



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2017 – 10:35 PM EST

PDB ID : 5LUQ
Title : Crystal Structure of Human DNA-dependent Protein Kinase Catalytic Subunit (DNA-PKcs)
Authors : Sibanda, B.L.; Chirgadze, D.Y.; Ascher, D.B.; Blundell, T.L.
Deposited on : 2016-09-09
Resolution : 4.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

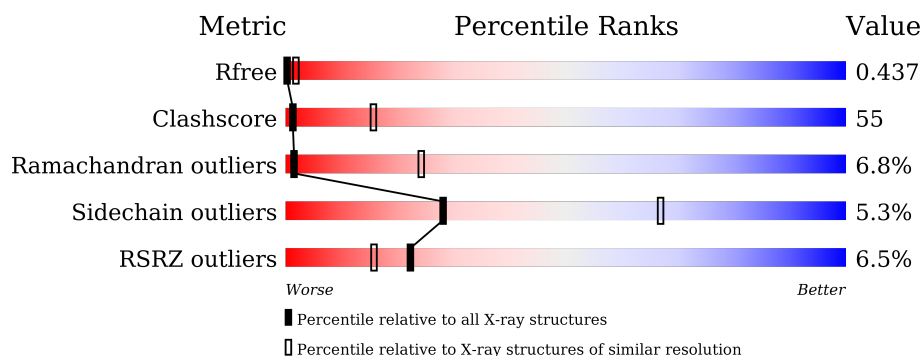
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1059 (5.00-3.60)
Clashscore	102246	1166 (5.00-3.60)
Ramachandran outliers	100387	1106 (5.00-3.60)
Sidechain outliers	100360	1089 (5.00-3.60)
RSRZ outliers	91569	1062 (5.00-3.60)

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

Mol	Chain	Length	Quality of chain
1	A	4128	
1	B	4128	
2	K	194	
2	S	194	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 59694 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-dependent protein kinase catalytic subunit,DNA-dependent Protein Kinase Catalytic Subunit,DNA-dependent protein kinase catalytic subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	3725	Total	C	N	O	S	Se	0	0	0
			29574	18907	5016	5460	81	110			
1	B	3725	Total	C	N	O	S	Se	0	0	0
			29574	18907	5016	5460	81	110			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	expression tag	UNP P78527
A	4128	MSE	-	expression tag	UNP P78527
B	1	MSE	-	expression tag	UNP P78527
B	4128	MSE	-	expression tag	UNP P78527

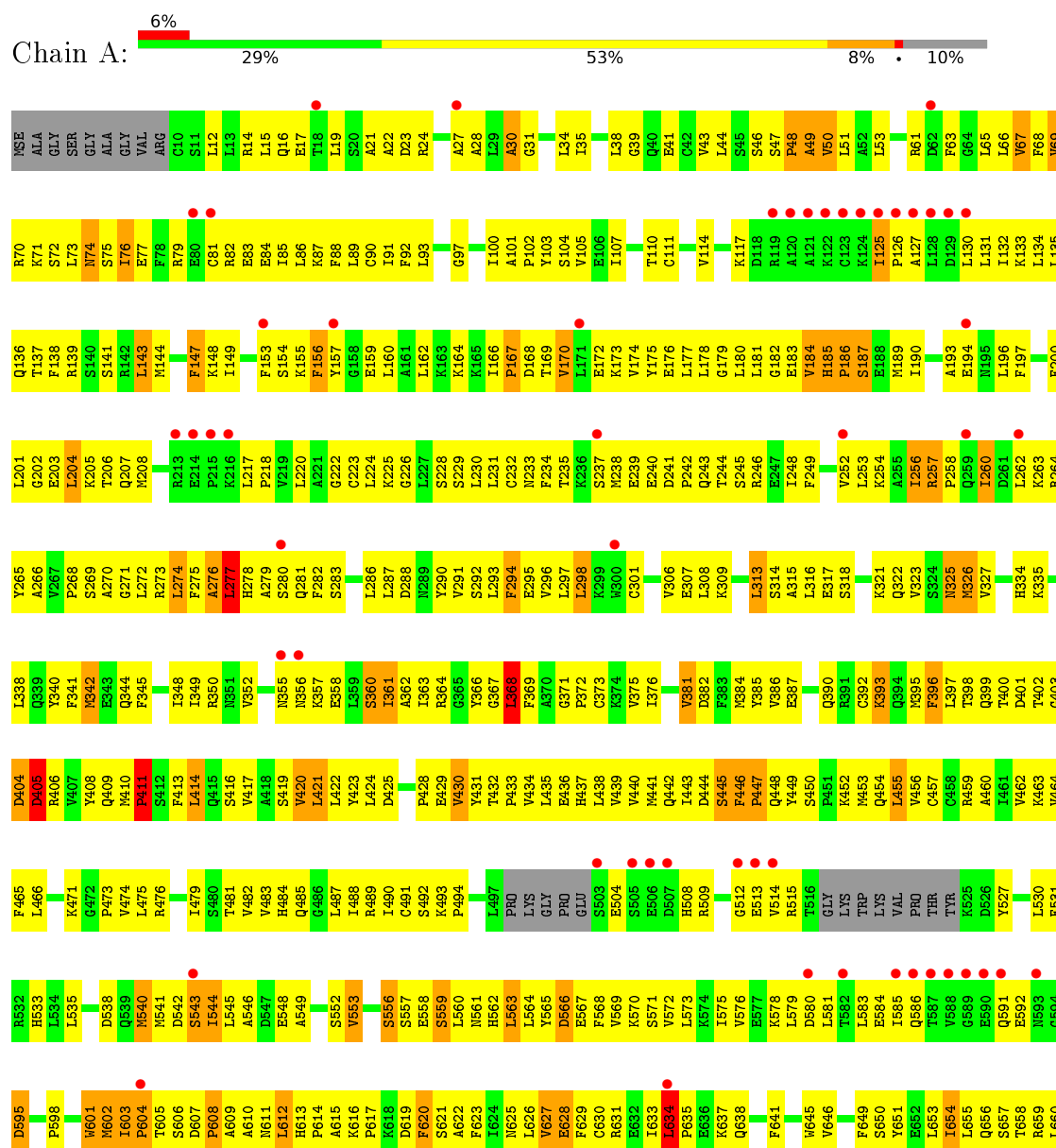
- Molecule 2 is a protein called C-terminal fragment of KU80 (KU80ct194).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	54	Total	C	N	O	Se	0	0	0
			273	164	54	54	1			
2	S	54	Total	C	N	O	Se	0	0	0
			273	164	54	54	1			

3 Residue-property plots

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

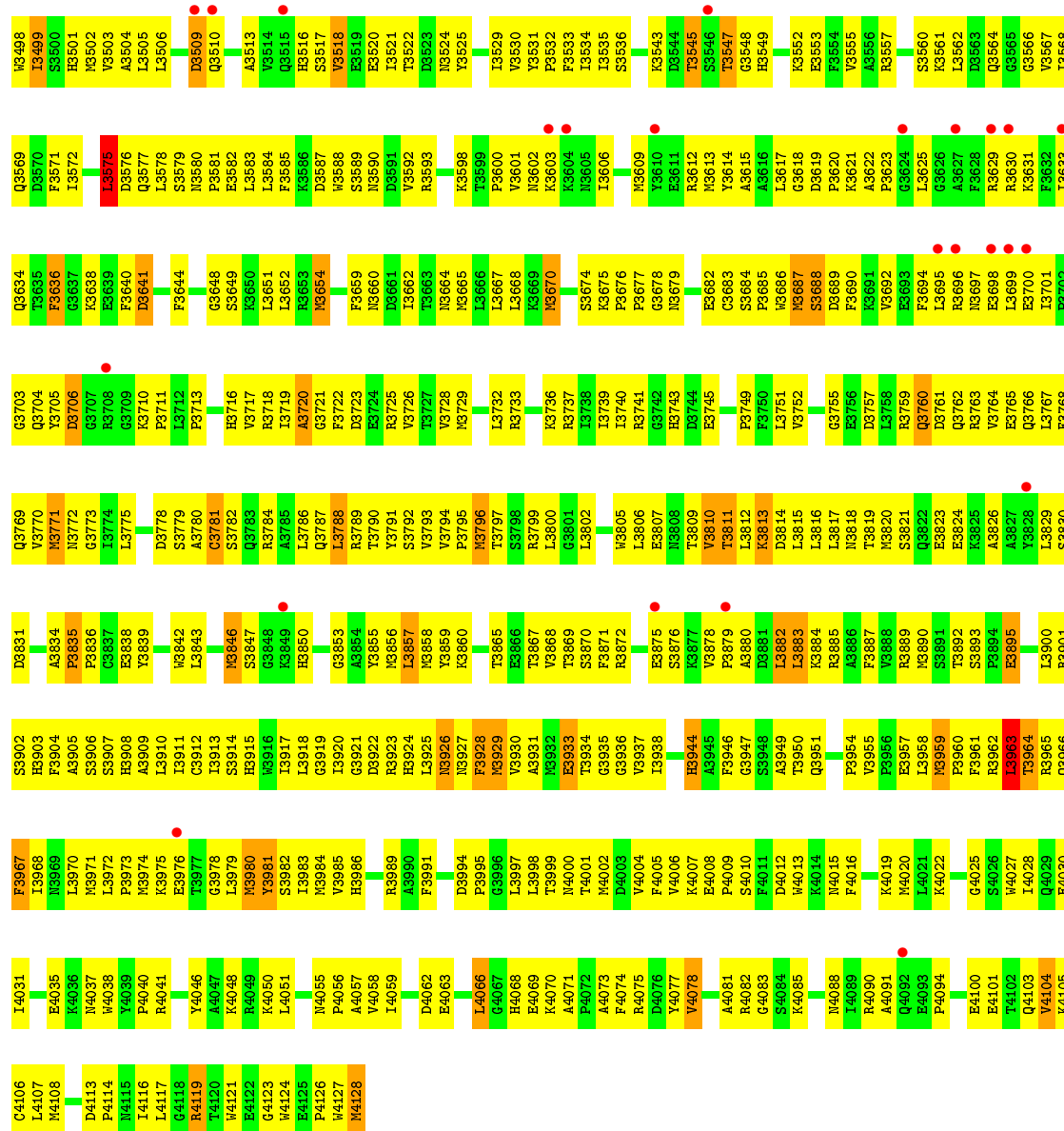
- Molecule 1: DNA-dependent protein kinase catalytic subunit,DNA-dependent Protein Kinase Catalytic Subunit,DNA-dependent protein kinase catalytic subunit



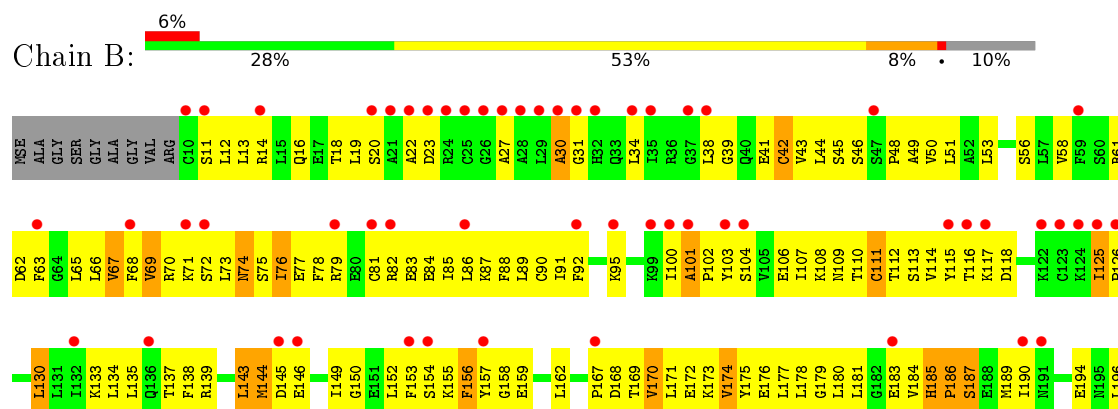
E1565	L1503	V1434	M1369	A1308	P1289	D1467	A1103	L1037	D977	P912	E849	P787	D723	P661
T1566	D1504	M1435	R1370	ALA	T1240	L1168	L1104	K1038	Q978	R913	E850	L768	E724	L662
L1567	L1505	L1436	V1371	GLU	Y1243	V1169	V1105	W1039	V979	R852	R851	Y789	L725	L663
M1568	S1506	Y1437	L1372	LNS	Y1243	M1171	L1106	LNS	T980	E916	R853	L793	L726	S664
L1569	C1507	G1438	V1373	CYS	P1247	L1172	M1108	K1042	R981	Q917	R854	L794	S728	Y667
E1570	K1508	P1439	V1374	PHE	F1248	L1173	E1109	G1043	Q982	Q918	R854	C795	C729	K668
L1571	D1440	D1440	T1375	GLY	S1249	L1174	E1109	L1044	L983	L919	R854	L796	L730	L668
L1572	L1510	A1441	L1376	THR	L1250	A1174	S1110	T1045	L984	S922	M858	D797	L731	L670
L1573	L1511	D1444	C1377	GLY	Q1251	A1174	L1111	P1046	P986	R924	L859	L799	F732	L671
M1574	S1512	R1445	E1378	ALA	Q1251	L1178	A1112	Q1049	L987	R924	L862	L733	F733	L672
D1576	G1513	L1448	E1378	ALA	T1253	A1252	L1113	P1053	V988	Q925	L862	L734	L734	R675
L1577	G1513	A1448	I1382	GLY	T1253	L1254	H1115	P1053	V989	T926	G863	S785	L736	M676
A1578	G1513	A1449	I1382	ASN	C1255	L1254	H1115	P1053	Q990	K927	Q864	T802	P737	A677
L1582	A1518	V1452	M1385	THR	W1256	Q1180	A1116	P1053	L991	V928	Q864	L800	L736	M676
M1583	F1519	I1386	I1386	CYS	L1257	CYS	D1117	T1056	L992	V928	Q864	L801	L736	A677
L1584	A1520	G1387	D1387	P1324	D1258	ARG	E1118	T1056	R993	R924	Q864	L801	L736	A677
A1584	A1454	A1454	D1388	P1324	D1258	ARG	E1118	T1056	R993	R924	Q864	L801	L736	A677
S1585	V1389	K1455	V1389	HIS	L1259	HIS	S1120	S1058	R993	R924	Q864	L801	L736	A677
G1522	V1389	K1455	V1389	HIS	L1259	HIS	S1120	S1058	R993	R924	Q864	L801	L736	A677
G1523	Q1390	K1456	Q1390	LEU	L1260	LEU	L1121	F1060	R993	R924	Q864	L801	L736	A677
V1587	V1391	Q1457	V1391	ILE	E1285	ILE	G1122	K1061	R993	R924	Q864	L801	L736	A677
D1588	L1458	L1458	M1392	GLU	C1266	GLU	T1123	L1063	R993	R924	Q864	L801	L736	A677
M1589	H1459	H1459	M1392	LEU	Y1287	LEU	T1123	L1063	R993	R924	Q864	L801	L736	A677
T1590	ARG	R1460	L1395	PHE	N1288	TRP	C1127	S1065	K1000	N937	S876	L808	L743	PHE
K1591	LEU	A1461	L1396	TRP	T1269	LNS	C1128	L1066	K1001	N937	S876	L808	L743	PHE
M1592	VAL	G1462	D1397	LNS	F1270	LNS	I1131	A1067	E1002	N938	D877	L808	L743	PHE
L1593	SER	L1463	C1398	PHE	F1270	LNS	I1131	A1067	E1002	N938	D877	L808	L743	PHE
S1594	LEU	L1464	C1398	VAL	I1271	VAL	D1132	L1068	Q1003	F940	M879	L808	L743	PHE
L1597	LEU	H1465	V1337	PRO	R1274	PRO	L1134	H1069	Q1004	N941	M879	L808	L743	PHE
M1598	LEU	H1466	V1338	LEU	R1275	LEU	C1135	N1071	T1006	N947	K881	L808	L743	PHE
G1599	ASN	L1467	V1339	GLY	V1276	PRO	R1136	A1072	V1007	N948	S882	L808	L743	PHE
M1600	PRO	L1468	K1403	GLY	G1277	PRO	L1137	F1073	A1008	N949	S882	L808	L743	PHE
L1601	ALA	P1469	K1404	GLY	A1278	GLY	L1138	A1074	L1009	P949	S884	L808	L743	PHE
D1602	VAL	S1470	A1405	ASN	L1279	ASN	K1139	R1075	E1011	G951	A886	L808	L743	PHE
Q1603	LEU	Q1471	L1406	ARG	L1279	ARG	K1140	L1076	E1011	G951	A886	L808	L743	PHE
S1604	SER	S1472	K1407	SER	L1282	PRO	K1141	G1077	A1012	G952	D887	L808	L743	PHE
F1605	ALA	L1475	M1408	PRO	G1283	ASN	H1142	A1078	I1013	G953	R888	L808	L743	PHE
L1606	SER	H1476	S1409	ASN	T1284	ASN	V1143	S1079	L1014	G954	E889	L808	L743	PHE
E1607	LEU	H1477	P1410	LEU	E1285	LEU	L1144	S1080	D1015	A955	K890	L808	L743	PHE
A1608	GLY	S1478	L1415	THR	E1286	THR	L1145	A1081	D1016	P956	R891	L808	L743	PHE
A1609	SER	V1479	L1416	LEU	Q1287	LEU	M1146	F1082	I1017	P957	L892	L808	L743	PHE
ASN	SER	E1482	E1416	VAL	S1289	ASP	A1148	N1084	D1019	N959	F894	L808	L743	PHE
GLN	GLN	E1482	T1447	VAL	L1290	VAL	K1149	I1085	P1020	Q960	A895	L808	L743	PHE
LYS	LYS	E1482	H1418	K1213	L1291	LEU	L1150	Y1086	V1021	L961	V896	L808	L743	PHE
HIS	G1548	Y1488	H1418	K1213	L1291	LEU	L1150	Y1086	V1021	L961	V896	L808	L743	PHE
GLN	S1549	K1489	L1419	E1214	E1214	LEU	R1151	R1087	D1022	Y962	P897	L808	L743	PHE
LYS	V1550	G1490	R1420	E1215	E1215	LEU	L1152	E1088	S1023	R963	F898	L808	L743	PHE
GLY	L1551	G1490	E1421	G1216	G1216	LEU	L1153	F1089	T1024	R964	R899	L808	L743	PHE
LEU	H1552	I1491	K1422	G1217	G1217	LEU	P1154	R1090	L1025	T965	E900	L808	L743	PHE
LYS	F1553	A1492	L1423	V1217	V1217	LEU	R1155	R1090	R1026	F966	M901	L808	L743	PHE
LEU	S1554	P1493	T1424	S1218	S1218	LEU	P1158	E1093	D1027	P967	K902	L808	L743	PHE
ALA	L1555	G1494	A1426	F1219	F1219	LEU	P1159	S1094	D1028	V968	P903	L808	L743	PHE
THR	G1556	D1495	Q1426	L1220	L1220	LEU	P1160	L1095	C1029	V969	V904	L808	L743	PHE
THR	E1557	E1496	S1427	I1301	I1301	LEU	L1161	V1096	G1030	R971	I905	L808	L743	PHE
ILE	L1558	Q1497	E1428	I1302	I1302	LEU	L1162	V1096	G1030	R971	I905	L808	L743	PHE
LEU	F1559	Q1498	E1429	M1303	M1303	LEU	L1163	Q1098	C1032	L972	L907	L808	L743	PHE
GLN	Y1560	G1499	E1430	H1304	H1304	LEU	L1164	F1099	I1033	A973	D908	L808	L743	PHE
HIS	L1560	G1499	E1430	H1304	H1304	LEU	L1164	F1099	I1033	A973	D908	L808	L743	PHE
TRP	F1563	P1501	C1432	H1306	H1306	LEU	L1165	V1100	R1034	C974	V909	L808	L743	PHE
LYS	S1564	S1502	A1433	L1368	L1368	LEU	L1166	E1102	F1036	V976	L911	L808	L743	PHE







• Molecule 1: DNA-dependent protein kinase catalytic subunit, DNA-dependent Protein Kinase Catalytic Subunit, DNA-dependent protein kinase catalytic subunit

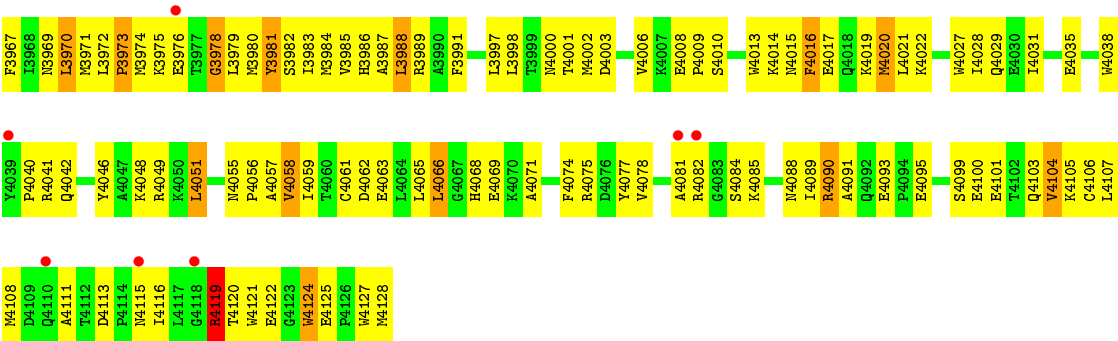


Y1107	M1108	E1109	S1110	L1111	A1112	L1113	A1114	H1115	E1118	K1119	S1120	L1121	G1122	T1123	C1127	D1128	D1129	A1130	I1131	D1132	H1133	L1134	C1135	I1136	L1137	I1138	E1139	K1140	K1141	L1142	V1143	S1144	L1145	N1146	K1147	A1148	K1149	K1150	R1151	L1152	L1153	P1154	R1155	G1156	F1157	P1158	P1159	S1162	L1163	C1164	L1165	L1166	D1167	V1168	K1170		
I1044	Y984	E985	P986	L987	V988	K989	S990	L991	P992	H993	Y994	L995	T996	N997	L1063	Y1064	S1065	L1066	A1067	L1068	H1069	P1070	M1071	L1134	C1135	I1136	L1137	I1138	E1139	K1140	K1141	L1142	V1143	S1144	L1145	N1146	K1147	A1148	K1149	K1150	R1151	L1152	L1153	P1154	R1155	G1156	F1157	P1158	P1159	S1162	L1163	C1164	L1165	L1166	D1167	V1168	K1170
S922	R852	L792	T731	F666	I603	L534	P473	S412	F345	K263	F197																																														
R852	L853	T793	F732	V667	I604	L535	V474	F413	R264	K263	F197																																														
R855	V855	C795	L733	K668	T605	S536	L475	L414	Y265	K264	F200																																														
V856	D857	L796	R734	L670	T607	S537	R476	Q415	A266	L201																																															
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W858	L798	C798	P737	L672	A609	M540	S480	A418	S269	K269	K205																																														
L859	L799	Y799	H738	T673	A610	P540	T481	V352	A270	T206	K206																																														
G860	L800	L800	N739	T673	N611	D542	V482	L420	G271	Q207	M208																																														
S861	R801	R801	N739	N676	L612	S543	V483	L421	L272	M208																																															
L862	T802	T802	I741	I680	H613	I544	H484	L422	R273	T209																																															
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R868	S806	S806	A751	PHE	P617	F550	I488	T426	L277	E214																																															
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L870	T809	T809	Y748	VAL	D619	S552	I490	P428	A279	P215																																															
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L877	VAL	VAL	N754	LYS	L626	E559	L497	L435	L287	G222																																															
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L888	L892	L892	L765	PHE	K637	L570	H508	F446	V306	C232																																															
L889	R893	R893	A766	F704	X637	S571	R509	P447	E307	N233																																															
L890	E900	E900	L773	L705	Q638	V572	A510	Q448	E307	F234																																															
L891	R901	R901	L774	L706	F641	L572	LVS	F449	L308	M238																																															
L892	L902	L902	L775	E713	T642	K578	S511	Y449	L313	E239																																															
L893	R903	R903	L776	L714	F642	L579	G512	S450	L313	E240																																															
L894	L904	L904	L777	A715	S650	D580	LVS	P396	S314	D241																																															
L895	L905	L905	L778	L716	V651	L581	TRP	L397	A315	P242																																															
L896	R906	R906	L779	K717	E652	T582	LVS	T398	L316	Q243																																															
L897	L907	L907	L780	L718	R653	L583	VAL	E459	E317	Q244																																															
L898	L908	L908	L781	L719	L654	E584	PRD	A460	Q394	S245																																															
L899	L909	L909	L782	L720	Q656	L593	THR	T402	L318	L244																																															
L900	L910	L910	L783	Y721	R657	Q591	D526	K463	L320	I248																																															
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L902	L912	L912	L785	L725	R659	N593	V528	F465	Q322	H250																																															
L903	L913	L913	L786	L726	L660	LVS	L530	A467	Q323	F249																																															
L904	L914	L914	L787	L727	P661	P598	L530	L468	V327	E256																																															
L905	L915	L915	L788	L728	L662	LVS	L530	L468	L256	R257																																															
L906	L916	L916	L789	L729	L663	V789	F531	L468	N330	R257																																															
L907	L917	L917	Y789	C729	I663	L730	H533	L468	H334	P258																																															
L908	L918	L918	Y790	L730	L663	L730	H533	L468	H334	P258																																															
L909	L919	L919	L791	L731	L663	L730	H533	L468	H334	P258																																															
L910	L920	L920	L792	L732	L663	L730	H533	L468	H334	P258																																															
L911	L921	L921	L793	L733	L663	L730	H533	L468	H334	P258																																															
L912	L922	L922	L794	L734	L663	L730	H533	L468	H334	P258																																															
L913	L923	L923	L795	L735	L663	L730	H533	L468	H334	P258																																															
L914	L924	L924	L796	L736	L663	L730	H533	L468	H334	P258																																															
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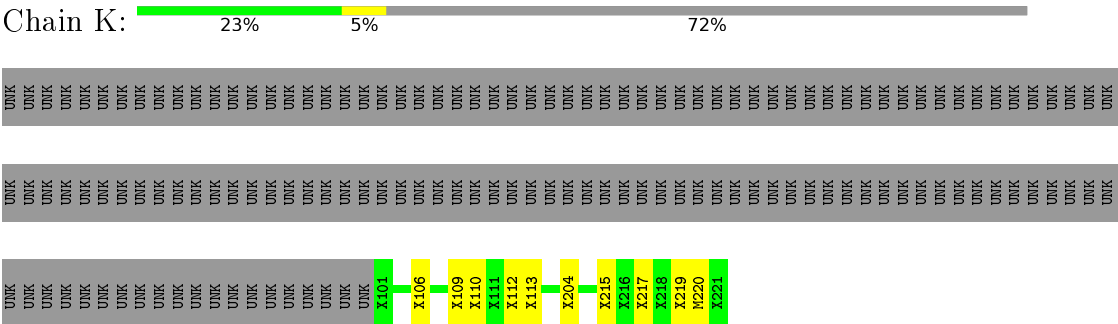
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	K1895	GLU	ASP	A1634	M1574	Q1509	Q1441	L1375	ALA	P1247	THR
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	Y1962	ARG	ARG	S1637	L1577	G1513	R1445	C1377	CYS	L1250	ARG
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S2027	G1964	ARG	ARG	L1639	V1579		R1447	P1379	GLY	A1252	LYS
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	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	S2270			
	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	E2208			
	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	I2271			
	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	G2272			
	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	I2273			
	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	I2274			
	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	Q2275			
	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	L2276			
	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	I2277			

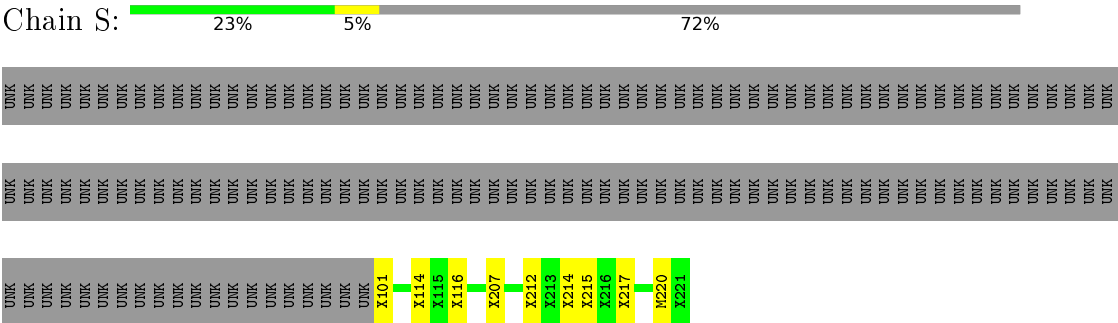
H3903	F3838	G3773	L3705	L3633	L3572	V3503	Y3442	SER	S294	L3230	L3103	K3029
F3904	F3839	L3774	D3706	Q3634	N3573	A3504	P3443	GLY	E295	L3231	Q3104	I3030
A3905	F3840	L3775	G3707	F3635	A3574	L3505	A3444	SER	Q296		N3105	K3031
S3906	F3841	D3778	G3708	F3636	L3575	L3506	L3445	SER	V297	C3234	F3168	S3032
S3907	F3842	S3779	G3709	G3637	D3576	D3507	V3446	SER	L3298	K3235	L3107	F3033
A3908	L3843	K3710	K3711	K3638	K3577	K3508	V3447	GLU	T3299		G3108	P3034
L3910	L3844	A3780	P3711	D3641	L3578	D3509	E3448	ASP	V3300	K3238	S3109	F3035
L3911	K3845	C3781	L3712		S3579	Q3510	K3449	SER	V3304	K3239	F3110	F3036
C3912	Q3783	S3782	F3713	G3648	N3580	A3511	K3450	GLU		K3240	Q3037	Q3038
L3913	K3784	K3783	H3716	G3649	V3512	V3513	L3451	LVS	L3307	K3241	Q3112	Q3039
S3914	S3847	K3785	V3717	F3650	K3582	A3514	K3452	V3373		K3242	L3113	L3040
H3915		A3786	R3718	L3651	L3583	V3515	K3453		K3341	L3243	Y3114	
H3916	H3850	L3786	R3719	L3652	K3584	Q3516	L3454	R3390		D3244		
L3917		Q3787	L3720	F3655	H3516	H3517	K3455		V3312		I3117	P3042
L3918	Y3855	L3788	A3720	K3656	S3517	S3518	I3456	Q3383	S3313	R3247	D3118	P3043
L3919	K3856	R3789	G3721	K3654	F3586	V3518	N3457	H3384	S3314	K3248	M3044	M3044
G3919	L3857	F3790	F3722	K3655	V3588	E3519	S3458	L3385	V3315	Q3249	L3120	L3045
L3920	K3858	K3791	D3723	L3656	S3589	K3520	N3459	L3316	L3316	K3250	L3121	K3046
	Y3859	S3792	D3724	S3657	N3590	L3521	E3460	V3389	S3317	N3251	H3122	S3047
R3923	K3860	K3793	R3725	D3658	D3591	T3522	A3461	Q3390	K3318	F3252	Q3123	K3048
N3926	G3861	V3794	R3726	F3659	V3592	D3523	K3462	E3393	K3319	S3253	S3124	L3049
N3927	A3862	P3795	F3735	K3660	K3593	Y3524	L3463	E3394	L3320	A3255	K3125	K3050
F3928	K3863	K3796	D3661	D3661	A3594	Y3525	K3464		L3321		L3051	L3052
N3929	R3864	T3797	K3729	L3662	E3595	P3526			A3322	K3256	L3052	
F3930	E3866		L3732	T3663	L3596	Q3527		Q3397	F3323	K3257	K3128	L3053
A3931	L3800	L3800	R3733		K3597	A3528	L3466	P3398	R3324	L3258	Q3130	
N3932	G3801	F3801	R3734	L3667	K3598	K3529	L3469	P3399	D3325	L3259	S3131	E3056
E3933	L3802	L3802	F3735	K3670	T3599	V3530	Q3470	S3400	Q3326	K3260	L3132	A3057
T3934	L3803	L3803	K3736		P3600	F3531	I3471		N3327	K3261	Q3133	D3058
G3935	K3804	K3804	R3737	S3674	V3601	P3532	L3472	C3403	L3328	L3262	Q3134	Q3059
	N3805	N3805	L3738	K3675	N3602	F3533	E3473	G3404	L3329	H3263	A3134	S3060
G3936	L3806	L3806	L3739	K3676	K3603	I3534	K3474	P3405	L3330	K3264	L3135	L3061
V3937	F3807	F3807	L3740	K3677	K3604	L3535	T3475	A3406	G3331	E3265	E3137	
N3938	N3808	N3808	R3741	P3677	N3605	S3536	P3476	A3407	T3332	S3266	L3138	F3064
L3940	G3877	G3877	G3742	K3678	E3537	S3537	E3477	G3408	T3333	K3267	Q3139	L3065
D3941	V3877	V3877	H3743	N3679	E3538	E3538	E3478		Y3334	T3268	E3140	
F3942	L3811	L3811	D3744		S3539	S3539	L3480	D3411			F3141	M3069
G3943	K3812	K3812	E3745	K3681	V3610	Y3540	S3481	A3412	D3271		L3142	E3070
H3944	D3813	D3813		E3682	F3611		S3482	Y3413	N3339	N3272	S3143	G3071
A3945	L3814	L3814	F3750	C3683	R3612	T3547	L3482	M3414	A3340	L3273	F3144	E3072
F3946	L3815	L3815	L3751	S3684	N3613	G3548	N3483	T3415	L3341	V3274	L3145	L3073
G3947	L3816	L3816	V3752	P3685	Y3614	H3549	T3484	L3416	S3342	S3275	S3146	Q3074
S3948	L3817	L3817	K3753	N3686	A3615	K3550	K3485		S3343	K3276	K3147	K3075
A3949	N3818	N3818	G3754	K3687	A3616	N3551	E3486	F3419	E3344	V3277	Q3148	A3076
T3950	S3888	S3888	L3758	S3688	L3617	K3552	I3487	C3420	P3345	Q3278	G3149	
L3953	F3887	F3887	R3759	D3689	D3618	K3553	S3488	D3421	A3346	S3279	N3150	L3080
P3954	N3889	N3889	Q3760	F3690	D3619	F3554	S3489	Q3422	C3347	S3280	L3151	Q3084
	S3891	S3891	D3761	K3691	P3620		V3490	Q3423	L3348	C3281	S3152	E3085
E3957	F3694	F3694	Q3762		K3621	L3558	C3492	R3425	E3350	L3283	Q3154	L3086
L3958	L3695	L3695	K3763	L3695	A3622	K3561	N3493	K3426	T3351	S3284	V3155	
M3959	A3826	A3826	V3764	K3696	G3624		Q3494	E3427		H3285	P3156	L3089
P3960	E3895	E3895	E3765	N3697	L3625	Q3564	F3495		K3355	K3286	L3157	Y3090
F3961	A3896	A3896	Q3766	E3698	G3626	G3565	L3496	S3432	A3356	R3287	L3158	L3091
L3962	L3897	L3897	L3767	L3699	G3627	G3566	S3497		K3357	K3288	GLU	L3092
	S3898	S3898	F3768	E3700	F3628	V3567	K3498	D3435	R3358	R3289	L3160	
L3963	A3899	A3899	Q3769	L3701	R3629	L3668	I3499		T3359	S3290	L3161	D3095
T3964	L3900	L3900	V3770	P3702	K3630	Q3569	S3500	E3438	LEU	Q3291	N3162	
R3965	R3901	R3901	K3771	G3703	H3501	D3570	GLU	L3438	GLU	S3228	G3163	A3099
Q3966	S3902	S3902	N3772	Q3704	P3632	F3571	N3502		LEU	S3229	V3164	



● Molecule 2: C-terminal fragment of KU80 (KU80ct194)



● Molecule 2: C-terminal fragment of KU80 (KU80ct194)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	169.12Å 132.64Å 296.59Å 90.00° 105.53° 90.00°	Depositor
Resolution (Å)	49.92 – 4.30 49.92 – 4.30	Depositor EDS
% Data completeness (in resolution range)	97.8 (49.92-4.30) 97.6 (49.92-4.30)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 4.29Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.386 , 0.437 0.384 , 0.437	Depositor DCC
R_{free} test set	1973 reflections (2.34%)	DCC
Wilson B-factor (Å ²)	184.6	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 187.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	59694	wwPDB-VP
Average B, all atoms (Å ²)	253.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.45	3/29743 (0.0%)	0.77	47/40014 (0.1%)
1	B	0.46	6/29743 (0.0%)	0.77	49/40014 (0.1%)
2	K	0.22	0/7	0.50	0/7
2	S	0.45	0/7	0.34	0/7
All	All	0.46	9/59500 (0.0%)	0.77	96/80042 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	B	0	6
All	All	0	14

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1069	HIS	C-N	-9.65	1.16	1.34
1	B	3794	VAL	C-N	-8.26	1.18	1.34
1	B	1069	HIS	C-N	7.70	1.48	1.34
1	B	4124	TRP	CB-CG	-6.16	1.39	1.50
1	A	601	TRP	CB-CG	-5.75	1.40	1.50
1	B	3981	TYR	CD1-CE1	-5.53	1.31	1.39
1	B	2546	TYR	CB-CG	-5.38	1.43	1.51
1	B	2546	TYR	CD2-CE2	-5.37	1.31	1.39
1	A	2362	VAL	CB-CG1	-5.04	1.42	1.52

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	726	LEU	CA-CB-CG	-10.22	91.80	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3456	LEU	CA-CB-CG	9.67	137.54	115.30
1	B	1009	LEU	CB-CG-CD1	-9.35	95.11	111.00
1	A	3456	LEU	CA-CB-CG	9.33	136.75	115.30
1	B	726	LEU	CA-CB-CG	-9.12	94.32	115.30
1	B	1010	LEU	CA-CB-CG	9.01	136.02	115.30
1	A	2926	LEU	CA-CB-CG	8.88	135.71	115.30
1	A	1010	LEU	CA-CB-CG	8.37	134.55	115.30
1	A	3882	LEU	CA-CB-CG	-8.14	96.57	115.30
1	B	2542	LEU	CA-CB-CG	7.94	133.56	115.30
1	A	3575	LEU	CA-CB-CG	7.75	133.12	115.30
1	A	1165	LEU	CA-CB-CG	7.67	132.95	115.30
1	A	2542	LEU	CA-CB-CG	7.53	132.63	115.30
1	B	1165	LEU	CA-CB-CG	7.50	132.54	115.30
1	A	1976	LEU	CB-CG-CD1	-7.38	98.45	111.00
1	B	1695	LEU	CA-CB-CG	7.22	131.91	115.30
1	B	4051	LEU	CA-CB-CG	6.89	131.15	115.30
1	A	3321	LEU	CB-CG-CD2	-6.88	99.31	111.00
1	A	3788	LEU	CA-CB-CG	-6.87	99.49	115.30
1	B	1717	LEU	CA-CB-CG	-6.85	99.53	115.30
1	A	1025	LEU	CA-CB-CG	-6.81	99.63	115.30
1	B	3397	GLN	CA-CB-CG	6.52	127.75	113.40
1	B	220	LEU	CA-CB-CG	6.52	130.29	115.30
1	B	515	ARG	NE-CZ-NH1	-6.47	117.07	120.30
1	A	3480	LEU	CA-CB-CG	6.27	129.73	115.30
1	A	455	LEU	CA-CB-CG	6.26	129.70	115.30
1	B	862	LEU	CB-CG-CD2	-6.26	100.36	111.00
1	A	3665	MSE	CB-CG-SE	6.25	131.43	112.70
1	B	1580	LEU	CA-CB-CG	6.24	129.65	115.30
1	A	1111	LEU	CA-CB-CG	-6.24	100.95	115.30
1	A	2241	LEU	CA-CB-CG	-6.19	101.07	115.30
1	B	1984	LEU	CA-CB-CG	6.17	129.49	115.30
1	B	2892	LEU	CA-CB-CG	6.14	129.43	115.30
1	B	1812	LEU	CA-CB-CG	6.14	129.43	115.30
1	A	1524	LEU	CA-CB-CG	6.13	129.41	115.30
1	A	1145	LEU	CA-CB-CG	6.13	129.40	115.30
1	B	2921	LEU	CA-CB-CG	6.09	129.30	115.30
1	B	3667	LEU	CA-CB-CG	6.07	129.26	115.30
1	B	3416	LEU	CA-CB-CG	6.03	129.16	115.30
1	A	718	MSE	CB-CG-SE	-6.02	94.64	112.70
1	B	942	LEU	CB-CG-CD1	-6.02	100.77	111.00
1	A	1648	LEU	CA-CB-CG	5.95	128.99	115.30
1	A	901	MSE	CA-CB-CG	-5.94	103.20	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1025	LEU	CA-CB-CG	-5.93	101.66	115.30
1	B	3988	LEU	CA-CB-CG	-5.87	101.80	115.30
1	A	204	LEU	CA-CB-CG	-5.84	101.87	115.30
1	B	913	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	B	3230	LEU	CA-CB-CG	5.79	128.61	115.30
1	A	1984	LEU	CA-CB-CG	5.75	128.52	115.30
1	A	3963	LEU	CA-CB-CG	5.75	128.52	115.30
1	B	942	LEU	CA-CB-CG	5.73	128.47	115.30
1	B	734	LEU	CA-CB-CG	-5.71	102.17	115.30
1	B	130	LEU	CB-CG-CD1	-5.69	101.33	111.00
1	B	545	LEU	CA-CB-CG	5.68	128.37	115.30
1	B	1686	LEU	CA-CB-CG	-5.66	102.29	115.30
1	B	3734	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	B	2097	LEU	CB-CG-CD2	-5.62	101.44	111.00
1	A	1752	LEU	CA-CB-CG	-5.56	102.50	115.30
1	B	612	LEU	CA-CB-CG	5.56	128.08	115.30
1	A	1812	LEU	CA-CB-CG	5.54	128.05	115.30
1	B	1643	MSE	CB-CG-SE	-5.52	96.14	112.70
1	B	583	LEU	CA-CB-CG	5.51	127.97	115.30
1	B	2539	LEU	CA-CB-CG	5.50	127.95	115.30
1	A	2921	LEU	CA-CB-CG	5.49	127.92	115.30
1	A	414	LEU	CA-CB-CG	-5.43	102.81	115.30
1	B	3788	LEU	CA-CB-CG	-5.38	102.94	115.30
1	A	2235	LEU	CA-CB-CG	5.37	127.65	115.30
1	A	1415	LEU	CA-CB-CG	-5.37	102.96	115.30
1	A	1976	LEU	CA-CB-CG	5.35	127.61	115.30
1	A	1915	LEU	CA-CB-CG	5.33	127.55	115.30
1	A	3667	LEU	CA-CB-CG	5.33	127.56	115.30
1	B	1572	LEU	CA-CB-CG	5.28	127.44	115.30
1	B	359	LEU	CA-CB-CG	5.25	127.39	115.30
1	A	313	LEU	CA-CB-CG	5.25	127.37	115.30
1	A	421	LEU	CA-CB-CG	5.24	127.35	115.30
1	B	1930	GLU	CA-CB-CG	5.22	124.89	113.40
1	B	421	LEU	CA-CB-CG	5.21	127.28	115.30
1	A	933	LEU	CA-CB-CG	-5.21	103.32	115.30
1	A	2808	LEU	CB-CG-CD1	-5.20	102.16	111.00
1	A	563	LEU	CB-CG-CD1	-5.17	102.20	111.00
1	A	3152	SER	C-N-CA	5.17	134.63	121.70
1	A	1095	LEU	CA-CB-CG	5.16	127.17	115.30
1	B	2926	LEU	CB-CG-CD2	-5.16	102.23	111.00
1	B	3575	LEU	CA-CB-CG	5.14	127.13	115.30
1	A	892	LEU	CA-CB-CG	-5.13	103.51	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2398	LEU	CA-CB-CG	5.12	127.09	115.30
1	A	1762	MSE	CB-CG-SE	5.12	128.06	112.70
1	B	2122	LEU	CA-CB-CG	5.12	127.07	115.30
1	A	2396	LEU	CB-CG-CD2	-5.11	102.31	111.00
1	A	758	LEU	CA-CB-CG	-5.07	103.65	115.30
1	B	564	LEU	CA-CB-CG	5.05	126.91	115.30
1	B	475	LEU	CA-CB-CG	5.04	126.89	115.30
1	B	871	LEU	CA-CB-CG	5.03	126.86	115.30
1	A	1582	LEU	CA-CB-CG	-5.01	103.77	115.30
1	B	670	LEU	CA-CB-CG	5.01	126.83	115.30
1	B	3159	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1323	SER	Peptide
1	A	2283	ASN	Peptide
1	A	2372	PRO	Peptide
1	A	3547	THR	Peptide
1	A	3980	MSE	Peptide
1	A	411	PRO	Peptide
1	A	4119	ARG	Peptide
1	A	634	LEU	Peptide
1	B	1323	SER	Peptide
1	B	2372	PRO	Peptide
1	B	3547	THR	Peptide
1	B	411	PRO	Peptide
1	B	4119	ARG	Peptide
1	B	634	LEU	Peptide

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	29574	0	29642	3223	0
1	B	29574	0	29642	3283	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	273	0	70	9	0
2	S	273	0	73	8	0
All	All	59694	0	59427	6514	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 55.

