:A:1124:HIS:HB3	1:A:1130:GLN:HG2	1.89	0.55
2:B:798:TYR:HE2	3:C:62:PHE:HZ	1.51	0.55
2:B:798:TYR:CE2	3:C:62:PHE:CZ	2.95	0.55
2:B:833:TYR:N	2:B:833:TYR:HD1	2.04	0.55
3:C:46:ILE:HG13	3:C:72:LEU:HD11	1.89	0.55
3:C:189:THR:HG22	3:C:190:ASP:H	1.71	0.55
3:C:256:ALA:O	3:C:259:LEU:N	2.40	0.55
7:G:34:VAL:CG1	7:G:45:ILE:HG21	2.28	0.55
13:N:0:DT:H1'	13:N:1:DA:C5'	2.37	0.55
1:A:49:LYS:HZ3	1:A:61:ILE:HG13	1.72	0.54
1:A:504:LEU:HD12	1:A:504:LEU:N	2.22	0.54
1:A:982:THR:HB	1:A:985:ASP:H	1.71	0.54
1:A:1420:ASP:O	1:A:1421:CYS:HB2	2.07	0.54
2:B:293:PRO:HG2	2:B:296:GLU:HB2	1.89	0.54
2:B:658:ILE:HG22	2:B:659:ALA:N	2.21	0.54
2:B:999:MET:HB3	2:B:1007:VAL:HG21	1.88	0.54
2:B:1156:ASP:HB3	2:B:1197:PRO:HA	1.88	0.54
4:D:51:ASN:O	4:D:52:LEU:O	2.25	0.54
4:D:167:LEU:O	4:D:170:THR:OG1	2.18	0.54
1:A:50:ILE:C	1:A:52:GLY:N	2.63	0.54
1:A:527:THR:CG2	1:A:650:GLN:HA	2.38	0.54
1:A:577:ILE:O	1:A:578:LEU:C	2.51	0.54
1:A:1011:GLN:NE2	1:A:1015:VAL:HG21	2.22	0.54
1:A:1118:VAL:HG12	1:A:1327:ILE:HG13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:446:LEU:O	2:B:447:ALA:HB3	2.07	0.54
2:B:467:GLY:N	2:B:475:SER:CB	2.64	0.54
3:C:27:LEU:HD13	3:C:228:PHE:HE2	1.72	0.54
3:C:129:ILE:HG23	3:C:130:GLY:N	2.22	0.54
8:H:25:ARG:HA	8:H:41:ASP:HA	1.89	0.54
8:H:55:LEU:HD22	8:H:144:ILE:CG2	2.36	0.54
12:L:36:SER:O	12:L:37:LYS:C	2.49	0.54
1:A:666:ILE:HD12	1:A:666:ILE:N	2.22	0.54
2:B:364:ILE:HG12	2:B:585:VAL:CG1	2.29	0.54
2:B:465:ASN:HD22	2:B:465:ASN:N	2.04	0.54
3:C:76:ASP:OD2	3:C:128:ASN:N	2.39	0.54
3:C:142:VAL:H	10:J:16:ASP:HB3	1.71	0.54
6:F:85:MET:HE2	6:F:93:ILE:CD1	2.37	0.54
6:F:86:THR:HG23	6:F:89:GLU:OE1	2.07	0.54
10:J:36:LEU:O	10:J:39:LEU:N	2.39	0.54
13:N:0:DT:H2''	13:N:1:DA:O5'	2.07	0.54
1:A:79:GLY:HA3	1:A:243:PRO:HG3	1.89	0.54
1:A:154:SER:HB3	1:A:162:VAL:HG21	1.90	0.54
1:A:518:LYS:HE2	1:A:624:SER:O	2.08	0.54
1:A:785:PRO:HG2	2:B:703:ILE:HD12	1.89	0.54
1:A:909:ASP:C	1:A:911:SER:H	2.16	0.54
1:A:1370:LEU:O	1:A:1374:VAL:HG23	2.07	0.54
2:B:95:ILE:HG13	2:B:130:VAL:HG22	1.88	0.54
2:B:339:THR:O	2:B:339:THR:HG22	2.07	0.54
2:B:431:TYR:CZ	2:B:447:ALA:HB2	2.42	0.54
2:B:806:THR:CG2	2:B:808:ALA:HB3	2.37	0.54
4:D:156:ASP:C	4:D:158:GLU:H	2.15	0.54
6:F:119:ARG:HH11	6:F:119:ARG:HG3	1.72	0.54
9:I:101:PHE:N	9:I:101:PHE:CD1	2.75	0.54
1:A:130:ASP:O	1:A:131:SER:C	2.50	0.54
1:A:299:HIS:C	1:A:301:ALA:H	2.15	0.54
1:A:441:PRO:HD2	1:A:498:ARG:NH2	2.23	0.54
2:B:129:PHE:CD2	2:B:166:PHE:HA	2.41	0.54
2:B:221:ASN:OD1	2:B:242:SER:HA	2.08	0.54
2:B:683:SER:O	2:B:687:GLU:HB2	2.07	0.54
2:B:1219:ASP:OD1	2:B:1219:ASP:O	2.25	0.54
3:C:140:ASN:O	3:C:141:GLY:O	2.26	0.54
10:J:27:GLU:O	10:J:29:GLU:N	2.40	0.54
10:J:43:ARG:HG3	10:J:45:CYS:SG	2.48	0.54
1:A:34:LYS:HZ1	1:A:57:ARG:NH1	2.05	0.54
1:A:670:ILE:HG23	1:A:805:LEU:HD21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1299:VAL:CG1	1:A:1300:LYS:N	2.71	0.54
1:A:1356:ILE:HD12	1:A:1368:MET:SD	2.48	0.54
2:B:29:ASP:O	2:B:30:SER:C	2.50	0.54
2:B:388:CYS:O	2:B:391:ASP:N	2.36	0.54
2:B:549:THR:HG22	2:B:550:ASP:N	2.15	0.54
3:C:145:CYS:HA	10:J:2:ILE:HD11	1.89	0.54
6:F:69:LEU:N	6:F:70:LYS:N	2.56	0.54
7:G:29:LYS:O	7:G:30:LEU:C	2.51	0.54
9:I:82:GLU:HB3	9:I:104:LEU:HD12	1.88	0.54
2:B:101:MET:O	2:B:102:VAL:HG23	2.07	0.54
2:B:283:VAL:O	2:B:286:PHE:N	2.41	0.54
2:B:830:TYR:O	2:B:831:SER:C	2.50	0.54
2:B:843:GLN:O	2:B:846:ILE:N	2.41	0.54
3:C:263:THR:C	3:C:265:MET:N	2.66	0.54
6:F:130:ILE:O	6:F:148:VAL:HG21	2.07	0.54
1:A:185:TRP:CZ3	1:A:200:ARG:HG2	2.42	0.54
1:A:317:LYS:O	1:A:318:SER:CB	2.56	0.54
1:A:332:LYS:O	1:A:334:GLY:N	2.40	0.54
1:A:471:ASN:O	1:A:474:VAL:HG12	2.08	0.54
1:A:715:GLU:OE2	1:A:774:ARG:NH1	2.41	0.54
1:A:741:ASN:HD21	1:A:743:VAL:HB	1.73	0.54
1:A:853:ASP:OD1	1:A:853:ASP:C	2.50	0.54
1:A:971:PHE:O	1:A:972:HIS:C	2.51	0.54
1:A:1063:MET:SD	1:A:1436:ILE:HG12	2.48	0.54
1:A:1365:TYR:O	1:A:1367:HIS:N	2.40	0.54
2:B:210:LYS:HA	2:B:481:GLN:O	2.07	0.54
2:B:521:LEU:HB3	2:B:633:VAL:CG1	2.37	0.54
2:B:1106:ARG:HH12	2:B:1110:PRO:HG2	1.71	0.54
3:C:37:MET:HA	3:C:41:ILE:CD1	2.38	0.54
4:D:64:VAL:O	4:D:66:ARG:N	2.40	0.54
7:G:138:THR:HG22	7:G:139:ILE:HG13	1.88	0.54
8:H:98:TYR:C	8:H:118:PHE:HD2	2.15	0.54
1:A:385:ILE:CG2	1:A:386:ASP:N	2.71	0.54
1:A:718:VAL:O	1:A:721:PHE:HB2	2.07	0.54
1:A:1118:VAL:HG23	1:A:1118:VAL:O	2.07	0.54
1:A:1445:ILE:HD11	7:G:68:ALA:HB1	1.89	0.54
2:B:46:GLN:HG3	2:B:47:GLN:N	2.21	0.54
2:B:520:GLY:N	2:B:748:ILE:HG22	2.22	0.54
2:B:911:ILE:O	2:B:911:ILE:HG22	2.07	0.54
3:C:175:ALA:HB3	10:J:43:ARG:HH22	1.71	0.54
8:H:116:TYR:HE2	8:H:140:ALA:HB1	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:31:VAL:O	11:K:74:ARG:HA	2.06	0.54
11:K:31:VAL:CG1	11:K:32:VAL:N	2.71	0.54
13:N:5:DA:C2	15:T:13:DA:C2	2.95	0.54
14:P:0:U:H2'	14:P:1:U:H5'	1.89	0.54
14:P:5:C:O2'	14:P:6:C:H5'	2.07	0.54
1:A:40:THR:HG22	1:A:41:MET:CG	2.29	0.54
1:A:58:LEU:CD1	1:A:59:GLY:N	2.63	0.54
1:A:89:PRO:HB2	1:A:204:THR:HG22	1.89	0.54
1:A:350:ARG:HB2	1:A:488:ASN:OD1	2.08	0.54
1:A:600:PRO:C	1:A:602:ASP:H	2.15	0.54
1:A:711:ARG:NH2	9:I:87:GLN:OE1	2.41	0.54
1:A:767:GLN:OE1	1:A:799:PHE:HB2	2.08	0.54
1:A:858:ASN:ND2	1:A:861:GLY:H	2.05	0.54
1:A:901:LEU:N	1:A:926:GLN:NE2	2.48	0.54
1:A:1114:PRO:O	1:A:1115:SER:O	2.26	0.54
1:A:1450:LEU:HD21	7:G:18:PHE:O	2.07	0.54
2:B:172:ILE:HG22	2:B:173:MET:N	2.22	0.54
2:B:412:LEU:HB3	2:B:466:TRP:HZ2	1.73	0.54
2:B:654:ARG:C	2:B:656:GLY:H	2.16	0.54
2:B:776:GLN:NE2	14:P:8:G:H5'	2.20	0.54
2:B:910:VAL:HG12	2:B:912:ILE:H	1.73	0.54
5:E:31:THR:O	5:E:35:VAL:HG23	2.07	0.54
5:E:145:THR:HG21	5:E:187:TYR:CE2	2.43	0.54
7:G:47:CYS:O	7:G:76:ALA:HB1	2.08	0.54
8:H:47:PHE:CD2	8:H:95:TYR:HD1	2.25	0.54
10:J:32:GLU:O	10:J:33:GLY:C	2.50	0.54
10:J:45:CYS:O	10:J:48:ARG:HG3	2.08	0.54
11:K:47:ARG:HD2	11:K:47:ARG:O	2.08	0.54
1:A:18:GLN:CB	2:B:1215:ARG:HB2	2.39	0.53
1:A:241:VAL:O	1:A:242:PRO:C	2.51	0.53
1:A:441:PRO:HD2	1:A:498:ARG:CZ	2.38	0.53
2:B:1182:CYS:O	2:B:1183:LYS:O	2.26	0.53
3:C:249:ASP:O	3:C:252:GLN:HB3	2.09	0.53
7:G:27:LYS:O	7:G:30:LEU:HB3	2.08	0.53
1:A:50:ILE:O	1:A:52:GLY:N	2.40	0.53
1:A:672:ASP:HB2	1:A:736:ASN:OD1	2.08	0.53
1:A:852:TYR:CE1	6:F:136:ARG:HG2	2.43	0.53
3:C:242:GLN:C	3:C:244:VAL:H	2.14	0.53
6:F:86:THR:HG23	6:F:89:GLU:CD	2.33	0.53
1:A:53:LEU:O	1:A:54:ASN:C	2.50	0.53
1:A:362:ASP:OD2	1:A:459:ARG:HD3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:VAL:CG2	1:A:460:VAL:HG22	2.36	0.53
1:A:618:GLU:O	1:A:619:LYS:C	2.52	0.53
1:A:1191:TRP:CD1	1:A:1256:GLU:HB2	2.44	0.53
2:B:38:PHE:HD1	2:B:811:TYR:CD2	2.27	0.53
2:B:547:VAL:HG12	2:B:612:GLU:OE2	2.08	0.53
2:B:803:LEU:CD1	2:B:1032:SER:HB3	2.38	0.53
2:B:1099:VAL:HG12	2:B:1100:ASP:H	1.72	0.53
3:C:34:ARG:HA	3:C:37:MET:HE3	1.91	0.53
9:I:55:THR:CG2	9:I:58:VAL:HG21	2.38	0.53
9:I:101:PHE:CE1	9:I:112:SER:HB2	2.43	0.53
1:A:38:PRO:HA	1:A:270:LEU:HD23	1.90	0.53
1:A:222:LEU:O	1:A:224:PHE:N	2.41	0.53
1:A:230:ARG:N	1:A:233:TRP:CE3	2.65	0.53
1:A:503:GLN:C	1:A:504:LEU:HD12	2.34	0.53
1:A:1006:ILE:HD12	5:E:163:GLU:HG3	1.90	0.53
2:B:705:MET:H	2:B:710:LEU:CD1	2.22	0.53
2:B:803:LEU:HD12	2:B:1032:SER:HB3	1.89	0.53
2:B:810:GLU:HB2	2:B:815:ARG:NH2	2.22	0.53
4:D:7:THR:HG21	4:D:32:GLU:OE2	2.08	0.53
4:D:198:LEU:O	4:D:200:ASN:N	2.40	0.53
7:G:9:LEU:HD12	7:G:10:ASN:H	1.73	0.53
11:K:41:THR:HG22	11:K:42:LEU:N	2.22	0.53
1:A:44:THR:O	1:A:45:GLN:HB2	2.09	0.53
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.44	0.53
1:A:224:PHE:HD2	1:A:229:SER:O	1.91	0.53
1:A:598:LEU:HD22	8:H:25:ARG:NH1	2.24	0.53
1:A:997:LEU:HD13	1:A:1018:PHE:CE2	2.43	0.53
2:B:293:PRO:HG2	2:B:296:GLU:HB3	1.89	0.53
3:C:187:LYS:C	3:C:189:THR:H	2.15	0.53
5:E:29:PHE:C	5:E:30:ILE:HG13	2.33	0.53
1:A:61:ILE:O	1:A:63:ARG:N	2.42	0.53
1:A:278:THR:O	1:A:278:THR:HG22	2.09	0.53
1:A:368:LYS:O	1:A:369:SER:C	2.51	0.53
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.39	0.53
1:A:699:ALA:CB	1:A:701:LEU:HG	2.39	0.53
1:A:852:TYR:CD2	1:A:1060:PRO:CB	2.92	0.53
1:A:1074:GLU:H	1:A:1075:PRO:HD2	1.73	0.53
1:A:1224:LEU:HD11	1:A:1240:CYS:HB2	1.90	0.53
2:B:388:CYS:O	2:B:390:LEU:N	2.42	0.53
2:B:449:ASN:C	2:B:451:LYS:H	2.17	0.53
2:B:705:MET:N	2:B:710:LEU:HD12	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1084:GLN:C	2:B:1085:ILE:HD12	2.34	0.53
3:C:9:LYS:O	3:C:10:ILE:C	2.52	0.53
3:C:166:GLU:OE1	12:L:70:ARG:NH2	2.32	0.53
7:G:87:VAL:HG23	7:G:103:VAL:HG21	1.91	0.53
1:A:34:LYS:H	1:A:57:ARG:NH2	2.07	0.53
1:A:248:PRO:O	1:A:260:ASP:HB2	2.09	0.53
1:A:1010:ALA:O	1:A:1011:GLN:C	2.52	0.53
1:A:1242:VAL:HG12	1:A:1243:VAL:N	2.24	0.53
2:B:448:ILE:O	2:B:450:ALA:N	2.42	0.53
2:B:975:GLN:O	2:B:990:ILE:HD12	2.09	0.53
3:C:254:LYS:C	3:C:256:ALA:N	2.65	0.53
4:D:18:VAL:HG13	4:D:18:VAL:O	2.09	0.53
7:G:73:LYS:HE2	7:G:74:TYR:O	2.08	0.53
9:I:26:LEU:CD2	9:I:37:GLU:HA	2.34	0.53
10:J:28:ASP:O	10:J:30:LEU:HG	2.09	0.53
1:A:504:LEU:HD11	6:F:91:ALA:HB1	1.91	0.53
1:A:556:TRP:C	1:A:558:GLY:H	2.17	0.53
1:A:1006:ILE:HD11	5:E:163:GLU:HG3	1.90	0.53
2:B:1115:THR:CG2	2:B:1117:GLN:HG3	2.39	0.53
4:D:13:ARG:C	4:D:17:LYS:HZ3	2.16	0.53
5:E:105:PHE:O	5:E:106:GLN:HB2	2.08	0.53
6:F:75:PRO:HG3	6:F:78:GLN:OE1	2.08	0.53
7:G:4:ILE:O	7:G:4:ILE:HG22	2.06	0.53
7:G:96:GLN:HG3	7:G:97:HIS:HD2	1.74	0.53
7:G:99:PHE:CE2	7:G:115:MET:HE2	2.44	0.53
15:T:24:DG:H2''	15:T:25:DT:C5'	2.38	0.53
1:A:42:ASP:HB3	1:A:45:GLN:N	2.24	0.53
1:A:652:VAL:O	1:A:653:VAL:C	2.52	0.53
2:B:172:ILE:HD13	2:B:178:ASN:CB	2.34	0.53
2:B:1156:ASP:O	2:B:1157:ALA:O	2.26	0.53
4:D:64:VAL:C	4:D:66:ARG:N	2.66	0.53
6:F:123:LYS:O	6:F:124:GLU:C	2.52	0.53
8:H:23:VAL:HG22	8:H:43:ASN:HA	1.90	0.53
8:H:58:THR:HG22	8:H:59:ILE:H	1.74	0.53
15:T:19:DT:C2'	15:T:20:DC:O5'	2.57	0.53
1:A:269:ILE:CD1	1:A:300:VAL:HG22	2.36	0.53
1:A:472:LEU:CD2	2:B:836:GLU:HG3	2.38	0.53
1:A:477:PRO:CG	1:A:521:MET:HG2	2.38	0.53
1:A:1102:LYS:O	1:A:1106:ASN:ND2	2.42	0.53
1:A:1313:LEU:O	1:A:1315:GLU:N	2.42	0.53
2:B:661:LEU:HD11	2:B:684:LEU:HD11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:745:PRO:C	2:B:747:MET:N	2.65	0.53
2:B:977:GLY:HA3	2:B:1099:VAL:CG2	2.39	0.53
2:B:1010:LEU:O	2:B:1011:ILE:HG12	2.08	0.53
2:B:1060:ARG:C	2:B:1062:HIS:H	2.16	0.53
3:C:35:ARG:NH1	11:K:41:THR:H	2.06	0.53
3:C:35:ARG:HH11	11:K:41:THR:CA	2.21	0.53
5:E:124:VAL:HG13	5:E:132:ILE:HD12	1.91	0.53
5:E:147:HIS:O	5:E:148:GLU:C	2.52	0.53
12:L:38:LEU:O	12:L:39:SER:CB	2.56	0.53
1:A:58:LEU:CG	1:A:59:GLY:N	2.72	0.52
1:A:353:ILE:HG21	1:A:487:MET:HG3	1.89	0.52
1:A:774:ARG:NH2	1:A:797:LYS:HG3	2.24	0.52
1:A:1139:GLU:O	1:A:1275:GLY:HA3	2.09	0.52
3:C:254:LYS:C	3:C:256:ALA:H	2.17	0.52
9:I:71:SER:OG	9:I:83:ASN:HB2	2.09	0.52
14:P:4:A:H2'	14:P:5:C:C6	2.44	0.52
1:A:92:HIS:O	1:A:93:VAL:C	2.52	0.52
1:A:384:ASN:OD1	1:A:388:LEU:HD12	2.09	0.52
1:A:626:ASN:O	1:A:631:HIS:CD2	2.61	0.52
1:A:961:ARG:HG2	1:A:965:GLN:HE21	1.73	0.52
1:A:1017:LEU:CB	5:E:205:SER:HA	2.39	0.52
1:A:1100:ARG:HH21	1:A:1351:GLU:CG	2.21	0.52
2:B:34:ILE:O	2:B:35:SER:C	2.53	0.52
4:D:17:LYS:CA	4:D:17:LYS:HE3	2.39	0.52
9:I:78:CYS:HB3	9:I:106:CYS:SG	2.49	0.52
10:J:5:VAL:O	10:J:6:ARG:O	2.26	0.52
10:J:14:VAL:CG1	10:J:50:ILE:HD11	2.39	0.52
15:T:15:DT:C6	15:T:16:DT:C7	2.80	0.52
1:A:334:GLY:O	1:A:335:ARG:C	2.52	0.52
1:A:466:SER:HB3	2:B:1103:ILE:HG12	1.91	0.52
1:A:600:PRO:HG2	1:A:601:LYS:H	1.74	0.52
1:A:1209:MET:SD	1:A:1236:LEU:HD22	2.49	0.52
1:A:1259:MET:C	1:A:1261:LYS:H	2.16	0.52
2:B:579:ARG:HG2	2:B:579:ARG:NH1	2.23	0.52
2:B:622:LYS:CE	9:I:59:VAL:HG22	2.31	0.52
2:B:860:MET:HG2	2:B:861:ASP:H	1.75	0.52
3:C:33:LEU:O	3:C:34:ARG:C	2.52	0.52
3:C:45:ALA:O	3:C:159:ALA:HA	2.09	0.52
1:A:34:LYS:CB	1:A:36:ARG:HE	2.22	0.52
1:A:220:THR:O	1:A:221:SER:C	2.53	0.52
1:A:353:ILE:HB	1:A:470:LEU:HD21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:PHE:CE2	1:A:565:ILE:HD12	2.44	0.52
1:A:598:LEU:O	1:A:599:SER:C	2.53	0.52
2:B:189:LEU:O	2:B:190:TYR:C	2.53	0.52
2:B:332:ASP:O	2:B:336:ARG:HG3	2.09	0.52
2:B:711:GLU:H	2:B:712:PRO:HD2	1.74	0.52
2:B:758:PHE:HZ	2:B:1031:LEU:HD22	1.74	0.52
6:F:69:LEU:N	6:F:70:LYS:HA	2.25	0.52
1:A:92:HIS:O	1:A:95:PHE:N	2.32	0.52
1:A:108:MET:SD	1:A:210:ILE:HD13	2.49	0.52
1:A:243:PRO:O	1:A:244:PRO:C	2.52	0.52
1:A:645:LEU:O	1:A:646:PHE:C	2.53	0.52
1:A:903:ASN:ND2	1:A:904:THR:N	2.45	0.52
1:A:1373:ASP:HA	1:A:1376:THR:HG22	1.91	0.52
2:B:224:GLN:O	2:B:238:ALA:HA	2.10	0.52
2:B:461:LEU:N	2:B:461:LEU:HD12	2.23	0.52
2:B:642:ASP:HB3	2:B:649:LYS:CG	2.40	0.52
2:B:785:TYR:CD1	2:B:785:TYR:C	2.87	0.52
2:B:797:TYR:HE1	2:B:854:LEU:CD2	2.22	0.52
4:D:185:CYS:HB2	4:D:211:LEU:CD2	2.37	0.52
6:F:140:ASP:C	6:F:140:ASP:OD1	2.53	0.52
9:I:60:GLN:NE2	9:I:107:SER:OG	2.41	0.52
11:K:21:ILE:HG23	11:K:31:VAL:CG1	2.40	0.52
14:P:0:U:C2'	14:P:1:U:H5'	2.40	0.52
1:A:244:PRO:HB2	1:A:245:PRO:CD	2.38	0.52
1:A:323:LYS:HZ3	14:P:1:U:H4'	1.75	0.52
1:A:404:TYR:HB2	1:A:433:GLU:HB2	1.92	0.52
1:A:1004:ASN:O	1:A:1008:GLN:HB2	2.10	0.52
1:A:1341:ILE:O	1:A:1344:GLY:N	2.43	0.52
2:B:22:SER:HA	2:B:654:ARG:HG3	1.91	0.52
2:B:269:ILE:HG21	2:B:282:ILE:HD13	1.91	0.52
3:C:74:SER:HB2	3:C:77:ILE:HG12	1.91	0.52
4:D:191:ALA:C	4:D:193:THR:N	2.68	0.52
1:A:34:LYS:O	1:A:35:ILE:HB	2.09	0.52
1:A:381:THR:HG23	1:A:382:PRO:CD	2.39	0.52
1:A:475:THR:CG2	1:A:476:SER:H	2.23	0.52
1:A:863:VAL:HG11	1:A:866:PHE:CE2	2.44	0.52
2:B:27:ALA:O	2:B:29:ASP:N	2.43	0.52
2:B:34:ILE:O	2:B:37:PHE:N	2.42	0.52
2:B:343:ILE:HG22	2:B:345:LYS:H	1.75	0.52
2:B:942:ARG:O	2:B:944:THR:N	2.43	0.52
2:B:1151:LEU:N	2:B:1151:LEU:HD12	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1177:HIS:O	2:B:1179:GLN:N	2.42	0.52
3:C:31:ASN:O	3:C:32:SER:C	2.50	0.52
5:E:168:TYR:C	5:E:169:ARG:HG3	2.34	0.52
6:F:90:ARG:CG	6:F:91:ALA:N	2.73	0.52
11:K:111:LEU:C	11:K:112:GLN:HE21	2.17	0.52
1:A:224:PHE:CE2	1:A:231:PRO:HG3	2.44	0.52
1:A:563:PRO:HG3	1:A:572:TRP:CE2	2.45	0.52
1:A:882:SER:HB3	1:A:953:ASN:OD1	2.10	0.52
1:A:1164:PRO:HG2	1:A:1165:GLU:HG3	1.92	0.52
1:A:1342:GLU:OE2	5:E:212:ARG:NH1	2.43	0.52
2:B:223:VAL:HG11	2:B:381:MET:HG2	1.92	0.52
2:B:431:TYR:CE2	2:B:447:ALA:HB2	2.45	0.52
2:B:731:VAL:HG12	2:B:732:SER:H	1.75	0.52
3:C:251:LEU:O	3:C:251:LEU:HD12	2.10	0.52
4:D:19:GLU:O	4:D:21:GLU:N	2.43	0.52
5:E:157:SER:HG	5:E:160:GLU:HG3	1.73	0.52
7:G:88:ASP:HA	7:G:144:ARG:HA	1.91	0.52
8:H:99:GLY:N	8:H:118:PHE:CD2	2.78	0.52
9:I:50:THR:HG22	9:I:51:ASN:N	2.25	0.52
9:I:61:ASP:C	9:I:63:GLY:N	2.66	0.52
1:A:23:SER:HA	1:A:233:TRP:NE1	2.25	0.52
1:A:34:LYS:HG2	1:A:36:ARG:NH2	2.25	0.52
2:B:233:PRO:HG2	2:B:234:ILE:CD1	2.38	0.52
2:B:1085:ILE:HG22	2:B:1086:PHE:N	2.25	0.52
3:C:18:VAL:O	3:C:19:ASP:C	2.53	0.52
11:K:53:ASP:HB3	11:K:56:VAL:HG23	1.92	0.52
1:A:172:PRO:HB3	1:A:185:TRP:CD2	2.45	0.52
1:A:613:ILE:HG22	1:A:614:PHE:HD2	1.75	0.52
1:A:647:GLY:O	1:A:651:LYS:HG3	2.10	0.52
1:A:800:VAL:HG11	1:A:808:LEU:HG	1.90	0.52
2:B:287:ARG:NH1	2:B:324:ILE:O	2.42	0.52
2:B:291:ILE:HD13	2:B:300:HIS:CD2	2.44	0.52
2:B:343:ILE:HG22	2:B:348:ARG:HG3	1.88	0.52
2:B:497:ARG:NH2	2:B:775:LYS:HZ3	2.07	0.52
2:B:746:SER:HB2	2:B:1046:PRO:HG2	1.92	0.52
2:B:896:ASP:OD2	12:L:58:LYS:HE3	2.10	0.52
2:B:1106:ARG:NH1	2:B:1110:PRO:CG	2.72	0.52
10:J:13:VAL:O	10:J:14:VAL:CG2	2.58	0.52
1:A:2:VAL:HG21	2:B:1157:ALA:HB1	1.92	0.51
1:A:335:ARG:N	1:A:339:ASN:HD22	2.07	0.51
1:A:573:SER:O	1:A:576:GLN:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:PRO:HG2	1:A:640:GLN:N	2.24	0.51
1:A:818:MET:HA	2:B:514:LEU:HB3	1.92	0.51
1:A:845:LEU:O	1:A:846:GLU:C	2.51	0.51
1:A:997:LEU:HD13	1:A:1018:PHE:HE2	1.74	0.51
1:A:1319:VAL:HG13	1:A:1320:PRO:HD2	1.92	0.51
2:B:227:LYS:HB2	2:B:395:GLN:OE1	2.10	0.51
2:B:843:GLN:O	2:B:846:ILE:HB	2.10	0.51
2:B:918:ILE:HD12	2:B:935:ARG:HD3	1.91	0.51
2:B:1050:ILE:HG22	2:B:1051:THR:N	2.25	0.51
4:D:175:PHE:HZ	7:G:85:GLU:HG3	1.74	0.51
5:E:153:HIS:O	5:E:154:ILE:CG1	2.58	0.51
7:G:1:MET:O	7:G:3:PHE:CD1	2.63	0.51
7:G:111:THR:HB	7:G:114:LEU:HB2	1.92	0.51
10:J:36:LEU:O	10:J:37:SER:C	2.53	0.51
10:J:64:ASN:CB	10:J:65:PRO:CD	2.86	0.51
1:A:37:PHE:HD1	1:A:37:PHE:H	1.58	0.51
1:A:590:ARG:HH11	1:A:590:ARG:CG	2.23	0.51
1:A:1005:GLU:O	1:A:1006:ILE:C	2.53	0.51
2:B:579:ARG:CB	2:B:586:TRP:HE1	2.22	0.51
2:B:814:PHE:C	2:B:816:GLU:N	2.68	0.51
2:B:1068:GLY:O	2:B:1069:PHE:O	2.29	0.51
2:B:1115:THR:HG22	2:B:1117:GLN:HG3	1.93	0.51
3:C:98:VAL:O	3:C:99:LEU:HD22	2.09	0.51
9:I:25:LEU:HB3	9:I:38:ALA:CB	2.40	0.51
1:A:93:VAL:HG21	1:A:301:ALA:O	2.11	0.51
1:A:549:MET:SD	1:A:577:ILE:HD11	2.50	0.51
1:A:840:ARG:O	1:A:841:LEU:C	2.53	0.51
1:A:867:ILE:HG22	1:A:871:ASP:H	1.75	0.51
1:A:1329:THR:H	1:A:1335:ILE:HD11	1.75	0.51
1:A:1349:TYR:CA	1:A:1372:VAL:HG21	2.39	0.51
2:B:343:ILE:CG2	2:B:348:ARG:N	2.73	0.51
2:B:885:MET:HA	2:B:936:ASP:HB2	1.93	0.51
2:B:1182:CYS:O	2:B:1182:CYS:SG	2.68	0.51
3:C:26:ASP:O	3:C:27:LEU:C	2.51	0.51
3:C:209:TYR:HD1	3:C:209:TYR:H	1.57	0.51
3:C:238:ILE:HG21	3:C:242:GLN:HB2	1.90	0.51
4:D:176:GLU:HB3	4:D:198:LEU:HD21	1.92	0.51
6:F:77:ASP:C	6:F:79:ARG:N	2.68	0.51
7:G:145:VAL:CG1	7:G:146:LYS:N	2.73	0.51
9:I:99:LEU:O	9:I:111:THR:HG23	2.10	0.51
1:A:90:VAL:HG13	1:A:297:GLN:CD	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:GLU:H	1:A:117:GLU:CD	2.17	0.51
1:A:393:ARG:O	1:A:394:ASN:C	2.52	0.51
1:A:481:ASP:OD1	1:A:483:ASP:OD2	2.28	0.51
1:A:547:LEU:HD22	11:K:58:PHE:CE1	2.45	0.51
1:A:1171:GLN:HA	1:A:1174:PHE:CE1	2.46	0.51
2:B:54:PHE:CZ	2:B:59:LEU:HD13	2.46	0.51
2:B:212:LEU:HD23	2:B:480:SER:HB2	1.92	0.51
2:B:860:MET:HG2	2:B:861:ASP:N	2.26	0.51
3:C:168:ALA:O	3:C:169:LYS:C	2.51	0.51
3:C:243:VAL:O	3:C:243:VAL:HG12	2.08	0.51
7:G:51:TYR:O	7:G:54:ILE:HG13	2.10	0.51
1:A:49:LYS:NZ	1:A:61:ILE:CG1	2.72	0.51
1:A:958:VAL:O	1:A:958:VAL:HG12	2.09	0.51
2:B:232:SER:CB	2:B:261:ARG:HH21	2.12	0.51
2:B:707:PRO:O	2:B:711:GLU:HG3	2.10	0.51
3:C:16:ASP:O	3:C:17:ASN:CG	2.54	0.51
7:G:3:PHE:CD1	7:G:80:LYS:NZ	2.75	0.51
9:I:51:ASN:O	9:I:54:GLU:HG3	2.11	0.51
12:L:70:ARG:HG2	12:L:70:ARG:HH11	1.76	0.51
14:P:3:G:H2'	14:P:4:A:C8	2.46	0.51
15:T:20:DC:C2'	15:T:21:DC:O5'	2.58	0.51
1:A:224:PHE:CD2	1:A:231:PRO:HG3	2.45	0.51
1:A:463:ILE:HD12	1:A:469:ARG:HD2	1.91	0.51
1:A:738:LYS:HB2	1:A:740:LEU:HG	1.93	0.51
3:C:226:ASP:O	3:C:227:THR:CB	2.58	0.51
5:E:112:TYR:CZ	5:E:136:ASN:HB2	2.45	0.51
10:J:13:VAL:C	10:J:14:VAL:HG23	2.36	0.51
11:K:53:ASP:C	11:K:55:LYS:H	2.19	0.51
1:A:40:THR:HG21	1:A:41:MET:HE2	1.92	0.51
1:A:244:PRO:CB	1:A:245:PRO:CD	2.89	0.51
1:A:567:LYS:NZ	8:H:46:LEU:HB2	2.25	0.51
1:A:873:MET:C	1:A:1058:VAL:CG2	2.84	0.51
1:A:1116:LEU:HD11	1:A:1118:VAL:HG13	1.92	0.51
2:B:515:HIS:O	2:B:518:HIS:HB2	2.10	0.51
3:C:215:GLU:O	3:C:216:GLY:C	2.53	0.51
5:E:177:ARG:HD3	5:E:215:MET:CG	2.41	0.51
7:G:74:TYR:H	7:G:74:TYR:HD2	1.59	0.51
9:I:106:CYS:O	9:I:107:SER:HB2	2.10	0.51
11:K:5:ASP:O	11:K:6:ARG:C	2.53	0.51
1:A:116:ASP:C	1:A:118:HIS:N	2.67	0.51
1:A:464:PRO:HG2	1:A:465:TYR:HD1	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:754:SER:H	1:A:757:ASN:ND2	1.93	0.51
1:A:984:LYS:O	1:A:988:LEU:HB2	2.09	0.51
1:A:1289:ARG:HD2	1:A:1303:GLU:OE2	2.10	0.51
2:B:484:ASN:HB3	2:B:486:TYR:HD1	1.74	0.51
2:B:542:MET:SD	2:B:747:MET:HE3	2.51	0.51
2:B:999:MET:HA	2:B:999:MET:CE	2.38	0.51
2:B:1002:THR:HG21	2:B:1006:ILE:CD1	2.30	0.51
4:D:135:GLY:C	4:D:137:ASN:H	2.18	0.51
5:E:14:ARG:O	5:E:17:ARG:HB3	2.11	0.51
5:E:112:TYR:OH	5:E:136:ASN:HB2	2.11	0.51
5:E:161:LYS:HD2	5:E:195:VAL:HG23	1.92	0.51
7:G:143:ILE:CG2	7:G:144:ARG:N	2.74	0.51
8:H:22:LYS:O	8:H:23:VAL:HG23	2.11	0.51
1:A:260:ASP:OD1	1:A:261:ASP:N	2.44	0.51
1:A:685:GLU:HG3	1:A:686:ALA:N	2.26	0.51
1:A:785:PRO:HG2	1:A:786:HIS:HD2	1.76	0.51
1:A:832:ALA:HB1	15:T:19:DT:OP1	2.10	0.51
1:A:836:TYR:CZ	1:A:840:ARG:HD2	2.45	0.51
1:A:966:ASN:O	1:A:967:ALA:C	2.54	0.51
2:B:95:ILE:CB	2:B:130:VAL:HG22	2.41	0.51
2:B:758:PHE:HB3	2:B:761:HIS:HD2	1.75	0.51
4:D:8:PHE:O	4:D:9:GLN:HB2	2.11	0.51
5:E:205:SER:O	5:E:206:GLY:C	2.53	0.51
7:G:18:PHE:HZ	7:G:68:ALA:HB2	1.76	0.51
9:I:101:PHE:HE1	9:I:112:SER:HB2	1.76	0.51
11:K:68:PHE:N	11:K:68:PHE:CD2	2.74	0.51
15:T:22:BRU:C2'	15:T:23:DG:O4'	2.59	0.51
2:B:237:VAL:HG12	2:B:238:ALA:N	2.26	0.51
2:B:311:LEU:O	2:B:312:GLU:C	2.54	0.51
3:C:112:ASN:HD22	3:C:112:ASN:N	2.09	0.51
3:C:166:GLU:O	3:C:167:HIS:HB2	2.09	0.51
4:D:192:LYS:HE3	4:D:204:ASP:OD1	2.11	0.51
6:F:147:SER:OG	6:F:150:GLU:HG3	2.10	0.51
7:G:125:SER:OG	7:G:128:PRO:HA	2.11	0.51
14:P:0:U:O2'	14:P:1:U:H5'	2.11	0.51
1:A:853:ASP:OD1	1:A:855:THR:HB	2.10	0.50
1:A:996:ASN:C	1:A:998:LEU:HD12	2.36	0.50
2:B:848:ARG:HD2	10:J:7:CYS:O	2.11	0.50
2:B:905:VAL:HG23	2:B:941:LEU:HD22	1.93	0.50
2:B:1081:LEU:O	2:B:1082:MET:C	2.54	0.50
3:C:175:ALA:HB3	10:J:43:ARG:NH2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:242:GLN:C	3:C:244:VAL:N	2.69	0.50
7:G:7:LEU:CD1	7:G:45:ILE:HD11	2.41	0.50
9:I:16:PRO:HB3	9:I:27:PHE:CD2	2.47	0.50
9:I:111:THR:CG2	9:I:112:SER:N	2.74	0.50
1:A:75:ASN:O	1:A:76:GLU:CB	2.58	0.50
1:A:306:ASN:HB2	1:A:324:SER:HB3	1.93	0.50
1:A:697:ALA:C	1:A:699:ALA:H	2.17	0.50
1:A:1074:GLU:HB3	1:A:1075:PRO:CD	2.40	0.50
1:A:1444:MET:CG	7:G:60:ARG:HA	2.38	0.50
2:B:642:ASP:HB3	2:B:649:LYS:HD2	1.92	0.50
2:B:796:LEU:HD12	2:B:852:ARG:O	2.11	0.50
2:B:957:ASN:O	2:B:958:GLN:C	2.54	0.50
2:B:1099:VAL:C	2:B:1101:ASP:H	2.19	0.50
3:C:77:ILE:C	3:C:79:GLN:H	2.19	0.50
3:C:145:CYS:HA	10:J:2:ILE:CD1	2.42	0.50
3:C:167:HIS:CD2	3:C:168:ALA:N	2.79	0.50
3:C:203:GLN:HG2	3:C:207:CYS:SG	2.51	0.50
3:C:239:PRO:O	3:C:240:VAL:C	2.53	0.50
5:E:124:VAL:HB	5:E:125:PRO:HD3	1.93	0.50
7:G:22:MET:O	7:G:23:LYS:C	2.54	0.50
7:G:79:PHE:HZ	7:G:106:MET:CE	2.20	0.50
8:H:139:ASN:O	8:H:140:ALA:HB2	2.11	0.50
9:I:85:PHE:CD2	9:I:85:PHE:N	2.67	0.50
11:K:31:VAL:HG12	11:K:32:VAL:H	1.75	0.50
11:K:69:ALA:O	11:K:70:ARG:HB3	2.10	0.50
1:A:203:SER:OG	1:A:206:GLU:HB2	2.11	0.50
1:A:262:LEU:O	1:A:264:PHE:N	2.45	0.50
1:A:608:ILE:C	1:A:610:GLY:N	2.68	0.50
1:A:960:ILE:O	1:A:961:ARG:C	2.54	0.50
2:B:129:PHE:HA	2:B:165:VAL:O	2.12	0.50
2:B:582:VAL:HG12	2:B:587:HIS:NE2	2.26	0.50
2:B:594:ALA:HA	2:B:617:ARG:NH1	2.26	0.50
2:B:803:LEU:HB2	2:B:1032:SER:OG	2.10	0.50
2:B:1162:ILE:HD11	2:B:1194:ILE:HD13	1.92	0.50
3:C:36:VAL:HG11	3:C:251:LEU:HB2	1.93	0.50
1:A:40:THR:C	1:A:41:MET:HG3	2.36	0.50
1:A:92:HIS:HB3	1:A:95:PHE:HB2	1.94	0.50
1:A:326:ARG:HH22	1:A:1407:GLU:CG	2.23	0.50
1:A:828:ALA:HB1	2:B:530:GLY:HA2	1.93	0.50
1:A:998:LEU:HD12	1:A:998:LEU:H	1.77	0.50
1:A:1144:LYS:HB2	1:A:1268:LEU:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:196:PRO:HG2	2:B:197:PHE:H	1.76	0.50
7:G:39:THR:HG22	7:G:41:LYS:H	1.76	0.50
11:K:60:ALA:O	11:K:73:LEU:HD12	2.11	0.50
11:K:110:ASN:C	11:K:111:LEU:HG	2.36	0.50
1:A:341:MET:HE1	2:B:1135:ARG:CZ	2.41	0.50
1:A:1100:ARG:NH2	1:A:1351:GLU:HG2	2.27	0.50
1:A:1402:PHE:O	1:A:1403:GLU:HB2	2.10	0.50
2:B:1096:ARG:O	2:B:1097:HIS:CB	2.59	0.50
3:C:167:HIS:CD2	3:C:168:ALA:H	2.29	0.50
7:G:117:GLN:C	7:G:119:LEU:H	2.18	0.50
8:H:84:ALA:CB	8:H:87:ARG:HB2	2.41	0.50
10:J:23:ASN:O	10:J:25:LEU:N	2.45	0.50
1:A:416:ARG:HG3	1:A:417:TYR:CE2	2.47	0.50
1:A:535:THR:HG22	1:A:536:LEU:N	2.26	0.50
1:A:1097:GLY:O	1:A:1100:ARG:HB3	2.11	0.50
1:A:1299:VAL:CG1	1:A:1300:LYS:H	2.25	0.50
2:B:386:LEU:O	2:B:387:LEU:C	2.55	0.50
2:B:516:ASN:ND2	2:B:516:ASN:H	2.10	0.50
2:B:1096:ARG:HA	2:B:1098:MET:HE2	1.92	0.50
2:B:1106:ARG:HG3	2:B:1107:ALA:N	2.25	0.50
4:D:51:ASN:ND2	4:D:54:GLU:OE2	2.45	0.50
5:E:153:HIS:O	5:E:154:ILE:HG13	2.10	0.50
5:E:161:LYS:C	5:E:163:GLU:N	2.68	0.50
6:F:111:LEU:C	6:F:113:GLY:N	2.57	0.50
1:A:33:ALA:O	1:A:83:HIS:HD2	1.95	0.50
1:A:172:PRO:HD3	1:A:185:TRP:HE1	1.77	0.50
1:A:356:ASP:OD2	11:K:65:HIS:CE1	2.65	0.50
2:B:1172:ILE:HG22	2:B:1172:ILE:O	2.11	0.50
3:C:255:VAL:O	3:C:255:VAL:HG12	2.12	0.50
9:I:82:GLU:O	9:I:104:LEU:HG	2.11	0.50
12:L:31:CYS:HB3	12:L:34:CYS:C	2.37	0.50
14:P:4:A:H2'	14:P:5:C:O4'	2.11	0.50
1:A:57:ARG:O	1:A:68:GLN:HG3	2.11	0.50
1:A:172:PRO:HG3	1:A:185:TRP:CZ2	2.47	0.50
1:A:241:VAL:HG13	1:A:266:LEU:HD13	1.94	0.50
1:A:408:ASP:C	1:A:410:GLY:H	2.18	0.50
1:A:870:GLU:HG2	5:E:208:TYR:CG	2.46	0.50
1:A:1152:ILE:HG13	9:I:44:TYR:HD2	1.77	0.50
1:A:1323:ASP:C	1:A:1325:THR:H	2.19	0.50
1:A:1324:PRO:HB2	5:E:142:VAL:HG11	1.93	0.50
1:A:1445:ILE:H	1:A:1445:ILE:CD1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:344:LYS:O	2:B:345:LYS:CB	2.58	0.50
2:B:744:HIS:CG	2:B:745:PRO:HD2	2.46	0.50
2:B:957:ASN:O	2:B:960:GLY:N	2.43	0.50
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.94	0.50
3:C:183:TRP:O	3:C:185:LYS:HG3	2.12	0.50
3:C:236:GLY:O	3:C:238:ILE:N	2.45	0.50
8:H:138:GLU:O	8:H:139:ASN:C	2.54	0.50
15:T:10:DA:H2''	15:T:11:DG:OP2	2.11	0.50
1:A:78:PRO:HB2	2:B:1201:LYS:HE3	1.92	0.50
1:A:277:GLU:C	1:A:279:LEU:H	2.19	0.50
1:A:920:LEU:HD23	1:A:920:LEU:C	2.37	0.50
1:A:1418:LEU:HD12	1:A:1419:ASP:H	1.77	0.50
2:B:174:LEU:HD22	2:B:202:TYR:CE1	2.47	0.50
2:B:388:CYS:C	2:B:390:LEU:N	2.69	0.50
2:B:744:HIS:HD2	2:B:746:SER:CB	2.25	0.50
2:B:1182:CYS:O	2:B:1183:LYS:C	2.54	0.50
7:G:80:LYS:O	7:G:82:PHE:CE1	2.65	0.50
8:H:113:ALA:HB2	8:H:126:GLU:HG3	1.93	0.50
9:I:86:PHE:CE1	9:I:100:PHE:HB2	2.46	0.50
1:A:29:ALA:HB1	2:B:1184:GLY:HA2	1.94	0.49
1:A:695:LYS:C	1:A:697:ALA:N	2.69	0.49
1:A:844:ALA:O	1:A:845:LEU:HD23	2.12	0.49
1:A:947:PHE:CD2	1:A:954:TRP:CE2	3.00	0.49
2:B:234:ILE:HD12	2:B:234:ILE:N	2.26	0.49
2:B:383:ASN:O	2:B:384:ARG:C	2.55	0.49
2:B:458:LYS:O	2:B:459:TYR:C	2.55	0.49