All (6514) 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)
1:B:2183:HIS:O	1:B:2187:VAL:HB	1.30	1.31
1:B:662:LEU:O	1:B:666:PHE:HB2	1.28	1.30
1:A:3521:ILE:O	1:A:3525:TYR:HB2	1.32	1.28
1:B:3683:CYS:SG	1:B:3736:LYS:NZ	2.12	1.23
1:B:2167:PRO:O	1:B:2171:LEU:HB2	1.39	1.18
1:B:1344:PHE:O	1:B:1348:LEU:HB2	1.41	1.18
1:A:3923:ARG:HG2	1:A:3962:ARG:HH22	1.07	1.17
1:B:1407:LYS:NZ	1:B:1460:ARG:O	1.77	1.16
1:B:3521:ILE:O	1:B:3525:TYR:HB2	1.43	1.16
1:A:2183:HIS:O	1:A:2187:VAL:HB	1.39	1.16
1:A:368:LEU:HD21	1:A:384:MSE:HB2	1.25	1.15
1:B:3868:VAL:O	1:B:3872:ARG:HB3	1.44	1.15
1:B:2872:ASP:O	1:B:2913:LYS:NZ	1.80	1.15
1:B:2477:LEU:O	1:B:2481:HIS:HB3	1.44	1.14
1:B:3467:ARG:O	1:B:3471:ILE:HB	1.46	1.14
1:B:1931:ASN:O	1:B:1938:ARG:NH2	1.80	1.13
1:B:974:CYS:HA	1:B:981:ARG:HD2	1.17	1.13
1:A:3167:ARG:HD3	1:A:3186:ARG:HG2	1.29	1.12
1:B:67:VAL:O	1:B:71:LYS:HB2	1.50	1.12
1:B:2100:LEU:HD21	1:B:2104:MSE:HE3	1.31	1.11
1:B:3099:ALA:O	1:B:3103:ILE:HB	1.47	1.11
1:A:3812:LEU:O	1:A:3816:LEU:HB2	1.49	1.11
1:A:560:LEU:HB3	1:A:616:LYS:HZ3	1.12	1.11
1:B:2960:GLU:OE2	1:B:3289:ARG:NH1	1.83	1.10
1:B:19:LEU:O	1:B:23:ASP:HB2	1.51	1.10
1:B:2891:ARG:HH22	1:B:3884:LYS:HD3	0.97	1.10
1:B:3581:PRO:HG2	1:B:3674:SER:HB2	1.34	1.09
1:A:3467:ARG:O	1:A:3471:ILE:HB	1.49	1.09
1:B:909:VAL:HG13	1:B:913:ARG:HH11	1.16	1.08
1:B:899:ARG:HH12	1:B:2570:PRO:HB2	1.17	1.08
1:B:3772:ASN:HB2	1:B:3787:GLN:HG3	1.36	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3868:VAL:O	1:A:3872:ARG:HB3	1.54	1.07
1:B:3117:ILE:HD12	1:B:3125:ARG:HH11	1.15	1.07
1:A:887:ASP:HB3	1:A:3889:ARG:HB3	1.35	1.04
1:B:2304:VAL:HG11	1:B:2344:LEU:HB3	1.40	1.04
1:B:3534:ILE:HG12	1:B:3704:GLN:HE22	1.22	1.03
1:B:2991:LYS:NZ	1:B:2995:GLU:OE2	1.91	1.03
1:A:2227:LYS:HD2	1:A:2235:LEU:HG	1.37	1.03
1:A:4082:ARG:HG3	1:A:4091:ALA:HB2	1.40	1.03
1:A:963:LYS:NZ	1:A:1006:THR:OG1	1.92	1.02
1:B:90:CYS:HB3	1:B:137:THR:HG22	1.40	1.02
1:A:327:VAL:HG22	1:A:338:LEU:HD13	1.38	1.02
1:B:2887:PRO:HB3	1:B:2922:ARG:HH11	1.24	1.02
1:B:4071:ALA:O	1:B:4075:ARG:HB3	1.58	1.01
1:B:3917:ILE:O	1:B:4048:LYS:NZ	1.92	1.01
1:A:1491:ILE:O	1:A:1497:ARG:NH1	1.93	1.00
1:B:3284:SER:HB2	1:B:3287:ARG:HH21	1.23	1.00
1:A:974:CYS:HA	1:A:981:ARG:HD2	1.41	1.00
1:A:1808:ASP:HB2	1:A:1814:PHE:HB3	1.41	0.99
1:B:2216:LEU:HD22	1:B:2249:LEU:HD11	1.43	0.99
1:B:2166:SER:O	1:B:2170:GLN:HB3	1.60	0.99
1:A:1471:GLN:O	1:A:1475:LEU:HB3	1.63	0.98
1:B:985:GLU:HG3	1:B:1031:ARG:HH22	1.25	0.98
1:B:2879:GLY:HA2	1:B:2886:GLN:HG2	1.42	0.98
1:B:3284:SER:HA	1:B:3287:ARG:HE	1.24	0.98
1:B:3699:LEU:O	1:B:3718:ARG:NH1	1.97	0.98
1:A:4103:GLN:O	1:A:4107:LEU:HB2	1.64	0.98
1:B:963:LYS:NZ	1:B:1006:THR:OG1	1.96	0.98
1:A:3819:THR:OG1	1:A:3889:ARG:NH1	1.96	0.97
1:B:1959:LEU:HD13	1:B:1998:MSE:HE3	1.44	0.97
1:A:357:LYS:HB3	1:A:360:SER:HB2	1.46	0.97
1:B:366:TYR:O	1:B:369:PHE:HB3	1.62	0.97
1:A:366:TYR:O	1:A:369:PHE:HB3	1.63	0.97
1:B:357:LYS:HB3	1:B:360:SER:HB2	1.44	0.97
1:B:2424:MSE:HG2	1:B:2433:LYS:HD2	1.47	0.96
1:B:3923:ARG:HG2	1:B:3962:ARG:HH22	1.30	0.96
1:A:2943:PHE:HD1	1:A:2944:THR:H	1.13	0.96
1:B:1093:GLU:N	1:B:1097:GLU:OE2	1.98	0.96
1:A:2070:GLU:HG3	1:A:2072:ARG:HG3	1.47	0.96
1:B:2243:GLU:HA	1:B:2246:LYS:HD2	1.46	0.96
1:A:2375:ALA:O	1:A:2379:MSE:HB3	1.66	0.96
1:B:1249:SER:O	1:B:1253:THR:HB	1.64	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1435:ASN:OD1	1:B:1489:LYS:NZ	1.99	0.96
1:B:3931:ALA:O	1:B:3935:GLY:HA2	1.63	0.96
1:A:3182:ILE:HB	1:A:3186:ARG:NH1	1.80	0.95
1:A:3923:ARG:O	1:A:3962:ARG:NH1	1.98	0.95
1:A:385:TYR:HD1	1:A:420:VAL:HG13	1.30	0.95
1:B:3819:THR:OG1	1:B:3889:ARG:NH1	2.00	0.95
1:B:2228:ARG:NH1	1:B:2269:ASP:OD1	1.98	0.95
1:A:560:LEU:HB3	1:A:616:LYS:NZ	1.81	0.95
1:A:2962:ARG:HB2	1:A:3253:SER:HB3	1.47	0.95
1:B:440:VAL:HB	1:B:483:VAL:HG12	1.46	0.95
1:B:2308:SER:HB3	1:B:2348:GLN:HG2	1.49	0.95
1:B:2538:ARG:HH11	1:B:2565:MSE:HB3	1.32	0.95
1:B:801:LYS:NZ	1:B:877:ASP:OD2	2.00	0.95
1:A:1685:ASP:HB2	1:A:1727:ARG:HH22	1.28	0.94
1:B:3887:PHE:HB3	1:B:3897:PHE:HE1	1.31	0.94
1:A:1010:LEU:HB2	1:A:1028:PHE:CD1	2.02	0.94
1:A:1733:THR:HG21	1:A:1877:LEU:HB3	1.47	0.94
1:A:3885:ARG:HE	1:A:3889:ARG:HD2	1.32	0.94
1:A:1883:ARG:HB2	1:A:1927:MSE:HE1	1.48	0.94
1:B:3923:ARG:HG2	1:B:3962:ARG:NH2	1.82	0.94
1:B:2416:LYS:O	1:B:2420:PHE:HB3	1.68	0.94
1:B:3772:ASN:HD22	1:B:3788:LEU:H	1.16	0.94
1:B:3722:PHE:HE1	1:B:3740:ILE:HG12	1.31	0.93
1:B:753:GLN:O	1:B:757:LYS:HB2	1.68	0.93
1:A:3923:ARG:HG2	1:A:3962:ARG:NH2	1.83	0.93
1:B:3920:ILE:HG13	1:B:3923:ARG:HD2	1.50	0.93
1:B:977:ASP:HB2	1:B:981:ARG:HB3	1.50	0.93
1:B:2891:ARG:NH2	1:B:3884:LYS:HD3	1.81	0.93
1:B:61:ARG:O	1:B:65:LEU:HB2	1.68	0.93
1:A:2443:MSE:HE3	1:A:2476:ILE:HB	1.48	0.93
1:A:3789:ARG:NH2	1:A:3806:LEU:HD22	1.83	0.93
1:B:1966:LEU:HD22	1:B:1991:PRO:HB3	1.50	0.93
1:A:964:ARG:HB2	1:A:1009:LEU:HD22	1.49	0.93
1:A:3521:ILE:O	1:A:3525:TYR:CB	2.16	0.93
1:A:473:PRO:HA	1:A:476:ARG:HH22	1.33	0.93
1:B:760:LEU:HD11	1:B:799:TYR:HB2	1.48	0.93
1:A:2549:LYS:HZ1	1:A:2557:LEU:HD22	1.30	0.92
1:B:659:ARG:HH22	1:B:662:LEU:HG	1.33	0.92
1:B:3462:ARG:HB2	1:B:3498:TRP:HB3	1.47	0.92
1:A:2330:VAL:HG21	1:A:2338:GLU:HB3	1.52	0.92
1:A:2457:PRO:HA	1:A:2460:GLU:HB2	1.52	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3872:ARG:HH11	1:A:3965:ARG:NH1	1.67	0.92
1:B:1949:ILE:HD12	1:B:1952:ILE:HG21	1.51	0.92
1:B:2330:VAL:HG22	1:B:2335:ASN:HA	1.51	0.92
1:B:756:PHE:HA	1:B:773:LEU:HD13	1.50	0.92
1:B:1343:GLU:O	1:B:1347:THR:OG1	1.88	0.92
1:B:1729:PHE:HE2	1:B:1870:LYS:HA	1.32	0.91
1:B:2390:HIS:HA	1:B:2397:CYS:HB2	1.52	0.91
1:A:3462:ARG:HB2	1:A:3498:TRP:HB3	1.49	0.91
1:B:970:LEU:HD22	1:B:1031:ARG:HH21	1.34	0.91
1:B:2330:VAL:HG21	1:B:2338:GLU:HB3	1.52	0.91
1:B:2011:ALA:HB3	1:B:2014:ALA:HB2	1.50	0.91
1:A:363:ILE:O	1:A:367:GLY:N	2.03	0.91
1:A:2375:ALA:O	1:A:2379:MSE:CB	2.19	0.91
1:A:616:LYS:O	1:A:620:PHE:HB2	1.71	0.91
1:B:808:GLU:HG2	1:B:852:ARG:HH21	1.31	0.91
1:B:1107:TYR:O	1:B:1110:SER:HB2	1.71	0.91
1:B:2361:ILE:HD12	1:B:2364:LEU:HD12	1.49	0.91
1:B:2559:THR:HG21	1:B:2808:LEU:HD13	1.53	0.91
1:B:1743:MSE:SE	1:B:1880:MSE:SE	2.90	0.90
1:A:3498:TRP:CD1	1:A:3502:MSE:HB2	2.05	0.90
1:B:1010:LEU:HD13	1:B:1028:PHE:HE1	1.36	0.90
1:B:3839:TYR:HE1	1:B:3867:THR:HB	1.36	0.90
1:B:429:GLU:O	1:B:431:TYR:N	2.04	0.90
1:A:1905:ILE:HG12	1:A:1951:VAL:HG11	1.51	0.90
1:A:1987:ARG:O	1:A:1991:PRO:HD3	1.71	0.90
1:A:2837:LEU:HD22	1:A:2868:LEU:HG	1.51	0.90
1:A:1106:ILE:O	1:A:1110:SER:N	2.05	0.89
1:A:1155:ARG:NH1	1:A:1155:ARG:O	2.04	0.89
1:B:4082:ARG:HG3	1:B:4091:ALA:HB2	1.54	0.89
1:B:2562:LEU:HD12	1:B:2812:LEU:HD21	1.53	0.89
1:A:1090:ARG:HH21	1:A:1100:VAL:HG11	1.35	0.89
1:A:2467:THR:HB	1:A:2518:GLN:HE22	1.35	0.89
1:A:2552:VAL:HG23	1:A:2852:PRO:HG2	1.54	0.89
1:B:1552:HIS:O	1:B:1555:HIS:ND1	2.05	0.89
1:B:2142:ILE:HA	1:B:2145:PHE:CD2	2.07	0.89
1:A:429:GLU:O	1:A:431:TYR:N	2.06	0.89
1:B:2352:HIS:HB3	1:B:2360:PHE:HB3	1.54	0.89
1:B:1651:LYS:HB2	1:B:1684:LEU:HD11	1.53	0.89
1:B:3887:PHE:HB3	1:B:3897:PHE:CE1	2.08	0.89
1:A:1931:ASN:O	1:A:1938:ARG:NH2	2.06	0.89
1:A:3816:LEU:HD13	1:A:3966:GLN:HE22	1.36	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3696:ARG:NH1	1:A:3720:ALA:O	2.05	0.88
1:B:3259:LEU:O	1:B:3263:HIS:HB2	1.73	0.88
1:B:2891:ARG:HD3	1:B:3972:LEU:HD22	1.55	0.88
1:A:1729:PHE:HE2	1:A:1870:LYS:HA	1.39	0.88
1:A:2957:LEU:HB3	1:A:3989:ARG:NH1	1.87	0.88
1:B:993:HIS:HB2	1:B:1038:LYS:HG2	1.55	0.88
1:B:3048:LYS:HD3	1:B:3061:LEU:HD23	1.55	0.88
1:B:3762:GLN:HA	1:B:3793:VAL:HG21	1.54	0.88
1:B:473:PRO:HA	1:B:476:ARG:HH22	1.36	0.88
1:A:2390:HIS:HA	1:A:2397:CYS:HB2	1.54	0.88
1:B:1241:LEU:HD11	1:B:1253:THR:HG21	1.54	0.88
1:B:2326:ILE:O	1:B:2330:VAL:HB	1.74	0.88
1:A:1010:LEU:HB2	1:A:1028:PHE:HD1	1.36	0.88
1:B:3923:ARG:O	1:B:3962:ARG:NH1	2.07	0.88
1:A:3589:SER:O	1:A:3593:ARG:HB2	1.74	0.88
1:A:3772:ASN:HB2	1:A:3787:GLN:HG3	1.55	0.88
1:A:801:LYS:HB2	1:A:805:LEU:HD12	1.56	0.88
1:B:1582:LEU:HD22	1:B:1600:MSE:HE1	1.52	0.88
1:A:3772:ASN:ND2	1:A:3788:LEU:O	2.06	0.88
1:A:90:CYS:HB3	1:A:137:THR:HG22	1.56	0.88
1:A:185:HIS:H	1:A:186:PRO:HD2	1.38	0.88
1:A:2022:PRO:HB2	1:A:2072:ARG:HH21	1.36	0.88
1:A:658:THR:HA	1:A:733:LEU:HD22	1.55	0.88
1:B:1018:VAL:HB	1:B:1074:LYS:HB2	1.54	0.88
1:B:741:ILE:O	1:B:744:ASP:N	2.05	0.88
1:B:662:LEU:O	1:B:666:PHE:CB	2.20	0.87
1:B:658:THR:HA	1:B:733:LEU:HD22	1.55	0.87
1:A:473:PRO:HA	1:A:476:ARG:NH2	1.88	0.87
1:A:535:LEU:HD21	1:A:623:PHE:HA	1.55	0.87
1:B:1808:ASP:HB2	1:B:1814:PHE:HB3	1.54	0.87
1:B:2546:TYR:CE1	1:B:2558:ALA:HB2	2.09	0.87
1:A:105:VAL:HG21	1:A:149:ILE:HD13	1.53	0.87
1:B:252:VAL:HG11	1:B:265:TYR:HB2	1.56	0.87
1:A:3003:ASN:ND2	1:A:3014:CYS:SG	2.47	0.87
1:A:2378:PHE:HE1	1:A:2408:MSE:HE1	1.40	0.87
1:B:2307:MSE:HB3	1:B:2348:GLN:HE22	1.39	0.87
1:A:2477:LEU:O	1:A:2481:HIS:HB3	1.74	0.87
1:B:591:GLN:OE1	1:B:1026:ARG:NH1	2.08	0.87
1:B:2253:TYR:HD1	1:B:2256:ILE:HD12	1.37	0.86
1:A:866:ILE:HD13	1:A:3129:LEU:HB3	1.57	0.86
1:B:3530:VAL:HG11	1:B:3702:PRO:HD3	1.55	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1107:TYR:O	1:A:1110:SER:HB2	1.74	0.86
1:A:3492:CYS:O	1:A:3495:PHE:HB3	1.74	0.86
1:B:2286:PRO:HB2	1:B:2289:ASP:HA	1.57	0.86
1:A:1407:LYS:O	1:A:1409:SER:N	2.08	0.86
1:A:1919:CYS:O	1:A:1923:PHE:HB2	1.76	0.86
1:A:793:LEU:HA	1:A:796:LEU:HG	1.58	0.86
1:A:2563:LEU:O	1:A:2567:SER:OG	1.93	0.86
1:B:2837:LEU:HA	1:B:2840:PHE:HD2	1.40	0.86
1:A:1603:GLN:OE1	1:A:1606:ARG:NH2	2.08	0.86
1:A:4071:ALA:O	1:A:4075:ARG:HB3	1.76	0.86
1:B:2253:TYR:HB2	1:B:2291:GLN:HG2	1.56	0.86
1:B:2443:MSE:SE	1:B:2476:ILE:HB	2.25	0.86
1:A:1749:ALA:HA	1:A:1752:LEU:HD12	1.55	0.86
1:B:3167:ARG:HH11	1:B:3167:ARG:HG3	1.40	0.86
1:B:658:THR:HG22	1:B:659:ARG:NH1	1.89	0.86
1:A:3326:GLN:HB2	1:A:3393:GLU:HG2	1.56	0.86
1:A:659:ARG:HH22	1:A:662:LEU:HG	1.41	0.86
1:A:1762:MSE:SE	1:A:1896:ILE:HG23	2.26	0.85
1:A:3581:PRO:HG2	1:A:3674:SER:HB2	1.58	0.85
1:B:1733:THR:HG21	1:B:1877:LEU:HB3	1.55	0.85
1:A:2142:ILE:HA	1:A:2145:PHE:CD2	2.11	0.85
1:B:745:VAL:HG11	1:B:776:TRP:HZ2	1.39	0.85
1:A:527:TYR:OH	1:A:615:ALA:O	1.93	0.85
1:A:1010:LEU:HA	1:A:1013:ILE:HG12	1.56	0.85
1:B:2358:ASP:HB2	1:B:2396:LEU:HD21	1.57	0.85
1:B:3326:GLN:HB2	1:B:3393:GLU:HG2	1.57	0.85
1:B:3868:VAL:O	1:B:3872:ARG:CB	2.24	0.85
1:A:3613:MSE:HE1	1:A:3617:LEU:HD12	1.56	0.85
1:A:4007:LYS:HG3	1:A:4041:ARG:HD2	1.55	0.85
1:B:3632:PHE:O	1:B:3637:GLY:N	2.08	0.85
1:A:2330:VAL:HG22	1:A:2335:ASN:HA	1.57	0.85
1:B:3487:ILE:HG21	1:B:3495:PHE:HB2	1.58	0.85
1:B:725:LEU:O	1:B:728:SER:OG	1.94	0.85
1:A:2043:PHE:O	1:A:2047:THR:OG1	1.93	0.85
1:B:2227:LYS:HD2	1:B:2235:LEU:HG	1.58	0.85
1:B:2375:ALA:O	1:B:2379:MSE:HB3	1.76	0.85
1:B:2478:MSE:O	1:B:2482:ASP:HB3	1.76	0.85
1:A:971:ARG:HG3	1:A:972:LEU:N	1.90	0.85
1:A:2007:ILE:HG22	1:A:2009:LYS:HB2	1.57	0.85
1:B:2070:GLU:HG3	1:B:2072:ARG:HG3	1.57	0.85
1:B:3589:SER:O	1:B:3593:ARG:HB2	1.77	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:974:CYS:HA	1:A:981:ARG:CD	2.07	0.84
1:B:1010:LEU:HB2	1:B:1028:PHE:HD1	1.40	0.84
1:B:2481:HIS:HE1	1:B:2485:ARG:NH1	1.75	0.84
1:B:3583:LEU:HD11	1:B:3733:ARG:HB3	1.57	0.84
1:A:2161:ALA:HA	1:A:2164:TRP:HD1	1.42	0.84
1:B:2300:PHE:CZ	1:B:2341:LEU:HB2	2.12	0.84
1:B:3811:THR:OG1	1:B:3813:LYS:NZ	2.09	0.84
1:A:2292:CYS:HB3	1:A:2300:PHE:HB2	1.57	0.84
1:A:2837:LEU:HA	1:A:2840:PHE:HD2	1.41	0.84
1:B:2196:TRP:CD2	1:B:2199:LEU:HD11	2.12	0.84
1:B:3182:ILE:HB	1:B:3186:ARG:NH1	1.91	0.84
1:A:286:LEU:HB2	1:A:290:TYR:HB2	1.59	0.84
1:B:978:GLN:HA	1:B:981:ARG:HE	1.42	0.84
1:B:3243:ILE:HG12	1:B:3258:LEU:HD11	1.58	0.84
1:B:3725:ARG:HH12	1:B:3737:ARG:NH2	1.74	0.84
1:B:3879:PRO:HA	1:B:3882:LEU:HB2	1.58	0.84
1:A:3174:ASP:H	1:A:3175:PRO:HD2	1.42	0.84
1:A:3868:VAL:HG11	1:A:4114:PRO:HB3	1.60	0.84
1:B:3117:ILE:HD12	1:B:3125:ARG:NH1	1.91	0.84
1:A:3092:LEU:HA	1:A:3192:LYS:HE3	1.58	0.84
1:A:361:ILE:HB	1:A:364:ARG:NH2	1.92	0.84
1:B:1162:SER:H	1:B:1165:LEU:HD12	1.42	0.84
1:B:2552:VAL:HG23	1:B:2852:PRO:HG2	1.57	0.84
1:B:3486:GLU:HG3	1:B:3487:ILE:H	1.43	0.84
1:B:3858:MSE:HE3	1:B:4119:ARG:HA	1.60	0.84
1:B:2161:ALA:HA	1:B:2164:TRP:HD1	1.43	0.84
1:B:2329:TYR:O	1:B:2333:ARG:N	2.11	0.84
1:A:1410:PRO:HB2	1:A:1414:ILE:HD12	1.58	0.84
1:A:1743:MSE:O	1:A:1747:LEU:HB2	1.78	0.83
1:A:1992:VAL:O	1:A:1996:VAL:HG22	1.78	0.83
1:A:2542:LEU:HB2	1:A:2546:TYR:HE2	1.42	0.83
1:B:3687:MSE:O	1:B:3689:ASP:N	2.11	0.83
1:B:2152:ASN:HB3	1:B:2153:THR:HA	1.60	0.83
1:B:3900:LEU:HD21	1:B:3935:GLY:HA3	1.59	0.83
1:B:4103:GLN:O	1:B:4107:LEU:HB2	1.77	0.83
1:A:2415:LEU:O	1:A:2419:ASP:HB2	1.78	0.83
1:A:968:VAL:HG23	1:A:971:ARG:HD3	1.60	0.83
1:B:2813:PHE:HD2	1:B:2859:GLN:HG3	1.43	0.83
1:B:3499:ILE:HG23	1:B:3535:ILE:HD13	1.60	0.83
1:B:971:ARG:HG3	1:B:972:LEU:N	1.93	0.83
1:A:352:VAL:HG23	1:A:357:LYS:H	1.43	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3521:ILE:O	1:B:3525:TYR:CB	2.27	0.83
1:B:2274:ILE:HD13	1:B:2318:ALA:HB2	1.60	0.83
1:A:4090:ARG:HH11	1:A:4106:CYS:HA	1.41	0.83
1:A:61:ARG:O	1:A:65:LEU:HB2	1.77	0.83
1:B:1073:PHE:HD1	1:B:1074:LYS:H	1.27	0.83
1:B:609:ALA:H	1:B:1798:LEU:HD12	1.43	0.83
1:B:3725:ARG:NH1	1:B:3737:ARG:HH22	1.76	0.83
2:K:106:UNK:O	2:K:110:UNK:N	2.11	0.83
1:A:2361:ILE:HD12	1:A:2364:LEU:HD12	1.61	0.83
1:A:2478:MSE:O	1:A:2482:ASP:HB3	1.78	0.83
1:B:658:THR:HG22	1:B:659:ARG:HH11	1.41	0.83
1:A:1886:LYS:HZ2	1:A:1924:THR:HB	1.44	0.83
1:B:215:PRO:HG3	1:B:251:PHE:HB3	1.59	0.83
1:B:2435:CYS:O	1:B:2439:ILE:HB	1.77	0.83
1:B:245:SER:HA	1:B:248:ILE:HD12	1.58	0.83
1:B:1087:ARG:HD3	1:B:1134:LEU:HB3	1.60	0.83
1:B:3012:GLU:HB2	1:B:3050:LYS:NZ	1.94	0.83
1:A:575:ILE:HA	1:A:578:LYS:HB2	1.61	0.83
1:B:3034:PRO:HG2	1:B:3037:GLN:HB2	1.61	0.83
1:A:1138:ILE:HD13	1:A:1150:LYS:HE2	1.60	0.82
1:A:3961:PHE:CE1	1:A:3963:LEU:HB2	2.14	0.82
1:A:3972:LEU:O	1:A:3974:MSE:N	2.10	0.82
1:B:2957:LEU:HD22	1:B:4100:GLU:HG3	1.61	0.82
1:B:1010:LEU:HB2	1:B:1028:PHE:CD1	2.14	0.82
1:B:598:PRO:HB3	1:B:1022:ASP:HB2	1.59	0.82
1:A:1751:GLU:O	1:A:1755:SER:N	2.11	0.82
1:B:3737:ARG:HH11	1:B:3739:ILE:HD11	1.43	0.82
1:B:3816:LEU:HD21	1:B:3883:LEU:HD13	1.59	0.82
1:A:1651:LYS:HB3	1:A:1680:ALA:HB1	1.59	0.82
1:A:2196:TRP:CD2	1:A:2199:LEU:HD11	2.14	0.82
1:A:1007:VAL:O	1:A:1011:GLU:HB2	1.79	0.82
1:A:2002:LYS:O	1:A:2004:TYR:N	2.12	0.82
1:A:1070:PRO:HB2	1:A:1073:PHE:CZ	2.14	0.82
1:A:2049:VAL:HA	1:A:2052:TYR:HD2	1.42	0.82
1:A:203:GLU:O	1:A:207:GLN:HB2	1.78	0.82
1:A:3722:PHE:HE1	1:A:3740:ILE:HG12	1.44	0.82
1:A:4057:ALA:HB3	1:A:4059:ILE:HB	1.60	0.82
1:B:3751:LEU:O	1:B:3802:LEU:HG	1.80	0.82
1:A:3789:ARG:HH22	1:A:3806:LEU:HD22	1.42	0.82
1:A:70:ARG:HD3	1:A:82:ARG:HD3	1.59	0.82
1:A:959:TYR:O	1:A:963:LYS:HB2	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2375:ALA:O	1:B:2379:MSE:CB	2.28	0.82
1:B:488:ILE:HG21	1:B:616:LYS:HD2	1.60	0.82
1:A:3152:SER:HB3	1:A:3153:SER:HB3	1.61	0.82
1:B:1346:THR:HG21	1:B:1401:ASN:HB3	1.62	0.82
1:B:1729:PHE:CE2	1:B:1870:LYS:HA	2.15	0.82
1:A:3820:MSE:HA	1:A:3882:LEU:HD22	1.62	0.81
1:A:978:GLN:HA	1:A:981:ARG:HE	1.44	0.81
1:B:2126:MSE:HG3	1:B:2129:LEU:HD12	1.61	0.81
1:B:2531:LEU:HG	1:B:2538:ARG:HB2	1.62	0.81
1:B:974:CYS:HA	1:B:981:ARG:CD	2.07	0.81
1:A:3872:ARG:O	1:A:3876:SER:OG	1.98	0.81
1:B:3449:LYS:HA	1:B:3452:LYS:HD2	1.62	0.81
1:B:956:PRO:HB2	1:B:957:PRO:HD3	1.62	0.81
1:A:1155:ARG:HH12	1:A:1159:PRO:HD3	1.45	0.81
1:A:1696:LEU:HA	1:A:1700:THR:HG21	1.61	0.81
1:A:3762:GLN:HA	1:A:3793:VAL:HG21	1.62	0.81
1:B:1744:LYS:HG3	1:B:1880:MSE:HE3	1.60	0.81
1:B:1729:PHE:CZ	1:B:1870:LYS:HG3	2.15	0.81
1:B:1930:GLU:N	1:B:1930:GLU:OE2	2.13	0.81
1:B:3044:MSE:O	1:B:3047:SER:OG	1.96	0.81
1:A:2167:PRO:O	1:A:2171:LEU:CB	2.28	0.81
1:B:1987:ARG:O	1:B:1991:PRO:HD3	1.80	0.81
1:A:2167:PRO:O	1:A:2171:LEU:HB2	1.79	0.81
1:B:3498:TRP:CD1	1:B:3502:MSE:HB2	2.14	0.81
1:B:3572:ILE:HA	1:B:3575:LEU:HD22	1.62	0.81
1:A:2538:ARG:NH1	1:A:2562:LEU:O	2.13	0.81
1:A:3269:ARG:NH1	1:A:3312:VAL:HA	1.96	0.81
1:B:1877:LEU:O	1:B:1920:TYR:OH	1.98	0.81
1:B:3238:MSE:SE	1:B:3242:MSE:SE	2.99	0.81
1:B:431:TYR:HA	1:B:434:VAL:HG12	1.63	0.81
1:A:1080:LEU:HD12	1:A:1081:ALA:H	1.46	0.81
1:B:2260:PHE:HD1	1:B:2274:ILE:HG22	1.46	0.81
1:B:916:GLU:HB3	1:B:930:ALA:HB1	1.63	0.81
1:A:741:ILE:O	1:A:744:ASP:N	2.09	0.81
1:B:2031:LEU:HB2	1:B:2033:ASP:HB2	1.61	0.81
1:A:1729:PHE:CZ	1:A:1870:LYS:HG3	2.16	0.81
1:A:2239:LYS:HG3	1:A:2279:ILE:HG23	1.62	0.81
1:A:3319:ASN:HD22	1:A:3407:ALA:HB1	1.45	0.81
1:A:382:ASP:O	1:A:386:VAL:HB	1.79	0.81
1:B:1017:ILE:HG21	1:B:1025:LEU:HD22	1.63	0.81
1:A:1594:SER:O	1:A:1598:ASN:HB2	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1090:ARG:HH21	1:B:1100:VAL:HG11	1.45	0.81
1:A:977:ASP:HB3	1:A:981:ARG:H	1.46	0.81
1:B:2379:MSE:HE1	1:B:2404:ARG:HD3	1.61	0.81
1:B:2446:LEU:O	1:B:2451:LEU:HB2	1.81	0.81
1:B:891:ARG:HE	1:B:894:PHE:HB3	1.46	0.81
1:A:970:LEU:CD2	1:A:1031:ARG:HH21	1.94	0.80
1:A:1552:HIS:O	1:A:1555:HIS:ND1	2.14	0.80
1:B:959:TYR:O	1:B:963:LYS:HB2	1.81	0.80
1:A:3872:ARG:HH11	1:A:3965:ARG:HH12	1.27	0.80
1:A:459:ARG:HG2	1:A:540:MSE:HE1	1.60	0.80
1:B:1729:PHE:HZ	1:B:1870:LYS:HG3	1.45	0.80
1:B:3530:VAL:HG21	1:B:3701:ILE:HA	1.63	0.80
1:A:2559:THR:HG21	1:A:2808:LEU:HD13	1.61	0.80
1:A:805:LEU:HD22	1:A:3125:ARG:HH11	1.45	0.80
1:B:1090:ARG:HH12	1:B:1096:VAL:HG13	1.45	0.80
1:B:893:SER:HB3	1:B:906:PHE:HB2	1.63	0.80
1:B:931:CYS:SG	1:B:984:TYR:OH	2.39	0.80
1:A:2243:GLU:HA	1:A:2246:LYS:HD2	1.63	0.80
1:B:266:ALA:HB2	1:B:308:LEU:HG	1.63	0.80
1:A:3638:LYS:HA	1:A:3641:ASP:HB2	1.63	0.80
1:A:369:PHE:CD1	1:A:416:SER:HA	2.17	0.80
1:A:619:ASP:O	1:A:622:ALA:N	2.14	0.80
1:B:2253:TYR:CD1	1:B:2256:ILE:HD12	2.16	0.80
1:A:725:LEU:O	1:A:728:SER:OG	1.99	0.80
1:B:1996:VAL:HG11	1:B:2048:GLY:HA2	1.63	0.80
1:A:3046:ARG:NH2	1:A:3181:ASP:OD2	2.14	0.80
1:A:939:MSE:SE	1:A:2783:ILE:HG12	2.30	0.80
1:A:627:VAL:HG12	1:A:628:GLU:H	1.46	0.80
1:B:295:GLU:HA	1:B:298:LEU:HD22	1.63	0.80
1:A:705:ALA:HB1	1:A:1385:ASN:HD21	1.46	0.79
1:A:1429:GLU:O	1:A:1433:ALA:HB2	1.81	0.79
1:B:16:GLN:O	1:B:20:SER:HB3	1.81	0.79
1:B:3255:ALA:O	1:B:3282:ARG:NH2	2.15	0.79
1:B:1112:ALA:HA	1:B:1115:HIS:CE1	2.17	0.79
1:B:2546:TYR:HE1	1:B:2558:ALA:HB2	1.43	0.79
1:A:2861:ILE:HG21	1:A:2889:GLY:HA2	1.61	0.79
1:B:286:LEU:HB2	1:B:290:TYR:HB2	1.65	0.79
1:B:3252:PHE:HA	1:B:3282:ARG:HD2	1.65	0.79
1:B:1918:LEU:HD11	1:B:1957:ASN:HB3	1.63	0.79
1:B:2423:VAL:O	1:B:2425:ARG:N	2.15	0.79
1:B:2837:LEU:HD22	1:B:2868:LEU:HG	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2987:THR:HB	1:B:2991:LYS:H	1.46	0.79
1:B:726:LEU:HA	1:B:729:CYS:SG	2.22	0.79
1:A:1886:LYS:HG3	1:A:1890:HIS:HE1	1.46	0.79
1:A:770:LEU:HD12	1:A:851:ILE:HD13	1.61	0.79
1:B:1410:PRO:HB2	1:B:1414:ILE:HD12	1.64	0.79
1:A:2474:TYR:HB3	1:A:2478:MSE:HE3	1.64	0.79
1:A:3989:ARG:HH21	1:A:4100:GLU:CB	1.95	0.79
1:B:12:LEU:HD22	1:B:38:LEU:HA	1.65	0.79
1:A:3450:MSE:SE	1:A:3464:LYS:HG2	2.33	0.79
1:B:637:LYS:O	1:B:641:PHE:HB3	1.81	0.79
1:A:2351:GLN:O	1:A:2355:THR:OG1	2.00	0.79
1:B:1718:ILE:HG23	1:B:1750:LEU:HD11	1.62	0.79
1:B:298:LEU:HD23	1:B:316:LEU:HD13	1.62	0.79
1:A:1000:LYS:O	1:A:1002:GLU:N	2.15	0.79
1:A:767:GLU:HG3	1:A:851:ILE:HD11	1.65	0.79
1:A:796:LEU:HA	1:A:799:TYR:CE2	2.18	0.79
1:B:1655:ILE:HG23	1:B:1677:SER:HB3	1.65	0.79
1:B:2121:ASP:HA	1:B:2126:MSE:HB3	1.63	0.79
1:B:2443:MSE:HB3	1:B:2480:ILE:HG12	1.65	0.79
1:A:162:LEU:HD21	1:A:196:LEU:HD13	1.65	0.79
1:A:3955:VAL:HG12	1:A:4027:TRP:HE1	1.47	0.79
1:B:527:TYR:OH	1:B:619:ASP:N	2.16	0.79
1:B:627:VAL:HG12	1:B:628:GLU:H	1.46	0.79
1:A:3314:SER:HA	1:A:3315:TYR:HB3	1.64	0.78
1:A:3397:GLN:HE22	1:A:3449:LYS:HD3	1.49	0.78
1:A:714:VAL:HG13	1:A:734:LEU:HD13	1.65	0.78
1:B:1011:GLU:OE2	1:B:1062:ARG:NE	2.17	0.78
1:B:1029:CYS:HB3	1:B:1085:ILE:HG13	1.63	0.78
1:A:2890:ILE:HG21	1:A:2922:ARG:HH12	1.49	0.78
1:B:1762:MSE:SE	1:B:1896:ILE:HG23	2.33	0.78
1:B:2100:LEU:O	1:B:2104:MSE:HB2	1.82	0.78
1:B:2153:THR:OG1	1:B:2154:GLU:N	2.14	0.78
1:A:3736:LYS:HB3	1:A:3752:VAL:HB	1.64	0.78
1:A:3868:VAL:O	1:A:3872:ARG:CB	2.29	0.78
1:B:1986:ARG:HH12	1:B:2036:LEU:HD22	1.46	0.78
1:A:15:LEU:HD23	1:A:2359:LYS:HZ3	1.48	0.78
1:A:2379:MSE:HE1	1:A:2404:ARG:HH11	1.49	0.78
1:A:903:PRO:HB2	1:A:2811:SER:HB2	1.65	0.78
1:B:1802:TYR:HA	1:B:1805:PHE:HD2	1.47	0.78
1:B:2911:ARG:HG2	1:B:2914:ALA:HB3	1.66	0.78
1:B:538:ASP:HB3	1:B:627:VAL:HG13	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3499:ILE:HG23	1:A:3535:ILE:HD13	1.63	0.78
1:A:3904:PHE:O	1:A:3907:SER:OG	2.01	0.78
1:B:3529:ILE:HG23	1:B:3532:PRO:HD2	1.63	0.78
1:B:439:VAL:HG11	1:B:479:ILE:HD13	1.65	0.78
1:A:2467:THR:HA	1:A:2470:ARG:HG3	1.64	0.78
1:A:376:ILE:HG13	1:A:381:VAL:HG21	1.65	0.78
1:B:808:GLU:CG	1:B:852:ARG:HH21	1.96	0.78
1:A:960:GLN:HG3	1:A:1009:LEU:HD21	1.65	0.78
1:B:3575:LEU:HG	1:B:3687:MSE:HG2	1.65	0.78
1:B:3923:ARG:NH2	1:B:3941:ASP:O	2.17	0.78
1:A:980:THR:HG23	1:A:984:TYR:HE1	1.49	0.78
1:B:281:GLN:HA	1:B:326:MSE:SE	2.34	0.78
1:A:1582:LEU:HD22	1:A:1600:MSE:HE1	1.66	0.77
1:A:3922:ASP:O	1:A:3927:ASN:ND2	2.17	0.77
1:B:2538:ARG:NH1	1:B:2565:MSE:HB3	1.98	0.77
1:B:3421:ASP:OD2	1:B:3464:LYS:NZ	2.16	0.77
1:A:87:LYS:HG2	1:A:133:LYS:HG3	1.66	0.77
1:A:1886:LYS:HG3	1:A:1890:HIS:CE1	2.19	0.77
1:A:2190:VAL:HG21	1:A:2241:LEU:HD13	1.66	0.77
1:A:3479:THR:O	1:A:3483:MSE:HB2	1.83	0.77
1:B:1407:LYS:O	1:B:1409:SER:N	2.14	0.77
1:B:2193:ILE:HA	1:B:2196:TRP:CZ2	2.20	0.77
1:B:909:VAL:HG13	1:B:913:ARG:NH1	1.96	0.77
1:A:1640:GLU:O	1:A:1644:ALA:HB2	1.85	0.77
1:A:1890:HIS:HB3	1:A:1937:ARG:HA	1.65	0.77
1:A:2253:TYR:CD1	1:A:2256:ILE:HD12	2.18	0.77
1:A:2879:GLY:HA2	1:A:2886:GLN:HG2	1.65	0.77
1:B:3684:SER:O	1:B:3688:SER:OG	2.01	0.77
1:B:3732:LEU:HD21	1:B:3926:ASN:HD21	1.48	0.77
1:A:1073:PHE:HD1	1:A:1074:LYS:H	1.30	0.77
1:A:1374:GLN:HB3	1:A:1377:CYS:HB3	1.64	0.77
1:A:1590:THR:O	1:A:1592:MSE:N	2.16	0.77
1:A:1718:ILE:HA	1:A:1725:GLN:HE21	1.50	0.77
1:A:1946:ASN:ND2	1:A:1993:GLU:OE2	2.17	0.77
1:B:2235:LEU:O	1:B:2239:LYS:N	2.16	0.77
1:B:2457:PRO:HA	1:B:2460:GLU:HB2	1.66	0.77
1:B:3137:GLU:OE1	1:B:3167:ARG:NH1	2.18	0.77
1:B:805:LEU:HD22	1:B:3125:ARG:NH1	2.00	0.77
1:B:979:VAL:HG21	1:B:2656:UNK:HA	1.66	0.77
1:A:2412:TYR:HE1	1:A:2415:LEU:HD23	1.48	0.77
1:A:2467:THR:HG22	1:A:2470:ARG:NH1	2.00	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:SER:O	1:A:556:SER:OG	2.02	0.77
1:A:977:ASP:HB2	1:A:981:ARG:HB3	1.64	0.77
1:B:1080:LEU:HD13	1:B:1127:CYS:HB3	1.66	0.77
1:A:2083:LEU:O	1:A:2087:GLU:N	2.17	0.77
1:A:2161:ALA:HA	1:A:2164:TRP:CD1	2.19	0.77
1:A:2847:THR:HB	1:A:2850:PHE:CD2	2.20	0.77
1:A:2891:ARG:NH2	1:A:3884:LYS:HD3	2.00	0.77
1:B:2300:PHE:HZ	1:B:2341:LEU:HB2	1.46	0.77
1:B:3148:GLN:HB2	1:B:3156:PRO:HB3	1.67	0.77
1:B:852:ARG:NH1	1:B:3111:MSE:SE	2.68	0.77
1:A:2049:VAL:HG11	1:A:2100:LEU:HD12	1.66	0.77
1:A:2890:ILE:HG21	1:A:2922:ARG:NH1	2.00	0.77
1:B:2459:VAL:HG21	1:B:2501:LEU:HD21	1.67	0.77
1:B:4057:ALA:HB3	1:B:4059:ILE:HB	1.65	0.77
1:A:2462:VAL:HB	1:A:2473:MSE:SE	2.35	0.77
1:A:3704:GLN:HB2	1:A:3796:MSE:HE2	1.66	0.77
1:A:3813:LYS:HE2	1:A:3926:ASN:HB2	1.67	0.77
1:A:67:VAL:O	1:A:71:LYS:HB2	1.83	0.77
1:B:2236:GLU:HA	1:B:2239:LYS:HB3	1.67	0.77
1:B:936:SER:HB3	1:B:2791:ILE:HG12	1.66	0.77
1:B:3152:SER:HB3	1:B:3153:SER:HB3	1.65	0.77
1:B:3923:ARG:CG	1:B:3962:ARG:HH22	1.97	0.77
1:B:385:TYR:HD1	1:B:420:VAL:HG13	1.49	0.77
1:B:446:PHE:HA	1:B:449:TYR:CE2	2.20	0.77
1:A:1343:GLU:O	1:A:1347:THR:HB	1.85	0.77
1:A:753:GLN:O	1:A:757:LYS:HB2	1.84	0.77
1:B:1350:ASN:HD21	1:B:1404:LYS:HG2	1.47	0.77
1:B:1919:CYS:O	1:B:1923:PHE:HB2	1.85	0.77
1:B:323:VAL:O	1:B:327:VAL:HB	1.84	0.77
1:B:1469:PRO:HA	1:B:1472:SER:HB3	1.67	0.77
1:A:1356:TRP:CZ2	1:A:1409:SER:HB3	2.20	0.76
1:A:2220:MSE:SE	1:A:2256:ILE:HD11	2.34	0.76
1:A:2239:LYS:O	1:A:2242:VAL:HB	1.85	0.76
1:A:2560:ASN:HB2	1:A:2800:ARG:HD3	1.66	0.76
1:B:2382:VAL:HG21	1:B:2404:ARG:HG3	1.64	0.76
1:B:3590:ASN:OD1	1:B:3593:ARG:NH2	2.18	0.76
1:A:1086:TYR:HE2	1:A:1090:ARG:HE	1.33	0.76
1:A:1930:GLU:OE1	1:A:1987:ARG:NH1	2.18	0.76
1:A:2809:PHE:HB3	1:A:2859:GLN:NE2	1.99	0.76
1:A:46:SER:H	1:A:51:LEU:HD13	1.49	0.76
1:B:16:GLN:O	1:B:20:SER:CB	2.32	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:942:LEU:HD22	1:B:2783:ILE:HG21	1.67	0.76
1:A:1081:ALA:O	1:A:1085:ILE:HG12	1.86	0.76
1:A:3057:ALA:HB1	1:A:3062:LEU:HD11	1.67	0.76
1:A:805:LEU:CD2	1:A:3125:ARG:HH11	1.99	0.76
1:B:1987:ARG:O	1:B:1990:PHE:N	2.18	0.76
1:A:2253:TYR:CE2	1:A:2287:PRO:HB3	2.19	0.76
1:A:890:LYS:HG3	1:A:891:ARG:HD3	1.66	0.76
1:B:2473:MSE:O	1:B:2476:ILE:HG12	1.85	0.76
1:B:3019:ILE:HG23	1:B:3021:SER:H	1.51	0.76
1:A:1966:LEU:HD22	1:A:1991:PRO:HB3	1.66	0.76
1:B:1594:SER:O	1:B:1598:ASN:HB2	1.85	0.76
1:B:2147:ALA:HB1	1:B:2151:ILE:HD12	1.67	0.76
1:B:2281:MSE:HE2	1:B:2322:VAL:HA	1.66	0.76
1:B:2883:SER:O	1:B:2886:GLN:HG3	1.84	0.76
1:A:2397:CYS:O	1:A:2401:VAL:HB	1.86	0.76
1:A:971:ARG:HG3	1:A:972:LEU:H	1.50	0.76
1:B:3479:THR:O	1:B:3483:MSE:HB2	1.86	0.76
1:B:891:ARG:HE	1:B:894:PHE:CB	1.99	0.76
1:A:3243:ILE:HD13	1:A:3262:LEU:HD22	1.65	0.76
1:A:385:TYR:CD1	1:A:420:VAL:HG13	2.18	0.76
1:A:638:GLN:HE22	1:A:669:LEU:HB2	1.51	0.76
1:B:1178:ARG:HB3	1:B:1179:PRO:HD3	1.68	0.76
1:B:185:HIS:H	1:B:186:PRO:HD2	1.49	0.76
1:B:2453:GLU:O	1:B:2457:PRO:HD3	1.85	0.76
1:A:1655:ILE:HD13	1:A:1681:ASP:HB3	1.68	0.76
1:A:2364:LEU:O	1:A:2368:THR:OG1	2.03	0.76
1:B:1138:ILE:HG21	1:B:1150:LYS:HE2	1.68	0.76
1:B:2891:ARG:HH22	1:B:3884:LYS:CD	1.88	0.76
1:B:3629:ARG:HH22	1:B:3638:LYS:NZ	1.84	0.76
1:B:576:VAL:HG13	1:B:601:TRP:HE3	1.51	0.76
1:A:3019:ILE:HG23	1:A:3021:SER:H	1.49	0.76
1:B:1091:GLU:HG2	1:B:1137:ILE:HG21	1.68	0.76
1:B:138:PHE:HD2	1:B:173:LYS:HE3	1.51	0.76
1:B:904:VAL:O	1:B:906:PHE:N	2.18	0.76
1:A:1700:THR:HA	1:A:1703:THR:HB	1.67	0.76
1:A:2313:LYS:HA	1:A:2316:TYR:CE2	2.21	0.76
1:B:1036:PHE:HA	1:B:1055:ASN:HD21	1.50	0.76
1:B:1070:PRO:HD3	1:B:1075:ARG:HD2	1.67	0.76
1:B:3534:ILE:HG12	1:B:3704:GLN:NE2	1.99	0.76
1:A:1007:VAL:O	1:A:1011:GLU:CB	2.33	0.75
1:A:1060:PHE:HA	1:A:1063:LEU:HD12	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:LEU:H	1:A:143:LEU:HD12	1.51	0.75
1:A:3176:MSE:HE2	1:A:3251:ASN:ND2	2.01	0.75
1:A:891:ARG:HG3	1:A:894:PHE:HB2	1.68	0.75
1:A:926:THR:O	1:A:930:ALA:HB3	1.85	0.75
1:A:3487:ILE:HG21	1:A:3495:PHE:HB2	1.67	0.75
1:A:661:PRO:HG2	1:A:733:LEU:HA	1.67	0.75
1:B:2062:ALA:HB1	1:B:2066:PHE:HE2	1.52	0.75
1:B:2542:LEU:HB2	1:B:2546:TYR:HE2	1.51	0.75
1:B:3520:GLU:OE1	1:B:3524:ASN:ND2	2.19	0.75
1:B:3872:ARG:O	1:B:3876:SER:OG	2.00	0.75
1:B:3989:ARG:HH21	1:B:4100:GLU:CG	1.99	0.75
1:A:2183:HIS:CE1	1:A:2237:ILE:HG21	2.21	0.75
1:A:3487:ILE:HD11	1:A:3498:TRP:HH2	1.51	0.75
1:B:19:LEU:O	1:B:23:ASP:CB	2.33	0.75
1:B:3284:SER:CB	1:B:3287:ARG:HH21	1.99	0.75
1:B:608:PRO:HG2	1:B:1798:LEU:HG	1.68	0.75
1:A:1637:SER:O	1:A:1640:GLU:N	2.19	0.75
1:A:1751:GLU:HG2	1:A:1870:LYS:HE2	1.68	0.75
1:A:3305:SER:HA	1:A:3308:ASP:HB3	1.68	0.75
1:A:1587:VAL:HB	1:A:1643:MSE:HE2	1.68	0.75
1:A:2449:VAL:HA	1:A:2452:ARG:HD2	1.67	0.75
1:A:1118:GLU:HG3	1:A:3743:HIS:HE1	1.51	0.75
1:A:3979:LEU:HA	1:A:3981:TYR:HB3	1.67	0.75
1:B:1039:TRP:HZ2	1:B:1049:GLN:HA	1.52	0.75
1:B:1356:TRP:CZ2	1:B:1409:SER:HB3	2.22	0.75
1:B:153:PHE:HB2	1:B:157:TYR:HE2	1.52	0.75
1:B:1992:VAL:O	1:B:1996:VAL:HG22	1.85	0.75
1:B:3414:MSE:SE	1:B:3450:MSE:SE	3.04	0.75
1:A:3269:ARG:NH1	1:A:3312:VAL:HG12	2.02	0.75
1:B:2458:VAL:HA	1:B:2461:PHE:CE2	2.22	0.75
1:B:2887:PRO:HG3	1:B:2921:LEU:HD13	1.68	0.75
1:B:3243:ILE:HG21	1:B:3262:LEU:HD22	1.68	0.75
1:A:2363:CYS:O	1:A:2367:VAL:HG12	1.87	0.75
1:B:1086:TYR:CD2	1:B:1090:ARG:HG2	2.22	0.75
1:B:3144:PHE:CD1	1:B:3160:LEU:HD11	2.21	0.75
1:B:3491:PRO:HB3	1:B:3711:PRO:HB3	1.69	0.75
1:A:2300:PHE:CZ	1:A:2341:LEU:HB2	2.22	0.74
1:A:2372:PRO:HB2	1:A:2374:LEU:HD13	1.68	0.74
1:B:353:ASP:O	1:B:1859:ASN:ND2	2.19	0.74
1:B:253:LEU:HD21	1:B:297:LEU:HA	1.68	0.74
1:B:2806:LYS:HD3	1:B:2855:VAL:HG13	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3583:LEU:HD11	1:A:3733:ARG:HB3	1.66	0.74
1:B:3012:GLU:HB2	1:B:3050:LYS:HZ1	1.51	0.74
1:B:385:TYR:HE1	1:B:421:LEU:HD23	1.52	0.74
1:B:1217:VAL:HG13	1:B:1274:ARG:HH12	1.50	0.74
1:B:1977:ILE:O	1:B:1979:GLU:N	2.17	0.74
1:B:2253:TYR:CZ	1:B:2287:PRO:HB3	2.22	0.74
1:B:2311:ARG:HG3	1:B:2363:CYS:HB2	1.70	0.74
1:B:971:ARG:HG3	1:B:972:LEU:H	1.52	0.74
1:A:1010:LEU:HD13	1:A:1028:PHE:HE1	1.51	0.74
1:A:3974:MSE:HB3	1:A:3976:GLU:H	1.52	0.74
1:A:766:ALA:O	1:A:768:VAL:N	2.17	0.74
1:B:4021:LEU:HD22	1:B:4028:ILE:HD12	1.68	0.74
1:B:714:VAL:HG12	1:B:734:LEU:HD11	1.69	0.74
1:B:978:GLN:O	1:B:981:ARG:HG2	1.88	0.74
1:A:2960:GLU:OE2	1:A:3289:ARG:NH1	2.19	0.74
1:B:1221:ILE:HG13	1:B:1274:ARG:HH11	1.53	0.74
1:B:3314:SER:HA	1:B:3315:TYR:HB3	1.68	0.74
1:B:3447:VAL:HG12	1:B:3468:LEU:HD22	1.69	0.74
1:B:616:LYS:HB3	1:B:617:PRO:HD2	1.68	0.74
1:A:1976:LEU:HD11	1:A:2031:LEU:HB3	1.69	0.74
1:B:2810:SER:HA	1:B:2813:PHE:CE2	2.23	0.74
1:B:3503:VAL:HG11	1:B:3535:ILE:HB	1.70	0.74
1:A:242:PRO:HB3	1:A:282:PHE:CD1	2.22	0.74
1:A:3323:PHE:O	1:A:3326:GLN:N	2.19	0.74
1:A:2549:LYS:NZ	1:A:2554:PHE:HA	2.02	0.74
1:B:1012:ALA:O	1:B:1015:ASP:HB3	1.87	0.74
1:B:3397:GLN:N	1:B:3397:GLN:OE1	2.19	0.74
1:B:3459:ASN:O	1:B:3462:ARG:HG2	1.87	0.74
1:B:4071:ALA:O	1:B:4075:ARG:CB	2.35	0.74
1:B:4084:SER:O	1:B:4088:ASN:N	2.21	0.74
1:B:793:LEU:HG	1:B:796:LEU:HD12	1.68	0.74
1:A:3575:LEU:O	1:A:3577:GLN:N	2.21	0.74
1:A:3762:GLN:NE2	1:A:3763:ARG:HH11	1.85	0.74
1:B:2260:PHE:CD1	1:B:2274:ILE:HG22	2.23	0.74
1:B:4089:ILE:HB	1:B:4090:ARG:NH2	2.02	0.74
1:A:2274:ILE:O	1:A:2277:LEU:N	2.21	0.74
1:A:2404:ARG:HG2	1:A:2408:MSE:HE3	1.68	0.74
1:A:940:PHE:CE2	1:A:2576:MSE:SE	2.91	0.74
1:A:273:ARG:HD2	1:A:314:SER:HB3	1.69	0.74
1:A:2877:SER:O	1:A:2879:GLY:N	2.21	0.74
1:A:726:LEU:HA	1:A:729:CYS:SG	2.28	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1871:MSE:HA	1:B:1874:TYR:HB2	1.70	0.74
1:B:2379:MSE:HE1	1:B:2404:ARG:NH1	2.03	0.74
1:B:3110:PHE:O	1:B:3114:TYR:HD1	1.69	0.74
1:B:968:VAL:HG23	1:B:971:ARG:HD3	1.70	0.74
1:A:3034:PRO:HG2	1:A:3037:GLN:HB2	1.69	0.73
1:A:432:THR:HG23	1:A:475:LEU:HD13	1.70	0.73
1:B:2068:ARG:O	1:B:2070:GLU:N	2.20	0.73
1:B:2253:TYR:CE2	1:B:2287:PRO:HB3	2.23	0.73
1:B:2379:MSE:SE	1:B:2404:ARG:HD3	2.38	0.73
1:B:3928:PHE:HD2	1:B:3962:ARG:HH21	1.35	0.73
1:A:1132:ASP:HA	1:A:1135:CYS:SG	2.28	0.73
1:A:3176:MSE:HE1	1:A:3179:TRP:HE3	1.54	0.73
1:B:1985:LYS:HD2	1:B:2037:SER:HB3	1.69	0.73
1:B:2507:ILE:HA	1:B:2510:LEU:HD12	1.69	0.73
1:B:1073:PHE:CE2	1:B:3745:GLU:HA	2.23	0.73
1:A:2142:ILE:HA	1:A:2145:PHE:HD2	1.51	0.73
1:A:2222:HIS:O	1:A:2225:HIS:N	2.16	0.73
1:A:760:LEU:HD13	1:A:802:THR:OG1	1.88	0.73
1:B:1342:MSE:HE2	1:B:1398:VAL:HG12	1.70	0.73
1:B:3493:TRP:HE3	1:B:3713:PRO:HB3	1.53	0.73
1:B:886:TRP:HD1	1:B:889:GLU:H	1.35	0.73
1:B:363:ILE:O	1:B:367:GLY:N	2.18	0.73
1:A:2872:ASP:O	1:A:2913:LYS:NZ	2.21	0.73
1:B:2404:ARG:NH1	1:B:2412:TYR:CZ	2.56	0.73
1:B:2917:PRO:HA	1:B:2920:VAL:HG12	1.70	0.73
1:B:3432:SER:HB2	1:B:3435:ASP:HB2	1.69	0.73
1:A:2253:TYR:HB2	1:A:2291:GLN:HG2	1.70	0.73
1:A:4066:LEU:HG	1:A:4075:ARG:HA	1.71	0.73
1:B:1142:HIS:O	1:B:1144:SER:N	2.20	0.73
1:B:174:VAL:O	1:B:178:LEU:HG	1.88	0.73
1:B:2851:PHE:HA	1:B:2854:PHE:CD2	2.24	0.73
1:B:3323:PHE:O	1:B:3326:GLN:HG2	1.88	0.73
1:A:1115:HIS:O	1:A:1119:LYS:N	2.22	0.73
1:A:170:VAL:HG23	1:A:173:LYS:HD3	1.71	0.73
1:A:2883:SER:O	1:A:2886:GLN:HG3	1.87	0.73
1:B:989:MSE:HE2	1:B:1031:ARG:HH12	1.54	0.73
1:B:2004:TYR:CD1	1:B:2054:TYR:HB3	2.23	0.73
1:B:3167:ARG:NH1	1:B:3167:ARG:HG3	2.02	0.73
1:B:4010:SER:O	1:B:4015:ASN:N	2.21	0.73
1:B:629:PHE:CZ	1:B:666:PHE:HD1	2.07	0.73
1:A:567:GLU:OE2	1:A:1798:LEU:HB3	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4010:SER:O	1:A:4015:ASN:N	2.22	0.73
1:A:70:ARG:HH22	1:A:117:LYS:HE3	1.54	0.73
1:B:1070:PRO:HB2	1:B:1073:PHE:CZ	2.24	0.73
1:B:153:PHE:HB2	1:B:157:TYR:CE2	2.24	0.73
1:B:2027:SER:HB2	1:B:2030:TYR:OH	1.87	0.73
1:B:2321:GLU:OE2	1:B:2325:LEU:HD22	1.89	0.73
1:B:3944:HIS:HA	1:B:4016:PHE:HZ	1.53	0.73
1:A:1984:LEU:O	1:A:1988:TYR:HB3	1.89	0.73
1:A:2571:ASP:O	1:A:2789:SER:OG	2.06	0.73
1:A:3167:ARG:O	1:A:3186:ARG:NH2	2.22	0.73
1:B:1014:LEU:HB2	1:B:1078:ALA:HB1	1.71	0.73
1:B:1890:HIS:HB3	1:B:1937:ARG:HA	1.69	0.73
1:A:1009:LEU:O	1:A:1012:ALA:N	2.22	0.73
1:A:1890:HIS:HB2	1:A:1937:ARG:HD2	1.71	0.73
1:A:19:LEU:O	1:A:23:ASP:HB2	1.89	0.73
1:A:2157:PHE:CE1	1:A:2203:THR:HB	2.23	0.73
1:A:2925:GLU:HB3	1:A:3121:LEU:HD11	1.70	0.73
1:B:730:LEU:HA	1:B:733:LEU:HD12	1.71	0.73
1:A:3048:LYS:HD3	1:A:3061:LEU:HD23	1.71	0.72
1:A:609:ALA:O	1:A:613:HIS:ND1	2.20	0.72
1:B:1651:LYS:O	1:B:1655:ILE:HD12	1.89	0.72
1:B:2918:PRO:HA	1:B:2921:LEU:HG	1.70	0.72
1:A:1087:ARG:HD3	1:A:1134:LEU:HD22	1.71	0.72
1:A:1374:GLN:O	1:A:1378:GLU:N	2.21	0.72
1:A:253:LEU:HD11	1:A:297:LEU:HB3	1.71	0.72
1:A:3276:TRP:HB3	1:A:3280:TYR:CZ	2.24	0.72
1:B:2896:ALA:HA	1:B:2899:ARG:NH2	2.04	0.72
1:B:3876:SER:HB3	1:B:4127:TRP:O	1.87	0.72
1:B:398:THR:HG22	1:B:1865:THR:HG21	1.70	0.72
1:B:535:LEU:HD22	1:B:626:LEU:HG	1.72	0.72
1:B:990:GLN:HA	1:B:993:HIS:CD2	2.24	0.72
1:A:1070:PRO:HG3	1:A:1075:ARG:HB2	1.70	0.72
1:A:1743:MSE:SE	1:A:1880:MSE:SE	3.07	0.72
1:B:1349:LEU:HD21	1:B:1359:LEU:HB2	1.70	0.72
1:B:1886:LYS:NZ	1:B:1948:ALA:HB2	2.05	0.72
1:B:2222:HIS:O	1:B:2225:HIS:N	2.19	0.72
1:B:471:LYS:HA	1:B:1553:PHE:HE2	1.53	0.72
1:A:2311:ARG:HG3	1:A:2363:CYS:HB2	1.69	0.72
1:A:3284:SER:HA	1:A:3287:ARG:HE	1.55	0.72
1:A:978:GLN:O	1:A:981:ARG:HG2	1.89	0.72
1:B:1014:LEU:HA	1:B:1025:LEU:HD13	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1115:HIS:O	1:B:1119:LYS:N	2.22	0.72
1:B:526:ASP:HB2	1:B:529:ASP:OD2	1.89	0.72
1:B:967:PRO:HA	1:B:970:LEU:HD23	1.69	0.72
1:A:1456:LYS:HA	1:A:1459:HIS:HD2	1.53	0.72
1:A:4082:ARG:HG3	1:A:4091:ALA:CB	2.19	0.72
1:A:1456:LYS:HA	1:A:1459:HIS:CD2	2.23	0.72
1:A:2260:PHE:O	1:A:2262:GLY:N	2.22	0.72
1:A:2542:LEU:HB2	1:A:2546:TYR:CE2	2.25	0.72
1:A:3045:ILE:O	1:A:3048:LYS:HB3	1.89	0.72
1:A:3130:GLN:HG3	1:A:3178:ILE:HG12	1.72	0.72
1:B:2860:ASP:HB3	1:B:2868:LEU:HD22	1.72	0.72
1:A:1871:MSE:HA	1:A:1874:TYR:HB2	1.71	0.72
1:A:2193:ILE:HA	1:A:2196:TRP:CZ2	2.24	0.72
1:A:737:PRO:HA	1:A:740:ILE:HD12	1.70	0.72
1:B:3583:LEU:O	1:B:3587:ASP:HB2	1.88	0.72
1:A:3015:SER:O	1:A:3019:ILE:N	2.21	0.72
1:A:349:ILE:HG12	1:A:364:ARG:HD2	1.72	0.72
1:A:434:VAL:HA	1:A:437:HIS:CE1	2.24	0.72
1:B:1802:TYR:O	1:B:1805:PHE:N	2.22	0.72
1:B:2177:ASN:HD22	1:B:2182:ILE:HG22	1.54	0.72
1:B:2563:LEU:O	1:B:2567:SER:OG	2.06	0.72
1:A:2300:PHE:HZ	1:A:2341:LEU:HB2	1.54	0.72
1:A:3592:VAL:HG22	1:A:3609:MSE:SE	2.40	0.72
1:B:2837:LEU:HA	1:B:2840:PHE:CD2	2.25	0.72
1:B:3579:SER:OG	1:B:3580:ASN:N	2.22	0.72
1:B:868:LYS:HA	1:B:871:LEU:HD12	1.71	0.72
1:A:358:GLU:HA	1:A:1858:LEU:HD22	1.71	0.72
1:A:871:LEU:HD11	1:A:3122:HIS:HE1	1.55	0.72
1:A:3256:MSE:HE2	1:A:3282:ARG:NH1	2.03	0.72
1:A:3432:SER:HB2	1:A:3435:ASP:HB2	1.72	0.72
1:B:1090:ARG:HA	1:B:1090:ARG:NE	2.05	0.72
1:B:721:TYR:CE1	1:B:1121:LEU:HD21	2.24	0.72
1:B:2313:LYS:HG3	1:B:2314:GLU:OE2	1.90	0.72
1:B:2961:ALA:HB1	1:B:3002:TYR:HD1	1.54	0.72
1:B:649:PHE:CE1	1:B:657:SER:HB2	2.25	0.72
1:A:1870:LYS:HG2	1:A:1871:MSE:HE2	1.71	0.71
1:B:2239:LYS:HG3	1:B:2279:ILE:HG23	1.72	0.71
1:B:3326:GLN:OE1	1:B:3393:GLU:HA	1.90	0.71
1:A:1306:ILE:HG12	1:A:1334:LYS:HB3	1.72	0.71
1:A:2323:LEU:HD21	1:A:2345:VAL:HG21	1.72	0.71
1:A:2423:VAL:HG13	1:A:2424:MSE:H	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2433:LYS:HG3	1:A:2436:LEU:HD12	1.70	0.71
1:B:1032:CYS:HB3	1:B:1036:PHE:CZ	2.25	0.71
1:B:3593:ARG:HA	1:B:3596:LEU:HD12	1.72	0.71
1:B:932:GLU:HG3	1:B:2636:UNK:HA	1.72	0.71
1:A:2312:TYR:HE2	1:A:2314:GLU:HG2	1.55	0.71
1:A:2453:GLU:O	1:A:2457:PRO:HD3	1.90	0.71
1:A:3503:VAL:HG11	1:A:3535:ILE:HB	1.72	0.71
1:A:3982:SER:O	1:A:3986:HIS:ND1	2.22	0.71
1:B:1349:LEU:HA	1:B:1353:PRO:HD2	1.71	0.71
1:B:1761:LEU:HD22	1:B:1860:GLU:HB3	1.73	0.71
1:B:2806:LYS:NZ	1:B:2858:ILE:HG21	2.06	0.71
1:B:602:MSE:SE	1:B:726:LEU:HD13	2.40	0.71
1:A:1977:ILE:O	1:A:1979:GLU:N	2.18	0.71
1:A:2070:GLU:HA	1:A:2071:GLN:HB2	1.72	0.71
1:A:922:SER:HB3	1:A:926:THR:HG23	1.72	0.71
1:A:967:PRO:HA	1:A:970:LEU:HD23	1.70	0.71
1:A:2281:MSE:HE2	1:A:2322:VAL:HA	1.73	0.71
1:A:2435:CYS:O	1:A:2439:ILE:HB	1.89	0.71
1:A:3677:PRO:O	1:A:3679:ASN:N	2.22	0.71
1:A:616:LYS:HB3	1:A:617:PRO:HD2	1.72	0.71
1:B:1762:MSE:HB2	1:B:1896:ILE:HG12	1.72	0.71
1:B:2883:SER:O	1:B:2885:GLN:N	2.22	0.71
1:B:2970:LYS:NZ	1:B:2974:GLU:OE2	2.22	0.71
1:B:3130:GLN:HG3	1:B:3178:ILE:HG12	1.73	0.71
1:B:2884:LEU:HB3	1:B:3895:GLU:HG3	1.73	0.71
1:B:491:CYS:SG	1:B:492:SER:N	2.62	0.71
1:B:560:LEU:HB3	1:B:616:LYS:HE2	1.73	0.71
1:A:2535:THR:O	1:A:2538:ARG:HG2	1.89	0.71
1:B:204:LEU:HD22	1:B:219:VAL:HG12	1.71	0.71
1:B:3471:ILE:HG23	1:B:3472:ILE:HG13	1.73	0.71
1:B:553:VAL:HB	1:B:637:LYS:HZ2	1.56	0.71
1:B:808:GLU:HG2	1:B:852:ARG:NH2	2.06	0.71
1:A:1256:TRP:O	1:A:1260:LEU:N	2.17	0.71
1:A:3257:LYS:HA	1:A:3260:LYS:HD2	1.73	0.71
1:A:3427:GLU:HB3	1:A:3439:LEU:HD22	1.71	0.71
1:A:3835:PRO:HA	1:A:3871:PHE:HE1	1.54	0.71
1:A:3875:GLU:HG2	1:A:4127:TRP:HB3	1.72	0.71
1:B:1702:LEU:O	1:B:1706:SER:HB3	1.91	0.71
1:B:3587:ASP:HB3	1:B:4022:LYS:HZ2	1.55	0.71
1:A:705:ALA:HB1	1:A:1385:ASN:ND2	2.05	0.71
1:A:1609:ALA:HB3	1:A:1806:ARG:NH2	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1745:LYS:O	1:A:1747:LEU:N	2.24	0.71
1:A:2538:ARG:HH12	1:A:2566:THR:H	1.36	0.71
1:A:396:PHE:CZ	1:A:397:LEU:HG	2.25	0.71
1:A:756:PHE:HA	1:A:773:LEU:HD13	1.73	0.71
1:B:2043:PHE:O	1:B:2047:THR:OG1	2.09	0.71
1:B:2200:ALA:HA	1:B:2203:THR:HG22	1.73	0.71
1:A:2152:ASN:HB3	1:A:2153:THR:HA	1.72	0.71
1:A:446:PHE:O	1:A:533:HIS:NE2	2.24	0.71
1:A:621:SER:HB3	1:A:659:ARG:NH2	2.06	0.71
1:B:1798:LEU:O	1:B:1802:TYR:HB2	1.90	0.71
1:B:3464:LYS:HG3	1:B:3468:LEU:HD11	1.72	0.71
1:B:454:GLN:HG3	1:B:533:HIS:HE1	1.54	0.71
1:A:1681:ASP:OD1	1:A:1682:THR:N	2.23	0.71
1:A:2478:MSE:O	1:A:2482:ASP:CB	2.37	0.71
1:A:3813:LYS:HG2	1:A:3926:ASN:HA	1.73	0.71
1:B:1267:TYR:O	1:B:1271:ILE:HG13	1.90	0.71
1:B:1464:LEU:HB2	1:B:1468:LEU:HD12	1.73	0.71
1:B:3155:VAL:HG21	1:B:3159:ARG:NH2	2.06	0.71
1:B:3875:GLU:O	1:B:3879:PRO:HD3	1.91	0.71
1:B:560:LEU:HD11	1:B:645:TRP:CZ2	2.26	0.71
1:A:1880:MSE:SE	1:A:1881:TYR:HD1	2.23	0.70
1:A:2260:PHE:CZ	1:A:2303:LEU:HA	2.25	0.70
1:A:2312:TYR:CE2	1:A:2314:GLU:HG2	2.25	0.70
1:A:660:LEU:O	1:A:664:SER:OG	2.08	0.70
1:A:941:MSE:HB2	1:A:958:MSE:HE3	1.73	0.70
1:B:1060:PHE:HA	1:B:1063:LEU:HD12	1.72	0.70
1:B:1138:ILE:HD13	1:B:1150:LYS:HE2	1.73	0.70
1:B:2161:ALA:HA	1:B:2164:TRP:CD1	2.25	0.70
1:B:2227:LYS:HG3	1:B:2232:ARG:HA	1.73	0.70
1:B:3772:ASN:ND2	1:B:3788:LEU:H	1.89	0.70
1:B:4048:LYS:O	1:B:4051:LEU:HB3	1.91	0.70
1:B:514:VAL:HG12	1:B:604:PRO:HG3	1.73	0.70
1:B:982:GLN:O	1:B:986:PRO:HD3	1.91	0.70
1:A:1655:ILE:HG23	1:A:1677:SER:HB3	1.73	0.70
1:A:3498:TRP:HD1	1:A:3502:MSE:HB2	1.56	0.70
1:B:3340:ALA:O	1:B:3343:SER:N	2.24	0.70
1:B:575:ILE:HD11	1:B:579:LEU:HD22	1.70	0.70
1:B:913:ARG:NE	1:B:916:GLU:OE2	2.24	0.70
1:A:1403:MSE:HE1	1:A:1419:LEU:HD21	1.73	0.70
1:A:2137:ILE:HB	1:A:2170:GLN:HE22	1.55	0.70
1:A:3989:ARG:HH21	1:A:4100:GLU:HB3	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2086:ASP:HB3	1:B:2090:ARG:HH21	1.55	0.70
1:B:2896:ALA:HA	1:B:2899:ARG:HH21	1.57	0.70
1:B:1472:SER:HA	1:B:1476:HIS:CD2	2.26	0.70
1:B:2161:ALA:HB1	1:B:2211:LEU:HD13	1.71	0.70
1:B:2260:PHE:O	1:B:2262:GLY:N	2.24	0.70
1:A:1593:VAL:O	1:A:1597:LEU:HB2	1.91	0.70
1:A:3044:MSE:O	1:A:3047:SER:OG	2.04	0.70
1:A:527:TYR:OH	1:A:619:ASP:N	2.22	0.70
1:B:989:MSE:HE2	1:B:1031:ARG:NH1	2.07	0.70
1:B:1155:ARG:NH2	1:B:1230:GLY:O	2.24	0.70
1:B:2379:MSE:CE	1:B:2404:ARG:HD3	2.20	0.70
1:A:446:PHE:H	1:A:446:PHE:HD1	1.36	0.70
1:B:1017:ILE:HB	1:B:1025:LEU:HB2	1.74	0.70
1:B:2412:TYR:HD2	1:B:2416:LYS:HE3	1.57	0.70
1:B:2936:TYR:HD2	1:B:3979:LEU:HD21	1.56	0.70
1:A:2030:TYR:HD1	1:A:2031:LEU:HG	1.57	0.70
1:A:3917:ILE:HG22	1:A:3918:LEU:HD22	1.72	0.70
1:B:1416:GLU:O	1:B:1420:ARG:HB2	1.91	0.70
1:B:2535:THR:O	1:B:2538:ARG:HG2	1.92	0.70
1:B:2945:SER:O	1:B:2949:THR:HG23	1.90	0.70
1:A:3592:VAL:HA	1:A:3609:MSE:SE	2.41	0.70
1:B:2112:GLN:OE1	1:B:2120:ARG:NH2	2.24	0.70
1:B:848:LEU:HA	1:B:851:ILE:HD12	1.74	0.70
1:A:1592:MSE:O	1:A:1594:SER:N	2.24	0.70
1:B:1445:ARG:HA	1:B:1448:LEU:HD12	1.74	0.70
1:B:2260:PHE:CE2	1:B:2303:LEU:HA	2.27	0.70
1:B:3498:TRP:HE1	1:B:3502:MSE:SE	2.25	0.70
1:B:3638:LYS:HA	1:B:3641:ASP:OD2	1.91	0.70
1:B:3772:ASN:HB2	1:B:3787:GLN:CG	2.19	0.70
1:B:932:GLU:HB3	1:B:2794:LEU:HD13	1.73	0.70
1:A:1014:LEU:HD13	1:A:1078:ALA:HB1	1.72	0.70
1:A:1918:LEU:HD22	1:A:1958:GLU:HB3	1.72	0.70
1:A:2239:LYS:HE2	1:A:2240:THR:HG22	1.73	0.70
1:A:527:TYR:CE1	1:A:615:ALA:HB1	2.26	0.70
1:B:177:LEU:O	1:B:180:LEU:N	2.25	0.70
1:B:19:LEU:HD22	1:B:30:ALA:HB1	1.72	0.70
1:B:970:LEU:CD2	1:B:1031:ARG:HH21	2.05	0.70
1:A:114:VAL:HG11	1:A:130:LEU:HD11	1.72	0.69
1:A:1249:SER:O	1:A:1253:THR:HB	1.92	0.69
1:A:1877:LEU:O	1:A:1920:TYR:OH	2.09	0.69
1:A:2781:PRO:HB2	1:A:2786:LYS:HD3	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3687:MSE:O	1:A:3689:ASP:N	2.25	0.69
1:A:990:GLN:HA	1:A:993:HIS:HD2	1.57	0.69
1:B:1985:LYS:O	1:B:1989:ASN:ND2	2.22	0.69
1:B:2253:TYR:HB2	1:B:2291:GLN:CG	2.22	0.69
1:B:2452:ARG:HA	1:B:2455:LEU:HD12	1.73	0.69
1:B:3284:SER:HB2	1:B:3287:ARG:NH2	2.04	0.69
1:B:3119:VAL:HG21	1:B:3899:ALA:HB1	1.74	0.69
1:B:3910:LEU:O	1:B:3914:SER:OG	2.07	0.69
1:B:629:PHE:HZ	1:B:666:PHE:HD1	1.40	0.69
1:A:1378:GLU:OE2	1:A:1382:ILE:HG23	1.92	0.69
1:A:1469:PRO:HA	1:A:1472:SER:HB3	1.74	0.69
1:B:436:GLU:OE2	1:B:475:LEU:HD12	1.93	0.69
1:B:743:LEU:O	1:B:746:ARG:NH1	2.25	0.69
1:A:1996:VAL:HG23	1:A:1997:PRO:CD	2.22	0.69
1:A:2071:GLN:HA	1:A:2074:PRO:HG2	1.73	0.69
1:A:2958:LEU:O	1:A:3289:ARG:NH2	2.25	0.69
1:A:718:MSE:HE3	1:A:731:THR:HG22	1.74	0.69
1:A:718:MSE:HE2	1:A:754:MSE:HG3	1.75	0.69
1:B:660:LEU:O	1:B:663:ILE:HG13	1.91	0.69
1:A:1583:MSE:SE	1:A:1643:MSE:SE	3.09	0.69
1:A:1651:LYS:O	1:A:1655:ILE:HD12	1.92	0.69
1:A:2038:GLU:OE1	1:A:2076:VAL:HG22	1.93	0.69
1:A:2153:THR:OG1	1:A:2154:GLU:N	2.18	0.69
1:B:1087:ARG:HD2	1:B:1137:ILE:HD11	1.74	0.69
1:B:1412:LYS:HA	1:B:1415:LEU:HD12	1.72	0.69
1:B:3979:LEU:HA	1:B:3981:TYR:HB3	1.74	0.69
1:B:512:GLY:HA2	1:B:602:MSE:HG3	1.73	0.69
1:B:629:PHE:CE2	1:B:668:LYS:HB2	2.28	0.69
1:A:334:HIS:CE1	1:A:338:LEU:HD21	2.28	0.69
1:B:2813:PHE:CD2	1:B:2859:GLN:HG3	2.25	0.69
1:B:272:LEU:HB3	1:B:319:PHE:CZ	2.27	0.69
1:B:722:LYS:HB3	1:B:727:ALA:HA	1.74	0.69
1:B:86:LEU:HD23	1:B:89:LEU:HD12	1.72	0.69
1:A:2216:LEU:HD22	1:A:2249:LEU:HD11	1.73	0.69
1:A:2452:ARG:HE	1:A:2498:ILE:HD11	1.57	0.69
1:A:3810:VAL:HG23	1:A:3815:LEU:HD11	1.74	0.69
1:B:170:VAL:HG23	1:B:173:LYS:HZ1	1.57	0.69
1:B:2413:PHE:CE1	1:B:2442:MSE:HB3	2.27	0.69
1:B:2430:GLU:HG3	1:B:2465:PRO:HB3	1.74	0.69
1:B:2884:LEU:C	1:B:2887:PRO:HD2	2.13	0.69
1:B:3574:ALA:HA	1:B:3577:GLN:HB2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1445:ARG:HA	1:A:1448:LEU:HD12	1.74	0.69
1:A:2304:VAL:HG13	1:A:2348:GLN:HE21	1.57	0.69
1:A:2329:TYR:O	1:A:2333:ARG:N	2.25	0.69
1:A:2464:HIS:H	1:A:2465:PRO:HD3	1.56	0.69
1:A:723:ASP:HB2	1:A:726:LEU:HD12	1.74	0.69
1:B:2196:TRP:HE1	1:B:2200:ALA:HB2	1.58	0.69
1:B:3654:MSE:SE	1:B:3659:PHE:HB3	2.42	0.69
1:B:65:LEU:O	1:B:69:VAL:HB	1.93	0.69
1:A:1059:LEU:HD22	1:A:1063:LEU:HD11	1.75	0.69
1:A:1018:VAL:HB	1:A:1074:LYS:HA	1.75	0.69
1:A:1507:CYS:SG	1:A:1508:LYS:N	2.65	0.69
1:A:1685:ASP:HB2	1:A:1727:ARG:NH2	2.06	0.69
1:A:2125:TRP:O	1:A:2127:LYS:N	2.25	0.69
1:A:19:LEU:HB2	1:A:34:LEU:HD13	1.75	0.69
1:A:368:LEU:HD23	1:A:372:PRO:HG2	1.74	0.69
1:A:3974:MSE:HB3	1:A:3976:GLU:HB3	1.74	0.69
1:A:462:VAL:HG11	1:A:540:MSE:SE	2.42	0.69
1:B:135:LEU:HD13	1:B:170:VAL:HB	1.75	0.69
1:B:2351:GLN:O	1:B:2355:THR:OG1	2.07	0.69
1:B:2555:LEU:O	1:B:2558:ALA:HB3	1.92	0.69
1:A:602:MSE:SE	1:A:726:LEU:HD13	2.42	0.69
1:B:414:LEU:HD23	1:B:460:ALA:HB1	1.74	0.69
1:B:434:VAL:HA	1:B:437:HIS:CE1	2.28	0.69
1:A:2187:VAL:O	1:A:2190:VAL:HG22	1.93	0.69
1:A:4121:TRP:HD1	1:A:4123:GLY:H	1.40	0.69
1:A:870:LEU:HA	1:A:873:VAL:HB	1.75	0.69
1:B:1086:TYR:HD2	1:B:1090:ARG:HG2	1.58	0.69
1:B:1955:VAL:HG12	1:B:1957:ASN:HB2	1.75	0.69
1:A:1569:THR:O	1:A:1573:LYS:HB2	1.93	0.69
1:A:3048:LYS:NZ	1:A:3089:LEU:HB3	2.08	0.69
1:A:934:LEU:HD21	1:A:962:TYR:CE1	2.28	0.69
1:B:1799:GLU:HA	1:B:1802:TYR:HB2	1.74	0.69
1:B:3587:ASP:HB3	1:B:4022:LYS:NZ	2.08	0.69
1:B:3772:ASN:ND2	1:B:3788:LEU:O	2.26	0.69
1:B:917:LEU:HD21	1:B:934:LEU:HD13	1.74	0.69
1:B:935:HIS:NE2	1:B:987:LEU:HG	2.09	0.69
1:A:970:LEU:HD22	1:A:1031:ARG:HH21	1.58	0.68
1:A:1763:THR:OG1	1:A:1864:ASP:OD2	2.09	0.68
1:A:3114:TYR:CE1	1:A:3128:LYS:HD3	2.28	0.68
1:A:977:ASP:HB3	1:A:981:ARG:N	2.08	0.68
1:B:999:LYS:HD3	1:B:1000:LYS:H	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1080:LEU:CD1	1:B:1127:CYS:HB3	2.23	0.68
1:B:2074:PRO:O	1:B:2077:HIS:N	2.26	0.68
1:B:2283:ASN:O	1:B:2287:PRO:HD3	1.92	0.68
1:B:2365:ASN:HD21	1:B:2382:VAL:HG11	1.58	0.68
1:B:2951:GLN:OE1	1:B:2972:TYR:OH	2.10	0.68
1:A:3312:VAL:O	1:A:3314:SER:N	2.26	0.68
1:B:3631:LYS:HB3	1:B:3682:GLU:HA	1.76	0.68
1:B:745:VAL:HG11	1:B:776:TRP:CZ2	2.27	0.68
1:A:1722:PHE:CD2	1:A:1754:GLN:HG2	2.29	0.68
1:B:3435:ASP:O	1:B:3439:LEU:CB	2.41	0.68
1:B:345:PHE:HD2	1:B:367:GLY:HA3	1.59	0.68
1:B:398:THR:O	1:B:401:ASP:N	2.24	0.68
1:A:2177:ASN:HD22	1:A:2182:ILE:HG22	1.57	0.68
1:A:2283:ASN:ND2	1:A:2284:ASP:OD2	2.26	0.68
1:B:1165:LEU:HA	1:B:1168:LEU:HD12	1.76	0.68
1:B:2242:VAL:HG12	1:B:2246:LYS:HE3	1.75	0.68
1:A:1937:ARG:O	1:A:1941:HIS:HB2	1.92	0.68
1:A:1917:LYS:HE2	1:A:1955:VAL:HB	1.74	0.68
1:A:2271:SER:HB2	1:A:2314:GLU:HG3	1.75	0.68
1:A:2900:LEU:HB2	1:A:2910:VAL:HA	1.75	0.68
1:A:3955:VAL:HG23	1:A:4121:TRP:CE3	2.28	0.68
1:B:1989:ASN:HB3	1:B:2040:MSE:HB3	1.75	0.68
1:B:2274:ILE:O	1:B:2277:LEU:N	2.27	0.68
1:B:4113:ASP:HB3	1:B:4116:ILE:HG13	1.75	0.68
1:B:721:TYR:HE1	1:B:1121:LEU:HD21	1.58	0.68
1:A:1382:ILE:HB	1:A:1386:ILE:HD11	1.75	0.68
1:A:940:PHE:CZ	1:A:2791:ILE:HG21	2.28	0.68
1:A:793:LEU:HG	1:A:796:LEU:HD12	1.75	0.68
1:B:1682:THR:OG1	1:B:1727:ARG:NH2	2.27	0.68
1:B:1981:LEU:O	1:B:1984:LEU:HG	1.93	0.68
1:B:2423:VAL:HG23	1:B:2426:HIS:HB3	1.76	0.68
1:A:3583:LEU:O	1:A:3587:ASP:HB2	1.92	0.68
1:A:3816:LEU:HD11	1:A:3883:LEU:HG	1.74	0.68
1:A:4066:LEU:HD23	1:A:4075:ARG:HG3	1.76	0.68
1:A:543:SER:C	1:A:545:LEU:H	1.95	0.68
1:B:1403:MSE:HE1	1:B:1419:LEU:HD21	1.75	0.68
1:B:1643:MSE:HA	1:B:1646:LEU:HG	1.74	0.68
1:B:3084:GLN:OE1	1:B:3084:GLN:N	2.21	0.68
1:B:3339:ASN:O	1:B:3341:LEU:N	2.26	0.68
1:B:3737:ARG:NH1	1:B:3739:ILE:HD11	2.07	0.68
1:B:3840:LYS:HE2	1:B:4122:GLU:HB3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:669:LEU:HD22	1:B:672:ILE:HG13	1.75	0.68
1:B:926:THR:O	1:B:930:ALA:HB3	1.92	0.68
1:A:2094:MSE:HE1	1:A:2143:ARG:HA	1.75	0.68
1:A:2936:TYR:HB3	1:A:3979:LEU:HD11	1.75	0.68
1:A:484:HIS:CD2	1:A:616:LYS:HE3	2.29	0.68
1:A:580:ASP:OD1	1:A:581:LEU:N	2.26	0.68
1:B:2477:LEU:HB3	1:B:2506:LEU:HD21	1.76	0.68
1:B:3031:TRP:CE3	1:B:3034:PRO:HD3	2.29	0.68
1:B:3981:TYR:OH	1:B:4101:GLU:HB3	1.93	0.68
1:A:1437:TYR:CD2	1:A:1444:ASP:OD2	2.47	0.68
1:A:3830:SER:HB2	1:A:3835:PRO:HG3	1.76	0.68
1:B:2260:PHE:CZ	1:B:2303:LEU:HA	2.29	0.68
1:B:574:LYS:O	1:B:577:GLU:HG2	1.94	0.68
1:A:1802:TYR:O	1:A:1805:PHE:N	2.27	0.68
1:A:265:TYR:O	1:A:268:PRO:HD2	1.94	0.68
1:A:3049:LEU:HD13	1:A:3184:THR:HB	1.76	0.68
1:A:3790:THR:HG22	1:A:3791:TYR:H	1.58	0.68
1:A:882:SER:HB2	1:A:3892:THR:H	1.59	0.68
1:A:3883:LEU:HD13	1:A:3970:LEU:HD13	1.74	0.68
1:B:1886:LYS:HZ3	1:B:1948:ALA:HB2	1.59	0.68
1:B:2316:TYR:CG	1:B:2317:ALA:N	2.62	0.68
1:B:655:LEU:O	1:B:659:ARG:HG2	1.93	0.68
1:A:1080:LEU:HD12	1:A:1081:ALA:N	2.08	0.67
1:A:260:ILE:HG22	1:A:264:ARG:HH12	1.59	0.67
1:B:2258:GLU:OE2	1:B:2295:GLN:NE2	2.22	0.67
1:B:2542:LEU:HB2	1:B:2546:TYR:CE2	2.29	0.67
1:B:3620:PRO:HA	1:B:3625:LEU:HD12	1.76	0.67
1:B:411:PRO:HA	1:B:414:LEU:HB3	1.75	0.67
1:B:968:VAL:HA	1:B:971:ARG:HG2	1.76	0.67
1:A:1403:MSE:HA	1:A:1406:LEU:HB2	1.76	0.67
1:A:172:GLU:O	1:A:176:GLU:HG3	1.94	0.67
1:A:990:GLN:HA	1:A:993:HIS:CD2	2.29	0.67
1:B:2390:HIS:HD1	1:B:2397:CYS:HG	1.41	0.67
1:B:2440:TYR:HD2	1:B:2476:ILE:HD12	1.58	0.67
1:B:899:ARG:NH1	1:B:2570:PRO:HB2	2.00	0.67
1:B:4063:GLU:HA	1:B:4066:LEU:HD22	1.75	0.67
1:A:323:VAL:O	1:A:327:VAL:HB	1.94	0.67
1:A:367:GLY:C	1:A:369:PHE:H	1.98	0.67
1:B:2776:ARG:HA	1:B:2776:ARG:NH1	2.08	0.67
1:B:797:ASP:HA	1:B:800:LEU:HD12	1.77	0.67
1:A:3788:LEU:HG	1:A:3789:ARG:H	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:ILE:HG13	1:A:381:VAL:CG2	2.24	0.67
1:A:848:LEU:HA	1:A:851:ILE:HD12	1.76	0.67
1:A:909:VAL:HG13	1:A:913:ARG:NH1	2.09	0.67
1:B:3761:ASP:HB3	1:B:3942:PHE:HB2	1.76	0.67
1:B:3797:THR:HG22	1:B:3800:LEU:HG	1.77	0.67
1:B:429:GLU:N	1:B:429:GLU:OE1	2.27	0.67
1:B:554:ASN:CG	1:B:637:LYS:HZ3	1.98	0.67
1:A:1163:LEU:HD13	1:A:1256:TRP:CD1	2.29	0.67
1:A:1723:PRO:C	1:A:1725:GLN:H	1.97	0.67
1:A:2239:LYS:HG3	1:A:2279:ILE:CG2	2.23	0.67
1:A:3174:ASP:OD2	1:A:3782:SER:HB3	1.94	0.67
1:A:3858:MSE:HB3	1:A:4119:ARG:NH2	2.10	0.67
1:A:3964:THR:O	1:A:3967:PHE:HD1	1.78	0.67
1:A:411:PRO:HA	1:A:414:LEU:HB3	1.76	0.67
1:A:571:SER:HB2	1:A:606:SER:H	1.59	0.67
1:B:446:PHE:HD1	1:B:446:PHE:H	1.42	0.67
1:B:969:LEU:O	1:B:973:ALA:CB	2.42	0.67
1:A:2538:ARG:HH11	1:A:2565:MSE:HB3	1.59	0.67
1:A:3959:MSE:HE1	1:A:4124:TRP:CD2	2.30	0.67
1:A:756:PHE:O	1:A:760:LEU:HG	1.95	0.67
1:B:1504:ASP:HA	1:B:1507:CYS:HB3	1.76	0.67
1:B:550:PHE:HZ	1:B:632:GLU:HG2	1.57	0.67
1:A:144:MSE:HE2	1:A:184:VAL:HG11	1.76	0.67
1:A:2477:LEU:HD13	1:A:2505:VAL:HG11	1.76	0.67
1:A:3974:MSE:HA	1:A:3975:LYS:HB3	1.75	0.67
1:A:767:GLU:HG2	1:A:846:ILE:O	1.94	0.67
1:B:1643:MSE:O	1:B:1646:LEU:N	2.27	0.67
1:A:1017:ILE:HD12	1:A:1025:LEU:HD22	1.77	0.67
1:A:1744:LYS:HA	1:A:1880:MSE:HE3	1.75	0.67
1:A:2223:VAL:HB	1:A:2238:ILE:HD12	1.76	0.67
1:A:2851:PHE:HA	1:A:2854:PHE:CD2	2.29	0.67
1:A:3344:GLU:O	1:A:3348:LEU:HG	1.94	0.67
1:A:3505:LEU:HD12	1:A:3509:ASP:HB3	1.76	0.67
1:A:3583:LEU:HD11	1:A:3733:ARG:HD3	1.77	0.67
1:A:4066:LEU:HD11	1:A:4078:VAL:HG11	1.77	0.67
1:B:2140:LEU:HA	1:B:2143:ARG:HD2	1.75	0.67
1:B:2420:PHE:HE1	1:B:2436:LEU:HD22	1.59	0.67
1:B:3812:LEU:HG	1:B:3813:LYS:N	2.08	0.67
1:B:406:ARG:O	1:B:409:GLN:N	2.26	0.67
1:B:463:LYS:O	1:B:466:LEU:HB3	1.94	0.67
1:B:865:GLN:N	1:B:865:GLN:OE1	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:LYS:NZ	1:A:1328:GLU:OE2	2.24	0.67
1:A:173:LYS:O	1:A:177:LEU:HG	1.94	0.67
1:A:2253:TYR:CZ	1:A:2287:PRO:HB3	2.30	0.67
1:B:1145:LEU:HB2	1:B:1149:LYS:NZ	2.10	0.67
1:B:1344:PHE:O	1:B:1348:LEU:CB	2.33	0.67
1:B:1483:LEU:HA	1:B:1500:LEU:HD21	1.75	0.67
1:B:1963:GLN:HE21	1:B:1995:GLU:HG2	1.60	0.67
1:B:2001:LYS:HA	1:B:2054:TYR:CE2	2.29	0.67
1:B:2440:TYR:CD2	1:B:2476:ILE:HD12	2.29	0.67
1:B:2854:PHE:CG	1:B:2882:ALA:HB2	2.30	0.67
1:B:327:VAL:HG22	1:B:338:LEU:HD22	1.77	0.67
1:B:985:GLU:HG3	1:B:1031:ARG:NH2	2.03	0.67
1:A:2033:ASP:O	1:A:2037:SER:OG	2.13	0.67
1:A:2224:PHE:CZ	1:A:2276:LEU:HD22	2.30	0.67
1:A:2806:LYS:HA	1:A:2809:PHE:CD2	2.30	0.67
1:A:3879:PRO:HB2	1:A:3966:GLN:OE1	1.94	0.67
1:B:1491:ILE:O	1:B:1497:ARG:NH1	2.27	0.67
1:B:1751:GLU:OE2	1:B:1884:LEU:HD13	1.95	0.67
1:B:1894:SER:O	1:B:1897:ASN:N	2.21	0.67
1:B:2507:ILE:HG12	1:B:2548:PRO:HB2	1.77	0.67
1:B:794:PRO:HA	1:B:869:ASN:HB3	1.77	0.67
1:A:1292:LYS:NZ	1:A:1361:LYS:NZ	2.44	0.66
1:A:1464:LEU:HB2	1:A:1468:LEU:HD12	1.75	0.66
1:A:1880:MSE:SE	1:A:1881:TYR:CD1	2.98	0.66
1:A:2066:PHE:HB3	1:A:2067:ARG:HG2	1.76	0.66
1:A:2913:LYS:O	1:A:2916:LEU:N	2.22	0.66
1:A:646:VAL:HG22	1:A:660:LEU:HD23	1.76	0.66
1:A:76:ILE:HG13	1:A:77:GLU:H	1.59	0.66
1:B:3007:GLU:O	1:B:3010:SER:OG	2.13	0.66
1:A:1036:PHE:CD1	1:A:1059:LEU:HD11	2.30	0.66
1:A:1214:GLU:HG2	1:A:1218:SER:HB3	1.77	0.66
1:A:2256:ILE:HD13	1:A:2276:LEU:HD11	1.77	0.66
1:A:3072:GLU:O	1:A:3076:ALA:HB2	1.96	0.66
1:A:3471:ILE:HG23	1:A:3472:ILE:HG13	1.75	0.66
1:A:610:ALA:HA	1:A:613:HIS:CE1	2.29	0.66
1:B:2323:LEU:HG	1:B:2341:LEU:HD21	1.77	0.66
1:B:3414:MSE:HE1	1:B:3450:MSE:HA	1.76	0.66
1:B:980:THR:CG2	1:B:984:TYR:HE2	2.09	0.66
1:A:3019:ILE:HG13	1:A:3020:ASP:H	1.60	0.66
1:A:3467:ARG:HG3	1:A:3471:ILE:HD12	1.77	0.66
1:A:931:CYS:SG	1:A:932:GLU:N	2.68	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1103:ALA:O	1:B:1106:ILE:HG12	1.95	0.66
1:B:2009:LYS:HG2	1:B:2011:ALA:H	1.58	0.66
1:B:3042:PRO:HA	1:B:3045:ILE:HG12	1.76	0.66
1:B:266:ALA:CB	1:B:308:LEU:HG	2.25	0.66
1:B:659:ARG:HH22	1:B:662:LEU:CG	2.05	0.66
1:A:1548:GLY:O	1:A:1552:HIS:ND1	2.28	0.66
1:A:2121:ASP:HA	1:A:2126:MSE:HB3	1.77	0.66
1:A:3040:TYR:HA	1:A:3043:TYR:CD2	2.31	0.66
1:A:3061:LEU:HD21	1:A:3089:LEU:HD13	1.76	0.66
1:A:3182:ILE:HB	1:A:3186:ARG:HH11	1.58	0.66
1:A:3579:SER:OG	1:A:3580:ASN:N	2.25	0.66
1:A:3725:ARG:HH12	1:A:3737:ARG:HH22	1.43	0.66
1:A:3875:GLU:O	1:A:3879:PRO:HD3	1.95	0.66
1:B:1113:LEU:HD13	1:B:1162:SER:HB3	1.76	0.66
1:B:1266:CYS:O	1:B:1269:THR:OG1	2.12	0.66
1:B:1364:CYS:HB3	1:B:1367:HIS:ND1	2.10	0.66
1:B:1952:ILE:HG23	1:B:1953:CYS:O	1.96	0.66
1:B:3606:ILE:HD13	1:B:3609:MSE:HE3	1.76	0.66
1:B:3820:MSE:HA	1:B:3882:LEU:HD22	1.77	0.66
1:B:776:TRP:CZ2	1:B:780:ILE:HD12	2.30	0.66
1:A:1702:LEU:O	1:A:1706:SER:HB3	1.95	0.66
1:A:3008:TRP:O	1:A:3011:LEU:N	2.22	0.66
1:A:3582:GLU:HB2	1:A:3674:SER:OG	1.95	0.66
1:A:2891:ARG:HD3	1:A:3972:LEU:HD22	1.77	0.66
1:A:886:TRP:HZ3	1:A:954:GLY:O	1.78	0.66
1:B:3160:LEU:O	1:B:3163:THR:HG22	1.96	0.66
1:B:638:GLN:OE1	1:B:638:GLN:N	2.25	0.66
1:A:657:SER:O	1:A:661:PRO:HD3	1.95	0.66
1:B:2137:ILE:O	1:B:2141:ASN:N	2.27	0.66
1:B:2167:PRO:HB2	1:B:2171:LEU:HD22	1.77	0.66
1:B:362:ALA:HB2	1:B:409:GLN:HE21	1.61	0.66
1:B:3721:GLY:O	1:B:3741:ARG:HB2	1.95	0.66
1:B:3842:TRP:CH2	1:B:3846:MSE:HE2	2.30	0.66
1:B:69:VAL:O	1:B:73:LEU:HG	1.96	0.66
1:A:1170:LYS:HA	1:A:1173:LEU:HD12	1.77	0.66
1:A:2886:GLN:HG3	1:A:2887:PRO:HD3	1.77	0.66
1:A:3493:TRP:CE3	1:A:3496:ILE:HG13	2.30	0.66
1:A:514:VAL:HA	1:A:604:PRO:HG3	1.78	0.66
1:B:4002:MSE:SE	1:B:4048:LYS:HE3	2.46	0.66
1:B:793:LEU:HA	1:B:796:LEU:HG	1.78	0.66
1:A:1306:ILE:CG1	1:A:1334:LYS:HB3	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1649:LEU:HA	1:A:1652:ILE:HD12	1.76	0.66
1:A:175:TYR:HE1	1:A:200:PHE:HB3	1.59	0.66
1:A:2254:ARG:HG3	1:A:2255:LEU:H	1.61	0.66
1:A:2549:LYS:HZ2	1:A:2554:PHE:HA	1.59	0.66
1:A:260:ILE:HG23	1:A:263:LYS:HD2	1.75	0.66
1:A:3323:PHE:O	1:A:3326:GLN:HG3	1.96	0.66
1:A:3703:GLY:O	1:A:3706:ASP:HB2	1.95	0.66
1:A:612:LEU:O	1:A:615:ALA:HB3	1.96	0.66
1:B:178:LEU:HB3	1:B:197:PHE:CZ	2.30	0.66
1:B:2462:VAL:HG21	1:B:2473:MSE:SE	2.46	0.66
1:B:3446:VAL:HA	1:B:3449:LYS:HD2	1.78	0.66
1:B:3486:GLU:HG3	1:B:3487:ILE:N	2.09	0.66
1:B:3725:ARG:HH12	1:B:3737:ARG:HH22	1.31	0.66
1:B:649:PHE:CZ	1:B:657:SER:HB2	2.31	0.66
1:A:3125:ARG:O	1:A:3128:LYS:N	2.29	0.66
1:A:3414:MSE:HG3	1:A:3456:LEU:HD21	1.76	0.66
1:A:3460:GLU:HA	1:A:3463:LEU:HD12	1.78	0.66
1:A:3619:ASP:HA	1:A:3622:ALA:HB3	1.76	0.66
1:A:680:ILE:HG12	1:A:701:TYR:CD1	2.30	0.66
1:B:186:PRO:HB2	1:B:189:MSE:HB3	1.78	0.66
1:B:1993:GLU:O	1:B:1997:PRO:HD2	1.96	0.66
1:B:2155:GLU:O	1:B:2157:PHE:N	2.29	0.66
1:B:2190:VAL:HG21	1:B:2241:LEU:HD13	1.76	0.66
1:B:2408:MSE:HE2	1:B:2408:MSE:HA	1.78	0.66
1:B:294:PHE:HZ	1:B:319:PHE:CD2	2.14	0.66
1:B:3887:PHE:HE2	1:B:3904:PHE:HD2	1.43	0.66
1:B:3944:HIS:CE1	1:B:4020:MSE:HE2	2.30	0.66
1:B:617:PRO:O	1:B:620:PHE:N	2.29	0.66
1:A:2382:VAL:HG21	1:A:2404:ARG:HG3	1.79	0.65
1:A:971:ARG:HB3	1:A:1027:ASP:OD2	1.96	0.65
1:B:1081:ALA:O	1:B:1085:ILE:HG12	1.95	0.65
1:B:3262:LEU:HD21	1:B:3274:VAL:HG12	1.78	0.65
1:B:403:GLY:C	1:B:405:ASP:H	1.98	0.65
1:A:2011:ALA:O	1:A:2013:GLU:N	2.28	0.65
1:A:2023:SER:HA	1:A:2070:GLU:OE2	1.96	0.65
1:A:2183:HIS:O	1:A:2187:VAL:CB	2.30	0.65
1:A:3042:PRO:HA	1:A:3045:ILE:HG12	1.77	0.65
1:A:2962:ARG:HE	1:A:3254:LEU:HA	1.60	0.65
1:A:3287:ARG:HH11	1:A:3331:GLY:HA3	1.61	0.65
1:A:446:PHE:CD1	1:A:447:PRO:HD3	2.30	0.65
1:B:717:LYS:NZ	1:B:1121:LEU:HD11	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1681:ASP:OD1	1:B:1682:THR:N	2.29	0.65
1:B:2478:MSE:O	1:B:2482:ASP:CB	2.44	0.65
1:B:3589:SER:O	1:B:3593:ARG:CB	2.44	0.65
1:A:135:LEU:HD13	1:A:173:LYS:HB3	1.78	0.65
1:A:1802:TYR:HA	1:A:1805:PHE:HD2	1.61	0.65
1:A:2794:LEU:HA	1:A:2797:VAL:HG22	1.78	0.65
1:A:3847:SER:HA	1:A:3857:LEU:HD13	1.77	0.65
1:B:2224:PHE:CZ	1:B:2276:LEU:HD22	2.32	0.65
1:B:2571:ASP:O	1:B:2789:SER:OG	2.14	0.65
1:B:2935:GLU:HG3	1:B:2936:TYR:H	1.62	0.65
1:B:253:LEU:HD11	1:B:297:LEU:HB3	1.78	0.65
1:B:3630:ARG:HG2	1:B:3686:TRP:NE1	2.11	0.65
1:B:393:LYS:HA	1:B:396:PHE:CD1	2.31	0.65
1:B:3998:LEU:O	1:B:4001:THR:OG1	2.13	0.65
1:B:649:PHE:O	1:B:652:GLU:N	2.15	0.65
1:A:1101:PHE:O	1:A:1104:LEU:HB2	1.97	0.65
1:A:1934:LEU:CD1	1:A:1937:ARG:H	2.09	0.65
1:A:3429:GLU:OE1	1:A:4046:TYR:OH	2.13	0.65
1:A:3946:PHE:CE2	1:A:4048:LYS:HD2	2.31	0.65
1:A:939:MSE:HE2	1:A:942:LEU:HD13	1.79	0.65
1:B:1349:LEU:HD23	1:B:1353:PRO:HG2	1.78	0.65
1:B:1816:ARG:HB3	1:B:1819:PHE:HE1	1.60	0.65
1:A:1121:LEU:HG	1:A:1122:GLY:N	2.11	0.65
1:A:1292:LYS:NZ	1:A:1361:LYS:HZ1	1.95	0.65
1:A:1423:ILE:HG13	1:A:1424:THR:H	1.60	0.65
1:A:1718:ILE:HG23	1:A:1750:LEU:HD21	1.78	0.65
1:A:2034:SER:O	1:A:2036:LEU:N	2.29	0.65
1:A:2182:ILE:O	1:A:2186:VAL:HG12	1.97	0.65
1:A:2253:TYR:HD1	1:A:2256:ILE:HD12	1.59	0.65
1:A:3480:LEU:O	1:A:3484:THR:OG1	2.14	0.65
1:B:1101:PHE:CG	1:B:1138:ILE:HG12	2.32	0.65
1:B:385:TYR:O	1:B:389:ILE:HB	1.95	0.65
1:B:753:GLN:O	1:B:757:LYS:CB	2.43	0.65
1:A:1737:ASN:C	1:A:1739:TYR:H	2.00	0.65
1:A:2049:VAL:O	1:A:2052:TYR:N	2.28	0.65
1:A:2507:ILE:HA	1:A:2510:LEU:HD12	1.78	0.65
1:A:2886:GLN:OE1	1:A:2921:LEU:HB2	1.97	0.65
1:B:471:LYS:HA	1:B:1553:PHE:CE2	2.31	0.65
1:B:173:LYS:O	1:B:177:LEU:HG	1.97	0.65
1:B:3677:PRO:O	1:B:3679:ASN:N	2.28	0.65
1:B:736:LEU:O	1:B:740:ILE:HG13	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:938:VAL:HG21	1:B:962:TYR:CZ	2.32	0.65
1:A:1346:THR:HG21	1:A:1401:ASN:HB3	1.79	0.65
1:A:2049:VAL:HA	1:A:2052:TYR:CD2	2.30	0.65
1:A:2058:ASP:HB3	1:A:2059:PRO:HD3	1.78	0.65
1:A:2240:THR:HG21	2:K:113:UNK:N	2.12	0.65
1:A:2274:ILE:HA	1:A:2277:LEU:HG	1.76	0.65
1:A:2304:VAL:HG13	1:A:2348:GLN:NE2	2.10	0.65
1:A:3630:ARG:HA	1:A:3686:TRP:CD1	2.32	0.65
1:A:393:LYS:HA	1:A:396:PHE:CD1	2.32	0.65
1:A:4004:VAL:O	1:A:4008:GLU:HB2	1.97	0.65
1:A:759:GLY:HA2	1:A:763:THR:OG1	1.95	0.65
1:A:895:ALA:HB3	1:A:904:VAL:HG21	1.78	0.65
1:B:1651:LYS:O	1:B:1654:GLN:HB2	1.97	0.65
1:B:2062:ALA:HB1	1:B:2066:PHE:CE2	2.30	0.65
1:B:2937:ASP:OD1	1:B:3979:LEU:HD12	1.96	0.65
1:A:1039:TRP:HZ2	1:A:1049:GLN:HA	1.62	0.65
1:A:1107:TYR:O	1:A:1111:LEU:N	2.29	0.65
1:A:1138:ILE:HG21	1:A:1150:LYS:HE2	1.78	0.65
1:A:1373:VAL:HB	1:A:1418:HIS:CE1	2.31	0.65
1:A:1437:TYR:CE2	1:A:1444:ASP:OD2	2.48	0.65
1:A:2854:PHE:CG	1:A:2882:ALA:HB2	2.32	0.65
1:A:660:LEU:O	1:A:663:ILE:HG13	1.96	0.65
1:A:757:LYS:HA	1:A:760:LEU:HD12	1.78	0.65
1:B:1249:SER:O	1:B:1253:THR:CB	2.44	0.65
1:B:220:LEU:O	1:B:224:LEU:HG	1.97	0.65
1:B:3141:PHE:HE1	1:B:3193:ILE:HG13	1.62	0.65
1:B:3705:TYR:HE2	1:B:3708:ARG:NH1	1.95	0.65
1:B:4099:SER:O	1:B:4103:GLN:NE2	2.27	0.65
1:A:1949:ILE:HD12	1:A:1952:ILE:HG21	1.79	0.65
1:A:2375:ALA:O	1:A:2379:MSE:HB2	1.96	0.65
1:A:3416:LEU:HD13	1:A:3446:VAL:HG12	1.78	0.65
1:A:909:VAL:HG13	1:A:913:ARG:HH11	1.62	0.65
1:A:940:PHE:HE2	1:A:2576:MSE:SE	2.29	0.65
1:B:2070:GLU:HB2	1:B:2072:ARG:N	2.12	0.65
1:B:2270:ASN:O	1:B:2274:ILE:HG23	1.95	0.65
1:B:2412:TYR:CD2	1:B:2416:LYS:HE3	2.31	0.65
1:B:3152:SER:HB2	1:B:3155:VAL:HB	1.77	0.65
1:B:3257:LYS:HA	1:B:3260:LYS:HD2	1.77	0.65
1:B:3704:GLN:HE21	1:B:3796:MSE:SE	2.30	0.65
1:B:3722:PHE:CD1	1:B:3740:ILE:HA	2.32	0.65
1:A:3176:MSE:HE1	1:A:3179:TRP:CE3	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3843:LEU:HD22	1:A:3858:MSE:HE1	1.79	0.65
1:B:2196:TRP:CG	1:B:2199:LEU:HD11	2.31	0.65
1:B:2413:PHE:CD2	1:B:2445:LYS:HG3	2.32	0.65
1:B:2883:SER:HA	1:B:2886:GLN:HE21	1.62	0.65
1:B:2936:TYR:CE1	1:B:2949:THR:HG21	2.32	0.65
1:B:3499:ILE:HG13	1:B:3531:TYR:CZ	2.32	0.65
1:B:3594:ALA:HB1	1:B:4028:ILE:HG21	1.79	0.65
1:B:4062:ASP:O	1:B:4066:LEU:HD13	1.97	0.65
1:B:416:SER:O	1:B:420:VAL:HB	1.97	0.65
1:A:3141:PHE:HE1	1:A:3193:ILE:HG13	1.62	0.64
1:A:757:LYS:HA	1:A:760:LEU:CD1	2.27	0.64
1:B:1094:SER:N	1:B:1097:GLU:OE2	2.28	0.64
1:B:1163:LEU:HD22	1:B:1260:LEU:HD11	1.79	0.64
1:B:217:LEU:HD22	1:B:264:ARG:HG3	1.79	0.64
1:B:446:PHE:CZ	1:B:530:LEU:HB3	2.32	0.64
1:A:1145:LEU:HD13	1:A:1149:LYS:HD3	1.80	0.64
1:A:1915:LEU:HD12	1:A:1916:ILE:HG13	1.78	0.64
1:A:3011:LEU:HD12	1:A:3047:SER:HB3	1.79	0.64
1:A:3421:ASP:OD2	1:A:3467:ARG:HD3	1.97	0.64
1:A:404:ASP:O	1:A:406:ARG:N	2.29	0.64
1:B:1655:ILE:HG13	1:B:1677:SER:HA	1.79	0.64
1:B:172:GLU:O	1:B:176:GLU:HG3	1.97	0.64
1:B:2538:ARG:NH1	1:B:2562:LEU:O	2.30	0.64
1:B:2539:LEU:HA	1:B:2542:LEU:HD23	1.79	0.64
1:B:3015:SER:O	1:B:3019:ILE:N	2.28	0.64
1:B:3931:ALA:O	1:B:3935:GLY:CA	2.43	0.64
1:A:1889:VAL:HG22	1:A:1900:PHE:CD2	2.33	0.64
1:A:2412:TYR:CE1	1:A:2415:LEU:HD23	2.32	0.64
1:B:1909:ASN:O	1:B:1912:THR:HG23	1.98	0.64
1:B:171:LEU:HD13	1:B:219:VAL:HG13	1.80	0.64
1:B:385:TYR:CE1	1:B:421:LEU:HD23	2.31	0.64
1:A:183:GLU:HA	1:A:233:ASN:HD21	1.62	0.64
1:A:2094:MSE:HE2	1:A:2142:ILE:HG22	1.79	0.64
1:A:2452:ARG:HG2	1:A:2498:ILE:HD11	1.79	0.64
1:A:3048:LYS:HZ2	1:A:3089:LEU:HB3	1.63	0.64
1:A:866:ILE:HB	1:A:3129:LEU:HD13	1.78	0.64
1:A:3503:VAL:HG21	1:A:3535:ILE:O	1.97	0.64
1:B:1649:LEU:HA	1:B:1652:ILE:HD12	1.78	0.64
1:B:2999:LEU:HD12	1:B:3002:TYR:HE2	1.63	0.64
1:B:3496:ILE:O	1:B:3498:TRP:N	2.31	0.64
1:B:4020:MSE:HE3	1:B:4027:TRP:NE1	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:710:PHE:O	1:B:714:VAL:HG23	1.96	0.64
1:A:1107:TYR:CE1	1:A:1111:LEU:HD13	2.33	0.64
1:A:1349:LEU:HD21	1:A:1359:LEU:HD13	1.78	0.64
1:A:2782:ASP:HA	1:A:2786:LYS:HB2	1.80	0.64
1:A:3046:ARG:HH22	1:A:3181:ASP:CG	1.99	0.64
1:A:3721:GLY:O	1:A:3741:ARG:HB2	1.97	0.64
1:B:1279:LEU:HG	1:B:1292:LYS:NZ	2.13	0.64
1:B:111:CYS:HA	1:B:134:LEU:HD22	1.80	0.64
1:B:3864:ARG:NH1	1:B:4115:ASN:OD1	2.30	0.64
1:A:1269:THR:HG22	1:A:1275:THR:HG21	1.78	0.64
1:A:1649:LEU:HD12	1:A:1652:ILE:HD12	1.78	0.64
1:A:3998:LEU:O	1:A:4002:MSE:HG3	1.97	0.64
1:A:512:GLY:HA3	1:A:726:LEU:HD22	1.79	0.64
1:A:743:LEU:HG	1:A:783:HIS:HE1	1.62	0.64
1:A:854:ARG:O	1:A:858:MSE:HB2	1.98	0.64
1:B:1039:TRP:CZ2	1:B:1049:GLN:HA	2.32	0.64
1:B:177:LEU:HA	1:B:180:LEU:HB2	1.79	0.64
1:B:2467:THR:HB	1:B:2518:GLN:HE22	1.62	0.64
1:B:2850:PHE:HB2	1:B:2853:PRO:HG2	1.80	0.64
1:B:2870:SER:O	1:B:2872:ASP:N	2.30	0.64
1:B:3974:MSE:SE	1:B:3976:GLU:HB3	2.47	0.64
1:B:85:ILE:O	1:B:89:LEU:HG	1.97	0.64
1:A:1165:LEU:HB3	1:A:1169:VAL:HG23	1.79	0.64
1:A:1345:THR:HG21	1:A:1368:LEU:HD13	1.78	0.64
1:A:1609:ALA:HB3	1:A:1806:ARG:HH22	1.61	0.64
1:A:1890:HIS:CE1	1:A:1941:HIS:HA	2.33	0.64
1:A:2307:MSE:HG2	1:A:2348:GLN:NE2	2.12	0.64
1:A:3589:SER:O	1:A:3593:ARG:CB	2.45	0.64
1:A:3676:PRO:O	1:A:3679:ASN:ND2	2.30	0.64
1:A:3425:ARG:NH2	1:A:4000:ASN:OD1	2.31	0.64
1:B:2276:LEU:HA	1:B:2279:ILE:HG12	1.80	0.64
1:B:2939:LEU:HD21	1:B:2994:TRP:CD2	2.33	0.64
1:A:720:GLN:HB3	1:A:1123:THR:HG21	1.78	0.64
1:A:1084:ASN:HD21	1:A:1131:ILE:HG22	1.63	0.64
1:A:2413:PHE:CE1	1:A:2442:MSE:HG2	2.33	0.64
1:A:2555:LEU:HD11	1:A:2803:ILE:HD11	1.79	0.64
1:A:3498:TRP:NE1	1:A:3502:MSE:SE	2.81	0.64
1:B:1973:LYS:O	1:B:1974:ASN:HB2	1.98	0.64
1:B:2423:VAL:HG13	1:B:2424:MSE:H	1.63	0.64
1:B:2433:LYS:NZ	1:B:2461:PHE:CZ	2.65	0.64
1:B:2555:LEU:HD12	1:B:2556:SER:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:LEU:HB3	1:B:319:PHE:HZ	1.63	0.64
1:B:3705:TYR:CE2	1:B:3708:ARG:NH1	2.66	0.64
1:B:393:LYS:HA	1:B:396:PHE:HD1	1.62	0.64
1:B:66:LEU:HD21	1:B:89:LEU:HD11	1.78	0.64
1:A:1700:THR:O	1:A:1702:LEU:N	2.30	0.64
1:A:884:VAL:HB	1:A:3892:THR:OG1	1.98	0.64
1:A:995:PHE:CD1	1:A:1003:SER:HA	2.33	0.64
1:B:101:ALA:HB3	1:B:102:PRO:HD3	1.80	0.64
1:B:1069:HIS:HB3	1:B:3741:ARG:CZ	2.28	0.64
1:B:1598:ASN:CG	1:B:1811:ARG:HG2	2.19	0.64
1:B:1696:LEU:HA	1:B:1700:THR:HG21	1.79	0.64
1:B:3282:ARG:HB2	1:B:3282:ARG:NH1	2.13	0.64
1:B:345:PHE:CD2	1:B:367:GLY:HA3	2.32	0.64
1:B:3816:LEU:O	1:B:3820:MSE:HB3	1.97	0.64
1:B:411:PRO:HG2	1:B:457:CYS:SG	2.37	0.64
1:A:14:ARG:HB3	1:A:2359:LYS:HE2	1.79	0.64
1:A:2253:TYR:HA	1:A:2256:ILE:HB	1.80	0.64
1:A:3855:TYR:HB3	1:A:4074:PHE:CZ	2.32	0.64
1:A:771:ASN:O	1:A:773:LEU:N	2.30	0.64
1:B:1471:GLN:O	1:B:1475:LEU:HB3	1.98	0.64
1:B:207:GLN:O	1:B:212:VAL:HG12	1.98	0.64
1:B:2379:MSE:HE1	1:B:2404:ARG:HH11	1.60	0.64
1:B:909:VAL:O	1:B:913:ARG:HG2	1.98	0.64
1:A:1039:TRP:CZ2	1:A:1049:GLN:HA	2.33	0.63
1:A:1939:LEU:HD13	1:A:1986:ARG:HH21	1.62	0.63
1:A:2194:LEU:HD13	1:A:2244:CYS:HB3	1.79	0.63
1:A:2929:LEU:HG	1:A:3784:ARG:HG2	1.79	0.63
1:A:3110:PHE:O	1:A:3114:TYR:HD1	1.81	0.63
1:A:3788:LEU:HG	1:A:3789:ARG:N	2.13	0.63
1:A:66:LEU:HD21	1:A:89:LEU:HD11	1.80	0.63
1:B:2912:GLY:HA2	1:B:2915:ARG:HH21	1.64	0.63
1:B:3725:ARG:NH1	1:B:3737:ARG:NH2	2.38	0.63
1:A:1640:GLU:O	1:A:1644:ALA:CB	2.46	0.63
1:A:2866:ALA:O	1:A:2869:LEU:N	2.31	0.63
1:A:3781:CYS:HA	1:A:3786:LEU:HD12	1.78	0.63
1:A:3985:VAL:HG11	1:A:4101:GLU:HG2	1.79	0.63
1:A:493:LYS:HB3	1:A:494:PRO:HD2	1.80	0.63
1:B:139:ARG:HA	1:B:173:LYS:HD3	1.80	0.63
1:B:1970:LYS:HE2	1:B:2017:GLY:HA3	1.80	0.63
1:B:4038:TRP:CH2	1:B:4040:PRO:HB3	2.32	0.63
1:A:1259:LEU:HD11	1:A:1337:VAL:HA	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2352:HIS:HB3	1:A:2360:PHE:HB3	1.78	0.63
1:B:2171:LEU:HG	1:B:2177:ASN:HD21	1.63	0.63
1:B:3687:MSE:C	1:B:3689:ASP:H	1.99	0.63
1:B:617:PRO:HB3	1:B:659:ARG:HG3	1.80	0.63
1:A:132:ILE:HA	1:A:135:LEU:HD12	1.80	0.63
1:A:1981:LEU:HD21	1:A:2031:LEU:O	1.98	0.63
1:A:1982:ILE:HA	1:A:1985:LYS:HE2	1.80	0.63
1:A:2281:MSE:SE	1:A:2286:PRO:HB3	2.48	0.63
1:A:2404:ARG:NH1	1:A:2412:TYR:CZ	2.67	0.63
1:A:3192:LYS:N	1:A:3192:LYS:HD2	2.13	0.63
1:B:995:PHE:CD1	1:B:1003:SER:HA	2.33	0.63
1:B:1296:PHE:O	1:B:1299:GLU:N	2.28	0.63
1:B:2145:PHE:HD1	1:B:2188:GLU:HG2	1.62	0.63
1:B:2433:LYS:HG3	1:B:2436:LEU:HD12	1.79	0.63
1:B:2933:ILE:HG23	1:B:3979:LEU:HB2	1.80	0.63
1:B:3974:MSE:HA	1:B:3975:LYS:HB3	1.80	0.63
1:B:744:ASP:C	1:B:746:ARG:H	2.01	0.63
1:B:984:TYR:O	1:B:988:VAL:HG13	1.99	0.63
1:A:1093:GLU:N	1:A:1097:GLU:OE2	2.22	0.63
1:A:720:GLN:HG3	1:A:1121:LEU:HD22	1.81	0.63
1:A:1424:THR:O	1:A:1427:SER:N	2.28	0.63
1:A:1685:ASP:CB	1:A:1727:ARG:HH22	2.06	0.63
1:A:278:HIS:O	1:A:281:GLN:HB3	1.98	0.63
1:A:2936:TYR:CD1	1:A:2949:THR:HG21	2.33	0.63
1:A:904:VAL:O	1:A:906:PHE:N	2.32	0.63
1:B:1006:THR:HG22	1:B:1010:LEU:HG	1.81	0.63
1:B:2022:PRO:HB2	1:B:2072:ARG:HH21	1.62	0.63
1:B:2144:LEU:HB3	1:B:2148:LYS:HE3	1.80	0.63
1:B:2449:VAL:HA	1:B:2452:ARG:HD2	1.80	0.63
1:B:3155:VAL:HG23	1:B:3158:LYS:HD2	1.80	0.63
1:B:3630:ARG:HG2	1:B:3686:TRP:HE1	1.63	0.63
1:B:473:PRO:HA	1:B:476:ARG:NH2	2.11	0.63
1:B:726:LEU:HD23	1:B:729:CYS:SG	2.38	0.63
1:A:1070:PRO:HB2	1:A:1073:PHE:CE1	2.34	0.63
1:A:1729:PHE:CE2	1:A:1870:LYS:HG3	2.33	0.63
1:A:345:PHE:HD2	1:A:367:GLY:HA3	1.64	0.63
1:B:1251:GLN:O	1:B:1255:CYS:HB2	1.98	0.63
1:B:2788:SER:O	1:B:2791:ILE:HB	1.98	0.63
1:B:3763:ARG:NH2	1:B:4009:PRO:HG3	2.13	0.63
1:B:3834:ALA:HB1	1:B:3838:GLU:OE1	1.98	0.63
1:B:766:ALA:O	1:B:768:VAL:N	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:ILE:HG22	1:A:257:ARG:HG3	1.80	0.63
1:A:3684:SER:OG	1:A:3685:PRO:HD3	1.98	0.63
1:A:414:LEU:HD23	1:A:460:ALA:HB1	1.80	0.63
1:A:988:VAL:O	1:A:992:ILE:HG23	1.99	0.63
1:B:1583:MSE:HE1	1:B:1640:GLU:OE2	1.98	0.63
1:B:1711:ARG:HG3	1:B:1712:ARG:N	2.13	0.63
1:B:3919:GLY:H	1:B:3946:PHE:H	1.47	0.63
1:B:942:LEU:HD11	1:B:991:LEU:HD11	1.80	0.63
1:A:1419:LEU:O	1:A:1421:GLU:N	2.31	0.63
1:A:1575:LEU:HD13	1:A:1604:SER:HB3	1.80	0.63
1:A:1952:ILE:HG12	1:A:1953:CYS:H	1.63	0.63
1:A:3816:LEU:HD13	1:A:3966:GLN:NE2	2.12	0.63
1:A:4050:LYS:HB3	1:A:4055:ASN:HD21	1.63	0.63
1:B:1100:VAL:O	1:B:1104:LEU:N	2.29	0.63
1:B:1279:LEU:HG	1:B:1292:LYS:HZ1	1.62	0.63
1:B:1306:ILE:HG12	1:B:1334:LYS:HB3	1.81	0.63
1:B:3167:ARG:HG2	1:B:3186:ARG:NE	2.14	0.63
1:B:3982:SER:O	1:B:3986:HIS:ND1	2.32	0.63
1:B:4088:ASN:OD1	1:B:4091:ALA:HB3	1.99	0.63
1:B:988:VAL:O	1:B:992:ILE:HG23	1.99	0.63
1:A:1887:ASP:OD1	1:A:1937:ARG:NH2	2.31	0.63
1:A:2256:ILE:HG21	1:A:2280:VAL:HG21	1.81	0.63
1:A:2327:LEU:O	1:A:2331:MSE:HG2	1.99	0.63
1:B:114:VAL:CG1	1:B:130:LEU:HD11	2.29	0.63
1:B:2226:PRO:O	1:B:2230:VAL:N	2.27	0.63
1:B:2799:GLN:HG3	1:B:2808:LEU:HD11	1.81	0.63
1:B:2936:TYR:HE1	1:B:2949:THR:HG21	1.64	0.63
1:B:3045:ILE:O	1:B:3048:LYS:HB2	1.99	0.63
1:B:4035:GLU:HG2	1:B:4038:TRP:CE3	2.34	0.63
1:B:559:SER:O	1:B:563:LEU:HG	1.98	0.63
1:A:999:LYS:HD3	1:A:1000:LYS:H	1.64	0.62
1:A:1029:CYS:HB3	1:A:1085:ILE:HG13	1.81	0.62
1:A:2379:MSE:SE	1:A:2408:MSE:SE	3.17	0.62
1:A:31:GLY:O	1:A:34:LEU:HB3	1.98	0.62
1:A:4048:LYS:O	1:A:4051:LEU:HB3	1.99	0.62
1:A:649:PHE:O	1:A:651:TYR:N	2.32	0.62
1:A:802:THR:O	1:A:806:SER:OG	2.15	0.62
1:A:935:HIS:O	1:A:938:VAL:HB	1.99	0.62
1:B:3250:ASN:OD1	1:B:3285:HIS:HB3	1.98	0.62
1:A:1745:LYS:C	1:A:1747:LEU:H	2.02	0.62
1:A:4056:PRO:HG2	1:A:4094:PRO:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1459:HIS:CE1	1:B:1510:LEU:HG	2.35	0.62
1:B:1604:SER:HB2	1:B:1632:TRP:HB3	1.80	0.62
1:B:2146:LEU:HA	1:B:2149:LEU:HG	1.80	0.62
1:B:3107:ILE:HA	1:B:3110:PHE:CE2	2.34	0.62
1:B:3778:ASP:OD2	1:B:3781:CYS:N	2.32	0.62
1:B:452:LYS:O	1:B:455:LEU:HG	1.99	0.62
1:B:585:ILE:HG22	1:B:586:GLN:H	1.64	0.62
1:A:101:ALA:HB3	1:A:102:PRO:HD3	1.81	0.62
1:A:2147:ALA:HB1	1:A:2151:ILE:HD12	1.82	0.62
1:A:2378:PHE:CE1	1:A:2408:MSE:HE1	2.29	0.62
1:A:956:PRO:HB2	1:A:957:PRO:HD3	1.79	0.62
1:B:3592:VAL:HG13	1:B:3609:MSE:SE	2.50	0.62
1:B:4046:TYR:CZ	1:B:4049:ARG:NH2	2.68	0.62
1:A:2074:PRO:O	1:A:2077:HIS:N	2.32	0.62
1:A:252:VAL:HG11	1:A:265:TYR:HB2	1.81	0.62
1:A:2900:LEU:HD12	1:A:2905:LEU:HD21	1.80	0.62
1:A:3176:MSE:HE2	1:A:3251:ASN:HD22	1.64	0.62
1:A:3256:MSE:HE2	1:A:3282:ARG:HH12	1.62	0.62
1:A:3762:GLN:NE2	1:A:3763:ARG:NH1	2.46	0.62
1:A:3812:LEU:O	1:A:3816:LEU:CB	2.38	0.62
1:B:1637:SER:O	1:B:1640:GLU:N	2.32	0.62
1:B:154:SER:OG	1:B:189:MSE:HG2	1.99	0.62
1:B:200:PHE:O	1:B:204:LEU:HG	1.98	0.62
1:B:2936:TYR:CD2	1:B:3979:LEU:HD21	2.33	0.62
1:B:2943:PHE:CD2	1:B:2944:THR:HG23	2.34	0.62
1:B:508:HIS:HD2	1:B:725:LEU:HD13	1.65	0.62
1:B:891:ARG:CD	1:B:905:ILE:HG12	2.30	0.62
1:A:2239:LYS:HD3	2:K:110:UNK:CB	2.30	0.62
1:A:2260:PHE:CD1	1:A:2274:ILE:HG22	2.35	0.62
1:A:2900:LEU:HB3	1:A:2905:LEU:HD11	1.80	0.62
1:A:3486:GLU:HG3	1:A:3487:ILE:H	1.65	0.62
1:A:870:LEU:HD11	1:A:3125:ARG:HG3	1.80	0.62
1:B:1080:LEU:HD12	1:B:1081:ALA:N	2.14	0.62
1:B:1708:GLU:HB2	1:B:1709:GLU:OE2	2.00	0.62
1:B:2386:LEU:O	1:B:2390:HIS:HB2	2.00	0.62
1:B:3824:GLU:HB3	1:B:3829:LEU:HD11	1.81	0.62
1:A:971:ARG:HD2	1:A:1024:THR:HG23	1.80	0.62
1:A:1033:ILE:HB	1:A:1085:ILE:HG22	1.81	0.62
1:A:1292:LYS:HZ2	1:A:1361:LYS:NZ	1.96	0.62
1:A:2239:LYS:HD2	1:A:2279:ILE:HD12	1.81	0.62
1:A:245:SER:HA	1:A:248:ILE:HD12	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2555:LEU:O	1:A:2558:ALA:HB3	1.99	0.62
1:A:2837:LEU:HA	1:A:2840:PHE:CD2	2.30	0.62
1:A:2869:LEU:HG	1:A:2893:LEU:HD12	1.80	0.62
1:B:1265:GLU:O	1:B:1269:THR:HG23	2.00	0.62
1:B:1293:ALA:HA	1:B:1296:PHE:HD2	1.65	0.62
1:B:3582:GLU:O	1:B:3586:LYS:HB3	2.00	0.62
1:B:3630:ARG:HG2	1:B:3686:TRP:CD1	2.35	0.62
1:B:3174:ASP:OD2	1:B:3779:SER:HA	2.00	0.62
1:B:3812:LEU:HA	1:B:3815:LEU:HD12	1.81	0.62
1:B:414:LEU:HA	1:B:417:VAL:HB	1.80	0.62
1:B:508:HIS:CD2	1:B:725:LEU:HD13	2.35	0.62
1:A:2847:THR:HB	1:A:2850:PHE:HD2	1.65	0.62
1:A:345:PHE:CD2	1:A:367:GLY:HA3	2.34	0.62
1:A:3810:VAL:CG2	1:A:3815:LEU:HD11	2.29	0.62
1:A:3931:ALA:O	1:A:3935:GLY:HA2	2.00	0.62
1:A:509:ARG:HB3	1:A:729:CYS:SG	2.40	0.62
1:B:1574:ASN:HB3	1:B:1582:LEU:HD21	1.82	0.62
1:B:2925:GLU:HA	1:B:3121:LEU:HD11	1.80	0.62
1:B:3393:GLU:OE1	1:B:3416:LEU:HD13	1.99	0.62
1:B:3872:ARG:HH11	1:B:3965:ARG:NH1	1.97	0.62
1:B:796:LEU:HA	1:B:799:TYR:CE2	2.34	0.62
1:B:870:LEU:HA	1:B:873:VAL:HB	1.81	0.62
1:A:1119:LYS:HZ1	1:A:1256:TRP:HZ2	1.47	0.62
1:A:1220:LEU:HD13	1:A:1274:ARG:HG3	1.82	0.62
1:A:1216:GLY:HA3	1:A:1271:ILE:HG22	1.80	0.62
1:A:1342:MSE:SE	1:A:1372:LEU:HB2	2.50	0.62
1:A:1429:GLU:O	1:A:1433:ALA:CB	2.46	0.62
1:A:1880:MSE:HE2	1:A:1884:LEU:HD11	1.81	0.62
1:A:2002:LYS:C	1:A:2004:TYR:H	2.03	0.62
1:A:2227:LYS:HA	1:A:2234:ASN:HD22	1.64	0.62
1:A:2416:LYS:HB3	1:A:2442:MSE:SE	2.49	0.62
1:A:3930:VAL:HG12	1:A:3937:VAL:HG22	1.81	0.62
1:A:398:THR:O	1:A:401:ASP:N	2.33	0.62
1:A:794:PRO:HA	1:A:869:ASN:HB3	1.81	0.62
1:A:801:LYS:NZ	1:A:877:ASP:OD2	2.29	0.62
1:B:1090:ARG:HA	1:B:1090:ARG:HE	1.64	0.62
1:B:1221:ILE:HG13	1:B:1274:ARG:NH1	2.14	0.62
1:B:2157:PHE:HE2	1:B:2199:LEU:CD1	2.12	0.62
1:B:2310:VAL:HG23	1:B:2315:VAL:HG21	1.81	0.62
1:B:2416:LYS:O	1:B:2420:PHE:CB	2.47	0.62
1:B:2776:ARG:HA	1:B:2776:ARG:HH11	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3019:ILE:HG13	1:B:3020:ASP:H	1.65	0.62
1:B:446:PHE:HA	1:B:449:TYR:HE2	1.62	0.62
1:A:1449:ALA:HA	1:A:1452:VAL:HB	1.80	0.62
1:A:2283:ASN:O	1:A:2287:PRO:HD3	2.00	0.62
1:A:3465:PHE:HA	1:A:3468:LEU:HD12	1.81	0.62
1:A:572:VAL:HG13	1:A:573:LEU:H	1.64	0.62
1:B:1269:THR:HG22	1:B:1275:THR:HG21	1.82	0.62
1:B:18:THR:O	1:B:22:ALA:HB3	1.99	0.62
1:B:232:CYS:SG	1:B:274:LEU:HD13	2.40	0.62
1:B:3228:SER:HA	1:B:3231:ILE:HD12	1.80	0.62
1:B:3513:ALA:O	1:B:3516:HIS:N	2.33	0.62
1:B:634:LEU:HB3	1:B:638:GLN:HE22	1.65	0.62
1:A:2874:ALA:HB1	1:A:2878:ALA:HB3	1.81	0.62
1:A:2913:LYS:O	1:A:2915:ARG:N	2.32	0.62
1:A:538:ASP:O	1:A:545:LEU:HD13	1.99	0.62
1:A:789:TYR:HA	1:A:793:LEU:HD12	1.82	0.62
1:B:3243:ILE:HD13	1:B:3262:LEU:HD22	1.82	0.62
1:B:358:GLU:HG3	1:B:359:LEU:H	1.64	0.62
1:A:1928:ALA:HB2	1:A:1941:HIS:CE1	2.35	0.61
1:A:242:PRO:O	1:A:246:ARG:HB3	2.00	0.61
1:A:753:GLN:O	1:A:757:LYS:CB	2.48	0.61
1:A:935:HIS:HB2	1:A:984:TYR:HE2	1.65	0.61
1:B:1280:GLN:HA	1:B:1361:LYS:NZ	2.15	0.61
1:B:1298:LEU:HA	1:B:1301:ILE:HB	1.82	0.61
1:B:1073:PHE:CZ	1:B:3745:GLU:HA	2.35	0.61
1:B:732:PHE:HB2	1:B:733:LEU:HD23	1.82	0.61
1:A:1604:SER:HB2	1:A:1632:TRP:HB3	1.82	0.61
1:A:202:GLY:O	1:A:206:THR:OG1	2.10	0.61
1:A:2399:GLU:O	1:A:2402:LEU:HG	2.00	0.61
1:A:2549:LYS:HZ1	1:A:2557:LEU:CD2	2.10	0.61