2:B:763:GLN:O	2:B:764:SER:C	2.55	0.49
2:B:802:PRO:HG2	2:B:805:THR:HG22	1.94	0.49
2:B:1189:ILE:HG22	2:B:1190:ASP:N	2.26	0.49
3:C:123:ASN:ND2	3:C:125:MET:HG2	2.27	0.49
3:C:232:VAL:HG21	3:C:244:VAL:CG2	2.39	0.49
4:D:151:PHE:CD1	4:D:151:PHE:N	2.78	0.49
5:E:16:PHE:HZ	5:E:20:LYS:HE2	1.73	0.49
5:E:144:ILE:HG13	5:E:145:THR:N	2.25	0.49
8:H:58:THR:HG22	8:H:59:ILE:N	2.27	0.49
12:L:47:ARG:HH21	12:L:54:ARG:HH21	1.59	0.49
1:A:26:GLU:O	1:A:27:VAL:C	2.54	0.49
1:A:35:ILE:HD12	1:A:241:VAL:HG21	1.94	0.49
1:A:207:ILE:O	1:A:208:LEU:C	2.55	0.49
1:A:482:PHE:C	1:A:484:GLY:N	2.70	0.49
1:A:954:TRP:HB3	1:A:955:PRO:HD2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:620:ARG:NH2	9:I:89:GLN:NE2	2.60	0.49
2:B:794:ASN:O	2:B:795:ILE:HD12	2.12	0.49
2:B:801:LYS:O	10:J:52:THR:CG2	2.60	0.49
2:B:824:ILE:CG2	2:B:1087:PHE:CE2	2.86	0.49
3:C:56:THR:HG22	3:C:57:VAL:N	2.18	0.49
4:D:145:MET:O	4:D:149:THR:N	2.44	0.49
5:E:26:ARG:HH22	5:E:133:GLU:CD	2.19	0.49
9:I:14:LEU:HA	9:I:28:GLU:O	2.12	0.49
10:J:48:ARG:HH21	10:J:49:MET:HE1	1.75	0.49
14:P:5:C:C2'	14:P:6:C:O4'	2.55	0.49
1:A:43:GLU:O	1:A:44:THR:CB	2.59	0.49
1:A:399:HIS:HB3	1:A:400:PRO:CD	2.34	0.49
1:A:403:LYS:O	1:A:404:TYR:CD2	2.66	0.49
1:A:629:LEU:O	1:A:633:VAL:HG23	2.13	0.49
2:B:129:PHE:HE2	2:B:166:PHE:HD1	1.60	0.49
2:B:258:LEU:HG	2:B:258:LEU:O	2.13	0.49
2:B:811:TYR:N	2:B:811:TYR:CD1	2.80	0.49
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.94	0.49
4:D:51:ASN:C	4:D:52:LEU:O	2.54	0.49
4:D:66:ARG:O	4:D:70:PHE:HB2	2.12	0.49
8:H:123:MET:HE1	8:H:142:LEU:HD11	1.93	0.49
1:A:577:ILE:HA	1:A:580:VAL:HG23	1.94	0.49
2:B:466:TRP:O	2:B:468:GLU:N	2.46	0.49
3:C:241:ASP:O	3:C:245:VAL:HG23	2.12	0.49
4:D:137:ASN:C	4:D:137:ASN:HD22	2.21	0.49
6:F:79:ARG:HG3	6:F:144:GLU:OE1	2.13	0.49
9:I:50:THR:HG21	9:I:52:ILE:HG12	1.94	0.49
1:A:152:VAL:HG12	1:A:153:PRO:HD2	1.94	0.49
1:A:367:PRO:HA	1:A:463:ILE:O	2.13	0.49
1:A:453:MET:C	1:A:455:MET:N	2.70	0.49
1:A:665:GLY:O	1:A:666:ILE:C	2.56	0.49
1:A:925:LEU:C	1:A:927:VAL:H	2.21	0.49
1:A:1118:VAL:HG23	1:A:1306:LEU:HB2	1.93	0.49
1:A:1334:ASP:O	1:A:1336:MET:N	2.45	0.49
2:B:460:ALA:C	2:B:462:ALA:H	2.20	0.49
2:B:526:GLU:CD	2:B:752:ALA:HB2	2.38	0.49
2:B:702:LEU:HD12	2:B:703:ILE:H	1.76	0.49
2:B:778:MET:CE	2:B:1094:ARG:CD	2.89	0.49
2:B:792:MET:HG3	2:B:855:PHE:CE1	2.48	0.49
2:B:798:TYR:CE2	3:C:62:PHE:CE2	3.01	0.49
3:C:70:ILE:O	3:C:70:ILE:HG22	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:27:LEU:HD22	4:D:173:HIS:HD2	1.76	0.49
4:D:51:ASN:O	4:D:52:LEU:C	2.55	0.49
4:D:52:LEU:O	4:D:54:GLU:N	2.44	0.49
5:E:195:VAL:HG22	5:E:213:ILE:HG13	1.94	0.49
8:H:103:LYS:HG2	8:H:104:PHE:H	1.78	0.49
1:A:30:ILE:HD11	2:B:1168:LEU:HD13	1.93	0.49
1:A:868:TYR:CD2	1:A:1058:VAL:HG21	2.41	0.49
1:A:1116:LEU:CB	1:A:1308:THR:HG21	2.42	0.49
2:B:401:PHE:HA	2:B:404:LYS:HG3	1.93	0.49
3:C:77:ILE:O	3:C:79:GLN:N	2.46	0.49
3:C:174:ALA:HB2	3:C:235:VAL:CG2	2.38	0.49
7:G:61:ILE:HG23	7:G:66:GLY:O	2.12	0.49
12:L:28:LYS:HB2	12:L:39:SER:HA	1.95	0.49
1:A:24:PRO:HB3	1:A:237:THR:HB	1.94	0.49
1:A:53:LEU:CD2	1:A:54:ASN:N	2.56	0.49
1:A:815:PHE:C	1:A:817:ALA:N	2.69	0.49
1:A:1095:THR:OG1	1:A:1113:THR:HB	2.13	0.49
2:B:51:PHE:HE2	2:B:172:ILE:HG23	1.77	0.49
2:B:205:ILE:N	2:B:205:ILE:HD12	2.27	0.49
2:B:222:ILE:O	2:B:240:ILE:HA	2.12	0.49
2:B:882:THR:O	2:B:883:LEU:HB2	2.13	0.49
2:B:911:ILE:HD11	2:B:941:LEU:CD1	2.37	0.49
3:C:258:ILE:HD12	3:C:258:ILE:N	2.26	0.49
4:D:130:LEU:C	4:D:132:GLN:N	2.70	0.49
5:E:156:LEU:HD12	5:E:195:VAL:CB	2.42	0.49
5:E:161:LYS:C	5:E:163:GLU:H	2.20	0.49
5:E:192:ARG:HG3	5:E:192:ARG:NH1	2.28	0.49
6:F:75:PRO:HG2	6:F:78:GLN:HB2	1.93	0.49
8:H:35:GLN:O	8:H:37:LYS:HG3	2.12	0.49
10:J:52:THR:O	10:J:53:HIS:C	2.56	0.49
11:K:111:LEU:C	11:K:112:GLN:HG2	2.37	0.49
1:A:265:LYS:NZ	1:A:322:VAL:HG13	2.28	0.49
1:A:464:PRO:O	1:A:465:TYR:O	2.30	0.49
1:A:701:LEU:HD23	9:I:115:LYS:HG3	1.95	0.49
1:A:815:PHE:O	1:A:816:HIS:C	2.53	0.49
2:B:95:ILE:HG13	2:B:129:PHE:O	2.12	0.49
2:B:280:ILE:CD1	2:B:334:ILE:HG12	2.41	0.49
2:B:1001:PHE:CZ	2:B:1073:TYR:HB2	2.48	0.49
3:C:252:GLN:O	3:C:253:LYS:C	2.54	0.49
4:D:63:LEU:HD13	4:D:133:THR:OG1	2.12	0.49
4:D:195:ILE:N	4:D:196:PRO:CD	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:65:HIS:CD2	11:K:66:PRO:HG2	2.48	0.49
1:A:341:MET:HE1	1:A:843:LYS:HZ3	1.77	0.49
1:A:595:THR:O	1:A:596:THR:HG23	2.12	0.49
1:A:683:ILE:HG21	1:A:801:GLU:HG3	1.94	0.49
1:A:853:ASP:OD1	1:A:855:THR:CB	2.61	0.49
2:B:693:ILE:HD13	2:B:701:ILE:HD13	1.95	0.49
2:B:769:TYR:C	2:B:771:SER:N	2.70	0.49
2:B:1065:GLN:NE2	2:B:1066:SER:H	2.11	0.49
2:B:1177:HIS:C	2:B:1179:GLN:H	2.21	0.49
3:C:46:ILE:CG2	3:C:157:CYS:HB3	2.41	0.49
4:D:52:LEU:CD2	4:D:147:TYR:HE2	2.25	0.49
4:D:145:MET:O	4:D:149:THR:HB	2.13	0.49
8:H:40:LEU:HD12	8:H:122:LEU:O	2.13	0.49
10:J:34:THR:O	10:J:35:ALA:C	2.56	0.49
11:K:7:PHE:CD1	11:K:7:PHE:C	2.90	0.49
13:N:3:DG:H1'	13:N:4:DT:C5'	2.42	0.49
1:A:18:GLN:O	2:B:1215:ARG:HG2	2.13	0.49
1:A:268:ASP:O	1:A:269:ILE:C	2.54	0.49
1:A:388:LEU:HD22	1:A:432:VAL:HG21	1.95	0.49
1:A:528:LEU:C	1:A:528:LEU:HD12	2.38	0.49
1:A:567:LYS:HD2	1:A:568:PRO:CD	2.43	0.49
1:A:1063:MET:HG3	1:A:1436:ILE:HG23	1.95	0.49
1:A:1208:THR:HG22	1:A:1210:GLY:H	1.77	0.49
1:A:1279:ILE:HD11	1:A:1316:VAL:HG21	1.93	0.49
1:A:1402:PHE:CD1	1:A:1403:GLU:HG3	2.48	0.49
2:B:405:ARG:HA	2:B:631:GLY:O	2.13	0.49
2:B:550:ASP:OD1	2:B:551:PRO:HD2	2.13	0.49
2:B:705:MET:HA	2:B:705:MET:HE3	1.94	0.49
2:B:1192:TYR:N	2:B:1192:TYR:CD1	2.80	0.49
3:C:74:SER:CB	3:C:77:ILE:HG12	2.43	0.49
3:C:114:TYR:CD2	3:C:140:ASN:HB2	2.47	0.49
6:F:77:ASP:O	6:F:78:GLN:HB2	2.12	0.49
9:I:103:CYS:CB	9:I:106:CYS:SG	3.01	0.49
10:J:2:ILE:CG2	10:J:3:VAL:N	2.75	0.49
12:L:43:THR:HG22	12:L:43:THR:O	2.13	0.49
1:A:42:ASP:C	1:A:44:THR:N	2.69	0.48
1:A:49:LYS:HZ1	1:A:61:ILE:CG1	2.26	0.48
1:A:289:ILE:C	1:A:291:GLU:N	2.70	0.48
1:A:331:GLY:O	1:A:332:LYS:O	2.31	0.48
1:A:351:THR:HG22	2:B:1103:ILE:HA	1.95	0.48
1:A:719:VAL:O	1:A:721:PHE:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1149:ALA:HB2	9:I:47:GLU:HA	1.95	0.48
2:B:181:LEU:HD22	2:B:189:LEU:HD22	1.95	0.48
3:C:29:MET:HE2	11:K:98:LEU:CD2	2.43	0.48
3:C:147:LEU:N	3:C:147:LEU:CD2	2.75	0.48
3:C:165:LYS:O	11:K:6:ARG:NH1	2.45	0.48
4:D:153:ARG:C	4:D:154:PHE:CD1	2.91	0.48
10:J:2:ILE:H	10:J:57:ILE:HG22	1.78	0.48
14:P:0:U:H2'	14:P:1:U:C5'	2.43	0.48
1:A:55:ASP:C	1:A:57:ARG:N	2.68	0.48
1:A:310:GLY:O	1:A:312:PRO:HD2	2.14	0.48
1:A:590:ARG:HB2	1:A:605:MET:HB3	1.95	0.48
1:A:903:ASN:ND2	1:A:903:ASN:C	2.64	0.48
1:A:1074:GLU:N	1:A:1075:PRO:HD2	2.28	0.48
2:B:95:ILE:HB	2:B:130:VAL:HG22	1.94	0.48
2:B:189:LEU:CA	2:B:192:LEU:HD12	2.25	0.48
2:B:281:PRO:O	2:B:283:VAL:N	2.46	0.48
3:C:75:MET:HE2	3:C:239:PRO:CG	2.43	0.48
4:D:146:GLN:O	4:D:147:TYR:C	2.55	0.48
9:I:75:CYS:SG	9:I:78:CYS:C	2.96	0.48
11:K:50:LEU:CD2	11:K:56:VAL:HG21	2.43	0.48
11:K:55:LYS:HB2	11:K:81:TYR:HE1	1.78	0.48
1:A:7:SER:HB2	2:B:1175:LEU:HD22	1.95	0.48
1:A:639:PRO:CG	1:A:640:GLN:H	2.25	0.48
1:A:723:ASN:C	1:A:725:ALA:N	2.69	0.48
1:A:881:GLN:O	1:A:953:ASN:HA	2.13	0.48
1:A:883:LEU:HD11	1:A:1017:LEU:HD11	1.96	0.48
1:A:1205:LYS:O	1:A:1206:ASP:C	2.56	0.48
1:A:1265:ASN:C	1:A:1267:MET:N	2.68	0.48
1:A:1327:ILE:HG22	5:E:147:HIS:HE1	1.77	0.48
2:B:777:ALA:HA	2:B:1095:LEU:HA	1.94	0.48
2:B:847:ASP:C	2:B:849:GLY:N	2.70	0.48
2:B:1147:LEU:C	2:B:1147:LEU:HD23	2.37	0.48
3:C:47:ASP:O	3:C:48:SER:HB2	2.13	0.48
5:E:177:ARG:O	5:E:212:ARG:CD	2.61	0.48
7:G:115:MET:CB	7:G:116:PRO:HD2	2.43	0.48
9:I:100:PHE:N	9:I:100:PHE:CD1	2.81	0.48
1:A:364:VAL:O	1:A:364:VAL:HG13	2.13	0.48
1:A:525:GLN:HB2	2:B:835:GLN:OE1	2.13	0.48
1:A:682:THR:CG2	1:A:728:LYS:HE3	2.43	0.48
1:A:968:GLN:C	1:A:970:THR:H	2.21	0.48
1:A:1010:ALA:HA	1:A:1013:ASP:OD2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1216:ILE:O	1:A:1219:THR:HB	2.12	0.48
1:A:1437:GLY:HA3	6:F:88:TYR:CD2	2.48	0.48
2:B:44:VAL:HG11	2:B:199:MET:HG2	1.94	0.48
2:B:696:GLU:O	2:B:699:GLU:HB2	2.13	0.48
2:B:996:ARG:HH21	3:C:175:ALA:HA	1.77	0.48
2:B:1002:THR:O	2:B:1003:ALA:C	2.56	0.48
2:B:1065:GLN:NE2	2:B:1066:SER:N	2.61	0.48
2:B:1079:LYS:HA	3:C:27:LEU:HD21	1.94	0.48
2:B:1224:PHE:CE2	5:E:171:LYS:HG3	2.35	0.48
5:E:13:TRP:O	5:E:16:PHE:HB3	2.13	0.48
5:E:124:VAL:HA	5:E:132:ILE:HD12	1.95	0.48
5:E:154:ILE:HG22	5:E:155:ARG:O	2.12	0.48
6:F:85:MET:CE	6:F:93:ILE:HD12	2.43	0.48
7:G:48:VAL:HG13	7:G:74:TYR:HD1	1.78	0.48
15:T:24:DG:C2'	15:T:25:DT:O5'	2.62	0.48
1:A:323:LYS:NZ	14:P:1:U:H4'	2.29	0.48
1:A:637:LYS:HB3	1:A:641:VAL:HG11	1.94	0.48
1:A:873:MET:HG2	1:A:957:PRO:HB3	1.95	0.48
1:A:1074:GLU:C	1:A:1076:ALA:N	2.69	0.48
1:A:1333:ILE:HG22	1:A:1334:ASP:N	2.27	0.48
2:B:911:ILE:O	2:B:912:ILE:HG13	2.14	0.48
3:C:73:GLN:NE2	3:C:74:SER:N	2.57	0.48
5:E:131:THR:HG21	5:E:191:LYS:NZ	2.28	0.48
8:H:26:ILE:HD13	8:H:49:VAL:HG11	1.94	0.48
11:K:91:CYS:O	11:K:94:ILE:HB	2.13	0.48
1:A:601:LYS:HB2	1:A:603:ASN:HD21	1.78	0.48
1:A:1017:LEU:HB3	5:E:205:SER:HA	1.94	0.48
1:A:1099:PRO:O	1:A:1102:LYS:HB3	2.14	0.48
1:A:1344:GLY:O	1:A:1345:ARG:C	2.56	0.48
1:A:1445:ILE:HG21	7:G:18:PHE:CD2	2.48	0.48
2:B:38:PHE:CD1	2:B:811:TYR:CD2	3.02	0.48
2:B:759:PRO:C	2:B:761:HIS:H	2.21	0.48
2:B:872:GLU:CD	2:B:914:LYS:HE2	2.38	0.48
2:B:877:PRO:C	2:B:878:GLN:HG3	2.38	0.48
2:B:1102:LYS:O	2:B:1103:ILE:C	2.56	0.48
3:C:66:ARG:NH1	3:C:144:ILE:O	2.47	0.48
8:H:111:LEU:HD23	8:H:127:GLY:O	2.13	0.48
10:J:58:GLU:HA	10:J:61:LEU:HD12	1.96	0.48
1:A:710:LEU:H	1:A:710:LEU:HD12	1.79	0.48
1:A:774:ARG:HB2	1:A:797:LYS:HB3	1.96	0.48
1:A:947:PHE:CD2	1:A:954:TRP:CZ2	3.01	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1110:ASN:OD1	1:A:1110:ASN:N	2.47	0.48
2:B:360:PHE:O	2:B:361:LEU:C	2.56	0.48
2:B:459:TYR:C	2:B:459:TYR:CD2	2.92	0.48
2:B:640:VAL:O	2:B:640:VAL:HG12	2.13	0.48
2:B:831:SER:HB3	2:B:994:TYR:OH	2.14	0.48
2:B:843:GLN:CG	11:K:6:ARG:HH21	2.27	0.48
2:B:1121:GLY:C	2:B:1123:SER:N	2.69	0.48
4:D:195:ILE:C	4:D:197:SER:H	2.22	0.48
7:G:25:TYR:HE2	7:G:29:LYS:HD2	1.79	0.48
11:K:35:PHE:CD1	11:K:71:PHE:CE1	3.01	0.48
13:N:5:DA:H2''	13:N:6:DC:OP2	2.13	0.48
1:A:84:ILE:O	1:A:84:ILE:CG2	2.61	0.48
1:A:295:LEU:O	1:A:298:PHE:HB3	2.13	0.48
1:A:577:ILE:O	1:A:579:SER:N	2.47	0.48
1:A:901:LEU:HA	1:A:907:THR:OG1	2.13	0.48
1:A:1070:GLN:O	1:A:1072:ILE:N	2.46	0.48
2:B:65:GLU:CG	2:B:66:ASP:H	2.09	0.48
2:B:282:ILE:HD12	2:B:382:ILE:HD13	1.94	0.48
2:B:376:PHE:CE2	2:B:569:TYR:HD2	2.32	0.48
2:B:1023:VAL:O	2:B:1024:ALA:C	2.57	0.48
3:C:100:THR:CG2	3:C:101:LEU:N	2.77	0.48
3:C:114:TYR:HB3	3:C:140:ASN:O	2.13	0.48
4:D:51:ASN:O	4:D:54:GLU:HB3	2.14	0.48
5:E:124:VAL:HG13	5:E:132:ILE:CG1	2.43	0.48
7:G:1:MET:O	7:G:3:PHE:CE1	2.67	0.48
7:G:91:VAL:HB	7:G:139:ILE:O	2.13	0.48
13:N:5:DA:H1'	13:N:6:DC:O5'	2.13	0.48
1:A:38:PRO:HB3	1:A:270:LEU:HG	1.95	0.48
1:A:53:LEU:CD2	1:A:54:ASN:HD22	2.27	0.48
1:A:313:GLN:O	1:A:314:ALA:HB3	2.13	0.48
1:A:773:LYS:H	1:A:773:LYS:HG3	1.45	0.48
1:A:847:ASP:OD1	1:A:848:ILE:HG13	2.14	0.48
1:A:935:GLN:O	1:A:936:LEU:C	2.56	0.48
2:B:361:LEU:N	2:B:362:PRO:CD	2.76	0.48
2:B:616:ILE:HG12	2:B:697:GLU:HA	1.96	0.48
3:C:66:ARG:NH2	10:J:5:VAL:CG2	2.76	0.48
4:D:194:LEU:C	4:D:195:ILE:HG13	2.39	0.48
8:H:38:LEU:HD13	8:H:125:LEU:CD1	2.44	0.48
1:A:7:SER:CB	2:B:1175:LEU:HD22	2.43	0.48
1:A:442:VAL:CB	1:A:489:LEU:HD11	2.40	0.48
1:A:858:ASN:C	1:A:858:ASN:ND2	2.59	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1066:VAL:O	1:A:1070:GLN:HG3	2.13	0.48
1:A:1441:PHE:HZ	6:F:89:GLU:HA	1.78	0.48
2:B:263:GLY:O	2:B:264:SER:C	2.56	0.48
2:B:308:TRP:CA	2:B:311:LEU:HD12	2.38	0.48
2:B:825:VAL:HG13	2:B:826:ALA:N	2.24	0.48
2:B:846:ILE:HG23	2:B:974:PRO:HG2	1.96	0.48
2:B:1178:ASN:O	2:B:1180:PHE:CD1	2.67	0.48
3:C:204:SER:C	3:C:206:ASN:N	2.70	0.48
5:E:48:ASP:CG	5:E:49:SER:N	2.69	0.48
7:G:111:THR:HG22	7:G:113:HIS:N	2.27	0.48
1:A:445:ASN:ND2	1:A:446:ARG:N	2.61	0.47
1:A:1114:PRO:HB2	1:A:1311:VAL:HG23	1.94	0.47
1:A:1291:VAL:HG13	1:A:1292:PRO:N	2.29	0.47
1:A:1389:PHE:CD1	1:A:1389:PHE:C	2.91	0.47
2:B:387:LEU:O	2:B:392:ARG:HB2	2.14	0.47
2:B:466:TRP:HA	2:B:466:TRP:CE3	2.49	0.47
2:B:882:THR:HG21	2:B:884:ARG:HB2	1.96	0.47
3:C:259:LEU:HD13	11:K:91:CYS:HB2	1.96	0.47
9:I:4:PHE:CD1	9:I:4:PHE:C	2.92	0.47
9:I:101:PHE:HB2	9:I:110:PHE:CE2	2.49	0.47
10:J:16:ASP:O	10:J:18:TRP:N	2.47	0.47
1:A:49:LYS:CE	1:A:61:ILE:HD12	2.42	0.47
1:A:64:ASN:O	1:A:65:LEU:C	2.56	0.47
1:A:108:MET:HB3	1:A:210:ILE:CD1	2.45	0.47
1:A:532:ARG:O	1:A:535:THR:HB	2.14	0.47
1:A:650:GLN:HB3	1:A:654:ASN:HD21	1.79	0.47
1:A:684:ALA:O	1:A:687:LYS:HB2	2.14	0.47
1:A:817:ALA:O	1:A:818:MET:C	2.56	0.47
1:A:967:ALA:O	1:A:968:GLN:O	2.32	0.47
1:A:993:LEU:HD23	1:A:1022:LEU:HD21	1.96	0.47
1:A:1236:LEU:C	1:A:1237:ILE:HG13	2.39	0.47
1:A:1279:ILE:O	1:A:1279:ILE:HG22	2.14	0.47
2:B:638:PHE:HB3	2:B:651:LEU:HD22	1.97	0.47
2:B:1065:GLN:NE2	2:B:1067:ARG:HG2	2.29	0.47
2:B:1115:THR:CG2	2:B:1117:GLN:CG	2.92	0.47
3:C:258:ILE:N	3:C:258:ILE:CD1	2.78	0.47
5:E:207:ARG:CB	5:E:207:ARG:HH11	2.26	0.47
12:L:27:LEU:O	12:L:28:LYS:HG2	2.14	0.47
1:A:500:GLU:OE2	2:B:1145:SER:CB	2.62	0.47
1:A:783:THR:HG22	1:A:784:LEU:HG	1.96	0.47
1:A:874:ASP:HA	1:A:1058:VAL:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1125:ALA:C	1:A:1127:ASP:H	2.22	0.47
1:A:1151:GLU:HA	9:I:44:TYR:O	2.13	0.47
2:B:683:SER:C	2:B:685:LEU:N	2.73	0.47
2:B:753:ALA:HA	2:B:756:ILE:CD1	2.44	0.47
3:C:8:VAL:HG12	3:C:9:LYS:N	2.29	0.47
3:C:213:PRO:HG2	3:C:214:ASN:H	1.79	0.47
4:D:159:THR:O	4:D:163:VAL:HG23	2.13	0.47
5:E:42:PHE:HZ	5:E:58:MET:HE3	1.78	0.47
5:E:67:GLU:O	5:E:70:SER:HB3	2.15	0.47
5:E:156:LEU:HD12	5:E:195:VAL:CG1	2.44	0.47
7:G:20:PRO:HG2	7:G:21:ARG:H	1.79	0.47
11:K:111:LEU:O	11:K:112:GLN:CB	2.62	0.47
1:A:84:ILE:HG22	1:A:239:LEU:HB3	1.94	0.47
1:A:335:ARG:O	1:A:336:ILE:C	2.55	0.47
1:A:409:SER:O	1:A:410:GLY:C	2.56	0.47
1:A:528:LEU:HG	1:A:529:CYS:N	2.30	0.47
1:A:639:PRO:CG	1:A:640:GLN:N	2.77	0.47
1:A:827:THR:O	1:A:831:THR:HB	2.13	0.47
1:A:901:LEU:H	1:A:926:GLN:HE21	1.58	0.47
1:A:1074:GLU:HB3	1:A:1075:PRO:HD3	1.95	0.47
1:A:1305:VAL:CG1	1:A:1306:LEU:N	2.77	0.47
2:B:258:LEU:HB2	2:B:385:LEU:HD21	1.97	0.47
2:B:637:LEU:O	2:B:690:VAL:HG13	2.14	0.47
2:B:641:GLU:C	2:B:643:ASP:H	2.21	0.47
2:B:1010:LEU:HD12	2:B:1010:LEU:HA	1.78	0.47
4:D:47:LEU:CD1	7:G:3:PHE:HD2	2.22	0.47
5:E:136:ASN:OD1	5:E:137:GLU:N	2.48	0.47
9:I:16:PRO:HB2	9:I:25:LEU:HD11	1.97	0.47
1:A:34:LYS:HZ1	1:A:57:ARG:CZ	2.28	0.47
1:A:242:PRO:HD3	2:B:1209:ALA:CB	2.44	0.47
1:A:699:ALA:O	1:A:700:ASN:CB	2.62	0.47
1:A:800:VAL:CG1	1:A:808:LEU:HG	2.43	0.47
1:A:964:ILE:O	1:A:967:ALA:HB3	2.14	0.47
1:A:1152:ILE:HG13	9:I:44:TYR:HB3	1.97	0.47
1:A:1405:THR:HB	1:A:1406:VAL:H	1.47	0.47
2:B:130:VAL:HB	2:B:167:ILE:HD12	1.97	0.47
2:B:558:LEU:O	2:B:560:GLU:N	2.46	0.47
2:B:658:ILE:CG2	2:B:662:MET:HE2	2.45	0.47
2:B:782:LEU:HD12	2:B:788:ARG:NH1	2.24	0.47
2:B:1034:VAL:O	2:B:1037:LEU:N	2.42	0.47
3:C:254:LYS:O	3:C:256:ALA:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:55:ARG:HD2	5:E:83:CYS:O	2.14	0.47
6:F:89:GLU:HB3	6:F:134:ILE:CD1	2.45	0.47
7:G:96:GLN:HG3	7:G:97:HIS:CD2	2.49	0.47
7:G:139:ILE:HG22	7:G:140:LYS:N	2.29	0.47
1:A:58:LEU:CD1	1:A:243:PRO:HB3	2.40	0.47
1:A:230:ARG:HB2	1:A:233:TRP:CE3	2.50	0.47
1:A:298:PHE:CZ	1:A:314:ALA:HB2	2.50	0.47
1:A:560:ILE:H	1:A:560:ILE:HG12	1.43	0.47
1:A:613:ILE:O	1:A:614:PHE:HB3	2.15	0.47
1:A:858:ASN:ND2	1:A:860:LEU:N	2.57	0.47
1:A:1120:LEU:CD1	1:A:1120:LEU:H	2.28	0.47
1:A:1277:GLU:C	1:A:1279:ILE:H	2.21	0.47
1:A:1327:ILE:O	1:A:1327:ILE:HG23	2.13	0.47
2:B:46:GLN:CG	2:B:47:GLN:H	2.21	0.47
2:B:205:ILE:O	2:B:206:ASN:C	2.57	0.47
2:B:522:VAL:CG1	2:B:537:LYS:HB3	2.45	0.47
2:B:542:MET:HE3	2:B:636:PRO:CG	2.43	0.47
2:B:820:GLY:C	2:B:1091:TYR:CE1	2.92	0.47
2:B:1099:VAL:O	2:B:1101:ASP:N	2.47	0.47
2:B:1106:ARG:HH11	2:B:1110:PRO:HG2	1.77	0.47
4:D:68:ARG:C	4:D:70:PHE:H	2.23	0.47
4:D:192:LYS:HG2	4:D:207:LEU:CD2	2.45	0.47
8:H:93:TYR:CD1	8:H:93:TYR:N	2.82	0.47
11:K:109:TRP:O	11:K:111:LEU:N	2.47	0.47
1:A:166:GLY:O	1:A:167:CYS:CB	2.63	0.47
1:A:415:LEU:HA	1:A:415:LEU:HD23	1.61	0.47
1:A:438:ASP:OD1	1:A:461:LYS:HA	2.14	0.47
1:A:506:ALA:O	1:A:509:LEU:HB2	2.14	0.47
1:A:658:LEU:CD1	2:B:831:SER:H	2.26	0.47
1:A:774:ARG:CZ	1:A:797:LYS:HG3	2.44	0.47
1:A:947:PHE:HD2	1:A:954:TRP:CZ2	2.32	0.47
1:A:1067:LEU:HD12	1:A:1367:HIS:CE1	2.49	0.47
1:A:1107:VAL:HG12	1:A:1107:VAL:O	2.13	0.47
1:A:1195:LEU:HD11	1:A:1267:MET:CE	2.45	0.47
1:A:1222:ASN:O	1:A:1223:ASP:HB3	2.14	0.47
1:A:1315:GLU:C	1:A:1317:MET:H	2.22	0.47
1:A:1454:MET:O	1:A:1454:MET:HG3	2.14	0.47
2:B:217:ARG:HD2	2:B:217:ARG:O	2.13	0.47
2:B:324:ILE:CG2	2:B:325:GLN:N	2.76	0.47
2:B:597:MET:C	2:B:599:THR:H	2.23	0.47
2:B:770:GLN:OE1	2:B:983:ARG:CA	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:864:LYS:N	2:B:872:GLU:OE1	2.47	0.47
2:B:1142:GLY:O	2:B:1144:ALA:N	2.47	0.47
2:B:1182:CYS:C	2:B:1183:LYS:O	2.56	0.47
3:C:22:LEU:HD13	3:C:230:MET:CE	2.45	0.47
4:D:20:GLU:HA	4:D:20:GLU:OE2	2.13	0.47
6:F:109:VAL:HG11	6:F:123:LYS:HD3	1.95	0.47
9:I:25:LEU:CB	9:I:38:ALA:HB2	2.44	0.47
1:A:456:MET:HE3	1:A:478:TYR:CE1	2.50	0.47
1:A:785:PRO:CG	2:B:703:ILE:HD12	2.45	0.47
1:A:806:ARG:NH1	2:B:729:ILE:HG13	2.29	0.47
1:A:1362:TYR:HD1	1:A:1363:VAL:H	1.61	0.47
2:B:37:PHE:CE2	2:B:542:MET:HA	2.47	0.47
2:B:115:GLN:HG2	2:B:193:LYS:HB2	1.96	0.47
2:B:185:THR:O	2:B:186:GLU:C	2.57	0.47
2:B:681:TRP:O	2:B:684:LEU:N	2.48	0.47
2:B:1087:PHE:HD2	2:B:1087:PHE:C	2.23	0.47
2:B:1207:LEU:HD23	2:B:1210:MET:HE3	1.96	0.47
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.50	0.47
5:E:42:PHE:CZ	5:E:58:MET:HE3	2.49	0.47
6:F:74:ILE:HG23	6:F:75:PRO:HD2	1.95	0.47
6:F:124:GLU:HB3	6:F:130:ILE:HG12	1.95	0.47
8:H:123:MET:HG2	8:H:124:ARG:N	2.29	0.47
11:K:82:ASP:O	11:K:85:ASP:HB2	2.15	0.47
1:A:31:SER:OG	1:A:82:GLY:HA2	2.15	0.47
1:A:42:ASP:O	1:A:44:THR:N	2.36	0.47
1:A:58:LEU:O	1:A:59:GLY:O	2.33	0.47
1:A:350:ARG:HG3	1:A:350:ARG:NH1	2.30	0.47
1:A:981:LEU:HD21	1:A:1038:THR:C	2.40	0.47
1:A:1013:ASP:C	1:A:1015:VAL:H	2.20	0.47
1:A:1157:ASP:C	1:A:1159:ARG:H	2.23	0.47
1:A:1260:LEU:CG	1:A:1260:LEU:O	2.63	0.47
1:A:1265:ASN:O	1:A:1268:LEU:N	2.46	0.47
2:B:683:SER:C	2:B:685:LEU:H	2.22	0.47
2:B:732:SER:HB2	2:B:734:HIS:CD2	2.49	0.47
2:B:799:PRO:HB3	2:B:818:PRO:HG2	1.96	0.47
2:B:839:MET:HE3	2:B:1010:LEU:HD21	1.97	0.47
2:B:889:THR:HG22	2:B:891:ASP:HB2	1.97	0.47
2:B:973:ILE:HG23	2:B:974:PRO:HD2	1.97	0.47
2:B:1087:PHE:CD2	2:B:1087:PHE:C	2.92	0.47
2:B:1110:PRO:HG3	2:B:1124:ARG:O	2.14	0.47
2:B:1125:ASP:O	2:B:1125:ASP:OD1	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1151:LEU:N	2:B:1151:LEU:CD1	2.77	0.47
2:B:1215:ARG:C	2:B:1216:LEU:HD23	2.39	0.47
5:E:17:ARG:O	5:E:20:LYS:HB2	2.15	0.47
8:H:113:ALA:HB1	8:H:125:LEU:O	2.15	0.47
9:I:4:PHE:HE1	9:I:6:PHE:CE2	2.32	0.47
9:I:58:VAL:O	9:I:58:VAL:HG12	2.15	0.47
1:A:399:HIS:CB	1:A:400:PRO:CD	2.91	0.47
1:A:1070:GLN:O	1:A:1071:SER:C	2.57	0.47
2:B:240:ILE:CD1	2:B:377:PHE:HE2	2.28	0.47
2:B:400:HIS:O	2:B:402:GLY:N	2.48	0.47
2:B:642:ASP:CA	2:B:649:LYS:HG3	2.44	0.47
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.97	0.47
2:B:861:ASP:OD1	2:B:862:GLN:N	2.48	0.47
2:B:862:GLN:CG	2:B:963:PHE:HD1	2.25	0.47
3:C:70:ILE:CD1	3:C:144:ILE:HD11	2.45	0.47
3:C:168:ALA:C	3:C:170:TRP:H	2.20	0.47
3:C:236:GLY:O	3:C:237:SER:C	2.58	0.47
4:D:46:GLU:C	4:D:47:LEU:O	2.58	0.47
5:E:90:VAL:O	5:E:90:VAL:HG22	2.15	0.47
6:F:90:ARG:HD3	6:F:155:LEU:HD12	1.94	0.47
11:K:67:PHE:C	11:K:68:PHE:CD2	2.93	0.47
12:L:28:LYS:HB2	12:L:39:SER:HB2	1.97	0.47
12:L:40:LEU:HD22	12:L:44:ASP:CB	2.45	0.47
1:A:114:LEU:HD13	1:A:171:GLN:NE2	2.30	0.46
1:A:262:LEU:HD12	1:A:328:ARG:NH2	2.30	0.46
1:A:350:ARG:HG3	1:A:350:ARG:HH11	1.80	0.46
1:A:534:LEU:HD13	1:A:656:TRP:CD2	2.49	0.46
1:A:1162:VAL:O	1:A:1162:VAL:HG12	2.15	0.46
1:A:1187:GLN:HG3	1:A:1188:GLN:H	1.81	0.46
2:B:129:PHE:HD2	2:B:166:PHE:HA	1.79	0.46
2:B:492:LEU:O	2:B:493:SER:C	2.58	0.46
2:B:1202:LEU:O	2:B:1206:GLU:HG3	2.16	0.46
3:C:76:ASP:O	3:C:79:GLN:HG2	2.16	0.46
3:C:213:PRO:O	3:C:214:ASN:CB	2.62	0.46
7:G:110:VAL:HG22	7:G:161:GLY:O	2.15	0.46
9:I:115:LYS:CD	9:I:117:LYS:HE3	2.38	0.46
10:J:31:ASP:O	10:J:32:GLU:C	2.57	0.46
1:A:47:ARG:HH12	1:A:254:GLU:HG2	1.80	0.46
1:A:252:PHE:HB2	1:A:256:GLN:CD	2.41	0.46
1:A:269:ILE:CD1	1:A:300:VAL:HA	2.40	0.46
1:A:577:ILE:O	1:A:580:VAL:N	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:877:HIS:O	1:A:878:ILE:CG1	2.63	0.46
1:A:1007:ILE:C	1:A:1009:ASN:H	2.23	0.46
1:A:1115:SER:O	1:A:1311:VAL:HG22	2.16	0.46
1:A:1118:VAL:HG12	1:A:1327:ILE:CD1	2.45	0.46
1:A:1215:ARG:O	1:A:1216:ILE:C	2.58	0.46
1:A:1325:THR:O	1:A:1325:THR:CG2	2.63	0.46
2:B:175:ARG:HH11	2:B:175:ARG:CG	2.20	0.46
2:B:459:TYR:CE1	2:B:469:GLN:HG2	2.51	0.46
2:B:1034:VAL:C	2:B:1036:ALA:N	2.73	0.46
2:B:1132:GLU:O	2:B:1135:ARG:HB3	2.15	0.46
3:C:67:LEU:HD13	3:C:157:CYS:SG	2.56	0.46
4:D:7:THR:O	4:D:7:THR:HG23	2.14	0.46
5:E:178:ILE:HG22	5:E:213:ILE:O	2.14	0.46
6:F:130:ILE:O	6:F:148:VAL:CG2	2.63	0.46
7:G:1:MET:SD	7:G:79:PHE:CE1	3.08	0.46
12:L:58:LYS:O	12:L:59:ALA:O	2.33	0.46
15:T:17:TT:H3R	15:T:19:DT:C5'	2.41	0.46
1:A:87:ALA:HB1	1:A:276:LEU:HD23	1.97	0.46
1:A:107:CYS:H	1:A:114:LEU:HD21	1.80	0.46
1:A:650:GLN:O	1:A:654:ASN:ND2	2.48	0.46
1:A:783:THR:HG21	1:A:815:PHE:CE2	2.50	0.46
1:A:816:HIS:CD2	2:B:764:SER:HB2	2.51	0.46
1:A:1142:THR:O	1:A:1143:LEU:C	2.58	0.46
1:A:1163:ILE:HG22	1:A:1164:PRO:HD2	1.98	0.46
1:A:1226:VAL:HG12	1:A:1227:ILE:N	2.29	0.46
2:B:806:THR:HG22	2:B:808:ALA:CB	2.45	0.46
2:B:1002:THR:CG2	2:B:1006:ILE:HD12	2.31	0.46
2:B:1197:PRO:O	2:B:1200:ALA:N	2.48	0.46
3:C:69:LEU:N	3:C:69:LEU:CD1	2.78	0.46
3:C:186:LEU:N	3:C:186:LEU:HD12	2.31	0.46
5:E:207:ARG:NH1	5:E:207:ARG:HB2	2.31	0.46
6:F:143:PHE:HD1	6:F:143:PHE:O	1.99	0.46
7:G:23:LYS:HG3	7:G:56:ILE:HD12	1.97	0.46
11:K:88:LYS:O	11:K:89:ASN:C	2.59	0.46
1:A:511:ILE:O	1:A:519:PRO:HA	2.16	0.46
1:A:709:THR:HG22	1:A:710:LEU:N	2.29	0.46
1:A:940:ARG:HB3	1:A:941:LYS:HE3	1.98	0.46
1:A:1149:ALA:CB	9:I:47:GLU:HA	2.45	0.46
2:B:130:VAL:HB	2:B:167:ILE:CD1	2.45	0.46
2:B:274:PRO:O	2:B:275:TYR:HB2	2.16	0.46
2:B:654:ARG:O	2:B:656:GLY:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1096:ARG:HH21	14:P:7:A:H4'	1.80	0.46
2:B:1177:HIS:CB	2:B:1179:GLN:HE21	2.26	0.46
3:C:35:ARG:HH12	11:K:41:THR:H	1.63	0.46
3:C:47:ASP:C	12:L:69:ALA:HB2	2.40	0.46
3:C:74:SER:HB2	3:C:77:ILE:CG1	2.45	0.46
3:C:263:THR:O	3:C:265:MET:N	2.49	0.46
5:E:136:ASN:OD1	5:E:138:ALA:N	2.48	0.46
7:G:27:LYS:HE2	7:G:54:ILE:HB	1.97	0.46
9:I:34:TYR:CE2	9:I:36:GLU:HB3	2.45	0.46
9:I:55:THR:HG22	9:I:58:VAL:CG2	2.43	0.46
11:K:55:LYS:HB3	11:K:81:TYR:CD1	2.50	0.46
14:P:5:C:C2'	14:P:6:C:H5'	2.45	0.46
1:A:325:ILE:HG21	2:B:1210:MET:CG	2.40	0.46
1:A:335:ARG:HB3	1:A:336:ILE:H	1.63	0.46
1:A:525:GLN:CB	2:B:835:GLN:HG2	2.44	0.46
1:A:699:ALA:HB1	9:I:114:GLN:HB2	1.98	0.46
1:A:871:ASP:OD2	1:A:873:MET:HB2	2.14	0.46
1:A:877:HIS:C	1:A:878:ILE:HG13	2.40	0.46
1:A:901:LEU:H	1:A:926:GLN:CD	2.20	0.46
1:A:942:PHE:C	1:A:942:PHE:CD2	2.93	0.46
1:A:1364:ASN:O	1:A:1366:ARG:HG3	2.16	0.46
2:B:185:THR:H	2:B:188:ASP:CB	2.29	0.46
2:B:363:HIS:O	2:B:364:ILE:CB	2.53	0.46
2:B:908:GLU:O	2:B:909:ASP:O	2.33	0.46
3:C:86:CYS:O	3:C:88:CYS:N	2.49	0.46
3:C:191:TYR:CD2	3:C:201:TRP:CD1	3.03	0.46
3:C:259:LEU:CD1	11:K:91:CYS:HB2	2.46	0.46
7:G:1:MET:HE1	7:G:80:LYS:C	2.40	0.46
9:I:15:TYR:N	9:I:15:TYR:CD1	2.84	0.46
11:K:65:HIS:HD2	11:K:67:PHE:N	1.94	0.46
1:A:77:CYS:C	1:A:78:PRO:O	2.55	0.46
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.81	0.46
1:A:537:ARG:NH1	8:H:120:GLY:O	2.48	0.46
1:A:722:LEU:O	1:A:725:ALA:HB3	2.14	0.46
1:A:841:LEU:O	1:A:845:LEU:HG	2.15	0.46
1:A:883:LEU:CD2	1:A:1021:LEU:HB2	2.46	0.46
1:A:1236:LEU:O	1:A:1237:ILE:HG13	2.16	0.46
1:A:1260:LEU:O	1:A:1260:LEU:HG	2.15	0.46
2:B:358:LYS:HA	2:B:366:GLN:HB3	1.98	0.46
3:C:242:GLN:HB3	3:C:246:ARG:HG3	1.97	0.46
4:D:53:SER:HB3	4:D:152:SER:CA	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:209:ARG:O	4:D:212:LYS:HB2	2.16	0.46
9:I:100:PHE:N	9:I:100:PHE:HD1	2.13	0.46
11:K:29:ASN:O	11:K:76:GLN:HG3	2.16	0.46
11:K:85:ASP:O	11:K:88:LYS:HB2	2.16	0.46
12:L:46:VAL:O	12:L:46:VAL:HG12	2.16	0.46
13:N:2:DA:H2"	13:N:3:DG:OP2	2.16	0.46
1:A:7:SER:C	1:A:9:ALA:N	2.72	0.46
1:A:144:THR:O	1:A:146:MET:HE2	2.15	0.46
1:A:195:ASP:O	1:A:196:GLU:HB3	2.16	0.46
1:A:367:PRO:O	1:A:368:LYS:C	2.59	0.46
1:A:420:ARG:O	1:A:421:ALA:C	2.58	0.46
1:A:458:HIS:NE2	1:A:478:TYR:OH	2.38	0.46
1:A:575:LYS:NZ	1:A:615:GLY:H	2.13	0.46
1:A:650:GLN:C	1:A:654:ASN:ND2	2.73	0.46
1:A:816:HIS:CD2	2:B:764:SER:H	2.34	0.46
1:A:853:ASP:OD1	1:A:855:THR:HG22	2.15	0.46
1:A:964:ILE:O	1:A:967:ALA:N	2.48	0.46
1:A:1019:CYS:O	1:A:1022:LEU:N	2.49	0.46
1:A:1116:LEU:HB3	1:A:1308:THR:CG2	2.45	0.46
2:B:48:LEU:O	2:B:49:ASP:C	2.58	0.46
2:B:51:PHE:O	2:B:54:PHE:HB3	2.16	0.46
2:B:118:ARG:HG2	2:B:204:ILE:HD13	1.97	0.46
2:B:228:LYS:CB	2:B:261:ARG:HH22	2.29	0.46
2:B:317:CYS:O	2:B:318:VAL:C	2.57	0.46
2:B:685:LEU:C	2:B:687:GLU:H	2.24	0.46
2:B:906:SER:O	2:B:907:GLY:O	2.33	0.46
2:B:1033:LYS:NZ	2:B:1068:GLY:O	2.48	0.46
3:C:89:GLU:O	3:C:90:ASP:HB3	2.15	0.46
3:C:160:LYS:O	3:C:161:LYS:O	2.34	0.46
4:D:24:ALA:C	4:D:26:THR:N	2.73	0.46
10:J:56:LEU:O	10:J:57:ILE:C	2.57	0.46