1:A:3008:TRP:HA	1:A:3050:LYS:HG2	1.82	0.61
1:A:3684:SER:O	1:A:3688:SER:OG	2.14	0.61
1:A:3809:THR:HA	1:A:3931:ALA:HA	1.82	0.61
1:A:713:GLU:O	1:A:717:LYS:HG2	2.00	0.61
1:B:1214:GLU:HB2	1:B:1218:SER:HB3	1.82	0.61
1:B:1374:GLN:O	1:B:1378:GLU:HB2	2.00	0.61
1:B:2142:ILE:HA	1:B:2145:PHE:HD2	1.62	0.61
1:B:592:GLU:HB3	1:B:601:TRP:HZ2	1.65	0.61
1:B:913:ARG:HG3	1:B:937:MSE:SE	2.50	0.61
1:A:1108:MSE:O	1:A:1112:ALA:N	2.32	0.61
1:A:83:GLU:HG3	1:A:130:LEU:HD13	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1996:VAL:HG23	1:A:1997:PRO:HD2	1.82	0.61
1:A:2274:ILE:HD13	1:A:2318:ALA:HB2	1.81	0.61
1:A:287:LEU:C	1:A:291:VAL:HB	2.21	0.61
1:A:3037:GLN:HG3	1:A:3040:TYR:HE2	1.65	0.61
1:A:3578:LEU:HD13	1:A:3683:CYS:SG	2.40	0.61
1:A:3924:HIS:H	1:A:3927:ASN:HD22	1.46	0.61
1:B:1403:MSE:HA	1:B:1406:LEU:HB2	1.81	0.61
1:B:2177:ASN:HD22	1:B:2182:ILE:CG2	2.12	0.61
1:B:2399:GLU:O	1:B:2402:LEU:HG	2.00	0.61
1:B:2957:LEU:HB3	1:B:3989:ARG:HH22	1.63	0.61
1:B:980:THR:HG22	1:B:984:TYR:HE2	1.66	0.61
1:A:2167:PRO:O	1:A:2171:LEU:HB3	2.01	0.61
1:A:2925:GLU:O	1:A:2927:ALA:N	2.30	0.61
1:A:440:VAL:HG21	1:A:1814:PHE:CZ	2.36	0.61
1:A:913:ARG:NE	1:A:916:GLU:OE2	2.32	0.61
1:B:1431:LEU:HD11	1:B:1479:VAL:HG22	1.81	0.61
1:B:2538:ARG:HH11	1:B:2565:MSE:CB	2.08	0.61
1:B:2961:ALA:HB1	1:B:3002:TYR:CD1	2.33	0.61
1:A:1086:TYR:CD2	1:A:1090:ARG:HG2	2.36	0.61
1:A:1574:ASN:HB3	1:A:1582:LEU:HD21	1.81	0.61
1:A:2936:TYR:O	1:A:2940:ARG:HB2	2.00	0.61
1:A:3630:ARG:HD2	1:A:3633:ILE:HG12	1.83	0.61
1:A:3962:ARG:CZ	1:A:3962:ARG:HB2	2.30	0.61
1:A:508:HIS:HD2	1:A:725:LEU:HD22	1.65	0.61
1:B:2220:MSE:SE	1:B:2256:ILE:HD11	2.51	0.61
1:B:2849:SER:HB3	1:B:2881:LEU:HD12	1.82	0.61
1:B:3152:SER:HB3	1:B:3153:SER:CB	2.31	0.61
1:B:3167:ARG:HD3	1:B:3186:ARG:HG2	1.82	0.61
1:A:1076:LEU:HD22	1:A:1111:LEU:HG	1.83	0.61
1:A:2517:LEU:HA	1:A:2520:ILE:HG22	1.82	0.61
1:A:3765:GLU:O	1:A:3768:PHE:HB2	2.00	0.61
1:A:3962:ARG:NH1	1:A:4124:TRP:CZ3	2.66	0.61
1:A:575:ILE:HG12	1:A:579:LEU:HB2	1.81	0.61
1:B:1378:GLU:O	1:B:1382:ILE:HG12	2.01	0.61
1:B:2011:ALA:O	1:B:2013:GLU:N	2.33	0.61
1:B:3435:ASP:O	1:B:3439:LEU:HB3	2.01	0.61
1:B:4082:ARG:CG	1:B:4091:ALA:HB2	2.30	0.61
1:B:612:LEU:O	1:B:616:LYS:N	2.31	0.61
1:A:1178:ARG:HB3	1:A:1179:PRO:HD3	1.82	0.61
1:A:2396:LEU:HA	1:A:2400:VAL:HG23	1.82	0.61
1:A:3885:ARG:O	1:A:3889:ARG:HB2	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:PHE:CE2	1:A:530:LEU:HB3	2.34	0.61
1:B:1108:MSE:O	1:B:1112:ALA:N	2.33	0.61
1:B:146:GLU:HB2	1:B:149:ILE:HB	1.83	0.61
1:B:3314:SER:HB3	1:B:3318:LYS:HE3	1.82	0.61
1:B:3493:TRP:HB3	1:B:3711:PRO:HA	1.81	0.61
1:B:3491:PRO:CB	1:B:3711:PRO:HB3	2.30	0.61
1:A:970:LEU:HD21	1:A:1031:ARG:HH21	1.65	0.61
1:A:1352:SER:HB3	1:A:1353:PRO:HD3	1.83	0.61
1:A:3414:MSE:HE1	1:A:3450:MSE:HA	1.82	0.61
1:A:3435:ASP:O	1:A:3439:LEU:CB	2.49	0.61
1:A:3797:THR:HG22	1:A:3800:LEU:HG	1.82	0.61
1:A:934:LEU:HA	1:A:937:MSE:HE3	1.83	0.61
1:B:1270:PHE:HZ	1:B:1347:THR:HB	1.66	0.61
1:B:2847:THR:HB	1:B:2850:PHE:HD2	1.65	0.61
1:B:3047:SER:O	1:B:3050:LYS:HG3	2.01	0.61
1:B:367:GLY:C	1:B:369:PHE:H	2.03	0.61
1:B:3729:MSE:HE2	1:B:3737:ARG:HB2	1.82	0.61
1:B:3835:PRO:HA	1:B:3871:PHE:HE1	1.65	0.61
1:B:3923:ARG:CD	1:B:3962:ARG:HH22	2.14	0.61
1:B:938:VAL:O	1:B:942:LEU:HB2	2.00	0.61
1:A:1142:HIS:O	1:A:1144:SER:N	2.30	0.61
1:A:1270:PHE:CZ	1:A:1347:THR:HG23	2.35	0.61
1:A:2204:GLY:HA2	1:A:2208:ASP:OD2	2.00	0.61
1:A:2479:TRP:CZ3	1:A:2480:ILE:HD13	2.36	0.61
1:A:349:ILE:CD1	1:A:368:LEU:HD12	2.31	0.61
1:A:3517:SER:HA	1:A:3520:GLU:HB2	1.81	0.61
1:A:3543:LYS:HE2	1:A:3545:THR:HG22	1.82	0.61
1:A:1248:PHE:HB3	1:A:3695:LEU:HD23	1.83	0.61
1:A:935:HIS:HB2	1:A:984:TYR:CE2	2.34	0.61
1:B:1352:SER:O	1:B:1354:GLU:N	2.33	0.61
1:B:1587:VAL:HG23	1:B:1647:ALA:HB2	1.82	0.61
1:B:206:THR:HA	1:B:209:THR:OG1	2.01	0.61
1:B:2814:SER:O	1:B:2818:LYS:HB2	2.00	0.61
1:A:114:VAL:HG12	1:A:130:LEU:HD21	1.81	0.61
1:A:1740:VAL:O	1:A:1743:MSE:HG3	1.99	0.61
1:A:239:GLU:HG3	1:A:240:GLU:HG3	1.83	0.61
1:A:273:ARG:HG3	1:A:274:LEU:N	2.15	0.61
1:A:2960:GLU:HG2	1:A:3252:PHE:CD2	2.36	0.61
1:A:2933:ILE:HD13	1:A:3976:GLU:HG3	1.83	0.61
1:A:437:HIS:O	1:A:440:VAL:HG22	2.00	0.61
1:A:484:HIS:CD2	1:A:556:SER:HB3	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:645:TRP:CE3	1:A:660:LEU:HD11	2.35	0.61
1:A:621:SER:HB3	1:A:659:ARG:CZ	2.31	0.61
1:B:2157:PHE:HE2	1:B:2199:LEU:HD13	1.66	0.61
1:B:2345:VAL:O	1:B:2349:LEU:HG	2.01	0.61
1:B:2943:PHE:C	1:B:2945:SER:H	2.04	0.61
1:B:3247:ARG:NE	1:B:3278:GLN:OE1	2.30	0.61
1:B:3614:TYR:O	1:B:3618:GLY:N	2.29	0.61
1:B:3631:LYS:HA	1:B:3634:GLN:HB3	1.83	0.61
1:A:177:LEU:O	1:A:180:LEU:N	2.34	0.60
1:A:2183:HIS:CE1	1:A:2237:ILE:HD13	2.36	0.60
1:A:2260:PHE:HD1	1:A:2274:ILE:HG22	1.65	0.60
1:A:3915:HIS:O	1:A:3918:LEU:N	2.33	0.60
1:A:446:PHE:HD1	1:A:447:PRO:HD3	1.65	0.60
1:A:637:LYS:O	1:A:641:PHE:HB3	2.01	0.60
1:B:1886:LYS:HE3	1:B:1924:THR:HG21	1.82	0.60
1:B:2274:ILE:HA	1:B:2277:LEU:HG	1.83	0.60
1:B:2481:HIS:HE1	1:B:2485:ARG:HH11	1.49	0.60
1:B:2575:PRO:HD2	1:B:2785:ILE:HD11	1.81	0.60
1:B:2806:LYS:HZ1	1:B:2858:ILE:HG21	1.64	0.60
1:B:3498:TRP:O	1:B:3498:TRP:CD1	2.54	0.60
1:B:659:ARG:NH2	1:B:662:LEU:HG	2.10	0.60
1:A:1118:GLU:HG3	1:A:3743:HIS:CE1	2.35	0.60
1:A:1087:ARG:HD2	1:A:1137:ILE:HD11	1.83	0.60
1:A:1155:ARG:O	1:A:1158:PRO:HD2	2.01	0.60
1:A:135:LEU:HD21	1:A:173:LYS:HD2	1.83	0.60
1:A:1885:PRO:O	1:A:1889:VAL:HG23	2.00	0.60
1:A:3117:ILE:HG13	1:A:3120:LEU:HB3	1.82	0.60
1:A:3283:LEU:HD11	1:A:3297:VAL:HG13	1.82	0.60
1:A:3788:LEU:HD13	1:A:3910:LEU:HD23	1.82	0.60
1:A:3947:GLY:O	1:A:3950:THR:N	2.34	0.60
1:B:1419:LEU:O	1:B:1421:GLU:N	2.34	0.60
1:B:1711:ARG:HG3	1:B:1712:ARG:H	1.65	0.60
1:B:175:TYR:HA	1:B:178:LEU:HD12	1.82	0.60
1:B:1903:SER:O	1:B:1906:THR:OG1	2.18	0.60
1:B:2316:TYR:CZ	1:B:2317:ALA:HB2	2.36	0.60
1:B:2989:ALA:O	1:B:2993:PHE:N	2.32	0.60
1:B:3595:GLU:HA	1:B:3598:LYS:HD2	1.81	0.60
1:B:627:VAL:HG12	1:B:628:GLU:N	2.15	0.60
1:B:775:GLU:O	1:B:779:TYR:HD2	1.84	0.60
1:A:1424:THR:OG1	1:A:1425:ALA:N	2.34	0.60
1:A:1452:VAL:HG11	1:A:1502:SER:HB3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1805:PHE:HA	1:A:1808:ASP:OD2	2.00	0.60
1:A:2167:PRO:HB2	1:A:2171:LEU:HD22	1.83	0.60
1:A:246:ARG:HA	1:A:249:PHE:HD2	1.66	0.60
1:A:2813:PHE:HA	1:A:2816:ILE:HG22	1.82	0.60
1:A:607:ASP:HA	1:A:610:ALA:HB3	1.81	0.60
1:B:1762:MSE:HE2	1:B:1899:VAL:HG11	1.83	0.60
1:B:2353:GLN:HG2	1:B:2361:ILE:HD13	1.83	0.60
1:B:242:PRO:HB3	1:B:282:PHE:CD1	2.35	0.60
1:B:2775:TYR:HB3	1:B:2776:ARG:NH2	2.16	0.60
1:B:3048:LYS:O	1:B:3052:LEU:N	2.31	0.60
1:B:3265:GLU:HA	1:B:3267:LYS:HE3	1.84	0.60
1:B:404:ASP:O	1:B:406:ARG:N	2.33	0.60
1:A:1761:LEU:HD22	1:A:1860:GLU:HB3	1.83	0.60
1:A:1981:LEU:O	1:A:1985:LYS:HG2	2.02	0.60
1:A:2088:LEU:O	1:A:2092:GLU:N	2.34	0.60
1:A:3876:SER:O	1:A:3879:PRO:HD2	2.00	0.60
1:A:390:GLN:O	1:A:393:LYS:HG2	2.01	0.60
1:B:108:LYS:HG2	1:B:138:PHE:HA	1.81	0.60
1:B:3065:ILE:HD13	1:B:3089:LEU:HD21	1.83	0.60
1:B:3954:PRO:HB3	1:B:4027:TRP:HA	1.82	0.60
1:B:3594:ALA:HB1	1:B:4028:ILE:HD13	1.83	0.60
1:A:1131:ILE:HA	1:A:1134:LEU:HG	1.84	0.60
1:A:1978:PHE:O	1:A:1981:LEU:HB3	2.01	0.60
1:A:1983:ASP:O	1:A:1987:ARG:HB2	2.02	0.60
1:A:2430:GLU:OE2	1:A:2461:PHE:HD1	1.83	0.60
1:A:2413:PHE:CD1	1:A:2442:MSE:HG2	2.36	0.60
1:A:908:ASP:HB3	1:A:2807:GLN:OE1	2.01	0.60
1:A:3181:ASP:O	1:A:3184:THR:OG1	2.13	0.60
1:A:4004:VAL:O	1:A:4008:GLU:CB	2.50	0.60
1:A:617:PRO:HB3	1:A:659:ARG:HG2	1.82	0.60
1:B:1259:LEU:HG	1:B:1337:VAL:HG22	1.83	0.60
1:B:1743:MSE:HG2	1:B:1747:LEU:HD12	1.83	0.60
1:B:224:LEU:HD22	1:B:248:ILE:HD11	1.83	0.60
1:B:327:VAL:HG22	1:B:338:LEU:HD13	1.83	0.60
1:B:3389:VAL:HG11	1:B:3419:PHE:CZ	2.35	0.60
1:B:3965:ARG:HE	1:B:3969:ASN:HD21	1.49	0.60
1:B:730:LEU:HD23	1:B:733:LEU:HD12	1.83	0.60
1:A:1100:VAL:O	1:A:1104:LEU:N	2.33	0.60
1:A:1935:GLU:HB2	1:A:1986:ARG:CZ	2.31	0.60
1:A:3155:VAL:N	1:A:3156:PRO:HD2	2.17	0.60
1:A:3725:ARG:NH1	1:A:3737:ARG:HH22	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:GLY:C	1:A:405:ASP:H	2.04	0.60
1:A:966:PHE:O	1:A:969:LEU:HB3	2.02	0.60
1:B:1742:CYS:HA	1:B:1745:LYS:HD2	1.83	0.60
1:B:2472:GLN:O	1:B:2476:ILE:HG23	2.02	0.60
1:B:3483:MSE:O	1:B:3516:HIS:NE2	2.35	0.60
1:B:3670:MSE:O	1:B:3674:SER:HB3	2.00	0.60
1:B:613:HIS:ND1	1:B:614:PRO:HD3	2.16	0.60
1:A:249:PHE:O	1:A:253:LEU:HG	2.01	0.60
1:A:3503:VAL:HG23	1:A:3536:SER:HA	1.83	0.60
1:A:3760:GLN:OE1	1:A:3760:GLN:N	2.34	0.60
1:A:566:ASP:OD2	1:A:1800:SER:HA	2.02	0.60
1:B:1066:LEU:HA	1:B:1069:HIS:CD2	2.36	0.60
1:B:1220:LEU:HD13	1:B:1274:ARG:HG3	1.81	0.60
1:B:1700:THR:OG1	1:B:1701:SER:N	2.33	0.60
1:B:1946:ASN:O	1:B:1949:ILE:HG22	2.02	0.60
1:B:2326:ILE:HG21	1:B:2341:LEU:HD23	1.82	0.60
1:B:3723:ASP:HB2	1:B:3741:ARG:HE	1.66	0.60
1:A:3152:SER:HB3	1:A:3153:SER:CB	2.32	0.60
1:A:3487:ILE:CG2	1:A:3495:PHE:HB2	2.31	0.60
1:A:752:LEU:HB2	1:A:756:PHE:CE1	2.37	0.60
1:A:936:SER:O	1:A:939:MSE:N	2.35	0.60
1:B:1130:ALA:O	1:B:1134:LEU:HG	2.01	0.60
1:B:1146:ASN:O	1:B:1150:LYS:HB3	2.02	0.60
1:B:2975:ALA:C	1:B:2977:ASN:H	2.05	0.60
1:B:3344:GLU:O	1:B:3348:LEU:HG	2.02	0.60
1:B:3928:PHE:HE2	1:B:3962:ARG:HE	1.47	0.60
1:B:3962:ARG:NH1	1:B:4124:TRP:CH2	2.70	0.60
1:B:649:PHE:HE1	1:B:653:LEU:H	1.49	0.60
1:A:1063:LEU:HD13	1:A:1082:PHE:CZ	2.37	0.60
1:A:1583:MSE:HE2	1:A:1639:LEU:HB2	1.83	0.60
1:A:2083:LEU:H	1:A:2086:ASP:HB2	1.67	0.60
1:A:2274:ILE:CG1	1:A:2314:GLU:HB3	2.32	0.60
1:A:2554:PHE:O	1:A:2557:LEU:N	2.35	0.60
1:A:3351:ILE:O	1:A:3355:LYS:HG2	2.02	0.60
1:A:416:SER:O	1:A:420:VAL:HB	2.01	0.60
1:A:999:LYS:HB3	1:A:1001:PHE:CE2	2.37	0.60
1:B:1520:ALA:O	1:B:1524:LEU:HD13	2.01	0.60
1:B:3916:TRP:CE3	1:B:3917:ILE:HD12	2.36	0.60
1:B:3950:THR:OG1	1:B:3957:GLU:O	2.09	0.60
1:A:2157:PHE:HE1	1:A:2203:THR:HB	1.66	0.60
1:A:2389:PHE:CD2	1:A:2396:LEU:HD22	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:PHE:CD1	1:A:297:LEU:HD13	2.37	0.60
1:A:3971:MSE:HE1	1:A:3980:MSE:SE	2.52	0.60
1:B:1762:MSE:HG2	1:B:1896:ILE:HA	1.83	0.60
1:B:2145:PHE:HZ	1:B:2185:MSE:HA	1.66	0.60
1:B:2981:TRP:O	1:B:2985:GLU:HB2	2.02	0.60
1:B:3444:ALA:HA	1:B:3475:TYR:OH	2.02	0.60
1:B:3571:PHE:O	1:B:3575:LEU:CB	2.49	0.60
1:A:2183:HIS:HE1	1:A:2237:ILE:HG21	1.67	0.59
1:A:2436:LEU:O	1:A:2439:ILE:HG22	2.02	0.59
1:A:933:LEU:HD11	1:A:2795:GLN:OE1	2.02	0.59
1:A:3498:TRP:HE1	1:A:3502:MSE:SE	2.35	0.59
1:A:3572:ILE:O	1:A:3575:LEU:HB2	2.01	0.59
1:A:3584:LEU:O	1:A:3588:TRP:HB3	2.02	0.59
1:A:396:PHE:CD2	1:A:441:MSE:HG3	2.37	0.59
1:A:414:LEU:HA	1:A:417:VAL:HB	1.84	0.59
1:A:722:LYS:HB3	1:A:727:ALA:HA	1.84	0.59
1:B:1166:LEU:HB3	1:B:1170:LYS:NZ	2.17	0.59
1:B:1569:THR:O	1:B:1573:LYS:HB2	2.02	0.59
1:B:1750:LEU:O	1:B:1754:GLN:HG3	2.02	0.59
1:B:18:THR:O	1:B:22:ALA:CB	2.49	0.59
1:B:3722:PHE:CE1	1:B:3740:ILE:HG12	2.23	0.59
1:B:913:ARG:HA	1:B:916:GLU:CD	2.23	0.59
1:A:1344:PHE:HA	1:A:1347:THR:HB	1.84	0.59
1:A:1438:GLY:O	1:A:1441:ALA:HB2	2.01	0.59
1:A:1916:ILE:HG23	1:A:1920:TYR:CE1	2.36	0.59
1:A:2139:PRO:O	1:A:2143:ARG:HD2	2.01	0.59
1:A:2352:HIS:HB2	1:A:2364:LEU:HD11	1.83	0.59
1:A:2549:LYS:NZ	1:A:2557:LEU:HD22	2.11	0.59
1:A:3047:SER:HB2	1:A:3050:LYS:HE2	1.84	0.59
1:A:3435:ASP:O	1:A:3439:LEU:HB3	2.02	0.59
1:A:3572:ILE:HA	1:A:3575:LEU:HG	1.82	0.59
1:A:3723:ASP:HB2	1:A:3741:ARG:HE	1.67	0.59
1:B:2430:GLU:HG3	1:B:2465:PRO:CB	2.32	0.59
1:B:850:GLU:OE2	1:B:854:ARG:NH2	2.34	0.59
1:B:977:ASP:HB3	1:B:981:ARG:H	1.67	0.59
1:A:1651:LYS:O	1:A:1654:GLN:HB2	2.02	0.59
1:A:2325:LEU:HG	1:A:2329:TYR:CE2	2.37	0.59
1:A:393:LYS:HA	1:A:396:PHE:HD1	1.67	0.59
1:A:3913:ILE:HD11	1:A:3984:MSE:HB3	1.83	0.59
1:A:3946:PHE:HE2	1:A:4048:LYS:HD2	1.68	0.59
1:A:913:ARG:CB	1:A:934:LEU:HD12	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:980:THR:O	1:A:984:TYR:HD1	1.85	0.59
1:B:1175:HIS:O	1:B:1179:PRO:HD3	2.01	0.59
1:B:610:ALA:HA	1:B:613:HIS:CE1	2.37	0.59
1:A:1029:CYS:SG	1:A:1085:ILE:HG13	2.42	0.59
1:A:1142:HIS:C	1:A:1144:SER:H	2.05	0.59
1:A:1894:SER:HB2	1:A:1896:ILE:HG13	1.83	0.59
1:A:1996:VAL:HG21	1:A:2047:THR:OG1	2.02	0.59
1:A:2510:LEU:HG	1:A:2522:ARG:HE	1.68	0.59
1:A:3090:TYR:HB2	1:A:3099:ALA:HB2	1.84	0.59
1:A:3080:LEU:HB3	1:A:3102:TYR:CE1	2.37	0.59
1:A:3439:LEU:O	1:A:3443:PRO:HD3	2.02	0.59
1:A:3583:LEU:HD13	1:A:3755:GLY:HA3	1.85	0.59
1:A:966:PHE:HB3	1:A:967:PRO:HD3	1.83	0.59
1:B:1005:ASP:OD1	1:B:1005:ASP:N	2.34	0.59
1:B:108:LYS:HB3	1:B:138:PHE:CD1	2.37	0.59
1:B:2129:LEU:HD22	1:B:2144:LEU:HD11	1.83	0.59
1:B:2330:VAL:CG2	1:B:2335:ASN:HA	2.28	0.59
1:B:2420:PHE:CZ	1:B:2436:LEU:HB3	2.37	0.59
1:B:2542:LEU:CB	1:B:2546:TYR:HE2	2.14	0.59
1:B:2886:GLN:CD	1:B:2887:PRO:HD3	2.23	0.59
1:B:3333:THR:OG1	1:B:3385:LEU:HB3	2.01	0.59
1:B:3887:PHE:HE1	1:B:3900:LEU:HB3	1.67	0.59
2:S:217:UNK:HA	2:S:220:MSE:SE	2.52	0.59
1:A:136:GLN:HA	1:A:139:ARG:HD3	1.84	0.59
1:A:2274:ILE:HG12	1:A:2314:GLU:HB3	1.83	0.59
1:A:2420:PHE:CZ	1:A:2436:LEU:HB3	2.37	0.59
1:A:3811:THR:HG22	1:A:3929:MSE:SE	2.53	0.59
1:A:4081:ALA:HA	1:A:4113:ASP:OD2	2.02	0.59
1:B:1908:GLY:HA3	1:B:1952:ILE:HG13	1.84	0.59
1:B:232:CYS:HG	1:B:275:PHE:HE1	1.50	0.59
1:B:3069:MSE:HA	1:B:3072:GLU:HB3	1.84	0.59
1:B:3389:VAL:O	1:B:3393:GLU:HG3	2.02	0.59
1:B:633:ILE:HG22	1:B:634:LEU:HD23	1.84	0.59
1:A:1416:GLU:O	1:A:1420:ARG:HB2	2.03	0.59
1:A:1711:ARG:HB3	1:A:1739:TYR:HE1	1.68	0.59
1:A:1925:GLU:O	1:A:1928:ALA:N	2.32	0.59
1:A:2326:ILE:O	1:A:2330:VAL:HB	2.03	0.59
1:A:3156:PRO:HB2	1:A:3197:LEU:HD12	1.84	0.59
1:A:3581:PRO:O	1:A:3585:PHE:HD1	1.85	0.59
1:B:1142:HIS:C	1:B:1144:SER:H	2.05	0.59
1:B:1368:LEU:HA	1:B:1371:VAL:HG12	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:GLU:OE2	1:B:264:ARG:NH2	2.36	0.59
1:B:2239:LYS:O	1:B:2242:VAL:HB	2.02	0.59
1:B:2281:MSE:SE	1:B:2286:PRO:HB3	2.52	0.59
1:B:2501:LEU:O	1:B:2505:VAL:HG23	2.02	0.59
1:B:2921:LEU:HD12	1:B:2922:ARG:N	2.17	0.59
1:B:3592:VAL:HA	1:B:3609:MSE:SE	2.53	0.59
1:A:1267:TYR:O	1:A:1271:ILE:HG13	2.03	0.59
1:A:1467:ILE:HG13	1:A:1468:LEU:HG	1.84	0.59
1:A:1962:TYR:O	1:A:1965:PHE:N	2.35	0.59
1:A:2299:TYR:O	1:A:2302:ALA:N	2.35	0.59
1:A:2319:ALA:O	1:A:2323:LEU:HD12	2.03	0.59
1:A:2851:PHE:HA	1:A:2854:PHE:CE2	2.38	0.59
1:A:2957:LEU:HB3	1:A:3989:ARG:HH12	1.63	0.59
1:A:253:LEU:HD21	1:A:297:LEU:HA	1.84	0.59
1:A:3031:TRP:CE3	1:A:3034:PRO:HD3	2.37	0.59
1:A:3492:CYS:O	1:A:3495:PHE:CB	2.50	0.59
1:A:3612:ARG:HD3	1:A:3799:ARG:NH2	2.17	0.59
1:A:3963:LEU:HD12	1:A:3967:PHE:HZ	1.66	0.59
1:A:940:PHE:CE1	1:A:2791:ILE:HG21	2.37	0.59
1:B:1594:SER:OG	1:B:1683:LYS:HD3	2.02	0.59
1:B:2040:MSE:HA	1:B:2043:PHE:HD1	1.68	0.59
1:B:2136:PRO:C	1:B:2139:PRO:HD2	2.22	0.59
1:B:2144:LEU:HB3	1:B:2148:LYS:CE	2.33	0.59
1:B:2291:GLN:O	1:B:2293:GLY:N	2.35	0.59
1:B:2638:UNK:O	1:B:2790:LEU:HD13	2.02	0.59
1:B:3000:ASP:O	1:B:3004:HIS:N	2.35	0.59
1:B:327:VAL:HG13	1:B:338:LEU:HD13	1.84	0.59
1:A:2270:ASN:O	1:A:2274:ILE:HG23	2.03	0.59
1:A:2543:ASN:HA	1:A:2546:TYR:HD2	1.67	0.59
1:A:2960:GLU:CD	1:A:3289:ARG:HH12	2.05	0.59
1:B:1655:ILE:HG12	1:B:1681:ASP:HB3	1.83	0.59
1:B:179:GLY:HA3	1:B:229:SER:HB3	1.84	0.59
1:B:2419:ASP:O	1:B:2422:GLN:HB3	2.02	0.59
1:B:2645:UNK:HA	1:B:2649:UNK:C	2.33	0.59
1:B:270:ALA:O	1:B:274:LEU:HG	2.03	0.59
1:B:3273:LEU:O	1:B:3277:VAL:HG12	2.03	0.59
1:B:4062:ASP:O	1:B:4065:LEU:HG	2.03	0.59
1:B:886:TRP:CH2	1:B:892:LEU:HD13	2.37	0.59
1:A:1060:PHE:O	1:A:1064:TYR:HD2	1.85	0.59
1:A:1437:TYR:O	1:A:1439:PRO:HD2	2.02	0.59
1:A:1571:LEU:HD13	1:A:1599:GLY:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1647:ALA:O	1:A:1651:LYS:HE3	2.02	0.59
1:A:194:GLU:HA	1:A:197:PHE:HD2	1.68	0.59
1:A:242:PRO:O	1:A:246:ARG:CB	2.50	0.59
1:A:2546:TYR:CE1	1:A:2558:ALA:HB2	2.38	0.59
1:A:2868:LEU:O	1:A:2872:ASP:HB2	2.03	0.59
1:A:3269:ARG:HH11	1:A:3312:VAL:HA	1.66	0.59
1:A:3638:LYS:O	1:A:3641:ASP:N	2.36	0.59
1:A:3811:THR:OG1	1:A:3811:THR:O	2.19	0.59
1:A:4006:VAL:HA	1:A:4012:ASP:OD2	2.03	0.59
1:A:980:THR:HG23	1:A:984:TYR:CE1	2.34	0.59
1:B:1018:VAL:HB	1:B:1074:LYS:CB	2.28	0.59
1:B:390:GLN:NE2	1:B:1723:PRO:HG2	2.18	0.59
1:B:2185:MSE:O	1:B:2189:ILE:HG13	2.02	0.59
1:B:197:PHE:CZ	1:B:230:LEU:HD22	2.37	0.59
1:B:3753:LYS:HD3	1:B:3758:LEU:HD21	1.85	0.59
1:B:392:CYS:HA	1:B:395:MSE:HB2	1.83	0.59
1:B:3909:ALA:HB2	1:B:3980:MSE:HE2	1.83	0.59
1:B:437:HIS:HA	1:B:1814:PHE:CZ	2.38	0.59
1:B:767:GLU:HG2	1:B:846:ILE:O	2.03	0.59
1:A:1866:GLN:O	1:A:1870:LYS:HB2	2.03	0.59
1:A:1992:VAL:HG21	1:A:2044:ASP:OD1	2.03	0.59
1:A:2330:VAL:CG2	1:A:2335:ASN:HA	2.31	0.59
1:A:3076:ALA:HB1	1:A:3080:LEU:HD11	1.85	0.59
1:A:3324:ARG:O	1:A:3328:ILE:HG13	2.02	0.59
1:A:3505:LEU:HB3	1:A:3510:GLN:OE1	2.03	0.59
1:B:1016:GLY:O	1:B:1019:ASP:HB2	2.03	0.59
1:B:1084:ASN:CG	1:B:1134:LEU:HD11	2.22	0.59
1:B:3908:HIS:O	1:B:3911:ILE:HG12	2.03	0.59
1:A:1736:PHE:O	1:A:1740:VAL:HG23	2.02	0.58
1:A:2462:VAL:CB	1:A:2473:MSE:SE	3.00	0.58
1:A:3585:PHE:HE2	1:A:3617:LEU:HD11	1.68	0.58
1:A:535:LEU:HD13	1:A:626:LEU:HD21	1.84	0.58
1:A:982:GLN:O	1:A:986:PRO:HD3	2.03	0.58
1:B:3149:GLY:HA3	1:B:3196:LYS:HE3	1.84	0.58
1:B:3351:ILE:HG23	1:B:3355:LYS:HE2	1.84	0.58
1:B:3516:HIS:CG	1:B:3517:SER:N	2.70	0.58
1:B:3503:VAL:HG22	1:B:3539:SER:HB2	1.84	0.58
1:B:673:THR:HG22	1:B:704:PHE:HE1	1.68	0.58
1:B:806:SER:O	1:B:809:THR:N	2.36	0.58
1:A:1102:GLU:HA	1:A:1150:LYS:NZ	2.18	0.58
1:A:1330:TYR:O	1:A:1334:LYS:HG2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2058:ASP:H	1:A:2061:PRO:HG2	1.68	0.58
1:A:2221:LYS:O	1:A:2225:HIS:ND1	2.36	0.58
1:A:2560:ASN:OD1	1:A:2800:ARG:NH1	2.36	0.58
1:A:2936:TYR:CD2	1:A:3979:LEU:HD21	2.38	0.58
1:A:3274:VAL:O	1:A:3277:VAL:HG22	2.04	0.58
1:A:3769:GLN:HA	1:A:3772:ASN:OD1	2.03	0.58
1:A:3813:LYS:CE	1:A:3926:ASN:HB2	2.31	0.58
1:A:3872:ARG:NH1	1:A:3965:ARG:HH12	1.98	0.58
1:A:437:HIS:CD2	1:A:438:LEU:N	2.70	0.58
1:B:1036:PHE:CD1	1:B:1059:LEU:HD11	2.38	0.58
1:B:111:CYS:HB2	1:B:134:LEU:HB3	1.86	0.58
1:B:1648:LEU:HD13	1:B:1688:LEU:HD21	1.85	0.58
1:B:1737:ASN:C	1:B:1739:TYR:H	2.06	0.58
1:B:2145:PHE:CZ	1:B:2185:MSE:HA	2.39	0.58
1:B:176:GLU:HG2	1:B:225:LYS:HD3	1.83	0.58
1:B:3190:LEU:HD21	1:B:3235:LYS:HG2	1.85	0.58
1:B:3637:GLY:O	1:B:3641:ASP:HB3	2.03	0.58
1:B:3583:LEU:HD21	1:B:3733:ARG:HD3	1.84	0.58
1:B:738:HIS:ND1	1:B:745:VAL:HG13	2.18	0.58
1:A:1386:ILE:HA	1:A:1389:VAL:HB	1.85	0.58
1:A:1454:ALA:O	1:A:1457:GLN:HB2	2.03	0.58
1:A:2378:PHE:O	1:A:2382:VAL:HG22	2.02	0.58
1:A:2942:ILE:HD12	1:A:2987:THR:HG22	1.85	0.58
1:A:3505:LEU:HA	1:A:3509:ASP:HB2	1.84	0.58
1:A:368:LEU:CD2	1:A:384:MSE:HB2	2.18	0.58
1:B:143:LEU:O	1:B:144:MSE:HB2	2.03	0.58
1:B:1918:LEU:HD13	1:B:1958:GLU:HB3	1.85	0.58
1:B:2003:LYS:O	1:B:2007:ILE:HG13	2.03	0.58
1:B:2157:PHE:HA	1:B:2160:TYR:CD2	2.38	0.58
1:B:2182:ILE:O	1:B:2186:VAL:HG12	2.03	0.58
1:B:2775:TYR:HB3	1:B:2776:ARG:CZ	2.33	0.58
1:B:2936:TYR:HA	1:B:2939:LEU:HB2	1.85	0.58
1:B:321:LYS:O	1:B:325:ASN:ND2	2.26	0.58
1:B:3427:GLU:HB3	1:B:3439:LEU:HD22	1.85	0.58
1:B:435:LEU:O	1:B:439:VAL:HG23	2.03	0.58
1:B:535:LEU:HD21	1:B:622:ALA:O	2.03	0.58
1:B:752:LEU:HA	1:B:755:ALA:HB3	1.84	0.58
1:A:1296:PHE:HD1	1:A:1299:GLU:OE2	1.86	0.58
1:A:1711:ARG:HB3	1:A:1739:TYR:CE1	2.37	0.58
1:A:1919:CYS:O	1:A:1923:PHE:CB	2.50	0.58
1:A:2884:LEU:HD22	1:A:3895:GLU:OE2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3099:ALA:O	1:A:3103:ILE:HB	2.02	0.58
1:A:3454:LEU:HA	1:A:3456:LEU:HD12	1.85	0.58
1:A:446:PHE:HA	1:A:449:TYR:CE2	2.39	0.58
1:A:613:HIS:ND1	1:A:614:PRO:HD3	2.18	0.58
1:A:633:ILE:HG22	1:A:637:LYS:HG2	1.86	0.58
1:A:727:ALA:O	1:A:731:THR:HG23	2.03	0.58
1:A:985:GLU:HB3	1:A:986:PRO:HD3	1.84	0.58
1:B:1963:GLN:NE2	1:B:1995:GLU:HG2	2.18	0.58
1:B:2070:GLU:HA	1:B:2071:GLN:HB2	1.85	0.58
1:B:2913:LYS:HG3	1:B:2914:ALA:N	2.18	0.58
1:B:571:SER:O	1:B:605:THR:OG1	2.19	0.58
1:A:1386:ILE:HB	1:A:1391:VAL:HG21	1.84	0.58
1:A:1959:LEU:HD13	1:A:1998:MSE:HE3	1.84	0.58
1:A:2420:PHE:CE1	1:A:2436:LEU:HB3	2.38	0.58
1:A:3092:LEU:HD22	1:A:3192:LYS:HE2	1.86	0.58
1:A:3587:ASP:HB3	1:A:4022:LYS:NZ	2.19	0.58
1:B:971:ARG:HD2	1:B:1024:THR:OG1	2.04	0.58
1:B:1583:MSE:HE3	1:B:1643:MSE:CB	2.33	0.58
1:B:503:SER:O	1:B:507:ASP:HB2	2.02	0.58
1:B:713:GLU:O	1:B:717:LYS:HG2	2.04	0.58
1:B:722:LYS:HD2	1:B:730:LEU:HB2	1.85	0.58
1:A:1648:LEU:HD22	1:A:1684:LEU:HD22	1.86	0.58
1:A:2275:GLN:O	1:A:2279:ILE:HG12	2.03	0.58
1:A:2962:ARG:NH2	1:A:3006:ALA:HB1	2.18	0.58
1:A:3092:LEU:HD22	1:A:3192:LYS:CE	2.33	0.58
1:A:3339:ASN:O	1:A:3341:LEU:N	2.36	0.58
1:A:450:SER:O	1:A:454:GLN:HB2	2.04	0.58
1:A:566:ASP:O	1:A:570:LYS:NZ	2.36	0.58
1:A:491:CYS:SG	1:A:615:ALA:HB2	2.43	0.58
1:B:1651:LYS:HB2	1:B:1684:LEU:CD1	2.29	0.58
1:B:2011:ALA:HB3	1:B:2014:ALA:CB	2.29	0.58
1:B:2126:MSE:HE2	1:B:2156:VAL:HG22	1.86	0.58
1:B:2167:PRO:O	1:B:2171:LEU:CB	2.33	0.58
1:B:2900:LEU:HD12	1:B:2905:LEU:HD11	1.84	0.58
1:B:572:VAL:HG13	1:B:573:LEU:H	1.67	0.58
1:A:1059:LEU:O	1:A:1063:LEU:HG	2.03	0.58
1:A:1101:PHE:CD2	1:A:1138:ILE:HG12	2.38	0.58
1:A:1327:GLY:O	1:A:1330:TYR:HB3	2.04	0.58
1:A:1594:SER:HA	1:A:1687:HIS:HE1	1.69	0.58
1:A:205:LYS:HA	1:A:208:MSE:HG2	1.84	0.58
1:A:2085:MSE:SE	1:A:2088:LEU:HD22	2.54	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2140:LEU:HA	1:A:2143:ARG:HD3	1.86	0.58
1:A:2454:LEU:O	1:A:2457:PRO:HD2	2.03	0.58
1:A:3910:LEU:O	1:A:3914:SER:OG	2.15	0.58
1:A:509:ARG:HD2	1:A:655:LEU:HD13	1.84	0.58
1:B:1063:LEU:HD13	1:B:1082:PHE:CE1	2.38	0.58
1:B:1086:TYR:HE2	1:B:1090:ARG:HE	1.51	0.58
1:B:1644:ALA:HA	1:B:1648:LEU:HD12	1.83	0.58
1:B:1925:GLU:OE2	1:B:1959:LEU:HG	2.03	0.58
1:B:204:LEU:HD13	1:B:223:CYS:HB2	1.84	0.58
1:B:2358:ASP:HB2	1:B:2396:LEU:CD2	2.30	0.58
1:B:903:PRO:HG2	1:B:2811:SER:HB2	1.85	0.58
1:B:3463:LEU:HD13	1:B:4000:ASN:HB2	1.86	0.58
1:B:410:MSE:HE1	1:B:445:SER:HB3	1.85	0.58
1:B:446:PHE:CD1	1:B:447:PRO:HD3	2.38	0.58
1:A:1074:LYS:O	1:A:1075:ARG:HG2	2.04	0.58
1:A:252:VAL:HG21	1:A:265:TYR:HB2	1.85	0.58
1:A:2920:VAL:HB	1:A:3036:TYR:OH	2.04	0.58
1:A:3464:LYS:O	1:A:3468:LEU:HG	2.03	0.58
1:A:3454:LEU:O	1:A:3494:GLN:NE2	2.34	0.58
1:A:3525:TYR:O	1:A:3529:ILE:HB	2.03	0.58
1:A:3631:LYS:HE2	1:A:3634:GLN:HG2	1.86	0.58
1:A:3879:PRO:HA	1:A:3882:LEU:HB2	1.86	0.58
1:A:617:PRO:O	1:A:620:PHE:N	2.36	0.58
1:B:1163:LEU:HA	1:B:1260:LEU:HD21	1.84	0.58
1:B:175:TYR:HE1	1:B:200:PHE:HB3	1.68	0.58
1:B:1606:ARG:HH11	1:B:1806:ARG:HB3	1.69	0.58
1:B:2167:PRO:HA	1:B:2171:LEU:HD13	1.86	0.58
1:B:419:SER:O	1:B:422:LEU:HB2	2.04	0.58
1:A:2338:GLU:O	1:A:2338:GLU:HG2	2.03	0.58
1:A:3047:SER:O	1:A:3050:LYS:HG3	2.04	0.58
1:A:3322:ALA:O	1:A:3325:ASP:HB3	2.04	0.58
1:A:352:VAL:HA	1:A:355:ASN:O	2.03	0.58
1:A:3772:ASN:O	1:A:3787:GLN:NE2	2.24	0.58
1:A:549:ALA:O	1:A:553:VAL:HG23	2.03	0.58
1:A:870:LEU:HD21	1:A:3129:LEU:HD11	1.86	0.58
1:B:2040:MSE:HA	1:B:2043:PHE:CD1	2.38	0.58
1:B:2481:HIS:O	1:B:2485:ARG:N	2.37	0.58
1:B:2477:LEU:CB	1:B:2506:LEU:HD21	2.34	0.58
1:B:3571:PHE:O	1:B:3575:LEU:HB2	2.03	0.58
1:B:3974:MSE:HB3	1:B:3976:GLU:HB3	1.86	0.58
1:B:510:ALA:O	1:B:513:GLU:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1010:LEU:HA	1:A:1013:ILE:CG1	2.30	0.58
1:A:1521:PHE:HB2	1:A:1589:ASN:OD1	2.04	0.58
1:A:2440:TYR:O	1:A:2443:MSE:HE2	2.04	0.58
1:A:2430:GLU:HG3	1:A:2465:PRO:HB3	1.86	0.58
1:A:435:LEU:HD11	1:A:475:LEU:HD21	1.85	0.58
1:A:627:VAL:HG12	1:A:628:GLU:N	2.17	0.58
1:A:806:SER:O	1:A:809:THR:N	2.26	0.58
1:B:1145:LEU:HB2	1:B:1149:LYS:HZ3	1.66	0.58
1:B:1883:ARG:HE	1:B:1923:PHE:HZ	1.50	0.58
1:B:3699:LEU:HB3	1:B:3718:ARG:HH12	1.69	0.58
1:B:669:LEU:O	1:B:671:SER:N	2.36	0.58
1:B:852:ARG:O	1:B:855:VAL:HB	2.04	0.58
1:A:2349:LEU:O	1:A:2353:GLN:HG3	2.02	0.57
1:A:2440:TYR:OH	1:A:2455:LEU:HG	2.04	0.57
1:A:2474:TYR:HE2	1:A:2518:GLN:HB3	1.69	0.57
1:A:2993:PHE:O	1:A:2997:ALA:N	2.25	0.57
1:A:3451:LEU:HG	1:A:3486:GLU:OE1	2.04	0.57
1:A:3649:SER:HA	1:A:3652:LEU:HG	1.86	0.57
1:A:3944:HIS:CG	1:A:3949:ALA:HA	2.39	0.57
1:A:3855:TYR:HB3	1:A:4074:PHE:HZ	1.66	0.57
1:A:488:ILE:O	1:A:612:LEU:HB2	2.04	0.57
1:A:852:ARG:O	1:A:855:VAL:HB	2.04	0.57
1:B:1810:PRO:O	1:B:1812:LEU:HG	2.03	0.57
1:B:2568:MSE:HG3	1:B:2569:SER:H	1.69	0.57
1:B:3104:GLN:HA	1:B:3107:ILE:HD12	1.86	0.57
1:B:3464:LYS:HE3	1:B:3468:LEU:HD21	1.86	0.57
1:B:3501:HIS:HA	1:B:4008:GLU:OE2	2.04	0.57
1:B:3981:TYR:CE1	1:B:4104:VAL:HB	2.39	0.57
1:B:647:TYR:HE1	1:B:1389:VAL:HA	1.68	0.57
1:A:1139:GLU:HG3	1:A:1175:HIS:NE2	2.18	0.57
1:A:1400:VAL:O	1:A:1404:LYS:HB2	2.04	0.57
1:A:1679:LEU:O	1:A:1683:LYS:HG3	2.04	0.57
1:A:2065:ARG:HD3	1:A:2100:LEU:HD11	1.86	0.57
1:A:2495:SER:O	1:A:2498:ILE:HB	2.04	0.57
1:A:2538:ARG:HH11	1:A:2565:MSE:CB	2.17	0.57
1:A:2782:ASP:HA	1:A:2786:LYS:CB	2.34	0.57
1:A:2950:LYS:HE2	1:A:4105:LYS:NZ	2.18	0.57
1:B:1761:LEU:O	1:B:1895:LYS:HB2	2.04	0.57
1:B:205:LYS:HA	1:B:208:MSE:HE3	1.86	0.57
1:B:2323:LEU:HD21	1:B:2345:VAL:HG21	1.86	0.57
1:B:2374:LEU:CD1	1:B:2377:ARG:HB2	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:ASP:HB3	1:B:282:PHE:CE2	2.39	0.57
1:B:2837:LEU:HD12	1:B:2867:ALA:HB3	1.86	0.57
1:B:571:SER:HB2	1:B:606:SER:H	1.68	0.57
1:B:781:ASP:OD2	1:B:862:LEU:HD21	2.03	0.57
1:B:966:PHE:O	1:B:969:LEU:HB3	2.03	0.57
1:B:986:PRO:O	1:B:989:MSE:N	2.37	0.57
1:B:997:ASN:HA	1:B:1042:LYS:HD3	1.86	0.57
1:A:1952:ILE:HG23	1:A:1953:CYS:O	2.04	0.57
1:A:2286:PRO:HD3	1:A:2325:LEU:HD23	1.85	0.57
1:A:2809:PHE:HB3	1:A:2859:GLN:CD	2.24	0.57
1:A:3287:ARG:NH1	1:A:3331:GLY:HA3	2.19	0.57
1:A:3496:ILE:O	1:A:3498:TRP:N	2.37	0.57
1:A:3686:TRP:CZ3	1:A:3687:MSE:HG3	2.39	0.57
1:A:75:SER:O	1:A:77:GLU:N	2.36	0.57
1:B:2094:MSE:HE1	1:B:2143:ARG:HA	1.85	0.57
1:B:2366:LYS:NZ	2:S:101:UNK:HA	2.19	0.57
1:B:2927:ALA:HB2	1:B:2930:TYR:HD2	1.68	0.57
1:B:3181:ASP:HA	1:B:3184:THR:HG23	1.86	0.57
1:B:3496:ILE:HG23	1:B:3499:ILE:HD11	1.86	0.57
1:B:3871:PHE:HB3	1:B:4127:TRP:CD1	2.39	0.57
1:B:450:SER:O	1:B:454:GLN:HB2	2.03	0.57
1:A:1063:LEU:HD13	1:A:1082:PHE:CE1	2.39	0.57
1:A:1655:ILE:HG12	1:A:1677:SER:O	2.05	0.57
1:A:1606:ARG:HA	1:A:1806:ARG:HD3	1.87	0.57
1:A:205:LYS:NZ	1:A:243:GLN:OE1	2.25	0.57
1:A:2562:LEU:O	1:A:2566:THR:HG22	2.04	0.57
1:A:3034:PRO:O	1:A:3038:GLU:HB3	2.05	0.57
1:A:2960:GLU:HG2	1:A:3252:PHE:CG	2.39	0.57
1:A:368:LEU:HA	1:A:372:PRO:HG2	1.86	0.57
1:A:756:PHE:O	1:A:759:GLY:N	2.36	0.57
1:A:871:LEU:HD21	1:A:3122:HIS:CE1	2.39	0.57
1:A:987:LEU:O	1:A:991:LEU:HD13	2.05	0.57
1:B:1000:LYS:O	1:B:1003:SER:N	2.30	0.57
1:B:1090:ARG:HH22	1:B:1096:VAL:C	2.07	0.57
1:B:1270:PHE:CZ	1:B:1347:THR:HB	2.38	0.57
1:B:358:GLU:HA	1:B:1858:LEU:HD22	1.85	0.57
1:B:1923:PHE:CE2	1:B:1927:MSE:HE1	2.40	0.57
1:B:1976:LEU:HD13	1:B:2031:LEU:CD2	2.34	0.57
1:B:2085:MSE:O	1:B:2089:ASN:ND2	2.37	0.57
1:B:16:GLN:O	1:B:20:SER:OG	2.21	0.57
1:B:2886:GLN:OE1	1:B:2921:LEU:HB2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3174:ASP:H	1:B:3175:PRO:HD2	1.67	0.57
1:B:3568:ILE:O	1:B:3571:PHE:N	2.38	0.57
1:B:473:PRO:CA	1:B:476:ARG:HH22	2.12	0.57
1:B:886:TRP:HD1	1:B:889:GLU:N	2.02	0.57
1:A:131:LEU:O	1:A:135:LEU:HG	2.05	0.57
1:A:2227:LYS:HZ1	1:A:2232:ARG:HB3	1.69	0.57
1:A:2503:LYS:O	1:A:2507:ILE:HB	2.04	0.57
1:A:805:LEU:CD2	1:A:3125:ARG:NH1	2.68	0.57
1:A:373:CYS:O	1:A:423:TYR:OH	2.20	0.57
1:A:4057:ALA:HB2	1:A:4090:ARG:O	2.04	0.57
1:B:1238:GLN:HE22	1:B:1297:PHE:HD1	1.51	0.57
1:B:1632:TRP:HA	1:B:1635:LYS:HD2	1.85	0.57
1:B:2190:VAL:O	1:B:2193:ILE:HG22	2.04	0.57
1:B:2210:VAL:HG13	1:B:2211:LEU:H	1.70	0.57
1:B:2321:GLU:O	1:B:2324:GLY:N	2.36	0.57
1:B:2555:LEU:HB2	1:B:2809:PHE:CE1	2.40	0.57
1:B:3767:LEU:O	1:B:3771:MSE:HG3	2.04	0.57
1:B:3765:GLU:O	1:B:3768:PHE:HB2	2.05	0.57
1:B:575:ILE:HD13	1:B:603:ILE:HB	1.86	0.57
1:B:923:ASP:O	1:B:927:LYS:HE2	2.03	0.57
1:A:2913:LYS:HG3	1:A:2914:ALA:N	2.19	0.57
1:A:4027:TRP:HB3	1:A:4031:ILE:HD11	1.85	0.57
1:A:409:GLN:HG3	1:A:413:PHE:CZ	2.39	0.57
1:A:414:LEU:HD22	1:A:442:GLN:HG2	1.85	0.57
1:A:704:PHE:HA	1:A:707:PHE:CD1	2.39	0.57
1:A:797:ASP:HA	1:A:800:LEU:HD12	1.86	0.57
1:B:1715:GLU:HA	1:B:1718:ILE:HB	1.85	0.57
1:B:2562:LEU:O	1:B:2566:THR:HG22	2.04	0.57
1:B:3817:LEU:HA	1:B:3820:MSE:HE3	1.87	0.57
1:B:610:ALA:HA	1:B:613:HIS:ND1	2.19	0.57
1:A:2157:PHE:CZ	1:A:2203:THR:HB	2.40	0.57
1:A:2196:TRP:CG	1:A:2199:LEU:HD11	2.39	0.57
1:A:2349:LEU:HD23	1:A:2364:LEU:HD22	1.86	0.57
1:A:737:PRO:O	1:A:741:ILE:HG12	2.04	0.57
1:A:968:VAL:CG2	1:A:971:ARG:HD3	2.33	0.57
1:B:1681:ASP:HB2	1:B:1717:LEU:HD22	1.86	0.57
1:B:361:ILE:HD13	1:B:1858:LEU:HD23	1.86	0.57
1:B:2216:LEU:HD13	1:B:2249:LEU:HD21	1.85	0.57
1:B:2289:ASP:O	1:B:2292:CYS:N	2.24	0.57
1:B:262:LEU:HD22	1:B:306:VAL:HG12	1.86	0.57
1:B:680:ILE:HG12	1:B:701:TYR:HD2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:798:GLY:HA2	1:B:873:VAL:HG11	1.87	0.57
1:B:969:LEU:O	1:B:973:ALA:HB3	2.05	0.57
1:A:182:GLY:O	1:A:233:ASN:ND2	2.36	0.57
1:A:1982:ILE:O	1:A:1986:ARG:HB2	2.04	0.57
1:A:257:ARG:H	1:A:258:PRO:CD	2.17	0.57
1:A:3907:SER:CB	1:A:3937:VAL:H	2.17	0.57
1:A:585:ILE:HG22	1:A:586:GLN:H	1.68	0.57
1:A:567:GLU:HB3	1:A:606:SER:HB3	1.87	0.57
1:B:1216:GLY:HA3	1:B:1271:ILE:CG2	2.35	0.57
1:B:2319:ALA:O	1:B:2323:LEU:HD12	2.04	0.57
1:B:990:GLN:HG3	1:B:2776:ARG:NH1	2.19	0.57
1:B:2801:ASP:HB2	1:B:2802:PRO:CD	2.35	0.57
1:B:3267:LYS:N	1:B:3271:ASP:OD2	2.37	0.57
1:B:3771:MSE:HE1	1:B:3917:ILE:HG21	1.85	0.57
1:A:1635:LYS:O	1:A:1639:LEU:HG	2.05	0.57
1:A:1809:ASP:O	1:A:1815:THR:HG22	2.05	0.57
1:A:1989:ASN:HB3	1:A:2040:MSE:HB3	1.86	0.57
1:A:2555:LEU:HD13	1:A:2809:PHE:CZ	2.39	0.57
1:A:2883:SER:O	1:A:2885:GLN:N	2.38	0.57
1:A:3498:TRP:HB2	1:A:3501:HIS:HB2	1.86	0.57
1:A:3631:LYS:O	1:A:3631:LYS:HD3	2.05	0.57
1:A:3687:MSE:C	1:A:3689:ASP:H	2.06	0.57
1:A:3839:TYR:HE1	1:A:3867:THR:HB	1.70	0.57
1:A:576:VAL:HG13	1:A:601:TRP:CE3	2.40	0.57
1:B:1274:ARG:O	1:B:1279:LEU:N	2.28	0.57
1:B:1350:ASN:ND2	1:B:1404:LYS:HG2	2.18	0.57
1:B:1494:GLY:HA2	1:B:1497:ARG:HG3	1.87	0.57
1:B:2194:LEU:HD13	1:B:2244:CYS:SG	2.45	0.57
1:B:2267:SER:HB2	1:B:2269:ASP:OD2	2.05	0.57
1:B:2927:ALA:CB	1:B:2930:TYR:HD2	2.18	0.57
1:B:3903:HIS:O	1:B:3907:SER:OG	2.15	0.57
1:B:527:TYR:CE1	1:B:531:PHE:HZ	2.21	0.57
1:B:752:LEU:HD13	1:B:776:TRP:CZ3	2.40	0.57
1:A:1006:THR:O	1:A:1010:LEU:HG	2.05	0.57
1:A:1146:ASN:O	1:A:1150:LYS:HB3	2.05	0.57
1:A:283:SER:HA	1:A:286:LEU:HG	1.85	0.57
1:A:3167:ARG:HG2	1:A:3186:ARG:CZ	2.35	0.57
1:A:3529:ILE:HG23	1:A:3532:PRO:HD2	1.86	0.57
1:A:3980:MSE:HB2	1:A:3983:ILE:HD12	1.86	0.57
1:A:575:ILE:HD11	1:A:579:LEU:HD13	1.87	0.57
1:A:891:ARG:HB2	1:A:905:ILE:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:SER:HA	1:B:181:LEU:HD22	1.87	0.57
1:B:2019:SER:O	1:B:2023:SER:OG	2.10	0.57
1:B:385:TYR:HD1	1:B:420:VAL:CG1	2.18	0.57
1:B:460:ALA:O	1:B:464:VAL:HG12	2.05	0.57
1:B:566:ASP:O	1:B:570:LYS:NZ	2.38	0.57
1:B:70:ARG:HD3	1:B:82:ARG:HD3	1.87	0.57
1:A:175:TYR:CE1	1:A:200:PHE:HB3	2.39	0.56
1:A:2324:GLY:HA2	1:A:2371:PHE:HB3	1.87	0.56
1:A:2911:ARG:HG2	1:A:2914:ALA:HB3	1.87	0.56
1:A:2930:TYR:HH	1:A:3902:SER:HG	1.48	0.56
1:A:3459:ASN:O	1:A:3462:ARG:HG2	2.05	0.56
1:A:3483:MSE:C	1:A:3516:HIS:HE2	2.08	0.56
1:B:1007:VAL:O	1:B:1011:GLU:HB3	2.04	0.56
1:B:1293:ALA:HA	1:B:1296:PHE:CD2	2.40	0.56
1:B:144:MSE:HE2	1:B:144:MSE:HA	1.86	0.56
1:B:2359:LYS:HA	1:B:2362:VAL:HG13	1.87	0.56
1:B:2481:HIS:CE1	1:B:2485:ARG:NH1	2.65	0.56
1:B:3167:ARG:HG2	1:B:3186:ARG:CZ	2.35	0.56
1:B:3238:MSE:O	1:B:3242:MSE:HG3	2.05	0.56
1:B:3629:ARG:HH22	1:B:3638:LYS:CE	2.18	0.56
1:B:647:TYR:O	1:B:650:SER:OG	2.12	0.56
1:B:909:VAL:CG1	1:B:913:ARG:HH11	2.05	0.56
1:A:1042:LYS:NZ	1:A:1044:ILE:HD12	2.20	0.56
1:A:1343:GLU:O	1:A:1347:THR:CB	2.52	0.56
1:A:2193:ILE:HA	1:A:2196:TRP:CE2	2.39	0.56
1:A:3493:TRP:CZ2	1:A:3496:ILE:HG21	2.40	0.56
1:A:4005:PHE:O	1:A:4009:PRO:HD3	2.05	0.56
1:A:488:ILE:HG13	1:A:612:LEU:HD12	1.86	0.56
1:B:1475:LEU:O	1:B:1479:VAL:HG23	2.04	0.56
1:B:2452:ARG:HE	1:B:2498:ILE:HD11	1.71	0.56
1:B:2877:SER:C	1:B:2879:GLY:H	2.08	0.56
1:B:2967:GLU:O	1:B:2971:GLN:NE2	2.38	0.56
1:B:3345:PRO:O	1:B:3347:CYS:N	2.34	0.56
1:B:3448:GLU:HG3	1:B:3449:LYS:HG3	1.87	0.56
1:B:3530:VAL:CG1	1:B:3702:PRO:HD3	2.31	0.56
1:A:1491:ILE:HG22	1:A:1497:ARG:HH22	1.70	0.56
1:A:1722:PHE:CE2	1:A:1754:GLN:HG2	2.39	0.56
1:A:205:LYS:HA	1:A:208:MSE:HE3	1.86	0.56
1:A:2086:ASP:HB3	1:A:2090:ARG:NH2	2.20	0.56
1:A:3425:ARG:HH12	1:A:3999:THR:HG22	1.70	0.56
1:A:4063:GLU:HA	1:A:4066:LEU:HD22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:LYS:HD2	1:A:730:LEU:HB2	1.88	0.56
1:B:1046:PRO:O	1:B:1049:GLN:HB3	2.05	0.56
1:B:1080:LEU:HB3	1:B:1111:LEU:CD2	2.36	0.56
1:B:1115:HIS:O	1:B:1118:GLU:C	2.44	0.56
1:B:1582:LEU:HD13	1:B:1600:MSE:SE	2.55	0.56
1:B:1987:ARG:O	1:B:1989:ASN:N	2.38	0.56
1:B:2364:LEU:O	1:B:2368:THR:OG1	2.11	0.56
1:B:2420:PHE:CE1	1:B:2439:ILE:HG21	2.40	0.56
1:B:2485:ARG:NH1	1:B:2530:ARG:CZ	2.68	0.56
1:B:265:TYR:O	1:B:268:PRO:HD2	2.05	0.56
1:B:2945:SER:O	1:B:2949:THR:N	2.36	0.56
1:B:3791:TYR:OH	1:B:3942:PHE:HE2	1.88	0.56
1:B:4046:TYR:CE2	1:B:4049:ARG:NH2	2.74	0.56
1:B:657:SER:O	1:B:661:PRO:HD3	2.04	0.56
1:B:642:PHE:CE2	1:B:710:PHE:HE2	2.23	0.56
1:A:1698:PHE:HD1	1:A:1699:PHE:N	2.03	0.56
1:A:2808:LEU:O	1:A:2812:LEU:HB2	2.06	0.56
1:A:3179:TRP:CH2	1:A:3258:LEU:HG	2.39	0.56
1:A:3907:SER:O	1:A:3911:ILE:HG23	2.05	0.56
1:A:369:PHE:CE1	1:A:419:SER:HB2	2.40	0.56
1:A:993:HIS:HB2	1:A:1038:LYS:HG2	1.86	0.56
1:B:2157:PHE:CE2	1:B:2199:LEU:HD13	2.40	0.56
1:B:242:PRO:HD3	1:B:282:PHE:CE2	2.41	0.56
1:B:3420:CYS:O	1:B:3423:GLN:HB3	2.05	0.56
1:B:368:LEU:HD22	1:B:420:VAL:HG22	1.87	0.56
1:B:53:LEU:O	1:B:56:SER:OG	2.22	0.56
1:B:634:LEU:HD22	1:B:667:TYR:CD1	2.40	0.56
1:B:66:LEU:CD2	1:B:89:LEU:HD11	2.34	0.56
1:B:893:SER:OG	1:B:906:PHE:HD2	1.88	0.56
1:A:852:ARG:NH1	1:A:3111:MSE:HE2	2.21	0.56
1:A:3762:GLN:HE22	1:A:3763:ARG:HH11	1.53	0.56
1:B:1000:LYS:O	1:B:1002:GLU:N	2.39	0.56
1:B:3279:SER:O	1:B:3283:LEU:HB2	2.05	0.56
1:B:3397:GLN:OE1	1:B:3398:PRO:HD2	2.06	0.56
1:B:737:PRO:O	1:B:741:ILE:HG13	2.06	0.56
1:B:778:ILE:HG13	1:B:858:MSE:SE	2.56	0.56
1:A:1516:GLU:O	1:A:1519:PHE:N	2.38	0.56
1:A:164:LYS:HB3	1:A:166:ILE:HG13	1.88	0.56
1:A:2080:VAL:HG12	1:A:2081:LEU:H	1.70	0.56
1:A:2236:GLU:HA	1:A:2239:LYS:HB3	1.88	0.56
1:A:2538:ARG:NH1	1:A:2565:MSE:HB3	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3448:GLU:OE2	1:A:3449:LYS:HE3	2.04	0.56
1:A:3751:LEU:O	1:A:3802:LEU:HG	2.05	0.56
1:A:381:VAL:HB	1:A:384:MSE:HG2	1.88	0.56
1:A:484:HIS:NE2	1:A:616:LYS:HE3	2.20	0.56
1:B:1017:ILE:HG23	1:B:1018:VAL:HG13	1.87	0.56
1:B:1374:GLN:O	1:B:1378:GLU:N	2.39	0.56
1:B:2265:PRO:HD3	1:B:2309:PHE:CZ	2.41	0.56
1:B:3277:VAL:HB	1:B:3321:LEU:HD21	1.88	0.56
1:B:797:ASP:HB3	1:B:870:LEU:HB3	1.88	0.56
1:B:909:VAL:HG22	1:B:2807:GLN:HG3	1.88	0.56
1:B:926:THR:O	1:B:930:ALA:CB	2.54	0.56
1:B:931:CYS:SG	1:B:932:GLU:N	2.78	0.56
1:B:964:ARG:HH12	1:B:968:VAL:HB	1.70	0.56
1:A:1032:CYS:O	1:A:1035:GLU:N	2.37	0.56
1:A:1148:ALA:O	1:A:1152:ARG:HG3	2.06	0.56
1:A:1598:ASN:O	1:A:1602:ASP:HB3	2.05	0.56
1:A:168:ASP:O	1:A:170:VAL:N	2.36	0.56
1:A:1861:SER:O	1:A:1864:ASP:HB3	2.06	0.56
1:A:1934:LEU:HD12	1:A:1937:ARG:H	1.70	0.56
1:A:2799:GLN:HB3	1:A:2808:LEU:HD11	1.86	0.56
1:A:2879:GLY:HA2	1:A:2886:GLN:CG	2.35	0.56
1:A:361:ILE:HG12	1:A:1858:LEU:CD2	2.36	0.56
1:A:3960:PRO:HG2	1:A:3961:PHE:CD2	2.41	0.56
1:A:654:ILE:HG13	1:A:655:LEU:H	1.70	0.56
1:B:1090:ARG:NH2	1:B:1097:GLU:HA	2.21	0.56
1:B:1431:LEU:O	1:B:1434:VAL:HG12	2.05	0.56
1:B:2116:ASP:HB3	1:B:2119:PRO:HD2	1.88	0.56
1:B:313:LEU:HD11	1:B:359:LEU:HD21	1.88	0.56
1:A:3590:ASN:OD1	1:A:3593:ARG:NH2	2.36	0.56
1:A:3575:LEU:C	1:A:3686:TRP:HH2	2.09	0.56
1:A:381:VAL:HB	1:A:384:MSE:CG	2.36	0.56
1:A:395:MSE:SE	1:A:413:PHE:CE2	3.09	0.56
1:B:1128:CYS:HA	1:B:1131:ILE:HG23	1.88	0.56
1:B:1587:VAL:HB	1:B:1643:MSE:HE2	1.86	0.56
1:B:2330:VAL:HG21	1:B:2338:GLU:CB	2.29	0.56
1:B:2450:GLU:O	1:B:2454:LEU:HG	2.06	0.56
1:B:2843:PHE:CE2	1:B:2853:PRO:HG3	2.41	0.56
1:B:3141:PHE:HZ	1:B:3192:LYS:HB2	1.71	0.56
1:B:3331:GLY:O	1:B:3335:ARG:HD2	2.05	0.56
1:B:3821:SER:OG	1:B:3826:ALA:O	2.22	0.56
1:B:993:HIS:CD2	1:B:2776:ARG:HD3	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1077:GLY:HA2	1:A:1080:LEU:HD21	1.86	0.56
1:A:155:LYS:O	1:A:159:GLU:HG3	2.05	0.56
1:A:2073:ASP:HB3	1:A:2091:HIS:CE1	2.41	0.56
1:A:2093:CYS:HB3	1:A:2143:ARG:HH21	1.71	0.56
1:A:2552:VAL:CG2	1:A:2852:PRO:HG2	2.31	0.56
1:A:294:PHE:O	1:A:298:LEU:HG	2.05	0.56
1:A:3705:TYR:OH	1:A:3765:GLU:OE1	2.20	0.56
1:B:2810:SER:HA	1:B:2813:PHE:CD2	2.41	0.56
1:B:2858:ILE:HD12	1:B:3894:PRO:HG2	1.86	0.56
1:B:3090:TYR:HB3	1:B:3095:ASP:OD2	2.05	0.56
1:B:3103:ILE:HD13	1:B:3139:GLN:OE1	2.06	0.56
1:B:3593:ARG:HD2	1:B:3660:ASN:O	2.04	0.56
1:B:1069:HIS:O	1:B:3741:ARG:HD3	2.05	0.56
1:B:3847:SER:HA	1:B:3857:LEU:HD13	1.86	0.56
1:B:3875:GLU:HG2	1:B:4127:TRP:HB3	1.88	0.56
1:B:3908:HIS:CD2	1:B:3912:CYS:SG	2.99	0.56
1:B:886:TRP:CZ2	1:B:892:LEU:HD13	2.41	0.56
1:B:892:LEU:HB2	1:B:907:LEU:HD22	1.87	0.56
1:A:179:GLY:HA3	1:A:229:SER:HB3	1.86	0.56
1:A:2171:LEU:HG	1:A:2177:ASN:ND2	2.21	0.56
1:A:2382:VAL:CG2	1:A:2404:ARG:HG3	2.36	0.56
1:A:3954:PRO:HG2	1:A:4027:TRP:HA	1.88	0.56
1:A:855:VAL:O	1:A:859:LEU:HG	2.05	0.56
1:B:1348:LEU:HD23	1:B:1352:SER:HB3	1.87	0.56
1:B:1799:GLU:HA	1:B:1802:TYR:CB	2.36	0.56
1:B:4125:GLU:HA	1:B:4127:TRP:HE3	1.70	0.56
1:A:131:LEU:HD21	1:A:170:VAL:HG23	1.86	0.56
1:A:2430:GLU:HG3	1:A:2465:PRO:CB	2.36	0.56
1:A:2869:LEU:HB3	1:A:2893:LEU:HG	1.88	0.56
1:B:1090:ARG:NH2	1:B:1096:VAL:O	2.38	0.56
1:B:1131:ILE:HG12	1:B:1132:ASP:N	2.19	0.56
1:B:1909:ASN:ND2	1:B:1951:VAL:O	2.38	0.56
1:B:2886:GLN:CG	1:B:2887:PRO:HD3	2.36	0.56
1:B:756:PHE:O	1:B:760:LEU:HG	2.06	0.56
1:B:759:GLY:HA3	1:B:773:LEU:CD1	2.36	0.56
1:B:964:ARG:NH1	1:B:968:VAL:HB	2.21	0.56
1:B:978:GLN:H	1:B:981:ARG:HD3	1.70	0.56
1:A:2842:ARG:O	1:A:2846:THR:HG23	2.06	0.55
1:A:759:GLY:HA3	1:A:773:LEU:HD11	1.88	0.55
1:B:176:GLU:HG2	1:B:225:LYS:CD	2.36	0.55
1:B:1805:PHE:HA	1:B:1808:ASP:OD2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1977:ILE:C	1:B:1979:GLU:H	2.02	0.55
1:B:2065:ARG:NH1	1:B:2097:LEU:HD21	2.21	0.55
1:B:2936:TYR:CE1	1:B:2940:ARG:HB2	2.40	0.55
1:B:3781:CYS:HA	1:B:3786:LEU:HD12	1.87	0.55
1:B:3900:LEU:HD11	1:B:3934:THR:O	2.05	0.55
1:B:3962:ARG:HB2	1:B:3962:ARG:CZ	2.35	0.55
1:A:2186:VAL:O	1:A:2190:VAL:HG13	2.06	0.55
1:A:2447:LYS:HA	1:A:2451:LEU:HD12	1.89	0.55
1:A:2918:PRO:HA	1:A:2921:LEU:HG	1.88	0.55
1:A:3584:LEU:O	1:A:3588:TRP:CB	2.55	0.55
1:A:714:VAL:HG12	1:A:715:ALA:N	2.21	0.55
1:B:2869:LEU:HG	1:B:2893:LEU:HD12	1.88	0.55
1:B:3989:ARG:HH21	1:B:4100:GLU:CD	2.09	0.55
1:B:392:CYS:SG	1:B:438:LEU:HD21	2.46	0.55
1:B:411:PRO:HG3	1:B:442:GLN:HE22	1.71	0.55
1:A:1231:GLN:H	1:A:1232:PRO:CD	2.20	0.55
1:A:1952:ILE:HG12	1:A:1953:CYS:N	2.21	0.55
1:A:2837:LEU:HD12	1:A:2867:ALA:HB3	1.89	0.55
1:A:3495:PHE:HZ	1:A:3521:ILE:HG13	1.71	0.55
1:A:3499:ILE:O	1:A:3503:VAL:HG12	2.07	0.55
1:A:4031:ILE:O	1:A:4035:GLU:N	2.37	0.55
1:A:4100:GLU:HG2	1:A:4101:GLU:H	1.71	0.55
1:A:805:LEU:HD22	1:A:3125:ARG:NH1	2.20	0.55
1:A:913:ARG:HA	1:A:916:GLU:CD	2.27	0.55
1:A:989:MSE:O	1:A:992:ILE:HG13	2.06	0.55
1:B:1292:LYS:O	1:B:1295:ALA:HB3	2.05	0.55
1:B:1583:MSE:HE3	1:B:1643:MSE:HB2	1.87	0.55
1:B:1726:SER:HB2	1:B:1866:GLN:HE22	1.71	0.55
1:B:1733:THR:OG1	1:B:1877:LEU:HD13	2.06	0.55
1:B:2026:SER:HB3	2:S:207:UNK:CB	2.37	0.55
1:B:2285:LEU:O	1:B:2288:TYR:N	2.39	0.55
1:B:2378:PHE:O	1:B:2382:VAL:HG22	2.06	0.55
1:B:658:THR:HA	1:B:733:LEU:CD2	2.32	0.55
1:B:968:VAL:HG22	1:B:972:LEU:HD23	1.87	0.55
1:A:204:LEU:HD13	1:A:223:CYS:HB2	1.87	0.55
1:A:2222:HIS:O	1:A:2226:PRO:HD2	2.07	0.55
1:A:3144:PHE:CD1	1:A:3160:LEU:HD11	2.42	0.55
1:A:960:GLN:HG2	1:A:961:LEU:HD22	1.89	0.55
1:B:1442:GLN:HE22	1:B:1495:ASP:HB3	1.70	0.55
1:B:3106:GLY:HA2	1:B:3109:SER:HB2	1.88	0.55
1:B:3283:LEU:HG	1:B:3300:VAL:HG21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3966:GLN:H	1:B:4128:MSE:C	2.10	0.55
1:B:4125:GLU:HA	1:B:4127:TRP:CE3	2.41	0.55
1:B:760:LEU:HD13	1:B:802:THR:OG1	2.06	0.55
1:B:985:GLU:O	1:B:988:VAL:HG22	2.06	0.55
1:A:1636:ASP:O	1:A:1640:GLU:HB2	2.06	0.55
1:A:1641:THR:O	1:A:1645:VAL:HG23	2.07	0.55
1:A:1897:ASN:HB3	1:A:1901:HIS:HE1	1.71	0.55
1:A:2210:VAL:HG13	1:A:2211:LEU:H	1.71	0.55
1:A:2236:GLU:HG2	2:K:110:UNK:CB	2.36	0.55
1:A:2575:PRO:HD2	1:A:2785:ILE:HD11	1.87	0.55
1:A:2890:ILE:HD12	1:A:2918:PRO:HB3	1.87	0.55
1:A:3994:ASP:OD2	1:A:3997:LEU:HD13	2.06	0.55
1:B:2031:LEU:C	1:B:2033:ASP:H	2.07	0.55
1:B:2375:ALA:O	1:B:2379:MSE:HB2	2.04	0.55
1:B:2542:LEU:O	1:B:2545:LEU:N	2.38	0.55
1:B:3282:ARG:HB2	1:B:3282:ARG:HH11	1.70	0.55
1:B:2957:LEU:HB3	1:B:3989:ARG:NH2	2.22	0.55
1:B:4066:LEU:HD11	1:B:4078:VAL:HG11	1.88	0.55
1:B:922:SER:C	1:B:924:ARG:H	2.09	0.55
1:A:1567:ILE:HG12	1:A:1571:LEU:HD11	1.87	0.55
1:A:2145:PHE:HD1	1:A:2188:GLU:HG2	1.71	0.55
1:A:2556:SER:O	1:A:2559:THR:OG1	2.25	0.55
1:A:3722:PHE:CD1	1:A:3740:ILE:HA	2.41	0.55
1:A:3981:TYR:OH	1:A:4101:GLU:HB3	2.07	0.55
1:A:543:SER:O	1:A:545:LEU:N	2.34	0.55
1:A:793:LEU:HA	1:A:796:LEU:CG	2.33	0.55
1:B:1678:LEU:O	1:B:1682:THR:HG22	2.07	0.55
1:B:1976:LEU:HD13	1:B:2031:LEU:HD23	1.89	0.55
1:B:2099:ALA:O	1:B:2102:LYS:HB2	2.06	0.55
1:B:2239:LYS:HG3	1:B:2279:ILE:HD12	1.89	0.55
1:B:2289:ASP:O	1:B:2291:GLN:N	2.39	0.55
1:B:2806:LYS:HZ2	1:B:2858:ILE:HG13	1.71	0.55
1:A:1069:HIS:O	1:A:3741:ARG:HD3	2.07	0.55
1:A:1392:MSE:HA	1:A:1395:LEU:HB3	1.89	0.55
1:A:1431:LEU:O	1:A:1434:VAL:HG12	2.07	0.55
1:A:1946:ASN:HA	1:A:1949:ILE:HG22	1.89	0.55
1:A:1982:ILE:HG23	1:A:1986:ARG:HE	1.71	0.55
1:A:2271:SER:OG	1:A:2272:VAL:N	2.40	0.55
1:A:3499:ILE:CG2	1:A:3535:ILE:HG21	2.36	0.55
1:B:1011:GLU:OE2	1:B:1062:ARG:CZ	2.55	0.55
1:B:1102:GLU:HA	1:B:1150:LYS:NZ	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2254:ARG:HB2	1:B:2295:GLN:OE1	2.06	0.55
1:B:279:ALA:HA	1:B:282:PHE:CE2	2.41	0.55
1:B:2895:GLU:O	1:B:2899:ARG:NH2	2.40	0.55
1:B:3578:LEU:HB3	1:B:3579:SER:HA	1.89	0.55
1:B:629:PHE:CZ	1:B:666:PHE:CD1	2.92	0.55
1:B:706:LEU:HB3	1:B:710:PHE:CZ	2.42	0.55
1:B:776:TRP:CE2	1:B:780:ILE:HD12	2.41	0.55
1:A:1016:GLY:O	1:A:1019:ASP:HB2	2.05	0.55
1:A:1083:ASN:HD21	1:A:1104:LEU:HD21	1.71	0.55
1:A:1400:VAL:O	1:A:1404:LYS:CB	2.55	0.55
1:A:1606:ARG:O	1:A:1806:ARG:NH1	2.39	0.55
1:A:1880:MSE:O	1:A:1883:ARG:N	2.39	0.55
1:A:1918:LEU:HD11	1:A:1957:ASN:HB3	1.89	0.55
1:A:2098:THR:HG22	1:A:2146:LEU:HD13	1.89	0.55
1:A:2410:GLU:HA	1:A:2413:PHE:CZ	2.41	0.55
1:A:2957:LEU:HD11	1:A:3985:VAL:HG11	1.87	0.55
1:A:3424:LEU:HD13	1:A:3472:ILE:HD11	1.87	0.55
1:A:3472:ILE:HG22	1:A:3473:GLU:H	1.71	0.55
1:A:3676:PRO:HG2	1:A:3677:PRO:HD3	1.89	0.55
1:A:3722:PHE:CE1	1:A:3740:ILE:HG12	2.34	0.55
1:A:446:PHE:N	1:A:446:PHE:HD1	2.03	0.55
1:A:446:PHE:CZ	1:A:530:LEU:HB3	2.41	0.55
1:A:743:LEU:HD21	1:A:784:VAL:HG21	1.89	0.55
1:B:1424:THR:OG1	1:B:1425:ALA:N	2.40	0.55
1:B:1867:ILE:HG23	1:B:1871:MSE:HE3	1.89	0.55
1:B:2157:PHE:CE1	1:B:2203:THR:HB	2.42	0.55
1:B:2929:LEU:HD22	1:B:3983:ILE:HG12	1.89	0.55
1:B:3592:VAL:HG22	1:B:3609:MSE:SE	2.57	0.55
1:B:3791:TYR:HH	1:B:3942:PHE:HE2	1.54	0.55
1:B:3964:THR:HB	1:B:4128:MSE:O	2.06	0.55
1:B:568:PHE:O	1:B:571:SER:N	2.39	0.55
1:B:612:LEU:CD2	1:B:1800:SER:HB3	2.36	0.55
1:B:612:LEU:HD12	1:B:613:HIS:N	2.22	0.55
1:A:1335:CYS:HA	1:A:1338:VAL:HG12	1.89	0.55
1:A:1423:ILE:O	1:A:1427:SER:OG	2.20	0.55
1:A:1573:LYS:O	1:A:1576:ASP:HB3	2.07	0.55
1:A:1909:ASN:O	1:A:1912:THR:HG23	2.07	0.55
1:A:2789:SER:O	1:A:2793:PRO:HD3	2.07	0.55
1:A:2878:ALA:O	1:A:2886:GLN:HB3	2.07	0.55
1:A:3487:ILE:HA	1:A:3490:VAL:HG22	1.89	0.55
1:A:3901:ARG:HG2	1:A:3901:ARG:HH11	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3981:TYR:HE1	1:A:4105:LYS:N	2.05	0.55
1:A:892:LEU:HD11	1:A:958:MSE:HB2	1.87	0.55
1:B:1087:ARG:HD3	1:B:1134:LEU:HD22	1.89	0.55
1:B:1167:ASP:O	1:B:1171:TRP:HB2	2.06	0.55
1:B:1561:SER:HA	1:B:1564:SER:HB2	1.89	0.55
1:B:2088:LEU:HD21	1:B:2095:ALA:HB2	1.89	0.55
1:B:2190:VAL:HA	1:B:2193:ILE:HG22	1.88	0.55
1:B:3435:ASP:O	1:B:3439:LEU:HB2	2.06	0.55
1:A:1217:VAL:O	1:A:1221:ILE:HG13	2.07	0.55
1:A:1344:PHE:CE1	1:A:1348:LEU:HG	2.42	0.55
1:A:1729:PHE:HZ	1:A:1870:LYS:HG3	1.67	0.55
1:A:2046:SER:HB2	1:A:2096:PRO:HG2	1.89	0.55
1:A:2074:PRO:O	1:A:2076:VAL:N	2.40	0.55
1:A:2167:PRO:CA	1:A:2171:LEU:HB2	2.36	0.55
1:A:2951:GLN:OE1	1:A:2972:TYR:OH	2.18	0.55
1:A:3614:TYR:O	1:A:3618:GLY:N	2.29	0.55
1:A:3778:ASP:OD2	1:A:3781:CYS:N	2.40	0.55
1:A:3816:LEU:O	1:A:3820:MSE:HB3	2.07	0.55
1:A:385:TYR:OH	1:A:424:LEU:HD21	2.07	0.55
1:A:4070:LYS:H	1:A:4074:PHE:HD2	1.55	0.55
1:A:508:HIS:CD2	1:A:725:LEU:HD22	2.42	0.55
1:B:1346:THR:HG21	1:B:1401:ASN:CB	2.35	0.55
1:B:174:VAL:HG12	1:B:178:LEU:HD11	1.87	0.55
1:B:2387:PRO:HA	1:B:2390:HIS:HB3	1.88	0.55
1:B:3631:LYS:HA	1:B:3634:GLN:CB	2.37	0.55
1:B:3806:LEU:O	1:B:3809:THR:HG22	2.07	0.55
1:B:3915:HIS:O	1:B:3918:LEU:N	2.40	0.55
1:B:2957:LEU:HD21	1:B:4101:GLU:CD	2.27	0.55
1:B:431:TYR:HA	1:B:434:VAL:CG1	2.36	0.55
1:B:756:PHE:O	1:B:759:GLY:N	2.40	0.55
1:A:1007:VAL:O	1:A:1011:GLU:HB3	2.07	0.54
1:A:1080:LEU:HD22	1:A:1127:CYS:HB2	1.87	0.54
1:A:1253:THR:HA	1:A:1257:LEU:HD12	1.89	0.54
1:A:86:LEU:HD13	1:A:134:LEU:HD21	1.88	0.54
1:A:2145:PHE:CD1	1:A:2188:GLU:HG2	2.41	0.54
1:A:220:LEU:O	1:A:224:LEU:HG	2.06	0.54
1:A:3699:LEU:HG	1:A:3701:ILE:HG12	1.88	0.54
1:A:752:LEU:HA	1:A:755:ALA:HB3	1.88	0.54
1:B:114:VAL:HG11	1:B:130:LEU:HD11	1.90	0.54
1:B:170:VAL:HG23	1:B:173:LYS:NZ	2.21	0.54
1:B:1927:MSE:HG2	1:B:1941:HIS:CD2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2213:ASN:HB2	1:B:2250:SER:HB2	1.90	0.54
1:B:2793:PRO:O	1:B:2797:VAL:HG22	2.05	0.54
1:B:2944:THR:HG21	1:B:2983:ASP:OD2	2.07	0.54
1:B:358:GLU:N	1:B:361:ILE:HG23	2.22	0.54
1:B:3872:ARG:NH1	1:B:3965:ARG:NH1	2.54	0.54
1:B:454:GLN:HG3	1:B:533:HIS:CE1	2.40	0.54
1:B:784:VAL:O	1:B:787:PRO:HD2	2.07	0.54
1:A:1008:ALA:HA	1:A:1011:GLU:OE1	2.07	0.54
1:A:1240:THR:HA	1:A:1243:TYR:HD2	1.72	0.54
1:A:3122:HIS:O	1:A:3125:ARG:N	2.40	0.54
1:B:1276:VAL:HG13	1:B:1358:LEU:HD12	1.88	0.54
1:B:1378:GLU:HB3	1:B:1379:PRO:HD3	1.89	0.54
1:B:1636:ASP:O	1:B:1640:GLU:HB2	2.07	0.54
1:B:1682:THR:HB	1:B:1724:MSE:SE	2.57	0.54
1:B:1797:LEU:HD13	1:B:1805:PHE:CE2	2.41	0.54
1:B:356:ASN:OD1	1:B:1859:ASN:HB2	2.06	0.54
1:B:2224:PHE:HB3	1:B:2272:VAL:CG1	2.38	0.54
1:B:197:PHE:CE2	1:B:230:LEU:HD22	2.42	0.54
1:B:2304:VAL:O	1:B:2348:GLN:NE2	2.40	0.54
1:B:2352:HIS:CG	1:B:2364:LEU:HD21	2.42	0.54
1:B:3493:TRP:CE3	1:B:3713:PRO:HB3	2.39	0.54
1:B:3704:GLN:NE2	1:B:3796:MSE:SE	2.90	0.54
1:B:3876:SER:O	1:B:3879:PRO:HD2	2.07	0.54
1:A:1259:LEU:HG	1:A:1337:VAL:HG22	1.90	0.54
1:A:1279:LEU:HG	1:A:1292:LYS:HZ3	1.72	0.54
1:A:1363:LEU:C	1:A:1365:ASN:H	2.11	0.54
1:A:1675:TYR:CZ	1:A:1679:LEU:HD11	2.42	0.54
1:A:2040:MSE:HA	1:A:2043:PHE:HD1	1.73	0.54
1:A:2056:SER:HA	1:A:2061:PRO:HG3	1.88	0.54
1:A:2065:ARG:HB3	1:A:2125:TRP:CD1	2.42	0.54
1:A:245:SER:HB2	1:A:272:LEU:HD11	1.89	0.54
1:A:2796:ALA:O	1:A:2800:ARG:HG3	2.06	0.54
1:A:2870:SER:O	1:A:2872:ASP:N	2.41	0.54
1:A:3273:LEU:HB3	1:A:3321:LEU:CD2	2.37	0.54
1:A:3413:TYR:HD2	1:A:3453:ALA:HB2	1.72	0.54
1:A:887:ASP:O	1:A:3889:ARG:HG2	2.07	0.54
1:A:3967:PHE:CD1	1:A:3968:ILE:N	2.75	0.54
1:B:2636:UNK:O	1:B:2640:UNK:CB	2.55	0.54
1:B:2801:ASP:HB2	1:B:2802:PRO:HD3	1.88	0.54
1:B:2894:GLU:HA	1:B:2898:LEU:HB2	1.88	0.54
1:B:3464:LYS:O	1:B:3468:LEU:HG	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3864:ARG:HD2	1:B:4115:ASN:OD1	2.08	0.54
1:A:1018:VAL:HB	1:A:1074:LYS:CA	2.37	0.54
1:A:1064:TYR:CD1	1:A:1106:ILE:HD11	2.42	0.54
1:A:1296:PHE:O	1:A:1299:GLU:N	2.39	0.54
1:A:1462:GLY:C	1:A:1464:LEU:H	2.11	0.54
1:A:1551:ILE:HA	1:A:1554:SER:HB3	1.89	0.54
1:A:15:LEU:HD23	1:A:2359:LYS:NZ	2.22	0.54
1:A:2164:TRP:HH2	1:A:2190:VAL:HG12	1.70	0.54
1:A:2923:TRP:CD1	1:A:2931:ARG:HD3	2.42	0.54
1:A:3294:SER:HB3	1:A:3341:LEU:HD22	1.90	0.54
1:B:963:LYS:HB3	1:B:1009:LEU:HD11	1.88	0.54
1:B:1216:GLY:HA3	1:B:1271:ILE:HG22	1.88	0.54
1:B:2462:VAL:HG11	1:B:2473:MSE:SE	2.58	0.54
1:B:2474:TYR:CE1	1:B:2509:GLY:HA3	2.42	0.54
1:B:3472:ILE:HG22	1:B:3473:GLU:H	1.73	0.54
1:B:409:GLN:HG3	1:B:413:PHE:CZ	2.41	0.54
1:B:514:VAL:HA	1:B:604:PRO:HG3	1.90	0.54
1:B:575:ILE:N	1:B:605:THR:OG1	2.40	0.54
1:A:1111:LEU:HA	1:A:1114:ALA:HB3	1.90	0.54
1:A:2461:PHE:HE1	1:A:2469:CYS:HG	1.55	0.54
1:A:2538:ARG:HH11	1:A:2565:MSE:CG	2.21	0.54
1:A:3008:TRP:H	1:A:3050:LYS:HG2	1.73	0.54
1:A:3114:TYR:OH	1:A:3128:LYS:HB3	2.07	0.54
1:A:401:ASP:HB2	1:A:1763:THR:OG1	2.07	0.54
1:A:759:GLY:HA3	1:A:773:LEU:CD1	2.38	0.54
1:B:1019:ASP:HB3	1:B:1020:PRO:HD2	1.89	0.54
1:B:1639:LEU:HD12	1:B:1640:GLU:N	2.23	0.54
1:B:3121:LEU:HB2	1:B:3124:SER:OG	2.08	0.54
1:B:3864:ARG:NH2	1:B:4119:ARG:HH21	2.05	0.54
1:B:4027:TRP:HB3	1:B:4031:ILE:HD11	1.90	0.54
1:B:649:PHE:C	1:B:651:TYR:N	2.61	0.54
1:B:659:ARG:HH22	1:B:662:LEU:CB	2.20	0.54
1:B:65:LEU:HD23	1:B:68:PHE:CE1	2.43	0.54
1:B:936:SER:HB3	1:B:2791:ILE:CG1	2.35	0.54
1:A:1424:THR:O	1:A:1426:GLN:N	2.41	0.54
1:A:138:PHE:CD2	1:A:177:LEU:HD22	2.42	0.54
1:A:1810:PRO:O	1:A:1811:ARG:HG2	2.08	0.54
1:A:269:SER:HB2	1:A:315:ALA:HB2	1.90	0.54
1:B:1693:VAL:O	1:B:1697:PRO:HD3	2.07	0.54
1:B:2039:GLU:HG2	1:B:2077:HIS:NE2	2.22	0.54
1:B:2220:MSE:SE	1:B:2276:LEU:HD11	2.58	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2363:CYS:O	1:B:2367:VAL:HG12	2.07	0.54
1:B:3907:SER:O	1:B:3911:ILE:HG23	2.08	0.54
1:B:633:ILE:O	1:B:637:LYS:HG2	2.08	0.54
1:B:897:PRO:HG2	1:B:898:PHE:CE1	2.43	0.54
1:A:1103:ALA:O	1:A:1106:ILE:HG12	2.07	0.54
1:A:2030:TYR:CD1	1:A:2031:LEU:HG	2.40	0.54
1:A:270:ALA:O	1:A:274:LEU:HG	2.08	0.54
1:A:2837:LEU:HD13	1:A:2868:LEU:N	2.23	0.54
1:A:3390:GLN:O	1:A:3394:GLU:HB2	2.08	0.54
1:A:3464:LYS:HE3	1:A:3468:LEU:HD21	1.88	0.54
1:A:3486:GLU:HG3	1:A:3487:ILE:N	2.22	0.54
1:A:3701:ILE:O	1:A:3701:ILE:HG13	2.08	0.54
1:A:3812:LEU:HG	1:A:3813:LYS:N	2.22	0.54
1:A:3963:LEU:HG	1:A:3967:PHE:HE1	1.71	0.54
1:A:69:VAL:HG12	1:A:70:ARG:N	2.22	0.54
1:B:2097:LEU:HA	1:B:2100:LEU:HB3	1.89	0.54
1:B:2224:PHE:HZ	1:B:2276:LEU:HD22	1.70	0.54
1:B:2386:LEU:HD11	1:B:2400:VAL:HG12	1.88	0.54
1:B:2543:ASN:HA	1:B:2546:TYR:HD2	1.72	0.54
1:B:3840:LYS:CE	1:B:4122:GLU:HB3	2.36	0.54
1:B:3858:MSE:HG2	1:B:4119:ARG:HD3	1.89	0.54
1:B:916:GLU:CB	1:B:930:ALA:HB1	2.36	0.54
1:A:1087:ARG:CD	1:A:1134:LEU:HD22	2.36	0.54
1:A:1406:LEU:HB3	1:A:1415:LEU:HD21	1.90	0.54
1:A:1609:ALA:HB2	1:A:1633:TRP:CZ2	2.42	0.54
1:A:2085:MSE:O	1:A:2088:LEU:HB3	2.08	0.54
1:A:2416:LYS:HD3	1:A:2442:MSE:SE	2.58	0.54
1:A:2935:GLU:HG3	1:A:2936:TYR:H	1.73	0.54
1:A:83:GLU:O	1:A:87:LYS:HG3	2.08	0.54
1:A:971:ARG:NE	1:A:1024:THR:OG1	2.40	0.54
1:A:966:PHE:CZ	1:A:988:VAL:HG12	2.43	0.54
1:B:2163:HIS:O	1:B:2167:PRO:HD3	2.07	0.54
1:B:2312:TYR:CE2	1:B:2313:LYS:HG2	2.43	0.54
1:B:2352:HIS:HB2	1:B:2364:LEU:HD11	1.89	0.54
1:B:2820:MSE:SE	1:B:2833:THR:HG21	2.58	0.54
1:B:3568:ILE:HD11	1:B:3691:LYS:HD2	1.90	0.54
1:B:649:PHE:C	1:B:651:TYR:H	2.10	0.54
1:B:789:TYR:HD2	1:B:865:GLN:HG3	1.71	0.54
1:B:855:VAL:O	1:B:859:LEU:HG	2.07	0.54
1:A:114:VAL:CG1	1:A:130:LEU:HD11	2.38	0.54
1:A:1886:LYS:HZ2	1:A:1924:THR:CB	2.17	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1907:GLU:OE2	1:A:1911:LEU:HD11	2.08	0.54
1:A:2177:ASN:HD22	1:A:2182:ILE:CG2	2.21	0.54
1:A:2304:VAL:HG11	1:A:2344:LEU:HB3	1.90	0.54
1:A:2412:TYR:CE1	1:A:2415:LEU:HB3	2.43	0.54
1:A:3039:THR:O	1:A:3042:PRO:HD2	2.08	0.54
1:A:262:LEU:HD13	1:A:306:VAL:HG12	1.88	0.54
1:A:3728:VAL:HG22	1:A:3736:LYS:HG3	1.89	0.54
1:A:3762:GLN:HE22	1:A:3763:ARG:NH1	2.05	0.54
1:B:87:LYS:HG2	1:B:133:LYS:HG3	1.89	0.54
1:B:1862:THR:O	1:B:1865:THR:HG22	2.07	0.54
1:B:2049:VAL:HG11	1:B:2100:LEU:HD12	1.90	0.54
1:B:2238:ILE:O	1:B:2242:VAL:HG23	2.08	0.54
1:B:2366:LYS:HZ2	2:S:101:UNK:HA	1.73	0.54
1:B:276:ALA:HA	1:B:280:SER:OG	2.08	0.54
1:B:2806:LYS:HA	1:B:2809:PHE:CD2	2.43	0.54
1:B:278:HIS:O	1:B:281:GLN:HB3	2.08	0.54
1:B:2990:GLU:O	1:B:2994:TRP:HB2	2.07	0.54
1:B:3048:LYS:NZ	1:B:3064:PHE:CE2	2.74	0.54
1:B:3240:MSE:O	1:B:3242:MSE:N	2.41	0.54
1:B:620:PHE:CE1	1:B:623:PHE:HD2	2.26	0.54
1:B:718:MSE:SE	1:B:731:THR:HG22	2.58	0.54
1:B:39:GLY:HA2	1:B:92:PHE:HZ	1.71	0.54
1:B:981:ARG:HA	1:B:984:TYR:HD2	1.71	0.54
1:A:1080:LEU:HD13	1:A:1127:CYS:CB	2.38	0.54
1:A:1087:ARG:HD3	1:A:1134:LEU:HB3	1.89	0.54
1:A:1166:LEU:HB3	1:A:1170:LYS:NZ	2.23	0.54
1:A:1582:LEU:O	1:A:1585:SER:HB3	2.08	0.54
1:A:1718:ILE:HG23	1:A:1750:LEU:HD11	1.89	0.54
1:A:2039:GLU:HG2	1:A:2077:HIS:NE2	2.23	0.54
1:A:2200:ALA:HA	1:A:2203:THR:HG22	1.89	0.54
1:A:2855:VAL:O	1:A:2859:GLN:HB2	2.08	0.54
1:A:3518:VAL:HA	1:A:3521:ILE:HG22	1.90	0.54
1:A:3857:LEU:HA	1:A:3859:TYR:CE2	2.43	0.54
1:A:2891:ARG:HH22	1:A:3884:LYS:HE2	1.73	0.54
1:A:508:HIS:HB3	1:A:725:LEU:HB3	1.90	0.54
1:B:2798:ALA:HB3	1:B:2799:GLN:NE2	2.23	0.54
1:B:3578:LEU:HD22	1:B:3683:CYS:SG	2.47	0.54
1:B:629:PHE:CZ	1:B:666:PHE:O	2.60	0.54
1:A:1008:ALA:O	1:A:1011:GLU:HB3	2.08	0.53
1:A:1175:HIS:O	1:A:1179:PRO:HD3	2.08	0.53
1:A:1804:MSE:O	1:A:1808:ASP:HB3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1939:LEU:CD1	1:A:1986:ARG:HG2	2.38	0.53
1:A:2148:LYS:HD2	1:A:2188:GLU:OE2	2.08	0.53
1:A:3122:HIS:HB3	1:A:3126:LEU:HD13	1.89	0.53
1:A:3502:MSE:HE3	1:A:3517:SER:HB3	1.89	0.53
1:A:3525:TYR:CE1	1:A:3561:LYS:HD2	2.43	0.53
1:A:3974:MSE:HA	1:A:3975:LYS:CB	2.38	0.53
1:A:414:LEU:HG	1:A:414:LEU:O	2.01	0.53
1:A:548:GLU:O	1:A:552:SER:OG	2.21	0.53
1:B:1348:LEU:HD23	1:B:1353:PRO:HD3	1.90	0.53
1:B:1733:THR:HB	1:B:1877:LEU:HD22	1.90	0.53
1:B:2813:PHE:HA	1:B:2816:ILE:HG22	1.89	0.53
1:B:3047:SER:HB2	1:B:3050:LYS:HE2	1.90	0.53
1:B:3690:PHE:CZ	1:B:3722:PHE:HD2	2.26	0.53
1:B:3917:ILE:O	1:B:4048:LYS:CE	2.56	0.53
1:B:3965:ARG:HG3	1:B:3969:ASN:OD1	2.09	0.53
2:S:217:UNK:O	2:S:220:MSE:HG2	2.08	0.53
1:A:1817:GLN:HA	1:A:1820:VAL:HG22	1.90	0.53
1:A:3794:VAL:HG11	1:A:3796:MSE:HE3	1.90	0.53
1:A:3819:THR:HG1	1:A:3889:ARG:HH12	1.46	0.53
1:A:3789:ARG:HD3	1:A:3938:ILE:HG21	1.89	0.53
1:B:1575:LEU:HD13	1:B:1604:SER:HB3	1.90	0.53
1:B:1648:LEU:HD22	1:B:1684:LEU:HD22	1.89	0.53
1:B:2049:VAL:HA	1:B:2052:TYR:HD2	1.71	0.53
1:B:2870:SER:HA	1:B:2897:LEU:HD22	1.89	0.53
1:B:294:PHE:O	1:B:297:LEU:HG	2.09	0.53
1:B:3469:LEU:O	1:B:3474:ARG:HG2	2.08	0.53
1:B:356:ASN:ND2	1:B:1859:ASN:H	2.07	0.53
1:B:3636:PHE:C	1:B:3638:LYS:H	2.12	0.53
1:B:3927:ASN:O	1:B:3940:ILE:HG22	2.08	0.53
1:B:629:PHE:HZ	1:B:666:PHE:O	1.91	0.53
1:B:762:TYR:C	1:B:764:PRO:HD3	2.29	0.53
1:A:1046:PRO:O	1:A:1049:GLN:HB3	2.08	0.53
1:A:2078:ASP:HB3	1:A:2135:ASN:ND2	2.23	0.53
1:A:2168:LEU:HD13	1:A:2214:ARG:CZ	2.37	0.53
1:A:368:LEU:HD23	1:A:372:PRO:CG	2.37	0.53
1:A:489:ARG:HH22	1:A:492:SER:HB3	1.72	0.53
1:A:661:PRO:HG2	1:A:733:LEU:CA	2.38	0.53
1:A:926:THR:O	1:A:930:ALA:CB	2.56	0.53
1:B:1590:THR:O	1:B:1592:MSE:N	2.41	0.53
1:B:1723:PRO:C	1:B:1725:GLN:H	2.12	0.53
1:B:2009:LYS:NZ	1:B:2011:ALA:HA	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2196:TRP:CE2	1:B:2199:LEU:HD11	2.44	0.53
1:B:3585:PHE:HD1	1:B:3613:MSE:HE1	1.73	0.53
1:B:3790:THR:HG22	1:B:3791:TYR:H	1.73	0.53
1:B:641:PHE:CE1	1:B:663:ILE:HG21	2.42	0.53
1:B:757:LYS:HA	1:B:760:LEU:HD12	1.90	0.53
1:A:1032:CYS:HB3	1:A:1036:PHE:CZ	2.44	0.53
1:A:1083:ASN:HB2	1:A:1107:TYR:HE2	1.74	0.53
1:A:1111:LEU:HD23	1:A:1128:CYS:SG	2.48	0.53
1:A:306:VAL:O	1:A:309:LYS:HG3	2.08	0.53
1:A:3141:PHE:HZ	1:A:3192:LYS:HB2	1.73	0.53
1:A:3300:VAL:HG23	1:A:3328:ILE:HD13	1.89	0.53
1:A:3462:ARG:HE	1:A:3501:HIS:CD2	2.27	0.53
1:A:361:ILE:HG13	1:A:362:ALA:N	2.23	0.53
1:A:3944:HIS:NE2	1:A:4020:MSE:HE3	2.23	0.53
1:A:47:SER:H	1:A:51:LEU:HD12	1.74	0.53
1:A:535:LEU:HB3	1:A:626:LEU:HD11	1.91	0.53
1:A:756:PHE:O	1:A:759:GLY:C	2.47	0.53
1:B:1267:TYR:OH	1:B:1340:ARG:NH2	2.41	0.53
1:B:1275:THR:HA	1:B:1279:LEU:HB2	1.90	0.53
1:B:1941:HIS:ND1	1:B:1941:HIS:O	2.40	0.53
1:B:2300:PHE:CE2	1:B:2341:LEU:HB2	2.44	0.53
1:B:3311:ASN:O	1:B:3313:SER:N	2.39	0.53
1:B:3458:SER:OG	1:B:3494:GLN:NE2	2.42	0.53
1:B:3530:VAL:HA	1:B:3533:PHE:CD2	2.43	0.53
1:B:3629:ARG:NH2	1:B:3638:LYS:NZ	2.53	0.53
1:B:3699:LEU:HG	1:B:3701:ILE:HG23	1.90	0.53
1:B:969:LEU:O	1:B:973:ALA:HB2	2.07	0.53
1:B:977:ASP:O	1:B:980:THR:HB	2.09	0.53
1:A:1221:ILE:HG12	1:A:1274:ARG:NH1	2.24	0.53
1:A:1288:SER:O	1:A:1290:LEU:N	2.42	0.53
1:A:1306:ILE:HG22	1:A:1381:SER:HB3	1.90	0.53
1:A:1758:LEU:HD13	1:A:1860:GLU:HG2	1.89	0.53
1:A:2094:MSE:HE1	1:A:2143:ARG:CA	2.38	0.53
1:A:2352:HIS:CG	1:A:2364:LEU:HD21	2.44	0.53
1:A:276:ALA:HA	1:A:280:SER:OG	2.09	0.53
1:A:3529:ILE:HG13	1:A:3532:PRO:HG2	1.89	0.53
1:A:567:GLU:HB3	1:A:606:SER:CB	2.39	0.53
1:B:1015:ASP:HA	1:B:1018:VAL:HG22	1.90	0.53
1:B:1044:ILE:O	1:B:1045:THR:OG1	2.25	0.53
1:B:3259:LEU:O	1:B:3263:HIS:CB	2.53	0.53
1:B:3605:ASN:O	1:B:3609:MSE:HG3	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:LEU:HD21	1:B:1813:SER:HB3	1.90	0.53
1:B:430:VAL:HG21	1:B:1682:THR:HG23	1.90	0.53
1:A:1348:LEU:O	1:A:1352:SER:N	2.35	0.53
1:A:2129:LEU:HB3	1:A:2156:VAL:HG13	1.90	0.53
1:A:3266:SER:HB2	1:A:3271:ASP:CG	2.29	0.53
1:A:3486:GLU:O	1:A:3489:SER:N	2.41	0.53
1:A:3617:LEU:HD13	1:A:3644:PHE:HD2	1.74	0.53
1:A:364:ARG:O	1:A:368:LEU:N	2.24	0.53
1:A:965:THR:HA	1:A:968:VAL:HG12	1.90	0.53
1:B:110:THR:O	1:B:114:VAL:HG23	2.07	0.53
1:B:1756:PRO:C	1:B:1758:LEU:H	2.11	0.53
1:B:2280:VAL:HG13	1:B:2287:PRO:HB2	1.91	0.53
1:B:3530:VAL:HG11	1:B:3700:GLU:O	2.09	0.53
1:B:4017:GLU:N	1:B:4017:GLU:OE1	2.39	0.53
1:B:69:VAL:HG12	1:B:70:ARG:N	2.24	0.53
1:B:884:VAL:HG11	1:B:3889:ARG:O	2.08	0.53
1:A:1004:GLN:O	1:A:1008:ALA:CB	2.56	0.53
1:A:1513:GLY:O	1:A:1517:LEU:HG	2.07	0.53
1:A:1567:ILE:O	1:A:1571:LEU:HG	2.09	0.53
1:A:1976:LEU:HD22	1:A:1981:LEU:HD22	1.91	0.53
1:A:2870:SER:C	1:A:2872:ASP:H	2.11	0.53
1:A:3464:LYS:HG3	1:A:3468:LEU:HD11	1.91	0.53
1:A:3493:TRP:HB2	1:A:3713:PRO:HG3	1.91	0.53
1:A:361:ILE:HD11	1:A:413:PHE:CZ	2.44	0.53
1:A:3818:ASN:O	1:A:3821:SER:HB3	2.08	0.53
1:A:947:GLN:HB2	1:A:949:PRO:HD3	1.89	0.53
1:B:1256:TRP:O	1:B:1260:LEU:HG	2.08	0.53
1:B:150:GLY:HA2	1:B:153:PHE:CE2	2.43	0.53
1:B:1914:THR:HG22	1:B:1955:VAL:HG21	1.89	0.53
1:B:1988:TYR:OH	1:B:2044:ASP:OD2	2.24	0.53
1:B:2349:LEU:HD23	1:B:2364:LEU:HD22	1.90	0.53
1:B:2798:ALA:O	1:B:2802:PRO:HD2	2.09	0.53
1:B:2890:ILE:HD12	1:B:2918:PRO:HB3	1.90	0.53
1:B:3459:ASN:ND2	1:B:3710:LYS:NZ	2.57	0.53
1:B:3588:TRP:O	1:B:3592:VAL:HG23	2.09	0.53
1:B:75:SER:O	1:B:77:GLU:N	2.41	0.53
1:A:995:PHE:HZ	1:A:1006:THR:HB	1.74	0.53
1:A:1067:ALA:HB1	1:A:1111:LEU:CD1	2.38	0.53
1:A:2094:MSE:HA	1:A:2094:MSE:HE3	1.90	0.53
1:A:313:LEU:O	1:A:316:LEU:N	2.42	0.53
1:A:321:LYS:O	1:A:325:ASN:ND2	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3280:TYR:O	1:A:3283:LEU:HB3	2.09	0.53
1:A:361:ILE:HG12	1:A:1858:LEU:HD23	1.91	0.53
1:A:3620:PRO:HG2	1:A:3641:ASP:OD2	2.08	0.53
1:A:4002:MSE:SE	1:A:4048:LYS:HE3	2.58	0.53
1:A:771:ASN:C	1:A:773:LEU:H	2.12	0.53
1:A:995:PHE:CE1	1:A:1003:SER:HA	2.43	0.53
1:B:1158:PRO:HB2	1:B:1159:PRO:HD3	1.91	0.53
1:B:1685:ASP:OD1	1:B:1717:LEU:HD13	2.09	0.53
1:B:179:GLY:O	1:B:183:GLU:HG3	2.08	0.53
1:B:2502:ALA:O	1:B:2506:LEU:HG	2.08	0.53
1:B:808:GLU:OE1	1:B:3114:TYR:HB3	2.08	0.53
1:B:3133:GLN:O	1:B:3137:GLU:HG2	2.09	0.53
1:B:3487:ILE:HD11	1:B:3498:TRP:HH2	1.74	0.53
1:B:3908:HIS:CG	1:B:3967:PHE:CZ	2.97	0.53
1:B:3997:LEU:H	1:B:3997:LEU:HD12	1.73	0.53
1:A:2186:VAL:HG21	1:A:2219:LEU:HD21	1.91	0.53
1:A:3024:PRO:HB2	1:A:3067:LYS:NZ	2.23	0.53
1:A:3251:ASN:ND2	1:A:3254:LEU:HB2	2.24	0.53
1:A:3578:LEU:HD11	1:A:3686:TRP:CZ3	2.43	0.53
1:A:3457:ASN:CG	1:A:3710:LYS:HZ2	2.12	0.53
1:B:1802:TYR:HA	1:B:1805:PHE:CD2	2.37	0.53
1:B:1916:ILE:O	1:B:1920:TYR:HD1	1.92	0.53
1:B:2009:LYS:HG2	1:B:2011:ALA:N	2.24	0.53
1:B:2379:MSE:SE	1:B:2408:MSE:SE	3.27	0.53
1:B:2532:PRO:HG2	1:B:2538:ARG:N	2.23	0.53
1:B:2870:SER:C	1:B:2872:ASP:H	2.04	0.53
1:B:2877:SER:O	1:B:2879:GLY:N	2.28	0.53
1:B:3080:LEU:HA	1:B:3086:LEU:HD22	1.91	0.53
1:B:3719:ILE:HG23	1:B:3720:ALA:H	1.73	0.53
1:B:3879:PRO:HG2	1:B:4128:MSE:HE3	1.91	0.53
1:B:3972:LEU:HB2	1:B:3974:MSE:HE2	1.91	0.53
1:B:3946:PHE:CE2	1:B:4048:LYS:HD2	2.44	0.53
1:B:531:PHE:CZ	1:B:619:ASP:HB2	2.43	0.53
1:B:550:PHE:CZ	1:B:632:GLU:HG2	2.42	0.53
1:A:1382:ILE:HD12	1:A:1386:ILE:HD11	1.91	0.53
1:A:139:ARG:O	1:A:141:SER:N	2.39	0.53
1:A:1982:ILE:HG23	1:A:1986:ARG:NE	2.24	0.53
1:A:2083:LEU:N	1:A:2086:ASP:HB2	2.24	0.53
1:A:2412:TYR:HD2	1:A:2416:LYS:HZ2	1.57	0.53
1:A:3238:MSE:O	1:A:3242:MSE:HG3	2.08	0.53
1:A:3498:TRP:NE1	1:A:3502:MSE:HB2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3696:ARG:O	1:A:3699:LEU:HB2	2.09	0.53
1:A:558:GLU:HA	1:A:561:ASN:ND2	2.24	0.53
1:A:562:HIS:HA	1:A:565:TYR:HB3	1.91	0.53
1:B:1349:LEU:CD2	1:B:1359:LEU:HB2	2.38	0.53
1:B:1652:ILE:HG13	1:B:1684:LEU:HD12	1.90	0.53
1:B:244:THR:O	1:B:248:ILE:HG13	2.09	0.53
1:B:2517:LEU:H	1:B:2517:LEU:HD23	1.73	0.53
1:B:3012:GLU:HB2	1:B:3050:LYS:HZ3	1.69	0.53
1:B:3425:ARG:NH1	1:B:4003:ASP:OD2	2.42	0.53
1:B:658:THR:N	1:B:733:LEU:HD13	2.24	0.53
1:A:1550:VAL:HG23	1:A:1551:ILE:H	1.74	0.52
1:A:1560:TYR:O	1:A:1563:PHE:N	2.30	0.52
1:A:1729:PHE:H	1:A:1730:PRO:HD2	1.74	0.52
1:A:3145:ILE:HG23	1:A:3196:LYS:HG2	1.91	0.52
1:A:3640:PHE:HB3	1:A:3644:PHE:CE2	2.44	0.52
1:A:659:ARG:NH2	1:A:662:LEU:HG	2.18	0.52
1:B:1733:THR:N	1:B:1734:PRO:HD3	2.24	0.52
1:B:1933:LEU:HD22	1:B:1937:ARG:HG2	1.90	0.52
1:B:2273:GLY:O	1:B:2276:LEU:HB3	2.09	0.52
1:B:2420:PHE:CE2	1:B:2424:MSE:HE3	2.44	0.52
1:B:3175:PRO:HB2	1:B:3178:ILE:HG13	1.90	0.52
1:B:357:LYS:HB2	1:B:361:ILE:HG22	1.89	0.52
1:B:385:TYR:CE2	1:B:424:LEU:HD21	2.44	0.52
1:B:986:PRO:O	1:B:990:GLN:HG2	2.10	0.52
1:A:1111:LEU:O	1:A:1114:ALA:HB3	2.09	0.52
1:A:2462:VAL:HG11	1:A:2473:MSE:HE1	1.91	0.52
1:A:3007:GLU:HA	1:A:3011:LEU:HB2	1.90	0.52
1:A:3051:LEU:HD22	1:A:3058:ASP:HB2	1.91	0.52
1:A:3170:ASP:O	1:A:3172:LYS:NZ	2.39	0.52
1:A:3397:GLN:NE2	1:A:3449:LYS:HD3	2.21	0.52
1:A:3498:TRP:O	1:A:3498:TRP:CD1	2.61	0.52
1:A:4081:ALA:HB2	1:A:4116:ILE:HD11	1.90	0.52
1:B:1096:VAL:HG23	1:B:1099:PHE:HE2	1.73	0.52
1:B:1356:TRP:HZ2	1:B:1409:SER:HB3	1.72	0.52
1:B:138:PHE:CD2	1:B:173:LYS:HE3	2.38	0.52
1:B:2223:VAL:HB	1:B:2238:ILE:HD12	1.92	0.52
1:B:245:SER:O	1:B:248:ILE:N	2.42	0.52
1:B:2461:PHE:O	1:B:2465:PRO:HD3	2.09	0.52
1:B:2999:LEU:HA	1:B:3002:TYR:CE2	2.44	0.52
1:B:3461:ALA:O	1:B:3464:LYS:N	2.41	0.52
1:B:396:PHE:CZ	1:B:397:LEU:HG	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:730:LEU:HA	1:B:733:LEU:CD1	2.39	0.52
1:B:933:LEU:O	1:B:936:SER:N	2.41	0.52
1:A:103:TYR:O	1:A:107:ILE:HG13	2.09	0.52
1:A:104:SER:HA	1:A:107:ILE:HD12	1.92	0.52
1:A:1520:ALA:O	1:A:1524:LEU:HD13	2.09	0.52
1:A:1725:GLN:OE1	1:A:1754:GLN:NE2	2.43	0.52
1:A:1760:GLU:CB	1:A:1894:SER:HA	2.40	0.52
1:A:175:TYR:HE1	1:A:200:PHE:CB	2.23	0.52
1:A:2281:MSE:SE	1:A:2286:PRO:CB	3.07	0.52
1:A:231:LEU:HB2	1:A:275:PHE:CZ	2.44	0.52
1:A:2395:THR:O	1:A:2399:GLU:HB2	2.09	0.52
1:A:2420:PHE:HE1	1:A:2436:LEU:HD22	1.75	0.52
1:A:3117:ILE:HD12	1:A:3125:ARG:NH1	2.23	0.52
1:A:4071:ALA:O	1:A:4075:ARG:CB	2.55	0.52
1:A:535:LEU:HD22	1:A:626:LEU:HG	1.91	0.52
1:B:1073:PHE:CD1	1:B:1074:LYS:N	2.74	0.52
1:B:1880:MSE:HE2	1:B:1884:LEU:HD21	1.92	0.52
1:B:217:LEU:N	1:B:218:PRO:HD2	2.23	0.52
1:B:249:PHE:HD1	1:B:265:TYR:CE1	2.27	0.52
1:B:3684:SER:OG	1:B:3685:PRO:HD3	2.10	0.52
1:B:580:ASP:OD1	1:B:581:LEU:N	2.42	0.52
1:B:70:ARG:HG3	1:B:78:PHE:HB3	1.90	0.52
1:B:922:SER:O	1:B:924:ARG:N	2.42	0.52
1:A:1369:MSE:HE1	1:A:1414:ILE:O	2.10	0.52
1:A:178:LEU:HB3	1:A:197:PHE:CZ	2.45	0.52
1:A:2542:LEU:CB	1:A:2546:TYR:HE2	2.18	0.52
1:A:3033:GLU:OE2	1:A:3079:GLU:OE2	2.27	0.52
1:A:307:GLU:H	1:A:307:GLU:CD	2.12	0.52
1:A:3416:LEU:CD1	1:A:3446:VAL:HG12	2.40	0.52
1:A:654:ILE:O	1:A:657:SER:N	2.42	0.52
1:A:703:CYS:O	1:A:707:PHE:HD1	1.92	0.52
1:A:947:GLN:C	1:A:949:PRO:HD3	2.30	0.52
1:B:1104:LEU:HD22	1:B:1135:CYS:SG	2.49	0.52
1:B:1698:PHE:HD1	1:B:1699:PHE:N	2.07	0.52
1:B:2464:HIS:H	1:B:2465:PRO:HD3	1.74	0.52
1:B:2824:LYS:O	1:B:2826:LEU:HG	2.09	0.52
1:B:937:MSE:O	1:B:941:MSE:HG3	2.08	0.52
1:A:1090:ARG:HH22	1:A:1096:VAL:HG22	1.74	0.52
1:A:2799:GLN:CB	1:A:2808:LEU:HD11	2.40	0.52
1:A:3331:GLY:O	1:A:3335:ARG:HD2	2.09	0.52
1:A:3503:VAL:CG2	1:A:3536:SER:HA	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3588:TRP:O	1:A:3592:VAL:HG23	2.08	0.52
1:A:3620:PRO:CB	1:A:3633:ILE:HG23	2.39	0.52
1:A:368:LEU:C	1:A:372:PRO:HG2	2.30	0.52
1:A:3769:GLN:O	1:A:3773:GLY:HA3	2.10	0.52
1:A:385:TYR:CE1	1:A:421:LEU:HD23	2.45	0.52
1:A:608:PRO:HB2	1:A:1800:SER:HB2	1.91	0.52
1:A:730:LEU:HA	1:A:733:LEU:HD12	1.90	0.52
1:B:1911:LEU:O	1:B:1913:LYS:N	2.37	0.52
1:B:1913:LYS:HG3	1:B:1916:ILE:HD12	1.91	0.52
1:B:1883:ARG:HB2	1:B:1923:PHE:CZ	2.44	0.52
1:B:194:GLU:HA	1:B:197:PHE:HD2	1.74	0.52
1:B:2002:LYS:O	1:B:2004:TYR:N	2.43	0.52
1:B:2308:SER:H	1:B:2348:GLN:NE2	2.08	0.52
1:B:2854:PHE:CZ	1:B:2881:LEU:HB2	2.45	0.52
1:B:2987:THR:HB	1:B:2991:LYS:N	2.20	0.52
1:B:3005:LEU:C	1:B:3254:LEU:HD21	2.28	0.52
1:B:3625:LEU:HD13	1:B:3633:ILE:HG13	1.91	0.52
1:B:1244:LEU:HD13	1:B:3698:GLU:OE2	2.10	0.52
1:B:88:PHE:O	1:B:91:ILE:HG13	2.09	0.52
1:B:981:ARG:CG	1:B:982:GLN:N	2.72	0.52
1:A:985:GLU:HG3	1:A:1031:ARG:NH2	2.25	0.52
1:A:1076:LEU:C	1:A:1078:ALA:H	2.12	0.52
1:A:1675:TYR:OH	1:A:1679:LEU:HD11	2.10	0.52
1:A:2405:VAL:O	1:A:2408:MSE:HB2	2.08	0.52
1:A:2854:PHE:CZ	1:A:2881:LEU:HB2	2.44	0.52
1:A:3251:ASN:HD21	1:A:3254:LEU:HD13	1.75	0.52
1:A:3464:LYS:HD2	1:A:3467:ARG:HD2	1.91	0.52
1:A:3602:ASN:HA	1:A:3606:ILE:HG12	1.92	0.52
1:A:3775:LEU:HB2	1:A:3787:GLN:NE2	2.24	0.52
1:A:446:PHE:HB2	1:A:533:HIS:CD2	2.44	0.52
1:A:476:ARG:O	1:A:479:ILE:HB	2.10	0.52
1:A:612:LEU:HD23	1:A:613:HIS:N	2.24	0.52
1:A:913:ARG:HB3	1:A:934:LEU:HD12	1.90	0.52
1:B:2002:LYS:C	1:B:2004:TYR:H	2.12	0.52
1:B:1993:GLU:HG2	1:B:2043:PHE:CD2	2.44	0.52
1:B:2210:VAL:HG13	1:B:2211:LEU:HG	1.90	0.52
1:B:2546:TYR:CE1	1:B:2558:ALA:CB	2.90	0.52
1:B:2546:TYR:HE1	1:B:2558:ALA:CB	2.20	0.52
1:B:2573:PRO:C	1:B:2575:PRO:HD3	2.30	0.52
1:B:3064:PHE:CG	1:B:3065:ILE:N	2.74	0.52
1:B:4077:TYR:CZ	1:B:4119:ARG:HG2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:567:GLU:O	1:B:571:SER:N	2.42	0.52
1:B:580:ASP:O	1:B:584:GLU:N	2.43	0.52
1:B:658:THR:CG2	1:B:659:ARG:HH11	2.17	0.52
1:B:631:ARG:HG2	1:B:669:LEU:HD11	1.91	0.52
1:A:1067:ALA:HB1	1:A:1111:LEU:HD11	1.91	0.52
1:A:3280:TYR:CD1	1:A:3328:ILE:HD11	2.44	0.52
1:A:408:TYR:HB2	1:A:453:MSE:HG2	1.91	0.52
1:A:736:LEU:O	1:A:740:ILE:HG13	2.10	0.52
1:A:967:PRO:O	1:A:970:LEU:N	2.42	0.52
1:B:1352:SER:HB3	1:B:1353:PRO:HD3	1.92	0.52
1:B:1399:CYS:O	1:B:1403:MSE:HG3	2.10	0.52
1:B:1885:PRO:O	1:B:1888:ASP:N	2.42	0.52
1:B:2031:LEU:CB	1:B:2033:ASP:HB2	2.37	0.52
1:B:2365:ASN:ND2	1:B:2382:VAL:HG11	2.24	0.52
1:B:2803:ILE:O	1:B:2805:ALA:N	2.43	0.52
1:B:2942:ILE:HG22	1:B:2943:PHE:CD1	2.45	0.52
1:B:3280:TYR:O	1:B:3283:LEU:HB3	2.09	0.52
1:B:3575:LEU:HG	1:B:3687:MSE:CG	2.36	0.52
1:B:3649:SER:HA	1:B:3652:LEU:HG	1.92	0.52
1:B:552:SER:O	1:B:556:SER:HB2	2.09	0.52
1:A:1733:THR:OG1	1:A:1877:LEU:HD13	2.09	0.52
1:A:433:PRO:HB2	1:A:1812:LEU:HA	1.91	0.52
1:A:2125:TRP:CZ2	1:A:2128:PHE:HB2	2.45	0.52
1:A:2427:ARG:HD3	1:A:2436:LEU:HD11	1.91	0.52
1:A:2538:ARG:HH11	1:A:2565:MSE:HG3	1.74	0.52
1:A:3461:ALA:O	1:A:3464:LYS:N	2.43	0.52
1:A:3496:ILE:HG23	1:A:3499:ILE:HD11	1.91	0.52
1:A:3964:THR:O	1:A:3967:PHE:CD1	2.59	0.52
1:A:653:LEU:HD12	1:A:656:GLN:HG3	1.92	0.52
1:B:1412:LYS:O	1:B:1415:LEU:HB2	2.10	0.52
1:A:14:ARG:HE	1:A:2396:LEU:CD1	2.23	0.52
1:A:2289:ASP:O	1:A:2291:GLN:N	2.43	0.52
1:A:2886:GLN:CG	1:A:2887:PRO:HD3	2.39	0.52
1:A:3109:SER:O	1:A:3112:GLN:HB3	2.10	0.52
1:A:3398:PRO:HG2	1:A:3399:PRO:HD3	1.92	0.52
1:A:872:THR:O	1:A:876:SER:HB2	2.09	0.52
1:B:1006:THR:HA	1:B:1009:LEU:HD12	1.91	0.52
1:B:2361:ILE:HA	1:B:2364:LEU:HG	1.92	0.52
1:B:3475:TYR:O	1:B:3479:THR:HG22	2.09	0.52
1:B:358:GLU:O	1:B:361:ILE:HG12	2.10	0.52
1:B:3840:LYS:O	1:B:3844:THR:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:627:VAL:CG1	1:B:628:GLU:H	2.17	0.52
1:B:865:GLN:HB2	1:B:869:ASN:OD1	2.10	0.52
1:A:1070:PRO:O	1:A:1072:ALA:N	2.43	0.52
1:A:1574:ASN:CG	1:A:1582:LEU:HD21	2.30	0.52
1:A:1711:ARG:O	1:A:1715:GLU:HG3	2.10	0.52
1:A:181:LEU:CD1	1:A:189:MSE:HE2	2.39	0.52
1:A:3856:MSE:O	1:A:3859:TYR:OH	2.10	0.52
1:A:493:LYS:HB3	1:A:494:PRO:CD	2.39	0.52
1:A:611:ASN:C	1:A:614:PRO:HD2	2.30	0.52
1:B:2058:ASP:C	1:B:2061:PRO:HD2	2.30	0.52
1:B:2097:LEU:HD23	1:B:2100:LEU:HD22	1.90	0.52
1:B:2154:GLU:O	1:B:2157:PHE:HB2	2.10	0.52
1:B:2183:HIS:O	1:B:2187:VAL:CB	2.26	0.52
1:B:2199:LEU:HA	1:B:2202:PRO:HD2	1.92	0.52
1:B:2440:TYR:O	1:B:2443:MSE:HE2	2.10	0.52
1:B:3058:ASP:OD1	1:B:3060:SER:N	2.43	0.52
1:B:3277:VAL:HG23	1:B:3324:ARG:CD	2.40	0.52
1:B:3487:ILE:HA	1:B:3490:VAL:HG22	1.92	0.52
1:B:359:LEU:O	1:B:362:ALA:HB3	2.10	0.52
1:B:413:PHE:O	1:B:417:VAL:HG23	2.10	0.52
1:B:658:THR:O	1:B:661:PRO:HD2	2.09	0.52
1:B:805:LEU:HA	1:B:808:GLU:OE1	2.10	0.52
1:A:1014:LEU:HA	1:A:1025:LEU:HD13	1.91	0.51
1:A:1010:LEU:HB2	1:A:1028:PHE:CE1	2.44	0.51
1:A:111:CYS:HA	1:A:134:LEU:HD22	1.91	0.51
1:A:1632:TRP:HA	1:A:1635:LYS:HD2	1.91	0.51
1:A:3311:ASN:O	1:A:3313:SER:N	2.43	0.51
1:A:3333:THR:OG1	1:A:3385:LEU:HB3	2.10	0.51
1:A:3912:CYS:HB2	1:A:3984:MSE:HE2	1.91	0.51
1:A:655:LEU:HD12	1:A:658:THR:HB	1.91	0.51
1:B:1106:ILE:O	1:B:1109:GLU:HB3	2.11	0.51
1:B:1132:ASP:HA	1:B:1135:CYS:SG	2.50	0.51
1:B:1524:LEU:HD11	1:B:1592:MSE:HE3	1.92	0.51
1:B:1640:GLU:HG2	1:B:1691:GLN:HG2	1.92	0.51
1:B:1747:LEU:HD23	1:B:1750:LEU:HD12	1.92	0.51
1:B:1758:LEU:HD22	1:B:1759:LEU:HD22	1.92	0.51
1:B:1957:ASN:O	1:B:1961:PHE:N	2.43	0.51
1:B:2454:LEU:O	1:B:2457:PRO:HD2	2.10	0.51
1:B:2575:PRO:C	1:B:2576:MSE:HG3	2.31	0.51
1:B:2884:LEU:O	1:B:2887:PRO:HD2	2.10	0.51
1:B:3781:CYS:SG	1:B:3786:LEU:HB2	2.50	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2933:ILE:HG12	1:B:3979:LEU:O	2.10	0.51
1:A:1101:PHE:CG	1:A:1138:ILE:HG12	2.45	0.51
1:A:1330:TYR:O	1:A:1333:SER:OG	2.28	0.51
1:A:1590:THR:HG23	1:A:1591:LYS:N	2.25	0.51
1:A:2003:LYS:O	1:A:2007:ILE:HG13	2.11	0.51
1:A:2185:MSE:O	1:A:2189:ILE:HG12	2.11	0.51
1:A:2298:GLU:HB3	1:A:2301:GLN:HB3	1.92	0.51
1:A:2379:MSE:HE3	1:A:2383:PHE:HD1	1.75	0.51
1:A:3462:ARG:HH21	1:A:3501:HIS:CD2	2.28	0.51
1:A:3505:LEU:O	1:A:3510:GLN:HB2	2.11	0.51
1:A:3516:HIS:CG	1:A:3517:SER:N	2.77	0.51
1:A:3585:PHE:CE2	1:A:3613:MSE:SE	3.13	0.51
1:A:3631:LYS:HD2	1:A:3682:GLU:HG2	1.91	0.51
1:A:3659:PHE:CD1	1:A:3662:ILE:HD12	2.45	0.51
1:A:3705:TYR:HD2	1:A:3792:SER:HB2	1.74	0.51
1:A:4088:ASN:OD1	1:A:4091:ALA:HB3	2.09	0.51
1:A:557:SER:O	1:A:560:LEU:N	2.42	0.51
1:A:760:LEU:HD11	1:A:799:TYR:HB2	1.92	0.51
1:A:939:MSE:CE	1:A:942:LEU:HD13	2.40	0.51
1:B:1213:LYS:O	1:B:1215:GLU:N	2.43	0.51
1:B:1263:ALA:O	1:B:1267:TYR:HD1	1.94	0.51
1:B:1905:ILE:HG12	1:B:1951:VAL:HG11	1.92	0.51
1:B:2177:ASN:HB3	1:B:2182:ILE:N	2.24	0.51
1:B:2307:MSE:HB3	1:B:2348:GLN:NE2	2.17	0.51
1:B:2374:LEU:HD13	1:B:2377:ARG:HB2	1.91	0.51
1:B:276:ALA:HB2	1:B:318:SER:OG	2.10	0.51
1:B:2796:ALA:O	1:B:2800:ARG:HG3	2.10	0.51
1:B:3343:SER:O	1:B:3345:PRO:HD3	2.10	0.51
1:B:613:HIS:CE1	1:B:614:PRO:HD3	2.45	0.51
1:B:886:TRP:HZ3	1:B:954:GLY:O	1.93	0.51
1:A:127:ALA:O	1:A:131:LEU:HB2	2.11	0.51
1:A:1376:LEU:HD23	1:A:1376:LEU:H	1.75	0.51
1:A:135:LEU:CD2	1:A:173:LYS:HD2	2.40	0.51
1:A:1970:LYS:NZ	1:A:2017:GLY:HA3	2.24	0.51
1:A:21:ALA:O	1:A:24:ARG:HB2	2.11	0.51
1:A:352:VAL:HB	1:A:357:LYS:HG2	1.92	0.51
1:A:3909:ALA:HB2	1:A:3980:MSE:HE3	1.92	0.51
1:A:576:VAL:HG13	1:A:601:TRP:HE3	1.76	0.51
1:A:17:GLU:OE2	1:A:61:ARG:NH1	2.43	0.51
1:A:649:PHE:HE1	1:A:653:LEU:H	1.57	0.51
1:A:659:ARG:HH22	1:A:662:LEU:CG	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:681:LYS:HD2	1:A:746:ARG:HE	1.75	0.51
1:B:1029:CYS:CB	1:B:1085:ILE:HG13	2.36	0.51
1:B:1275:THR:HA	1:B:1279:LEU:CB	2.41	0.51
1:B:1579:VAL:HG12	1:B:1635:LYS:HG2	1.91	0.51
1:B:208:MSE:SE	1:B:220:LEU:HD21	2.61	0.51
1:B:2874:ALA:O	1:B:2877:SER:N	2.44	0.51
1:B:3107:ILE:HG23	1:B:3110:PHE:CZ	2.45	0.51
1:B:384:MSE:O	1:B:385:TYR:HB3	2.11	0.51
1:B:649:PHE:O	1:B:651:TYR:N	2.43	0.51
1:A:1072:ALA:HB1	1:A:1076:LEU:HD11	1.92	0.51
1:A:1266:CYS:O	1:A:1269:THR:OG1	2.25	0.51
1:A:1750:LEU:O	1:A:1754:GLN:HG3	2.10	0.51
1:A:2203:THR:O	1:A:2208:ASP:N	2.43	0.51
1:A:2452:ARG:HG2	1:A:2498:ILE:CD1	2.40	0.51
1:A:2450:GLU:O	1:A:2454:LEU:HG	2.11	0.51
1:A:266:ALA:CB	1:A:308:LEU:HG	2.41	0.51
1:A:3283:LEU:HD21	1:A:3297:VAL:HG22	1.92	0.51
1:A:3772:ASN:HB3	1:A:3788:LEU:H	1.74	0.51
1:A:906:PHE:O	1:A:909:VAL:N	2.35	0.51
1:B:111:CYS:O	1:B:134:LEU:HD13	2.10	0.51
1:B:1298:LEU:O	1:B:1302:ALA:HB2	2.10	0.51
1:B:2436:LEU:O	1:B:2439:ILE:HG22	2.10	0.51
1:B:2957:LEU:CB	1:B:3989:ARG:HH22	2.22	0.51
1:B:3493:TRP:NE1	1:B:3708:ARG:O	2.40	0.51
1:B:3794:VAL:HB	1:B:3802:LEU:H	1.76	0.51
1:B:3967:PHE:O	1:B:3970:LEU:HD23	2.10	0.51
1:B:4013:TRP:CZ3	1:B:4014:LYS:HB2	2.45	0.51
1:A:1503:LEU:O	1:A:1507:CYS:HB3	2.11	0.51
1:A:3588:TRP:HD1	1:A:3612:ARG:HD2	1.75	0.51
1:A:4019:LYS:HA	1:A:4019:LYS:HE2	1.93	0.51
1:A:413:PHE:O	1:A:417:VAL:HG23	2.11	0.51
1:A:863:GLY:HA2	1:A:866:ILE:HD11	1.91	0.51
1:B:1405:ALA:O	1:B:1410:PRO:HD3	2.10	0.51
1:B:1970:LYS:CE	1:B:2017:GLY:HA3	2.40	0.51
1:B:2094:MSE:SE	1:B:2143:ARG:HG3	2.60	0.51
1:B:2355:THR:O	1:B:2356:MSE:HG3	2.11	0.51
1:B:407:VAL:O	1:B:411:PRO:HD3	2.10	0.51
1:B:941:MSE:HE3	1:B:958:MSE:CG	2.40	0.51
1:A:1465:HIS:HA	1:A:1469:PRO:CD	2.41	0.51
1:A:2037:SER:O	1:A:2041:SER:HB3	2.10	0.51
1:A:2114:GLU:HG3	1:A:2116:ASP:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2224:PHE:HZ	1:A:2276:LEU:HD22	1.73	0.51
1:A:3147:LYS:O	1:A:3151:LEU:HG	2.10	0.51
1:A:3189:PHE:O	1:A:3193:ILE:HB	2.10	0.51
1:A:3813:LYS:HB3	1:A:3925:LEU:HG	1.93	0.51
1:A:4062:ASP:HB3	1:A:4078:VAL:HG21	1.93	0.51
1:A:543:SER:C	1:A:545:LEU:N	2.63	0.51
1:A:609:ALA:HB2	1:A:1800:SER:OG	2.11	0.51
1:A:619:ASP:O	1:A:621:SER:N	2.44	0.51
1:B:1266:CYS:HA	1:B:1344:PHE:CE1	2.46	0.51
1:B:1879:VAL:C	1:B:1882:SER:H	2.14	0.51
1:B:3134:ALA:O	1:B:3138:ILE:HG12	2.11	0.51
1:B:3298:LEU:HD11	1:B:3351:ILE:HD13	1.93	0.51
1:B:3525:TYR:CZ	1:B:3533:PHE:HE1	2.29	0.51
1:B:3954:PRO:HB2	1:B:4027:TRP:CD1	2.45	0.51
1:B:511:SER:HB2	1:B:515:ARG:HG2	1.93	0.51
1:A:1378:GLU:O	1:A:1382:ILE:HG12	2.11	0.51
1:A:1865:THR:HA	1:A:1868:THR:OG1	2.10	0.51
1:A:1876:ILE:O	1:A:1876:ILE:HG12	2.11	0.51
1:A:1993:GLU:O	1:A:1997:PRO:HD2	2.10	0.51
1:A:19:LEU:HD22	1:A:30:ALA:HB1	1.93	0.51
1:A:3173:MSE:HG2	1:A:3174:ASP:OD1	2.11	0.51