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.61	0.46
1:A:65:LEU:O	1:A:66:LYS:C	2.59	0.46
1:A:443:LEU:O	1:A:489:LEU:HD12	2.16	0.46
1:A:630:ILE:O	1:A:631:HIS:C	2.58	0.46
1:A:847:ASP:O	1:A:858:ASN:HA	2.16	0.46
1:A:1010:ALA:O	1:A:1013:ASP:HB2	2.15	0.46
1:A:1116:LEU:N	1:A:1308:THR:CG2	2.73	0.46
2:B:114:PRO:HG2	2:B:115:GLN:N	2.27	0.46
2:B:181:LEU:HD22	2:B:189:LEU:CD2	2.46	0.46
2:B:1029:CYS:HA	2:B:1089:PRO:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:47:ASP:HA	3:C:169:LYS:NZ	2.30	0.46
7:G:79:PHE:CE2	7:G:105:PRO:HG2	2.51	0.46
7:G:99:PHE:CD1	7:G:99:PHE:C	2.93	0.46
9:I:112:SER:O	9:I:114:GLN:N	2.48	0.46
10:J:43:ARG:O	10:J:47:ARG:HB2	2.16	0.46
1:A:58:LEU:HD11	1:A:80:HIS:H	1.81	0.46
1:A:71:GLN:O	1:A:73:GLY:N	2.43	0.46
1:A:146:MET:HA	1:A:171:GLN:HB2	1.98	0.46
1:A:182:VAL:HG22	1:A:201:VAL:HA	1.97	0.46
1:A:211:PHE:HA	1:A:214:ILE:HG13	1.98	0.46
1:A:324:SER:O	1:A:327:ALA:HB3	2.15	0.46
1:A:552:TRP:HE3	1:A:651:LYS:HB3	1.81	0.46
1:A:722:LEU:HD21	1:A:794:PRO:HB3	1.98	0.46
1:A:909:ASP:O	1:A:911:SER:N	2.49	0.46
1:A:1115:SER:HB3	1:A:1330:ASN:HD21	1.80	0.46
1:A:1283:VAL:HG12	1:A:1284:MET:H	1.78	0.46
2:B:469:GLN:HB2	2:B:470:LYS:H	1.45	0.46
2:B:502:ILE:HD12	2:B:502:ILE:N	2.19	0.46
2:B:558:LEU:C	2:B:560:GLU:N	2.74	0.46
2:B:979:LYS:HG2	2:B:1095:LEU:HD13	1.98	0.46
3:C:27:LEU:HD13	3:C:228:PHE:CE2	2.50	0.46
3:C:37:MET:HA	3:C:41:ILE:HD11	1.98	0.46
4:D:53:SER:HB3	4:D:152:SER:HA	1.97	0.46
4:D:213:GLU:O	4:D:217:LEU:HG	2.16	0.46
6:F:119:ARG:HG3	6:F:119:ARG:NH1	2.31	0.46
7:G:27:LYS:O	7:G:28:THR:C	2.57	0.46
1:A:326:ARG:HG2	1:A:327:ALA:N	2.30	0.46
1:A:779:PHE:O	1:A:780:VAL:C	2.59	0.46
1:A:809:THR:H	1:A:812:GLU:HB2	1.81	0.46
2:B:29:ASP:HB3	2:B:658:ILE:HD11	1.97	0.46
2:B:897:GLY:O	2:B:898:LEU:HD23	2.16	0.46
2:B:942:ARG:NH2	15:T:25:DT:OP2	2.48	0.46
2:B:990:ILE:HG22	2:B:991:GLY:N	2.31	0.46
3:C:66:ARG:HH21	10:J:5:VAL:HG23	1.76	0.46
6:F:95:GLY:O	6:F:96:THR:C	2.59	0.46
7:G:20:PRO:CG	7:G:21:ARG:H	2.29	0.46
7:G:56:ILE:O	7:G:57:GLN:HB2	2.16	0.46
1:A:262:LEU:C	1:A:264:PHE:N	2.72	0.45
1:A:298:PHE:O	1:A:301:ALA:HB3	2.16	0.45
1:A:919:ILE:O	1:A:920:LEU:C	2.59	0.45
1:A:963:ILE:HD13	1:A:1049:ILE:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1111:MET:HE1	1:A:1330:ASN:OD1	2.16	0.45
1:A:1209:MET:HE1	1:A:1236:LEU:HB3	1.97	0.45
1:A:1219:THR:HG21	1:A:1271:ILE:HD11	1.98	0.45
2:B:642:ASP:CA	2:B:649:LYS:HA	2.41	0.45
2:B:828:ALA:O	2:B:834:ASN:ND2	2.49	0.45
3:C:23:SER:O	3:C:24:ASN:HB3	2.16	0.45
4:D:7:THR:O	4:D:9:GLN:N	2.49	0.45
4:D:173:HIS:O	4:D:177:VAL:HG23	2.16	0.45
6:F:109:VAL:HG12	6:F:110:ASP:N	2.30	0.45
7:G:14:HIS:HD1	7:G:15:PRO:HD2	1.76	0.45
8:H:26:ILE:CD1	8:H:49:VAL:HG11	2.45	0.45
11:K:19:LEU:HD21	11:K:35:PHE:CE2	2.51	0.45
12:L:27:LEU:HD23	12:L:27:LEU:N	2.31	0.45
1:A:37:PHE:N	1:A:37:PHE:HD1	2.10	0.45
1:A:70:CYS:O	1:A:70:CYS:SG	2.74	0.45
1:A:119:ASN:O	1:A:122:MET:HB3	2.16	0.45
1:A:298:PHE:HZ	1:A:314:ALA:HB2	1.80	0.45
1:A:567:LYS:HG3	1:A:568:PRO:CD	2.36	0.45
1:A:569:LYS:O	1:A:571:LEU:HD13	2.15	0.45
1:A:719:VAL:C	1:A:721:PHE:N	2.74	0.45
1:A:774:ARG:H	1:A:774:ARG:HG2	1.42	0.45
1:A:825:ILE:O	1:A:826:ASP:C	2.57	0.45
1:A:847:ASP:HB3	1:A:1398:MET:HE1	1.98	0.45
1:A:874:ASP:O	1:A:875:ALA:C	2.59	0.45
1:A:1111:MET:CE	1:A:1330:ASN:OD1	2.63	0.45
1:A:1362:TYR:CD1	1:A:1362:TYR:C	2.92	0.45
2:B:225:VAL:HA	2:B:237:VAL:O	2.16	0.45
2:B:230:ALA:N	2:B:231:PRO:HD2	2.31	0.45
2:B:244:LEU:C	2:B:246:LYS:N	2.71	0.45
2:B:259:TYR:HD1	2:B:259:TYR:H	1.65	0.45
2:B:485:ARG:NH2	2:B:782:LEU:HD11	2.31	0.45
2:B:658:ILE:HG22	2:B:662:MET:HE2	1.98	0.45
2:B:764:SER:HB3	2:B:765:PRO:CD	2.46	0.45
2:B:770:GLN:C	2:B:772:ALA:H	2.24	0.45
2:B:842:ASN:HD22	2:B:845:SER:CB	2.30	0.45
2:B:844:SER:O	2:B:847:ASP:N	2.49	0.45
2:B:1084:GLN:OE1	3:C:189:THR:HG22	2.16	0.45
3:C:31:ASN:O	3:C:34:ARG:N	2.49	0.45
1:A:75:ASN:HA	2:B:1116:ARG:HH22	1.81	0.45
1:A:525:GLN:HG3	2:B:835:GLN:HG2	1.97	0.45
1:A:567:LYS:HE3	8:H:46:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:LEU:HD23	1:A:612:ILE:CD1	2.46	0.45
1:A:929:LEU:HD23	1:A:983:ILE:HG21	1.98	0.45
2:B:654:ARG:C	2:B:656:GLY:N	2.74	0.45
2:B:770:GLN:CD	2:B:983:ARG:CA	2.85	0.45
2:B:899:ILE:O	2:B:952:VAL:HG21	2.16	0.45
2:B:981:ALA:HB2	2:B:987:LYS:HA	1.98	0.45
2:B:983:ARG:HD2	2:B:1091:TYR:CD2	2.50	0.45
9:I:14:LEU:HD22	9:I:28:GLU:O	2.17	0.45
10:J:2:ILE:H	10:J:57:ILE:CG2	2.29	0.45
11:K:40:HIS:O	11:K:41:THR:C	2.59	0.45
1:A:453:MET:C	1:A:455:MET:H	2.23	0.45
1:A:963:ILE:HD13	1:A:1049:ILE:CG1	2.47	0.45
2:B:210:LYS:HD3	2:B:481:GLN:O	2.17	0.45
2:B:286:PHE:CD1	2:B:297:ILE:HG23	2.51	0.45
2:B:361:LEU:O	2:B:363:HIS:O	2.33	0.45
2:B:365:THR:HG23	2:B:367:LEU:N	2.25	0.45
2:B:776:GLN:O	2:B:1095:LEU:HA	2.16	0.45
2:B:977:GLY:HA3	2:B:1099:VAL:HG21	1.97	0.45
2:B:980:PHE:CA	2:B:1095:LEU:HD11	2.46	0.45
2:B:1011:ILE:O	2:B:1011:ILE:HG22	2.16	0.45
2:B:1064:TYR:O	2:B:1065:GLN:C	2.59	0.45
4:D:17:LYS:HE3	4:D:17:LYS:N	2.32	0.45
5:E:135:PHE:CD2	5:E:140:LEU:HD21	2.48	0.45
7:G:44:TYR:O	7:G:78:VAL:HG12	2.17	0.45
10:J:56:LEU:O	10:J:59:LYS:N	2.45	0.45
1:A:81:PHE:CZ	2:B:1208:MET:HB2	2.52	0.45
1:A:224:PHE:CE2	1:A:231:PRO:HA	2.52	0.45
1:A:367:PRO:HB3	1:A:465:TYR:O	2.16	0.45
1:A:723:ASN:O	1:A:724:GLU:C	2.60	0.45
1:A:742:ASN:O	1:A:743:VAL:C	2.59	0.45
1:A:745:GLN:HA	1:A:748:MET:HE3	1.99	0.45
1:A:746:MET:HE3	2:B:1018:PRO:HG2	1.98	0.45
1:A:834:THR:HG21	1:A:1077:THR:HA	1.99	0.45
1:A:886:ILE:HG13	1:A:943:LEU:CD1	2.46	0.45
1:A:976:THR:HG23	8:H:136:LYS:NZ	2.32	0.45
1:A:977:LYS:HB3	1:A:978:PRO:HD2	1.98	0.45
1:A:1406:VAL:O	1:A:1407:GLU:C	2.59	0.45
2:B:326:ASP:O	2:B:327:ARG:C	2.58	0.45
2:B:882:THR:HG22	2:B:884:ARG:HB2	1.99	0.45
3:C:18:VAL:HG23	3:C:240:VAL:HB	1.98	0.45
3:C:66:ARG:HH21	10:J:5:VAL:H	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:55:ARG:O	5:E:57:MET:N	2.50	0.45
5:E:124:VAL:HG13	5:E:132:ILE:CB	2.44	0.45
5:E:124:VAL:N	5:E:125:PRO:HD2	2.32	0.45
8:H:99:GLY:N	8:H:118:PHE:HD2	2.14	0.45
12:L:49:LYS:O	12:L:50:ASP:CB	2.64	0.45
1:A:58:LEU:CD1	1:A:80:HIS:H	2.29	0.45
1:A:60:SER:C	1:A:61:ILE:HG13	2.41	0.45
1:A:116:ASP:C	1:A:118:HIS:H	2.25	0.45
1:A:350:ARG:HA	1:A:487:MET:O	2.17	0.45
1:A:350:ARG:HA	1:A:468:PHE:HE1	1.81	0.45
1:A:382:PRO:HD3	1:A:428:TYR:CE2	2.51	0.45
1:A:794:PRO:C	1:A:796:SER:H	2.23	0.45
1:A:874:ASP:CA	1:A:1058:VAL:HG22	2.46	0.45
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.98	0.45
2:B:39:ARG:NH2	2:B:665:GLU:CG	2.78	0.45
2:B:197:PHE:HZ	2:B:816:GLU:HG2	1.82	0.45
2:B:283:VAL:O	2:B:284:ILE:C	2.59	0.45
3:C:161:LYS:O	3:C:170:TRP:NE1	2.49	0.45
3:C:256:ALA:C	3:C:258:ILE:N	2.74	0.45
5:E:20:LYS:O	5:E:21:GLU:C	2.59	0.45
7:G:17:PHE:C	7:G:19:GLY:H	2.24	0.45
10:J:2:ILE:HG22	10:J:3:VAL:N	2.32	0.45
1:A:40:THR:CG2	1:A:41:MET:HE2	2.47	0.45
1:A:401:GLY:O	1:A:435:HIS:CD2	2.70	0.45
1:A:417:TYR:O	1:A:418:SER:C	2.59	0.45
1:A:741:ASN:ND2	1:A:744:LYS:H	2.14	0.45
1:A:1227:ILE:HG22	1:A:1228:TRP:H	1.81	0.45
1:A:1325:THR:O	1:A:1325:THR:HG22	2.17	0.45
2:B:496:ARG:HB3	2:B:496:ARG:HH11	1.80	0.45
2:B:1033:LYS:NZ	2:B:1070:GLU:OE1	2.47	0.45
2:B:1073:TYR:OH	3:C:179:GLU:HG3	2.17	0.45
3:C:154:LYS:C	3:C:155:LEU:HD23	2.41	0.45
4:D:146:GLN:O	4:D:149:THR:HG22	2.16	0.45
4:D:162:ALA:O	4:D:163:VAL:C	2.59	0.45
5:E:85:GLU:OE2	5:E:92:THR:HG21	2.17	0.45
5:E:128:PRO:HA	5:E:129:PRO:C	2.42	0.45
7:G:59:GLY:CA	7:G:70:PHE:CD2	2.98	0.45
8:H:4:THR:HG22	8:H:5:LEU:H	1.82	0.45
8:H:61:SER:HB2	8:H:139:ASN:HB3	1.98	0.45
8:H:62:SER:C	8:H:64:ASN:N	2.69	0.45
11:K:53:ASP:C	11:K:55:LYS:N	2.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:LYS:HA	1:A:435:HIS:HD1	1.80	0.45
1:A:548:ASN:HA	11:K:60:ALA:HB1	1.99	0.45
1:A:590:ARG:HH21	1:A:620:LYS:CB	2.23	0.45
1:A:666:ILE:O	1:A:669:THR:OG1	2.31	0.45
2:B:19:GLU:O	2:B:20:ASP:C	2.60	0.45
2:B:39:ARG:HG2	2:B:39:ARG:HH11	1.82	0.45
2:B:43:LEU:HD13	2:B:812:LEU:HD23	1.99	0.45
2:B:237:VAL:HG22	2:B:257:LYS:HA	1.98	0.45
2:B:240:ILE:HG23	2:B:240:ILE:O	2.17	0.45
2:B:245:GLU:C	2:B:246:LYS:HG3	2.41	0.45
2:B:446:LEU:N	2:B:446:LEU:HD23	2.32	0.45
2:B:593:PRO:O	2:B:594:ALA:C	2.60	0.45
2:B:879:ARG:O	2:B:880:THR:HB	2.17	0.45
2:B:1152:MET:O	2:B:1153:GLU:C	2.60	0.45
2:B:1223:ASP:O	2:B:1224:PHE:HB2	2.17	0.45
3:C:8:VAL:HG12	3:C:9:LYS:H	1.82	0.45
3:C:55:THR:O	3:C:55:THR:HG22	2.16	0.45
3:C:99:LEU:CD1	3:C:118:LEU:HB3	2.43	0.45
4:D:29:LEU:O	4:D:30:GLY:C	2.59	0.45
4:D:187:THR:HG22	4:D:188:ALA:H	1.82	0.45
8:H:95:TYR:HE2	8:H:97:MET:HG3	1.77	0.45
9:I:34:TYR:HD2	9:I:35:VAL:CA	2.28	0.45
11:K:111:LEU:C	11:K:112:GLN:CG	2.88	0.45
1:A:262:LEU:C	1:A:264:PHE:H	2.24	0.45
1:A:672:ASP:O	1:A:673:GLY:C	2.60	0.45
1:A:936:LEU:O	1:A:939:ASP:HB2	2.16	0.45
1:A:1015:VAL:O	1:A:1016:THR:C	2.59	0.45
1:A:1120:LEU:HD13	1:A:1304:TRP:O	2.17	0.45
1:A:1334:ASP:C	1:A:1336:MET:N	2.73	0.45
1:A:1451:VAL:O	1:A:1454:MET:HG2	2.17	0.45
2:B:27:ALA:C	2:B:29:ASP:N	2.73	0.45
2:B:806:THR:HG21	2:B:808:ALA:HB3	1.98	0.45
2:B:948:ILE:HG22	2:B:949:VAL:O	2.16	0.45
2:B:980:PHE:CE2	2:B:1094:ARG:HG3	2.51	0.45
2:B:1031:LEU:HD23	2:B:1044:ALA:HB2	1.97	0.45
3:C:88:CYS:SG	3:C:91:HIS:HA	2.57	0.45
4:D:30:GLY:O	4:D:31:GLN:C	2.59	0.45
9:I:61:ASP:O	9:I:63:GLY:N	2.50	0.45
11:K:50:LEU:HD11	11:K:75:ILE:CD1	2.47	0.45
15:T:24:DG:H2''	15:T:25:DT:H5'	1.99	0.45
1:A:326:ARG:CG	1:A:327:ALA:N	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:PHE:HE2	1:A:375:THR:HG23	1.81	0.45
1:A:590:ARG:HB3	1:A:605:MET:N	2.31	0.45
1:A:925:LEU:C	1:A:927:VAL:N	2.75	0.45
2:B:18:PHE:N	2:B:19:GLU:N	2.65	0.45
2:B:229:ALA:HB1	2:B:231:PRO:HD2	1.99	0.45
2:B:298:LEU:HD13	2:B:314:LEU:HD13	1.98	0.45
2:B:604:ARG:C	2:B:606:LYS:H	2.25	0.45
2:B:789:MET:HE2	2:B:953:LEU:HD22	1.99	0.45
2:B:976:ILE:O	2:B:990:ILE:HB	2.16	0.45
2:B:998:ASP:HB3	2:B:1076:HIS:HE1	1.82	0.45
2:B:1106:ARG:HD3	2:B:1126:GLY:O	2.17	0.45
4:D:39:ASN:HD22	4:D:41:GLN:HB2	1.81	0.45
4:D:66:ARG:O	4:D:67:ARG:C	2.60	0.45
5:E:30:ILE:CG2	5:E:31:THR:N	2.79	0.45
7:G:87:VAL:CG2	7:G:103:VAL:HG21	2.47	0.45
7:G:99:PHE:CZ	7:G:143:ILE:HD13	2.52	0.45
11:K:98:LEU:O	11:K:101:LEU:N	2.50	0.45
12:L:30:ILE:HG22	12:L:31:CYS:N	2.32	0.45
1:A:244:PRO:O	1:A:245:PRO:C	2.60	0.44
1:A:500:GLU:O	1:A:504:LEU:HD13	2.17	0.44
1:A:1041:ALA:O	1:A:1044:TRP:HB3	2.17	0.44
2:B:189:LEU:O	2:B:192:LEU:HB2	2.16	0.44
2:B:226:PHE:CD1	2:B:398:ARG:NH2	2.85	0.44
2:B:681:TRP:C	2:B:683:SER:N	2.75	0.44
2:B:806:THR:C	2:B:808:ALA:N	2.69	0.44
2:B:834:ASN:ND2	2:B:1013:ASN:HB2	2.32	0.44
4:D:13:ARG:C	4:D:17:LYS:NZ	2.76	0.44
4:D:25:ALA:C	4:D:27:LEU:H	2.25	0.44
4:D:151:PHE:H	4:D:151:PHE:HD1	1.63	0.44
4:D:156:ASP:C	4:D:158:GLU:N	2.75	0.44
5:E:18:THR:O	5:E:19:VAL:C	2.59	0.44
7:G:106:MET:CG	7:G:107:LYS:N	2.80	0.44
7:G:117:GLN:C	7:G:119:LEU:N	2.75	0.44
1:A:174:ILE:HG22	1:A:175:ARG:N	2.33	0.44
1:A:381:THR:HG22	1:A:383:TYR:N	2.32	0.44
1:A:811:GLN:O	1:A:812:GLU:C	2.60	0.44
1:A:964:ILE:O	1:A:965:GLN:C	2.60	0.44
1:A:1132:LYS:O	1:A:1135:ARG:N	2.50	0.44
1:A:1315:GLU:C	1:A:1317:MET:N	2.71	0.44
1:A:1339:LEU:HD13	5:E:147:HIS:CD2	2.52	0.44
2:B:848:ARG:NH1	10:J:8:PHE:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:899:ILE:HD12	2:B:911:ILE:HG23	1.99	0.44
3:C:39:ALA:HA	3:C:164:ALA:CB	2.44	0.44
3:C:112:ASN:CB	3:C:114:TYR:CE1	3.00	0.44
3:C:191:TYR:HD2	3:C:201:TRP:CD1	2.34	0.44
8:H:10:PHE:HA	8:H:29:ALA:O	2.17	0.44
1:A:71:GLN:C	1:A:73:GLY:N	2.71	0.44
1:A:71:GLN:HG3	1:A:72:GLU:N	2.33	0.44
1:A:494:SER:O	1:A:497:THR:N	2.45	0.44
1:A:779:PHE:CE1	1:A:785:PRO:CD	2.93	0.44
2:B:51:PHE:CD2	2:B:173:MET:HB3	2.52	0.44
2:B:101:MET:C	2:B:102:VAL:HG23	2.42	0.44
2:B:310:MET:O	2:B:313:MET:HB2	2.18	0.44
2:B:352:ALA:O	2:B:353:LYS:C	2.61	0.44
2:B:604:ARG:NH1	2:B:691:GLU:OE2	2.50	0.44
2:B:656:GLY:O	2:B:657:HIS:C	2.60	0.44
2:B:694:ASP:O	2:B:698:GLU:HB2	2.17	0.44
2:B:766:ARG:HH22	2:B:1020:ARG:HH11	1.65	0.44
2:B:910:VAL:HG12	2:B:911:ILE:N	2.32	0.44
3:C:181:ASP:CG	3:C:186:LEU:HD13	2.42	0.44
7:G:34:VAL:O	7:G:36:GLY:N	2.51	0.44
8:H:39:THR:O	8:H:123:MET:HA	2.18	0.44
11:K:92:ASN:O	11:K:93:SER:C	2.60	0.44
12:L:61:THR:CG2	12:L:63:ARG:HG2	2.47	0.44
1:A:261:ASP:O	1:A:262:LEU:C	2.60	0.44
1:A:329:LEU:HD12	1:A:1406:VAL:HG22	2.00	0.44
1:A:474:VAL:HG22	1:A:478:TYR:CE1	2.50	0.44
1:A:679:ILE:O	1:A:683:ILE:HG13	2.17	0.44
1:A:826:ASP:HB2	1:A:830:LYS:HD3	2.00	0.44
1:A:870:GLU:HG2	5:E:208:TYR:CD2	2.52	0.44
1:A:886:ILE:HG13	1:A:943:LEU:HD12	1.99	0.44
1:A:897:TYR:HB3	1:A:936:LEU:HD12	1.99	0.44
1:A:967:ALA:HA	1:A:1044:TRP:CZ3	2.52	0.44
1:A:1410:PHE:HD2	2:B:1212:ILE:HD12	1.83	0.44
2:B:197:PHE:CZ	2:B:816:GLU:HG2	2.52	0.44
2:B:228:LYS:HB2	2:B:261:ARG:HH22	1.82	0.44
2:B:258:LEU:O	2:B:258:LEU:CG	2.64	0.44
2:B:265:SER:O	2:B:266:ALA:CB	2.65	0.44
2:B:309:GLN:CD	9:I:52:ILE:HD11	2.42	0.44
2:B:424:LEU:O	2:B:428:ILE:HG13	2.17	0.44
2:B:580:VAL:HG22	2:B:624:LEU:CB	2.45	0.44
2:B:785:TYR:CD1	2:B:786:ASN:N	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1060:ARG:C	2:B:1062:HIS:N	2.75	0.44
3:C:77:ILE:HG22	3:C:78:GLU:N	2.33	0.44
3:C:83:SER:OG	3:C:160:LYS:HD3	2.16	0.44
3:C:184:ASN:ND2	3:C:187:LYS:HA	2.32	0.44
5:E:177:ARG:HD3	5:E:215:MET:HG3	1.99	0.44
8:H:91:ASP:C	8:H:93:TYR:N	2.74	0.44
9:I:32:CYS:SG	9:I:33:SER:N	2.90	0.44
10:J:41:LEU:HD23	10:J:41:LEU:N	2.32	0.44
15:T:16:DT:C2'	15:T:17:TT:O2P	2.54	0.44
1:A:107:CYS:O	1:A:111:GLY:HA2	2.17	0.44
1:A:399:HIS:CG	1:A:400:PRO:N	2.85	0.44
1:A:715:GLU:O	1:A:716:ASP:C	2.61	0.44
1:A:744:LYS:HG2	1:A:748:MET:HE2	1.99	0.44
1:A:935:GLN:C	1:A:937:VAL:N	2.74	0.44
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	1.98	0.44
1:A:1394:THR:HG22	1:A:1395:GLY:N	2.33	0.44
2:B:45:SER:O	2:B:46:GLN:C	2.60	0.44
2:B:372:SER:O	2:B:376:PHE:HD1	2.00	0.44
2:B:597:MET:HA	2:B:597:MET:HE3	2.00	0.44
2:B:838:SER:HA	2:B:989:THR:O	2.18	0.44
2:B:844:SER:O	2:B:847:ASP:HB2	2.18	0.44
2:B:1069:PHE:CD1	2:B:1069:PHE:N	2.77	0.44
3:C:10:ILE:HG22	3:C:11:ARG:O	2.18	0.44
5:E:60:PHE:CE2	5:E:80:VAL:HB	2.53	0.44
1:A:106:VAL:HA	1:A:114:LEU:HD21	2.00	0.44
1:A:166:GLY:O	1:A:167:CYS:SG	2.76	0.44
1:A:463:ILE:HD12	1:A:469:ARG:CD	2.47	0.44
1:A:786:HIS:N	1:A:786:HIS:CD2	2.84	0.44
1:A:868:TYR:CE1	1:A:1064:VAL:CG1	2.97	0.44
1:A:940:ARG:HG2	1:A:940:ARG:NH1	2.33	0.44
1:A:979:SER:HG	1:A:981:LEU:HG	1.82	0.44
1:A:1334:ASP:C	1:A:1336:MET:H	2.26	0.44
2:B:45:SER:OG	2:B:46:GLN:N	2.47	0.44
2:B:193:LYS:HZ1	12:L:32:ALA:HB1	1.80	0.44
2:B:309:GLN:HG3	9:I:52:ILE:CD1	2.48	0.44
2:B:566:LEU:O	2:B:567:GLU:C	2.60	0.44
2:B:792:MET:H	2:B:857:ARG:HA	1.83	0.44
2:B:1000:PRO:O	2:B:1007:VAL:HG23	2.18	0.44
2:B:1001:PHE:CD1	2:B:1001:PHE:C	2.96	0.44
7:G:8:SER:HB3	7:G:73:LYS:HD2	2.00	0.44
10:J:57:ILE:CA	10:J:60:PHE:HD2	2.24	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ILE:CG2	1:A:84:ILE:HD12	2.47	0.44
1:A:91:PHE:HB2	1:A:297:GLN:HE22	1.82	0.44
1:A:666:ILE:HD11	2:B:1086:PHE:HE1	1.82	0.44
1:A:767:GLN:HA	1:A:799:PHE:HA	1.99	0.44
1:A:867:ILE:HG22	1:A:872:GLY:N	2.33	0.44
1:A:896:ARG:HH22	1:A:1030:ARG:HH21	1.65	0.44
1:A:1343:ALA:HB1	5:E:149:LEU:HB2	1.99	0.44
2:B:30:SER:HB3	2:B:743:ILE:O	2.17	0.44
2:B:327:ARG:O	2:B:331:LEU:HD13	2.18	0.44
2:B:377:PHE:CD2	2:B:381:MET:HE2	2.53	0.44
2:B:558:LEU:O	2:B:561:TRP:N	2.49	0.44
2:B:593:PRO:C	2:B:595:ARG:N	2.74	0.44
2:B:642:ASP:CB	2:B:649:LYS:HG3	2.47	0.44
2:B:948:ILE:HD12	2:B:969:ARG:HH12	1.82	0.44
3:C:38:ILE:HA	3:C:173:ALA:HB2	2.00	0.44
3:C:79:GLN:O	3:C:127:ARG:NH1	2.51	0.44
4:D:153:ARG:HB3	4:D:154:PHE:CD1	2.53	0.44
4:D:173:HIS:ND1	4:D:174:PRO:HD2	2.33	0.44
5:E:14:ARG:HH21	5:E:141:VAL:CG1	2.31	0.44
6:F:100:GLN:O	6:F:103:MET:HB2	2.18	0.44
7:G:96:GLN:HB3	7:G:121:PHE:CE2	2.53	0.44
9:I:82:GLU:HB3	9:I:104:LEU:CD1	2.48	0.44
11:K:43:GLY:HA3	11:K:61:TYR:CE1	2.52	0.44
11:K:57:LEU:N	11:K:76:GLN:O	2.51	0.44
1:A:58:LEU:HD11	1:A:243:PRO:HB2	1.96	0.44
1:A:502:SER:C	1:A:503:GLN:NE2	2.76	0.44
1:A:600:PRO:C	1:A:602:ASP:N	2.73	0.44
1:A:696:GLU:O	1:A:696:GLU:HG2	2.17	0.44
1:A:842:VAL:O	1:A:843:LYS:C	2.60	0.44
1:A:1036:ARG:HH11	1:A:1036:ARG:CG	2.31	0.44
1:A:1068:ALA:O	1:A:1069:ALA:C	2.61	0.44
1:A:1095:THR:O	1:A:1096:SER:CB	2.66	0.44
2:B:490:SER:O	2:B:491:THR:C	2.59	0.44
2:B:641:GLU:HB3	2:B:643:ASP:OD2	2.17	0.44
2:B:1110:PRO:HG3	2:B:1125:ASP:HB3	2.00	0.44
3:C:58:LEU:HD22	3:C:58:LEU:N	2.33	0.44
4:D:53:SER:HB3	4:D:153:ARG:N	2.31	0.44
4:D:170:THR:HG21	4:D:172:LEU:CD1	2.48	0.44
5:E:16:PHE:O	5:E:17:ARG:C	2.60	0.44
11:K:83:PRO:O	11:K:84:LYS:C	2.61	0.44
15:T:22:BRU:H2'	15:T:23:DG:H8	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:SER:CB	1:A:233:TRP:NE1	2.81	0.44
1:A:32:VAL:O	1:A:32:VAL:HG23	2.17	0.44
1:A:1005:GLU:O	1:A:1009:ASN:HB2	2.18	0.44
1:A:1147:THR:HA	1:A:1197:LEU:HD23	1.99	0.44
2:B:616:ILE:N	2:B:616:ILE:CD1	2.81	0.44
2:B:833:TYR:CZ	11:K:66:PRO:HG3	2.53	0.44
2:B:880:THR:HB	2:B:934:LYS:HD2	1.98	0.44
2:B:1099:VAL:HG13	2:B:1100:ASP:N	2.30	0.44
3:C:255:VAL:HG12	11:K:91:CYS:HB3	1.99	0.44
5:E:93:MET:SD	5:E:97:VAL:HG23	2.58	0.44
6:F:138:LEU:HA	6:F:138:LEU:HD23	1.74	0.44
10:J:48:ARG:HE	10:J:49:MET:HE2	1.83	0.44
12:L:48:CYS:SG	12:L:49:LYS:N	2.91	0.44
1:A:35:ILE:HG22	1:A:84:ILE:HD12	1.98	0.43
1:A:541:ILE:N	1:A:572:TRP:O	2.42	0.43
1:A:577:ILE:C	1:A:579:SER:H	2.26	0.43
1:A:682:THR:HA	1:A:685:GLU:HG2	2.00	0.43
1:A:1019:CYS:O	1:A:1022:LEU:HB3	2.18	0.43
2:B:307:ASP:O	2:B:308:TRP:C	2.61	0.43
2:B:370:PHE:HD2	2:B:373:ARG:HD2	1.83	0.43
2:B:410:GLY:O	2:B:411:PRO:C	2.61	0.43
2:B:591:ARG:O	2:B:592:ASN:C	2.60	0.43
2:B:681:TRP:O	2:B:683:SER:N	2.51	0.43
2:B:859:TYR:OH	2:B:941:LEU:CD1	2.59	0.43
3:C:69:LEU:HD12	3:C:69:LEU:H	1.79	0.43
4:D:63:LEU:O	4:D:129:LEU:HD11	2.18	0.43
5:E:191:LYS:O	5:E:193:GLY:N	2.50	0.43
7:G:1:MET:O	7:G:1:MET:CE	2.66	0.43
7:G:45:ILE:HD13	7:G:45:ILE:HA	1.88	0.43
13:N:0:DT:H71	13:N:1:DA:N6	2.33	0.43
1:A:164:ARG:CG	1:A:165:GLY:N	2.77	0.43
1:A:632:VAL:O	1:A:633:VAL:C	2.60	0.43
1:A:973:ILE:HD13	1:A:1036:ARG:O	2.17	0.43
2:B:54:PHE:O	2:B:58:THR:HB	2.17	0.43
2:B:172:ILE:CG2	2:B:173:MET:N	2.82	0.43
2:B:903:VAL:HG12	2:B:904:ARG:N	2.33	0.43
3:C:221:TYR:CE1	3:C:222:LYS:HG3	2.52	0.43
1:A:35:ILE:O	1:A:35:ILE:CG2	2.63	0.43
1:A:208:LEU:HD21	1:A:212:LYS:HE3	2.00	0.43
1:A:273:ASN:O	1:A:274:ILE:C	2.60	0.43
1:A:699:ALA:HB1	1:A:701:LEU:HG	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:821:ARG:HD2	1:A:825:ILE:CD1	2.45	0.43
1:A:1007:ILE:C	1:A:1009:ASN:N	2.74	0.43
1:A:1037:LEU:HD12	1:A:1042:PHE:HD1	1.82	0.43
1:A:1057:VAL:CG1	1:A:1058:VAL:N	2.81	0.43
1:A:1155:ASP:OD2	1:A:1161:THR:HG23	2.18	0.43
1:A:1213:GLY:O	1:A:1216:ILE:N	2.51	0.43
2:B:179:CYS:O	2:B:180:TYR:C	2.61	0.43
2:B:231:PRO:O	2:B:232:SER:HB2	2.18	0.43
2:B:235:SER:HA	2:B:261:ARG:NH1	2.33	0.43
2:B:433:GLN:O	2:B:437:GLU:HG3	2.19	0.43
2:B:758:PHE:O	2:B:759:PRO:C	2.60	0.43
2:B:908:GLU:O	2:B:909:ASP:C	2.61	0.43
2:B:1196:ILE:O	2:B:1196:ILE:HG13	2.17	0.43
3:C:53:THR:O	3:C:153:LEU:HA	2.17	0.43
4:D:29:LEU:HD13	7:G:82:PHE:CZ	2.53	0.43
5:E:61:GLN:HG2	5:E:62:ALA:N	2.33	0.43
7:G:21:ARG:HD3	7:G:21:ARG:HA	1.66	0.43
8:H:18:GLY:O	8:H:19:ARG:HB2	2.19	0.43
8:H:89:LEU:C	8:H:91:ASP:N	2.67	0.43
10:J:14:VAL:O	10:J:14:VAL:CG1	2.60	0.43
1:A:543:LEU:O	1:A:544:ASP:C	2.60	0.43
1:A:584:ASN:O	1:A:637:LYS:HE3	2.18	0.43
1:A:618:GLU:O	1:A:620:LYS:N	2.52	0.43
1:A:710:LEU:HD12	1:A:710:LEU:N	2.33	0.43
1:A:754:SER:O	1:A:755:PHE:C	2.62	0.43
1:A:795:GLU:CD	1:A:795:GLU:H	2.27	0.43
1:A:975:HIS:HA	1:A:1036:ARG:HG3	2.00	0.43
1:A:1121:GLU:O	1:A:1122:PRO:C	2.61	0.43
1:A:1211:GLN:O	1:A:1212:VAL:C	2.61	0.43
1:A:1226:VAL:HG13	1:A:1239:ARG:O	2.19	0.43
1:A:1226:VAL:HG13	1:A:1240:CYS:HB3	2.01	0.43
2:B:60:GLN:HE22	2:B:94:LYS:HA	1.82	0.43
2:B:360:PHE:CD2	2:B:361:LEU:HB2	2.53	0.43
2:B:865:LYS:C	2:B:866:TYR:CD1	2.96	0.43
3:C:94:LYS:HB2	3:C:94:LYS:HE3	1.83	0.43
3:C:124:LEU:O	3:C:125:MET:HB2	2.18	0.43
4:D:40:HIS:C	4:D:42:GLY:N	2.76	0.43
7:G:13:LEU:O	7:G:67:SER:HA	2.18	0.43
8:H:47:PHE:CD2	8:H:47:PHE:O	2.72	0.43
9:I:56:ALA:O	9:I:57:GLY:C	2.61	0.43
9:I:68:LEU:HB3	9:I:84:VAL:HG23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:53:HIS:C	10:J:53:HIS:CD2	2.96	0.43
15:T:16:DT:H73	15:T:17:TT:H5A1	1.98	0.43
1:A:108:MET:O	1:A:109:HIS:HB2	2.19	0.43
1:A:1280:GLU:O	1:A:1281:ARG:C	2.61	0.43
1:A:1364:ASN:HD22	1:A:1365:TYR:N	2.16	0.43
2:B:34:ILE:O	2:B:37:PHE:HB3	2.18	0.43
2:B:802:PRO:HB3	2:B:1091:TYR:CD2	2.53	0.43
2:B:899:ILE:HD13	2:B:905:VAL:HG11	2.00	0.43
2:B:1047:PHE:CD1	2:B:1047:PHE:N	2.76	0.43
2:B:1099:VAL:C	2:B:1101:ASP:N	2.77	0.43
2:B:1200:ALA:O	2:B:1203:LEU:HB3	2.18	0.43
3:C:123:ASN:ND2	3:C:125:MET:SD	2.91	0.43
7:G:138:THR:O	7:G:139:ILE:O	2.37	0.43
10:J:53:HIS:CD2	10:J:54:VAL:N	2.86	0.43
11:K:58:PHE:HB3	11:K:76:GLN:HB3	2.00	0.43
12:L:70:ARG:HG2	12:L:70:ARG:NH1	2.33	0.43
15:T:11:DG:H2"	15:T:12:DT:OP2	2.18	0.43
15:T:16:DT:C7	15:T:17:TT:C5A	2.93	0.43
1:A:89:PRO:HB3	1:A:208:LEU:HD12	2.00	0.43
1:A:406:ILE:HG13	1:A:431:LYS:HB2	2.00	0.43
1:A:450:LEU:HB3	1:A:838:GLN:HE21	1.79	0.43
1:A:509:LEU:HD23	1:A:509:LEU:HA	1.81	0.43
1:A:727:ASP:C	1:A:729:ALA:N	2.76	0.43
1:A:755:PHE:O	1:A:756:ILE:C	2.61	0.43
1:A:897:TYR:N	1:A:897:TYR:CD1	2.87	0.43
1:A:1130:GLN:O	1:A:1134:ILE:HG13	2.19	0.43
1:A:1349:TYR:O	1:A:1350:LYS:C	2.60	0.43
1:A:1350:LYS:O	1:A:1354:ASN:ND2	2.52	0.43
1:A:1437:GLY:O	1:A:1438:THR:C	2.61	0.43
1:A:1444:MET:HE3	1:A:1444:MET:HB2	1.93	0.43
2:B:39:ARG:HG2	2:B:39:ARG:NH1	2.34	0.43
2:B:644:GLU:C	2:B:646:LEU:H	2.27	0.43
2:B:798:TYR:HE2	3:C:62:PHE:CE2	2.35	0.43
2:B:865:LYS:NZ	2:B:869:SER:HA	2.34	0.43
2:B:980:PHE:HD2	2:B:1094:ARG:HA	1.84	0.43
2:B:980:PHE:HE2	2:B:1094:ARG:CG	2.31	0.43
3:C:47:ASP:HA	3:C:169:LYS:HZ2	1.83	0.43
4:D:153:ARG:C	4:D:154:PHE:CG	2.96	0.43
8:H:82:PRO:C	8:H:84:ALA:N	2.77	0.43
11:K:58:PHE:HB3	11:K:76:GLN:HE21	1.83	0.43
11:K:85:ASP:O	11:K:86:ALA:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ARG:CZ	2:B:1192:TYR:HE2	2.31	0.43
1:A:43:GLU:O	1:A:44:THR:HB	2.19	0.43
1:A:402:ALA:HB1	1:A:433:GLU:O	2.19	0.43
1:A:427:GLN:HB2	1:A:430:TRP:CE2	2.53	0.43
1:A:623:GLY:C	1:A:625:SER:H	2.27	0.43
1:A:742:ASN:O	1:A:745:GLN:N	2.52	0.43
1:A:826:ASP:O	1:A:827:THR:C	2.60	0.43
1:A:1116:LEU:C	1:A:1116:LEU:HD12	2.42	0.43
2:B:90:ILE:HD11	2:B:432:MET:SD	2.59	0.43
2:B:329:THR:O	2:B:332:ASP:HB3	2.19	0.43
2:B:472:ALA:C	2:B:474:SER:H	2.17	0.43
2:B:546:SER:OG	2:B:631:GLY:N	2.43	0.43
2:B:603:LEU:HD13	2:B:608:ASP:CB	2.45	0.43
2:B:618:ASP:O	2:B:619:ILE:C	2.61	0.43
2:B:1106:ARG:NH1	2:B:1110:PRO:CD	2.81	0.43
3:C:67:LEU:HD11	3:C:155:LEU:HD12	1.99	0.43
3:C:83:SER:O	3:C:85:ASP:N	2.52	0.43
3:C:120:ILE:HD13	3:C:124:LEU:HD21	2.01	0.43
4:D:14:ARG:O	4:D:15:LEU:HB3	2.19	0.43
4:D:52:LEU:C	4:D:54:GLU:N	2.76	0.43
5:E:157:SER:OG	5:E:159:ASP:HB2	2.17	0.43
11:K:88:LYS:O	11:K:91:CYS:N	2.47	0.43
1:A:75:ASN:O	1:A:76:GLU:HB2	2.19	0.43
1:A:96:ILE:O	1:A:97:ALA:C	2.62	0.43
1:A:494:SER:O	1:A:495:GLU:C	2.62	0.43
1:A:907:THR:HG23	1:A:908:LEU:N	2.33	0.43
1:A:1291:VAL:CG1	1:A:1292:PRO:N	2.81	0.43
2:B:114:PRO:O	2:B:115:GLN:C	2.61	0.43
2:B:299:GLU:HB3	2:B:571:PRO:HG3	1.99	0.43
2:B:336:ARG:NH2	2:B:345:LYS:CE	2.78	0.43
2:B:552:MET:C	2:B:554:ILE:H	2.26	0.43
2:B:654:ARG:HG3	2:B:654:ARG:HH11	1.83	0.43
2:B:784:ASN:O	2:B:788:ARG:HG3	2.19	0.43
2:B:842:ASN:O	2:B:846:ILE:HG13	2.19	0.43
3:C:70:ILE:HD11	3:C:144:ILE:HG12	2.01	0.43
3:C:141:GLY:HA2	10:J:16:ASP:HB3	2.00	0.43
4:D:59:ILE:O	4:D:60:LYS:C	2.60	0.43
4:D:176:GLU:C	4:D:178:ALA:N	2.61	0.43
4:D:193:THR:O	4:D:196:PRO:HD3	2.19	0.43
5:E:9:ILE:HD11	5:E:53:PRO:HD3	2.01	0.43
9:I:59:VAL:C	9:I:61:ASP:N	2.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ILE:HD13	1:A:241:VAL:HG21	2.00	0.43
1:A:56:PRO:O	1:A:57:ARG:HG3	2.19	0.43
1:A:260:ASP:O	1:A:261:ASP:C	2.61	0.43
1:A:899:VAL:CG1	1:A:908:LEU:HD21	2.49	0.43
1:A:984:LYS:O	1:A:985:ASP:C	2.61	0.43
1:A:1163:ILE:CG2	1:A:1164:PRO:HD2	2.49	0.43
2:B:460:ALA:C	2:B:462:ALA:N	2.77	0.43
2:B:726:ALA:O	2:B:727:LYS:O	2.36	0.43
2:B:1007:VAL:HG22	2:B:1008:PRO:CD	2.36	0.43
2:B:1106:ARG:HH12	2:B:1110:PRO:CG	2.31	0.43
2:B:1115:THR:HG21	2:B:1117:GLN:CD	2.44	0.43
3:C:262:LEU:HD23	3:C:262:LEU:HA	1.84	0.43
4:D:138:ASN:C	4:D:140:ASP:N	2.77	0.43
8:H:27:GLU:HG2	8:H:39:THR:HG23	2.00	0.43
8:H:116:TYR:HB2	8:H:123:MET:HB3	2.00	0.43
9:I:85:PHE:CD1	9:I:99:LEU:HD13	2.54	0.43
1:A:414:ASP:OD1	1:A:414:ASP:C	2.62	0.43
1:A:603:ASN:O	1:A:604:GLY:C	2.62	0.43
1:A:662:PHE:HB3	2:B:829:CYS:HB2	2.01	0.43
1:A:682:THR:HG23	1:A:728:LYS:CE	2.49	0.43
1:A:817:ALA:O	1:A:820:GLY:N	2.52	0.43
1:A:1212:VAL:O	1:A:1216:ILE:HG13	2.19	0.43
1:A:1220:PHE:O	1:A:1221:LYS:HB2	2.18	0.43
1:A:1327:ILE:HG22	5:E:147:HIS:CE1	2.54	0.43
1:A:1348:LEU:CG	1:A:1372:VAL:HG22	2.47	0.43
1:A:1377:THR:O	1:A:1378:GLN:C	2.61	0.43
2:B:809:MET:O	2:B:812:LEU:N	2.49	0.43
2:B:821:GLN:HE22	2:B:851:PHE:N	2.17	0.43
2:B:1072:MET:CE	2:B:1087:PHE:HD1	2.32	0.43
2:B:1084:GLN:OE1	3:C:189:THR:CG2	2.67	0.43
3:C:170:TRP:O	3:C:171:GLY:C	2.59	0.43
5:E:177:ARG:HD3	5:E:215:MET:HG2	2.01	0.43
7:G:77:VAL:O	7:G:77:VAL:HG12	2.16	0.43
15:T:26:DC:C2'	15:T:27:DA:O5'	2.67	0.43
1:A:34:LYS:NZ	1:A:57:ARG:NH1	2.66	0.42
1:A:230:ARG:O	1:A:231:PRO:C	2.61	0.42
1:A:908:LEU:CD1	1:A:983:ILE:HD11	2.49	0.42
1:A:1193:LEU:HD22	1:A:1260:LEU:CD1	2.47	0.42
1:A:1446:ASP:HB2	6:F:133:VAL:CG2	2.49	0.42
2:B:54:PHE:HA	2:B:58:THR:HB	2.01	0.42
2:B:460:ALA:O	2:B:462:ALA:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:579:ARG:N	2:B:589:VAL:HG13	2.34	0.42
2:B:641:GLU:C	2:B:643:ASP:N	2.76	0.42
2:B:1138:MET:HE3	2:B:1143:ALA:HB3	2.01	0.42
3:C:187:LYS:C	3:C:189:THR:N	2.77	0.42
3:C:216:GLY:O	3:C:217:ASP:C	2.62	0.42
5:E:9:ILE:C	5:E:11:ARG:N	2.76	0.42
6:F:88:TYR:CD1	6:F:88:TYR:N	2.87	0.42
8:H:59:ILE:O	8:H:60:ALA:HB3	2.18	0.42
1:A:12:ARG:NE	2:B:1192:TYR:CE2	2.83	0.42
1:A:34:LYS:CB	1:A:36:ARG:HH21	2.31	0.42
1:A:211:PHE:O	1:A:212:LYS:C	2.62	0.42
1:A:276:LEU:O	1:A:279:LEU:HB2	2.19	0.42
1:A:407:ARG:HG2	1:A:430:TRP:CZ2	2.54	0.42
1:A:665:GLY:C	1:A:667:GLY:N	2.76	0.42
1:A:742:ASN:O	1:A:745:GLN:HB2	2.18	0.42
1:A:867:ILE:CG2	1:A:872:GLY:N	2.82	0.42
1:A:1053:PHE:O	1:A:1055:ARG:N	2.53	0.42
1:A:1225:PHE:HE2	1:A:1227:ILE:HD11	1.84	0.42
2:B:312:GLU:O	2:B:315:LYS:HB2	2.20	0.42
2:B:487:THR:O	2:B:490:SER:HB3	2.19	0.42
2:B:604:ARG:O	2:B:606:LYS:N	2.52	0.42
2:B:952:VAL:HG12	2:B:953:LEU:N	2.34	0.42
2:B:1159:ARG:NE	2:B:1193:GLN:HE21	2.15	0.42
4:D:7:THR:HB	7:G:42:PHE:CZ	2.54	0.42
4:D:50:LEU:HD11	4:D:58:VAL:HG21	2.01	0.42
5:E:116:ILE:HG22	5:E:117:THR:N	2.34	0.42
6:F:93:ILE:HD11	6:F:134:ILE:CD1	2.40	0.42
6:F:118:LEU:O	6:F:122:MET:HG3	2.18	0.42
1:A:58:LEU:HG	1:A:244:PRO:HD2	2.00	0.42
1:A:218:ASP:HA	1:A:221:SER:OG	2.19	0.42
1:A:332:LYS:HA	1:A:337:ARG:HD2	2.02	0.42
1:A:353:ILE:HD11	1:A:480:ALA:HB1	2.00	0.42
1:A:709:THR:HG21	9:I:93:LYS:O	2.18	0.42
1:A:731:ARG:O	1:A:735:VAL:HG23	2.18	0.42
1:A:858:ASN:HD22	1:A:861:GLY:H	1.67	0.42
1:A:897:TYR:HD2	1:A:936:LEU:CD1	2.30	0.42
1:A:1225:PHE:CE2	1:A:1227:ILE:HD11	2.54	0.42
1:A:1336:MET:HE2	1:A:1381:LEU:HG	1.98	0.42
1:A:1373:ASP:O	1:A:1376:THR:N	2.49	0.42
1:A:1445:ILE:HD12	7:G:59:GLY:O	2.19	0.42
2:B:102:VAL:HG12	2:B:104:GLU:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:196:PRO:HG2	2:B:197:PHE:N	2.34	0.42
2:B:521:LEU:HD13	2:B:633:VAL:HB	2.01	0.42
2:B:792:MET:HE2	2:B:857:ARG:NH2	2.34	0.42
3:C:20:PHE:CE1	3:C:22:LEU:HD12	2.54	0.42
3:C:116:LYS:HD3	3:C:140:ASN:HB3	2.01	0.42
3:C:179:GLU:O	3:C:180:TYR:HB3	2.18	0.42
5:E:90:VAL:HG23	5:E:120:ALA:HA	2.02	0.42
6:F:120:ILE:O	6:F:123:LYS:HB3	2.19	0.42
7:G:91:VAL:HG23	7:G:141:SER:O	2.18	0.42
7:G:106:MET:HG2	7:G:107:LYS:N	2.33	0.42
7:G:137:ILE:HG21	7:G:143:ILE:HD11	2.01	0.42
8:H:31:THR:O	8:H:31:THR:HG22	2.18	0.42
8:H:55:LEU:HD22	8:H:144:ILE:HG21	2.00	0.42
11:K:84:LYS:O	11:K:87:LEU:HB3	2.19	0.42
12:L:61:THR:HG22	12:L:63:ARG:HG2	2.02	0.42
1:A:231:PRO:C	1:A:233:TRP:H	2.28	0.42
1:A:299:HIS:C	1:A:301:ALA:N	2.73	0.42
1:A:388:LEU:O	1:A:392:VAL:HG23	2.19	0.42
1:A:407:ARG:HG2	1:A:430:TRP:CH2	2.54	0.42
1:A:437:MET:O	1:A:438:ASP:C	2.62	0.42
1:A:848:ILE:HA	1:A:857:ARG:O	2.20	0.42
2:B:419:THR:O	2:B:419:THR:HG22	2.19	0.42
2:B:582:VAL:HG12	2:B:582:VAL:O	2.19	0.42
2:B:769:TYR:O	2:B:770:GLN:C	2.61	0.42
2:B:778:MET:SD	2:B:794:ASN:HB3	2.59	0.42
2:B:873:THR:HG22	2:B:874:PHE:N	2.34	0.42
2:B:1169:MET:O	2:B:1170:THR:C	2.61	0.42
2:B:1187:ASN:OD1	2:B:1189:ILE:N	2.43	0.42
3:C:98:VAL:C	3:C:99:LEU:CD2	2.93	0.42
3:C:144:ILE:O	3:C:145:CYS:HB3	2.19	0.42
3:C:239:PRO:O	3:C:241:ASP:N	2.53	0.42
4:D:40:HIS:CG	4:D:41:GLN:N	2.87	0.42
5:E:63:ASN:HA	5:E:64:PRO:HD3	1.86	0.42
6:F:98:ALA:O	6:F:99:LEU:C	2.62	0.42
8:H:127:GLY:O	8:H:128:ASN:CB	2.65	0.42
10:J:13:VAL:O	10:J:14:VAL:HG23	2.19	0.42
10:J:48:ARG:HD2	10:J:48:ARG:C	2.45	0.42
13:N:4:DT:H5'	13:N:4:DT:C6	2.55	0.42
15:T:17:TT:H1'	15:T:17:TT:C5R	2.48	0.42
1:A:283:GLY:O	1:A:285:PRO:CD	2.68	0.42
1:A:499:ALA:O	1:A:503:GLN:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:ASP:O	1:A:527:THR:C	2.61	0.42
1:A:723:ASN:O	1:A:725:ALA:N	2.53	0.42
1:A:849:MET:HE3	1:A:1061:GLY:O	2.19	0.42
1:A:935:GLN:O	1:A:938:LYS:N	2.52	0.42
1:A:1100:ARG:NH2	1:A:1351:GLU:CG	2.81	0.42
1:A:1283:VAL:CG1	1:A:1284:MET:N	2.80	0.42
2:B:294:ASP:O	2:B:296:GLU:N	2.49	0.42
2:B:365:THR:HG23	2:B:367:LEU:CG	2.45	0.42
2:B:377:PHE:C	2:B:379:GLY:N	2.76	0.42
2:B:582:VAL:O	2:B:582:VAL:CG1	2.67	0.42
2:B:610:ASN:O	2:B:612:GLU:N	2.52	0.42
2:B:640:VAL:HB	2:B:738:PHE:O	2.20	0.42
2:B:986:GLN:OE1	2:B:986:GLN:HA	2.19	0.42
2:B:1023:VAL:O	2:B:1026:LEU:HB2	2.20	0.42
3:C:208:GLU:C	3:C:210:GLU:N	2.75	0.42
4:D:131:GLU:O	4:D:132:GLN:HG2	2.19	0.42
5:E:168:TYR:CB	5:E:170:LEU:HG	2.49	0.42
7:G:98:GLY:HA3	7:G:110:VAL:O	2.20	0.42
11:K:95:ILE:O	11:K:98:LEU:N	2.53	0.42
15:T:16:DT:C6	15:T:17:TT:C5A	2.92	0.42
1:A:24:PRO:O	1:A:28:ARG:HG3	2.19	0.42
1:A:218:ASP:O	1:A:219:PHE:C	2.60	0.42
1:A:219:PHE:CE2	1:A:231:PRO:HD2	2.54	0.42
1:A:288:ALA:HA	1:A:291:GLU:OE2	2.20	0.42
1:A:340:LEU:HD23	2:B:1199:ALA:HB3	2.01	0.42
1:A:402:ALA:HB1	1:A:434:ARG:HA	2.02	0.42
1:A:482:PHE:O	1:A:484:GLY:N	2.48	0.42
1:A:586:ILE:CD1	1:A:633:VAL:HG22	2.50	0.42
1:A:857:ARG:HD3	1:A:861:GLY:O	2.20	0.42
1:A:1365:TYR:O	1:A:1366:ARG:C	2.62	0.42
1:A:1423:GLY:O	1:A:1426:GLU:HB2	2.20	0.42
2:B:101:MET:O	2:B:102:VAL:CG2	2.68	0.42
2:B:604:ARG:O	2:B:607:GLY:N	2.53	0.42
2:B:758:PHE:HB2	2:B:1024:ALA:HB1	2.01	0.42
2:B:844:SER:O	2:B:845:SER:C	2.63	0.42
2:B:984:HIS:NE2	2:B:1025:HIS:HA	2.34	0.42
3:C:20:PHE:HE1	3:C:22:LEU:HD12	1.83	0.42
3:C:22:LEU:HD13	3:C:230:MET:HE3	2.02	0.42
6:F:89:GLU:O	6:F:90:ARG:C	2.62	0.42
8:H:102:TYR:CE2	8:H:117:SER:HB2	2.54	0.42
10:J:57:ILE:O	10:J:60:PHE:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ASN:OD1	2:B:884:ARG:HD2	2.20	0.42
1:A:322:VAL:O	1:A:322:VAL:HG12	2.16	0.42
1:A:507:VAL:N	1:A:508:PRO:CD	2.82	0.42
1:A:767:GLN:HB2	1:A:799:PHE:HD1	1.84	0.42
1:A:1402:PHE:O	1:A:1402:PHE:CG	2.73	0.42
2:B:128:LEU:HB2	2:B:168:GLY:O	2.20	0.42
2:B:223:VAL:HG21	2:B:380:TYR:HE2	1.85	0.42
2:B:300:HIS:CE1	2:B:376:PHE:CE1	3.07	0.42
2:B:336:ARG:NE	2:B:348:ARG:HH11	2.17	0.42
2:B:488:TYR:O	2:B:489:SER:C	2.62	0.42
2:B:542:MET:HB3	2:B:636:PRO:HD2	2.01	0.42
2:B:769:TYR:O	2:B:771:SER:N	2.52	0.42
2:B:970:THR:HG22	2:B:971:THR:N	2.35	0.42
3:C:235:VAL:HG13	10:J:13:VAL:CG2	2.50	0.42
4:D:119:ARG:HD3	4:D:221:TYR:CD2	2.55	0.42
4:D:163:VAL:O	4:D:166:LEU:HB3	2.19	0.42
5:E:154:ILE:H	5:E:196:VAL:HG13	1.84	0.42
6:F:150:GLU:O	6:F:151:LEU:C	2.61	0.42
8:H:62:SER:HB2	8:H:64:ASN:HD22	1.83	0.42
9:I:7:CYS:HB2	9:I:34:TYR:CD1	2.54	0.42
10:J:8:PHE:N	10:J:49:MET:HE3	2.33	0.42
11:K:30:ALA:HA	11:K:75:ILE:O	2.20	0.42
1:A:47:ARG:O	1:A:48:ALA:HB2	2.20	0.42
1:A:55:ASP:HA	1:A:58:LEU:HB3	2.02	0.42
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.99	0.42
1:A:242:PRO:HD3	2:B:1209:ALA:HB1	2.02	0.42
1:A:503:GLN:HB2	1:A:504:LEU:HD12	2.00	0.42
1:A:574:GLY:C	1:A:576:GLN:N	2.77	0.42
1:A:657:LEU:O	1:A:657:LEU:HD12	2.20	0.42
1:A:1115:SER:O	1:A:1116:LEU:HB3	2.20	0.42
1:A:1334:ASP:O	1:A:1337:GLU:N	2.52	0.42
1:A:1396:ALA:O	1:A:1397:LEU:C	2.63	0.42
2:B:179:CYS:O	2:B:181:LEU:N	2.52	0.42
2:B:185:THR:O	2:B:188:ASP:HB2	2.20	0.42
2:B:570:VAL:HA	2:B:571:PRO:HD2	1.73	0.42
2:B:807:ARG:O	2:B:811:TYR:HE1	2.01	0.42
2:B:1072:MET:O	2:B:1081:LEU:HG	2.19	0.42
2:B:1197:PRO:O	2:B:1198:TYR:C	2.62	0.42
3:C:97:VAL:HG11	3:C:130:GLY:HA3	2.01	0.42
3:C:105:GLY:O	3:C:149:LYS:O	2.38	0.42
3:C:173:ALA:O	3:C:174:ALA:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:14:HIS:O	7:G:15:PRO:C	2.63	0.42
7:G:20:PRO:CD	7:G:21:ARG:H	2.32	0.42
15:T:17:TT:H2R2	15:T:17:TT:H2'1	2.02	0.42
1:A:470:LEU:HD22	1:A:487:MET:HE3	2.02	0.42
1:A:1032:LEU:O	1:A:1036:ARG:HD3	2.20	0.42
1:A:1208:THR:O	1:A:1209:MET:C	2.62	0.42
2:B:33:VAL:HG12	2:B:681:TRP:HZ3	1.85	0.42
2:B:281:PRO:O	2:B:282:ILE:C	2.62	0.42
2:B:386:LEU:O	2:B:388:CYS:N	2.53	0.42
2:B:798:TYR:CE2	3:C:62:PHE:HZ	2.33	0.42
2:B:1196:ILE:HD12	2:B:1200:ALA:HB3	2.01	0.42
3:C:69:LEU:CD1	3:C:69:LEU:H	2.33	0.42
3:C:101:LEU:HD13	3:C:118:LEU:CD2	2.31	0.42
3:C:174:ALA:O	3:C:175:ALA:CB	2.67	0.42
4:D:195:ILE:HG22	4:D:198:LEU:HG	2.01	0.42
5:E:22:MET:HE3	5:E:26:ARG:CZ	2.50	0.42
5:E:29:PHE:O	5:E:30:ILE:CG1	2.66	0.42
6:F:116:ASP:OD1	6:F:116:ASP:C	2.63	0.42
8:H:91:ASP:O	8:H:93:TYR:N	2.52	0.42
1:A:14:VAL:HG21	2:B:1216:LEU:CD1	2.36	0.42
1:A:204:THR:O	1:A:206:GLU:N	2.53	0.42
1:A:606:LEU:O	1:A:613:ILE:HB	2.20	0.42
1:A:608:ILE:HG13	1:A:613:ILE:HD12	2.01	0.42
1:A:682:THR:O	1:A:682:THR:HG22	2.20	0.42
1:A:699:ALA:O	1:A:700:ASN:HB3	2.19	0.42
1:A:722:LEU:HD22	1:A:799:PHE:CG	2.55	0.42
1:A:1017:LEU:HB2	5:E:205:SER:HA	2.01	0.42
1:A:1280:GLU:O	1:A:1281:ARG:O	2.38	0.42
2:B:176:SER:O	2:B:182:SER:HB3	2.20	0.42
2:B:258:LEU:C	2:B:258:LEU:HD12	2.45	0.42
2:B:278:GLN:HE22	2:B:337:ARG:HH21	1.67	0.42
2:B:806:THR:HG22	2:B:808:ALA:HB3	2.02	0.42
2:B:842:ASN:ND2	2:B:845:SER:OG	2.53	0.42
2:B:1074:ASN:OD1	2:B:1076:HIS:N	2.53	0.42
3:C:18:VAL:O	3:C:20:PHE:CD2	2.70	0.42
3:C:204:SER:C	3:C:206:ASN:H	2.28	0.42
3:C:236:GLY:C	3:C:238:ILE:H	2.27	0.42
4:D:122:GLU:HA	4:D:125:SER:OG	2.19	0.42
4:D:141:LEU:HD12	4:D:141:LEU:HA	1.79	0.42
5:E:46:TYR:CE2	5:E:58:MET:HA	2.55	0.42
8:H:95:TYR:CE2	8:H:97:MET:CG	2.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:98:TYR:C	8:H:98:TYR:CD1	2.95	0.42
10:J:19:GLU:O	10:J:23:ASN:HB2	2.20	0.42
11:K:49:GLU:OE2	11:K:97:LYS:HE3	2.20	0.42
12:L:55:ILE:O	12:L:56:LEU:HB2	2.19	0.42
1:A:471:ASN:OD1	1:A:471:ASN:C	2.63	0.41
1:A:483:ASP:HA	2:B:988:GLY:HA2	2.01	0.41
1:A:498:ARG:O	1:A:499:ALA:C	2.61	0.41
1:A:846:GLU:HB2	1:A:847:ASP:H	1.73	0.41
1:A:869:GLY:O	1:A:870:GLU:HB2	2.19	0.41
1:A:1340:GLY:O	1:A:1341:ILE:C	2.63	0.41
2:B:100:PRO:CD	2:B:180:TYR:HE1	2.26	0.41
2:B:114:PRO:C	2:B:116:GLU:N	2.77	0.41
2:B:364:ILE:CG1	2:B:585:VAL:HG13	2.33	0.41
2:B:882:THR:HG21	2:B:935:ARG:HA	2.01	0.41
2:B:1034:VAL:C	2:B:1036:ALA:H	2.27	0.41
2:B:1177:HIS:C	2:B:1179:GLN:N	2.78	0.41
3:C:174:ALA:O	10:J:10:CYS:O	2.37	0.41
3:C:179:GLU:CG	3:C:180:TYR:N	2.79	0.41
4:D:180:LEU:HD23	4:D:180:LEU:HA	1.78	0.41
7:G:20:PRO:CG	7:G:21:ARG:N	2.83	0.41
7:G:24:GLN:O	7:G:25:TYR:C	2.61	0.41
8:H:128:ASN:O	8:H:128:ASN:OD1	2.37	0.41
9:I:80:SER:OG	9:I:105:SER:HB2	2.19	0.41
10:J:13:VAL:C	10:J:14:VAL:CG2	2.93	0.41
1:A:49:LYS:HZ2	1:A:60:SER:HA	1.84	0.41
1:A:230:ARG:N	1:A:233:TRP:HE3	2.11	0.41
1:A:244:PRO:HG2	1:A:245:PRO:CD	2.49	0.41
1:A:516:SER:O	1:A:517:ASN:C	2.63	0.41
1:A:562:THR:HA	1:A:563:PRO:HD3	1.85	0.41
1:A:600:PRO:O	1:A:602:ASP:N	2.53	0.41
1:A:661:GLY:O	1:A:662:PHE:HB2	2.20	0.41
1:A:1116:LEU:HB2	1:A:1329:THR:OG1	2.20	0.41
2:B:549:THR:CG2	2:B:550:ASP:H	2.15	0.41
2:B:999:MET:HE2	2:B:1011:ILE:HD11	2.00	0.41
2:B:1216:LEU:HD23	2:B:1216:LEU:N	2.35	0.41
4:D:14:ARG:N	4:D:17:LYS:HZ3	2.18	0.41
4:D:177:VAL:O	4:D:177:VAL:HG12	2.21	0.41
4:D:195:ILE:C	4:D:197:SER:N	2.78	0.41
5:E:84:ASP:O	5:E:86:PRO:HD3	2.21	0.41
8:H:43:ASN:CG	8:H:46:LEU:HG	2.46	0.41
1:A:336:ILE:HG22	1:A:337:ARG:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:ARG:NH2	2:B:1108:ARG:HH12	2.17	0.41
1:A:699:ALA:HB3	1:A:701:LEU:HG	2.01	0.41
1:A:988:LEU:HA	1:A:988:LEU:HD23	1.85	0.41
1:A:1170:ILE:H	1:A:1170:ILE:HG13	1.50	0.41
1:A:1209:MET:O	1:A:1210:GLY:C	2.63	0.41
2:B:27:ALA:C	2:B:29:ASP:H	2.29	0.41
2:B:244:LEU:O	2:B:246:LYS:N	2.54	0.41
2:B:251:ILE:O	2:B:251:ILE:HG22	2.19	0.41
2:B:554:ILE:O	2:B:554:ILE:HG22	2.20	0.41
2:B:597:MET:C	2:B:599:THR:N	2.75	0.41
2:B:604:ARG:NH2	2:B:613:VAL:O	2.54	0.41
2:B:661:LEU:C	2:B:663:ALA:N	2.78	0.41
2:B:758:PHE:HE1	2:B:1027:ILE:HG22	1.82	0.41
2:B:834:ASN:HA	2:B:838:SER:O	2.20	0.41
2:B:1001:PHE:C	2:B:1072:MET:HG2	2.45	0.41
2:B:1181:GLU:O	2:B:1182:CYS:HB2	2.20	0.41
3:C:31:ASN:ND2	3:C:35:ARG:HD2	2.35	0.41
4:D:29:LEU:HD22	7:G:82:PHE:CD2	2.55	0.41
6:F:82:THR:HA	6:F:83:PRO:HD3	1.74	0.41
6:F:96:THR:O	6:F:99:LEU:HB3	2.20	0.41
8:H:62:SER:O	8:H:64:ASN:N	2.50	0.41
10:J:64:ASN:ND2	10:J:65:PRO:HD3	2.35	0.41
1:A:68:GLN:C	1:A:70:CYS:N	2.62	0.41
1:A:91:PHE:HB2	1:A:297:GLN:NE2	2.35	0.41
1:A:92:HIS:CD2	1:A:304:MET:HE1	2.50	0.41
1:A:167:CYS:SG	1:A:167:CYS:O	2.78	0.41
1:A:274:ILE:O	1:A:275:SER:C	2.63	0.41
1:A:418:SER:C	1:A:420:ARG:N	2.78	0.41
1:A:537:ARG:HH12	8:H:122:LEU:HG	1.86	0.41
1:A:730:GLY:C	1:A:732:LEU:N	2.77	0.41
1:A:866:PHE:HE1	5:E:211:TYR:H	1.67	0.41
1:A:899:VAL:CG2	1:A:1029:ARG:HG2	2.51	0.41
1:A:1376:THR:HG23	1:A:1377:THR:H	1.86	0.41
2:B:96:TYR:HB2	2:B:129:PHE:HB2	2.03	0.41
2:B:203:PHE:N	2:B:203:PHE:CD1	2.88	0.41
2:B:237:VAL:CG1	2:B:238:ALA:N	2.82	0.41
2:B:280:ILE:CG2	2:B:285:ILE:HG13	2.50	0.41
2:B:728:ARG:HH12	2:B:1047:PHE:HB3	1.84	0.41
2:B:828:ALA:HB2	2:B:1085:ILE:HG23	2.01	0.41
2:B:1214:PRO:HG2	2:B:1214:PRO:O	2.21	0.41
3:C:82:TYR:CD1	3:C:161:LYS:HD3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:118:THR:HG22	4:D:118:THR:O	2.20	0.41
4:D:135:GLY:O	4:D:137:ASN:N	2.53	0.41
5:E:42:PHE:O	5:E:43:LYS:C	2.63	0.41
5:E:58:MET:O	5:E:59:SER:C	2.63	0.41
6:F:82:THR:HG22	6:F:84:TYR:N	2.23	0.41
6:F:147:SER:O	6:F:148:VAL:C	2.63	0.41
7:G:34:VAL:O	7:G:35:GLU:C	2.61	0.41
7:G:115:MET:CB	7:G:116:PRO:CD	2.99	0.41
1:A:18:GLN:H	2:B:1215:ARG:HB2	1.85	0.41
1:A:283:GLY:O	1:A:285:PRO:HD3	2.20	0.41
1:A:341:MET:HE2	1:A:843:LYS:HZ3	1.73	0.41
1:A:408:ASP:O	1:A:410:GLY:N	2.45	0.41
1:A:497:THR:O	1:A:498:ARG:C	2.63	0.41
1:A:527:THR:HG21	1:A:650:GLN:HG2	2.02	0.41
1:A:608:ILE:CG1	1:A:613:ILE:HD12	2.51	0.41
1:A:767:GLN:HE21	1:A:774:ARG:HB3	1.85	0.41
1:A:826:ASP:OD1	1:A:827:THR:N	2.53	0.41
1:A:867:ILE:O	1:A:868:TYR:C	2.63	0.41
1:A:958:VAL:HG22	1:A:1052:GLN:HB3	2.03	0.41
1:A:1118:VAL:O	1:A:1305:VAL:HG13	2.20	0.41
2:B:54:PHE:CE2	2:B:59:LEU:HD13	2.56	0.41
2:B:120:ARG:HG2	2:B:955:THR:HG21	2.02	0.41
2:B:234:ILE:O	2:B:261:ARG:NH2	2.53	0.41
2:B:312:GLU:O	2:B:313:MET:C	2.63	0.41
2:B:467:GLY:CA	2:B:475:SER:HB3	2.50	0.41
2:B:542:MET:HB3	2:B:636:PRO:CD	2.48	0.41
2:B:555:ILE:HD11	2:B:587:HIS:CE1	2.55	0.41
2:B:758:PHE:N	2:B:759:PRO:CD	2.83	0.41
3:C:18:VAL:CG2	3:C:240:VAL:HB	2.51	0.41
3:C:87:PHE:H	3:C:87:PHE:HD1	1.66	0.41
5:E:78:LEU:HD21	5:E:80:VAL:CG2	2.44	0.41
8:H:42:ILE:HG23	8:H:95:TYR:CE1	2.47	0.41
8:H:123:MET:HE1	8:H:142:LEU:CD1	2.50	0.41
9:I:55:THR:HG21	9:I:109:ILE:HD13	2.02	0.41
1:A:284:ALA:O	1:A:286:HIS:N	2.45	0.41
1:A:472:LEU:O	1:A:475:THR:CB	2.63	0.41
1:A:568:PRO:HG2	1:A:569:LYS:H	1.85	0.41
1:A:909:ASP:C	1:A:911:SER:N	2.77	0.41
2:B:29:ASP:CB	2:B:658:ILE:HD13	2.48	0.41
2:B:129:PHE:HE2	2:B:166:PHE:CD1	2.37	0.41
2:B:240:ILE:HG23	2:B:254:LEU:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:247:GLY:C	2:B:249:ARG:N	2.76	0.41
2:B:303:TYR:N	2:B:303:TYR:CD2	2.87	0.41
2:B:324:ILE:HD13	2:B:330:ALA:HA	2.03	0.41
2:B:805:THR:HB	2:B:809:MET:SD	2.60	0.41
2:B:1069:PHE:O	2:B:1070:GLU:HG2	2.19	0.41
2:B:1074:ASN:OD1	2:B:1074:ASN:C	2.63	0.41
2:B:1187:ASN:HD21	2:B:1190:ASP:HB3	1.86	0.41
3:C:48:SER:N	12:L:69:ALA:HB2	2.35	0.41
4:D:30:GLY:O	4:D:32:GLU:N	2.54	0.41
4:D:40:HIS:C	4:D:42:GLY:H	2.28	0.41
5:E:191:LYS:O	5:E:192:ARG:C	2.63	0.41
7:G:122:ASN:ND2	7:G:125:SER:HB3	2.36	0.41
8:H:44:VAL:HG13	8:H:48:PRO:HA	2.03	0.41
9:I:84:VAL:HG13	9:I:84:VAL:O	2.20	0.41
11:K:87:LEU:O	11:K:88:LYS:C	2.62	0.41
11:K:110:ASN:O	11:K:111:LEU:CD2	2.61	0.41
1:A:152:VAL:HG12	1:A:153:PRO:CD	2.50	0.41
1:A:270:LEU:C	1:A:270:LEU:HD12	2.45	0.41
1:A:332:LYS:H	1:A:337:ARG:HB3	1.85	0.41
1:A:335:ARG:CA	1:A:339:ASN:HD22	2.33	0.41
1:A:380:VAL:HG23	1:A:430:TRP:O	2.21	0.41
1:A:568:PRO:HB2	3:C:221:TYR:CZ	2.55	0.41
1:A:765:VAL:HG23	1:A:802:ASN:O	2.21	0.41
1:A:1018:PHE:O	1:A:1021:LEU:HB3	2.20	0.41
1:A:1067:LEU:C	1:A:1067:LEU:CD1	2.93	0.41
1:A:1353:TYR:HD1	1:A:1368:MET:HE1	1.85	0.41
1:A:1397:LEU:O	1:A:1400:CYS:HB3	2.20	0.41
1:A:1443:VAL:C	1:A:1444:MET:HG3	2.45	0.41
2:B:33:VAL:O	2:B:36:ALA:HB3	2.20	0.41
2:B:96:TYR:HE1	2:B:131:ASP:OD2	2.02	0.41
2:B:336:ARG:HH22	2:B:345:LYS:CE	2.11	0.41
2:B:377:PHE:O	2:B:380:TYR:N	2.53	0.41
2:B:615:MET:HB2	2:B:615:MET:HE3	1.76	0.41
2:B:871:THR:HG22	2:B:872:GLU:N	2.35	0.41
2:B:911:ILE:HG22	2:B:966:VAL:HG21	2.03	0.41
2:B:911:ILE:CG2	2:B:966:VAL:HG11	2.50	0.41
2:B:1060:ARG:HA	2:B:1060:ARG:HD2	1.54	0.41
2:B:1065:GLN:NE2	2:B:1067:ARG:H	2.10	0.41
2:B:1162:ILE:C	2:B:1171:VAL:HG21	2.45	0.41
4:D:26:THR:C	4:D:28:GLN:N	2.78	0.41
7:G:9:LEU:HD12	7:G:10:ASN:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:101:VAL:N	7:G:108:VAL:O	2.52	0.41
8:H:24:CYS:HB2	8:H:44:VAL:HG21	2.01	0.41
8:H:83:GLN:C	8:H:85:GLY:N	2.78	0.41
10:J:2:ILE:C	10:J:53:HIS:CE1	2.98	0.41
12:L:49:LYS:O	12:L:50:ASP:HB3	2.21	0.41
1:A:19:PHE:HB3	1:A:1413:GLY:HA2	2.02	0.41
1:A:19:PHE:HE1	1:A:1396:ALA:HB3	1.85	0.41
1:A:95:PHE:O	1:A:98:LYS:N	2.53	0.41
1:A:263:THR:O	1:A:263:THR:HG22	2.20	0.41
1:A:345:VAL:HG11	2:B:1130:PHE:HB2	2.03	0.41
1:A:417:TYR:N	1:A:417:TYR:CD2	2.88	0.41
1:A:474:VAL:O	1:A:477:PRO:HD2	2.20	0.41
1:A:545:GLN:C	1:A:547:LEU:N	2.76	0.41
1:A:577:ILE:O	1:A:580:VAL:HG23	2.21	0.41
1:A:608:ILE:C	1:A:610:GLY:H	2.29	0.41
1:A:621:THR:O	1:A:629:LEU:HB2	2.20	0.41
1:A:756:ILE:O	1:A:757:ASN:C	2.63	0.41
1:A:806:ARG:HH12	2:B:729:ILE:HD12	1.83	0.41
1:A:1011:GLN:O	1:A:1015:VAL:HG23	2.21	0.41
1:A:1265:ASN:C	1:A:1267:MET:H	2.28	0.41
1:A:1377:THR:O	1:A:1379:GLY:N	2.53	0.41
1:A:1404:GLU:O	1:A:1407:GLU:HB2	2.20	0.41
2:B:355:ILE:O	2:B:359:GLU:HB2	2.21	0.41
2:B:530:GLY:O	2:B:531:GLN:C	2.63	0.41
2:B:552:MET:C	2:B:554:ILE:N	2.79	0.41
2:B:570:VAL:HG23	2:B:573:GLN:HB3	2.03	0.41
2:B:936:ASP:OD1	2:B:938:SER:N	2.48	0.41
2:B:992:ILE:HG12	2:B:993:THR:N	2.35	0.41
2:B:1121:GLY:O	2:B:1122:ARG:C	2.62	0.41
3:C:35:ARG:HH11	11:K:41:THR:HA	1.85	0.41
3:C:123:ASN:HD22	3:C:125:MET:HG2	1.85	0.41
5:E:35:VAL:C	5:E:37:LEU:N	2.79	0.41
6:F:143:PHE:CD1	6:F:143:PHE:O	2.74	0.41
10:J:28:ASP:O	10:J:29:GLU:C	2.64	0.41
11:K:6:ARG:O	11:K:8:GLU:N	2.54	0.41
12:L:27:LEU:HD13	12:L:37:LYS:HG2	2.03	0.41
1:A:7:SER:OG	2:B:1193:GLN:NE2	2.54	0.41
1:A:21:LEU:HG	1:A:1413:GLY:O	2.21	0.41
1:A:268:ASP:HB3	1:A:299:HIS:ND1	2.35	0.41
1:A:285:PRO:O	1:A:287:HIS:N	2.53	0.41
1:A:604:GLY:O	1:A:605:MET:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:666:ILE:CD1	1:A:667:GLY:H	2.29	0.41
1:A:667:GLY:HA3	3:C:192:TRP:HH2	1.84	0.41
1:A:890:ASP:H	1:A:1296:GLY:HA3	1.86	0.41
1:A:907:THR:HG23	1:A:908:LEU:H	1.86	0.41
1:A:974:ASP:C	1:A:976:THR:N	2.78	0.41
1:A:1053:PHE:C	1:A:1055:ARG:N	2.77	0.41
1:A:1070:GLN:C	1:A:1072:ILE:N	2.78	0.41
1:A:1129:GLU:O	1:A:1130:GLN:C	2.62	0.41
1:A:1328:TYR:HD1	1:A:1335:ILE:CD1	2.34	0.41
1:A:1398:MET:C	1:A:1400:CYS:N	2.76	0.41
1:A:1450:LEU:HD11	6:F:108:PHE:CZ	2.56	0.41
2:B:216:GLU:OE1	2:B:537:LYS:HE3	2.21	0.41
2:B:310:MET:HE1	2:B:387:LEU:CD1	2.51	0.41
2:B:336:ARG:HG2	2:B:348:ARG:CD	2.26	0.41
2:B:591:ARG:O	2:B:593:PRO:HD3	2.20	0.41
2:B:597:MET:O	2:B:599:THR:N	2.54	0.41
2:B:610:ASN:HA	2:B:611:PRO:HD3	1.96	0.41
2:B:780:VAL:HG21	10:J:56:LEU:HD11	2.03	0.41
2:B:828:ALA:HB2	2:B:1085:ILE:CG2	2.51	0.41
2:B:1040:ASN:O	2:B:1042:GLY:N	2.54	0.41
2:B:1085:ILE:CG2	2:B:1086:PHE:N	2.84	0.41
3:C:112:ASN:HB2	3:C:114:TYR:HE1	1.85	0.41
4:D:33:PHE:CE2	7:G:80:LYS:NZ	2.74	0.41
4:D:35:LEU:HD13	4:D:173:HIS:ND1	2.36	0.41
4:D:63:LEU:HD22	4:D:63:LEU:HA	1.84	0.41
5:E:177:ARG:O	5:E:212:ARG:HD3	2.18	0.41
7:G:18:PHE:CZ	7:G:68:ALA:HB2	2.55	0.41
7:G:112:LYS:O	7:G:115:MET:HG3	2.21	0.41
8:H:107:VAL:O	8:H:111:LEU:HB2	2.21	0.41
10:J:7:CYS:SG	10:J:49:MET:CE	3.09	0.41
10:J:32:GLU:O	10:J:35:ALA:N	2.54	0.41
11:K:6:ARG:C	11:K:8:GLU:H	2.28	0.41
11:K:31:VAL:CG1	11:K:32:VAL:H	2.30	0.41
11:K:68:PHE:HD2	11:K:68:PHE:N	2.18	0.41
11:K:111:LEU:O	11:K:112:GLN:HB3	2.21	0.41
1:A:55:ASP:N	1:A:56:PRO:CD	2.80	0.41
1:A:89:PRO:HB2	1:A:204:THR:HG21	2.03	0.41
1:A:162:VAL:HG12	1:A:163:SER:N	2.36	0.41
1:A:204:THR:O	1:A:205:GLU:C	2.64	0.41
1:A:351:THR:HB	2:B:1103:ILE:HD11	2.02	0.41
1:A:590:ARG:O	1:A:591:PHE:CB	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:710:LEU:HD13	9:I:94:ASP:O	2.21	0.41
1:A:780:VAL:HG23	2:B:699:GLU:OE1	2.20	0.41
1:A:786:HIS:O	1:A:787:PHE:CD2	2.74	0.41
1:A:839:ARG:O	1:A:840:ARG:C	2.60	0.41
1:A:871:ASP:OD1	1:A:871:ASP:C	2.63	0.41
1:A:920:LEU:C	1:A:920:LEU:CD2	2.93	0.41
1:A:1059:HIS:O	1:A:1060:PRO:C	2.64	0.41
1:A:1385:THR:C	1:A:1387:HIS:N	2.77	0.41
2:B:236:HIS:C	2:B:237:VAL:HG23	2.46	0.41
2:B:309:GLN:O	2:B:310:MET:C	2.64	0.41
2:B:708:GLU:O	2:B:709:ASP:C	2.63	0.41
2:B:841:MET:SD	2:B:846:ILE:HD11	2.61	0.41
2:B:842:ASN:HB3	2:B:845:SER:OG	2.20	0.41
7:G:44:TYR:CD2	7:G:105:PRO:HB2	2.56	0.41
7:G:101:VAL:HG12	7:G:102:GLN:N	2.36	0.41
1:A:93:VAL:CG2	1:A:301:ALA:HA	2.47	0.40
1:A:362:ASP:HB3	1:A:508:PRO:HG3	2.03	0.40
1:A:388:LEU:CD2	1:A:432:VAL:HB	2.51	0.40
1:A:420:ARG:HB3	1:A:423:ASP:HB3	2.02	0.40
1:A:1115:SER:HB3	1:A:1330:ASN:ND2	2.35	0.40
1:A:1115:SER:OG	1:A:1116:LEU:N	2.54	0.40
1:A:1345:ARG:O	1:A:1346:ALA:C	2.63	0.40
1:A:1448:GLU:C	1:A:1450:LEU:N	2.78	0.40
2:B:1016:ALA:O	2:B:1020:ARG:HG3	2.21	0.40
5:E:8:ASN:OD1	5:E:8:ASN:O	2.39	0.40
8:H:82:PRO:O	8:H:83:GLN:HB2	2.21	0.40
8:H:107:VAL:O	8:H:108:SER:O	2.39	0.40
9:I:95:THR:HG22	9:I:96:SER:N	2.35	0.40
11:K:68:PHE:HD1	11:K:70:ARG:NH1	2.19	0.40
12:L:27:LEU:HB3	12:L:37:LYS:HD3	2.03	0.40
15:T:16:DT:H73	15:T:17:TT:C5A	2.50	0.40
1:A:23:SER:O	1:A:26:GLU:N	2.54	0.40
1:A:110:CYS:HB3	1:A:167:CYS:SG	2.62	0.40
1:A:233:TRP:C	1:A:235:ILE:H	2.29	0.40
1:A:805:LEU:HD11	2:B:1052:VAL:HG21	2.02	0.40
1:A:1029:ARG:HG3	1:A:1029:ARG:HH11	1.86	0.40
1:A:1131:ALA:O	1:A:1132:LYS:C	2.64	0.40
1:A:1215:ARG:HD2	1:A:1215:ARG:HA	1.92	0.40
1:A:1446:ASP:O	1:A:1447:GLU:C	2.63	0.40
2:B:175:ARG:HG2	2:B:175:ARG:NH1	2.21	0.40
2:B:455:SER:O	2:B:456:GLY:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:581:PHE:HA	2:B:585:VAL:O	2.21	0.40
2:B:1110:PRO:O	2:B:1119:VAL:HG13	2.22	0.40
2:B:1115:THR:HG21	2:B:1117:GLN:CG	2.51	0.40
3:C:152:GLU:HG2	3:C:153:LEU:H	1.86	0.40
7:G:37:SER:OG	7:G:45:ILE:HB	2.20	0.40
7:G:154:VAL:CG1	7:G:155:SER:N	2.83	0.40
8:H:7:ASP:O	8:H:8:ASP:HB2	2.20	0.40
11:K:43:GLY:HA2	11:K:71:PHE:CZ	2.56	0.40
11:K:68:PHE:CD1	11:K:70:ARG:NH1	2.89	0.40
1:A:349:ALA:C	2:B:1128:LEU:CD1	2.95	0.40
1:A:845:LEU:HD22	1:A:1374:VAL:HG21	2.03	0.40
1:A:1116:LEU:CB	1:A:1308:THR:CG2	3.00	0.40
1:A:1193:LEU:HB2	1:A:1260:LEU:HD11	2.03	0.40
1:A:1239:ARG:NH1	1:A:1239:ARG:HB3	2.36	0.40
1:A:1342:GLU:CG	5:E:198:ILE:HD13	2.51	0.40
1:A:1430:LEU:HB2	1:A:1432:GLN:HG3	2.04	0.40
2:B:640:VAL:HG23	2:B:740:HIS:HA	2.02	0.40
2:B:893:LEU:HD22	2:B:897:GLY:C	2.46	0.40
2:B:1134:GLU:H	2:B:1134:GLU:CD	2.28	0.40
4:D:202:ILE:O	4:D:202:ILE:HG23	2.22	0.40
5:E:35:VAL:O	5:E:37:LEU:N	2.53	0.40
7:G:1:MET:HG3	7:G:85:GLU:OE2	2.21	0.40
7:G:123:ALA:C	7:G:125:SER:H	2.29	0.40
8:H:11:GLN:O	8:H:28:ALA:HB1	2.21	0.40
11:K:103:THR:C	11:K:105:PHE:H	2.30	0.40
12:L:55:ILE:H	12:L:55:ILE:HG12	1.37	0.40
15:T:25:DT:H2''	15:T:26:DC:H5'	2.04	0.40
1:A:68:GLN:HE22	1:A:80:HIS:CG	2.39	0.40
1:A:73:GLY:O	1:A:74:MET:C	2.64	0.40
1:A:208:LEU:CD2	1:A:212:LYS:HE3	2.51	0.40
1:A:353:ILE:HG21	1:A:487:MET:CG	2.51	0.40
1:A:478:TYR:O	1:A:479:ASN:HB3	2.21	0.40
1:A:543:LEU:O	1:A:545:GLN:N	2.53	0.40
1:A:630:ILE:HG23	1:A:642:CYS:SG	2.62	0.40
1:A:897:TYR:HB3	1:A:936:LEU:CD1	2.51	0.40
1:A:1215:ARG:HA	1:A:1218:GLN:HG2	2.03	0.40
1:A:1434:ALA:HB3	1:A:1436:ILE:HD12	2.04	0.40
2:B:465:ASN:N	2:B:465:ASN:ND2	2.69	0.40
2:B:511:PRO:O	2:B:512:ARG:C	2.64	0.40
2:B:551:PRO:HG2	2:B:552:MET:H	1.86	0.40
2:B:744:HIS:CD2	2:B:746:SER:OG	2.71	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:902:GLY:O	12:L:65:VAL:HG11	2.21	0.40
2:B:977:GLY:HA3	2:B:1099:VAL:HB	2.04	0.40
2:B:1109:GLY:O	2:B:1110:PRO:C	2.64	0.40
2:B:1162:ILE:HG23	2:B:1168:LEU:O	2.22	0.40
2:B:1201:LYS:O	2:B:1204:PHE:HB2	2.22	0.40
7:G:15:PRO:HG2	7:G:66:GLY:HA3	2.04	0.40
7:G:18:PHE:CA	7:G:22:MET:HE3	2.42	0.40
8:H:48:PRO:C	8:H:49:VAL:HG23	2.46	0.40
8:H:125:LEU:HD12	8:H:125:LEU:HA	1.97	0.40
9:I:33:SER:O	9:I:35:VAL:HG23	2.22	0.40
1:A:61:ILE:CG2	1:A:62:ASP:H	2.20	0.40
1:A:324:SER:O	1:A:325:ILE:C	2.63	0.40
1:A:335:ARG:HH12	2:B:1202:LEU:HD13	1.81	0.40
1:A:571:LEU:HD22	8:H:46:LEU:HD11	2.02	0.40
1:A:635:ARG:HA	1:A:635:ARG:HH11	1.86	0.40
1:A:722:LEU:HD21	1:A:794:PRO:CB	2.52	0.40
1:A:1366:ARG:HH11	1:A:1366:ARG:HG2	1.87	0.40
2:B:23:ALA:O	2:B:654:ARG:HD2	2.21	0.40
2:B:31:TRP:O	2:B:32:ALA:C	2.64	0.40
2:B:333:PHE:O	2:B:334:ILE:C	2.64	0.40
2:B:371:GLU:N	2:B:371:GLU:CD	2.80	0.40
2:B:373:ARG:CG	2:B:566:LEU:HD23	2.51	0.40
2:B:408:LEU:O	2:B:412:LEU:HG	2.21	0.40
2:B:487:THR:O	2:B:488:TYR:C	2.64	0.40
2:B:687:GLU:O	2:B:688:GLY:C	2.64	0.40
2:B:1208:MET:O	2:B:1211:ASN:N	2.46	0.40
3:C:133:ILE:CD1	3:C:237:SER:CA	2.99	0.40
5:E:24:LYS:CG	5:E:25:ASP:N	2.84	0.40
7:G:1:MET:O	7:G:1:MET:HE2	2.22	0.40
8:H:118:PHE:O	8:H:119:GLY:C	2.64	0.40
11:K:10:PHE:N	11:K:10:PHE:HD2	2.19	0.40
11:K:110:ASN:C	11:K:111:LEU:CG	2.94	0.40
15:T:26:DC:H2''	15:T:27:DA:O5'	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	
1	A	1410/1733 (81%)	947 (67%)	306 (22%)	157 (11%)	0	6
2	B	1096/1224 (90%)	754 (69%)	222 (20%)	120 (11%)	0	7
3	C	264/318 (83%)	164 (62%)	62 (24%)	38 (14%)	0	3
4	D	173/221 (78%)	118 (68%)	38 (22%)	17 (10%)	0	9
5	E	212/215 (99%)	153 (72%)	42 (20%)	17 (8%)	1	12
6	F	84/155 (54%)	65 (77%)	13 (16%)	6 (7%)	1	14
7	G	169/171 (99%)	128 (76%)	30 (18%)	11 (6%)	1	15
8	H	131/146 (90%)	87 (66%)	26 (20%)	18 (14%)	0	3
9	I	114/122 (93%)	77 (68%)	26 (23%)	11 (10%)	0	9
10	J	63/70 (90%)	34 (54%)	12 (19%)	17 (27%)	0	0
11	K	112/120 (93%)	82 (73%)	20 (18%)	10 (9%)	0	10
12	L	44/70 (63%)	18 (41%)	13 (30%)	13 (30%)	0	0
All	All	3872/4565 (85%)	2627 (68%)	810 (21%)	435 (11%)	0	6