1:A:3173:MSE:HB3	1:A:3175:PRO:HD2	1.93	0.51
1:A:3518:VAL:O	1:A:3522:THR:OG1	2.10	0.51
1:A:514:VAL:HG11	1:A:610:ALA:O	2.10	0.51
1:A:917:LEU:HD22	1:A:969:LEU:HG	1.93	0.51
1:A:969:LEU:O	1:A:973:ALA:HB2	2.10	0.51
1:B:153:PHE:O	1:B:157:TYR:HD2	1.94	0.51
1:B:1975:LEU:HA	1:B:1976:LEU:HB3	1.91	0.51
1:B:3142:ILE:O	1:B:3145:ILE:HG22	2.11	0.51
1:B:3451:LEU:HD21	1:B:3483:MSE:HG2	1.93	0.51
1:B:3583:LEU:O	1:B:3587:ASP:CB	2.58	0.51
1:B:887:ASP:O	1:B:3889:ARG:HB3	2.11	0.51
1:B:798:GLY:HA2	1:B:873:VAL:CG1	2.41	0.51
1:A:1073:PHE:CD1	1:A:1074:LYS:N	2.76	0.51
1:A:1894:SER:C	1:A:1896:ILE:N	2.64	0.51
1:A:2952:ILE:O	1:A:2955:SER:OG	2.18	0.51
1:A:3044:MSE:HE3	1:A:3060:SER:OG	2.11	0.51
1:A:3354:ASP:O	1:A:3357:ARG:HB2	2.11	0.51
1:A:371:GLY:O	1:A:375:VAL:N	2.44	0.51
1:A:3780:ALA:HB1	1:A:3784:ARG:NH1	2.26	0.51
1:A:3954:PRO:CG	1:A:4027:TRP:HA	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:LEU:C	1:A:423:TYR:H	2.13	0.51
1:A:901:MSE:HG2	1:A:2819:GLU:HG2	1.92	0.51
1:A:968:VAL:HA	1:A:971:ARG:HG2	1.93	0.51
1:B:1729:PHE:H	1:B:1730:PRO:HD2	1.75	0.51
1:B:19:LEU:HB2	1:B:34:LEU:HD22	1.92	0.51
1:B:2038:GLU:HB3	1:B:2076:VAL:HG21	1.93	0.51
1:B:2365:ASN:HB2	1:B:2400:VAL:HG13	1.93	0.51
1:B:2470:ARG:HB3	1:B:2474:TYR:CE2	2.45	0.51
1:B:273:ARG:HE	1:B:314:SER:HB3	1.76	0.51
1:B:2923:TRP:HD1	1:B:2926:LEU:HD21	1.76	0.51
1:B:3448:GLU:HA	1:B:3451:LEU:HD22	1.91	0.51
1:B:3450:MSE:HG2	1:B:3464:LYS:HG2	1.93	0.51
1:B:3723:ASP:HB2	1:B:3741:ARG:NE	2.26	0.51
1:B:981:ARG:HG2	1:B:982:GLN:N	2.26	0.51
1:A:2274:ILE:HD11	1:A:2314:GLU:HB3	1.92	0.51
1:A:2375:ALA:HB1	1:A:2411:LEU:HD22	1.93	0.51
1:A:2936:TYR:O	1:A:2940:ARG:CB	2.58	0.51
1:A:3705:TYR:CD2	1:A:3792:SER:HB2	2.46	0.51
1:A:3905:ALA:O	1:A:3908:HIS:N	2.44	0.51
1:A:479:ILE:O	1:A:483:VAL:HG13	2.11	0.51
1:A:963:LYS:HB3	1:A:1009:LEU:HD11	1.93	0.51
1:B:1132:ASP:O	1:B:1135:CYS:N	2.44	0.51
1:B:125:ILE:H	1:B:126:PRO:CD	2.24	0.51
1:B:1700:THR:O	1:B:1702:LEU:N	2.44	0.51
1:B:178:LEU:HB3	1:B:197:PHE:HZ	1.75	0.51
1:B:287:LEU:C	1:B:291:VAL:HB	2.30	0.51
1:B:2928:LYS:HD2	1:B:3783:GLN:HB3	1.93	0.51
1:B:306:VAL:HG23	1:B:308:LEU:H	1.75	0.51
1:B:3696:ARG:O	1:B:3699:LEU:HB2	2.11	0.51
1:B:3751:LEU:HD13	1:B:3805:TRP:HB2	1.92	0.51
1:B:3883:LEU:HG	1:B:3970:LEU:HD13	1.93	0.51
1:B:3989:ARG:HH21	1:B:4100:GLU:CB	2.24	0.51
1:B:714:VAL:CG1	1:B:734:LEU:HD21	2.41	0.51
1:B:83:GLU:HG3	1:B:130:LEU:HD13	1.91	0.51
1:B:913:ARG:HE	1:B:916:GLU:CD	2.14	0.51
1:A:1004:GLN:O	1:A:1008:ALA:HB2	2.11	0.51
1:A:100:ILE:O	1:A:104:SER:N	2.44	0.51
1:A:2205:VAL:HB	1:A:2206:PRO:HD3	1.92	0.51
1:A:2356:MSE:SE	1:A:2360:PHE:CZ	3.14	0.51
1:A:273:ARG:HG3	1:A:274:LEU:H	1.76	0.51
1:A:3614:TYR:CE1	1:A:3618:GLY:HA3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:MSE:HG2	1:A:541:MSE:H	1.76	0.51
1:A:743:LEU:HD22	1:A:746:ARG:HH12	1.76	0.51
1:A:877:ASP:O	1:A:879:MSE:N	2.44	0.51
1:B:716:VAL:HG11	1:B:1121:LEU:HD13	1.93	0.51
1:B:1122:GLY:O	1:B:1123:THR:OG1	2.23	0.51
1:B:2495:SER:O	1:B:2498:ILE:HB	2.10	0.51
1:B:2890:ILE:HG21	1:B:2922:ARG:HH12	1.76	0.51
1:B:2943:PHE:O	1:B:2945:SER:N	2.41	0.51
1:B:3518:VAL:HG13	1:B:3554:PHE:CZ	2.46	0.51
1:B:3572:ILE:HA	1:B:3575:LEU:HB3	1.93	0.51
1:B:3568:ILE:HD11	1:B:3691:LYS:CD	2.41	0.51
1:B:3901:ARG:HG2	1:B:3901:ARG:HH11	1.75	0.51
1:B:4077:TYR:OH	1:B:4119:ARG:HG2	2.11	0.51
1:B:538:ASP:CB	1:B:627:VAL:HG13	2.39	0.51
1:B:63:PHE:CD1	1:B:89:LEU:HD13	2.46	0.51
1:B:947:GLN:C	1:B:949:PRO:HD3	2.32	0.51
1:A:1342:MSE:HE2	1:A:1398:VAL:HG12	1.93	0.50
1:A:1347:THR:O	1:A:1351:THR:OG1	2.27	0.50
1:A:1472:SER:HA	1:A:1476:HIS:CD2	2.46	0.50
1:A:1521:PHE:O	1:A:1524:LEU:HB2	2.11	0.50
1:A:2323:LEU:HD11	1:A:2345:VAL:HG21	1.93	0.50
1:A:2464:HIS:H	1:A:2465:PRO:CD	2.24	0.50
1:A:2443:MSE:SE	1:A:2480:ILE:HG21	2.61	0.50
1:A:2501:LEU:O	1:A:2505:VAL:HG23	2.10	0.50
1:A:2884:LEU:C	1:A:2887:PRO:HD2	2.32	0.50
1:A:3167:ARG:HG2	1:A:3186:ARG:NE	2.26	0.50
1:A:3280:TYR:CZ	1:A:3304:VAL:HG23	2.46	0.50
1:A:3979:LEU:CA	1:A:3981:TYR:HB3	2.39	0.50
1:A:4038:TRP:CH2	1:A:4040:PRO:HB3	2.46	0.50
1:A:406:ARG:O	1:A:409:GLN:N	2.27	0.50
1:A:575:ILE:HD11	1:A:579:LEU:HD22	1.93	0.50
1:A:84:GLU:O	1:A:88:PHE:HD1	1.94	0.50
1:A:87:LYS:HG2	1:A:133:LYS:CG	2.38	0.50
1:B:2152:ASN:CB	1:B:2153:THR:HA	2.36	0.50
1:B:217:LEU:O	1:B:221:ALA:HB2	2.10	0.50
1:B:2204:GLY:HA2	1:B:2208:ASP:OD2	2.12	0.50
1:B:3487:ILE:CG2	1:B:3495:PHE:HB2	2.37	0.50
1:B:3505:LEU:HD12	1:B:3509:ASP:HB3	1.91	0.50
1:B:2928:LYS:HG3	1:B:3783:GLN:O	2.11	0.50
1:B:3820:MSE:HB2	1:B:3882:LEU:HD13	1.94	0.50
1:B:3915:HIS:ND1	1:B:3920:ILE:HD12	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:886:TRP:CD1	1:B:889:GLU:N	2.69	0.50
1:B:928:VAL:O	1:B:932:GLU:HB2	2.11	0.50
1:B:929:ALA:O	1:B:933:LEU:HB2	2.11	0.50
1:A:1017:ILE:HG23	1:A:1018:VAL:HG13	1.92	0.50
1:A:1063:LEU:O	1:A:1066:LEU:HB3	2.11	0.50
1:A:1584:GLN:O	1:A:1588:ASP:OD1	2.29	0.50
1:A:1789:GLY:O	1:A:1793:THR:HG23	2.12	0.50
1:A:3011:LEU:HB3	1:A:3047:SER:HB3	1.94	0.50
1:A:3768:PHE:O	1:A:3771:MSE:N	2.44	0.50
1:A:3981:TYR:CE1	1:A:4104:VAL:HB	2.46	0.50
1:A:489:ARG:O	1:A:489:ARG:CZ	2.59	0.50
1:B:1376:LEU:HG	1:B:1377:CYS:N	2.26	0.50
1:B:1596:VAL:O	1:B:1600:MSE:HG3	2.11	0.50
1:B:2031:LEU:C	1:B:2033:ASP:N	2.64	0.50
1:B:2390:HIS:ND1	1:B:2397:CYS:SG	2.74	0.50
1:B:2462:VAL:CB	1:B:2473:MSE:SE	3.09	0.50
1:B:2935:GLU:O	1:B:2939:LEU:HG	2.10	0.50
1:B:348:ILE:HG23	1:B:357:LYS:HG3	1.93	0.50
1:B:3705:TYR:HE2	1:B:3708:ARG:HH12	1.60	0.50
1:B:3762:GLN:OE1	1:B:3795:PRO:HG3	2.11	0.50
1:B:390:GLN:O	1:B:393:LYS:HG2	2.11	0.50
1:B:411:PRO:O	1:B:415:GLN:HB2	2.12	0.50
1:B:419:SER:HA	1:B:422:LEU:HG	1.94	0.50
1:B:743:LEU:O	1:B:746:ARG:HG2	2.11	0.50
1:B:796:LEU:HD22	1:B:799:TYR:HE2	1.76	0.50
1:A:1042:LYS:HZ1	1:A:1044:ILE:HD12	1.76	0.50
1:A:1350:ASN:ND2	1:A:1404:LYS:HG2	2.27	0.50
1:A:1698:PHE:CD1	1:A:1699:PHE:N	2.79	0.50
1:A:173:LYS:HA	1:A:176:GLU:OE1	2.11	0.50
1:A:1815:THR:C	1:A:1816:ARG:HE	2.14	0.50
1:A:2095:ALA:HB3	1:A:2096:PRO:HD3	1.92	0.50
1:A:2190:VAL:HA	1:A:2193:ILE:HG22	1.93	0.50
1:A:2216:LEU:O	1:A:2220:MSE:HG3	2.11	0.50
1:A:2254:ARG:HG3	1:A:2255:LEU:N	2.27	0.50
1:A:2339:GLU:O	1:A:2343:GLU:HG3	2.10	0.50
1:A:237:SER:O	1:A:278:HIS:HB3	2.10	0.50
1:A:3007:GLU:OE2	1:A:3046:ARG:HD3	2.10	0.50
1:A:3108:GLN:HA	1:A:3111:MSE:HG3	1.94	0.50
1:A:3780:ALA:HB1	1:A:3784:ARG:HH12	1.77	0.50
1:A:703:CYS:O	1:A:706:LEU:HB2	2.11	0.50
1:B:1036:PHE:CZ	1:B:1082:PHE:HE2	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1076:LEU:HD11	1:B:1114:ALA:HB1	1.93	0.50
1:B:1238:GLN:HB2	1:B:1239:PRO:HD3	1.94	0.50
1:B:1469:PRO:HA	1:B:1472:SER:CB	2.38	0.50
1:B:2088:LEU:O	1:B:2092:GLU:N	2.43	0.50
1:B:2145:PHE:CE1	1:B:2188:GLU:HB3	2.47	0.50
1:B:3072:GLU:HG3	1:B:3080:LEU:HD11	1.94	0.50
1:B:3789:ARG:NH2	1:B:3806:LEU:HD22	2.26	0.50
1:B:410:MSE:HE1	1:B:445:SER:CB	2.42	0.50
1:A:1265:GLU:O	1:A:1269:THR:HG23	2.10	0.50
1:A:1751:GLU:HG2	1:A:1870:LYS:CE	2.39	0.50
1:A:1856:THR:O	1:A:1860:GLU:HB2	2.12	0.50
1:A:1882:SER:C	1:A:1885:PRO:HD2	2.32	0.50
1:A:2000:ARG:HG2	1:A:2001:LYS:HG3	1.92	0.50
1:A:2097:LEU:HD13	1:A:2143:ARG:HG2	1.93	0.50
1:A:2379:MSE:O	1:A:2383:PHE:HB2	2.11	0.50
1:A:2386:LEU:HD11	1:A:2400:VAL:HG12	1.94	0.50
1:A:232:CYS:SG	1:A:274:LEU:HD13	2.51	0.50
1:A:2956:ALA:HA	1:A:2965:TYR:OH	2.11	0.50
1:A:367:GLY:C	1:A:369:PHE:N	2.64	0.50
1:A:568:PHE:CZ	1:A:653:LEU:HG	2.47	0.50
1:A:767:GLU:O	1:A:771:ASN:HB2	2.10	0.50
1:A:964:ARG:N	1:A:1009:LEU:HD13	2.26	0.50
1:B:1162:SER:N	1:B:1165:LEU:HD12	2.20	0.50
1:B:1220:LEU:HD13	1:B:1274:ARG:CG	2.41	0.50
1:B:1503:LEU:O	1:B:1507:CYS:HB3	2.11	0.50
1:B:1956:PHE:HB3	1:B:1998:MSE:HE1	1.93	0.50
1:B:2129:LEU:HD13	1:B:2156:VAL:HG13	1.93	0.50
1:B:2220:MSE:SE	1:B:2256:ILE:CD1	3.10	0.50
1:B:3962:ARG:HD3	1:B:4124:TRP:CE3	2.46	0.50
1:B:554:ASN:O	1:B:557:SER:HB2	2.11	0.50
1:B:852:ARG:CZ	1:B:3111:MSE:SE	3.09	0.50
1:A:1102:GLU:O	1:A:1105:VAL:HG22	2.12	0.50
1:A:1107:TYR:HE1	1:A:1111:LEU:HD13	1.75	0.50
1:A:1678:LEU:O	1:A:1682:THR:HG22	2.12	0.50
1:A:1922:ALA:HA	1:A:1925:GLU:OE2	2.11	0.50
1:A:1886:LYS:NZ	1:A:1924:THR:HB	2.23	0.50
1:A:3593:ARG:HD2	1:A:3660:ASN:O	2.12	0.50
1:A:3763:ARG:O	1:A:3767:LEU:HB2	2.12	0.50
1:A:3901:ARG:HG2	1:A:3901:ARG:NH1	2.26	0.50
1:A:3962:ARG:HD3	1:A:4124:TRP:CE3	2.47	0.50
1:A:3981:TYR:O	1:A:3985:VAL:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:LEU:O	1:A:490:ILE:HG22	2.11	0.50
1:B:1039:TRP:HH2	1:B:1052:SER:HB3	1.76	0.50
1:B:1101:PHE:O	1:B:1104:LEU:HB2	2.12	0.50
1:B:3151:LEU:O	1:B:3156:PRO:HD3	2.11	0.50
1:B:3810:VAL:HG23	1:B:3815:LEU:HD11	1.93	0.50
1:B:385:TYR:CD1	1:B:420:VAL:HG13	2.40	0.50
1:B:527:TYR:CE1	1:B:615:ALA:HA	2.46	0.50
1:B:67:VAL:O	1:B:71:LYS:CB	2.41	0.50
1:A:1502:SER:O	1:A:1505:LEU:N	2.43	0.50
1:A:175:TYR:OH	1:A:204:LEU:HD11	2.10	0.50
1:A:2166:SER:O	1:A:2170:GLN:HB3	2.12	0.50
1:A:288:ASP:N	1:A:288:ASP:OD1	2.43	0.50
1:A:3674:SER:O	1:A:3677:PRO:HD2	2.12	0.50
1:A:4007:LYS:CG	1:A:4041:ARG:HD2	2.35	0.50
1:A:801:LYS:O	1:A:805:LEU:HB2	2.11	0.50
1:A:85:ILE:O	1:A:89:LEU:HG	2.10	0.50
1:A:913:ARG:HB2	1:A:934:LEU:HD12	1.93	0.50
1:A:954:GLY:O	1:A:957:PRO:HD2	2.12	0.50
1:B:1406:LEU:O	1:B:1415:LEU:HD21	2.12	0.50
1:B:1406:LEU:HA	1:B:1410:PRO:HG3	1.94	0.50
1:B:2352:HIS:CD2	1:B:2364:LEU:HD21	2.47	0.50
1:B:2430:GLU:OE1	1:B:2433:LYS:HE3	2.11	0.50
1:B:2936:TYR:CZ	1:B:2940:ARG:HD2	2.47	0.50
1:B:3648:GLY:O	1:B:3651:LEU:HB2	2.11	0.50
1:B:3766:GLN:O	1:B:3770:VAL:HG23	2.11	0.50
1:B:512:GLY:CA	1:B:602:MSE:HG3	2.40	0.50
1:B:68:PHE:O	1:B:72:SER:OG	2.10	0.50
1:B:722:LYS:HB3	1:B:727:ALA:CA	2.42	0.50
1:B:734:LEU:C	1:B:737:PRO:HD2	2.32	0.50
1:A:1036:PHE:CZ	1:A:1082:PHE:HE2	2.30	0.50
1:A:1741:ASP:O	1:A:1745:LYS:HG3	2.11	0.50
1:A:2318:ALA:O	1:A:2322:VAL:HB	2.12	0.50
1:A:3049:LEU:HA	1:A:3188:PHE:CZ	2.46	0.50
1:A:334:HIS:O	1:A:338:LEU:HD11	2.12	0.50
1:A:3525:TYR:CZ	1:A:3533:PHE:HE1	2.30	0.50
1:A:3998:LEU:O	1:A:4001:THR:OG1	2.28	0.50
1:A:676:ASN:O	1:A:680:ILE:HG13	2.11	0.50
1:A:743:LEU:HG	1:A:783:HIS:CE1	2.44	0.50
1:A:66:LEU:CD2	1:A:89:LEU:HD11	2.42	0.50
1:B:1357:LYS:HG3	1:B:1360:LYS:NZ	2.26	0.50
1:B:152:LEU:O	1:B:156:PHE:HD1	1.95	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1696:LEU:HD23	1:B:1700:THR:HG21	1.92	0.50
1:B:1756:PRO:O	1:B:1758:LEU:N	2.34	0.50
1:B:1894:SER:O	1:B:1896:ILE:N	2.44	0.50
1:B:1972:GLU:CD	1:B:1987:ARG:HH12	2.14	0.50
1:B:2320:ALA:HB1	1:B:2370:SER:OG	2.10	0.50
1:B:2389:PHE:CD2	1:B:2396:LEU:HD22	2.46	0.50
1:B:2536:LEU:O	1:B:2539:LEU:HB2	2.11	0.50
1:B:3726:VAL:HG21	1:B:3736:LYS:HD3	1.93	0.50
1:B:368:LEU:HA	1:B:372:PRO:HG2	1.94	0.50
1:B:4066:LEU:HD23	1:B:4075:ARG:HG3	1.94	0.50
1:B:888:ARG:HA	1:B:907:LEU:HD21	1.94	0.50
1:A:1086:TYR:HD2	1:A:1090:ARG:HG2	1.76	0.50
1:A:1106:ILE:O	1:A:1109:GLU:HB3	2.12	0.50
1:A:1298:LEU:HA	1:A:1301:ILE:HB	1.94	0.50
1:A:1433:ALA:O	1:A:1437:TYR:CD2	2.65	0.50
1:A:1604:SER:HA	1:A:1632:TRP:CE3	2.47	0.50
1:A:1956:PHE:HB3	1:A:1998:MSE:CE	2.41	0.50
1:A:2512:ASP:H	1:A:2519:LEU:HD12	1.76	0.50
1:A:2814:SER:O	1:A:2818:LYS:HB2	2.11	0.50
1:A:293:LEU:O	1:A:296:VAL:HG12	2.12	0.50
1:A:3464:LYS:O	1:A:3467:ARG:HB3	2.12	0.50
1:A:3498:TRP:HD1	1:A:3498:TRP:O	1.95	0.50
1:A:3789:ARG:CZ	1:A:3806:LEU:HD22	2.40	0.50
1:A:4066:LEU:HD21	1:A:4078:VAL:HG21	1.94	0.50
1:A:741:ILE:O	1:A:743:LEU:N	2.45	0.50
1:A:969:LEU:O	1:A:973:ALA:CB	2.60	0.50
1:B:1074:LYS:O	1:B:1075:ARG:HG3	2.12	0.50
1:B:1586:SER:HB3	1:B:1643:MSE:HE1	1.94	0.50
1:B:1736:PHE:O	1:B:1740:VAL:HG23	2.11	0.50
1:B:1816:ARG:HB3	1:B:1819:PHE:CE1	2.45	0.50
1:B:2080:VAL:HG12	1:B:2081:LEU:H	1.75	0.50
1:B:2212:ALA:O	1:B:2215:LEU:N	2.44	0.50
1:B:175:TYR:HD2	1:B:222:GLY:HA3	1.76	0.50
1:B:898:PHE:CE2	1:B:2566:THR:HG21	2.47	0.50
1:B:2879:GLY:HA2	1:B:2886:GLN:CG	2.29	0.50
1:B:2960:GLU:O	1:B:2965:TYR:CD1	2.65	0.50
1:B:2964:ASP:O	1:B:2968:ALA:HB2	2.12	0.50
1:B:3179:TRP:CZ2	1:B:3258:LEU:HG	2.47	0.50
1:B:3383:GLN:HG3	1:B:3438:GLU:OE2	2.12	0.50
1:B:3510:GLN:O	1:B:3512:VAL:N	2.34	0.50
1:B:3572:ILE:HD13	1:B:3575:LEU:HD22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:966:PHE:CE2	1:B:988:VAL:HG12	2.47	0.50
1:A:1655:ILE:CD1	1:A:1681:ASP:HB3	2.40	0.50
1:A:1747:LEU:O	1:A:1750:LEU:N	2.41	0.50
1:A:1935:GLU:HB2	1:A:1986:ARG:NH2	2.27	0.50
1:A:2171:LEU:CG	1:A:2177:ASN:HD21	2.25	0.50
1:A:2416:LYS:O	1:A:2420:PHE:HB3	2.12	0.50
1:A:2538:ARG:HH22	1:A:2566:THR:CG2	2.25	0.50
1:A:3495:PHE:CZ	1:A:3521:ILE:HG13	2.47	0.50
1:A:3865:THR:O	1:A:3869:THR:OG1	2.14	0.50
1:A:629:PHE:HA	1:A:634:LEU:HD21	1.91	0.50
1:B:1299:GLU:OE2	1:B:1367:HIS:HB2	2.12	0.50
1:B:12:LEU:HD13	1:B:42:CYS:SG	2.52	0.50
1:B:1348:LEU:O	1:B:1352:SER:N	2.34	0.50
1:B:1455:CYS:O	1:B:1458:LEU:HB2	2.11	0.50
1:B:1882:SER:C	1:B:1885:PRO:HD2	2.33	0.50
1:B:2922:ARG:HD3	1:B:2930:TYR:HD1	1.77	0.50
1:B:3141:PHE:CZ	1:B:3192:LYS:HB2	2.47	0.50
1:B:3277:VAL:HG23	1:B:3324:ARG:HD2	1.94	0.50
1:B:3507:ASP:CG	1:B:3540:TYR:HA	2.32	0.50
1:B:3503:VAL:HG21	1:B:3535:ILE:O	2.12	0.50
1:A:1014:LEU:HB2	1:A:1078:ALA:CB	2.41	0.49
1:A:2135:ASN:N	1:A:2136:PRO:CD	2.75	0.49
1:A:2196:TRP:HE1	1:A:2200:ALA:HB2	1.77	0.49
1:A:232:CYS:HG	1:A:275:PHE:HE1	1.60	0.49
1:A:2373:PRO:HA	1:A:2378:PHE:HZ	1.77	0.49
1:A:242:PRO:HD3	1:A:282:PHE:CD2	2.47	0.49
1:A:3397:GLN:HB3	1:A:3398:PRO:CD	2.42	0.49
1:A:3989:ARG:HH21	1:A:4100:GLU:HB2	1.77	0.49
1:A:4090:ARG:NH1	1:A:4106:CYS:HA	2.20	0.49
1:A:569:VAL:HG13	1:A:570:LYS:H	1.77	0.49
1:B:1553:PHE:O	1:B:1557:GLU:HB2	2.12	0.49
1:B:2157:PHE:O	1:B:2160:TYR:N	2.45	0.49
1:B:2373:PRO:HB3	1:B:2407:GLY:O	2.11	0.49
1:B:2485:ARG:HH11	1:B:2530:ARG:CZ	2.25	0.49
1:B:294:PHE:CZ	1:B:319:PHE:CD2	2.96	0.49
1:B:2939:LEU:HD21	1:B:2994:TRP:CE2	2.47	0.49
1:B:3484:THR:HA	1:B:3516:HIS:HE2	1.77	0.49
1:B:2957:LEU:CA	1:B:3989:ARG:HH22	2.24	0.49
1:B:3858:MSE:HG3	1:B:4119:ARG:NE	2.27	0.49
1:B:428:PRO:HB3	1:B:1679:LEU:HD13	1.94	0.49
1:B:661:PRO:HG2	1:B:733:LEU:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1905:ILE:HG23	1:A:1951:VAL:HG21	1.94	0.49
1:A:2066:PHE:HB3	1:A:2067:ARG:CG	2.41	0.49
1:A:2168:LEU:HD13	1:A:2214:ARG:NE	2.27	0.49
1:A:2177:ASN:ND2	1:A:2182:ILE:HA	2.28	0.49
1:A:2255:LEU:HA	1:A:2258:GLU:HB2	1.94	0.49
1:A:2936:TYR:HB3	1:A:3979:LEU:CD1	2.41	0.49
1:A:3531:TYR:HB3	1:A:3532:PRO:HD3	1.93	0.49
1:A:3578:LEU:HD11	1:A:3686:TRP:HZ3	1.77	0.49
1:A:455:LEU:HD13	1:A:459:ARG:CZ	2.42	0.49
1:A:476:ARG:HA	1:A:479:ILE:HD12	1.93	0.49
1:A:617:PRO:HB3	1:A:659:ARG:CG	2.41	0.49
1:A:63:PHE:O	1:A:66:LEU:HG	2.13	0.49
1:A:730:LEU:O	1:A:734:LEU:HG	2.12	0.49
1:B:114:VAL:HG12	1:B:130:LEU:HD21	1.94	0.49
1:B:1927:MSE:C	1:B:1929:GLY:H	2.15	0.49
1:B:1965:PHE:O	1:B:1968:SER:OG	2.18	0.49
1:B:2220:MSE:HB3	1:B:2224:PHE:CZ	2.47	0.49
1:B:2447:LYS:N	1:B:2448:PRO:HD2	2.28	0.49
1:B:2458:VAL:HA	1:B:2461:PHE:CD2	2.45	0.49
1:B:2961:ALA:HB1	1:B:3002:TYR:HB2	1.94	0.49
1:B:3272:TRP:CE3	1:B:3307:LEU:HD21	2.46	0.49
1:B:3280:TYR:CZ	1:B:3304:VAL:HG23	2.47	0.49
1:B:3774:ILE:HG22	1:B:3775:LEU:HD23	1.94	0.49
1:B:805:LEU:HD23	1:B:808:GLU:OE2	2.13	0.49
1:A:1119:LYS:NZ	1:A:1256:TRP:HZ2	2.10	0.49
1:A:1389:VAL:HG12	1:A:1389:VAL:O	2.12	0.49
1:A:1469:PRO:HA	1:A:1472:SER:CB	2.42	0.49
1:A:1574:ASN:CB	1:A:1582:LEU:HD21	2.40	0.49
1:A:2393:LEU:HD13	1:A:2426:HIS:CD2	2.46	0.49
1:A:282:PHE:CD1	1:A:283:SER:N	2.80	0.49
1:A:3005:LEU:O	1:A:3180:ASP:OD2	2.30	0.49
1:A:3012:GLU:HB2	1:A:3050:LYS:NZ	2.27	0.49
1:A:39:GLY:O	1:A:43:VAL:HG23	2.12	0.49
1:A:47:SER:N	1:A:51:LEU:HD12	2.27	0.49
1:A:884:VAL:HG22	1:A:888:ARG:HG2	1.93	0.49
1:A:965:THR:HA	1:A:968:VAL:CG1	2.42	0.49
1:A:986:PRO:O	1:A:990:GLN:HG2	2.12	0.49
1:B:1010:LEU:HD13	1:B:1028:PHE:CE1	2.28	0.49
1:B:1907:GLU:O	1:B:1911:LEU:HG	2.11	0.49
1:B:2328:ARG:O	1:B:2332:GLU:HG2	2.13	0.49
1:B:319:PHE:O	1:B:323:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3326:GLN:CB	1:B:3393:GLU:HG2	2.38	0.49
1:B:3493:TRP:CD1	1:B:3710:LYS:O	2.65	0.49
1:B:3923:ARG:HB3	1:B:3962:ARG:HH12	1.78	0.49
1:B:533:HIS:O	1:B:537:SER:HB3	2.13	0.49
1:B:941:MSE:HE3	1:B:958:MSE:HG3	1.95	0.49
1:A:1121:LEU:HG	1:A:1122:GLY:H	1.75	0.49
1:A:1491:ILE:N	1:A:1497:ARG:HH12	2.10	0.49
1:A:390:GLN:NE2	1:A:1723:PRO:HG2	2.28	0.49
1:A:1811:ARG:O	1:A:1815:THR:HG23	2.12	0.49
1:A:1751:GLU:OE2	1:A:1884:LEU:HD13	2.11	0.49
1:A:2280:VAL:HG13	1:A:2287:PRO:HB2	1.93	0.49
1:A:2420:PHE:CE1	1:A:2439:ILE:HG21	2.46	0.49
1:A:2927:ALA:HB2	1:A:3121:LEU:HD22	1.93	0.49
1:A:3174:ASP:N	1:A:3175:PRO:HD2	2.17	0.49
1:A:318:SER:O	1:A:321:LYS:HB2	2.12	0.49
1:A:3620:PRO:HB3	1:A:3633:ILE:HD12	1.94	0.49
1:A:481:THR:HG23	1:A:559:SER:OG	2.13	0.49
1:A:680:ILE:HG12	1:A:701:TYR:CE1	2.48	0.49
1:A:86:LEU:HD13	1:A:134:LEU:CD2	2.42	0.49
1:B:103:TYR:O	1:B:107:ILE:HG13	2.13	0.49
1:B:1086:TYR:CE2	1:B:1090:ARG:HG2	2.48	0.49
1:B:1139:GLU:HG3	1:B:1175:HIS:CD2	2.47	0.49
1:B:1702:LEU:O	1:B:1706:SER:CB	2.61	0.49
1:B:2193:ILE:HA	1:B:2196:TRP:CE2	2.48	0.49
1:B:2847:THR:HB	1:B:2850:PHE:CD2	2.47	0.49
1:B:3163:THR:OG1	1:B:3167:ARG:NH2	2.43	0.49
1:B:3323:PHE:CE1	1:B:3324:ARG:HG3	2.48	0.49
1:B:334:HIS:O	1:B:338:LEU:HD11	2.12	0.49
1:B:560:LEU:HD11	1:B:645:TRP:HZ2	1.74	0.49
1:B:954:GLY:O	1:B:957:PRO:HD2	2.11	0.49
1:A:1145:LEU:HD22	1:A:1149:LYS:HZ3	1.78	0.49
1:A:1155:ARG:HH12	1:A:1159:PRO:CD	2.21	0.49
1:A:1158:PRO:HB2	1:A:1159:PRO:HD3	1.95	0.49
1:A:1475:LEU:O	1:A:1478:SER:HB3	2.13	0.49
1:A:1808:ASP:OD1	1:A:1809:ASP:N	2.45	0.49
1:A:2027:SER:HB2	1:A:2030:TYR:OH	2.12	0.49
1:A:2144:LEU:C	1:A:2148:LYS:HE3	2.33	0.49
1:A:2944:THR:HG21	1:A:2983:ASP:OD2	2.12	0.49
1:A:2970:LYS:NZ	1:A:3013:TYR:OH	2.44	0.49
1:A:808:GLU:OE1	1:A:3114:TYR:HB3	2.13	0.49
1:A:396:PHE:CG	1:A:397:LEU:N	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4012:ASP:C	1:A:4016:PHE:HB2	2.33	0.49
1:A:745:VAL:HG11	1:A:776:TRP:HZ2	1.78	0.49
1:A:767:GLU:CG	1:A:851:ILE:HD11	2.40	0.49
1:B:1645:VAL:HG22	1:B:1709:GLU:OE1	2.13	0.49
1:B:1945:TYR:CD1	1:B:1948:ALA:HB3	2.47	0.49
1:B:2094:MSE:O	1:B:2098:THR:HG23	2.13	0.49
1:B:2358:ASP:O	1:B:2361:ILE:HG22	2.12	0.49
1:B:2423:VAL:HG22	1:B:2424:MSE:N	2.27	0.49
1:B:2806:LYS:NZ	1:B:2858:ILE:HG13	2.26	0.49
1:B:2913:LYS:O	1:B:2915:ARG:N	2.45	0.49
1:B:3259:LEU:HD21	1:B:3279:SER:HB2	1.94	0.49
1:B:3696:ARG:HB2	1:B:3699:LEU:HB2	1.95	0.49
1:B:3825:LYS:HB2	1:B:3829:LEU:HD13	1.93	0.49
1:B:437:HIS:CD2	1:B:438:LEU:N	2.80	0.49
1:B:407:VAL:O	1:B:449:TYR:HE1	1.95	0.49
1:B:604:PRO:HG2	1:B:607:ASP:OD1	2.13	0.49
1:B:638:GLN:HG3	1:B:667:TYR:CD2	2.48	0.49
1:B:708:VAL:HG22	1:B:744:ASP:OD2	2.12	0.49
1:B:855:VAL:HG12	1:B:859:LEU:HD11	1.93	0.49
1:B:964:ARG:O	1:B:967:PRO:HD2	2.11	0.49
1:B:978:GLN:HA	1:B:981:ARG:NE	2.21	0.49
1:B:977:ASP:HB3	1:B:981:ARG:N	2.26	0.49
1:A:1060:PHE:HB3	1:A:1064:TYR:HE2	1.78	0.49
1:A:203:GLU:O	1:A:207:GLN:CB	2.55	0.49
1:A:2320:ALA:CA	1:A:2367:VAL:HG23	2.42	0.49
1:A:2352:HIS:CD2	1:A:2364:LEU:HD21	2.48	0.49
1:A:2960:GLU:HG3	1:A:3289:ARG:HH22	1.77	0.49
1:A:3356:ALA:CB	1:A:3384:HIS:HB3	2.43	0.49
1:A:704:PHE:O	1:A:707:PHE:HB2	2.11	0.49
1:A:871:LEU:HD11	1:A:3122:HIS:CE1	2.42	0.49
1:B:1107:TYR:O	1:B:1111:LEU:N	2.40	0.49
1:B:2452:ARG:HG2	1:B:2498:ILE:HD11	1.94	0.49
1:B:3266:SER:HB2	1:B:3271:ASP:OD1	2.12	0.49
1:B:352:VAL:HG23	1:B:357:LYS:H	1.77	0.49
1:B:3793:VAL:O	1:B:3795:PRO:HD3	2.12	0.49
1:B:63:PHE:CE1	1:B:89:LEU:HD22	2.47	0.49
1:B:903:PRO:O	1:B:905:ILE:HG13	2.12	0.49
1:B:992:ILE:HD13	1:B:1031:ARG:HB3	1.95	0.49
1:A:1102:GLU:O	1:A:1105:VAL:HG13	2.13	0.49
1:A:1643:MSE:O	1:A:1646:LEU:N	2.46	0.49
1:A:1723:PRO:C	1:A:1725:GLN:N	2.66	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2097:LEU:HA	1:A:2100:LEU:HB3	1.94	0.49
1:A:2148:LYS:NZ	1:A:2188:GLU:HG2	2.27	0.49
1:A:21:ALA:HA	1:A:24:ARG:HG3	1.94	0.49
1:A:2511:ILE:HA	1:A:2519:LEU:HD12	1.94	0.49
1:A:2542:LEU:HD12	1:A:2543:ASN:N	2.28	0.49
1:A:2567:SER:O	1:A:2571:ASP:HB2	2.11	0.49
1:A:899:ARG:HH22	1:A:2570:PRO:CB	2.25	0.49
1:A:933:LEU:HD22	1:A:2795:GLN:HA	1.93	0.49
1:A:3152:SER:HB2	1:A:3155:VAL:HB	1.94	0.49
1:A:892:LEU:H	1:A:907:LEU:HD22	1.78	0.49
1:B:1033:ILE:HA	1:B:1036:PHE:CD2	2.48	0.49
1:B:1960:LYS:HA	1:B:1963:GLN:OE1	2.13	0.49
1:B:2222:HIS:O	1:B:2226:PRO:HD2	2.12	0.49
1:B:2854:PHE:CE1	1:B:2878:ALA:HA	2.48	0.49
1:B:2999:LEU:HD12	1:B:3002:TYR:CE2	2.46	0.49
1:B:3003:ASN:O	1:B:3006:ALA:N	2.46	0.49
1:B:3163:THR:O	1:B:3167:ARG:HB2	2.13	0.49
1:B:3501:HIS:O	1:B:3505:LEU:HD13	2.12	0.49
1:B:3576:ASP:C	1:B:3578:LEU:HG	2.33	0.49
1:B:3667:LEU:HA	1:B:3670:MSE:HG2	1.92	0.49
1:B:3906:SER:O	1:B:3910:LEU:HD13	2.12	0.49
1:B:388:LEU:HG	1:B:420:VAL:HG21	1.94	0.49
1:B:479:ILE:O	1:B:483:VAL:HG13	2.12	0.49
1:B:789:TYR:CD2	1:B:865:GLN:HG3	2.47	0.49
1:A:1044:ILE:O	1:A:1045:THR:OG1	2.28	0.49
1:A:134:LEU:O	1:A:137:THR:OG1	2.25	0.49
1:A:1407:LYS:HG2	1:A:1462:GLY:N	2.28	0.49
1:A:2245:TRP:CE3	1:A:2245:TRP:HA	2.48	0.49
1:A:2365:ASN:HA	1:A:2368:THR:HB	1.94	0.49
1:A:2412:TYR:CD2	1:A:2416:LYS:HG3	2.47	0.49
1:A:270:ALA:HA	1:A:273:ARG:HG2	1.95	0.49
1:A:3052:LEU:HD13	1:A:3061:LEU:HG	1.94	0.49
1:A:3179:TRP:CZ2	1:A:3258:LEU:HG	2.46	0.49
1:A:3510:GLN:OE1	1:A:3513:ALA:HB2	2.13	0.49
1:A:3525:TYR:OH	1:A:3561:LYS:HB2	2.13	0.49
1:A:3885:ARG:HG3	1:A:3889:ARG:HD3	1.95	0.49
1:A:3929:MSE:O	1:A:3938:ILE:HG13	2.12	0.49
1:A:729:CYS:HA	1:A:732:PHE:CE2	2.48	0.49
1:B:1007:VAL:HA	1:B:1010:LEU:CD1	2.43	0.49
1:B:1220:LEU:O	1:B:1223:THR:OG1	2.26	0.49
1:B:1280:GLN:HA	1:B:1361:LYS:HZ2	1.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1459:HIS:NE2	1:B:1509:GLN:O	2.46	0.49
1:B:1751:GLU:O	1:B:1755:SER:N	2.42	0.49
1:B:1726:SER:HB2	1:B:1869:LYS:HD2	1.94	0.49
1:B:3117:ILE:CD1	1:B:3125:ARG:HH11	2.06	0.49
1:B:3293:CYS:O	1:B:3297:VAL:HB	2.13	0.49
1:B:3570:ASP:O	1:B:3573:ASN:HB3	2.13	0.49
1:B:3657:SER:O	1:B:3660:ASN:HB2	2.13	0.49
1:B:3971:MSE:HE2	1:B:3976:GLU:OE2	2.13	0.49
1:B:712:LYS:O	1:B:716:VAL:HG23	2.13	0.49
1:B:63:PHE:HD1	1:B:89:LEU:HD13	1.78	0.49
1:A:1139:GLU:HG3	1:A:1175:HIS:CD2	2.48	0.49
1:A:1684:LEU:HA	1:A:1687:HIS:HD2	1.77	0.49
1:A:175:TYR:HB2	1:A:222:GLY:C	2.33	0.49
1:A:2274:ILE:CD1	1:A:2314:GLU:HB3	2.43	0.49
1:A:3103:ILE:HD13	1:A:3139:GLN:OE1	2.13	0.49
1:A:3984:MSE:SE	1:A:4108:MSE:HE2	2.63	0.49
1:A:442:GLN:HA	1:A:445:SER:OG	2.12	0.49
1:B:1493:PRO:HG2	1:B:1495:ASP:HB2	1.94	0.49
1:B:2161:ALA:CB	1:B:2211:LEU:HD13	2.39	0.49
1:B:2357:GLU:OE1	1:B:2388:LYS:NZ	2.42	0.49
1:B:249:PHE:HB3	1:B:297:LEU:HD13	1.93	0.49
1:B:2778:GLY:O	1:B:2781:PRO:HD2	2.13	0.49
1:B:3522:THR:O	1:B:3526:PRO:HD3	2.13	0.49
1:B:3974:MSE:CG	1:B:3976:GLU:HB3	2.43	0.49
1:B:4041:ARG:HB2	1:B:4042:GLN:OE1	2.12	0.49
1:B:793:LEU:HA	1:B:796:LEU:HB2	1.94	0.49
1:B:891:ARG:HD2	1:B:905:ILE:HG12	1.94	0.49
1:A:1113:LEU:HA	1:A:1116:ALA:HB3	1.94	0.49
1:A:1695:LEU:HA	1:A:1698:PHE:CE2	2.48	0.49
1:A:1762:MSE:HE3	1:A:1864:ASP:OD1	2.13	0.49
1:A:3045:ILE:O	1:A:3048:LYS:HE2	2.13	0.49
1:A:3186:ARG:HD3	1:A:3242:MSE:SE	2.63	0.49
1:A:3247:ARG:HH21	1:A:3277:VAL:HG23	1.78	0.49
1:A:3651:LEU:HA	1:A:3654:MSE:HB2	1.95	0.49
1:A:3962:ARG:NH1	1:A:4124:TRP:CH2	2.81	0.49
1:A:903:PRO:HD2	1:A:904:VAL:HG23	1.95	0.49
1:A:927:LYS:HD3	1:A:976:VAL:HG12	1.94	0.49
1:B:1219:PHE:O	1:B:1223:THR:HG23	2.13	0.49
1:B:2467:THR:HA	1:B:2470:ARG:HG3	1.93	0.49
1:B:2842:ARG:O	1:B:2846:THR:HG23	2.11	0.49
1:B:2887:PRO:CB	1:B:2922:ARG:HH11	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3034:PRO:CG	1:B:3037:GLN:HB2	2.39	0.49
1:B:485:GLN:HA	1:B:488:ILE:HG12	1.94	0.49
1:B:567:GLU:HB3	1:B:606:SER:CB	2.43	0.49
1:B:990:GLN:HA	1:B:993:HIS:HD2	1.77	0.49
1:A:174:VAL:O	1:A:178:LEU:HG	2.13	0.48
1:A:181:LEU:HD13	1:A:189:MSE:HE2	1.95	0.48
1:A:2990:GLU:O	1:A:2994:TRP:HD1	1.96	0.48
1:A:3468:LEU:HD13	1:A:3483:MSE:HE1	1.93	0.48
1:A:3547:THR:HG21	1:A:3552:LYS:HB2	1.94	0.48
1:A:3648:GLY:O	1:A:3651:LEU:HB2	2.13	0.48
1:A:760:LEU:HD23	1:A:803:SER:HB3	1.95	0.48
1:A:901:MSE:HE1	1:A:2539:LEU:CD2	2.43	0.48
1:A:925:GLN:OE1	1:A:925:GLN:N	2.39	0.48
1:B:1059:LEU:O	1:B:1063:LEU:HG	2.13	0.48
1:B:13:LEU:O	1:B:16:GLN:HG2	2.13	0.48
1:B:1976:LEU:HG	1:B:1978:PHE:H	1.77	0.48
1:B:1959:LEU:CD1	1:B:1998:MSE:HE3	2.32	0.48
1:B:20:SER:HB2	1:B:65:LEU:HD22	1.95	0.48
1:B:2602:UNK:CB	1:B:2793:PRO:HG3	2.43	0.48
1:B:3061:LEU:HD21	1:B:3089:LEU:HD13	1.95	0.48
1:B:3155:VAL:N	1:B:3156:PRO:HD2	2.28	0.48
1:B:3972:LEU:O	1:B:3974:MSE:HG2	2.13	0.48
1:B:4085:LYS:HA	1:B:4088:ASN:CB	2.43	0.48
1:B:613:HIS:O	1:B:617:PRO:HG2	2.13	0.48
1:A:1122:GLY:O	1:A:1123:THR:OG1	2.29	0.48
1:A:1170:LYS:HD3	1:A:1267:TYR:CG	2.48	0.48
1:A:14:ARG:HD2	1:A:2358:ASP:OD2	2.13	0.48
1:A:1722:PHE:H	1:A:1723:PRO:CD	2.26	0.48
1:A:1869:LYS:O	1:A:1873:TYR:HD1	1.96	0.48
1:A:2110:PRO:HB2	1:A:2111:PRO:HD3	1.95	0.48
1:A:2171:LEU:HG	1:A:2177:ASN:HD21	1.78	0.48
1:A:2193:ILE:HD11	1:A:2245:TRP:CZ2	2.48	0.48
1:A:3247:ARG:NH2	1:A:3277:VAL:HG23	2.27	0.48
1:A:3684:SER:HB3	1:A:3726:VAL:CG1	2.42	0.48
1:A:3950:THR:OG1	1:A:3957:GLU:O	2.22	0.48
1:A:3963:LEU:HG	1:A:3967:PHE:CE1	2.47	0.48
1:A:3974:MSE:HB3	1:A:3976:GLU:N	2.23	0.48
1:A:398:THR:HG22	1:A:1865:THR:HG21	1.94	0.48
1:A:4103:GLN:H	1:A:4103:GLN:CD	2.17	0.48
1:A:531:PHE:CE2	1:A:619:ASP:HB2	2.47	0.48
1:B:1076:LEU:C	1:B:1078:ALA:H	2.16	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1238:GLN:NE2	1:B:1298:LEU:HG	2.28	0.48
1:B:1365:ASN:HA	1:B:1368:LEU:HD21	1.94	0.48
1:B:1708:GLU:HB2	1:B:1709:GLU:CD	2.33	0.48
1:B:1996:VAL:CG1	1:B:2048:GLY:HA2	2.37	0.48
1:B:2322:VAL:O	1:B:2326:ILE:HG12	2.13	0.48
1:B:280:SER:HB3	1:B:322:GLN:HB2	1.95	0.48
1:B:3228:SER:O	1:B:3231:ILE:HB	2.13	0.48
1:B:3284:SER:HA	1:B:3287:ARG:NE	2.09	0.48
1:B:3788:LEU:HD13	1:B:3907:SER:HA	1.96	0.48
1:B:3901:ARG:NH1	1:B:3901:ARG:HG2	2.27	0.48
1:B:4066:LEU:HG	1:B:4075:ARG:HA	1.95	0.48
1:B:575:ILE:HG12	1:B:579:LEU:HB2	1.95	0.48
1:B:669:LEU:HD13	1:B:672:ILE:HD12	1.95	0.48
1:A:2213:ASN:HB2	1:A:2250:SER:HB2	1.95	0.48
1:A:940:PHE:HZ	1:A:2791:ILE:HG21	1.73	0.48
1:A:583:LEU:HD23	1:A:592:GLU:OE2	2.13	0.48
1:A:848:LEU:HA	1:A:851:ILE:CD1	2.44	0.48
1:B:1299:GLU:HA	1:B:1302:ALA:CB	2.44	0.48
1:B:1330:TYR:O	1:B:1333:SER:OG	2.27	0.48
1:B:1889:VAL:HG13	1:B:1900:PHE:CD2	2.48	0.48
1:B:2031:LEU:HB2	1:B:2033:ASP:CB	2.40	0.48
1:B:2059:PRO:O	1:B:2062:ALA:HB3	2.13	0.48
1:B:2291:GLN:NE2	1:B:2294:ILE:HG13	2.28	0.48
1:B:2299:TYR:O	1:B:2302:ALA:N	2.46	0.48
1:B:2387:PRO:O	1:B:2390:HIS:HB3	2.12	0.48
1:B:2459:VAL:HG11	1:B:2505:VAL:HG22	1.95	0.48
1:B:249:PHE:O	1:B:253:LEU:HG	2.13	0.48
1:B:2549:LYS:HD2	1:B:2554:PHE:HB3	1.95	0.48
1:B:2851:PHE:O	1:B:2855:VAL:HG23	2.13	0.48
1:B:293:LEU:O	1:B:296:VAL:HG12	2.12	0.48
1:B:856:VAL:HG21	1:B:3110:PHE:CE1	2.48	0.48
1:B:3398:PRO:HG2	1:B:3399:PRO:HD3	1.94	0.48
1:B:358:GLU:HG3	1:B:359:LEU:N	2.27	0.48
1:B:3989:ARG:HE	1:B:4100:GLU:CB	2.26	0.48
1:B:611:ASN:C	1:B:614:PRO:HD2	2.33	0.48
1:B:758:LEU:O	1:B:762:TYR:HB3	2.13	0.48
1:B:884:VAL:HG22	1:B:888:ARG:HG2	1.95	0.48
1:B:892:LEU:HD12	1:B:892:LEU:O	2.13	0.48
1:B:996:THR:O	1:B:1042:LYS:HG2	2.12	0.48
1:A:1001:PHE:CD1	1:A:1002:GLU:N	2.82	0.48
1:A:1075:ARG:O	1:A:1078:ALA:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1029:CYS:CB	1:A:1085:ILE:HG13	2.43	0.48
1:A:1231:GLN:H	1:A:1232:PRO:HD3	1.78	0.48
1:A:1387:GLY:HA2	1:A:1392:MSE:SE	2.63	0.48
1:A:1889:VAL:HG22	1:A:1900:PHE:CE2	2.49	0.48
1:A:2122:LEU:HA	1:A:2127:LYS:HE2	1.96	0.48
1:A:2166:SER:N	1:A:2167:PRO:HD2	2.28	0.48
1:A:2161:ALA:HB1	1:A:2211:LEU:HD13	1.95	0.48
1:A:2573:PRO:C	1:A:2575:PRO:HD3	2.32	0.48
1:A:2778:GLY:O	1:A:2781:PRO:HD2	2.14	0.48
1:A:3020:ASP:HB3	1:A:3027:LEU:HD12	1.95	0.48
1:A:3612:ARG:O	1:A:3615:ALA:HB3	2.14	0.48
1:A:4117:LEU:HB3	1:A:4126:PRO:HB2	1.96	0.48
1:B:1741:ASP:O	1:B:1745:LYS:HG3	2.14	0.48
1:B:1884:LEU:HB2	1:B:1885:PRO:HD3	1.95	0.48
1:B:2086:ASP:CB	1:B:2090:ARG:HH21	2.24	0.48
1:B:2148:LYS:HD3	1:B:2160:TYR:HE1	1.78	0.48
1:B:2227:LYS:HD2	1:B:2235:LEU:CG	2.35	0.48
1:B:3076:ALA:O	1:B:3080:LEU:HG	2.14	0.48
1:B:3498:TRP:NE1	1:B:3502:MSE:HB2	2.28	0.48
1:B:3764:VAL:O	1:B:3768:PHE:HD1	1.96	0.48
1:B:3972:LEU:O	1:B:3974:MSE:N	2.46	0.48
1:B:706:LEU:HA	1:B:709:LYS:HB2	1.94	0.48
1:B:793:LEU:HA	1:B:796:LEU:CG	2.43	0.48
1:A:1389:VAL:O	1:A:1390:GLN:HB2	2.13	0.48
1:A:2196:TRP:CE2	1:A:2199:LEU:HD11	2.47	0.48
1:A:2241:LEU:HA	1:A:2244:CYS:SG	2.53	0.48
1:A:19:LEU:HA	1:A:22:ALA:HB3	1.95	0.48
1:A:2386:LEU:HD13	1:A:2401:VAL:HA	1.95	0.48
1:A:2437:ASP:HB3	1:A:2472:GLN:HG2	1.95	0.48
1:A:2532:PRO:O	1:A:2565:MSE:HE2	2.14	0.48
1:A:322:GLN:HA	1:A:325:ASN:HB2	1.95	0.48
1:A:3409:VAL:HB	1:A:3413:TYR:CE2	2.48	0.48
1:A:49:ALA:O	1:A:53:LEU:HB2	2.12	0.48
1:A:88:PHE:O	1:A:91:ILE:HG13	2.13	0.48
1:A:979:VAL:O	1:A:982:GLN:HB3	2.12	0.48
1:B:1228:GLY:O	1:B:1282:LEU:HD11	2.14	0.48
1:B:1698:PHE:CD1	1:B:1699:PHE:N	2.82	0.48
1:B:2063:THR:HA	1:B:2066:PHE:HB2	1.95	0.48
1:B:2085:MSE:O	1:B:2088:LEU:HB3	2.13	0.48
1:B:2837:LEU:HD22	1:B:2868:LEU:CG	2.41	0.48
1:B:3045:ILE:HB	1:B:3048:LYS:HZ1	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3420:CYS:SG	1:B:3421:ASP:N	2.86	0.48
1:B:3629:ARG:HH22	1:B:3638:LYS:HE3	1.78	0.48
1:B:3771:MSE:O	1:B:3775:LEU:HG	2.14	0.48
1:B:3881:ASP:HA	1:B:3884:LYS:HD2	1.96	0.48
1:B:417:VAL:O	1:B:421:LEU:HG	2.14	0.48
1:B:629:PHE:CD2	1:B:668:LYS:HE2	2.48	0.48
1:B:741:ILE:O	1:B:743:LEU:N	2.46	0.48
1:A:1136:ARG:HG2	1:A:1171:TRP:CH2	2.48	0.48
1:A:1385:ASN:O	1:A:1389:VAL:HG23	2.13	0.48
1:A:1430:GLU:HA	1:A:1433:ALA:HB3	1.95	0.48
1:A:3464:LYS:CD	1:A:3467:ARG:HD2	2.43	0.48
1:A:3617:LEU:HD13	1:A:3644:PHE:CD2	2.49	0.48
1:A:3762:GLN:OE1	1:A:3795:PRO:HG3	2.13	0.48
1:A:4085:LYS:HA	1:A:4088:ASN:CB	2.43	0.48
1:A:65:LEU:HD23	1:A:68:PHE:CE1	2.48	0.48
1:A:934:LEU:C	1:A:934:LEU:HD23	2.33	0.48
1:A:978:GLN:HA	1:A:981:ARG:NE	2.23	0.48
1:B:1390:GLN:O	1:B:1393:ALA:HB3	2.14	0.48
1:B:1414:ILE:O	1:B:1418:HIS:HB2	2.13	0.48
1:B:1571:LEU:HD22	1:B:1600:MSE:HA	1.96	0.48
1:B:1890:HIS:NE2	1:B:1941:HIS:HA	2.29	0.48
1:B:1894:SER:C	1:B:1896:ILE:N	2.66	0.48
1:B:2231:PHE:CE1	1:B:2233:HIS:HB2	2.49	0.48
1:B:2782:ASP:HA	1:B:2786:LYS:HB3	1.96	0.48
1:B:3319:ASN:O	1:B:3323:PHE:HD2	1.95	0.48
1:B:3427:GLU:OE1	1:B:3435:ASP:HB3	2.14	0.48
1:B:3495:PHE:CZ	1:B:3521:ILE:HG13	2.49	0.48
1:B:3575:LEU:HD21	1:B:3687:MSE:SE	2.63	0.48
1:B:361:ILE:HA	1:B:364:ARG:HG2	1.94	0.48
1:B:3629:ARG:NH2	1:B:3634:GLN:HA	2.28	0.48
1:B:3538:GLU:HG2	1:B:3759:ARG:NH1	2.29	0.48
1:B:3981:TYR:O	1:B:3985:VAL:HG23	2.14	0.48
1:B:46:SER:H	1:B:51:LEU:HD13	1.78	0.48
1:B:749:VAL:N	1:B:750:PRO:CD	2.77	0.48
1:B:757:LYS:HA	1:B:760:LEU:CD1	2.44	0.48
1:B:938:VAL:HG21	1:B:962:TYR:OH	2.13	0.48
1:A:1340:ARG:NH1	1:A:1343:GLU:HG2	2.29	0.48
1:A:1465:HIS:HA	1:A:1469:PRO:HD2	1.95	0.48
1:A:2230:VAL:HB	1:A:2234:ASN:HD21	1.79	0.48
1:A:2467:THR:HB	1:A:2518:GLN:NE2	2.16	0.48
1:A:2890:ILE:CG2	1:A:2922:ARG:HH12	2.23	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:GLU:HA	1:A:298:LEU:HD12	1.96	0.48
1:A:3454:LEU:HD12	1:A:3490:VAL:HG11	1.95	0.48
1:A:358:GLU:N	1:A:361:ILE:HG23	2.29	0.48
1:A:449:TYR:CZ	1:A:457:CYS:SG	3.05	0.48
1:B:1007:VAL:O	1:B:1011:GLU:CB	2.61	0.48
1:B:1055:ASN:HA	1:B:1059:LEU:HG	1.94	0.48
1:B:1080:LEU:HB2	1:B:1131:ILE:HG22	1.94	0.48
1:B:1165:LEU:HB3	1:B:1169:VAL:HG23	1.96	0.48
1:B:86:LEU:HD13	1:B:134:LEU:HD21	1.95	0.48
1:B:1387:GLY:HA2	1:B:1392:MSE:HB2	1.94	0.48
1:B:1692:ALA:O	1:B:1695:LEU:HB2	2.14	0.48
1:B:1711:ARG:O	1:B:1715:GLU:HG3	2.12	0.48
1:B:1946:ASN:O	1:B:1949:ILE:N	2.35	0.48
1:B:1970:LYS:HB3	1:B:1971:PRO:HD3	1.95	0.48
1:B:1978:PHE:O	1:B:1981:LEU:HB3	2.13	0.48
1:B:2462:VAL:HB	1:B:2473:MSE:SE	2.63	0.48
1:B:3463:LEU:HD21	1:B:4001:THR:HA	1.96	0.48
1:B:3582:GLU:HB2	1:B:3674:SER:OG	2.14	0.48
1:B:3675:LYS:N	1:B:3676:PRO:HD2	2.29	0.48
1:B:3916:TRP:HE3	1:B:3917:ILE:HD12	1.77	0.48
1:B:4103:GLN:H	1:B:4103:GLN:CD	2.16	0.48
1:B:901:MSE:HE1	1:B:2535:THR:HG21	1.96	0.48
1:A:1066:LEU:HA	1:A:1069:HIS:CD2	2.49	0.48
1:A:1086:TYR:HE2	1:A:1090:ARG:NE	2.08	0.48
1:A:1105:VAL:HB	1:A:1153:LEU:HD22	1.95	0.48
1:A:1080:LEU:HD13	1:A:1127:CYS:HB3	1.96	0.48
1:A:1651:LYS:HD2	1:A:1684:LEU:CG	2.44	0.48
1:A:1737:ASN:O	1:A:1739:TYR:N	2.44	0.48
1:A:2224:PHE:CE2	1:A:2259:LYS:HD3	2.48	0.48
1:A:2467:THR:CB	1:A:2518:GLN:HE22	2.17	0.48
1:A:2890:ILE:HD13	1:A:2922:ARG:HH12	1.78	0.48
1:A:2911:ARG:CG	1:A:2914:ALA:HB3	2.43	0.48
1:A:3806:LEU:O	1:A:3809:THR:HG22	2.14	0.48
1:A:3917:ILE:O	1:A:4048:LYS:NZ	2.46	0.48
1:A:440:VAL:HG12	1:A:483:VAL:HG12	1.94	0.48
1:A:634:LEU:HD22	1:A:667:TYR:HD1	1.79	0.48
1:A:722:LYS:HB3	1:A:727:ALA:CA	2.44	0.48
1:A:883:TYR:CE2	1:A:961:LEU:HD12	2.49	0.48
1:B:1306:ILE:CG1	1:B:1334:LYS:HB3	2.42	0.48
1:B:1916:ILE:HG23	1:B:1920:TYR:CE1	2.49	0.48
1:B:2073:ASP:N	1:B:2074:PRO:CD	2.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2142:ILE:HG12	1:B:2145:PHE:CE2	2.49	0.48
1:B:2164:TRP:HH2	1:B:2190:VAL:HG12	1.79	0.48
1:B:2304:VAL:HG13	1:B:2348:GLN:NE2	2.28	0.48
1:B:2877:SER:C	1:B:2879:GLY:N	2.67	0.48
1:B:2915:ARG:HG3	1:B:2915:ARG:HH11	1.78	0.48
1:B:3145:ILE:HG12	1:B:3196:LYS:HG2	1.95	0.48
1:B:3175:PRO:HG2	1:B:3178:ILE:HD11	1.95	0.48
1:B:345:PHE:O	1:B:349:ILE:HG13	2.13	0.48
1:B:3825:LYS:HD2	1:B:3829:LEU:HA	1.95	0.48
1:B:3835:PRO:HA	1:B:3871:PHE:CE1	2.47	0.48
1:B:3913:ILE:O	1:B:3917:ILE:HD13	2.14	0.48
1:B:429:GLU:OE2	1:B:1595:ALA:HB2	2.13	0.48
1:B:645:TRP:CZ3	1:B:659:ARG:CB	2.97	0.48
1:B:994:TRP:HA	1:B:994:TRP:CE3	2.48	0.48
1:A:1042:LYS:HE3	1:A:1044:ILE:HG21	1.95	0.48
1:A:1072:ALA:CB	1:A:1114:ALA:HB1	2.44	0.48
1:A:1165:LEU:O	1:A:1168:LEU:N	2.46	0.48
1:A:1175:HIS:O	1:A:1178:ARG:HB3	2.13	0.48
1:A:1434:VAL:HB	1:A:1448:LEU:HD11	1.94	0.48
1:A:2193:ILE:CD1	1:A:2245:TRP:CZ2	2.97	0.48
1:A:2256:ILE:HG12	1:A:2276:LEU:HD21	1.96	0.48
1:A:2232:ARG:NH2	1:A:2313:LYS:NZ	2.62	0.48
1:A:2820:MSE:HE3	1:A:2829:LYS:HB3	1.96	0.48
1:A:280:SER:O	1:A:322:GLN:HG2	2.14	0.48
1:A:3638:LYS:C	1:A:3641:ASP:H	2.16	0.48
1:A:542:ASP:HA	1:A:545:LEU:CD1	2.44	0.48
1:A:611:ASN:O	1:A:614:PRO:HD2	2.13	0.48
1:A:509:ARG:CB	1:A:729:CYS:SG	3.02	0.48
1:A:889:GLU:OE2	1:A:950:GLU:HG2	2.13	0.48
1:B:1109:GLU:O	1:B:1113:LEU:HB3	2.14	0.48
1:B:1303:MSE:O	1:B:1307:ILE:HG13	2.13	0.48
1:B:1476:HIS:CE1	1:B:1507:CYS:HA	2.49	0.48
1:B:1574:ASN:CB	1:B:1582:LEU:HD21	2.42	0.48
1:B:1923:PHE:HE2	1:B:1927:MSE:HE1	1.79	0.48
1:B:19:LEU:HA	1:B:22:ALA:HB3	1.96	0.48
1:B:2146:LEU:HD22	1:B:2149:LEU:HD11	1.95	0.48
1:B:231:LEU:HD23	1:B:234:PHE:HB3	1.94	0.48
1:B:3460:GLU:HA	1:B:3463:LEU:HD12	1.96	0.48
1:B:39:GLY:O	1:B:43:VAL:HG23	2.13	0.48
1:B:446:PHE:HD2	1:B:533:HIS:CB	2.25	0.48
1:B:641:PHE:CZ	1:B:645:TRP:NE1	2.82	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:929:ALA:O	1:B:933:LEU:CB	2.62	0.48
1:A:1373:VAL:C	1:A:1375:THR:H	2.16	0.48
1:A:1723:PRO:O	1:A:1725:GLN:N	2.47	0.48
1:A:1984:LEU:HD12	1:A:1985:LYS:N	2.29	0.48
1:A:2004:TYR:CE1	1:A:2054:TYR:O	2.67	0.48
1:A:2328:ARG:O	1:A:2332:GLU:HG3	2.13	0.48
1:A:2854:PHE:HZ	1:A:2881:LEU:HB2	1.77	0.48
1:A:290:TYR:CD1	1:A:293:LEU:HD13	2.48	0.48
1:A:2979:GLN:O	1:A:2982:VAL:HG22	2.14	0.48
1:A:3008:TRP:CG	1:A:3257:LYS:NZ	2.81	0.48
1:A:3326:GLN:CB	1:A:3393:GLU:HG2	2.37	0.48
1:A:3806:LEU:HG	1:A:3807:GLU:O	2.13	0.48
1:A:3900:LEU:HD11	1:A:3934:THR:O	2.13	0.48
1:A:3980:MSE:HA	1:A:3983:ILE:HG13	1.94	0.48
1:B:1025:LEU:HA	1:B:1025:LEU:HD12	1.60	0.48
1:B:1087:ARG:CD	1:B:1134:LEU:HD22	2.44	0.48
1:B:1253:THR:HA	1:B:1257:LEU:HD12	1.95	0.48
1:B:2222:HIS:O	1:B:2224:PHE:N	2.47	0.48
1:B:2913:LYS:HG3	1:B:2914:ALA:H	1.76	0.48
1:B:2912:GLY:HA2	1:B:2915:ARG:NH2	2.28	0.48
1:B:3571:PHE:O	1:B:3575:LEU:HB3	2.13	0.48
1:B:3758:LEU:HD22	1:B:3761:ASP:OD2	2.13	0.48
1:B:3862:ALA:O	1:B:3865:THR:OG1	2.27	0.48
1:B:3816:LEU:HD11	1:B:3883:LEU:HD22	1.96	0.48
1:A:157:TYR:HA	1:A:160:LEU:HG	1.96	0.47
1:A:1762:MSE:SE	1:A:1867:ILE:HG21	2.64	0.47
1:A:1918:LEU:HD11	1:A:1957:ASN:ND2	2.29	0.47
1:A:1977:ILE:C	1:A:1979:GLU:H	2.13	0.47
1:A:2074:PRO:CB	1:A:2136:PRO:HB3	2.43	0.47
1:A:2358:ASP:N	1:A:2358:ASP:OD1	2.46	0.47
1:A:2390:HIS:ND1	1:A:2397:CYS:SG	2.64	0.47
1:A:2538:ARG:HG3	1:A:2539:LEU:N	2.28	0.47
1:A:3128:LYS:C	1:A:3130:GLN:H	2.15	0.47
1:A:3425:ARG:NH1	1:A:3999:THR:HG22	2.29	0.47
1:A:3725:ARG:HH12	1:A:3737:ARG:NH2	2.11	0.47
1:A:3870:SER:OG	1:A:3871:PHE:N	2.46	0.47
1:A:65:LEU:O	1:A:69:VAL:HB	2.14	0.47
1:B:1018:VAL:HB	1:B:1074:LYS:CA	2.44	0.47
1:B:1036:PHE:CZ	1:B:1082:PHE:CE2	3.02	0.47
1:B:1268:ASN:HA	1:B:1271:ILE:HD12	1.95	0.47
1:B:1299:GLU:C	1:B:1302:ALA:H	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1946:ASN:HA	1:B:1949:ILE:HG22	1.96	0.47
1:B:2193:ILE:HG13	1:B:2196:TRP:CZ2	2.49	0.47
1:B:2382:VAL:CG2	1:B:2404:ARG:HG3	2.40	0.47
1:B:2538:ARG:HG3	1:B:2539:LEU:N	2.28	0.47
1:B:2782:ASP:HA	1:B:2786:LYS:CB	2.44	0.47
1:B:3003:ASN:ND2	1:B:3010:SER:HB2	2.28	0.47
1:B:3110:PHE:HB2	1:B:3114:TYR:HE1	1.78	0.47
1:B:3136:THR:O	1:B:3140:GLU:HB2	2.14	0.47
1:B:3268:THR:H	1:B:3271:ASP:HB3	1.79	0.47
1:B:3525:TYR:HA	1:B:3529:ILE:HG21	1.96	0.47
1:B:3531:TYR:HB3	1:B:3532:PRO:HD3	1.95	0.47
1:B:3789:ARG:CZ	1:B:3806:LEU:HD22	2.44	0.47
1:B:3896:ALA:O	1:B:3899:ALA:HB3	2.14	0.47
1:B:4062:ASP:HA	1:B:4065:LEU:CD2	2.44	0.47
1:B:645:TRP:CZ3	1:B:659:ARG:HB3	2.49	0.47
1:B:76:ILE:HG13	1:B:77:GLU:H	1.79	0.47
1:B:942:LEU:HD11	1:B:991:LEU:CD1	2.44	0.47
1:B:989:MSE:HB2	1:B:990:GLN:NE2	2.29	0.47
1:A:1073:PHE:CZ	1:A:3745:GLU:HA	2.49	0.47
1:A:1716:GLN:O	1:A:1719:VAL:N	2.40	0.47
1:A:1733:THR:N	1:A:1734:PRO:CD	2.77	0.47
1:A:2291:GLN:NE2	1:A:2294:ILE:HG21	2.29	0.47
1:A:290:TYR:O	1:A:294:PHE:HD1	1.97	0.47
1:A:31:GLY:HA3	1:A:81:CYS:SG	2.54	0.47
1:A:335:LYS:HA	1:A:338:LEU:HD12	1.94	0.47
1:A:3493:TRP:CZ3	1:A:3496:ILE:HG13	2.49	0.47
1:A:3954:PRO:HG3	1:A:4030:GLU:HB2	1.95	0.47
1:A:419:SER:O	1:A:422:LEU:HB2	2.15	0.47
1:A:935:HIS:NE2	1:A:987:LEU:HG	2.29	0.47
1:B:1438:GLY:O	1:B:1441:ALA:HB2	2.14	0.47
1:B:1869:LYS:O	1:B:1873:TYR:HD1	1.96	0.47
1:B:2420:PHE:HZ	1:B:2436:LEU:HB3	1.76	0.47
1:B:2482:ASP:HA	1:B:2485:ARG:HB3	1.95	0.47
1:B:2911:ARG:O	1:B:2915:ARG:NE	2.47	0.47
1:B:3522:THR:HA	1:B:3525:TYR:HB3	1.96	0.47
1:B:3842:TRP:HH2	1:B:3846:MSE:HE2	1.73	0.47
1:B:58:VAL:O	1:B:62:ASP:HB2	2.14	0.47
1:B:650:SER:HA	1:B:652:GLU:OE2	2.13	0.47
1:B:659:ARG:HH12	1:B:662:LEU:CD2	2.28	0.47
1:B:922:SER:O	1:B:926:THR:OG1	2.28	0.47
1:A:292:SER:O	1:A:296:VAL:HB	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2960:GLU:HA	1:A:3251:ASN:O	2.14	0.47
1:A:3301:LEU:HB2	1:A:3328:ILE:CG2	2.44	0.47
1:A:3606:ILE:HD13	1:A:3609:MSE:HE3	1.96	0.47
1:A:3493:TRP:CE3	1:A:3713:PRO:HB3	2.49	0.47
1:B:1111:LEU:HD22	1:B:1131:ILE:HD13	1.96	0.47
1:B:1397:ASP:O	1:B:1400:VAL:HB	2.13	0.47
1:B:1501:PRO:O	1:B:1505:LEU:HB2	2.14	0.47
1:B:187:SER:O	1:B:190:ILE:HG22	2.13	0.47
1:B:2440:TYR:O	1:B:2440:TYR:CG	2.67	0.47
1:B:3334:TYR:CE1	1:B:3426:LYS:HD3	2.49	0.47
1:B:3797:THR:CG2	1:B:3800:LEU:HG	2.43	0.47
1:B:634:LEU:O	1:B:669:LEU:HD12	2.14	0.47
1:B:714:VAL:HG11	1:B:734:LEU:HD21	1.96	0.47
1:A:2003:LYS:HG2	1:A:2006:GLU:OE1	2.14	0.47
1:A:14:ARG:HH12	1:A:2392:VAL:HG21	1.79	0.47
1:A:2776:ARG:CZ	1:A:2776:ARG:HA	2.44	0.47
1:A:2841:ASN:OD1	1:A:2844:LEU:HD12	2.15	0.47
1:A:2917:PRO:HB2	1:A:2918:PRO:HD3	1.95	0.47
1:A:2940:ARG:HD3	1:A:3975:LYS:CD	2.44	0.47
1:A:3487:ILE:HG21	1:A:3524:ASN:HD21	1.78	0.47
1:A:368:LEU:CA	1:A:372:PRO:HG2	2.44	0.47
1:A:3878:VAL:HB	1:A:3879:PRO:HD3	1.96	0.47
1:A:403:GLY:O	1:A:405:ASP:N	2.44	0.47
1:A:455:LEU:O	1:A:459:ARG:HG3	2.15	0.47
1:A:69:VAL:O	1:A:73:LEU:HG	2.13	0.47
1:A:718:MSE:O	1:A:722:LYS:HB2	2.15	0.47
1:A:892:LEU:HD21	1:A:958:MSE:HG3	1.96	0.47
1:B:1080:LEU:HB2	1:B:1131:ILE:CG2	2.45	0.47
1:B:1472:SER:OG	1:B:1473:THR:N	2.48	0.47
1:B:612:LEU:HD21	1:B:1800:SER:HB3	1.96	0.47
1:B:2155:GLU:HB3	1:B:2156:VAL:H	1.40	0.47
1:B:2186:VAL:O	1:B:2190:VAL:HG13	2.13	0.47
1:B:2193:ILE:HG12	1:B:2193:ILE:O	2.14	0.47
1:B:2200:ALA:CA	1:B:2203:THR:HG22	2.41	0.47
1:B:2212:ALA:O	1:B:2215:LEU:HB3	2.15	0.47
1:B:2257:PHE:CE1	1:B:2299:TYR:HB3	2.49	0.47
1:B:3498:TRP:HD1	1:B:3502:MSE:HB2	1.77	0.47
1:B:3514:VAL:HG21	1:B:3551:ASN:HB3	1.95	0.47
1:B:3839:TYR:HB2	1:B:3871:PHE:CE1	2.49	0.47
1:B:887:ASP:O	1:B:3889:ARG:NE	2.47	0.47
1:B:411:PRO:O	1:B:415:GLN:CB	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:927:LYS:O	1:B:931:CYS:SG	2.73	0.47
1:A:1216:GLY:HA3	1:A:1271:ILE:CG2	2.45	0.47
1:A:1292:LYS:H	1:A:1292:LYS:HG3	1.52	0.47
1:A:1508:LYS:C	1:A:1510:LEU:H	2.18	0.47
1:A:1809:ASP:HA	1:A:1815:THR:HA	1.96	0.47
1:A:2549:LYS:HZ3	1:A:2554:PHE:HA	1.75	0.47
1:A:3008:TRP:CE3	1:A:3050:LYS:HB2	2.50	0.47
1:A:3114:TYR:CE2	1:A:3125:ARG:NH2	2.83	0.47
1:A:3775:LEU:HB3	1:A:3781:CYS:SG	2.53	0.47
1:A:3834:ALA:HB1	1:A:3838:GLU:OE1	2.14	0.47
1:A:749:VAL:N	1:A:750:PRO:HD3	2.30	0.47
1:B:1001:PHE:CD1	1:B:1002:GLU:N	2.81	0.47
1:B:1090:ARG:HH12	1:B:1096:VAL:CG1	2.22	0.47
1:B:205:LYS:HE3	1:B:243:GLN:HB3	1.96	0.47
1:B:2508:GLN:HG2	1:B:2508:GLN:O	2.14	0.47
1:B:2539:LEU:HG	1:B:2816:ILE:HG13	1.95	0.47
1:B:2603:UNK:CB	1:B:2793:PRO:HB2	2.44	0.47
1:B:3128:LYS:O	1:B:3132:VAL:HG13	2.14	0.47
1:B:3160:LEU:HA	1:B:3160:LEU:HD12	1.75	0.47
1:B:3330:LEU:C	1:B:3332:THR:H	2.17	0.47
1:B:3820:MSE:O	1:B:3824:GLU:N	2.41	0.47
1:B:428:PRO:O	1:B:430:VAL:HG23	2.14	0.47
1:B:539:GLN:HG3	1:B:626:LEU:O	2.14	0.47
1:B:756:PHE:O	1:B:759:GLY:C	2.52	0.47
1:B:801:LYS:HB2	1:B:805:LEU:HD12	1.96	0.47
1:B:927:LYS:HE3	1:B:928:VAL:HG13	1.96	0.47
1:A:1213:LYS:O	1:A:1215:GLU:N	2.48	0.47
1:A:82:ARG:NH2	1:A:130:LEU:HD22	2.30	0.47
1:A:1372:LEU:HG	1:A:1373:VAL:N	2.29	0.47
1:A:1396:PRO:O	1:A:1400:VAL:HG23	2.14	0.47
1:A:2164:TRP:CH2	1:A:2190:VAL:HG12	2.49	0.47
1:A:2325:LEU:HG	1:A:2329:TYR:CD2	2.49	0.47
1:A:238:MSE:HG3	1:A:239:GLU:HG2	1.96	0.47
1:A:3524:ASN:O	1:A:3529:ILE:HD13	2.14	0.47
1:A:3719:ILE:HG23	1:A:3720:ALA:H	1.79	0.47
1:A:3846:MSE:O	1:A:3857:LEU:HD22	2.14	0.47
1:A:410:MSE:HE2	1:A:441:MSE:CE	2.44	0.47
1:A:4077:TYR:CG	1:A:4119:ARG:NH1	2.82	0.47
1:A:977:ASP:O	1:A:980:THR:HB	2.14	0.47
1:B:1290:LEU:HD12	1:B:1294:VAL:HG21	1.97	0.47
1:B:1570:GLU:HA	1:B:1573:LYS:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1726:SER:CB	1:B:1866:GLN:HE22	2.27	0.47
1:B:2420:PHE:CZ	1:B:2424:MSE:HE3	2.49	0.47
1:B:2803:ILE:O	1:B:2803:ILE:HG12	2.14	0.47
1:B:2884:LEU:O	1:B:2888:VAL:HG23	2.15	0.47
1:B:2989:ALA:HB1	1:B:2993:PHE:CD2	2.49	0.47
1:B:3128:LYS:C	1:B:3130:GLN:H	2.17	0.47
1:B:324:SER:HB3	1:B:370:ALA:O	2.15	0.47
1:B:3762:GLN:HA	1:B:3793:VAL:CG2	2.36	0.47
1:B:458:CYS:SG	1:B:540:MSE:SE	3.23	0.47
1:B:749:VAL:N	1:B:750:PRO:HD3	2.30	0.47
2:K:215:UNK:O	2:K:219:UNK:N	2.48	0.47
1:A:1013:ILE:O	1:A:1016:GLY:N	2.48	0.47
1:A:1033:ILE:CG1	1:A:1089:PHE:HE2	2.27	0.47
1:A:1715:GLU:HA	1:A:1718:ILE:HB	1.95	0.47
1:A:1816:ARG:HD3	1:A:1819:PHE:CE1	2.49	0.47
1:A:2224:PHE:HB3	1:A:2272:VAL:HG13	1.96	0.47
1:A:2257:PHE:CD1	1:A:2299:TYR:HB3	2.49	0.47
1:A:2313:LYS:HA	1:A:2316:TYR:CD2	2.50	0.47
1:A:2390:HIS:CE1	1:A:2397:CYS:HG	2.33	0.47
1:A:2538:ARG:HD2	1:A:2562:LEU:HD22	1.96	0.47
1:A:282:PHE:CD1	1:A:282:PHE:C	2.88	0.47
1:A:2861:ILE:HD13	1:A:2889:GLY:HA2	1.96	0.47
1:A:2939:LEU:HD21	1:A:2994:TRP:CD1	2.49	0.47
1:A:2936:TYR:HD1	1:A:2949:THR:HG21	1.80	0.47
1:A:3090:TYR:O	1:A:3092:LEU:N	2.48	0.47
1:A:3284:SER:HB2	1:A:3287:ARG:HH21	1.79	0.47
1:A:3757:ASP:OD2	1:A:3759:ARG:HD3	2.14	0.47
1:A:4083:GLY:O	1:A:4088:ASN:ND2	2.44	0.47
1:A:4085:LYS:HA	1:A:4088:ASN:HB2	1.97	0.47
1:A:527:TYR:O	1:A:531:PHE:CE2	2.67	0.47
1:A:729:CYS:HA	1:A:732:PHE:CD2	2.50	0.47
1:B:1492:ALA:HB1	1:B:1493:PRO:CD	2.45	0.47
1:B:2549:LYS:HD2	1:B:2554:PHE:CB	2.44	0.47
1:B:3187:CYS:O	1:B:3190:LEU:N	2.48	0.47
1:B:3503:VAL:HG23	1:B:3536:SER:HA	1.96	0.47
1:B:3834:ALA:H	1:B:3835:PRO:HD3	1.79	0.47
1:B:3887:PHE:CE1	1:B:3900:LEU:HB3	2.47	0.47
1:B:3919:GLY:N	1:B:3946:PHE:H	2.09	0.47
1:A:1116:ALA:O	1:A:1119:LYS:HG2	2.14	0.47
1:A:1162:SER:H	1:A:1165:LEU:HD12	1.80	0.47
1:A:1689:LYS:O	1:A:1693:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1879:VAL:O	1:A:1882:SER:HB3	2.15	0.47
1:A:2023:SER:HB2	1:A:2024:TYR:CD1	2.49	0.47
1:A:2216:LEU:HD13	1:A:2249:LEU:HD21	1.97	0.47
1:A:2462:VAL:HG11	1:A:2473:MSE:CE	2.44	0.47
1:A:2936:TYR:HD2	1:A:3979:LEU:HD11	1.78	0.47
1:A:3447:VAL:HG11	1:A:3475:TYR:OH	2.15	0.47
1:A:3741:ARG:HG2	1:A:3741:ARG:NH1	2.29	0.47
1:A:3820:MSE:CB	1:A:3882:LEU:HD13	2.44	0.47
1:A:557:SER:O	1:A:560:LEU:HG	2.14	0.47
1:A:63:PHE:O	1:A:67:VAL:HG23	2.14	0.47
1:B:1076:LEU:HD11	1:B:1114:ALA:CB	2.45	0.47
1:B:170:VAL:HG23	1:B:173:LYS:CE	2.44	0.47
1:B:1718:ILE:HA	1:B:1725:GLN:OE1	2.14	0.47
1:B:1737:ASN:O	1:B:1739:TYR:N	2.46	0.47
1:B:1705:GLY:HA2	1:B:1739:TYR:OH	2.15	0.47
1:B:1760:GLU:HB2	1:B:1894:SER:HA	1.97	0.47
1:B:1945:TYR:OH	1:B:1959:LEU:HD12	2.15	0.47
1:B:2187:VAL:O	1:B:2190:VAL:HG22	2.14	0.47
1:B:2320:ALA:HA	1:B:2367:VAL:HG23	1.96	0.47
1:B:2809:PHE:HB3	1:B:2859:GLN:OE1	2.14	0.47
1:B:3011:LEU:O	1:B:3014:CYS:HB2	2.14	0.47
1:B:3196:LYS:C	1:B:3199:PRO:HD2	2.35	0.47
1:B:3499:ILE:HG13	1:B:3531:TYR:OH	2.15	0.47
1:B:3792:SER:OG	1:B:3804:GLU:HB2	2.14	0.47
1:B:2933:ILE:HG21	1:B:3976:GLU:HG3	1.96	0.47
1:B:895:ALA:HB2	1:B:904:VAL:HG21	1.96	0.47
1:B:966:PHE:CD1	1:B:969:LEU:HD13	2.50	0.47
1:B:986:PRO:C	1:B:990:GLN:HE21	2.18	0.47
2:K:217:UNK:O	2:K:220:MSE:HG2	2.15	0.47
1:A:1575:LEU:O	1:A:1635:LYS:NZ	2.39	0.47
1:A:1729:PHE:CE2	1:A:1873:TYR:CE1	3.03	0.47
1:A:174:VAL:HG12	1:A:178:LEU:HD11	1.96	0.47
1:A:2134:GLY:H	1:A:2137:ILE:HD11	1.80	0.47
1:A:2404:ARG:NH1	1:A:2412:TYR:CE1	2.82	0.47
1:A:2430:GLU:OE2	1:A:2461:PHE:CD1	2.65	0.47
1:A:3420:CYS:HB2	1:A:3446:VAL:HG11	1.96	0.47
1:A:3467:ARG:CG	1:A:3471:ILE:HD12	2.45	0.47
1:A:3920:ILE:HG13	1:A:3923:ARG:CD	2.45	0.47
1:A:3944:HIS:CD2	1:A:4020:MSE:HE3	2.49	0.47
1:A:4069:GLU:OE2	1:A:4070:LYS:HG3	2.15	0.47
1:A:3985:VAL:HG22	1:A:4104:VAL:HG21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:PHE:O	1:A:72:SER:OG	2.23	0.47
1:A:798:GLY:HA2	1:A:873:VAL:HG11	1.96	0.47
1:B:1118:GLU:O	1:B:1120:SER:N	2.47	0.47
1:B:2385:LEU:HG	1:B:2389:PHE:CE2	2.49	0.47
1:B:3040:TYR:HA	1:B:3043:TYR:CD2	2.50	0.47
1:B:3122:HIS:O	1:B:3125:ARG:N	2.47	0.47
1:B:3247:ARG:HD3	1:B:3281:CYS:SG	2.55	0.47
1:B:3251:ASN:HD21	1:B:3254:LEU:HD13	1.80	0.47
1:B:3659:PHE:CD1	1:B:3662:ILE:HD12	2.50	0.47
1:B:3459:ASN:ND2	1:B:3710:LYS:HZ3	2.12	0.47
1:B:704:PHE:HA	1:B:707:PHE:CD1	2.50	0.47
1:B:858:MSE:O	1:B:861:SER:N	2.48	0.47
1:A:1036:PHE:CZ	1:A:1082:PHE:CE2	3.03	0.47
1:A:1131:ILE:HG12	1:A:1132:ASP:N	2.29	0.47
1:A:1701:SER:OG	1:A:1702:LEU:N	2.48	0.47
1:A:1970:LYS:HZ1	1:A:2018:ASP:N	2.13	0.47
1:A:205:LYS:O	1:A:208:MSE:HG2	2.15	0.47
1:A:241:ASP:HB2	1:A:282:PHE:HE2	1.80	0.47
1:A:257:ARG:H	1:A:258:PRO:HD2	1.78	0.47
1:A:3080:LEU:HD13	1:A:3102:TYR:OH	2.15	0.47
1:A:3386:SER:HA	1:A:3389:VAL:HG12	1.97	0.47
1:A:3393:GLU:OE1	1:A:3416:LEU:HD23	2.15	0.47
1:A:3510:GLN:CD	1:A:3513:ALA:HB2	2.35	0.47
1:A:3583:LEU:HD11	1:A:3733:ARG:CB	2.42	0.47
1:A:384:MSE:O	1:A:385:TYR:HB3	2.15	0.47
1:A:2891:ARG:HH21	1:A:3884:LYS:HD3	1.76	0.47
1:A:667:TYR:O	1:A:669:LEU:N	2.47	0.47
1:A:776:TRP:CZ2	1:A:780:ILE:HD12	2.50	0.47
1:A:928:VAL:HG23	1:A:929:ALA:N	2.29	0.47
1:B:963:LYS:HG3	1:B:1009:LEU:CD1	2.45	0.47
1:B:1036:PHE:HD1	1:B:1059:LEU:HD11	1.79	0.47
1:B:1068:LEU:HD11	1:B:1110:SER:OG	2.15	0.47
1:B:1302:ALA:O	1:B:1306:ILE:HB	2.15	0.47
1:B:2239:LYS:CG	1:B:2279:ILE:HD12	2.45	0.47
1:B:2254:ARG:HB2	1:B:2295:GLN:HB2	1.97	0.47
1:B:2407:GLY:O	1:B:2409:THR:HG23	2.15	0.47
1:B:2379:MSE:HG2	1:B:2408:MSE:SE	2.65	0.47
1:B:2987:THR:O	1:B:2990:GLU:HB2	2.14	0.47
1:B:3160:LEU:HB3	1:B:3164:TRP:CZ3	2.50	0.47
1:B:3243:ILE:HG23	1:B:3258:LEU:HD12	1.96	0.47
1:B:3244:ASP:O	1:B:3247:ARG:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3503:VAL:CG2	1:B:3536:SER:HA	2.45	0.47
1:B:3720:ALA:HB2	1:B:3743:HIS:HB2	1.96	0.47
1:B:3944:HIS:ND1	1:B:3949:ALA:HA	2.29	0.47
1:B:777:SER:HB2	1:B:858:MSE:HE1	1.97	0.47
1:B:943:GLY:O	1:B:945:ALA:N	2.45	0.47
1:B:987:LEU:O	1:B:991:LEU:HD13	2.15	0.47
1:A:1251:GLN:HE21	1:A:1329:ARG:NH1	2.13	0.47
1:A:125:ILE:H	1:A:126:PRO:CD	2.28	0.47
1:A:1292:LYS:O	1:A:1295:ALA:HB3	2.15	0.47
1:A:1335:CYS:SG	1:A:1382:ILE:HG21	2.55	0.47
1:A:474:VAL:HG11	1:A:1564:SER:HB2	1.97	0.47
1:A:1685:ASP:CB	1:A:1727:ARG:NH2	2.74	0.47
1:A:1745:LYS:C	1:A:1747:LEU:N	2.68	0.47
1:A:1598:ASN:ND2	1:A:1811:ARG:HB3	2.30	0.47
1:A:2260:PHE:HA	1:A:2273:GLY:HA3	1.96	0.47
1:A:234:PHE:O	1:A:235:THR:OG1	2.22	0.47
1:A:2637:UNK:O	1:A:2641:UNK:CB	2.63	0.47
1:A:2856:SER:O	1:A:2859:GLN:HB3	2.15	0.47
1:A:3011:LEU:HD11	1:A:3043:TYR:O	2.15	0.47
1:A:3053:LEU:HD11	1:A:3187:CYS:HB3	1.96	0.47
1:A:3147:LYS:O	1:A:3151:LEU:N	2.48	0.47
1:A:3533:PHE:CD1	1:A:3562:LEU:HB3	2.50	0.47
1:A:544:ILE:O	1:A:548:GLU:HB2	2.14	0.47
1:A:927:LYS:O	1:A:931:CYS:SG	2.73	0.47
1:B:133:LYS:O	1:B:137:THR:HG23	2.15	0.47
1:B:1349:LEU:CA	1:B:1353:PRO:HD2	2.44	0.47
1:B:1350:ASN:HD22	1:B:1404:LYS:HE3	1.79	0.47
1:B:1583:MSE:SE	1:B:1643:MSE:SE	3.32	0.47
1:B:1952:ILE:HG12	1:B:1953:CYS:H	1.79	0.47
1:B:2097:LEU:CD2	1:B:2100:LEU:HD22	2.45	0.47
1:B:257:ARG:N	1:B:258:PRO:CD	2.77	0.47
1:B:260:ILE:O	1:B:264:ARG:HG2	2.15	0.47
1:B:2970:LYS:O	1:B:2974:GLU:HG2	2.14	0.47
1:B:3059:GLN:CD	1:B:3059:GLN:H	2.17	0.47
1:B:3284:SER:CA	1:B:3287:ARG:HE	2.12	0.47
1:B:3298:LEU:HD11	1:B:3351:ILE:CD1	2.45	0.47
1:B:3585:PHE:HE1	1:B:3617:LEU:HD11	1.79	0.47
1:B:3904:PHE:CE1	1:B:3967:PHE:HE1	2.32	0.47
1:B:3965:ARG:HE	1:B:3969:ASN:ND2	2.14	0.47
1:B:3981:TYR:HA	1:B:4108:MSE:HE1	1.96	0.47
1:B:912:PRO:HB2	1:B:913:ARG:CZ	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1059:LEU:O	1:A:1062:ARG:N	2.48	0.46
1:A:1583:MSE:HE2	1:A:1639:LEU:HD13	1.97	0.46
1:A:1601:LEU:O	1:A:1605:PHE:HB2	2.14	0.46
1:A:1687:HIS:HB3	1:A:1691:GLN:NE2	2.30	0.46
1:A:358:GLU:OE1	1:A:1858:LEU:HD13	2.15	0.46
1:A:2323:LEU:HD13	1:A:2371:PHE:CZ	2.50	0.46
1:A:2473:MSE:O	1:A:2476:ILE:HG12	2.14	0.46
1:A:2514:ASN:H	1:A:2515:PRO:CD	2.29	0.46
1:A:242:PRO:HD3	1:A:282:PHE:CE2	2.50	0.46
1:A:3620:PRO:HB2	1:A:3633:ILE:HG23	1.95	0.46
1:A:3699:LEU:O	1:A:3718:ARG:NH1	2.47	0.46
1:A:3887:PHE:HZ	1:A:3904:PHE:CD2	2.33	0.46
1:A:3928:PHE:C	1:A:3928:PHE:CD1	2.88	0.46
1:A:443:ILE:HD11	1:A:465:PHE:HE2	1.80	0.46
1:A:797:ASP:HA	1:A:800:LEU:HB2	1.96	0.46
1:A:934:LEU:HD21	1:A:962:TYR:CZ	2.49	0.46
1:B:1563:PHE:CD1	1:B:1567:ILE:HG13	2.50	0.46
1:B:2404:ARG:NH1	1:B:2412:TYR:CE2	2.83	0.46
1:B:2439:ILE:HG21	1:B:2439:ILE:HD13	1.64	0.46
1:B:2554:PHE:O	1:B:2557:LEU:N	2.48	0.46
1:B:277:LEU:HD22	1:B:278:HIS:CD2	2.51	0.46
1:B:361:ILE:HB	1:B:364:ARG:NH2	2.30	0.46
1:B:3457:ASN:O	1:B:3710:LYS:NZ	2.47	0.46
1:B:3722:PHE:HD1	1:B:3740:ILE:HA	1.80	0.46
1:B:4081:ALA:HA	1:B:4113:ASP:OD2	2.13	0.46
1:B:670:LEU:HG	1:B:740:ILE:HG23	1.97	0.46
1:B:732:PHE:CE1	1:B:768:VAL:HG12	2.50	0.46
1:B:965:THR:HA	1:B:968:VAL:HG12	1.95	0.46
1:A:1010:LEU:O	1:A:1013:ILE:N	2.39	0.46
1:A:1373:VAL:O	1:A:1375:THR:N	2.41	0.46
1:A:186:PRO:O	1:A:189:MSE:HB3	2.16	0.46
1:A:1976:LEU:HD11	1:A:2031:LEU:CB	2.44	0.46
1:A:2186:VAL:O	1:A:2189:ILE:HG13	2.15	0.46
1:A:2199:LEU:HA	1:A:2202:PRO:HD2	1.97	0.46
1:A:2418:LYS:O	1:A:2421:VAL:HG12	2.15	0.46
1:A:2554:PHE:O	1:A:2557:LEU:HB2	2.16	0.46
1:A:2900:LEU:HD23	1:A:2910:VAL:HA	1.97	0.46
1:A:3008:TRP:CA	1:A:3050:LYS:HG2	2.44	0.46
1:A:348:ILE:O	1:A:364:ARG:HD3	2.16	0.46
1:A:3674:SER:C	1:A:3677:PRO:HD2	2.35	0.46
1:A:3931:ALA:HB3	1:A:3936:GLY:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4069:GLU:HA	1:A:4070:LYS:HA	1.64	0.46
1:B:1231:GLN:H	1:B:1232:PRO:CD	2.28	0.46
1:B:1259:LEU:HD11	1:B:1337:VAL:HA	1.97	0.46
1:B:135:LEU:O	1:B:139:ARG:HG3	2.15	0.46
1:B:401:ASP:HB2	1:B:1763:THR:HB	1.98	0.46
1:B:1874:TYR:OH	1:B:1884:LEU:HD12	2.15	0.46
1:B:2289:ASP:O	1:B:2290:PRO:C	2.53	0.46
1:B:381:VAL:O	1:B:384:MSE:HG2	2.14	0.46
1:B:763:THR:HG21	1:B:769:GLY:HA3	1.97	0.46
1:A:135:LEU:HD22	1:A:173:LYS:HB2	1.97	0.46
1:A:1376:LEU:HG	1:A:1377:CYS:N	2.30	0.46
1:A:1495:ASP:O	1:A:1498:GLN:HB2	2.15	0.46
1:A:1696:LEU:HD23	1:A:1700:THR:HG21	1.97	0.46
1:A:1985:LYS:HD2	1:A:2037:SER:HB3	1.98	0.46
1:A:2233:HIS:O	1:A:2237:ILE:HG13	2.15	0.46
1:A:2823:PHE:CG	1:A:2824:LYS:N	2.83	0.46
1:A:2949:THR:O	1:A:2952:ILE:N	2.46	0.46
1:A:3141:PHE:CE1	1:A:3189:PHE:HA	2.51	0.46
1:A:3762:GLN:HA	1:A:3793:VAL:CG2	2.41	0.46
1:A:385:TYR:HE1	1:A:421:LEU:HD23	1.79	0.46
1:A:399:GLN:OE1	1:A:405:ASP:HB2	2.16	0.46
1:A:436:GLU:OE2	1:A:475:LEU:CD1	2.63	0.46
1:A:777:SER:O	1:A:781:ASP:N	2.48	0.46
1:B:1455:CYS:O	1:B:1458:LEU:N	2.49	0.46
1:B:1602:ASP:HB2	1:B:1810:PRO:HB3	1.98	0.46
1:B:2009:LYS:HG3	1:B:2012:ARG:NH1	2.30	0.46
1:B:2067:ARG:O	1:B:2068:ARG:HB2	2.14	0.46
1:B:222:GLY:O	1:B:225:LYS:N	2.49	0.46
1:B:3616:ALA:O	1:B:3617:LEU:HD23	2.16	0.46
1:B:4002:MSE:SE	1:B:4048:LYS:CE	3.12	0.46
1:B:3855:TYR:HB3	1:B:4074:PHE:HZ	1.80	0.46
1:B:431:TYR:N	1:B:431:TYR:CD1	2.79	0.46
1:B:487:LEU:HD21	1:B:530:LEU:HB2	1.97	0.46
1:B:543:SER:O	1:B:545:LEU:N	2.37	0.46
1:B:789:TYR:HB2	1:B:865:GLN:HE21	1.81	0.46
1:A:1395:LEU:N	1:A:1396:PRO:HD2	2.30	0.46
1:A:1476:HIS:CE1	1:A:1507:CYS:HA	2.50	0.46
1:A:1589:ASN:O	1:A:1590:THR:HG22	2.16	0.46
1:A:1604:SER:CB	1:A:1632:TRP:HE3	2.28	0.46
1:A:1602:ASP:HB2	1:A:1810:PRO:HB3	1.96	0.46
1:A:1874:TYR:HD2	1:A:1885:PRO:HG3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2177:ASN:HB3	1:A:2182:ILE:N	2.30	0.46
1:A:2240:THR:HG21	2:K:112:UNK:HA	1.98	0.46
1:A:2310:VAL:HG23	1:A:2315:VAL:HG21	1.98	0.46
1:A:2834:GLN:O	1:A:2837:LEU:HG	2.15	0.46
1:A:350:ARG:NH1	1:A:387:GLU:OE1	2.49	0.46
1:A:730:LEU:HA	1:A:730:LEU:HD23	1.82	0.46
1:A:764:PRO:HB3	1:A:770:LEU:HD11	1.97	0.46
1:A:849:GLU:H	1:A:849:GLU:CD	2.18	0.46
1:B:70:ARG:HH12	1:B:117:LYS:HD2	1.80	0.46
1:B:158:GLY:O	1:B:162:LEU:HD13	2.15	0.46
1:B:1809:ASP:O	1:B:1815:THR:HG22	2.14	0.46
1:B:1917:LYS:HE2	1:B:1953:CYS:O	2.14	0.46
1:B:2312:TYR:CZ	1:B:2313:LYS:HG2	2.50	0.46
1:B:241:ASP:HB3	1:B:282:PHE:HE2	1.78	0.46
1:B:3160:LEU:HD23	1:B:3164:TRP:CH2	2.51	0.46
1:B:3283:LEU:O	1:B:3283:LEU:HD22	2.16	0.46
1:B:3740:ILE:HD12	1:B:3750:PHE:CE1	2.51	0.46
1:B:3816:LEU:O	1:B:3820:MSE:CB	2.64	0.46
1:B:3463:LEU:HD13	1:B:4000:ASN:CB	2.45	0.46
1:B:852:ARG:HH12	1:B:3111:MSE:HG2	1.79	0.46
1:B:892:LEU:HD11	1:B:958:MSE:HG3	1.98	0.46
1:B:898:PHE:CD2	1:B:2566:THR:HG21	2.50	0.46
1:A:964:ARG:CB	1:A:1009:LEU:HD22	2.35	0.46
1:A:1012:ALA:O	1:A:1015:ASP:HB3	2.15	0.46
1:A:993:HIS:HB2	1:A:1038:LYS:CG	2.45	0.46
1:A:1072:ALA:HB1	1:A:1076:LEU:CD1	2.46	0.46
1:A:1494:GLY:O	1:A:1498:GLN:HG3	2.15	0.46
1:A:1593:VAL:O	1:A:1597:LEU:CB	2.62	0.46
1:A:429:GLU:HG2	1:A:1594:SER:HB2	1.97	0.46
1:A:1636:ASP:HA	1:A:1639:LEU:HD11	1.98	0.46
1:A:1651:LYS:HD2	1:A:1684:LEU:HG	1.98	0.46
1:A:1897:ASN:HB3	1:A:1901:HIS:CE1	2.50	0.46
1:A:1934:LEU:HD11	1:A:1937:ARG:H	1.80	0.46
1:A:1933:LEU:H	1:A:1938:ARG:NH2	2.13	0.46
1:A:2923:TRP:CD1	1:A:2926:LEU:HD23	2.50	0.46
1:A:3121:LEU:O	1:A:3124:SER:HB2	2.14	0.46
1:A:3297:VAL:HG11	1:A:3332:THR:HG23	1.97	0.46
1:B:1423:ILE:HG13	1:B:1424:THR:H	1.81	0.46
1:B:1447:ARG:O	1:B:1451:VAL:HG23	2.15	0.46
1:B:1592:MSE:O	1:B:1596:VAL:HG12	2.16	0.46
1:B:1865:THR:O	1:B:1869:LYS:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:LEU:HB3	1:B:197:PHE:CE1	2.49	0.46
1:B:2383:PHE:CE1	1:B:2412:TYR:HD1	2.34	0.46
1:B:2413:PHE:HD2	1:B:2445:LYS:HG3	1.76	0.46
1:B:3334:TYR:HE1	1:B:3426:LYS:HD3	1.81	0.46
1:B:3813:LYS:HE3	1:B:3926:ASN:HB2	1.98	0.46
1:B:368:LEU:HD21	1:B:384:MSE:SE	2.66	0.46
1:B:4057:ALA:C	1:B:4059:ILE:N	2.69	0.46
1:B:4085:LYS:HA	1:B:4088:ASN:HB3	1.98	0.46
1:B:648:SER:O	1:B:651:TYR:HB2	2.15	0.46
1:A:1917:LYS:HD2	1:A:1953:CYS:HB3	1.98	0.46
1:A:2177:ASN:HB2	1:A:2182:ILE:HG23	1.97	0.46
1:A:2232:ARG:O	1:A:2234:ASN:N	2.49	0.46
1:A:2260:PHE:CZ	1:A:2306:ASN:HB2	2.51	0.46
1:A:2371:PHE:CG	1:A:2372:PRO:HD3	2.51	0.46
1:A:2555:LEU:HD12	1:A:2556:SER:H	1.79	0.46
1:A:2776:ARG:O	1:A:2780:LEU:HD23	2.15	0.46
1:A:2575:PRO:HB3	1:A:2789:SER:N	2.31	0.46
1:A:3463:LEU:HD13	1:A:4000:ASN:HB2	1.97	0.46
1:A:3549:HIS:NE2	1:A:3553:GLU:HG3	2.30	0.46
1:A:3578:LEU:HB3	1:A:3579:SER:HA	1.97	0.46
1:A:3722:PHE:CE1	1:A:3740:ILE:HA	2.51	0.46
1:A:3817:LEU:HD23	1:A:3820:MSE:CE	2.45	0.46
1:A:3944:HIS:HA	1:A:4016:PHE:HZ	1.81	0.46
1:A:3966:GLN:HG2	1:A:4128:MSE:O	2.15	0.46
1:A:434:VAL:HG23	1:A:437:HIS:CE1	2.51	0.46
1:A:471:LYS:HG3	1:A:1553:PHE:HZ	1.81	0.46
1:A:512:GLY:HA2	1:A:602:MSE:CE	2.45	0.46
1:A:649:PHE:C	1:A:651:TYR:H	2.18	0.46
1:A:749:VAL:N	1:A:750:PRO:CD	2.79	0.46
1:A:89:LEU:HA	1:A:92:PHE:CD2	2.50	0.46
1:B:1565:GLU:HG2	1:B:1566:THR:HG23	1.97	0.46
1:B:2142:ILE:O	1:B:2145:PHE:HB2	2.16	0.46
1:B:2159:PRO:HA	1:B:2162:LYS:HB2	1.98	0.46
1:B:2539:LEU:HB3	1:B:2816:ILE:CD1	2.46	0.46
1:B:3092:LEU:O	1:B:3192:LYS:NZ	2.42	0.46
1:B:3167:ARG:CD	1:B:3186:ARG:HG2	2.45	0.46
1:B:3578:LEU:HD13	1:B:3683:CYS:SG	2.56	0.46
1:B:3701:ILE:HG13	1:B:3701:ILE:O	2.15	0.46
1:B:12:LEU:HD12	1:B:58:VAL:HG21	1.97	0.46
1:B:617:PRO:CB	1:B:659:ARG:HD2	2.45	0.46
1:A:1138:ILE:HD13	1:A:1150:LYS:CE	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1382:ILE:HB	1:A:1386:ILE:CD1	2.44	0.46
1:A:1633:TRP:HA	1:A:1636:ASP:OD2	2.15	0.46
1:A:2004:TYR:C	1:A:2004:TYR:CD1	2.88	0.46
1:A:2097:LEU:HA	1:A:2097:LEU:HD23	1.77	0.46
1:A:2190:VAL:O	1:A:2193:ILE:HG22	2.16	0.46
1:A:2220:MSE:O	1:A:2223:VAL:HG12	2.16	0.46
1:A:2252:PRO:HA	1:A:2254:ARG:NH1	2.31	0.46
1:A:231:LEU:HD23	1:A:234:PHE:HB3	1.98	0.46
1:A:2433:LYS:HG3	1:A:2436:LEU:CD1	2.42	0.46
1:A:2861:ILE:HD12	1:A:2892:LEU:HD23	1.97	0.46
1:A:852:ARG:HH12	1:A:3110:PHE:HE1	1.61	0.46
1:A:3971:MSE:HE1	1:A:3980:MSE:HE1	1.97	0.46
1:A:4066:LEU:HD21	1:A:4078:VAL:CG2	2.46	0.46
1:A:608:PRO:HG2	1:A:1798:LEU:HD12	1.97	0.46
1:B:1119:LYS:NZ	1:B:1256:TRP:HE1	2.13	0.46
1:B:1449:ALA:HA	1:B:1452:VAL:HB	1.96	0.46
1:B:2002:LYS:C	1:B:2004:TYR:N	2.68	0.46
1:B:2374:LEU:N	1:B:2378:PHE:HE1	2.14	0.46
1:B:2926:LEU:HD22	1:B:2931:ARG:NE	2.31	0.46
1:B:2962:ARG:HG3	1:B:3253:SER:OG	2.16	0.46
1:B:3173:MSE:HG2	1:B:3174:ASP:OD1	2.15	0.46
1:B:3323:PHE:O	1:B:3326:GLN:N	2.48	0.46
1:B:3630:ARG:HD2	1:B:3633:ILE:HG12	1.98	0.46
1:B:3878:VAL:HB	1:B:3879:PRO:HD3	1.98	0.46
1:B:598:PRO:HG3	1:B:1022:ASP:O	2.16	0.46
1:B:655:LEU:HA	1:B:655:LEU:HD12	1.60	0.46
1:A:1132:ASP:O	1:A:1135:CYS:N	2.49	0.46
1:A:1378:GLU:O	1:A:1381:SER:N	2.49	0.46
1:A:1521:PHE:HA	1:A:1524:LEU:HD22	1.98	0.46
1:A:1652:ILE:HA	1:A:1655:ILE:HD12	1.97	0.46
1:A:2011:ALA:HB3	1:A:2014:ALA:HB2	1.98	0.46
1:A:2221:LYS:O	1:A:2225:HIS:CE1	2.69	0.46
1:A:2385:LEU:HG	1:A:2389:PHE:CZ	2.51	0.46
1:A:2828:GLU:O	1:A:2832:ILE:HG13	2.15	0.46
1:A:3024:PRO:N	1:A:3025:PRO:HD3	2.31	0.46
1:A:3059:GLN:H	1:A:3059:GLN:CD	2.19	0.46
1:A:3292:GLY:O	1:A:3297:VAL:HG23	2.15	0.46
1:A:3593:ARG:HH11	1:A:3593:ARG:HG2	1.81	0.46
1:A:3771:MSE:SE	1:A:3991:PHE:HE1	2.49	0.46
1:A:4077:TYR:CZ	1:A:4119:ARG:HD2	2.51	0.46
1:A:513:GLU:OE1	1:A:655:LEU:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1690:GLY:O	1:B:1694:THR:HG22	2.16	0.46
1:B:2000:ARG:HG2	1:B:2001:LYS:HG3	1.97	0.46
1:B:2369:LYS:HE3	1:B:2406:GLU:OE1	2.16	0.46
1:B:239:GLU:C	1:B:242:PRO:HD2	2.36	0.46
1:B:2869:LEU:HB3	1:B:2893:LEU:HG	1.96	0.46
1:B:3052:LEU:HD11	1:B:3092:LEU:HG	1.97	0.46
1:B:3241:LYS:C	1:B:3243:ILE:H	2.18	0.46
1:B:3272:TRP:CZ3	1:B:3307:LEU:HD21	2.51	0.46
1:B:3439:LEU:O	1:B:3443:PRO:HD3	2.16	0.46
1:B:3499:ILE:CG2	1:B:3535:ILE:HD13	2.41	0.46
1:B:3868:VAL:HG13	1:B:3872:ARG:HB2	1.98	0.46
1:B:575:ILE:HB	1:B:605:THR:CA	2.46	0.46
1:A:67:VAL:HG22	1:A:110:THR:HG21	1.97	0.46
1:A:1455:CYS:O	1:A:1458:LEU:HB2	2.16	0.46
1:A:1563:PHE:CE1	1:A:1567:ILE:HG13	2.51	0.46
1:A:1652:ILE:HG21	1:A:1716:GLN:OE1	2.15	0.46
1:A:1760:GLU:HB2	1:A:1894:SER:HA	1.97	0.46
1:A:2100:LEU:O	1:A:2104:MSE:HB2	2.16	0.46
1:A:2164:TRP:HH2	1:A:2190:VAL:CG1	2.29	0.46
1:A:2183:HIS:C	1:A:2187:VAL:HB	2.26	0.46
1:A:2255:LEU:HD12	1:A:2258:GLU:HB2	1.98	0.46
1:A:2232:ARG:HH22	1:A:2313:LYS:NZ	2.13	0.46
1:A:2517:LEU:HD23	1:A:2517:LEU:H	1.80	0.46
1:A:2801:ASP:HB2	1:A:2802:PRO:HD3	1.98	0.46
1:A:3092:LEU:O	1:A:3192:LYS:NZ	2.45	0.46
1:A:805:LEU:HD13	1:A:3117:ILE:HD13	1.98	0.46
1:A:295:GLU:CD	1:A:341:PHE:HE1	2.19	0.46
1:A:3694:PHE:CD2	1:A:3697:ASN:HA	2.51	0.46
1:A:431:TYR:CD1	1:A:431:TYR:N	2.84	0.46
1:A:878:GLU:C	1:A:880:MSE:H	2.19	0.46
1:A:971:ARG:CG	1:A:972:LEU:N	2.69	0.46
1:A:973:ALA:HB1	1:A:977:ASP:OD2	2.16	0.46
1:B:1747:LEU:HA	1:B:1747:LEU:HD23	1.77	0.46
1:B:172:GLU:HG2	1:B:221:ALA:HB3	1.98	0.46
1:B:2312:TYR:CG	1:B:2313:LYS:N	2.83	0.46
1:B:2900:LEU:HD23	1:B:2910:VAL:HA	1.98	0.46
1:B:3141:PHE:HA	1:B:3144:PHE:CE2	2.51	0.46
1:B:3091:LEU:O	1:B:3192:LYS:HE2	2.15	0.46
1:B:3408:GLY:O	1:B:3411:ASP:HB2	2.16	0.46
1:B:3534:ILE:H	1:B:3534:ILE:HD12	1.79	0.46
1:B:3829:LEU:HA	1:B:3829:LEU:HD12	1.60	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:THR:C	1:B:400:THR:N	2.68	0.46
1:B:403:GLY:C	1:B:405:ASP:N	2.67	0.46
1:B:560:LEU:CB	1:B:616:LYS:HG2	2.46	0.46
1:A:2069:ARG:HG2	2:K:204:UNK:CB	2.46	0.46
1:A:1133:HIS:CG	1:A:1133:HIS:O	2.68	0.46
1:A:1856:THR:HB	1:A:1860:GLU:OE1	2.16	0.46
1:A:1927:MSE:HE3	1:A:1927:MSE:HB2	1.62	0.46
1:A:2129:LEU:HD22	1:A:2144:LEU:HD11	1.96	0.46
1:A:2313:LYS:HA	1:A:2316:TYR:HE2	1.79	0.46
1:A:3583:LEU:HD21	1:A:3733:ARG:NH1	2.31	0.46
1:A:3780:ALA:CB	1:A:3784:ARG:HH12	2.29	0.46
1:A:3819:THR:O	1:A:3823:GLU:HG2	2.16	0.46
1:A:3900:LEU:HA	1:A:3900:LEU:HD12	1.80	0.46
1:A:4062:ASP:O	1:A:4066:LEU:HD13	2.16	0.46
1:A:982:GLN:O	1:A:986:PRO:CD	2.63	0.46
1:B:1430:GLU:OE1	1:B:1448:LEU:HA	2.16	0.46
1:B:1810:PRO:O	1:B:1811:ARG:HD2	2.16	0.46
1:B:1889:VAL:HG22	1:B:1900:PHE:CD2	2.51	0.46
1:B:1911:LEU:HD13	1:B:1916:ILE:HG22	1.97	0.46
1:B:2135:ASN:N	1:B:2136:PRO:CD	2.79	0.46
1:B:2161:ALA:O	1:B:2164:TRP:HB2	2.16	0.46
1:B:2241:LEU:H	1:B:2241:LEU:HG	1.53	0.46
1:B:2352:HIS:O	1:B:2360:PHE:HD2	1.99	0.46
1:B:2373:PRO:HA	1:B:2378:PHE:HZ	1.80	0.46
1:B:2386:LEU:O	1:B:2390:HIS:CB	2.64	0.46
1:B:257:ARG:H	1:B:258:PRO:CD	2.29	0.46
1:B:3483:MSE:O	1:B:3516:HIS:CE1	2.69	0.46
1:B:3872:ARG:O	1:B:3876:SER:CB	2.64	0.46
1:B:408:TYR:C	1:B:408:TYR:CD1	2.90	0.46
1:B:2957:LEU:HB3	1:B:4100:GLU:OE2	2.16	0.46
1:B:504:GLU:O	1:B:508:HIS:CG	2.69	0.46
1:B:578:LYS:O	1:B:581:LEU:HB2	2.16	0.46
1:B:620:PHE:HE1	1:B:623:PHE:HD2	1.64	0.46
1:B:752:LEU:HB2	1:B:756:PHE:CE1	2.51	0.46
1:A:1426:GLN:O	1:A:1430:GLU:HG3	2.16	0.45
1:A:1802:TYR:HA	1:A:1805:PHE:CD2	2.48	0.45
1:A:2035:THR:O	1:A:2039:GLU:HG3	2.16	0.45
1:A:2147:ALA:O	1:A:2151:ILE:N	2.49	0.45
1:A:2223:VAL:HG21	1:A:2238:ILE:HB	1.98	0.45
1:A:2356:MSE:HE2	1:A:2359:LYS:HD2	1.97	0.45
1:A:252:VAL:HB	1:A:265:TYR:HD1	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2874:ALA:O	1:A:2878:ALA:N	2.50	0.45
1:A:2921:LEU:HD12	1:A:2922:ARG:N	2.31	0.45
1:A:3326:GLN:OE1	1:A:3393:GLU:OE2	2.34	0.45
1:A:3413:TYR:CD1	1:A:3449:LYS:HB3	2.51	0.45
1:A:3564:GLN:C	1:A:3566:GLY:H	2.19	0.45
1:A:382:ASP:O	1:A:386:VAL:CB	2.58	0.45
1:A:3997:LEU:O	1:A:4001:THR:HG23	2.17	0.45
1:A:752:LEU:HB2	1:A:756:PHE:HE1	1.79	0.45
1:A:93:LEU:HD23	1:A:93:LEU:HA	1.78	0.45
1:B:1014:LEU:HB2	1:B:1078:ALA:CB	2.43	0.45
1:B:1630:ASP:HA	1:B:1633:TRP:HE3	1.81	0.45
1:B:1879:VAL:HG23	1:B:1920:TYR:CD2	2.51	0.45
1:B:1989:ASN:HB3	1:B:2040:MSE:SE	2.66	0.45
1:B:2373:PRO:HA	1:B:2378:PHE:CZ	2.51	0.45
1:B:2389:PHE:CG	1:B:2396:LEU:HD22	2.51	0.45
1:B:2405:VAL:O	1:B:2408:MSE:HB2	2.16	0.45
1:B:2538:ARG:NH1	1:B:2562:LEU:HA	2.31	0.45
1:B:2908:LYS:HA	1:B:2908:LYS:HD3	1.72	0.45
1:B:3582:GLU:OE2	1:B:3675:LYS:HG3	2.16	0.45
1:B:3703:GLY:H	1:B:3717:VAL:HG13	1.80	0.45
1:B:3866:GLU:HA	1:B:3869:THR:OG1	2.16	0.45
1:B:3954:PRO:CB	1:B:4027:TRP:HA	2.46	0.45
1:B:406:ARG:HB3	1:B:408:TYR:CD2	2.51	0.45
1:B:528:VAL:HA	1:B:531:PHE:CE2	2.51	0.45
1:B:634:LEU:O	1:B:638:GLN:NE2	2.49	0.45
1:B:756:PHE:CD2	1:B:773:LEU:HB3	2.51	0.45
1:A:992:ILE:HD13	1:A:1035:GLU:HB2	1.98	0.45
1:A:1076:LEU:HD21	1:A:1114:ALA:HB1	1.99	0.45
1:A:1334:LYS:HA	1:A:1334:LYS:HD3	1.82	0.45
1:A:1386:ILE:HB	1:A:1391:VAL:CG2	2.45	0.45
1:A:1460:ARG:HD2	1:A:1460:ARG:H	1.81	0.45
1:A:356:ASN:OD1	1:A:1859:ASN:HB2	2.16	0.45
1:A:1894:SER:O	1:A:1897:ASN:N	2.33	0.45
1:A:1966:LEU:HD22	1:A:1991:PRO:CB	2.42	0.45
1:A:2423:VAL:O	1:A:2425:ARG:N	2.50	0.45
1:A:264:ARG:O	1:A:268:PRO:HD3	2.15	0.45
1:A:2785:ILE:O	1:A:2785:ILE:HG12	2.16	0.45
1:A:2806:LYS:O	1:A:2806:LYS:HG2	2.15	0.45
1:A:3141:PHE:HA	1:A:3144:PHE:CE2	2.51	0.45
1:A:3530:VAL:HA	1:A:3533:PHE:CD2	2.51	0.45
1:A:44:LEU:HG	1:A:44:LEU:H	1.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:760:LEU:O	1:A:764:PRO:HG3	2.16	0.45
1:A:968:VAL:O	1:A:971:ARG:HG2	2.16	0.45
1:B:1559:PHE:CE1	1:B:1592:MSE:HE2	2.52	0.45
1:B:1875:LYS:HG3	1:B:1876:ILE:HB	1.99	0.45
1:B:2157:PHE:CD1	1:B:2157:PHE:C	2.90	0.45
1:B:2316:TYR:O	1:B:2319:ALA:HB3	2.17	0.45
1:B:2893:LEU:O	1:B:2897:LEU:N	2.47	0.45
1:B:3243:ILE:HG12	1:B:3258:LEU:CD1	2.40	0.45
1:B:3393:GLU:O	1:B:3397:GLN:OE1	2.34	0.45
1:B:3808:ASN:HB3	1:B:3933:GLU:HG2	1.98	0.45
1:B:3920:ILE:HD13	1:B:3961:PHE:HA	1.98	0.45
1:B:4090:ARG:HD3	1:B:4090:ARG:HA	1.71	0.45
1:B:2957:LEU:HD21	1:B:4101:GLU:HG3	1.97	0.45
1:B:392:CYS:SG	1:B:438:LEU:HD11	2.57	0.45
1:B:637:LYS:O	1:B:641:PHE:CB	2.58	0.45
1:B:657:SER:O	1:B:660:LEU:HB2	2.16	0.45
1:B:910:PHE:HE2	1:B:941:MSE:SE	2.49	0.45
1:A:1099:PHE:CG	1:A:1100:VAL:N	2.84	0.45
1:A:1416:GLU:HB3	1:A:1420:ARG:HD2	1.97	0.45
1:A:1604:SER:HA	1:A:1632:TRP:HE3	1.80	0.45
1:A:1939:LEU:HD13	1:A:1986:ARG:NH2	2.30	0.45
1:A:19:LEU:O	1:A:23:ASP:CB	2.62	0.45
1:A:2074:PRO:HB3	1:A:2136:PRO:HB3	1.98	0.45
1:A:2126:MSE:HE2	1:A:2126:MSE:HB2	1.79	0.45
1:A:2260:PHE:HZ	1:A:2306:ASN:HB2	1.82	0.45
1:A:252:VAL:C	1:A:254:LYS:H	2.20	0.45
1:A:313:LEU:HD22	1:A:317:GLU:OE2	2.16	0.45
1:A:3291:GLN:NE2	1:A:3294:SER:OG	2.50	0.45
1:A:3477:GLU:HA	1:A:3480:LEU:HG	1.98	0.45
1:A:3513:ALA:O	1:A:3516:HIS:N	2.49	0.45
1:A:3771:MSE:HE1	1:A:3917:ILE:HG21	1.97	0.45
1:A:3612:ARG:HD3	1:A:3799:ARG:HH21	1.82	0.45
1:A:3853:GLY:C	1:A:3855:TYR:H	2.18	0.45
1:A:2940:ARG:HD3	1:A:3975:LYS:HD2	1.97	0.45
1:A:3981:TYR:CE1	1:A:4105:LYS:HA	2.51	0.45
1:B:1014:LEU:HD23	1:B:1028:PHE:CE2	2.51	0.45
1:B:11:SER:OG	1:B:41:GLU:OE1	2.34	0.45
1:B:706:LEU:CD2	1:B:1385:ASN:HD22	2.29	0.45
1:B:1651:LYS:CE	1:B:1684:LEU:HD21	2.46	0.45
1:B:1801:VAL:HG12	1:B:1805:PHE:CE2	2.52	0.45
1:B:226:GLY:O	1:B:230:LEU:HD23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:ARG:HA	1:B:264:ARG:HD3	1.75	0.45
1:B:2912:GLY:O	1:B:2915:ARG:CZ	2.65	0.45
1:B:3459:ASN:CG	1:B:3710:LYS:HZ3	2.19	0.45
1:B:488:ILE:HG21	1:B:616:LYS:CD	2.38	0.45
1:B:617:PRO:HB3	1:B:659:ARG:CG	2.46	0.45
1:B:789:TYR:HD2	1:B:865:GLN:CG	2.29	0.45
1:A:1727:ARG:NH1	1:A:1728:GLU:OE1	2.50	0.45
1:A:1685:ASP:HA	1:A:1728:GLU:OE2	2.16	0.45
1:A:185:HIS:N	1:A:186:PRO:HD2	2.18	0.45
1:A:2286:PRO:HD2	1:A:2329:TYR:CE2	2.50	0.45
1:A:244:THR:O	1:A:248:ILE:HG13	2.16	0.45
1:A:249:PHE:CG	1:A:297:LEU:HD13	2.52	0.45
1:A:2539:LEU:HA	1:A:2542:LEU:HD23	1.98	0.45
1:A:2563:LEU:O	1:A:2567:SER:CB	2.65	0.45
1:A:2553:HIS:ND1	1:A:2803:ILE:HD12	2.32	0.45
1:A:3141:PHE:HZ	1:A:3192:LYS:CB	2.30	0.45
1:A:3868:VAL:HG12	1:A:3872:ARG:HE	1.81	0.45
1:A:4059:ILE:HD11	1:A:4082:ARG:HD2	1.99	0.45
1:A:443:ILE:HD11	1:A:465:PHE:CE2	2.52	0.45
1:A:48:PRO:O	1:A:50:VAL:N	2.50	0.45
1:B:1093:GLU:O	1:B:1096:VAL:HG12	2.17	0.45
1:B:1577:LEU:HD12	1:B:1578:ALA:HB2	1.99	0.45
1:B:1879:VAL:O	1:B:1882:SER:N	2.48	0.45
1:B:2038:GLU:OE1	1:B:2076:VAL:HG22	2.17	0.45
1:B:2271:SER:OG	1:B:2272:VAL:N	2.50	0.45
1:B:396:PHE:CG	1:B:397:LEU:N	2.83	0.45
1:B:4108:MSE:O	1:B:4111:ALA:N	2.44	0.45
1:B:433:PRO:CB	1:B:1812:LEU:HB3	2.47	0.45
1:B:764:PRO:CB	1:B:848:LEU:HD11	2.46	0.45
1:A:1090:ARG:NH2	1:A:1100:VAL:HG11	2.17	0.45
1:A:1363:LEU:HA	1:A:1363:LEU:HD23	1.70	0.45
1:A:1479:VAL:O	1:A:1482:GLU:HB2	2.15	0.45
1:A:1894:SER:O	1:A:1896:ILE:N	2.49	0.45
1:A:2137:ILE:HG22	1:A:2141:ASN:HD21	1.82	0.45
1:A:2164:TRP:HZ3	1:A:2186:VAL:HG23	1.81	0.45
1:A:2196:TRP:NE1	1:A:2200:ALA:HB2	2.31	0.45
1:A:2538:ARG:NH1	1:A:2566:THR:N	2.64	0.45
1:A:933:LEU:HD21	1:A:2795:GLN:NE2	2.31	0.45
1:A:2808:LEU:O	1:A:2811:SER:OG	2.31	0.45
1:A:3764:VAL:O	1:A:3768:PHE:HD1	2.00	0.45
1:A:910:PHE:H	1:A:912:PRO:HD2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1468:LEU:O	1:B:1472:SER:N	2.50	0.45
1:B:1686:LEU:HA	1:B:1686:LEU:HD23	1.56	0.45
1:B:437:HIS:HA	1:B:1814:PHE:CE2	2.52	0.45
1:B:1971:PRO:O	1:B:1972:GLU:HG2	2.16	0.45
1:B:2028:LEU:HB2	1:B:2030:TYR:CE2	2.52	0.45
1:B:2193:ILE:CD1	1:B:2245:TRP:CZ2	2.99	0.45
1:B:2524:PHE:HA	1:B:2527:HIS:HB3	1.98	0.45
1:B:2937:ASP:OD2	1:B:3976:GLU:HB2	2.16	0.45
1:B:3005:LEU:HG	1:B:3005:LEU:H	1.60	0.45
1:B:3048:LYS:HB2	1:B:3048:LYS:HE3	1.77	0.45
1:B:3160:LEU:HB3	1:B:3164:TRP:CH2	2.52	0.45
1:B:3454:LEU:HA	1:B:3454:LEU:HD23	1.59	0.45
1:B:3881:ASP:OD1	1:B:3884:LYS:NZ	2.47	0.45
1:B:4066:LEU:CD2	1:B:4075:ARG:HG3	2.46	0.45
1:B:733:LEU:HD23	1:B:733:LEU:N	2.31	0.45
1:B:906:PHE:HA	1:B:909:VAL:HB	1.98	0.45
1:A:971:ARG:HD2	1:A:1024:THR:CG2	2.44	0.45
1:A:1147:LYS:O	1:A:1151:ARG:NE	2.50	0.45
1:A:1161:ALA:O	1:A:1260:LEU:HD13	2.17	0.45
1:A:1917:LYS:HD2	1:A:1953:CYS:SG	2.57	0.45
1:A:2327:LEU:HA	1:A:2330:VAL:HG12	1.98	0.45
1:A:2379:MSE:HE1	1:A:2404:ARG:NH1	2.26	0.45
1:A:2427:ARG:HB3	1:A:2433:LYS:HB2	1.98	0.45
1:A:260:ILE:HG22	1:A:264:ARG:NH1	2.27	0.45
1:A:2806:LYS:HA	1:A:2809:PHE:CE2	2.50	0.45
1:A:2950:LYS:HE2	1:A:4105:LYS:HZ1	1.80	0.45
1:A:3944:HIS:CE1	1:A:4020:MSE:HE3	2.52	0.45
1:A:4013:TRP:HB2	1:A:4040:PRO:HG2	1.98	0.45
1:A:706:LEU:HD21	1:A:1388:ASP:OD2	2.15	0.45
1:A:763:THR:HG21	1:A:769:GLY:HA3	1.99	0.45
1:A:977:ASP:CB	1:A:981:ARG:H	2.24	0.45
1:B:1299:GLU:HA	1:B:1302:ALA:HB3	1.99	0.45
1:B:1652:ILE:HG12	1:B:1717:LEU:HD11	1.99	0.45
1:B:279:ALA:HA	1:B:282:PHE:CD2	2.52	0.45
1:B:2913:LYS:O	1:B:2916:LEU:N	2.25	0.45
1:B:3268:THR:O	1:B:3271:ASP:HB3	2.17	0.45
1:B:3518:VAL:HA	1:B:3521:ILE:HG22	1.98	0.45
1:B:3880:ALA:HB1	1:B:3969:ASN:HB3	1.99	0.45
1:B:3890:MSE:O	1:B:3891:SER:OG	2.33	0.45
1:B:3916:TRP:CZ3	1:B:3917:ILE:HD12	2.52	0.45
1:B:542:ASP:HA	1:B:545:LEU:CD1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:560:LEU:HA	1:B:563:LEU:HB2	1.99	0.45
1:B:586:GLN:OE1	1:B:1088:GLU:HG2	2.17	0.45
1:B:763:THR:N	1:B:764:PRO:HD3	2.31	0.45
1:B:982:GLN:O	1:B:986:PRO:CD	2.64	0.45
1:A:1147:LYS:HG2	1:A:1180:GLN:HG2	1.97	0.45
1:A:1996:VAL:HG23	1:A:1997:PRO:HD3	1.98	0.45
1:A:2004:TYR:OH	1:A:2055:SER:HB3	2.16	0.45
1:A:2077:HIS:HB3	1:A:2081:LEU:HG	1.99	0.45
1:A:2236:GLU:HG3	1:A:2236:GLU:H	1.46	0.45
1:A:2485:ARG:HA	1:A:2499:PHE:HE2	1.82	0.45
1:A:3077:ILE:O	1:A:3081:HIS:CG	2.70	0.45
1:A:313:LEU:HD13	1:A:317:GLU:OE2	2.16	0.45
1:A:3244:ASP:O	1:A:3247:ARG:HB3	2.16	0.45
1:A:3458:SER:OG	1:A:3494:GLN:NE2	2.49	0.45
1:A:3572:ILE:HD13	1:A:3575:LEU:HD12	1.97	0.45
1:A:3575:LEU:C	1:A:3577:GLN:H	2.18	0.45
1:A:3619:ASP:N	1:A:3620:PRO:CD	2.80	0.45
1:A:3670:MSE:HE3	1:A:3670:MSE:HB2	1.78	0.45
1:A:3834:ALA:H	1:A:3835:PRO:HD3	1.81	0.45
1:A:3955:VAL:HG12	1:A:4027:TRP:NE1	2.24	0.45
1:A:3958:LEU:O	1:A:3958:LEU:HD12	2.17	0.45
1:A:4077:TYR:OH	1:A:4116:ILE:HA	2.17	0.45
1:A:575:ILE:N	1:A:605:THR:OG1	2.50	0.45
1:A:65:LEU:HD23	1:A:68:PHE:CZ	2.52	0.45
1:A:799:TYR:O	1:A:801:LYS:N	2.50	0.45
1:A:916:GLU:HA	1:A:919:LEU:HG	1.99	0.45
1:B:1039:TRP:CH2	1:B:1052:SER:HB3	2.51	0.45
1:B:1269:THR:CG2	1:B:1275:THR:HG21	2.46	0.45
1:B:1378:GLU:HB3	1:B:1379:PRO:CD	2.46	0.45
1:B:1517:LEU:HD13	1:B:1585:SER:HB2	1.99	0.45
1:B:1876:ILE:O	1:B:1877:LEU:HG	2.16	0.45
1:B:215:PRO:HB3	1:B:251:PHE:CD2	2.51	0.45
1:B:2265:PRO:HD3	1:B:2309:PHE:HZ	1.79	0.45
1:B:2459:VAL:HG13	1:B:2505:VAL:HG13	1.98	0.45
1:B:2462:VAL:CG2	1:B:2473:MSE:SE	3.13	0.45
1:B:3312:VAL:O	1:B:3314:SER:N	2.50	0.45
1:B:3315:TYR:CG	1:B:3316:LEU:N	2.84	0.45
1:B:348:ILE:HG23	1:B:357:LYS:HE3	1.98	0.45
1:B:3813:LYS:CE	1:B:3926:ASN:HB2	2.46	0.45
1:B:3812:LEU:O	1:B:3816:LEU:HB2	2.16	0.45
1:B:743:LEU:HD23	1:B:783:HIS:HE1	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:901:MSE:HG3	1:B:2819:GLU:HB2	1.98	0.45
1:B:980:THR:HG23	1:B:984:TYR:HE2	1.80	0.45
1:A:1027:ASP:O	1:A:1031:ARG:HG2	2.17	0.45
1:A:1033:ILE:HG13	1:A:1089:PHE:HE2	1.82	0.45
1:A:1737:ASN:C	1:A:1739:TYR:N	2.69	0.45
1:A:2222:HIS:O	1:A:2224:PHE:N	2.49	0.45
1:A:2327:LEU:HD12	1:A:2371:PHE:HB2	1.98	0.45
1:A:3273:LEU:HD13	1:A:3321:LEU:HD13	1.99	0.45
1:A:3516:HIS:CE1	1:A:3517:SER:HG	2.34	0.45
1:A:3784:ARG:HB2	1:A:3786:LEU:HG	1.99	0.45
1:A:3820:MSE:HB2	1:A:3882:LEU:HD13	1.98	0.45
1:A:3967:PHE:CG	1:A:3968:ILE:N	2.84	0.45
1:A:436:GLU:O	1:A:440:VAL:HG13	2.17	0.45
1:A:460:ALA:O	1:A:464:VAL:HG12	2.17	0.45
1:A:557:SER:HA	1:A:560:LEU:CD2	2.47	0.45
1:A:933:LEU:HD12	1:A:933:LEU:HA	1.56	0.45
1:B:2196:TRP:NE1	1:B:2200:ALA:HB2	2.30	0.45
1:B:2402:LEU:HA	1:B:2405:VAL:HG22	1.97	0.45
1:B:252:VAL:C	1:B:254:LYS:H	2.20	0.45
1:B:3168:TYR:HB3	1:B:3169:PRO:HD3	1.99	0.45
1:B:3181:ASP:HA	1:B:3184:THR:CG2	2.45	0.45
1:B:3438:GLU:HB3	1:B:3442:TYR:HE2	1.82	0.45
1:B:3525:TYR:OH	1:B:3561:LYS:HB2	2.17	0.45
1:B:3594:ALA:CB	1:B:4028:ILE:HD13	2.45	0.45
1:B:3961:PHE:CE1	1:B:3963:LEU:HB2	2.51	0.45
1:B:4077:TYR:HB2	1:B:4119:ARG:NH2	2.32	0.45
1:B:63:PHE:O	1:B:66:LEU:HG	2.17	0.45
1:B:759:GLY:HA3	1:B:773:LEU:HD11	1.98	0.45
1:A:1402:LEU:O	1:A:1406:LEU:HD23	2.17	0.45
1:A:1685:ASP:HB3	1:A:1728:GLU:OE1	2.16	0.45
1:A:1858:LEU:O	1:A:1861:SER:HB2	2.16	0.45
1:A:1762:MSE:HG2	1:A:1864:ASP:OD1	2.17	0.45
1:A:1911:LEU:HD13	1:A:1916:ILE:CG2	2.45	0.45
1:A:1975:LEU:HA	1:A:1976:LEU:HD23	1.98	0.45
1:A:2226:PRO:O	1:A:2230:VAL:N	2.43	0.45
1:A:2253:TYR:HE1	1:A:2280:VAL:HG22	1.82	0.45
1:A:2439:ILE:C	1:A:2441:LYS:H	2.20	0.45
1:A:2777:HIS:O	1:A:2781:PRO:HD3	2.17	0.45
1:A:3930:VAL:HA	1:A:3937:VAL:HG13	1.98	0.45
1:A:513:GLU:HG2	1:A:653:LEU:HD11	1.99	0.45
1:A:16:GLN:OE1	1:A:61:ARG:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:VAL:HG12	1:B:130:LEU:HD11	1.98	0.45
1:B:1598:ASN:ND2	1:B:1811:ARG:HG2	2.32	0.45
1:B:1886:LYS:NZ	1:B:1944:ALA:O	2.47	0.45
1:B:2039:GLU:HG2	1:B:2077:HIS:CE1	2.52	0.45
1:B:2087:GLU:OE2	1:B:2138:VAL:HG12	2.17	0.45
1:B:262:LEU:H	1:B:262:LEU:HG	1.60	0.45
1:B:3110:PHE:C	1:B:3114:TYR:HD1	2.20	0.45
1:B:321:LYS:O	1:B:325:ASN:HB2	2.17	0.45
1:B:3498:TRP:HB2	1:B:3501:HIS:HB2	1.99	0.45
1:B:3550:LYS:HZ3	1:B:3554:PHE:HD2	1.58	0.45
1:B:3863:ASN:O	1:B:3867:THR:HG23	2.16	0.45
1:B:396:PHE:CZ	1:B:437:HIS:CD2	3.05	0.45
1:B:4056:PRO:HD2	1:B:4059:ILE:HG22	1.99	0.45
1:B:468:LEU:HD22	1:B:475:LEU:CD2	2.46	0.45