All (435) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	THR
1	A	48	ALA
1	A	57	ARG
1	A	62	ASP
1	A	65	LEU
1	A	93	VAL
1	A	130	ASP
1	A	154	SER
1	A	167	CYS
1	A	223	GLY
1	A	250	ILE
1	A	255	SER

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Mol	Chain	Res	Type
1	A	286	HIS
1	A	311	GLN
1	A	312	PRO
1	A	318	SER
1	A	335	ARG
1	A	385	ILE
1	A	423	ASP
1	A	536	LEU
1	A	567	LYS
1	A	619	LYS
1	A	636	GLU
1	A	666	ILE
1	A	789	LYS
1	A	847	ASP
1	A	968	GLN
1	A	969	GLN
1	A	986	ILE
1	A	1002	GLY
1	A	1014	ALA
1	A	1036	ARG
1	A	1114	PRO
1	A	1115	SER
1	A	1122	PRO
1	A	1212	VAL
1	A	1223	ASP
1	A	1281	ARG
1	A	1314	SER
1	A	1341	ILE
1	A	1365	TYR
1	A	1366	ARG
1	A	1377	THR
1	A	1378	GLN
1	A	1392	SER
1	A	1438	THR
2	B	45	SER
2	B	46	GLN
2	B	108	VAL
2	B	115	GLN
2	B	186	GLU
2	B	258	LEU
2	B	259	TYR
2	B	266	ALA

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Mol	Chain	Res	Type
2	B	345	LYS
2	B	367	LEU
2	B	467	GLY
2	B	470	LYS
2	B	474	SER
2	B	613	VAL
2	B	643	ASP
2	B	709	ASP
2	B	727	LYS
2	B	731	VAL
2	B	751	VAL
2	B	831	SER
2	B	881	ASN
2	B	907	GLY
2	B	909	ASP
2	B	943	SER
2	B	958	GLN
2	B	1046	PRO
2	B	1069	PHE
2	B	1155	SER
2	B	1156	ASP
2	B	1157	ALA
2	B	1171	VAL
2	B	1175	LEU
2	B	1178	ASN
2	B	1181	GLU
2	B	1182	CYS
2	B	1183	LYS
3	C	4	GLU
3	C	56	THR
3	C	78	GLU
3	C	141	GLY
3	C	149	LYS
3	C	156	THR
3	C	161	LYS
3	C	184	ASN
3	C	209	TYR
3	C	214	ASN
3	C	215	GLU
4	D	5	THR
4	D	8	PHE
4	D	9	GLN

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Mol	Chain	Res	Type
4	D	19	GLU
4	D	20	GLU
4	D	52	LEU
4	D	177	VAL
4	D	192	LYS
4	D	199	ASN
5	E	3	GLN
5	E	59	SER
5	E	73	PRO
5	E	106	GLN
5	E	130	ALA
6	F	81	THR
7	G	62	LEU
7	G	63	PRO
7	G	139	ILE
8	H	62	SER
8	H	82	PRO
8	H	108	SER
8	H	128	ASN
8	H	140	ALA
9	I	3	THR
9	I	9	ASP
9	I	79	HIS
10	J	2	ILE
10	J	6	ARG
10	J	32	GLU
10	J	64	ASN
11	K	7	PHE
11	K	110	ASN
12	L	35	SER
12	L	50	ASP
12	L	59	ALA
12	L	60	ARG
1	A	42	ASP
1	A	54	ASN
1	A	59	GLY
1	A	66	LYS
1	A	69	THR
1	A	74	MET
1	A	76	GLU
1	A	84	ILE
1	A	96	ILE