1:B:633:ILE:HG22	1:B:634:LEU:CD2	2.46	0.45
1:B:912:PRO:O	1:B:916:GLU:HG3	2.16	0.45
1:B:927:LYS:HE2	1:B:927:LYS:HB3	1.80	0.45
1:A:1300:SER:O	1:A:1304:HIS:ND1	2.36	0.45
1:A:1305:ASP:OD1	1:A:1306:ILE:N	2.50	0.45
1:A:111:CYS:HB3	1:A:134:LEU:HB3	1.98	0.45
1:A:1357:LYS:HG2	1:A:1357:LYS:O	2.17	0.45
1:A:1464:LEU:O	1:A:1468:LEU:N	2.43	0.45
1:A:1645:VAL:HG22	1:A:1709:GLU:OE1	2.17	0.45
1:A:1806:ARG:O	1:A:1810:PRO:HD3	2.17	0.45
1:A:1915:LEU:CD1	1:A:1916:ILE:HG13	2.46	0.45
1:A:1991:PRO:HD2	1:A:1992:VAL:H	1.81	0.45
1:A:2356:MSE:SE	1:A:2360:PHE:CE1	3.20	0.45
1:A:275:PHE:O	1:A:277:LEU:N	2.50	0.45
1:A:2972:TYR:CE2	1:A:2991:LYS:NZ	2.84	0.45
1:A:2959:ALA:O	1:A:3251:ASN:HA	2.17	0.45
1:A:3425:ARG:NH2	1:A:3467:ARG:NH1	2.65	0.45
1:A:763:THR:OG1	1:A:770:LEU:HD23	2.17	0.45
1:B:1032:CYS:HB3	1:B:1036:PHE:HZ	1.77	0.45
1:B:1301:ILE:HA	1:B:1304:HIS:HB2	1.99	0.45
1:B:1583:MSE:HE3	1:B:1643:MSE:HB3	1.98	0.45
1:B:1655:ILE:CG1	1:B:1681:ASP:HB3	2.47	0.45
1:B:2070:GLU:HG3	1:B:2072:ARG:CG	2.38	0.45
1:B:2164:TRP:HH2	1:B:2190:VAL:CG1	2.30	0.45
1:B:2219:LEU:HA	1:B:2219:LEU:HD23	1.76	0.45
1:B:2220:MSE:HE1	1:B:2256:ILE:HD11	1.98	0.45
1:B:2313:LYS:O	1:B:2316:TYR:HE1	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2555:LEU:HD22	1:B:2809:PHE:CE2	2.52	0.45
1:B:2883:SER:HA	1:B:2886:GLN:NE2	2.30	0.45
1:B:3493:TRP:CZ2	1:B:3496:ILE:HG21	2.52	0.45
1:B:362:ALA:HB2	1:B:409:GLN:NE2	2.29	0.45
1:A:1249:SER:HA	1:A:3698:GLU:OE2	2.17	0.44
1:A:1249:SER:O	1:A:1253:THR:CB	2.63	0.44
1:A:437:HIS:CE1	1:A:1813:SER:HG	2.35	0.44
1:A:2145:PHE:CE2	1:A:2185:MSE:SE	3.20	0.44
1:A:2203:THR:HG23	1:A:2245:TRP:HH2	1.82	0.44
1:A:2634:UNK:O	1:A:2637:UNK:N	2.50	0.44
1:A:3186:ARG:O	1:A:3189:PHE:HB2	2.17	0.44
1:A:3751:LEU:HD13	1:A:3805:TRP:HB2	1.98	0.44
1:A:3872:ARG:O	1:A:3876:SER:CB	2.65	0.44
1:A:3961:PHE:HE1	1:A:3963:LEU:HB2	1.76	0.44
1:A:4025:GLY:O	1:A:4028:ILE:HG22	2.17	0.44
1:A:4090:ARG:HD3	1:A:4090:ARG:HA	1.83	0.44
1:A:601:TRP:HE3	1:A:601:TRP:H	1.65	0.44
1:A:865:GLN:OE1	1:A:865:GLN:N	2.49	0.44
1:A:868:LYS:HA	1:A:871:LEU:HD12	1.99	0.44
1:A:909:VAL:HG12	1:A:937:MSE:SE	2.67	0.44
1:B:989:MSE:HG2	1:B:1031:ARG:NH1	2.32	0.44
1:B:109:ASN:HA	1:B:112:THR:HG22	1.99	0.44
1:B:1137:ILE:O	1:B:1140:LYS:HD2	2.18	0.44
1:B:1438:GLY:HA2	1:B:1491:ILE:HD11	1.99	0.44
1:B:2147:ALA:O	1:B:2151:ILE:HG13	2.17	0.44
1:B:2960:GLU:O	1:B:2965:TYR:HD1	2.00	0.44
1:B:2970:LYS:CE	1:B:2974:GLU:OE2	2.65	0.44
1:B:805:LEU:HD13	1:B:3117:ILE:CD1	2.46	0.44
1:B:3479:THR:OG1	1:B:3483:MSE:SE	2.85	0.44
1:B:3862:ALA:O	1:B:3866:GLU:HG3	2.17	0.44
1:B:4121:TRP:CG	1:B:4122:GLU:N	2.85	0.44
1:B:550:PHE:CE1	1:B:633:ILE:HA	2.52	0.44
1:B:82:ARG:NH1	1:B:114:VAL:HG13	2.32	0.44
1:A:1358:LEU:HD23	1:A:1358:LEU:O	2.17	0.44
1:A:1684:LEU:HD23	1:A:1687:HIS:HD2	1.83	0.44
1:A:187:SER:O	1:A:190:ILE:HG22	2.16	0.44
1:A:1918:LEU:HD11	1:A:1957:ASN:HD22	1.81	0.44
1:A:2227:LYS:C	1:A:2229:ALA:H	2.21	0.44
1:A:2866:ALA:O	1:A:2869:LEU:HB2	2.17	0.44
1:A:3172:LYS:HG3	1:A:3178:ILE:HG21	1.99	0.44
1:A:3427:GLU:HG3	1:A:3439:LEU:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:GLU:OE1	1:A:1798:LEU:HD13	2.18	0.44
1:A:74:ASN:HB3	1:A:75:SER:H	1.44	0.44
1:B:1701:SER:OG	1:B:1702:LEU:N	2.51	0.44
1:B:2004:TYR:CG	1:B:2054:TYR:HB3	2.52	0.44
1:B:2007:ILE:HG22	1:B:2009:LYS:CB	2.47	0.44
1:B:2093:CYS:C	1:B:2096:PRO:HD2	2.37	0.44
1:B:2442:MSE:H	1:B:2442:MSE:HG2	1.62	0.44
1:B:3619:ASP:N	1:B:3620:PRO:CD	2.80	0.44
1:B:3912:CYS:HB3	1:B:3961:PHE:CG	2.52	0.44
1:B:3764:VAL:HG13	1:B:3918:LEU:HD21	1.99	0.44
1:B:3974:MSE:HB3	1:B:3976:GLU:N	2.32	0.44
1:B:414:LEU:O	1:B:414:LEU:HG	2.14	0.44
1:B:732:PHE:HB2	1:B:733:LEU:CD2	2.47	0.44
1:B:84:GLU:O	1:B:88:PHE:HD2	2.01	0.44
1:B:91:ILE:O	1:B:95:LYS:HG3	2.17	0.44
1:B:89:LEU:HA	1:B:92:PHE:CD2	2.52	0.44
1:B:934:LEU:O	1:B:938:VAL:HG23	2.17	0.44
1:B:955:ALA:O	1:B:959:TYR:CB	2.66	0.44
1:A:1282:LEU:HD12	1:A:1282:LEU:HA	1.69	0.44
1:A:1476:HIS:HB2	1:A:1511:ALA:HB2	2.00	0.44
1:A:1583:MSE:HE1	1:A:1640:GLU:CD	2.37	0.44
1:A:1752:LEU:HD23	1:A:1752:LEU:HA	1.74	0.44
1:A:433:PRO:CB	1:A:1812:LEU:HA	2.48	0.44
1:A:185:HIS:H	1:A:186:PRO:CD	2.19	0.44
1:A:172:GLU:HA	1:A:222:GLY:HA3	1.99	0.44
1:A:2277:LEU:O	1:A:2280:VAL:HB	2.17	0.44
1:A:2310:VAL:O	1:A:2315:VAL:HG21	2.18	0.44
1:A:2320:ALA:HB2	1:A:2367:VAL:HA	1.99	0.44
1:A:3501:HIS:O	1:A:3505:LEU:HD13	2.18	0.44
1:A:3578:LEU:HD22	1:A:3683:CYS:SG	2.57	0.44
1:A:3739:ILE:CD1	1:A:3749:PRO:HB3	2.48	0.44
1:A:385:TYR:OH	1:A:421:LEU:HD23	2.18	0.44
1:A:409:GLN:HG3	1:A:413:PHE:CE2	2.53	0.44
1:A:456:VAL:O	1:A:459:ARG:HB2	2.18	0.44
1:B:1005:ASP:HB2	1:B:1006:THR:H	1.51	0.44
1:B:1119:LYS:HZ3	1:B:1256:TRP:HE1	1.64	0.44
1:B:1342:MSE:HG2	1:B:1402:LEU:HD23	1.99	0.44
1:B:1651:LYS:HD2	1:B:1684:LEU:HD21	2.00	0.44
1:B:2416:LYS:HE2	1:B:2439:ILE:HG12	1.99	0.44
1:B:307:GLU:O	1:B:308:LEU:HD13	2.17	0.44
1:B:3156:PRO:HB2	1:B:3197:LEU:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3477:GLU:O	1:B:3481:SER:HB2	2.17	0.44
1:B:3972:LEU:C	1:B:3974:MSE:HG2	2.38	0.44
1:B:4056:PRO:O	1:B:4058:VAL:N	2.51	0.44
1:B:487:LEU:HD23	1:B:530:LEU:HD12	1.99	0.44
1:B:527:TYR:HH	1:B:619:ASP:N	2.12	0.44
1:B:654:ILE:HG21	1:B:726:LEU:HB3	1.99	0.44
1:B:734:LEU:HD23	1:B:734:LEU:HA	1.52	0.44
1:A:1147:LYS:CG	1:A:1180:GLN:HG2	2.47	0.44
1:A:1583:MSE:SE	1:A:1643:MSE:HE3	2.67	0.44
1:A:1802:TYR:O	1:A:1805:PHE:HB2	2.17	0.44
1:A:1908:GLY:CA	1:A:1952:ILE:HG13	2.47	0.44
1:A:2506:LEU:H	1:A:2506:LEU:HG	1.56	0.44
1:A:939:MSE:SE	1:A:2783:ILE:HG23	2.67	0.44
1:A:334:HIS:ND1	1:A:338:LEU:HD21	2.31	0.44
1:A:3443:PRO:C	1:A:3445:LEU:H	2.20	0.44
1:A:352:VAL:HG23	1:A:357:LYS:N	2.23	0.44
1:A:368:LEU:O	1:A:420:VAL:HG23	2.17	0.44
1:A:3717:VAL:HG22	1:A:3718:ARG:H	1.83	0.44
1:A:3583:LEU:CD1	1:A:3733:ARG:HB3	2.43	0.44
1:A:3903:HIS:ND1	1:A:3934:THR:OG1	2.51	0.44
1:A:3966:GLN:HG2	1:A:4128:MSE:C	2.38	0.44
1:A:487:LEU:HG	1:A:530:LEU:HD13	2.00	0.44
1:A:658:THR:N	1:A:733:LEU:HD13	2.33	0.44
1:B:1101:PHE:HA	1:B:1104:LEU:HD12	1.98	0.44
1:B:1272:GLY:C	1:B:1274:ARG:H	2.21	0.44
1:B:1373:VAL:HG13	1:B:1374:GLN:HG2	2.00	0.44
1:B:1692:ALA:HA	1:B:1695:LEU:HD12	1.98	0.44
1:B:1949:ILE:HD12	1:B:1952:ILE:CG2	2.35	0.44
1:B:1958:GLU:HA	1:B:1961:PHE:HB3	2.00	0.44
1:B:2359:LYS:H	1:B:2359:LYS:HG3	1.62	0.44
1:B:2307:MSE:HE1	1:B:2367:VAL:HG11	1.98	0.44
1:B:2917:PRO:HB2	1:B:2918:PRO:HD3	1.99	0.44
1:B:481:THR:O	1:B:485:GLN:HG2	2.17	0.44
1:B:65:LEU:O	1:B:69:VAL:CB	2.64	0.44
1:B:669:LEU:C	1:B:671:SER:N	2.70	0.44
1:B:771:ASN:O	1:B:773:LEU:N	2.51	0.44
1:B:797:ASP:OD2	1:B:869:ASN:HB2	2.18	0.44
1:A:1076:LEU:O	1:A:1078:ALA:N	2.51	0.44
1:A:1086:TYR:CE1	1:A:1089:PHE:HB2	2.53	0.44
1:A:1115:HIS:O	1:A:1118:GLU:C	2.56	0.44
1:A:1151:ARG:O	1:A:1154:PRO:HD2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:PHE:HB2	1:A:157:TYR:HE2	1.82	0.44
1:A:189:MSE:HE3	1:A:193:ALA:HB2	1.99	0.44
1:A:2145:PHE:CE1	1:A:2188:GLU:HB3	2.53	0.44
1:A:224:LEU:HD22	1:A:248:ILE:HD11	2.00	0.44
1:A:2379:MSE:HE1	1:A:2404:ARG:HD3	1.99	0.44
1:A:3125:ARG:HH21	1:A:3128:LYS:HD2	1.82	0.44
1:A:3835:PRO:HA	1:A:3871:PHE:CE1	2.43	0.44
1:A:432:THR:HB	1:A:433:PRO:CD	2.48	0.44
1:A:863:GLY:CA	1:A:866:ILE:HD11	2.47	0.44
1:B:1025:LEU:CD1	1:B:1028:PHE:HD2	2.30	0.44
1:B:1108:MSE:HB2	1:B:1132:ASP:OD1	2.17	0.44
1:B:2058:ASP:HB3	1:B:2059:PRO:HD3	1.98	0.44
1:B:2205:VAL:HB	1:B:2206:PRO:HD3	1.99	0.44
1:B:2539:LEU:O	1:B:2542:LEU:HG	2.18	0.44
1:B:602:MSE:SE	1:B:726:LEU:CD1	3.14	0.44
1:B:63:PHE:O	1:B:67:VAL:HG23	2.18	0.44
1:B:729:CYS:O	1:B:733:LEU:HG	2.17	0.44
1:B:954:GLY:O	1:B:958:MSE:HB3	2.17	0.44
1:B:971:ARG:CG	1:B:972:LEU:N	2.71	0.44
1:A:1340:ARG:O	1:A:1343:GLU:HB3	2.18	0.44
1:A:1433:ALA:O	1:A:1437:TYR:CG	2.71	0.44
1:A:1455:CYS:O	1:A:1458:LEU:N	2.50	0.44
1:A:1504:ASP:HA	1:A:1507:CYS:SG	2.57	0.44
1:A:430:VAL:HG11	1:A:1682:THR:HG21	2.00	0.44
1:A:2147:ALA:CB	1:A:2151:ILE:HD12	2.47	0.44
1:A:2167:PRO:C	1:A:2171:LEU:HB2	2.37	0.44
1:A:2164:TRP:CE3	1:A:2189:ILE:HD12	2.52	0.44
1:A:2253:TYR:CE1	1:A:2280:VAL:HG22	2.53	0.44
1:A:2320:ALA:HA	1:A:2367:VAL:HG23	1.99	0.44
1:A:249:PHE:HD1	1:A:265:TYR:CE1	2.36	0.44
1:A:268:PRO:O	1:A:271:GLY:N	2.51	0.44
1:A:3045:ILE:HG21	1:A:3064:PHE:CZ	2.52	0.44
1:A:3073:LEU:H	1:A:3073:LEU:HG	1.63	0.44
1:A:3155:VAL:HG11	1:A:3159:ARG:CZ	2.47	0.44
1:A:3168:TYR:HB3	1:A:3169:PRO:HD3	2.00	0.44
1:A:3283:LEU:HD22	1:A:3283:LEU:O	2.17	0.44
1:A:3305:SER:HA	1:A:3308:ASP:CB	2.45	0.44
1:A:3345:PRO:HB2	1:A:3346:ALA:H	1.58	0.44
1:A:3534:ILE:HG13	1:A:3569:GLN:OE1	2.17	0.44
1:A:530:LEU:HG	1:A:530:LEU:H	1.44	0.44
1:B:1485:SER:HA	1:B:1488:TYR:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1568:ASN:N	1:B:1568:ASN:OD1	2.51	0.44
1:B:180:LEU:HD23	1:B:183:GLU:OE1	2.17	0.44
1:B:1906:THR:O	1:B:1910:GLU:HB2	2.18	0.44
1:B:2083:LEU:HD22	1:B:2184:TYR:HD2	1.82	0.44
1:B:901:MSE:HE1	1:B:2535:THR:CG2	2.47	0.44
1:B:2536:LEU:HA	1:B:2539:LEU:HB2	1.99	0.44
1:B:2817:LEU:HA	1:B:2820:MSE:HE2	1.99	0.44
1:B:2936:TYR:HD2	1:B:3979:LEU:CD2	2.28	0.44
1:B:3103:ILE:HD11	1:B:3138:ILE:HG21	2.00	0.44
1:B:3243:ILE:HG22	1:B:3278:GLN:HE21	1.83	0.44
1:B:3631:LYS:HG3	1:B:3685:PRO:HG2	1.99	0.44
1:B:3720:ALA:HB3	1:B:3741:ARG:O	2.17	0.44
1:B:3771:MSE:O	1:B:3774:ILE:HB	2.17	0.44
1:B:4013:TRP:CE3	1:B:4014:LYS:HB2	2.53	0.44
1:B:4074:PHE:O	1:B:4077:TYR:HB3	2.17	0.44
1:B:3984:MSE:SE	1:B:4108:MSE:HE2	2.68	0.44
1:B:612:LEU:O	1:B:615:ALA:HB3	2.18	0.44
1:B:625:ASN:HA	1:B:666:PHE:CE1	2.53	0.44
1:B:886:TRP:HH2	1:B:958:MSE:HB2	1.82	0.44
1:B:894:PHE:O	1:B:940:PHE:CZ	2.71	0.44
1:A:1076:LEU:HD23	1:A:1076:LEU:HA	1.65	0.44
1:A:1072:ALA:HB1	1:A:1076:LEU:HG	2.00	0.44
1:A:82:ARG:HD2	1:A:114:VAL:CG1	2.48	0.44
1:A:1387:GLY:HA2	1:A:1392:MSE:HG3	1.99	0.44
1:A:1582:LEU:HA	1:A:1582:LEU:HD23	1.77	0.44
1:A:1722:PHE:HE2	1:A:1754:GLN:HA	1.81	0.44
1:A:1946:ASN:O	1:A:1949:ILE:N	2.31	0.44
1:A:2028:LEU:HB2	1:A:2030:TYR:HE2	1.82	0.44
1:A:2068:ARG:O	1:A:2070:GLU:N	2.50	0.44
1:A:2453:GLU:HA	1:A:2456:ASN:ND2	2.33	0.44
1:A:321:LYS:C	1:A:325:ASN:HD22	2.20	0.44
1:A:3247:ARG:HB2	1:A:3278:GLN:NE2	2.32	0.44
1:A:2936:TYR:CD2	1:A:3979:LEU:HD11	2.52	0.44
1:A:452:LYS:O	1:A:455:LEU:HG	2.17	0.44
1:A:760:LEU:CD2	1:A:803:SER:HB3	2.47	0.44
1:A:948:MSE:N	1:A:949:PRO:HD3	2.33	0.44
1:B:1087:ARG:NE	1:B:1134:LEU:HD22	2.33	0.44
1:B:1424:THR:O	1:B:1426:GLN:N	2.51	0.44
1:B:1913:LYS:HB2	1:B:1916:ILE:HB	2.00	0.44
1:B:197:PHE:O	1:B:201:LEU:HG	2.16	0.44
1:B:2177:ASN:HB2	1:B:2182:ILE:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2211:LEU:H	1:B:2211:LEU:HG	1.49	0.44
1:B:2224:PHE:CE2	1:B:2259:LYS:HD3	2.53	0.44
1:B:175:TYR:HB3	1:B:226:GLY:HA3	1.98	0.44
1:B:2318:ALA:O	1:B:2322:VAL:HB	2.18	0.44
1:B:2505:VAL:O	1:B:2508:GLN:N	2.50	0.44
1:B:320:LEU:O	1:B:323:VAL:HB	2.17	0.44
1:B:3413:TYR:CD1	1:B:3449:LYS:HB3	2.53	0.44
1:B:3699:LEU:HA	1:B:3699:LEU:HD12	1.83	0.44
1:B:563:LEU:O	1:B:566:ASP:HB2	2.18	0.44
1:B:571:SER:HB2	1:B:605:THR:H	1.83	0.44
1:B:638:GLN:NE2	1:B:667:TYR:HB3	2.32	0.44
1:B:653:LEU:HD23	1:B:653:LEU:HA	1.50	0.44
1:B:727:ALA:O	1:B:731:THR:HG23	2.18	0.44
1:B:78:PHE:O	1:B:81:CYS:N	2.51	0.44
1:B:966:PHE:CE1	1:B:969:LEU:HD13	2.53	0.44
1:A:1022:ASP:CG	1:A:1023:SER:H	2.21	0.44
1:A:1032:CYS:HB3	1:A:1036:PHE:CE2	2.52	0.44
1:A:993:HIS:ND1	1:A:1038:LYS:HE2	2.33	0.44
1:A:2183:HIS:HE1	1:A:2237:ILE:HD13	1.82	0.44
1:A:2271:SER:HB2	1:A:2314:GLU:CG	2.47	0.44
1:A:2461:PHE:CE1	1:A:2462:VAL:HG23	2.52	0.44
1:A:271:GLY:O	1:A:274:LEU:HD12	2.18	0.44
1:A:294:PHE:HZ	1:A:341:PHE:CZ	2.36	0.44
1:A:3155:VAL:HG11	1:A:3159:ARG:NH1	2.32	0.44
1:A:3186:ARG:HA	1:A:3189:PHE:CD2	2.52	0.44
1:A:3266:SER:HB2	1:A:3271:ASP:OD1	2.17	0.44
1:A:3276:TRP:HB3	1:A:3280:TYR:CE2	2.52	0.44
1:A:3455:LYS:H	1:A:3455:LYS:HG3	1.62	0.44
1:A:366:TYR:C	1:A:369:PHE:HB3	2.36	0.44
1:A:3857:LEU:HG	1:A:3859:TYR:CD2	2.53	0.44
1:A:82:ARG:HH21	1:A:83:GLU:HG3	1.83	0.44
1:B:1334:LYS:HD3	1:B:1334:LYS:HA	1.45	0.44
1:B:1369:MSE:SE	1:B:1418:HIS:ND1	3.01	0.44
1:B:1471:GLN:OE1	1:B:1471:GLN:N	2.51	0.44
1:B:1684:LEU:HA	1:B:1684:LEU:HD23	1.71	0.44
1:B:1761:LEU:HD13	1:B:1860:GLU:OE1	2.18	0.44
1:B:1999:GLU:HB3	1:B:2051:SER:HB3	2.00	0.44
1:B:2093:CYS:CA	1:B:2096:PRO:HD2	2.48	0.44
1:B:2164:TRP:C	1:B:2167:PRO:HD2	2.38	0.44
1:B:2213:ASN:CG	1:B:2250:SER:HB2	2.38	0.44
1:B:2232:ARG:O	1:B:2234:ASN:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2854:PHE:HZ	1:B:2881:LEU:HB2	1.81	0.44
1:B:2886:GLN:HG3	1:B:2887:PRO:HD3	1.99	0.44
1:B:2916:LEU:HB3	1:B:2917:PRO:HD3	2.00	0.44
1:B:3475:TYR:HB2	1:B:3479:THR:H	1.83	0.44
1:B:3636:PHE:C	1:B:3638:LYS:N	2.71	0.44
1:B:3819:THR:HG1	1:B:3889:ARG:NH1	2.10	0.44
1:B:3974:MSE:HB3	1:B:3976:GLU:CB	2.48	0.44
1:B:3975:LYS:HE3	1:B:3975:LYS:HB2	1.81	0.44
1:B:848:LEU:HD12	1:B:848:LEU:HA	1.78	0.44
1:B:928:VAL:HG23	1:B:929:ALA:N	2.33	0.44
1:A:1014:LEU:HD23	1:A:1028:PHE:HE2	1.83	0.44
1:A:1733:THR:HG23	1:A:1881:TYR:CE2	2.53	0.44
1:A:2021:GLY:N	1:A:2022:PRO:HD2	2.32	0.44
1:A:2004:TYR:CD1	1:A:2054:TYR:HB3	2.52	0.44
1:A:3720:ALA:HB3	1:A:3741:ARG:O	2.18	0.44
1:A:3960:PRO:HG2	1:A:3961:PHE:CE2	2.52	0.44
1:A:446:PHE:N	1:A:447:PRO:CD	2.81	0.44
1:A:447:PRO:HD2	1:A:448:GLN:H	1.82	0.44
1:B:1017:ILE:HD12	1:B:1025:LEU:HD23	2.00	0.44
1:B:1070:PRO:O	1:B:1073:PHE:CE2	2.71	0.44
1:B:1368:LEU:HA	1:B:1371:VAL:CG1	2.48	0.44
1:B:1937:ARG:O	1:B:1941:HIS:HB2	2.18	0.44
1:B:2028:LEU:HB2	1:B:2030:TYR:HE2	1.81	0.44
1:B:2164:TRP:CH2	1:B:2190:VAL:HG12	2.53	0.44
1:B:2316:TYR:CE2	1:B:2317:ALA:HB2	2.53	0.44
1:B:2473:MSE:O	1:B:2477:LEU:HG	2.17	0.44
1:B:271:GLY:O	1:B:274:LEU:HD12	2.18	0.44
1:B:290:TYR:O	1:B:294:PHE:HB3	2.17	0.44
1:B:2983:ASP:O	1:B:2986:PRO:HD2	2.18	0.44
1:B:856:VAL:HG21	1:B:3110:PHE:CZ	2.53	0.44
1:B:3109:SER:O	1:B:3112:GLN:HB3	2.17	0.44
1:B:3842:TRP:HA	1:B:3845:LYS:HB2	2.00	0.44
1:B:393:LYS:O	1:B:397:LEU:HB2	2.18	0.44
1:B:12:LEU:HD21	1:B:41:GLU:HB2	2.00	0.44
1:B:13:LEU:HD22	1:B:61:ARG:HD2	2.00	0.44
1:B:927:LYS:HE3	1:B:928:VAL:CG1	2.47	0.44
1:A:1017:ILE:HB	1:A:1025:LEU:HB2	2.00	0.43
1:A:1073:PHE:HD1	1:A:1074:LYS:N	2.06	0.43
1:A:1163:LEU:HA	1:A:1260:LEU:HD21	2.00	0.43
1:A:1471:GLN:O	1:A:1475:LEU:CB	2.51	0.43
1:A:1804:MSE:HE1	1:A:1822:ARG:HH11	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1762:MSE:SE	1:A:1896:ILE:HG12	2.67	0.43
1:A:1945:TYR:O	1:A:1948:ALA:HB3	2.18	0.43
1:A:266:ALA:HB2	1:A:308:LEU:HG	1.99	0.43
1:A:3092:LEU:HD22	1:A:3192:LYS:HE3	2.00	0.43
1:A:3259:LEU:HD21	1:A:3279:SER:HB2	1.99	0.43
1:A:360:SER:O	1:A:363:ILE:HB	2.18	0.43
1:A:3810:VAL:O	1:A:3929:MSE:HG3	2.18	0.43
1:A:3887:PHE:HZ	1:A:3904:PHE:CE2	2.36	0.43
1:A:3908:HIS:O	1:A:3911:ILE:HG12	2.17	0.43
1:A:3915:HIS:CD2	1:A:3920:ILE:HD12	2.53	0.43
1:A:3961:PHE:CZ	1:A:3963:LEU:HD13	2.53	0.43
1:A:12:LEU:HD21	1:A:41:GLU:HB2	2.00	0.43
1:A:646:VAL:HG11	1:A:710:PHE:CG	2.54	0.43
1:A:764:PRO:HB2	1:A:848:LEU:HD11	2.00	0.43
1:A:992:ILE:CD1	1:A:1035:GLU:HB2	2.48	0.43
1:B:1015:ASP:HA	1:B:1018:VAL:CG2	2.47	0.43
1:B:1079:SER:O	1:B:1082:PHE:HB3	2.17	0.43
1:B:1153:LEU:HB3	1:B:1154:PRO:HD3	2.01	0.43
1:B:1218:SER:OG	1:B:1219:PHE:N	2.51	0.43
1:B:13:LEU:HA	1:B:16:GLN:HG2	2.00	0.43
1:B:1876:ILE:O	1:B:1876:ILE:HG12	2.17	0.43
1:B:217:LEU:HB3	1:B:264:ARG:HG3	2.00	0.43
1:B:2554:PHE:O	1:B:2557:LEU:HB2	2.18	0.43
1:B:280:SER:O	1:B:322:GLN:HG2	2.17	0.43
1:B:2923:TRP:CD1	1:B:2931:ARG:HD3	2.53	0.43
1:B:2979:GLN:H	1:B:2979:GLN:CD	2.22	0.43
1:B:3107:ILE:HG22	1:B:3111:MSE:HE2	1.98	0.43
1:B:3454:LEU:HD21	1:B:3461:ALA:HB2	1.99	0.43
1:B:3610:TYR:O	1:B:3613:MSE:HB3	2.18	0.43
1:B:3631:LYS:HB2	1:B:3685:PRO:HB2	2.00	0.43
1:B:3872:ARG:NH1	1:B:3965:ARG:HH12	2.16	0.43
1:B:70:ARG:HG3	1:B:78:PHE:CB	2.48	0.43
1:B:733:LEU:O	1:B:737:PRO:HG3	2.18	0.43
1:A:1067:ALA:HA	1:A:1079:SER:HB2	2.00	0.43
1:A:1073:PHE:CE1	1:A:3745:GLU:HA	2.53	0.43
1:A:1354:GLU:C	1:A:1356:TRP:H	2.21	0.43
1:A:1583:MSE:HE1	1:A:1640:GLU:OE2	2.17	0.43
1:A:1733:THR:N	1:A:1734:PRO:HD3	2.33	0.43
1:A:1747:LEU:HD13	1:A:1880:MSE:HE1	2.00	0.43
1:A:1950:SER:O	1:A:2000:ARG:NH1	2.51	0.43
1:A:2373:PRO:HA	1:A:2378:PHE:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2415:LEU:HD11	1:A:2419:ASP:OD2	2.17	0.43
1:A:2795:GLN:O	1:A:2799:GLN:HG2	2.18	0.43
1:A:2860:ASP:HB3	1:A:2868:LEU:HD22	2.00	0.43
1:A:2963:SER:O	1:A:2967:GLU:HG2	2.18	0.43
1:A:3547:THR:HB	1:A:3548:GLY:O	2.18	0.43
1:A:3921:GLY:C	1:A:3923:ARG:N	2.71	0.43
1:A:733:LEU:H	1:A:733:LEU:HG	1.61	0.43
1:A:681:LYS:HD2	1:A:746:ARG:NE	2.33	0.43
1:A:739:ASN:OD1	1:A:776:TRP:HA	2.19	0.43
1:A:784:VAL:O	1:A:787:PRO:HD2	2.18	0.43
1:B:1010:LEU:HA	1:B:1013:ILE:HG12	1.99	0.43
1:B:1039:TRP:CG	1:B:1055:ASN:HB2	2.53	0.43
1:B:1087:ARG:HD3	1:B:1134:LEU:CB	2.38	0.43
1:B:1945:TYR:O	1:B:1946:ASN:C	2.56	0.43
1:B:1945:TYR:O	1:B:1948:ALA:N	2.50	0.43
1:B:2110:PRO:HB2	1:B:2111:PRO:HD3	1.99	0.43
1:B:2286:PRO:HB2	1:B:2289:ASP:CA	2.40	0.43
1:B:2464:HIS:H	1:B:2465:PRO:CD	2.31	0.43
1:B:2927:ALA:HB2	1:B:2930:TYR:CD2	2.52	0.43
1:B:3110:PHE:CD1	1:B:3111:MSE:N	2.86	0.43
1:B:358:GLU:CG	1:B:359:LEU:N	2.81	0.43
1:B:3847:SER:HA	1:B:3857:LEU:HD22	2.00	0.43
1:B:3880:ALA:O	1:B:3884:LYS:HG3	2.18	0.43
1:B:4113:ASP:O	1:B:4116:ILE:N	2.47	0.43
1:B:451:PRO:O	1:B:454:GLN:HB3	2.18	0.43
1:B:572:VAL:HG13	1:B:573:LEU:N	2.33	0.43
1:A:1365:ASN:O	1:A:1369:MSE:HG2	2.17	0.43
1:A:1577:LEU:HD12	1:A:1578:ALA:HB2	2.01	0.43
1:A:1996:VAL:HG21	1:A:2047:THR:CB	2.48	0.43
1:A:2358:ASP:O	1:A:2361:ILE:HG22	2.18	0.43
1:A:3033:GLU:HB3	1:A:3038:GLU:OE1	2.19	0.43
1:A:342:MSE:O	1:A:345:PHE:HB2	2.18	0.43
1:A:348:ILE:HG23	1:A:357:LYS:HE3	1.99	0.43
1:A:3829:LEU:HA	1:A:3829:LEU:HD12	1.70	0.43
1:A:929:ALA:O	1:A:933:LEU:HB2	2.18	0.43
1:A:939:MSE:O	1:A:942:LEU:HB3	2.19	0.43
1:A:966:PHE:CE1	1:A:988:VAL:HG12	2.54	0.43
1:B:1107:TYR:CD2	1:B:1131:ILE:HD12	2.53	0.43
1:B:1147:LYS:O	1:B:1151:ARG:NE	2.52	0.43
1:B:1356:TRP:HA	1:B:1356:TRP:CE3	2.52	0.43
1:B:1550:VAL:HG23	1:B:1551:ILE:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1722:PHE:HB3	1:B:1723:PRO:HD3	1.99	0.43
1:B:2126:MSE:HE2	1:B:2156:VAL:CG2	2.48	0.43
1:B:2171:LEU:HG	1:B:2177:ASN:ND2	2.30	0.43
1:B:2323:LEU:CD2	1:B:2345:VAL:HG21	2.48	0.43
1:B:2408:MSE:HA	1:B:2408:MSE:CE	2.41	0.43
1:B:275:PHE:O	1:B:277:LEU:N	2.52	0.43
1:B:2788:SER:HA	1:B:2791:ILE:HG13	2.01	0.43
1:B:2923:TRP:CD1	1:B:2926:LEU:HD21	2.53	0.43
1:B:2937:ASP:OD1	1:B:3976:GLU:HA	2.18	0.43
1:B:3008:TRP:H	1:B:3050:LYS:HG2	1.83	0.43
1:B:352:VAL:HG23	1:B:357:LYS:HG2	2.01	0.43
1:B:554:ASN:O	1:B:558:GLU:OE2	2.37	0.43
1:B:620:PHE:HE2	1:B:641:PHE:CE2	2.37	0.43
1:B:717:LYS:HA	1:B:717:LYS:HD3	1.84	0.43
1:B:785:MSE:HB3	1:B:785:MSE:HE2	1.68	0.43
1:A:1087:ARG:HD3	1:A:1134:LEU:CD2	2.45	0.43
1:A:1652:ILE:CD1	1:A:1713:VAL:HG13	2.48	0.43
1:A:2915:ARG:O	1:A:2938:VAL:HG21	2.19	0.43
1:A:3008:TRP:N	1:A:3050:LYS:HG2	2.33	0.43
1:A:3583:LEU:HA	1:A:3583:LEU:HD23	1.85	0.43
1:A:732:PHE:HB2	1:A:733:LEU:CD2	2.48	0.43
1:B:1633:TRP:NE1	1:B:1697:PRO:HG2	2.33	0.43
1:B:139:ARG:HG3	1:B:173:LYS:HZ2	1.84	0.43
1:B:1856:THR:O	1:B:1860:GLU:HB2	2.18	0.43
1:B:2356:MSE:SE	1:B:2360:PHE:CZ	3.21	0.43
1:B:2926:LEU:HD12	1:B:3123:GLN:CD	2.38	0.43
1:B:3271:ASP:OD2	1:B:3272:TRP:CD1	2.72	0.43
1:B:3480:LEU:HD22	1:B:3516:HIS:HB3	1.99	0.43
1:B:3498:TRP:NE1	1:B:3502:MSE:SE	2.99	0.43
1:B:3682:GLU:C	1:B:3685:PRO:HD2	2.38	0.43
1:B:389:ILE:HG22	1:B:390:GLN:N	2.33	0.43
1:B:3904:PHE:HE1	1:B:3967:PHE:HE1	1.66	0.43
1:B:485:GLN:O	1:B:488:ILE:HG12	2.19	0.43
1:B:575:ILE:HD12	1:B:604:PRO:O	2.18	0.43
1:B:74:ASN:HB3	1:B:75:SER:H	1.45	0.43
1:B:910:PHE:CE2	1:B:941:MSE:SE	3.22	0.43
1:B:981:ARG:HA	1:B:984:TYR:CD2	2.52	0.43
1:A:1014:LEU:HB2	1:A:1078:ALA:HA	2.01	0.43
1:A:1056:THR:OG1	1:A:1057:LYS:N	2.51	0.43
1:A:1087:ARG:NE	1:A:1134:LEU:HD22	2.32	0.43
1:A:1645:VAL:HG12	1:A:1646:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1942:CYS:HB2	1:A:1990:PHE:CD1	2.54	0.43
1:A:226:GLY:O	1:A:230:LEU:HD23	2.19	0.43
1:A:2359:LYS:O	1:A:2362:VAL:HG22	2.18	0.43
1:A:2365:ASN:HB2	1:A:2400:VAL:HG13	1.99	0.43
1:A:2461:PHE:HE1	1:A:2469:CYS:SG	2.42	0.43
1:A:2463:SER:O	1:A:2464:HIS:ND1	2.51	0.43
1:A:2794:LEU:HA	1:A:2797:VAL:CG2	2.46	0.43
1:A:241:ASP:HB2	1:A:282:PHE:CE2	2.53	0.43
1:A:3052:LEU:HD23	1:A:3188:PHE:CZ	2.54	0.43
1:A:3253:SER:HA	1:A:3256:MSE:HB2	2.00	0.43
1:A:3683:CYS:SG	1:A:3736:LYS:NZ	2.90	0.43
1:A:3759:ARG:C	1:A:3761:ASP:H	2.21	0.43
1:A:448:GLN:O	1:A:449:TYR:CD1	2.71	0.43
1:A:572:VAL:HG13	1:A:573:LEU:N	2.29	0.43
1:A:963:LYS:HB3	1:A:1009:LEU:CD1	2.48	0.43
1:B:1401:ASN:O	1:B:1404:LYS:HB3	2.19	0.43
1:B:1916:ILE:O	1:B:1920:TYR:CD1	2.71	0.43
1:B:2040:MSE:HE2	1:B:2040:MSE:HB3	1.96	0.43
1:B:2066:PHE:HB3	1:B:2067:ARG:HG2	2.00	0.43
1:B:2311:ARG:HG3	1:B:2363:CYS:CB	2.43	0.43
1:B:2908:LYS:NZ	1:B:2986:PRO:CG	2.81	0.43
1:B:273:ARG:HA	1:B:318:SER:OG	2.19	0.43
1:B:3443:PRO:C	1:B:3445:LEU:H	2.21	0.43
1:B:3656:LEU:O	1:B:3659:PHE:HB2	2.19	0.43
1:B:3908:HIS:CD2	1:B:3967:PHE:CZ	3.06	0.43
1:B:657:SER:C	1:B:733:LEU:HD13	2.38	0.43
1:B:714:VAL:O	1:B:717:LYS:N	2.52	0.43
1:A:1332:TYR:CZ	1:A:1386:ILE:HG22	2.54	0.43
1:A:1565:GLU:HG2	1:A:1566:THR:HG23	2.00	0.43
1:A:1687:HIS:HB3	1:A:1691:GLN:HE22	1.83	0.43
1:A:185:HIS:O	1:A:186:PRO:C	2.56	0.43
1:A:2012:ARG:HA	1:A:2012:ARG:HD3	1.69	0.43
1:A:2216:LEU:HD22	1:A:2249:LEU:HD21	2.01	0.43
1:A:2227:LYS:HZ2	1:A:2232:ARG:C	2.21	0.43
1:A:2473:MSE:O	1:A:2477:LEU:HG	2.17	0.43
1:A:224:LEU:HD13	1:A:248:ILE:HD13	2.01	0.43
1:A:2538:ARG:NH1	1:A:2566:THR:H	2.08	0.43
1:A:2804:ILE:O	1:A:2806:LYS:N	2.46	0.43
1:A:3506:LEU:HD11	1:A:3555:VAL:HG13	2.00	0.43
1:A:3835:PRO:HB2	1:A:3836:PRO:HD3	2.00	0.43
1:A:3842:TRP:CZ3	1:A:3843:LEU:HD23	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:PRO:CA	1:A:476:ARG:HH22	2.18	0.43
1:A:680:ILE:HG12	1:A:701:TYR:HD1	1.79	0.43
1:B:112:THR:O	1:B:116:THR:OG1	2.25	0.43
1:B:1165:LEU:O	1:B:1168:LEU:N	2.50	0.43
1:B:1174:ALA:O	1:B:1178:ARG:HB2	2.18	0.43
1:B:1256:TRP:O	1:B:1259:LEU:N	2.51	0.43
1:B:1266:CYS:O	1:B:1270:PHE:CD2	2.72	0.43
1:B:1354:GLU:C	1:B:1356:TRP:H	2.22	0.43
1:B:1885:PRO:O	1:B:1886:LYS:C	2.57	0.43
1:B:1920:TYR:O	1:B:1923:PHE:HB3	2.18	0.43
1:B:2083:LEU:HD13	1:B:2184:TYR:HE2	1.83	0.43
1:B:2482:ASP:CG	1:B:2485:ARG:HH21	2.21	0.43
1:B:2517:LEU:HA	1:B:2520:ILE:HG22	2.00	0.43
1:B:2557:LEU:HB3	1:B:2561:PHE:CZ	2.53	0.43
1:B:334:HIS:ND1	1:B:338:LEU:HD21	2.33	0.43
1:B:3564:GLN:C	1:B:3566:GLY:H	2.22	0.43
1:B:3572:ILE:CA	1:B:3575:LEU:HB3	2.49	0.43
1:B:390:GLN:NE2	1:B:1724:MSE:HB2	2.33	0.43
1:B:3789:ARG:HB3	1:B:3938:ILE:CG2	2.49	0.43
1:B:3944:HIS:NE2	1:B:3948:SER:O	2.51	0.43
1:B:2936:TYR:CD2	1:B:3979:LEU:HD11	2.54	0.43
1:B:4075:ARG:O	1:B:4078:VAL:HG22	2.19	0.43
1:B:553:VAL:HB	1:B:637:LYS:NZ	2.31	0.43
1:B:669:LEU:HA	1:B:669:LEU:HD23	1.74	0.43
1:B:913:ARG:CB	1:B:934:LEU:HD12	2.48	0.43
1:A:2239:LYS:NZ	2:K:109:UNK:O	2.35	0.43
2:S:212:UNK:O	2:S:215:UNK:N	2.52	0.43
1:A:1112:ALA:HA	1:A:1115:HIS:CE1	2.54	0.43
1:A:1153:LEU:HB3	1:A:1154:PRO:HD3	2.00	0.43
1:A:1253:THR:HB	1:A:1254:LEU:HG	2.00	0.43
1:A:1330:TYR:CE1	1:A:1334:LYS:HE3	2.53	0.43
1:A:1433:ALA:HB1	1:A:1437:TYR:CZ	2.53	0.43
1:A:474:VAL:HG21	1:A:1564:SER:OG	2.19	0.43
1:A:1808:ASP:CB	1:A:1814:PHE:HB3	2.30	0.43
1:A:2009:LYS:O	1:A:2010:GLU:HG3	2.18	0.43
1:A:2192:THR:HA	1:A:2195:SER:OG	2.19	0.43
1:A:257:ARG:N	1:A:258:PRO:CD	2.81	0.43
1:A:2876:VAL:HG22	1:A:3035:PHE:CZ	2.53	0.43
1:A:3272:TRP:CE3	1:A:3307:LEU:HD21	2.53	0.43
1:A:3283:LEU:HG	1:A:3300:VAL:CG2	2.48	0.43
1:A:3344:GLU:HB2	1:A:3348:LEU:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3359:ILE:CG2	1:A:3391:ALA:HB3	2.48	0.43
1:A:3427:GLU:OE1	1:A:3435:ASP:HB3	2.19	0.43
1:A:3445:LEU:O	1:A:3449:LYS:NZ	2.42	0.43
1:A:562:HIS:O	1:A:562:HIS:ND1	2.50	0.43
1:A:742:GLU:HB3	1:A:783:HIS:CG	2.54	0.43
1:B:1091:GLU:CG	1:B:1137:ILE:HD13	2.49	0.43
1:B:1214:GLU:O	1:B:1218:SER:OG	2.23	0.43
1:B:1349:LEU:HA	1:B:1353:PRO:CD	2.45	0.43
1:B:1353:PRO:HA	1:B:1358:LEU:CB	2.48	0.43
1:B:1725:GLN:O	1:B:1725:GLN:HG2	2.18	0.43
1:B:1989:ASN:HB3	1:B:2040:MSE:HE2	2.01	0.43
1:B:1991:PRO:HA	1:B:1994:VAL:HG12	2.00	0.43
1:B:2071:GLN:HA	1:B:2074:PRO:HG2	2.01	0.43
1:B:2257:PHE:CD1	1:B:2299:TYR:HB3	2.54	0.43
1:B:2437:ASP:O	1:B:2440:TYR:HB3	2.18	0.43
1:B:2515:PRO:HG2	1:B:2518:GLN:HE22	1.84	0.43
1:B:2548:PRO:O	1:B:2550:ILE:HG13	2.19	0.43
1:B:2987:THR:OG1	1:B:2991:LYS:HB2	2.19	0.43
1:B:3179:TRP:HZ2	1:B:3258:LEU:HG	1.83	0.43
1:B:3287:ARG:NH1	1:B:3328:ILE:HA	2.33	0.43
1:B:3319:ASN:O	1:B:3323:PHE:CD2	2.71	0.43
1:B:3499:ILE:HD13	1:B:3499:ILE:HA	1.76	0.43
1:B:3498:TRP:HE1	1:B:3502:MSE:CG	2.32	0.43
1:B:3630:ARG:O	1:B:3634:GLN:N	2.50	0.43
1:B:3696:ARG:HB2	1:B:3699:LEU:CB	2.48	0.43
1:B:744:ASP:C	1:B:746:ARG:N	2.70	0.43
1:B:767:GLU:HG3	1:B:851:ILE:HD11	2.01	0.43
1:B:892:LEU:HD23	1:B:907:LEU:HD13	2.01	0.43
1:B:963:LYS:CG	1:B:1009:LEU:HD11	2.49	0.43
1:A:1116:ALA:CB	1:A:1164:CYS:HB3	2.49	0.43
1:A:1508:LYS:NZ	1:A:1516:GLU:HG3	2.33	0.43
1:A:175:TYR:CZ	1:A:204:LEU:HD11	2.54	0.43
1:A:2312:TYR:O	1:A:2315:VAL:HG22	2.19	0.43
1:A:901:MSE:HE1	1:A:2539:LEU:HD21	2.00	0.43
1:A:2837:LEU:HG	1:A:2837:LEU:H	1.51	0.43
1:A:3252:PHE:HA	1:A:3282:ARG:CZ	2.48	0.43
1:A:342:MSE:O	1:A:342:MSE:HG2	2.17	0.43
1:A:3955:VAL:O	1:A:3955:VAL:HG13	2.18	0.43
1:A:3884:LYS:N	1:A:3970:LEU:HD12	2.34	0.43
1:A:4066:LEU:CD2	1:A:4075:ARG:HG3	2.45	0.43
1:A:595:ASP:CG	1:A:1026:ARG:HG3	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:PHE:HZ	1:A:653:LEU:HG	1.84	0.43
1:A:798:GLY:O	1:A:801:LYS:HE2	2.19	0.43
1:A:937:MSE:HA	1:A:940:PHE:CD1	2.53	0.43
1:A:984:TYR:O	1:A:988:VAL:HG13	2.19	0.43
1:B:1038:LYS:HA	1:B:1038:LYS:HD2	1.85	0.43
1:B:993:HIS:CB	1:B:1038:LYS:HG2	2.37	0.43
1:B:1871:MSE:CA	1:B:1874:TYR:HB2	2.45	0.43
1:B:14:ARG:O	1:B:18:THR:HG23	2.18	0.43
1:B:2138:VAL:HA	1:B:2141:ASN:ND2	2.34	0.43
1:B:224:LEU:O	1:B:228:SER:OG	2.34	0.43
1:B:2276:LEU:O	1:B:2279:ILE:HB	2.18	0.43
1:B:197:PHE:CE1	1:B:230:LEU:HD22	2.53	0.43
1:B:2401:VAL:O	1:B:2405:VAL:HG13	2.19	0.43
1:B:2433:LYS:O	1:B:2436:LEU:N	2.44	0.43
1:B:2443:MSE:HB3	1:B:2480:ILE:CG1	2.43	0.43
1:B:2510:LEU:HG	1:B:2522:ARG:HE	1.84	0.43
1:B:2575:PRO:HG3	1:B:2789:SER:OG	2.18	0.43
1:B:2989:ALA:HA	1:B:2992:ASP:HB2	1.99	0.43
1:B:3329:LEU:HA	1:B:3329:LEU:HD23	1.80	0.43
1:B:3503:VAL:HG21	1:B:3535:ILE:C	2.39	0.43
1:B:3531:TYR:CD2	1:B:3707:GLY:HA3	2.53	0.43
1:B:3788:LEU:HD12	1:B:3788:LEU:HA	1.74	0.43
1:B:458:CYS:HA	1:B:461:ILE:HD12	2.01	0.43
1:B:766:ALA:HB1	1:B:768:VAL:HG23	2.00	0.43
1:B:948:MSE:N	1:B:949:PRO:HD3	2.34	0.43
1:A:175:TYR:HA	1:A:178:LEU:HD12	2.00	0.43
1:A:1883:ARG:HG3	1:A:1884:LEU:N	2.33	0.43
1:A:1949:ILE:CD1	1:A:1952:ILE:HG21	2.48	0.43
1:A:2379:MSE:SE	1:A:2404:ARG:HD3	2.69	0.43
1:A:2439:ILE:O	1:A:2441:LYS:N	2.52	0.43
1:A:3155:VAL:N	1:A:3156:PRO:CD	2.82	0.43
1:A:3314:SER:HB2	1:A:3315:TYR:O	2.19	0.43
1:A:3495:PHE:HA	1:A:3498:TRP:CZ2	2.54	0.43
1:A:3651:LEU:HA	1:A:3654:MSE:HE3	2.01	0.43
1:A:514:VAL:CG1	1:A:610:ALA:HB1	2.49	0.43
1:A:745:VAL:HG11	1:A:776:TRP:CZ2	2.54	0.43
1:A:763:THR:N	1:A:764:PRO:HD3	2.34	0.43
1:A:905:ILE:O	1:A:906:PHE:HB2	2.18	0.43
1:A:981:ARG:CG	1:A:982:GLN:N	2.81	0.43
1:A:996:THR:O	1:A:1042:LYS:HG2	2.19	0.43
1:B:103:TYR:O	1:B:106:GLU:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1222:ASN:O	1:B:1225:GLU:HB2	2.18	0.43
1:B:125:ILE:H	1:B:126:PRO:HD2	1.84	0.43
1:B:130:LEU:HD12	1:B:130:LEU:HA	1.65	0.43
1:B:173:LYS:O	1:B:174:VAL:C	2.57	0.43
1:B:2253:TYR:HA	1:B:2256:ILE:HB	2.01	0.43
1:B:2526:SER:O	1:B:2530:ARG:HB3	2.19	0.43
1:B:2841:ASN:HD22	1:B:2871:LEU:HD23	1.84	0.43
1:B:2943:PHE:CE2	1:B:2944:THR:HG23	2.54	0.43
1:B:3262:LEU:HD12	1:B:3266:SER:OG	2.18	0.43
1:B:3424:LEU:CD1	1:B:3439:LEU:HD11	2.49	0.43
1:B:3480:LEU:HB3	1:B:3516:HIS:HB2	2.01	0.43
1:B:3525:TYR:O	1:B:3529:ILE:HB	2.19	0.43
1:B:3174:ASP:OD2	1:B:3783:GLN:HG3	2.19	0.43
1:B:385:TYR:HA	1:B:388:LEU:HB3	2.00	0.43
1:B:3984:MSE:O	1:B:3987:ALA:HB3	2.18	0.43
1:B:4020:MSE:HE3	1:B:4027:TRP:HE1	1.84	0.43
1:B:933:LEU:HD11	1:B:2795:GLN:OE1	2.19	0.43
1:B:892:LEU:HD11	1:B:958:MSE:CG	2.49	0.43
1:A:1133:HIS:ND1	1:A:1136:ARG:HD2	2.34	0.43
1:A:184:VAL:O	1:A:185:HIS:CG	2.72	0.43
1:A:2399:GLU:HA	1:A:2402:LEU:HD23	2.01	0.43
1:A:3167:ARG:HG2	1:A:3186:ARG:NH2	2.33	0.43
1:A:3141:PHE:CE1	1:A:3193:ILE:HG13	2.49	0.43
1:A:3617:LEU:CD1	1:A:3644:PHE:HD2	2.30	0.43
1:A:3908:HIS:CD2	1:A:3912:CYS:SG	3.12	0.43
1:A:3951:GLN:NE2	1:A:4068:HIS:CE1	2.87	0.43
1:A:3917:ILE:O	1:A:4048:LYS:HE2	2.19	0.43
1:A:4074:PHE:O	1:A:4077:TYR:HB3	2.19	0.43
1:A:435:LEU:O	1:A:439:VAL:HG23	2.19	0.43
1:A:47:SER:O	1:A:51:LEU:HB2	2.19	0.43
1:A:634:LEU:HD22	1:A:667:TYR:CD1	2.53	0.43
1:A:70:ARG:CD	1:A:82:ARG:HD3	2.38	0.43
1:A:939:MSE:HA	1:A:939:MSE:HE3	2.01	0.43
1:B:1017:ILE:HA	1:B:1021:VAL:O	2.18	0.43
1:B:1027:ASP:O	1:B:1031:ARG:HG2	2.19	0.43
1:B:1296:PHE:CE1	1:B:1362:ASP:HB2	2.53	0.43
1:B:1296:PHE:CZ	1:B:1362:ASP:HB2	2.54	0.43
1:B:1449:ALA:O	1:B:1453:SER:OG	2.28	0.43
1:B:1874:TYR:CE1	1:B:1881:TYR:CG	3.06	0.43
1:B:2167:PRO:CB	1:B:2171:LEU:HD22	2.47	0.43
1:B:2461:PHE:HA	1:B:2464:HIS:ND1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2871:LEU:O	1:B:2873:PRO:HD3	2.19	0.43
1:B:2879:GLY:CA	1:B:2886:GLN:HG2	2.31	0.43
1:B:3020:ASP:OD2	1:B:3024:PRO:HA	2.18	0.43
1:B:3179:TRP:CG	1:B:3179:TRP:O	2.71	0.43
1:B:3266:SER:HB3	1:B:3271:ASP:HB2	2.01	0.43
1:B:3575:LEU:HB2	1:B:3686:TRP:CZ3	2.54	0.43
1:B:348:ILE:O	1:B:364:ARG:HD3	2.19	0.43
1:B:3830:SER:O	1:B:3833:ARG:N	2.50	0.43
1:B:2858:ILE:HG23	1:B:3894:PRO:HG3	2.00	0.43
1:B:396:PHE:CE1	1:B:397:LEU:HG	2.54	0.43
1:B:3989:ARG:HE	1:B:4100:GLU:HB3	1.83	0.43
1:B:4003:ASP:O	1:B:4006:VAL:HG22	2.19	0.43
1:B:408:TYR:O	1:B:411:PRO:HD2	2.19	0.43
1:B:560:LEU:HA	1:B:563:LEU:HD12	2.00	0.43
1:B:719:LYS:HE3	1:B:750:PRO:HB2	2.01	0.43
1:A:971:ARG:HD2	1:A:1024:THR:OG1	2.18	0.42
1:A:1073:PHE:HD1	1:A:1074:LYS:CG	2.31	0.42
1:A:1305:ASP:OD1	1:A:1334:LYS:HD2	2.18	0.42
1:A:1913:LYS:O	1:A:1915:LEU:N	2.52	0.42
1:A:194:GLU:HA	1:A:197:PHE:CD2	2.51	0.42
1:A:2299:TYR:O	1:A:2302:ALA:HB3	2.19	0.42
1:A:2645:UNK:HA	1:A:2649:UNK:O	2.20	0.42
1:A:3076:ALA:HB1	1:A:3080:LEU:CD1	2.48	0.42
1:A:3144:PHE:HZ	1:A:3193:ILE:HD11	1.84	0.42
1:A:3049:LEU:HA	1:A:3188:PHE:HZ	1.82	0.42
1:A:3619:ASP:O	1:A:3625:LEU:HB2	2.19	0.42
1:A:3675:LYS:N	1:A:3676:PRO:HD2	2.33	0.42
1:A:3690:PHE:CD1	1:A:3692:VAL:HG23	2.54	0.42
1:A:3906:SER:O	1:A:3910:LEU:HD13	2.18	0.42
1:A:3955:VAL:CG1	1:A:4027:TRP:HE1	2.25	0.42
1:A:4113:ASP:HB3	1:A:4116:ILE:HG13	2.00	0.42
1:A:446:PHE:CD1	1:A:446:PHE:N	2.75	0.42
1:A:892:LEU:HG	1:A:958:MSE:SE	2.69	0.42
1:B:1033:ILE:HD11	1:B:1089:PHE:HE2	1.84	0.42
1:B:1455:CYS:HA	1:B:1458:LEU:HD12	2.00	0.42
1:B:146:GLU:HG3	1:B:149:ILE:HD12	2.00	0.42
1:B:1574:ASN:CG	1:B:1582:LEU:HD21	2.40	0.42
1:B:1718:ILE:CG2	1:B:1750:LEU:HD11	2.40	0.42
1:B:1812:LEU:HD13	1:B:1814:PHE:HD2	1.84	0.42
1:B:1981:LEU:HA	1:B:1984:LEU:CD2	2.48	0.42
1:B:2452:ARG:O	1:B:2455:LEU:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2804:ILE:O	1:B:2806:LYS:N	2.50	0.42
1:B:3104:GLN:O	1:B:3107:ILE:HB	2.19	0.42
1:B:3252:PHE:CE2	1:B:3289:ARG:NH2	2.87	0.42
1:B:3390:GLN:O	1:B:3394:GLU:HB2	2.18	0.42
1:B:3483:MSE:O	1:B:3486:GLU:HG2	2.19	0.42
1:B:3525:TYR:HA	1:B:3529:ILE:CG2	2.49	0.42
1:B:381:VAL:HB	1:B:384:MSE:SE	2.68	0.42
1:B:3985:VAL:O	1:B:3988:LEU:N	2.51	0.42
1:B:4077:TYR:CG	1:B:4119:ARG:NH2	2.87	0.42
1:B:4093:GLU:O	1:B:4095:GLU:HG2	2.19	0.42
1:B:432:THR:HB	1:B:433:PRO:CD	2.48	0.42
1:B:856:VAL:HG11	1:B:3110:PHE:CZ	2.54	0.42
1:B:963:LYS:O	1:B:967:PRO:HD3	2.20	0.42
1:B:993:HIS:C	1:B:993:HIS:ND1	2.73	0.42
1:A:1812:LEU:O	1:A:1815:THR:HG23	2.19	0.42
1:A:361:ILE:HG21	1:A:1858:LEU:HD23	2.01	0.42
1:A:1882:SER:O	1:A:1885:PRO:HD2	2.19	0.42
1:A:2070:GLU:CG	1:A:2072:ARG:HG3	2.33	0.42
1:A:2251:ILE:HG23	1:A:2288:TYR:HD2	1.84	0.42
1:A:2358:ASP:HB3	1:A:2389:PHE:CE1	2.54	0.42
1:A:2552:VAL:HG22	1:A:2553:HIS:ND1	2.35	0.42
1:A:262:LEU:H	1:A:262:LEU:HG	1.62	0.42
1:A:2943:PHE:O	1:A:2945:SER:N	2.45	0.42
1:A:293:LEU:HA	1:A:296:VAL:HG12	2.00	0.42
1:A:3174:ASP:HA	1:A:3249:GLN:NE2	2.34	0.42
1:A:3397:GLN:HE21	1:A:3413:TYR:HD1	1.63	0.42
1:A:3435:ASP:O	1:A:3439:LEU:HB2	2.18	0.42
1:A:3583:LEU:HD22	1:A:3587:ASP:OD2	2.19	0.42
1:A:349:ILE:HD12	1:A:368:LEU:HD12	1.99	0.42
1:A:3806:LEU:HG	1:A:3807:GLU:N	2.33	0.42
1:B:1157:PHE:HB3	1:B:1169:VAL:HG22	2.02	0.42
1:B:1263:ALA:HB1	1:B:1267:TYR:HE1	1.84	0.42
1:B:1389:VAL:O	1:B:1389:VAL:HG12	2.19	0.42
1:B:138:PHE:HD2	1:B:173:LYS:CE	2.25	0.42
1:B:1583:MSE:HE2	1:B:1639:LEU:C	2.40	0.42
1:B:1727:ARG:O	1:B:1730:PRO:HD2	2.19	0.42
1:B:1992:VAL:HG11	1:B:2044:ASP:OD1	2.19	0.42
1:B:2125:TRP:CZ3	1:B:2129:LEU:HD21	2.55	0.42
1:B:2255:LEU:HD12	1:B:2258:GLU:HB2	2.01	0.42
1:B:2291:GLN:O	1:B:2294:ILE:N	2.53	0.42
1:B:2325:LEU:O	1:B:2329:TYR:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2320:ALA:CA	1:B:2367:VAL:HG23	2.49	0.42
1:B:2776:ARG:H	1:B:2776:ARG:HG2	1.59	0.42
1:B:3047:SER:HB2	1:B:3050:LYS:CE	2.48	0.42
1:B:346:TYR:HA	1:B:349:ILE:HD12	2.01	0.42
1:B:3470:GLN:HG2	1:B:3474:ARG:HH11	1.83	0.42
1:B:367:GLY:C	1:B:369:PHE:N	2.69	0.42
1:B:3987:ALA:O	1:B:3991:PHE:HD1	2.01	0.42
1:B:4019:LYS:HA	1:B:4019:LYS:HE2	2.01	0.42
1:B:44:LEU:H	1:B:44:LEU:HG	1.71	0.42
1:B:487:LEU:CD2	1:B:530:LEU:HB2	2.49	0.42
1:B:560:LEU:HB2	1:B:616:LYS:HG2	2.01	0.42
1:B:775:GLU:O	1:B:779:TYR:CD2	2.70	0.42
1:B:970:LEU:CD2	1:B:1031:ARG:NH2	2.78	0.42
2:S:212:UNK:C	2:S:214:UNK:N	2.82	0.42
1:A:131:LEU:HD23	1:A:135:LEU:HD11	2.02	0.42
1:A:1345:THR:HG22	1:A:1349:LEU:HD12	2.01	0.42
1:A:143:LEU:CD1	1:A:143:LEU:H	2.25	0.42
1:A:14:ARG:HH12	1:A:2392:VAL:HG11	1.83	0.42
1:A:1798:LEU:O	1:A:1802:TYR:HB2	2.19	0.42
1:A:1955:VAL:HA	1:A:2003:LYS:HZ2	1.85	0.42
1:A:2167:PRO:HA	1:A:2171:LEU:H	1.84	0.42
1:A:2300:PHE:HZ	1:A:2341:LEU:HD22	1.83	0.42
1:A:2462:VAL:HG13	1:A:2470:ARG:HE	1.84	0.42
1:A:901:MSE:SE	1:A:2536:LEU:HD21	2.69	0.42
1:A:3069:MSE:HA	1:A:3072:GLU:HB3	2.02	0.42
1:A:3465:PHE:HD1	1:A:3483:MSE:SE	2.52	0.42
1:A:3557:ARG:O	1:A:3560:SER:HB3	2.19	0.42
1:A:3587:ASP:HB3	1:A:4022:LYS:HZ2	1.85	0.42
1:A:3640:PHE:O	1:A:3644:PHE:CG	2.72	0.42
1:A:3568:ILE:HG21	1:A:3699:LEU:HD21	2.01	0.42
1:A:3972:LEU:HD12	1:A:3974:MSE:HE3	2.01	0.42
1:A:568:PHE:O	1:A:571:SER:N	2.52	0.42
1:A:658:THR:HA	1:A:733:LEU:CD2	2.38	0.42
1:B:1163:LEU:CD2	1:B:1260:LEU:HD11	2.47	0.42
1:B:1353:PRO:HG3	1:B:1358:LEU:HB3	2.02	0.42
1:B:2012:ARG:HA	1:B:2012:ARG:HD3	1.79	0.42
1:B:2171:LEU:CD2	1:B:2177:ASN:HD21	2.32	0.42
1:B:2424:MSE:HA	1:B:2436:LEU:HD12	2.01	0.42
1:B:294:PHE:CE2	1:B:298:LEU:HD21	2.55	0.42
1:B:808:GLU:CD	1:B:3114:TYR:HB3	2.40	0.42
1:B:3624:GLY:O	1:B:3625:LEU:HD23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2928:LYS:HB3	1:B:3784:ARG:CG	2.49	0.42
1:B:3754:GLY:HA2	1:B:3800:LEU:HB2	2.02	0.42
1:B:3946:PHE:HE2	1:B:4048:LYS:HD2	1.84	0.42
1:B:403:GLY:O	1:B:405:ASP:N	2.52	0.42
1:B:557:SER:O	1:B:560:LEU:HG	2.19	0.42
1:B:932:GLU:O	1:B:935:HIS:HB3	2.18	0.42
1:B:892:LEU:HD11	1:B:958:MSE:CB	2.49	0.42
1:A:1475:LEU:O	1:A:1479:VAL:HG23	2.20	0.42
1:A:153:PHE:HA	1:A:156:PHE:CD2	2.54	0.42
1:A:1632:TRP:N	1:A:1632:TRP:CD1	2.86	0.42
1:A:177:LEU:HA	1:A:180:LEU:HD12	2.01	0.42
1:A:1968:SER:O	1:A:1971:PRO:HD2	2.19	0.42
1:A:1999:GLU:OE1	1:A:2051:SER:HB2	2.20	0.42
1:A:2023:SER:HB2	1:A:2024:TYR:CE1	2.54	0.42
1:A:2386:LEU:HA	1:A:2386:LEU:HD23	1.75	0.42
1:A:2473:MSE:HE2	1:A:2473:MSE:HB3	1.90	0.42
1:A:2797:VAL:HG12	1:A:2800:ARG:NH1	2.34	0.42
1:A:2926:LEU:HD22	1:A:2931:ARG:NE	2.34	0.42
1:A:3272:TRP:CZ3	1:A:3307:LEU:HD11	2.55	0.42
1:A:3247:ARG:NE	1:A:3278:GLN:OE1	2.50	0.42
1:A:3315:TYR:CG	1:A:3316:LEU:N	2.88	0.42
1:A:438:LEU:HA	1:A:438:LEU:HD12	1.87	0.42
1:A:560:LEU:CB	1:A:616:LYS:HZ3	2.05	0.42
1:B:1064:TYR:CD1	1:B:1106:ILE:HD11	2.55	0.42
1:B:1300:SER:O	1:B:1304:HIS:ND1	2.35	0.42
1:B:1493:PRO:O	1:B:1497:ARG:HG2	2.20	0.42
1:B:1596:VAL:HG13	1:B:1597:LEU:H	1.83	0.42
1:B:1608:ARG:NE	1:B:1608:ARG:O	2.51	0.42
1:B:2360:PHE:O	1:B:2364:LEU:HG	2.19	0.42
1:B:2379:MSE:HE1	1:B:2404:ARG:CD	2.42	0.42
1:B:2424:MSE:HA	1:B:2436:LEU:CD1	2.49	0.42
1:B:3005:LEU:O	1:B:3254:LEU:HD21	2.20	0.42
1:B:3118:ASP:N	1:B:3118:ASP:OD1	2.51	0.42
1:B:3251:ASN:ND2	1:B:3254:LEU:HD13	2.35	0.42
1:B:3324:ARG:O	1:B:3328:ILE:HG13	2.20	0.42
1:B:3479:THR:O	1:B:3483:MSE:CB	2.63	0.42
1:B:3570:ASP:HA	1:B:3573:ASN:HB3	2.02	0.42
1:B:3612:ARG:O	1:B:3615:ALA:HB3	2.19	0.42
1:B:3705:TYR:HD2	1:B:3792:SER:HB2	1.84	0.42
1:B:3775:LEU:HD13	1:B:3781:CYS:SG	2.59	0.42
1:B:3704:GLN:HG3	1:B:3796:MSE:SE	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3819:THR:O	1:B:3823:GLU:HG2	2.18	0.42
1:B:3501:HIS:ND1	1:B:4008:GLU:OE1	2.52	0.42
1:B:436:GLU:O	1:B:439:VAL:HB	2.20	0.42
1:B:493:LYS:HB3	1:B:494:PRO:HD2	2.00	0.42
1:B:742:GLU:HA	1:B:745:VAL:HG23	2.01	0.42
1:B:766:ALA:C	1:B:768:VAL:H	2.17	0.42
1:B:88:PHE:HB3	1:B:92:PHE:CZ	2.55	0.42
1:B:971:ARG:O	1:B:974:CYS:HB3	2.19	0.42
1:A:1019:ASP:HB2	1:A:1021:VAL:HG23	2.00	0.42
1:A:1238:GLN:HG3	1:A:1298:LEU:HD21	2.01	0.42
1:A:1469:PRO:HG3	1:A:1510:LEU:HD21	2.00	0.42
1:A:1718:ILE:CG2	1:A:1750:LEU:HD11	2.48	0.42
1:A:1970:LYS:HZ3	1:A:2017:GLY:HA3	1.85	0.42
1:A:2136:PRO:C	1:A:2139:PRO:HD2	2.39	0.42
1:A:2322:VAL:HG12	1:A:2323:LEU:N	2.35	0.42
1:A:2357:GLU:CD	1:A:2388:LYS:HZ1	2.22	0.42
1:A:2367:VAL:O	1:A:2371:PHE:HE1	2.03	0.42
1:A:2408:MSE:O	1:A:2409:THR:OG1	2.31	0.42
1:A:2548:PRO:O	1:A:2550:ILE:HG13	2.18	0.42
1:A:2869:LEU:HD23	1:A:2893:LEU:HA	2.01	0.42
1:A:2961:ALA:HB3	1:A:3254:LEU:CD1	2.49	0.42
1:A:3343:SER:O	1:A:3345:PRO:HD3	2.19	0.42
1:A:367:GLY:O	1:A:369:PHE:N	2.52	0.42
1:A:3766:GLN:O	1:A:3770:VAL:HG23	2.20	0.42
1:A:4037:ASN:O	1:A:4037:ASN:ND2	2.53	0.42
1:A:463:LYS:O	1:A:466:LEU:HB3	2.19	0.42
1:A:481:THR:O	1:A:485:GLN:HG2	2.18	0.42
1:A:560:LEU:HA	1:A:563:LEU:HD12	2.01	0.42
1:A:678:LYS:HB2	1:A:743:LEU:HD13	2.02	0.42
1:A:736:LEU:HA	1:A:739:ASN:HB2	2.02	0.42
1:A:866:ILE:HG21	1:A:3129:LEU:HD22	2.02	0.42
1:A:924:ARG:H	1:A:924:ARG:HG2	1.74	0.42
1:B:1726:SER:O	1:B:1729:PHE:HB3	2.19	0.42
1:B:177:LEU:H	1:B:177:LEU:HG	1.63	0.42
1:B:1890:HIS:HE1	1:B:1941:HIS:CD2	2.38	0.42
1:B:1952:ILE:HG12	1:B:1953:CYS:N	2.35	0.42
1:B:224:LEU:HD13	1:B:248:ILE:HD13	2.00	0.42
1:B:2555:LEU:HD12	1:B:2556:SER:N	2.32	0.42
1:B:2646:UNK:HA	1:B:2778:GLY:HA3	2.00	0.42
1:B:2794:LEU:HA	1:B:2794:LEU:HD23	1.80	0.42
1:B:3119:VAL:HG21	1:B:3899:ALA:CB	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:ASN:CG	1:B:1859:ASN:H	2.23	0.42
1:B:3629:ARG:NH2	1:B:3638:LYS:HZ1	2.17	0.42
1:B:3631:LYS:HD2	1:B:3681:LYS:O	2.19	0.42
1:B:3791:TYR:OH	1:B:3942:PHE:CE2	2.70	0.42
1:B:3824:GLU:O	1:B:3829:LEU:HD13	2.19	0.42
1:B:3850:HIS:H	1:B:3850:HIS:CD2	2.37	0.42
1:B:2957:LEU:HD21	1:B:4101:GLU:CG	2.50	0.42
1:B:575:ILE:HG13	1:B:579:LEU:HD13	2.01	0.42
1:B:957:PRO:O	1:B:961:LEU:HB2	2.20	0.42
1:A:154:SER:OG	1:A:181:LEU:HD13	2.19	0.42
1:A:1700:THR:OG1	1:A:1701:SER:N	2.48	0.42
1:A:172:GLU:HG3	1:A:173:LYS:N	2.35	0.42
1:A:1915:LEU:HD12	1:A:1916:ILE:N	2.34	0.42
1:A:1890:HIS:CB	1:A:1937:ARG:HD2	2.46	0.42
1:A:1970:LYS:NZ	1:A:2017:GLY:CA	2.83	0.42
1:A:2311:ARG:O	1:A:2311:ARG:HG2	2.19	0.42
1:A:2813:PHE:HA	1:A:2816:ILE:CG2	2.47	0.42
1:A:3034:PRO:C	1:A:3036:TYR:H	2.23	0.42
1:A:3101:TYR:HE2	1:A:3102:TYR:CE1	2.38	0.42
1:A:3198:THR:OG1	1:A:3199:PRO:HD3	2.19	0.42
1:A:3530:VAL:HG11	1:A:3700:GLU:O	2.18	0.42
1:A:3771:MSE:O	1:A:3775:LEU:HG	2.20	0.42
1:A:3923:ARG:CG	1:A:3962:ARG:HH22	2.00	0.42
1:A:396:PHE:CZ	1:A:437:HIS:CD2	3.07	0.42
1:A:402:THR:HB	1:A:1763:THR:HB	2.02	0.42
1:A:655:LEU:HA	1:A:658:THR:OG1	2.18	0.42
1:A:774:GLU:OE2	1:A:854:ARG:HB2	2.19	0.42
1:A:899:ARG:HH22	1:A:2570:PRO:HB2	1.83	0.42
1:A:952:GLY:C	1:A:954:GLY:H	2.23	0.42
1:B:1166:LEU:HB3	1:B:1170:LYS:HZ1	1.83	0.42
1:B:1270:PHE:HZ	1:B:1347:THR:C	2.23	0.42
1:B:1437:TYR:O	1:B:1439:PRO:HD2	2.20	0.42
1:B:1718:ILE:HG23	1:B:1750:LEU:CD1	2.40	0.42
1:B:1751:GLU:H	1:B:1751:GLU:HG3	1.57	0.42
1:B:1763:THR:N	1:B:1864:ASP:OD2	2.52	0.42
1:B:1889:VAL:HG22	1:B:1900:PHE:CE2	2.54	0.42
1:B:1927:MSE:C	1:B:1929:GLY:N	2.72	0.42
1:B:2074:PRO:HB2	1:B:2075:THR:H	1.75	0.42
1:B:2168:LEU:HG	1:B:2168:LEU:H	1.56	0.42
1:B:898:PHE:HD2	1:B:2566:THR:OG1	2.02	0.42
1:B:2602:UNK:CB	1:B:2790:LEU:HD23	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2823:PHE:CG	1:B:2824:LYS:N	2.86	0.42
1:B:2900:LEU:HD12	1:B:2905:LEU:HD21	2.02	0.42
1:B:3034:PRO:C	1:B:3036:TYR:H	2.23	0.42
1:B:3039:THR:O	1:B:3042:PRO:HD2	2.19	0.42
1:B:3141:PHE:HZ	1:B:3192:LYS:CB	2.31	0.42
1:B:3167:ARG:NH1	1:B:3167:ARG:CG	2.71	0.42
1:B:3255:ALA:HB1	1:B:3282:ARG:CZ	2.49	0.42
1:B:3585:PHE:CD1	1:B:3613:MSE:HE1	2.53	0.42
1:B:3588:TRP:NE1	1:B:3609:MSE:O	2.39	0.42
1:B:3763:ARG:HH21	1:B:4009:PRO:HG3	1.85	0.42
1:B:627:VAL:CG1	1:B:628:GLU:N	2.81	0.42
1:B:890:LYS:HD3	1:B:890:LYS:HA	1.85	0.42
1:A:1002:GLU:O	1:A:1005:ASP:OD2	2.38	0.42
1:A:1069:HIS:H	1:A:1070:PRO:CD	2.32	0.42
1:A:1093:GLU:HB3	1:A:1096:VAL:CG1	2.50	0.42
1:A:1360:LYS:HG3	1:A:1360:LYS:H	1.52	0.42
1:A:1372:LEU:HG	1:A:1418:HIS:HE1	1.85	0.42
1:A:136:GLN:HG2	1:A:139:ARG:HH11	1.84	0.42
1:A:170:VAL:CG2	1:A:173:LYS:HD3	2.47	0.42
1:A:1817:GLN:NE2	1:A:1821:ASP:HB2	2.35	0.42
1:A:1960:LYS:HB2	1:A:1998:MSE:SE	2.70	0.42
1:A:197:PHE:CZ	1:A:230:LEU:HD22	2.54	0.42
1:A:2065:ARG:HB3	1:A:2125:TRP:HD1	1.82	0.42
1:A:2292:CYS:CB	1:A:2300:PHE:HB2	2.38	0.42
1:A:2375:ALA:HB1	1:A:2411:LEU:CD2	2.49	0.42
1:A:2384:PHE:C	1:A:2387:PRO:HD2	2.39	0.42
1:A:2411:LEU:HG	1:A:2412:TYR:N	2.34	0.42
1:A:2433:LYS:O	1:A:2436:LEU:N	2.46	0.42
1:A:2434:VAL:O	1:A:2438:ILE:HG13	2.19	0.42
1:A:2990:GLU:O	1:A:2994:TRP:CD1	2.72	0.42
1:A:3181:ASP:HA	1:A:3184:THR:HG23	2.02	0.42
1:A:3450:MSE:O	1:A:3454:LEU:HG	2.20	0.42
1:A:3513:ALA:O	1:A:3518:VAL:HB	2.20	0.42
1:A:3503:VAL:HG21	1:A:3535:ILE:C	2.40	0.42
1:A:3575:LEU:O	1:A:3686:TRP:HH2	2.03	0.42
1:A:3619:ASP:N	1:A:3620:PRO:HD2	2.34	0.42
1:A:3745:GLU:O	1:A:3745:GLU:HG2	2.20	0.42
1:A:3839:TYR:CE2	1:A:3843:LEU:HD11	2.54	0.42
1:A:3955:VAL:HG22	1:A:3957:GLU:HG3	2.01	0.42
1:A:580:ASP:O	1:A:584:GLU:N	2.53	0.42
1:A:649:PHE:C	1:A:651:TYR:N	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:742:GLU:OE1	1:A:783:HIS:CD2	2.72	0.42
1:A:929:ALA:O	1:A:933:LEU:CB	2.67	0.42
1:A:927:LYS:HE2	1:A:976:VAL:HG12	2.02	0.42
1:B:963:LYS:HG3	1:B:1009:LEU:HD11	2.00	0.42
1:B:1580:LEU:HD13	1:B:1639:LEU:HB3	2.00	0.42
1:B:1655:ILE:HD12	1:B:1655:ILE:H	1.85	0.42
1:B:1679:LEU:O	1:B:1683:LYS:HG3	2.19	0.42
1:B:1756:PRO:C	1:B:1758:LEU:N	2.71	0.42
1:B:2255:LEU:HD13	1:B:2258:GLU:OE1	2.20	0.42
1:B:2405:VAL:HB	1:B:2439:ILE:CD1	2.49	0.42
1:B:2411:LEU:HG	1:B:2412:TYR:N	2.35	0.42
1:B:2474:TYR:O	1:B:2478:MSE:HG3	2.19	0.42
1:B:2520:ILE:HG13	1:B:2524:PHE:CE2	2.55	0.42
1:B:2637:UNK:O	1:B:2641:UNK:CB	2.67	0.42
1:B:2933:ILE:HG22	1:B:2937:ASP:OD2	2.20	0.42
1:B:3258:LEU:HA	1:B:3258:LEU:HD22	1.75	0.42
1:B:3427:GLU:HG3	1:B:3439:LEU:HD13	2.01	0.42
1:B:3522:THR:OG1	1:B:3558:ILE:HD11	2.20	0.42
1:B:3816:LEU:HD23	1:B:3816:LEU:HA	1.84	0.42
1:B:38:LEU:HD13	1:B:62:ASP:OD2	2.20	0.42
1:B:558:GLU:HA	1:B:561:ASN:ND2	2.35	0.42
1:B:576:VAL:HG13	1:B:601:TRP:CE3	2.41	0.42
2:S:114:UNK:O	2:S:116:UNK:N	2.53	0.42
1:A:1463:LEU:O	1:A:1467:ILE:HG12	2.20	0.42
1:A:1498:GLN:C	1:A:1501:PRO:HD2	2.40	0.42
1:A:1608:ARG:NE	1:A:1608:ARG:O	2.52	0.42
1:A:1655:ILE:HD13	1:A:1681:ASP:CB	2.45	0.42
1:A:1889:VAL:HG22	1:A:1900:PHE:CG	2.54	0.42
1:A:2066:PHE:CD1	1:A:2128:PHE:HE1	2.38	0.42
1:A:2210:VAL:HG13	1:A:2211:LEU:HG	2.01	0.42
1:A:2300:PHE:CE2	1:A:2341:LEU:HB2	2.54	0.42
1:A:2943:PHE:CE1	1:A:2984:GLY:HA2	2.55	0.42
1:A:3690:PHE:HD1	1:A:3692:VAL:HG23	1.84	0.42
1:A:3872:ARG:HD2	1:A:3965:ARG:NH1	2.35	0.42
1:A:3982:SER:HB3	1:A:3986:HIS:HE1	1.83	0.42
1:A:453:MSE:SE	1:A:456:VAL:HG11	2.70	0.42
1:A:35:ILE:HG21	1:A:84:GLU:HB3	2.02	0.42
1:A:781:ASP:OD2	1:A:862:LEU:HD21	2.20	0.42
1:A:961:LEU:HA	1:A:961:LEU:HD13	1.81	0.42
1:B:107:ILE:O	1:B:110:THR:HB	2.20	0.42
1:B:1551:ILE:HA	1:B:1554:SER:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1686:LEU:CD2	1:B:1727:ARG:NH1	2.83	0.42
1:B:1861:SER:O	1:B:1864:ASP:HB3	2.20	0.42
1:B:2135:ASN:N	1:B:2136:PRO:HD3	2.35	0.42
1:B:2166:SER:O	1:B:2170:GLN:CB	2.50	0.42
1:B:2171:LEU:CG	1:B:2177:ASN:HD21	2.29	0.42
1:B:2326:ILE:HA	1:B:2326:ILE:HD13	1.89	0.42
1:B:2443:MSE:N	1:B:2444:PRO:HD2	2.35	0.42
1:B:2531:LEU:HA	1:B:2531:LEU:HD12	1.89	0.42
1:B:2541:ALA:O	1:B:2545:LEU:HG	2.20	0.42
1:B:2905:LEU:HB2	1:B:2906:PRO:CD	2.50	0.42
1:B:2875:ALA:HB2	1:B:2921:LEU:HD23	2.01	0.42
1:B:3283:LEU:HD13	1:B:3287:ARG:CZ	2.50	0.42
1:B:3283:LEU:HD13	1:B:3287:ARG:NE	2.34	0.42
1:B:3529:ILE:HG22	1:B:3529:ILE:O	2.19	0.42
1:B:3694:PHE:CD2	1:B:3697:ASN:HA	2.54	0.42
1:B:3577:GLN:HG3	1:B:3800:LEU:CD2	2.50	0.42
1:B:3885:ARG:O	1:B:3888:VAL:HG12	2.20	0.42
1:B:617:PRO:HB3	1:B:659:ARG:CD	2.50	0.42
1:B:792:ILE:O	1:B:796:LEU:HG	2.19	0.42
1:B:886:TRP:CH2	1:B:958:MSE:HB2	2.54	0.42
1:B:980:THR:HG22	1:B:984:TYR:CE2	2.52	0.42
1:A:1127:CYS:O	1:A:1131:ILE:HG23	2.20	0.42
1:A:1279:LEU:HG	1:A:1292:LYS:NZ	2.33	0.42
1:A:1651:LYS:HB2	1:A:1684:LEU:CD1	2.50	0.42
1:A:1686:LEU:HD23	1:A:1727:ARG:CZ	2.50	0.42
1:A:1939:LEU:O	1:A:1942:CYS:N	2.53	0.42
1:A:1981:LEU:O	1:A:1984:LEU:HG	2.19	0.42
1:A:2166:SER:N	1:A:2167:PRO:CD	2.82	0.42
1:A:2154:GLU:N	1:A:2199:LEU:HD22	2.34	0.42
1:A:2233:HIS:HA	1:A:2236:GLU:CD	2.40	0.42
1:A:2913:LYS:HG3	1:A:2914:ALA:H	1.82	0.42
1:A:3454:LEU:HD21	1:A:3461:ALA:HB2	2.01	0.42
1:A:3789:ARG:HH22	1:A:3806:LEU:CD2	2.23	0.42
1:A:403:GLY:C	1:A:405:ASP:N	2.71	0.42
1:A:575:ILE:HD13	1:A:603:ILE:HB	2.01	0.42
1:A:758:LEU:HA	1:A:758:LEU:HD12	1.91	0.42
1:A:971:ARG:HD2	1:A:1024:THR:CB	2.50	0.42
1:B:1007:VAL:HA	1:B:1010:LEU:HD11	2.02	0.42
1:B:1017:ILE:HB	1:B:1025:LEU:CB	2.47	0.42
1:B:1349:LEU:CD2	1:B:1353:PRO:HG2	2.49	0.42
1:B:1467:ILE:HG13	1:B:1468:LEU:HG	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2327:LEU:HA	1:B:2330:VAL:HG12	2.01	0.42
1:B:2877:SER:O	1:B:2880:CYS:N	2.36	0.42
1:B:3053:LEU:HD23	1:B:3053:LEU:HA	1.55	0.42
1:B:3293:CYS:HA	1:B:3297:VAL:CG2	2.50	0.42
1:B:62:ASP:O	1:B:66:LEU:HD23	2.20	0.42
1:B:642:PHE:HE2	1:B:710:PHE:HE2	1.66	0.42
1:B:992:ILE:HA	1:B:995:PHE:CE2	2.54	0.42
1:A:1015:ASP:HA	1:A:1018:VAL:HG22	2.01	0.42
1:A:1083:ASN:HD21	1:A:1104:LEU:CD2	2.32	0.42
1:A:1303:MSE:HB2	1:A:1371:VAL:HG23	2.01	0.42
1:A:147:PHE:CD2	1:A:148:LYS:HG3	2.55	0.42
1:A:1715:GLU:O	1:A:1719:VAL:HG23	2.19	0.42
1:A:2035:THR:HG22	1:A:2076:VAL:HG13	2.02	0.42
1:A:2276:LEU:O	1:A:2279:ILE:HB	2.19	0.42
1:A:2387:PRO:O	1:A:2390:HIS:HB3	2.20	0.42
1:A:2472:GLN:O	1:A:2476:ILE:HG12	2.19	0.42
1:A:2538:ARG:NH1	1:A:2565:MSE:HG3	2.35	0.42
1:A:2520:ILE:HD12	1:A:2607:UNK:CB	2.50	0.42
1:A:2843:PHE:HE2	1:A:2853:PRO:HG3	1.85	0.42
1:A:281:GLN:HA	1:A:326:MSE:SE	2.70	0.42
1:A:3280:TYR:CG	1:A:3328:ILE:HD11	2.55	0.42
1:A:356:ASN:CG	1:A:1859:ASN:HB2	2.40	0.42
1:A:393:LYS:HA	1:A:396:PHE:CE1	2.54	0.42
1:A:429:GLU:N	1:A:429:GLU:OE1	2.53	0.42
1:A:436:GLU:OE2	1:A:475:LEU:HD11	2.19	0.42
1:A:654:ILE:HG23	1:A:722:LYS:NZ	2.35	0.42
1:A:846:ILE:HG23	1:A:854:ARG:NH1	2.35	0.42
1:B:1335:CYS:HA	1:B:1338:VAL:HG12	2.01	0.42
1:B:149:ILE:O	1:B:152:LEU:HG	2.20	0.42
1:B:1681:ASP:HB2	1:B:1717:LEU:CD2	2.50	0.42
1:B:1809:ASP:N	1:B:1810:PRO:HD3	2.35	0.42
1:B:2385:LEU:HG	1:B:2389:PHE:CZ	2.55	0.42
1:B:2398:LEU:O	1:B:2402:LEU:HD23	2.20	0.42
1:B:3148:GLN:HE22	1:B:3160:LEU:HD22	1.85	0.42
1:B:3283:LEU:HG	1:B:3300:VAL:CG2	2.49	0.42
1:B:3978:GLY:O	1:B:3979:LEU:HD23	2.19	0.42
1:B:446:PHE:HD2	1:B:533:HIS:CG	2.37	0.42
1:B:617:PRO:HB3	1:B:659:ARG:HD2	2.02	0.42
1:B:913:ARG:O	1:B:917:LEU:HG	2.20	0.42
1:B:977:ASP:HB3	1:B:980:THR:HG22	2.02	0.42
1:A:1080:LEU:HD23	1:A:1128:CYS:SG	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1060:PHE:CD2	1:A:1099:PHE:HZ	2.38	0.41
1:A:82:ARG:NH1	1:A:114:VAL:HG13	2.35	0.41
1:A:1747:LEU:O	1:A:1748:ASP:C	2.58	0.41
1:A:1763:THR:N	1:A:1864:ASP:OD2	2.43	0.41
1:A:2082:GLU:HB2	1:A:2086:ASP:CB	2.50	0.41
1:A:2534:ASN:HB3	1:A:2537:ASP:HB2	2.01	0.41
1:A:279:ALA:HA	1:A:282:PHE:CD2	2.55	0.41
1:A:2943:PHE:CD1	1:A:2944:THR:N	2.79	0.41
1:A:3386:SER:O	1:A:3390:GLN:HB2	2.19	0.41
1:A:345:PHE:O	1:A:348:ILE:N	2.53	0.41
1:A:381:VAL:HB	1:A:384:MSE:SE	2.70	0.41
1:A:398:THR:HA	1:A:400:THR:HG22	2.02	0.41
1:A:3995:PRO:O	1:A:3999:THR:OG1	2.17	0.41
1:A:417:VAL:O	1:A:420:VAL:HG12	2.20	0.41
1:A:513:GLU:OE1	1:A:653:LEU:HD11	2.19	0.41
1:A:489:ARG:HA	1:A:612:LEU:HB2	2.02	0.41
1:B:2047:THR:O	1:B:2050:GLN:HB2	2.20	0.41
1:B:2190:VAL:HG21	1:B:2241:LEU:CD1	2.47	0.41
1:B:2843:PHE:HE2	1:B:2853:PRO:HG3	1.84	0.41
1:B:3585:PHE:O	1:B:3589:SER:OG	2.30	0.41
1:B:3577:GLN:HA	1:B:3800:LEU:HD22	2.02	0.41
1:B:368:LEU:HD13	1:B:388:LEU:HD23	2.00	0.41
1:B:454:GLN:CG	1:B:533:HIS:HE1	2.29	0.41
1:A:100:ILE:HG22	1:A:100:ILE:O	2.20	0.41
1:A:1503:LEU:HA	1:A:1503:LEU:HD23	1.88	0.41
1:A:1569:THR:O	1:A:1573:LYS:CB	2.67	0.41
1:A:1711:ARG:HG3	1:A:1712:ARG:N	2.35	0.41
1:A:1722:PHE:O	1:A:1725:GLN:HB3	2.20	0.41
1:A:2263:LYS:HB3	1:A:2264:ASP:H	1.61	0.41
1:A:2458:VAL:HG12	1:A:2473:MSE:HG3	2.01	0.41
1:A:2482:ASP:HB2	1:A:2485:ARG:NH2	2.35	0.41
1:A:2502:ALA:O	1:A:2506:LEU:HG	2.19	0.41
1:A:3351:ILE:HG23	1:A:3355:LYS:CE	2.49	0.41
1:A:3454:LEU:HD21	1:A:3461:ALA:CB	2.50	0.41
1:A:3505:LEU:HD12	1:A:3509:ASP:CB	2.45	0.41
1:A:560:LEU:HA	1:A:563:LEU:CG	2.50	0.41
1:A:997:ASN:HA	1:A:1042:LYS:HD3	2.03	0.41
1:B:1354:GLU:C	1:B:1356:TRP:N	2.74	0.41
1:B:2010:GLU:C	1:B:2012:ARG:N	2.73	0.41
1:B:2166:SER:N	1:B:2167:PRO:HD2	2.35	0.41
1:B:2193:ILE:HD12	1:B:2245:TRP:CZ2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2277:LEU:O	1:B:2280:VAL:HB	2.20	0.41
1:B:2337:LEU:HD12	1:B:2337:LEU:HA	1.86	0.41
1:B:2359:LYS:O	1:B:2362:VAL:HG22	2.20	0.41
1:B:2365:ASN:HA	1:B:2368:THR:HB	2.00	0.41
1:B:2473:MSE:HB3	1:B:2473:MSE:HE2	1.82	0.41
1:B:271:GLY:HA2	1:B:274:LEU:HD11	2.02	0.41
1:B:2837:LEU:HD13	1:B:2868:LEU:N	2.35	0.41
1:B:2886:GLN:H	1:B:2886:GLN:HG3	1.48	0.41
1:B:3241:LYS:O	1:B:3243:ILE:N	2.41	0.41
1:B:3929:MSE:HB3	1:B:3938:ILE:HD12	2.02	0.41
1:B:389:ILE:HG23	1:B:434:VAL:HG21	2.00	0.41
1:B:43:VAL:O	1:B:45:SER:N	2.52	0.41
1:A:999:LYS:HD2	1:A:1001:PHE:CE2	2.55	0.41
1:A:1163:LEU:HD23	1:A:1260:LEU:HD11	2.03	0.41
1:A:1251:GLN:O	1:A:1255:CYS:HB2	2.20	0.41
1:A:1582:LEU:O	1:A:1583:MSE:C	2.59	0.41
1:A:1684:LEU:HA	1:A:1684:LEU:HD23	1.82	0.41
1:A:1695:LEU:O	1:A:1700:THR:HB	2.20	0.41
1:A:2103:HIS:HA	1:A:2106:ARG:HB2	2.02	0.41
1:A:2168:LEU:HD13	1:A:2214:ARG:NH2	2.35	0.41
1:A:2462:VAL:HA	1:A:2465:PRO:HD3	2.02	0.41
1:A:2443:MSE:CE	1:A:2476:ILE:HB	2.34	0.41
1:A:2841:ASN:HD22	1:A:2871:LEU:HG	1.86	0.41
1:A:3011:LEU:O	1:A:3011:LEU:HD13	2.19	0.41
1:A:3056:GLU:HA	1:A:3092:LEU:HD11	2.02	0.41
1:A:3621:LYS:HB3	1:A:3638:LYS:HE2	2.02	0.41
1:A:349:ILE:HG12	1:A:364:ARG:HB2	2.01	0.41
1:A:398:THR:C	1:A:400:THR:N	2.74	0.41
1:A:513:GLU:OE2	1:A:655:LEU:HD23	2.21	0.41
1:A:592:GLU:HB3	1:A:601:TRP:HZ2	1.84	0.41
1:A:922:SER:OG	1:A:925:GLN:OE1	2.19	0.41
1:A:955:ALA:O	1:A:959:TYR:HB3	2.19	0.41
1:B:1025:LEU:HD12	1:B:1028:PHE:HD2	1.84	0.41
1:B:1164:CYS:O	1:B:1164:CYS:SG	2.77	0.41
1:B:113:SER:O	1:B:116:THR:HB	2.20	0.41
1:B:1648:LEU:O	1:B:1652:ILE:HD12	2.20	0.41
1:B:162:LEU:HD21	1:B:196:LEU:HD13	2.01	0.41
1:B:19:LEU:HB2	1:B:34:LEU:HD13	2.02	0.41
1:B:2160:TYR:HA	1:B:2163:HIS:CD2	2.55	0.41
1:B:2213:ASN:CB	1:B:2250:SER:HB2	2.50	0.41
1:B:2367:VAL:HG22	1:B:2371:PHE:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2396:LEU:H	1:B:2396:LEU:HD12	1.85	0.41
1:B:259:GLN:C	1:B:260:ILE:HG13	2.41	0.41
1:B:2647:UNK:HA	1:B:2775:TYR:HD1	1.85	0.41
1:B:2806:LYS:HD3	1:B:2855:VAL:CG1	2.43	0.41
1:B:61:ARG:O	1:B:65:LEU:CB	2.54	0.41
1:B:646:VAL:HG11	1:B:710:PHE:CZ	2.54	0.41
1:B:850:GLU:CD	1:B:854:ARG:HH21	2.21	0.41
1:A:1060:PHE:HB3	1:A:1064:TYR:CE2	2.56	0.41
1:A:1640:GLU:HG2	1:A:1691:GLN:HG2	2.01	0.41
1:A:166:ILE:HG22	1:A:167:PRO:HD2	2.02	0.41
1:A:1729:PHE:HZ	1:A:1870:LYS:HZ3	1.69	0.41
1:A:1997:PRO:HA	1:A:2000:ARG:N	2.36	0.41
1:A:2813:PHE:O	1:A:2816:ILE:HG22	2.20	0.41
1:A:3151:LEU:HA	1:A:3152:SER:HA	1.85	0.41
1:A:449:TYR:CD2	1:A:454:GLN:HA	2.55	0.41
1:A:488:ILE:HD12	1:A:616:LYS:HD3	2.02	0.41
1:A:51:LEU:H	1:A:51:LEU:HG	1.62	0.41
1:A:741:ILE:HB	1:A:744:ASP:CG	2.40	0.41
1:A:851:ILE:O	1:A:855:VAL:HG23	2.19	0.41
1:B:1006:THR:O	1:B:1010:LEU:HG	2.21	0.41
1:B:1092:GLU:O	1:B:1093:GLU:HB2	2.20	0.41
1:B:1289:SER:OG	1:B:1289:SER:O	2.39	0.41
1:B:1735:ARG:O	1:B:1736:PHE:HB2	2.20	0.41
1:B:1761:LEU:HD23	1:B:1762:MSE:N	2.36	0.41
1:B:1931:ASN:OD1	1:B:1932:GLN:N	2.53	0.41
1:B:1945:TYR:HD1	1:B:1948:ALA:HB3	1.86	0.41
1:B:2003:LYS:HA	1:B:2006:GLU:HB2	2.03	0.41
1:B:2066:PHE:HB3	1:B:2067:ARG:HA	2.02	0.41
1:B:2386:LEU:HA	1:B:2386:LEU:HD23	1.80	0.41
1:B:2870:SER:C	1:B:2872:ASP:N	2.71	0.41
1:B:2995:GLU:O	1:B:2998:SER:HB3	2.20	0.41
1:B:3778:ASP:OD1	1:B:3780:ALA:N	2.53	0.41
1:B:3944:HIS:CG	1:B:3949:ALA:HA	2.55	0.41
1:B:4028:ILE:HA	1:B:4031:ILE:HD12	2.02	0.41
1:B:3953:LEU:HD13	1:B:4069:GLU:HB3	2.01	0.41
1:A:1025:LEU:HD12	1:A:1025:LEU:HA	1.78	0.41
1:A:2083:LEU:HA	1:A:2083:LEU:HD23	1.81	0.41
1:A:2163:HIS:O	1:A:2167:PRO:HD3	2.21	0.41
1:A:2239:LYS:HE2	1:A:2240:THR:CG2	2.45	0.41
1:A:249:PHE:HZ	1:A:272:LEU:HD12	1.86	0.41
1:A:2512:ASP:HB2	1:A:2515:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3002:TYR:CE1	1:A:3003:ASN:HB3	2.55	0.41
1:A:3048:LYS:HZ3	1:A:3089:LEU:HB3	1.85	0.41
1:A:3135:LEU:O	1:A:3138:ILE:HB	2.20	0.41
1:A:3640:PHE:HB3	1:A:3644:PHE:CD2	2.56	0.41
1:A:3687:MSE:C	1:A:3689:ASP:N	2.70	0.41
1:A:3710:LYS:HA	1:A:3710:LYS:HD3	1.95	0.41
1:A:703:CYS:O	1:A:707:PHE:CD1	2.73	0.41
1:B:1076:LEU:HA	1:B:1076:LEU:HD23	1.75	0.41
1:B:1255:CYS:SG	1:B:1333:SER:HB3	2.60	0.41
1:B:1366:THR:O	1:B:1369:MSE:HB2	2.20	0.41
1:B:1608:ARG:HD3	1:B:1631:SER:H	1.86	0.41
1:B:2129:LEU:HD13	1:B:2156:VAL:CG1	2.51	0.41
1:B:2427:ARG:HB3	1:B:2433:LYS:HB2	2.02	0.41
1:B:2634:UNK:O	1:B:2637:UNK:N	2.53	0.41
1:B:2789:SER:O	1:B:2793:PRO:HD3	2.21	0.41
1:B:2970:LYS:HE3	1:B:2974:GLU:OE2	2.21	0.41
1:B:3006:ALA:HB2	1:B:3254:LEU:HD11	2.03	0.41
1:B:3026:ASP:O	1:B:3030:ILE:HG13	2.20	0.41
1:B:3072:GLU:HA	1:B:3076:ALA:HA	2.03	0.41
1:B:31:GLY:O	1:B:34:LEU:HB3	2.20	0.41
1:B:368:LEU:C	1:B:372:PRO:HG2	2.41	0.41
1:B:3974:MSE:CB	1:B:3976:GLU:HB3	2.49	0.41
1:B:394:GLN:O	1:B:398:THR:HG23	2.20	0.41
1:B:476:ARG:HA	1:B:479:ILE:CG1	2.50	0.41
1:B:567:GLU:OE2	1:B:1798:LEU:HD22	2.21	0.41
1:B:633:ILE:HG23	1:B:637:LYS:CE	2.51	0.41
1:B:906:PHE:O	1:B:909:VAL:HB	2.21	0.41
1:A:1014:LEU:O	1:A:1078:ALA:HB2	2.19	0.41
1:A:1116:ALA:HB2	1:A:1164:CYS:HB3	2.03	0.41
1:A:1220:LEU:HD13	1:A:1274:ARG:CG	2.49	0.41
1:A:1359:LEU:HD11	1:A:1365:ASN:OD1	2.20	0.41
1:A:197:PHE:CE2	1:A:230:LEU:HD22	2.56	0.41
1:A:2412:TYR:HD2	1:A:2416:LYS:NZ	2.17	0.41
1:A:246:ARG:CA	1:A:249:PHE:HD2	2.32	0.41
1:A:2520:ILE:HG23	1:A:2521:ILE:N	2.36	0.41
1:A:2887:PRO:HG3	1:A:2921:LEU:HD13	2.03	0.41
1:A:2858:ILE:CD1	1:A:2888:VAL:HB	2.51	0.41
1:A:2962:ARG:HH22	1:A:3006:ALA:HB1	1.85	0.41
1:A:3614:TYR:CD1	1:A:3618:GLY:HA3	2.56	0.41
1:A:3622:ALA:HB1	1:A:3623:PRO:HD2	2.02	0.41
1:A:3723:ASP:HB2	1:A:3741:ARG:NE	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3766:GLN:O	1:A:3769:GLN:HG2	2.21	0.41
1:A:3920:ILE:HG13	1:A:3923:ARG:HD3	2.02	0.41
1:A:2936:TYR:HD2	1:A:3979:LEU:HD21	1.83	0.41
1:A:504:GLU:O	1:A:508:HIS:CG	2.74	0.41
1:A:752:LEU:O	1:A:756:PHE:HD1	2.02	0.41
1:A:75:SER:HA	1:A:79:ARG:HG3	2.01	0.41
1:A:923:ASP:O	1:A:927:LYS:HE3	2.20	0.41
1:B:989:MSE:SE	1:B:1030:GLY:O	2.89	0.41
1:B:717:LYS:HZ3	1:B:1121:LEU:HD11	1.83	0.41
1:B:168:ASP:O	1:B:170:VAL:N	2.47	0.41
1:B:1880:MSE:O	1:B:1883:ARG:N	2.51	0.41
1:B:204:LEU:HG	1:B:204:LEU:H	1.53	0.41
1:B:204:LEU:HD22	1:B:219:VAL:CG1	2.46	0.41
1:B:2066:PHE:CD1	1:B:2128:PHE:HE1	2.39	0.41
1:B:2164:TRP:CZ3	1:B:2186:VAL:HG23	2.55	0.41
1:B:2542:LEU:HD13	1:B:2546:TYR:CE2	2.56	0.41
1:B:3329:LEU:O	1:B:3332:THR:OG1	2.32	0.41
1:B:3494:GLN:O	1:B:3498:TRP:CZ3	2.73	0.41
1:B:3736:LYS:HB3	1:B:3752:VAL:HB	2.02	0.41
1:B:3772:ASN:HA	1:B:3775:LEU:HG	2.02	0.41
1:B:431:TYR:CA	1:B:434:VAL:HG12	2.44	0.41
1:B:527:TYR:CD1	1:B:531:PHE:HZ	2.38	0.41
1:A:1165:LEU:O	1:A:1166:LEU:C	2.59	0.41
1:A:1168:LEU:O	1:A:1171:TRP:HB3	2.21	0.41
1:A:1364:CYS:C	1:A:1366:THR:N	2.74	0.41
1:A:1500:LEU:HB3	1:A:1501:PRO:HD3	2.03	0.41
1:A:160:LEU:O	1:A:164:LYS:HG2	2.20	0.41
1:A:1816:ARG:HD3	1:A:1819:PHE:HE1	1.86	0.41
1:A:1949:ILE:HD12	1:A:1949:ILE:HA	1.88	0.41
1:A:1992:VAL:HG23	1:A:1993:GLU:N	2.35	0.41
1:A:2040:MSE:HA	1:A:2043:PHE:CD1	2.55	0.41
1:A:2070:GLU:HB2	1:A:2072:ARG:N	2.36	0.41
1:A:217:LEU:N	1:A:218:PRO:HD2	2.36	0.41
1:A:2219:LEU:HB3	1:A:2238:ILE:HG21	2.02	0.41
1:A:2238:ILE:O	1:A:2242:VAL:HG23	2.21	0.41
1:A:2344:LEU:O	1:A:2347:LYS:HB2	2.21	0.41
1:A:2541:ALA:O	1:A:2545:LEU:HG	2.20	0.41
1:A:2824:LYS:HB3	1:A:2825:THR:H	1.69	0.41
1:A:2863:CYS:O	1:A:2865:HIS:N	2.54	0.41
1:A:2920:VAL:O	1:A:2923:TRP:HB3	2.21	0.41
1:A:3033:GLU:OE2	1:A:3079:GLU:CD	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3356:ALA:HB1	1:A:3384:HIS:HB3	2.02	0.41
1:A:3502:MSE:CE	1:A:3517:SER:HB3	2.51	0.41
1:A:3529:ILE:HG22	1:A:3529:ILE:O	2.21	0.41
1:A:3676:PRO:CG	1:A:3677:PRO:HD3	2.50	0.41
1:A:3928:PHE:O	1:A:3928:PHE:CD1	2.74	0.41
1:A:396:PHE:CE1	1:A:437:HIS:CD2	3.08	0.41
1:A:474:VAL:HG11	1:A:1564:SER:CB	2.50	0.41
1:A:481:THR:HG22	1:A:482:VAL:N	2.35	0.41
1:A:560:LEU:O	1:A:563:LEU:N	2.54	0.41
1:A:704:PHE:HA	1:A:707:PHE:CG	2.56	0.41
1:A:508:HIS:CD2	1:A:725:LEU:HD13	2.55	0.41
1:A:959:TYR:O	1:A:963:LYS:CB	2.62	0.41
1:A:980:THR:CG2	1:A:984:TYR:CE1	3.01	0.41
1:B:1273:GLU:HG2	1:B:1276:VAL:HB	2.02	0.41
1:B:1513:GLY:O	1:B:1517:LEU:HG	2.19	0.41
1:B:1909:ASN:ND2	1:B:1909:ASN:N	2.69	0.41
1:B:1911:LEU:HD22	1:B:1916:ILE:HG21	2.03	0.41
1:B:1946:ASN:ND2	1:B:1993:GLU:OE2	2.40	0.41
1:B:1996:VAL:HG23	1:B:1997:PRO:CD	2.51	0.41
1:B:2062:ALA:O	1:B:2066:PHE:N	2.53	0.41
1:B:2412:TYR:CG	1:B:2412:TYR:O	2.73	0.41
1:B:2565:MSE:SE	1:B:2565:MSE:O	2.88	0.41
1:B:2787:HIS:HB3	1:B:2790:LEU:HD12	2.02	0.41
1:B:2870:SER:HA	1:B:2897:LEU:CD2	2.51	0.41
1:B:2925:GLU:HB3	1:B:3121:LEU:HD21	2.02	0.41
1:B:2975:ALA:C	1:B:2977:ASN:N	2.74	0.41
1:B:3136:THR:O	1:B:3140:GLU:CB	2.68	0.41
1:B:3259:LEU:HD11	1:B:3275:SER:O	2.21	0.41
1:B:3291:GLN:O	1:B:3294:SER:OG	2.39	0.41
1:B:3492:CYS:HB2	1:B:3713:PRO:HG3	2.03	0.41
1:B:4002:MSE:O	1:B:4006:VAL:HG13	2.21	0.41
1:B:4082:ARG:HG3	1:B:4091:ALA:CB	2.37	0.41
1:B:752:LEU:HA	1:B:755:ALA:CB	2.50	0.41
1:B:989:MSE:CG	1:B:1031:ARG:NH1	2.83	0.41
1:A:1111:LEU:N	1:A:1111:LEU:HD12	2.35	0.41
1:A:1894:SER:C	1:A:1896:ILE:H	2.24	0.41
1:A:2138:VAL:HB	1:A:2139:PRO:HD3	2.03	0.41
1:A:2330:VAL:CG2	1:A:2338:GLU:HB3	2.35	0.41
1:A:2423:VAL:HG22	1:A:2424:MSE:N	2.36	0.41
1:A:2640:UNK:O	1:A:2641:UNK:C	2.68	0.41
1:A:265:TYR:C	1:A:268:PRO:HD2	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2999:LEU:HD12	1:A:3002:TYR:HE2	1.86	0.41
1:A:3048:LYS:HE2	1:A:3048:LYS:HB3	1.68	0.41
1:A:3190:LEU:O	1:A:3194:GLU:HB2	2.21	0.41
1:A:4070:LYS:HB3	1:A:4073:ALA:HB3	2.02	0.41
1:B:1463:LEU:O	1:B:1463:LEU:HD23	2.21	0.41
1:B:1548:GLY:O	1:B:1552:HIS:ND1	2.53	0.41
1:B:1606:ARG:NH1	1:B:1806:ARG:HB3	2.36	0.41
1:B:1880:MSE:CE	1:B:1884:LEU:HD11	2.51	0.41
1:B:1874:TYR:HD2	1:B:1885:PRO:HG3	1.85	0.41
1:B:2009:LYS:CG	1:B:2010:GLU:H	2.34	0.41
1:B:2083:LEU:HD23	1:B:2083:LEU:HA	1.82	0.41
1:B:2164:TRP:CE3	1:B:2215:LEU:HG	2.55	0.41
1:B:2367:VAL:O	1:B:2371:PHE:HE1	2.04	0.41
1:B:2371:PHE:CG	1:B:2372:PRO:HD3	2.56	0.41
1:B:2440:TYR:CE2	1:B:2443:MSE:SE	3.24	0.41
1:B:2943:PHE:C	1:B:2945:SER:N	2.73	0.41
1:B:3031:TRP:CD2	1:B:3034:PRO:HD3	2.56	0.41
1:B:3148:GLN:NE2	1:B:3197:LEU:HD12	2.36	0.41
1:B:3839:TYR:CE1	1:B:3867:THR:HB	2.29	0.41
1:B:46:SER:H	1:B:51:LEU:CD1	2.34	0.41
1:B:476:ARG:HA	1:B:479:ILE:HG13	2.03	0.41
1:B:634:LEU:CB	1:B:638:GLN:HE22	2.32	0.41
1:B:70:ARG:NH2	1:B:79:ARG:HG2	2.35	0.41
1:B:911:LEU:O	1:B:915:THR:HG23	2.20	0.41
1:A:1005:ASP:HB2	1:A:1006:THR:H	1.63	0.41
1:A:995:PHE:HZ	1:A:1006:THR:HG1	1.69	0.41
1:A:1013:ILE:HG21	1:A:1028:PHE:HB2	2.02	0.41
1:A:1147:LYS:CD	1:A:1180:GLN:HG2	2.50	0.41
1:A:1369:MSE:CE	1:A:1418:HIS:HB2	2.51	0.41
1:A:1431:LEU:HD11	1:A:1479:VAL:HG22	2.01	0.41
1:A:1938:ARG:O	1:A:1941:HIS:HB3	2.21	0.41
1:A:2439:ILE:HG12	1:A:2442:MSE:CE	2.51	0.41
1:A:2445:LYS:HD3	1:A:2445:LYS:HA	1.78	0.41
1:A:2514:ASN:H	1:A:2515:PRO:HD3	1.86	0.41
1:A:2884:LEU:HD12	1:A:2884:LEU:H	1.86	0.41
1:A:2943:PHE:HE1	1:A:2984:GLY:HA2	1.86	0.41
1:A:3425:ARG:NH1	1:A:3999:THR:CG2	2.84	0.41
1:A:3567:VAL:HG22	1:A:3571:PHE:CZ	2.56	0.41
1:A:3736:LYS:HD2	1:A:3752:VAL:HG21	2.03	0.41
1:A:3779:SER:O	1:A:3782:SER:N	2.54	0.41
1:A:3972:LEU:HD12	1:A:3974:MSE:CE	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:ILE:O	1:B:104:SER:HB3	2.20	0.41
1:B:1145:LEU:HD13	1:B:1149:LYS:HD3	2.02	0.41
1:B:1359:LEU:O	1:B:1362:ASP:OD1	2.39	0.41
1:B:1374:GLN:HA	1:B:1374:GLN:OE1	2.21	0.41
1:B:1583:MSE:HE3	1:B:1643:MSE:SE	2.70	0.41
1:B:1949:ILE:O	1:B:1952:ILE:HG22	2.20	0.41
1:B:1981:LEU:HA	1:B:1984:LEU:HD23	2.01	0.41
1:B:2386:LEU:HD12	1:B:2404:ARG:HE	1.84	0.41
1:B:3147:LYS:O	1:B:3151:LEU:HG	2.20	0.41
1:B:3155:VAL:HG21	1:B:3159:ARG:HH21	1.83	0.41
1:B:3231:ILE:HG23	1:B:3235:LYS:HE3	2.02	0.41
1:B:3319:ASN:ND2	1:B:3400:SER:HA	2.35	0.41
1:B:3575:LEU:CD2	1:B:3687:MSE:SE	3.18	0.41
1:B:3632:PHE:HE2	1:B:3683:CYS:SG	2.43	0.41
1:B:3705:TYR:CD2	1:B:3792:SER:HB2	2.56	0.41
1:B:4106:CYS:O	1:B:4108:MSE:N	2.54	0.41
1:B:804:ALA:O	1:B:806:SER:N	2.53	0.41
1:B:922:SER:C	1:B:924:ARG:N	2.74	0.41
1:B:978:GLN:N	1:B:981:ARG:HD3	2.34	0.41
1:A:1069:HIS:N	1:A:1070:PRO:CD	2.84	0.41
1:A:1385:ASN:O	1:A:1388:ASP:N	2.46	0.41
1:A:15:LEU:HA	1:A:2359:LYS:NZ	2.36	0.41
1:A:1874:TYR:CD2	1:A:1885:PRO:HG3	2.56	0.41
1:A:178:LEU:HB3	1:A:197:PHE:CE1	2.56	0.41
1:A:2165:LEU:HD11	1:A:2211:LEU:HD22	2.03	0.41
1:A:2239:LYS:CD	1:A:2279:ILE:HD12	2.49	0.41
1:A:2646:UNK:CB	1:A:2779:ASP:HA	2.51	0.41
1:A:2797:VAL:HG23	1:A:2798:ALA:N	2.36	0.41
1:A:2876:VAL:HG13	1:A:3035:PHE:CE1	2.56	0.41
1:A:295:GLU:HA	1:A:298:LEU:HB2	2.02	0.41
1:A:298:LEU:O	1:A:301:CYS:HB3	2.21	0.41
1:A:3027:LEU:HB3	1:A:3031:TRP:CZ2	2.56	0.41
1:A:3311:ASN:HB3	1:A:3312:VAL:H	1.62	0.41
1:A:3356:ALA:HB2	1:A:3384:HIS:HB3	2.03	0.41
1:A:340:TYR:O	1:A:344:GLN:HG3	2.21	0.41
1:A:3741:ARG:HG2	1:A:3741:ARG:HH11	1.84	0.41
1:A:3850:HIS:H	1:A:3850:HIS:CD2	2.39	0.41
1:A:3887:PHE:O	1:A:3890:MSE:HG2	2.20	0.41
1:B:1165:LEU:O	1:B:1166:LEU:C	2.60	0.41
1:B:1338:VAL:HA	1:B:1341:ILE:HD12	2.03	0.41
1:B:153:PHE:CD1	1:B:154:SER:N	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1752:LEU:C	1:B:1754:GLN:H	2.23	0.41
1:B:185:HIS:N	1:B:186:PRO:HD2	2.27	0.41
1:B:2009:LYS:HE2	1:B:2012:ARG:HH11	1.86	0.41
1:B:214:GLU:HB3	1:B:215:PRO:HD2	2.02	0.41
1:B:2220:MSE:O	1:B:2221:LYS:C	2.59	0.41
1:B:175:TYR:CD2	1:B:222:GLY:HA3	2.54	0.41
1:B:2849:SER:O	1:B:2850:PHE:CD1	2.74	0.41
1:B:3151:LEU:HA	1:B:3152:SER:HA	1.73	0.41
1:B:3186:ARG:HH11	1:B:3186:ARG:HG3	1.85	0.41
1:B:3292:GLY:HA2	1:B:3296:GLN:HG2	2.03	0.41
1:B:3503:VAL:HG22	1:B:3539:SER:CB	2.51	0.41
1:B:3694:PHE:O	1:B:3697:ASN:N	2.54	0.41
1:B:3950:THR:OG1	1:B:4065:LEU:HD22	2.20	0.41
1:B:553:VAL:O	1:B:556:SER:HB3	2.21	0.41
1:B:613:HIS:CG	1:B:614:PRO:HD3	2.56	0.41
1:B:806:SER:O	1:B:808:GLU:N	2.54	0.41
1:B:850:GLU:CD	1:B:854:ARG:NH2	2.75	0.41
1:A:960:GLN:CG	1:A:1009:LEU:HD21	2.44	0.41
1:A:1342:MSE:HE3	1:A:1402:LEU:HD23	2.03	0.41
1:A:1678:LEU:O	1:A:1681:ASP:OD1	2.38	0.41
1:A:1692:ALA:HA	1:A:1695:LEU:HD12	2.02	0.41
1:A:1955:VAL:HA	1:A:2003:LYS:NZ	2.36	0.41
1:A:2256:ILE:CD1	1:A:2276:LEU:HD11	2.49	0.41
1:A:2442:MSE:O	1:A:2451:LEU:HD21	2.21	0.41
1:A:2536:LEU:HA	1:A:2536:LEU:HD23	1.81	0.41
1:A:2826:LEU:O	1:A:2830:ASN:HB2	2.21	0.41
1:A:3174:ASP:N	1:A:3175:PRO:CD	2.84	0.41
1:A:3301:LEU:HB2	1:A:3328:ILE:HG21	2.03	0.41
1:A:3454:LEU:C	1:A:3456:LEU:H	2.25	0.41
1:A:34:LEU:HD11	1:A:38:LEU:HD11	2.03	0.41
1:A:3629:ARG:O	1:A:3686:TRP:NE1	2.51	0.41
1:A:3630:ARG:HA	1:A:3686:TRP:NE1	2.36	0.41
1:A:3683:CYS:O	1:A:3687:MSE:HB2	2.21	0.41
1:A:591:GLN:HB3	1:A:1026:ARG:HD3	2.03	0.41
1:A:617:PRO:O	1:A:659:ARG:HD2	2.21	0.41
1:A:671:SER:O	1:A:675:ARG:HB2	2.21	0.41
1:A:776:TRP:CE2	1:A:780:ILE:HD12	2.55	0.41
1:A:846:ILE:HG23	1:A:854:ARG:HH12	1.86	0.41
1:B:1010:LEU:HD12	1:B:1011:GLU:H	1.85	0.41
1:B:115:TYR:O	1:B:118:ASP:HB3	2.21	0.41
1:B:1452:VAL:HG11	1:B:1502:SER:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:LYS:O	1:B:159:GLU:HG3	2.21	0.41
1:B:2044:ASP:O	1:B:2048:GLY:HA3	2.20	0.41
1:B:2795:GLN:O	1:B:2799:GLN:HG2	2.21	0.41
1:B:2915:ARG:O	1:B:2938:VAL:HG21	2.21	0.41
1:B:2991:LYS:O	1:B:2995:GLU:HG2	2.21	0.41
1:B:3593:ARG:HD3	1:B:3663:THR:HG21	2.03	0.41
1:B:3600:PRO:C	1:B:3602:ASN:N	2.75	0.41
1:B:3601:VAL:O	1:B:3605:ASN:HB2	2.21	0.41
1:B:3654:MSE:SE	1:B:3659:PHE:CB	3.17	0.41
1:B:3839:TYR:HB2	1:B:3871:PHE:CZ	2.56	0.41
1:B:3920:ILE:CG1	1:B:3923:ARG:HD2	2.35	0.41
1:B:710:PHE:O	1:B:711:GLY:C	2.59	0.41
1:B:892:LEU:CD2	1:B:907:LEU:HD13	2.50	0.41
1:A:127:ALA:O	1:A:131:LEU:CB	2.69	0.40
1:A:1462:GLY:O	1:A:1464:LEU:N	2.54	0.40
1:A:1507:CYS:SG	1:A:1508:LYS:HG2	2.61	0.40
1:A:1710:LEU:HD23	1:A:1710:LEU:HA	1.68	0.40
1:A:1960:LYS:HG2	1:A:1963:GLN:OE1	2.20	0.40
1:A:197:PHE:O	1:A:201:LEU:HG	2.21	0.40
1:A:2120:ARG:NE	1:A:2120:ARG:HA	2.36	0.40
1:A:225:LYS:O	1:A:228:SER:OG	2.31	0.40
1:A:2775:TYR:N	1:A:2775:TYR:CD1	2.89	0.40
1:A:2576:MSE:HE3	1:A:2788:SER:HB2	2.02	0.40
1:A:3024:PRO:N	1:A:3025:PRO:CD	2.84	0.40
1:A:3076:ALA:O	1:A:3080:LEU:HG	2.21	0.40
1:A:3065:ILE:HD13	1:A:3089:LEU:HD21	2.02	0.40
1:A:3008:TRP:HB2	1:A:3257:LYS:NZ	2.36	0.40
1:A:3503:VAL:HG13	1:A:3504:ALA:H	1.87	0.40
1:A:3636:PHE:O	1:A:3640:PHE:HB2	2.21	0.40
1:A:3664:ASN:O	1:A:3668:LEU:HB2	2.21	0.40
1:A:4059:ILE:HD13	1:A:4059:ILE:HG21	1.82	0.40
1:A:4066:LEU:HG	1:A:4075:ARG:CA	2.44	0.40
1:A:797:ASP:OD1	1:A:800:LEU:HD12	2.21	0.40
1:A:913:ARG:HE	1:A:916:GLU:CD	2.24	0.40
1:B:1032:CYS:O	1:B:1035:GLU:N	2.54	0.40
1:B:1142:HIS:C	1:B:1144:SER:N	2.73	0.40
1:B:1291:LEU:HB3	1:B:1292:LYS:H	1.65	0.40
1:B:1426:GLN:O	1:B:1430:GLU:HG3	2.21	0.40
1:B:1651:LYS:HB3	1:B:1680:ALA:HB1	2.02	0.40
1:B:2042:GLN:HG3	1:B:2046:SER:HB3	2.03	0.40
1:B:2226:PRO:HA	1:B:2229:ALA:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2298:GLU:HB3	1:B:2301:GLN:HB3	2.03	0.40
1:B:2368:THR:HA	1:B:2371:PHE:CE1	2.56	0.40
1:B:2374:LEU:O	1:B:2374:LEU:HD12	2.21	0.40
1:B:2374:LEU:H	1:B:2378:PHE:HE1	1.69	0.40
1:B:2481:HIS:CE1	1:B:2485:ARG:HD3	2.56	0.40
1:B:2852:PRO:O	1:B:2855:VAL:HB	2.22	0.40
1:B:281:GLN:HG3	1:B:326:MSE:HE1	2.02	0.40
1:B:4058:VAL:HG12	1:B:4061:CYS:HB3	2.03	0.40
1:B:783:HIS:C	1:B:785:MSE:H	2.24	0.40
1:B:805:LEU:H	1:B:805:LEU:HG	1.71	0.40
1:B:952:GLY:C	1:B:954:GLY:H	2.25	0.40
1:B:979:VAL:O	1:B:982:GLN:HB3	2.21	0.40
1:A:1350:ASN:OD1	1:A:1405:ALA:HA	2.20	0.40
1:A:1797:LEU:HA	1:A:1797:LEU:HD23	1.83	0.40
1:A:2296:SER:OG	1:A:2297:SER:N	2.52	0.40
1:A:2260:PHE:CE2	1:A:2303:LEU:HA	2.57	0.40
1:A:2308:SER:HA	1:A:2352:HIS:NE2	2.36	0.40
1:A:2424:MSE:HA	1:A:2436:LEU:CD1	2.51	0.40
1:A:979:VAL:HG21	1:A:2656:UNK:HA	2.02	0.40
1:A:2882:ALA:HB1	1:A:2885:GLN:HB2	2.03	0.40
1:A:3052:LEU:HG	1:A:3092:LEU:CD2	2.50	0.40
1:A:3125:ARG:HA	1:A:3125:ARG:HD3	1.57	0.40
1:A:3811:THR:O	1:A:3814:ASP:N	2.54	0.40
1:A:385:TYR:CZ	1:A:424:LEU:HD21	2.56	0.40
1:A:3880:ALA:HB1	1:A:3884:LYS:NZ	2.36	0.40
1:A:463:LYS:O	1:A:466:LEU:N	2.54	0.40
1:A:513:GLU:HA	1:A:653:LEU:HD21	2.03	0.40
1:A:654:ILE:CG2	1:A:729:CYS:HB2	2.51	0.40
1:A:757:LYS:HA	1:A:760:LEU:HD11	2.01	0.40
1:A:766:ALA:O	1:A:768:VAL:HG23	2.22	0.40
1:A:971:ARG:CG	1:A:972:LEU:H	2.27	0.40
1:B:104:SER:HA	1:B:107:ILE:HD12	2.02	0.40
1:B:1087:ARG:CD	1:B:1134:LEU:HB3	2.40	0.40
1:B:82:ARG:HD2	1:B:114:VAL:HG13	2.03	0.40
1:B:1229:CYS:SG	1:B:1282:LEU:HG	2.61	0.40
1:B:1357:LYS:HG3	1:B:1360:LYS:HZ1	1.86	0.40
1:B:1419:LEU:HD23	1:B:1419:LEU:HA	1.81	0.40
1:B:1465:HIS:HA	1:B:1469:PRO:CD	2.51	0.40
1:B:2077:HIS:O	1:B:2081:LEU:HG	2.21	0.40
1:B:2200:ALA:O	1:B:2204:GLY:N	2.55	0.40
1:B:2349:LEU:HA	1:B:2364:LEU:HD13	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2480:ILE:HA	1:B:2480:ILE:HD12	1.83	0.40
1:B:280:SER:C	1:B:322:GLN:HG2	2.42	0.40
1:B:2939:LEU:HD11	1:B:2994:TRP:CZ3	2.56	0.40
1:B:2960:GLU:HG2	1:B:3289:ARG:HH22	1.86	0.40
1:B:3602:ASN:O	1:B:3606:ILE:HB	2.21	0.40
1:B:3824:GLU:HG2	1:B:3882:LEU:HD21	2.03	0.40
1:B:4063:GLU:O	1:B:4066:LEU:HB2	2.20	0.40
1:B:487:LEU:O	1:B:490:ILE:HG22	2.20	0.40
1:B:491:CYS:HB2	1:B:527:TYR:CD1	2.56	0.40
1:B:560:LEU:O	1:B:563:LEU:N	2.54	0.40
1:B:560:LEU:HA	1:B:563:LEU:CG	2.52	0.40
1:B:593:ASN:ND2	1:B:1084:ASN:HB2	2.37	0.40
1:B:86:LEU:HD13	1:B:134:LEU:CD2	2.52	0.40
1:B:934:LEU:HD21	1:B:962:TYR:OH	2.22	0.40
1:A:1424:THR:HA	1:A:1427:SER:HB2	2.02	0.40
1:A:1597:LEU:HA	1:A:1600:MSE:HB2	2.03	0.40
1:A:1604:SER:OG	1:A:1605:PHE:N	2.54	0.40
1:A:178:LEU:HD13	1:A:197:PHE:CE1	2.57	0.40
1:A:2420:PHE:CZ	1:A:2424:MSE:HG3	2.57	0.40
1:A:2531:LEU:HA	1:A:2531:LEU:HD12	1.91	0.40
1:A:257:ARG:N	1:A:258:PRO:HD2	2.37	0.40
1:A:294:PHE:CG	1:A:295:GLU:N	2.89	0.40
1:A:2960:GLU:O	1:A:2965:TYR:CD1	2.74	0.40
1:A:294:PHE:O	1:A:297:LEU:HG	2.21	0.40
1:A:2989:ALA:O	1:A:2993:PHE:N	2.49	0.40
1:A:3173:MSE:HB3	1:A:3174:ASP:H	1.58	0.40
1:A:2960:GLU:CG	1:A:3289:ARG:HH22	2.34	0.40
1:A:3495:PHE:CE1	1:A:3521:ILE:HA	2.56	0.40
1:A:3762:GLN:HE21	1:A:3763:ARG:HH11	1.67	0.40
1:A:3771:MSE:SE	1:A:3991:PHE:CE1	3.24	0.40
1:A:4062:ASP:C	1:A:4066:LEU:HD22	2.42	0.40
1:B:1014:LEU:HD23	1:B:1028:PHE:HE2	1.86	0.40
1:B:1741:ASP:HB3	1:B:1745:LYS:HE3	2.03	0.40
1:B:2088:LEU:HG	1:B:2095:ALA:H	1.87	0.40
1:B:2065:ARG:CZ	1:B:2097:LEU:HD21	2.52	0.40
1:B:2957:LEU:HD22	1:B:3989:ARG:NH2	2.36	0.40
1:B:3356:ALA:CB	1:B:3384:HIS:HB3	2.51	0.40
1:B:3447:VAL:HG21	1:B:3475:TYR:CE2	2.56	0.40
1:B:3479:THR:HG23	1:B:3480:LEU:HD23	2.03	0.40
1:B:3606:ILE:HG22	1:B:3610:TYR:CE2	2.56	0.40
1:B:3896:ALA:HA	1:B:3899:ALA:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3907:SER:HB2	1:B:3937:VAL:H	1.86	0.40
1:B:3964:THR:O	1:B:3967:PHE:HB3	2.21	0.40
1:B:3974:MSE:HA	1:B:3975:LYS:CB	2.47	0.40
1:B:4055:ASN:HA	1:B:4056:PRO:HD3	1.91	0.40
1:B:480:SER:O	1:B:484:HIS:HB2	2.21	0.40
1:B:542:ASP:HA	1:B:545:LEU:HD12	2.04	0.40
1:B:661:PRO:CG	1:B:733:LEU:HA	2.51	0.40
1:B:667:TYR:O	1:B:669:LEU:N	2.39	0.40
1:B:676:ASN:O	1:B:680:ILE:HG13	2.21	0.40
1:B:75:SER:HA	1:B:79:ARG:HG3	2.03	0.40
1:B:932:GLU:HB3	1:B:2794:LEU:CD1	2.45	0.40
1:A:1056:THR:O	1:A:1059:LEU:HB2	2.22	0.40
1:A:1106:ILE:HA	1:A:1109:GLU:HB3	2.04	0.40
1:A:1084:ASN:ND2	1:A:1131:ILE:HG22	2.33	0.40
1:A:136:GLN:HG2	1:A:139:ARG:NH1	2.37	0.40
1:A:1492:ALA:HB1	1:A:1493:PRO:HD2	2.02	0.40
1:A:1524:LEU:HG	1:A:1559:PHE:CD1	2.56	0.40
1:A:1583:MSE:HB3	1:A:1584:GLN:H	1.70	0.40
1:A:2142:ILE:O	1:A:2145:PHE:HB2	2.22	0.40
1:A:2640:UNK:O	1:A:2643:UNK:N	2.54	0.40
1:A:286:LEU:HD22	1:A:290:TYR:HD2	1.87	0.40
1:A:3011:LEU:HD11	1:A:3043:TYR:C	2.42	0.40
1:A:3448:GLU:O	1:A:3451:LEU:HB2	2.21	0.40
1:A:3425:ARG:NH2	1:A:3467:ARG:HH12	2.18	0.40
1:A:3812:LEU:HD22	1:A:3928:PHE:CE1	2.57	0.40
1:A:3930:VAL:HA	1:A:3937:VAL:HA	2.02	0.40
1:A:396:PHE:CE1	1:A:437:HIS:NE2	2.90	0.40
1:B:1128:CYS:O	1:B:1131:ILE:HG23	2.21	0.40
1:B:1682:THR:CB	1:B:1724:MSE:SE	3.18	0.40
1:B:2007:ILE:HD13	1:B:2007:ILE:HG21	1.72	0.40
1:B:2065:ARG:HD3	1:B:2100:LEU:HD11	2.02	0.40
1:B:2485:ARG:HH11	1:B:2530:ARG:NH2	2.18	0.40
1:B:262:LEU:HD22	1:B:306:VAL:CG1	2.51	0.40
1:B:2813:PHE:CD1	1:B:2814:SER:N	2.90	0.40
1:B:3176:MSE:HG2	1:B:3249:GLN:HG2	2.03	0.40
1:B:3230:LEU:O	1:B:3234:CYS:HB2	2.22	0.40
1:B:3564:GLN:C	1:B:3566:GLY:N	2.73	0.40
1:B:3736:LYS:HB2	1:B:3736:LYS:HE3	1.87	0.40
1:B:3860:LYS:O	1:B:3864:ARG:HG3	2.22	0.40
1:B:3959:MSE:SE	1:B:4124:TRP:CZ3	3.25	0.40
1:B:3981:TYR:HE1	1:B:4105:LYS:N	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:MSE:HE3	1:B:410:MSE:HB3	1.84	0.40
1:B:435:LEU:HD12	1:B:436:GLU:N	2.36	0.40
1:B:484:HIS:O	1:B:488:ILE:HG23	2.22	0.40
1:B:506:GLU:O	1:B:509:ARG:HG2	2.20	0.40
1:B:544:ILE:O	1:B:546:ALA:N	2.55	0.40
1:B:611:ASN:O	1:B:614:PRO:HD2	2.20	0.40
1:B:742:GLU:HB3	1:B:783:HIS:CD2	2.56	0.40
1:B:763:THR:HB	1:B:770:LEU:HD23	2.02	0.40
1:A:1639:LEU:HD12	1:A:1640:GLU:N	2.37	0.40
1:A:1727:ARG:O	1:A:1730:PRO:HD2	2.21	0.40
1:A:1602:ASP:HB2	1:A:1810:PRO:CB	2.52	0.40
1:A:1916:ILE:HG23	1:A:1920:TYR:HE1	1.85	0.40
1:A:2065:ARG:CZ	1:A:2097:LEU:HD21	2.50	0.40
1:A:2307:MSE:O	1:A:2310:VAL:O	2.40	0.40
1:A:2325:LEU:HD12	1:A:2325:LEU:HA	1.82	0.40
1:A:2926:LEU:HB2	1:A:3123:GLN:CD	2.42	0.40
1:A:3042:PRO:HA	1:A:3045:ILE:CG1	2.49	0.40
1:A:3144:PHE:CZ	1:A:3193:ILE:HD11	2.57	0.40
1:A:323:VAL:O	1:A:327:VAL:CB	2.66	0.40
1:A:2960:GLU:HG2	1:A:3252:PHE:CB	2.51	0.40
1:A:3251:ASN:HD21	1:A:3254:LEU:HD22	1.87	0.40
1:A:2929:LEU:HD21	1:A:3784:ARG:HB3	2.04	0.40
1:A:882:SER:HB2	1:A:3892:THR:CB	2.52	0.40
1:A:3933:GLU:C	1:A:3935:GLY:H	2.24	0.40
1:A:442:GLN:OE1	1:A:457:CYS:HB3	2.22	0.40
1:B:1017:ILE:HD12	1:B:1025:LEU:CD2	2.52	0.40
1:B:101:ALA:O	1:B:104:SER:OG	2.17	0.40
1:B:1353:PRO:HA	1:B:1358:LEU:HB3	2.03	0.40
1:B:1571:LEU:HD13	1:B:1599:GLY:O	2.21	0.40
1:B:1737:ASN:C	1:B:1739:TYR:N	2.73	0.40
1:B:1762:MSE:CB	1:B:1896:ILE:HG12	2.48	0.40
1:B:1916:ILE:HG23	1:B:1920:TYR:HE1	1.85	0.40
1:B:2379:MSE:HE3	1:B:2383:PHE:HD1	1.87	0.40
1:B:2461:PHE:CE1	1:B:2462:VAL:HG23	2.57	0.40
1:B:2894:GLU:CD	1:B:3973:PRO:HG2	2.41	0.40
1:B:2950:LYS:O	1:B:2954:GLN:HB2	2.22	0.40
1:B:3159:ARG:C	1:B:3161:LEU:H	2.25	0.40
1:B:350:ARG:NH1	1:B:387:GLU:CD	2.74	0.40
1:B:3605:ASN:HB3	1:B:3609:MSE:CE	2.52	0.40
1:B:376:ILE:HG13	1:B:381:VAL:HG21	2.03	0.40
1:B:3775:LEU:HB3	1:B:3781:CYS:SG	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3870:SER:OG	1:B:3871:PHE:N	2.54	0.40
1:B:509:ARG:HB3	1:B:729:CYS:SG	2.62	0.40
1:B:567:GLU:HB3	1:B:606:SER:HB2	2.04	0.40
1:B:869:ASN:O	1:B:873:VAL:HG23	2.21	0.40
1:B:971:ARG:CG	1:B:972:LEU:H	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3631/4128 (88%)	2664 (73%)	724 (20%)	243 (7%)	1	25
1	B	3631/4128 (88%)	2657 (73%)	723 (20%)	251 (7%)	1	24
2	K	1/194 (0%)	1 (100%)	0	0	100	100
2	S	1/194 (0%)	1 (100%)	0	0	100	100
All	All	7264/8644 (84%)	5323 (73%)	1447 (20%)	494 (7%)	1	24

All (494) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	ALA
1	A	76	ILE
1	A	147	PHE
1	A	167	PRO
1	A	184	VAL
1	A	185	HIS
1	A	276	ALA
1	A	325	ASN
1	A	405	ASP
1	A	428	PRO

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Mol	Chain	Res	Type
1	A	430	VAL
1	A	544	ILE
1	A	546	ALA
1	A	566	ASP
1	A	635	PRO
1	A	650	SER
1	A	742	GLU
1	A	755	ALA
1	A	767	GLU
1	A	885	ALA
1	A	897	PRO
1	A	903	PRO
1	A	905	ILE
1	A	958	MSE
1	A	1001	PHE
1	A	1005	ASP
1	A	1053	PRO
1	A	1094	SER
1	A	1110	SER
1	A	1141	LYS
1	A	1143	VAL
1	A	1271	ILE
1	A	1324	PRO
1	A	1425	ALA
1	A	1583	MSE
1	A	1591	LYS
1	A	1593	VAL
1	A	1733	THR
1	A	1746	PHE
1	A	1762	MSE
1	A	1978	PHE
1	A	2003	LYS
1	A	2012	ARG
1	A	2029	SER
1	A	2030	TYR
1	A	2058	ASP
1	A	2068	ARG
1	A	2069	ARG
1	A	2074	PRO
1	A	2075	THR
1	A	2126	MSE
1	A	2155	GLU