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Mol	Chain	Res	Type
1	A	219	PHE
1	A	244	PRO
1	A	253	ASN
1	A	283	GLY
1	A	300	VAL
1	A	322	VAL
1	A	331	GLY
1	A	332	LYS
1	A	336	ILE
1	A	409	SER
1	A	418	SER
1	A	424	ILE
1	A	439	ASN
1	A	465	TYR
1	A	543	LEU
1	A	544	ASP
1	A	597	LEU
1	A	720	ARG
1	A	753	GLY
1	A	780	VAL
1	A	852	TYR
1	A	871	ASP
1	A	979	SER
1	A	1071	SER
1	A	1096	SER
1	A	1116	LEU
1	A	1165	GLU
1	A	1233	ASP
1	A	1280	GLU
1	A	1335	ILE
1	A	1389	PHE
1	A	1402	PHE
1	A	1405	THR
2	B	28	GLU
2	B	124	TYR
2	B	184	ALA
2	B	260	GLY
2	B	264	SER
2	B	282	ILE
2	B	283	VAL
2	B	389	ALA
2	B	401	PHE

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Mol	Chain	Res	Type
2	B	450	ALA
2	B	540	SER
2	B	559	SER
2	B	605	ARG
2	B	619	ILE
2	B	629	ASP
2	B	655	LYS
2	B	708	GLU
2	B	746	SER
2	B	752	ALA
2	B	754	SER
2	B	792	MET
2	B	951	GLN
2	B	1011	ILE
2	B	1041	GLU
2	B	1065	GLN
2	B	1096	ARG
2	B	1100	ASP
2	B	1167	GLY
2	B	1186	ASP
2	B	1188	LYS
3	C	10	ILE
3	C	51	VAL
3	C	84	ARG
3	C	87	PHE
3	C	110	THR
3	C	175	ALA
3	C	213	PRO
3	C	216	GLY
4	D	21	GLU
4	D	65	GLU
4	D	131	GLU
4	D	196	PRO
5	E	36	GLU
5	E	74	ASP
5	E	115	ASN
5	E	192	ARG
5	E	206	GLY
6	F	112	GLU
7	G	19	GLY
7	G	35	GLU
7	G	154	VAL