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Mol	Chain	Res	Type
1	A	2177	ASN
1	A	2248	CYS
1	A	2261	SER
1	A	2286	PRO
1	A	2287	PRO
1	A	2290	PRO
1	A	2357	GLU
1	A	2373	PRO
1	A	2424	MSE
1	A	2464	HIS
1	A	2785	ILE
1	A	2878	ALA
1	A	2926	LEU
1	A	2927	ALA
1	A	3173	MSE
1	A	3313	SER
1	A	3345	PRO
1	A	3576	ASP
1	A	3600	PRO
1	A	3603	LYS
1	A	3688	SER
1	A	3716	HIS
1	A	3835	PRO
1	A	3933	GLU
1	B	76	ILE
1	B	167	PRO
1	B	184	VAL
1	B	185	HIS
1	B	238	MSE
1	B	260	ILE
1	B	276	ALA
1	B	395	MSE
1	B	405	ASP
1	B	430	VAL
1	B	540	MSE
1	B	546	ALA
1	B	566	ASP
1	B	635	PRO
1	B	670	LEU
1	B	742	GLU
1	B	746	ARG
1	B	767	GLU

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Mol	Chain	Res	Type
1	B	784	VAL
1	B	871	LEU
1	B	885	ALA
1	B	897	PRO
1	B	903	PRO
1	B	923	ASP
1	B	1001	PHE
1	B	1005	ASP
1	B	1073	PHE
1	B	1093	GLU
1	B	1110	SER
1	B	1119	LYS
1	B	1122	GLY
1	B	1141	LYS
1	B	1143	VAL
1	B	1214	GLU
1	B	1271	ILE
1	B	1324	PRO
1	B	1408	MSE
1	B	1591	LYS
1	B	1762	MSE
1	B	1957	ASN
1	B	1974	ASN
1	B	1978	PHE
1	B	2012	ARG
1	B	2029	SER
1	B	2058	ASP
1	B	2068	ARG
1	B	2069	ARG
1	B	2074	PRO
1	B	2075	THR
1	B	2155	GLU
1	B	2156	VAL
1	B	2177	ASN
1	B	2248	CYS
1	B	2261	SER
1	B	2263	LYS
1	B	2286	PRO
1	B	2287	PRO
1	B	2290	PRO
1	B	2373	PRO
1	B	2424	MSE