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Mol	Chain	Res	Type
8	H	17	PRO
8	H	21	ASN
8	H	59	ILE
8	H	77	ARG
8	H	81	PRO
8	H	90	ALA
9	I	11	ASN
9	I	47	GLU
9	I	57	GLY
9	I	106	CYS
10	J	14	VAL
10	J	17	LYS
10	J	24	LEU
10	J	28	ASP
10	J	29	GLU
10	J	33	GLY
11	K	15	GLY
11	K	29	ASN
11	K	88	LYS
12	L	53	HIS
1	A	8	SER
1	A	43	GLU
1	A	61	ILE
1	A	70	CYS
1	A	73	GLY
1	A	169	ASN
1	A	232	GLU
1	A	245	PRO
1	A	263	THR
1	A	278	THR
1	A	333	GLU
1	A	386	ASP
1	A	483	ASP
1	A	846	GLU
1	A	1013	ASP
1	A	1164	PRO
1	A	1221	LYS
1	A	1277	GLU
2	B	48	LEU
2	B	65	GLU
2	B	114	PRO
2	B	257	LYS

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Mol	Chain	Res	Type
2	B	364	ILE
2	B	365	THR
2	B	369	GLY
2	B	449	ASN
2	B	460	ALA
2	B	461	LEU
2	B	571	PRO
2	B	591	ARG
2	B	641	GLU
2	B	711	GLU
2	B	764	SER
2	B	818	PRO
2	B	867	GLY
2	B	878	GLN
2	B	880	THR
2	B	891	ASP
2	B	894	ASP
2	B	1108	ARG
3	C	81	GLU
3	C	148	ARG
3	C	164	ALA
3	C	212	PRO
3	C	237	SER
3	C	240	VAL
3	C	264	GLN
4	D	53	SER
5	E	44	ALA
5	E	45	LYS
7	G	20	PRO
7	G	64	THR
8	H	32	THR
8	H	36	CYS
8	H	84	ALA
8	H	92	ASP
8	H	135	LEU
9	I	78	CYS
10	J	8	PHE
10	J	9	SER
10	J	27	GLU
10	J	55	ASP
11	K	53	ASP
11	K	112	GLN

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Mol	Chain	Res	Type
1	A	131	SER
1	A	399	HIS
1	A	400	PRO
1	A	591	PHE
1	A	601	LYS
1	A	605	MET
1	A	759	ALA
1	A	825	ILE
1	A	1054	LEU
1	A	1133	LEU
1	A	1224	LEU
1	A	1397	LEU
1	A	1448	GLU
2	B	22	SER
2	B	30	SER
2	B	61	ASP
2	B	94	LYS
2	B	180	TYR
2	B	309	GLN
2	B	466	TRP
2	B	682	SER
2	B	728	ARG
2	B	844	SER
2	B	869	SER
2	B	945	GLU
3	C	48	SER
3	C	138	GLU
3	C	139	GLY
3	C	142	VAL
3	C	167	HIS
3	C	208	GLU
4	D	47	LEU
5	E	148	GLU
6	F	154	ASP
8	H	44	VAL
9	I	34	TYR
9	I	107	SER
10	J	45	CYS
11	K	70	ARG
12	L	26	THR
12	L	28	LYS
12	L	39	SER

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Mol	Chain	Res	Type
12	L	56	LEU
1	A	5	GLN
1	A	55	ASP
1	A	111	GLY
1	A	205	GLU
1	A	517	ASN
1	A	639	PRO
1	A	649	ILE
1	A	673	GLY
1	A	775	ILE
1	A	910	PRO
1	A	940	ARG
1	A	958	VAL
1	A	972	HIS
1	A	1124	HIS
1	A	1309	ASP
1	A	1386	ARG
1	A	1395	GLY
2	B	598	GLU
2	B	734	HIS
2	B	848	ARG
2	B	1017	ILE
2	B	1061	GLU
2	B	1214	PRO
3	C	6	PRO
4	D	12	ARG
6	F	89	GLU
6	F	150	GLU
6	F	151	LEU
7	G	81	PRO
8	H	78	SER
12	L	40	LEU
12	L	52	GLY
12	L	54	ARG
1	A	196	GLU
1	A	492	PRO
1	A	599	SER
1	A	626	ASN
1	A	648	ASN
1	A	755	PHE
1	A	1016	THR
1	A	1127	ASP

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Mol	Chain	Res	Type
1	A	1260	LEU
1	A	1302	PRO
1	A	1369	ALA
2	B	56	ASP
2	B	206	ASN
2	B	387	LEU
2	B	611	PRO
2	B	1112	GLN
3	C	95	CYS
4	D	146	GLN
5	E	43	LYS
7	G	115	MET
10	J	18	TRP
11	K	104	ASN
12	L	55	ILE
1	A	197	PRO
1	A	380	VAL
1	A	719	VAL
2	B	511	PRO
2	B	551	PRO
2	B	712	PRO
2	B	832	GLY
3	C	18	VAL
3	C	172	PRO
10	J	57	ILE
1	A	1158	PRO
2	B	102	VAL
5	E	76	GLY
9	I	62	ILE
11	K	66	PRO
1	A	35	ILE
1	A	661	GLY
2	B	688	GLY
2	B	729	ILE
2	B	903	VAL
3	C	129	ILE
3	C	217	ASP
1	A	99	ILE
1	A	357	PRO
1	A	396	PRO
1	A	652	VAL
2	B	55	VAL

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Mol	Chain	Res	Type
7	G	34	VAL
5	E	38	PRO
5	E	129	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1244/1520 (82%)	1124 (90%)	120 (10%)	8	28
2	B	967/1061 (91%)	885 (92%)	82 (8%)	10	33
3	C	235/274 (86%)	216 (92%)	19 (8%)	11	34
4	D	159/200 (80%)	134 (84%)	25 (16%)	2	15
5	E	196/197 (100%)	189 (96%)	7 (4%)	31	53
6	F	77/137 (56%)	69 (90%)	8 (10%)	7	25
7	G	152/152 (100%)	139 (91%)	13 (9%)	10	33
8	H	119/128 (93%)	112 (94%)	7 (6%)	18	42
9	I	110/116 (95%)	99 (90%)	11 (10%)	7	26
10	J	60/65 (92%)	54 (90%)	6 (10%)	7	26
11	K	99/102 (97%)	87 (88%)	12 (12%)	5	21
12	L	40/57 (70%)	36 (90%)	4 (10%)	7	26
All	All	3458/4009 (86%)	3144 (91%)	314 (9%)	9	30

All (314) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	11	LEU
1	A	32	VAL
1	A	34	LYS
1	A	37	PHE
1	A	38	PRO
1	A	62	ASP

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Mol	Chain	Res	Type
1	A	67	CYS
1	A	70	CYS
1	A	93	VAL
1	A	108	MET
1	A	142	CYS
1	A	198	GLU
1	A	200	ARG
1	A	215	SER
1	A	221	SER
1	A	227	VAL
1	A	236	LEU
1	A	245	PRO
1	A	270	LEU
1	A	275	SER
1	A	302	THR
1	A	308	ILE
1	A	312	PRO
1	A	320	ARG
1	A	321	PRO
1	A	326	ARG
1	A	335	ARG
1	A	344	ARG
1	A	345	VAL
1	A	350	ARG
1	A	379	VAL
1	A	381	THR
1	A	385	ILE
1	A	388	LEU
1	A	396	PRO
1	A	406	ILE
1	A	407	ARG
1	A	408	ASP
1	A	412	ARG
1	A	425	GLN
1	A	442	VAL
1	A	443	LEU
1	A	445	ASN
1	A	450	LEU
1	A	451	HIS
1	A	460	VAL
1	A	461	LYS
1	A	462	VAL

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Mol	Chain	Res	Type
1	A	466	SER
1	A	469	ARG
1	A	481	ASP
1	A	493	GLN
1	A	497	THR
1	A	512	VAL
1	A	515	GLN
1	A	560	ILE
1	A	562	THR
1	A	618	GLU
1	A	629	LEU
1	A	635	ARG
1	A	666	ILE
1	A	670	ILE
1	A	711	ARG
1	A	768	GLN
1	A	774	ARG
1	A	779	PHE
1	A	821	ARG
1	A	827	THR
1	A	845	LEU
1	A	858	ASN
1	A	859	SER
1	A	886	ILE
1	A	890	ASP
1	A	907	THR
1	A	929	LEU
1	A	940	ARG
1	A	941	LYS
1	A	969	GLN
1	A	983	ILE
1	A	992	ASP
1	A	1001	ARG
1	A	1006	ILE
1	A	1017	LEU
1	A	1029	ARG
1	A	1035	TYR
1	A	1067	LEU
1	A	1110	ASN
1	A	1116	LEU
1	A	1120	LEU
1	A	1122	PRO

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Mol	Chain	Res	Type
1	A	1127	ASP
1	A	1146	VAL
1	A	1152	ILE
1	A	1170	ILE
1	A	1187	GLN
1	A	1206	ASP
1	A	1264	GLU
1	A	1271	ILE
1	A	1291	VAL
1	A	1295	THR
1	A	1298	TYR
1	A	1329	THR
1	A	1332	PHE
1	A	1333	ILE
1	A	1359	ASP
1	A	1371	LEU
1	A	1372	VAL
1	A	1376	THR
1	A	1378	GLN
1	A	1385	THR
1	A	1386	ARG
1	A	1405	THR
1	A	1408	ILE
1	A	1418	LEU
1	A	1425	SER
1	A	1432	GLN
1	A	1442	ASP
1	A	1443	VAL
1	A	1445	ILE
2	B	35	SER
2	B	57	TYR
2	B	63	ILE
2	B	100	PRO
2	B	104	GLU
2	B	106	ASP
2	B	175	ARG
2	B	180	TYR
2	B	188	ASP
2	B	194	GLU
2	B	223	VAL
2	B	258	LEU
2	B	267	ARG

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Mol	Chain	Res	Type
2	B	268	THR
2	B	323	VAL
2	B	365	THR
2	B	371	GLU
2	B	378	LEU
2	B	393	LYS
2	B	396	ASP
2	B	399	ASP
2	B	427	ASP
2	B	463	THR
2	B	466	TRP
2	B	498	THR
2	B	502	ILE
2	B	513	GLN
2	B	516	ASN
2	B	557	PHE
2	B	582	VAL
2	B	593	PRO
2	B	603	LEU
2	B	628	THR
2	B	635	ARG
2	B	644	GLU
2	B	649	LYS
2	B	682	SER
2	B	737	THR
2	B	742	GLU
2	B	748	ILE
2	B	755	ILE
2	B	787	VAL
2	B	795	ILE
2	B	816	GLU
2	B	825	VAL
2	B	830	TYR
2	B	833	TYR
2	B	835	GLN
2	B	837	ASP
2	B	839	MET
2	B	844	SER
2	B	878	GLN
2	B	901	PRO
2	B	909	ASP
2	B	953	LEU

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Mol	Chain	Res	Type
2	B	997	GLU
2	B	999	MET
2	B	1002	THR
2	B	1006	ILE
2	B	1010	LEU
2	B	1047	PHE
2	B	1060	ARG
2	B	1069	PHE
2	B	1084	GLN
2	B	1085	ILE
2	B	1095	LEU
2	B	1099	VAL
2	B	1103	ILE
2	B	1106	ARG
2	B	1120	GLU
2	B	1122	ARG
2	B	1133	MET
2	B	1159	ARG
2	B	1160	VAL
2	B	1162	ILE
2	B	1169	MET
2	B	1170	THR
2	B	1176	ASN
2	B	1183	LYS
2	B	1202	LEU
2	B	1212	ILE
2	B	1216	LEU
3	C	4	GLU
3	C	22	LEU
3	C	57	VAL
3	C	77	ILE
3	C	89	GLU
3	C	99	LEU
3	C	108	GLU
3	C	129	ILE
3	C	140	ASN
3	C	147	LEU
3	C	163	ILE
3	C	166	GLU
3	C	172	PRO
3	C	193	TYR
3	C	214	ASN

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Mol	Chain	Res	Type
3	C	233	GLU
3	C	240	VAL
3	C	259	LEU
3	C	266	ASP
4	D	8	PHE
4	D	13	ARG
4	D	17	LYS
4	D	19	GLU
4	D	22	GLU
4	D	47	LEU
4	D	63	LEU
4	D	70	PHE
4	D	126	ILE
4	D	137	ASN
4	D	139	LYS
4	D	148	LEU
4	D	149	THR
4	D	151	PHE
4	D	152	SER
4	D	156	ASP
4	D	170	THR
4	D	174	PRO
4	D	187	THR
4	D	192	LYS
4	D	193	THR
4	D	206	GLU
4	D	208	GLU
4	D	216	ASN
4	D	221	TYR
5	E	40	GLU
5	E	60	PHE
5	E	74	ASP
5	E	78	LEU
5	E	114	ASN
5	E	132	ILE
5	E	175	LEU
6	F	79	ARG
6	F	90	ARG
6	F	103	MET
6	F	111	LEU
6	F	116	ASP
6	F	143	PHE

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Mol	Chain	Res	Type
6	F	148	VAL
6	F	153	VAL
7	G	1	MET
7	G	11	ILE
7	G	13	LEU
7	G	17	PHE
7	G	45	ILE
7	G	74	TYR
7	G	77	VAL
7	G	78	VAL
7	G	80	LYS
7	G	88	ASP
7	G	115	MET
7	G	126	ASN
7	G	171	ILE
8	H	42	ILE
8	H	86	ASP
8	H	93	TYR
8	H	102	TYR
8	H	106	GLU
8	H	130	ARG
8	H	143	LEU
9	I	8	ARG
9	I	9	ASP
9	I	15	TYR
9	I	34	TYR
9	I	59	VAL
9	I	78	CYS
9	I	85	PHE
9	I	86	PHE
9	I	94	ASP
9	I	99	LEU
9	I	101	PHE
10	J	7	CYS
10	J	9	SER
10	J	10	CYS
10	J	16	ASP
10	J	44	TYR
10	J	46	CYS
11	K	5	ASP
11	K	10	PHE
11	K	12	LEU

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Mol	Chain	Res	Type
11	K	25	THR
11	K	41	THR
11	K	47	ARG
11	K	50	LEU
11	K	61	TYR
11	K	78	THR
11	K	111	LEU
11	K	112	GLN
11	K	113	THR
12	L	27	LEU
12	L	51	CYS
12	L	55	ILE
12	L	65	VAL

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

Mol	Chain	Res	Type
1	A	5	GLN
1	A	54	ASN
1	A	64	ASN
1	A	68	GLN
1	A	71	GLN
1	A	83	HIS
1	A	160	GLN
1	A	225	ASN
1	A	256	GLN
1	A	339	ASN
1	A	358	ASN
1	A	390	GLN
1	A	439	ASN
1	A	493	GLN
1	A	515	GLN
1	A	517	ASN
1	A	525	GLN
1	A	545	GLN
1	A	603	ASN
1	A	631	HIS
1	A	654	ASN
1	A	698	GLN
1	A	741	ASN
1	A	757	ASN
1	A	768	GLN

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Mol	Chain	Res	Type
1	A	786	HIS
1	A	838	GLN
1	A	858	ASN
1	A	903	ASN
1	A	926	GLN
1	A	1009	ASN
1	A	1033	GLN
1	A	1040	GLN
1	A	1106	ASN
1	A	1140	HIS
1	A	1171	GLN
1	A	1265	ASN
1	A	1364	ASN
1	A	1378	GLN
1	A	1387	HIS
1	A	1432	GLN
2	B	46	GLN
2	B	53	GLN
2	B	60	GLN
2	B	178	ASN
2	B	215	GLN
2	B	236	HIS
2	B	325	GLN
2	B	363	HIS
2	B	366	GLN
2	B	465	ASN
2	B	499	ASN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	538	ASN
2	B	657	HIS
2	B	734	HIS
2	B	744	HIS
2	B	763	GLN
2	B	776	GLN
2	B	794	ASN
2	B	821	GLN
2	B	842	ASN
2	B	843	GLN
2	B	975	GLN
2	B	1015	HIS

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Mol	Chain	Res	Type
2	B	1065	GLN
2	B	1076	HIS
2	B	1084	GLN
2	B	1117	GLN
2	B	1176	ASN
2	B	1179	GLN
2	B	1193	GLN
3	C	73	GLN
3	C	112	ASN
3	C	123	ASN
3	C	167	HIS
3	C	231	ASN
4	D	39	ASN
4	D	40	HIS
4	D	132	GLN
4	D	137	ASN
4	D	157	GLN
5	E	8	ASN
5	E	101	GLN
5	E	104	ASN
5	E	114	ASN
5	E	146	HIS
5	E	147	HIS
7	G	53	ASN
7	G	97	HIS
7	G	122	ASN
7	G	126	ASN
8	H	64	ASN
8	H	137	GLN
9	I	12	ASN
9	I	89	GLN
9	I	90	GLN
10	J	53	HIS
10	J	64	ASN
11	K	44	ASN
11	K	65	HIS
11	K	76	GLN
11	K	104	ASN
11	K	110	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	9/11 (81%)	1 (11%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	7	A

There are no RNA pucker outliers to report.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
15	TT	T	17	15	40,43,44	5.03	10 (25%)	58,69,72	2.62	16 (27%)
15	BRU	T	22	15,14	18,21,22	0.81	1 (5%)	25,30,33	1.00	1 (4%)

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
15	TT	T	17	15	-	10/18/105/106	0/5/6/6
15	BRU	T	22	15,14	-	2/7/21/22	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	17	TT	C5T-C6T	-21.42	1.31	1.55
15	T	17	TT	C5-C6	-20.81	1.32	1.55
15	T	17	TT	C6T-N1T	-4.83	1.39	1.46
15	T	17	TT	C1'-N1	3.95	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	17	TT	C6-N1	-3.85	1.40	1.46
15	T	17	TT	C5T-C4T	-3.75	1.45	1.51
15	T	17	TT	C6T-C6	3.15	1.65	1.56
15	T	22	BRU	O5'-C5'	-2.45	1.37	1.44
15	T	17	TT	O4-C4	2.31	1.26	1.22
15	T	17	TT	C2T-N1T	2.21	1.40	1.36
15	T	17	TT	C5-C4	-2.06	1.47	1.51

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	17	TT	C2R-C1R-N1T	8.38	126.91	115.59
15	T	17	TT	C5T-C5-C6	7.72	97.39	88.36
15	T	17	TT	C5-C6-C6T	-6.66	79.03	89.26
15	T	17	TT	C5-C6-N1	6.29	123.99	115.65
15	T	17	TT	N3T-C2T-N1T	-4.65	111.92	116.78
15	T	17	TT	C5-C5T-C6T	-4.51	83.09	88.36
15	T	17	TT	C5T-C6T-N1T	4.03	120.99	115.65
15	T	17	TT	O4R-C4R-C5R	3.83	121.61	109.33
15	T	17	TT	C5A-C5-C5T	-3.83	105.32	116.61
15	T	17	TT	C3R-C2R-C1R	-3.66	93.64	102.60
15	T	17	TT	O4R-C1R-N1T	3.22	112.47	108.65
15	T	17	TT	O4-C4-C5	2.93	125.44	122.71
15	T	22	BRU	C6-C5-C4	-2.88	117.75	120.67
15	T	17	TT	O3R-C3R-C4R	-2.61	100.18	110.07
15	T	17	TT	C5-C4-N3	-2.42	114.05	116.09
15	T	17	TT	C5T-C6T-C6	2.38	92.93	89.26
15	T	17	TT	C6-C6T-N1T	2.14	126.50	118.51

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	T	17	TT	C3R-C4R-C5R-O5R
15	T	17	TT	O3'-C7-O5R-C5R
15	T	17	TT	C2'-C1'-N1-C6
15	T	17	TT	C2'-C1'-N1-C2
15	T	17	TT	O4'-C1'-N1-C6
15	T	17	TT	O4'-C4'-C5'-O5'
15	T	17	TT	O4'-C1'-N1-C2
15	T	17	TT	O4R-C4R-C5R-O5R
15	T	22	BRU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
15	T	17	TT	O4R-C1R-N1T-C6T
15	T	22	BRU	C3'-C4'-C5'-O5'
15	T	17	TT	O4R-C1R-N1T-C2T

There are no ring outliers.

2 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	T	17	TT	23	0
15	T	22	BRU	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	2
3	C	1

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Mol	Chain	Number of breaks
1	A	1
6	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	18:PHE	C	19:GLU	N	3.98
1	C	2:SER	C	3:GLU	N	3.88
1	A	1175:SER	C	1176:LEU	N	3.69
1	F	69:LEU	C	70:LYS	N	3.59
1	B	337:ARG	C	338:GLY	N	2.64

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.