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Mol	Chain	Res	Type
1	B	2785	ILE
1	B	2878	ALA
1	B	2884	LEU
1	B	3240	MSE
1	B	3241	LYS
1	B	3313	SER
1	B	3340	ALA
1	B	3600	PRO
1	B	3603	LYS
1	B	3688	SER
1	B	3711	PRO
1	B	3835	PRO
1	A	97	GLY
1	A	169	THR
1	A	170	VAL
1	A	186	PRO
1	A	187	SER
1	A	260	ILE
1	A	602	MSE
1	A	608	PRO
1	A	746	ARG
1	A	772	ALA
1	A	871	LEU
1	A	923	ASP
1	A	957	PRO
1	A	1000	LYS
1	A	1075	ARG
1	A	1093	GLU
1	A	1112	ALA
1	A	1119	LYS
1	A	1122	GLY
1	A	1169	VAL
1	A	1214	GLU
1	A	1231	GLN
1	A	1237	ALA
1	A	1290	LEU
1	A	1590	THR
1	A	1700	THR
1	A	1724	MSE
1	A	1745	LYS
1	A	1934	LEU
1	A	1957	ASN

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Mol	Chain	Res	Type
1	A	1963	GLN
1	A	2002	LYS
1	A	2011	ALA
1	A	2016	ASN
1	A	2072	ARG
1	A	2168	LEU
1	A	2282	ALA
1	A	2423	VAL
1	A	2514	ASN
1	A	2824	LYS
1	A	2884	LEU
1	A	3311	ASN
1	A	3312	VAL
1	A	3340	ALA
1	A	3456	LEU
1	A	3575	LEU
1	A	3678	GLY
1	A	3973	PRO
1	B	325	ASN
1	B	394	GLN
1	B	428	PRO
1	B	545	LEU
1	B	654	ILE
1	B	671	SER
1	B	712	LYS
1	B	755	ALA
1	B	958	MSE
1	B	1053	PRO
1	B	1075	ARG
1	B	1094	SER
1	B	1290	LEU
1	B	1420	ARG
1	B	1425	ALA
1	B	1709	GLU
1	B	1733	THR
1	B	1811	ARG
1	B	2002	LYS
1	B	2030	TYR
1	B	2072	ARG
1	B	2168	LEU
1	B	2423	VAL
1	B	2570	PRO

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Mol	Chain	Res	Type
1	B	2801	ASP
1	B	2824	LYS
1	B	2871	LEU
1	B	2926	LEU
1	B	2944	THR
1	B	3064	PHE
1	B	3242	MSE
1	B	3345	PRO
1	B	3403	CYS
1	B	3456	LEU
1	B	3499	ILE
1	B	3678	GLY
1	B	3826	ALA
1	B	3933	GLU
1	A	28	ALA
1	A	30	ALA
1	A	48	PRO
1	A	404	ASP
1	A	425	ASP
1	A	604	PRO
1	A	628	GLU
1	A	654	ILE
1	A	1045	THR
1	A	1077	GLY
1	A	1238	GLN
1	A	1289	SER
1	A	1408	MSE
1	A	1420	ARG
1	A	1722	PHE
1	A	1811	ARG
1	A	1962	TYR
1	A	2034	SER
1	A	2096	PRO
1	A	2206	PRO
1	A	2263	LYS
1	A	2280	VAL
1	A	2371	PHE
1	A	2823	PHE
1	A	2914	ALA
1	A	3314	SER
1	A	3545	THR
1	A	3598	LYS

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Mol	Chain	Res	Type
1	A	3796	MSE
1	A	3826	ALA
1	A	3857	LEU
1	A	3978	GLY
1	B	27	ALA
1	B	48	PRO
1	B	101	ALA
1	B	125	ILE
1	B	144	MSE
1	B	186	PRO
1	B	257	ARG
1	B	368	LEU
1	B	404	ASP
1	B	425	ASP
1	B	513	GLU
1	B	650	SER
1	B	957	PRO
1	B	1215	GLU
1	B	1231	GLN
1	B	1237	ALA
1	B	1238	GLN
1	B	1492	ALA
1	B	1565	GLU
1	B	1583	MSE
1	B	1700	THR
1	B	1722	PHE
1	B	1917	LYS
1	B	2003	LYS
1	B	2011	ALA
1	B	2080	VAL
1	B	2096	PRO
1	B	2206	PRO
1	B	2357	GLU
1	B	2371	PHE
1	B	2465	PRO
1	B	2514	ASN
1	B	2575	PRO
1	B	2795	GLN
1	B	2823	PHE
1	B	2927	ALA
1	B	3174	ASP
1	B	3311	ASN

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Mol	Chain	Res	Type
1	B	3601	VAL
1	B	3716	HIS
1	B	3796	MSE
1	B	4120	THR
1	A	27	ALA
1	A	125	ILE
1	A	257	ARG
1	A	277	LEU
1	A	515	ARG
1	A	543	SER
1	A	712	LYS
1	A	784	VAL
1	A	878	GLU
1	A	949	PRO
1	A	1073	PHE
1	A	1463	LEU
1	A	1492	ALA
1	A	1565	GLU
1	A	1647	ALA
1	A	1723	PRO
1	A	2010	GLU
1	A	2080	VAL
1	A	2176	ASN
1	A	2542	LEU
1	A	2795	GLN
1	A	2871	LEU
1	A	2873	PRO
1	A	2879	GLY
1	A	3064	PHE
1	A	3240	MSE
1	A	3443	PRO
1	A	3472	ILE
1	A	3760	GLN
1	A	3860	LYS
1	B	49	ALA
1	B	69	VAL
1	B	169	THR
1	B	277	LEU
1	B	411	PRO
1	B	604	PRO
1	B	910	PHE
1	B	947	GLN

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Mol	Chain	Res	Type
1	B	1000	LYS
1	B	1045	THR
1	B	1069	HIS
1	B	1077	GLY
1	B	1112	ALA
1	B	1348	LEU
1	B	1590	THR
1	B	1723	PRO
1	B	1757	MSE
1	B	1891	ALA
1	B	1895	LYS
1	B	1934	LEU
1	B	1962	TYR
1	B	1987	ARG
1	B	2098	THR
1	B	2464	HIS
1	B	3075	LYS
1	B	3486	GLU
1	B	3497	SER
1	B	3637	GLY
1	B	3654	MSE
1	B	3720	ALA
1	B	3760	GLN
1	B	3847	SER
1	B	3860	LYS
1	B	3973	PRO
1	A	368	LEU
1	A	540	MSE
1	A	598	PRO
1	A	634	LEU
1	A	900	GLU
1	A	1069	HIS
1	A	1364	CYS
1	A	1510	LEU
1	A	1891	ALA
1	A	1895	LYS
1	A	2448	PRO
1	A	2465	PRO
1	A	2569	SER
1	A	2805	ALA
1	A	3091	LEU
1	A	3654	MSE

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Mol	Chain	Res	Type
1	A	3720	ALA
1	A	3732	LEU
1	A	4058	VAL
1	B	30	ALA
1	B	74	ASN
1	B	745	VAL
1	B	763	THR
1	B	878	GLU
1	B	997	ASN
1	B	1071	ASN
1	B	1169	VAL
1	B	1247	PRO
1	B	1346	THR
1	B	1423	ILE
1	B	1593	VAL
1	B	1631	SER
1	B	1701	SER
1	B	1707	LEU
1	B	1812	LEU
1	B	1963	GLN
1	B	2016	ASN
1	B	2280	VAL
1	B	2289	ASP
1	B	2292	CYS
1	B	2879	GLY
1	B	2914	ALA
1	B	3129	LEU
1	B	3243	ILE
1	B	3312	VAL
1	B	3472	ILE
1	B	3978	GLY
1	A	74	ASN
1	A	298	LEU
1	A	627	VAL
1	A	763	THR
1	A	1520	ALA
1	A	2289	ASP
1	A	2942	ILE
1	A	3117	ILE
1	A	3317	SER
1	A	3499	ILE
1	A	3711	PRO

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Mol	Chain	Res	Type
1	A	3981	TYR
1	B	187	SER
1	B	298	LEU
1	B	323	VAL
1	B	427	VAL
1	B	627	VAL
1	B	718	MSE
1	B	748	TYR
1	B	1364	CYS
1	B	1738	ASN
1	B	2291	GLN
1	B	2873	PRO
1	B	2976	LEU
1	B	3443	PRO
1	B	4068	HIS
1	A	256	ILE
1	A	411	PRO
1	A	553	VAL
1	A	1637	SER
1	A	2076	VAL
1	A	2505	VAL
1	A	2552	VAL
1	A	2575	PRO
1	A	3025	PRO
1	A	3601	VAL
1	B	50	VAL
1	B	67	VAL
1	B	170	VAL
1	B	2552	VAL
1	B	4058	VAL
1	A	50	VAL
1	A	69	VAL
1	A	1382	ILE
1	A	2156	VAL
1	A	3174	ASP
1	B	948	MSE
1	B	1382	ILE
1	B	2448	PRO
1	B	3331	GLY
1	A	67	VAL
1	A	381	VAL
1	A	447	PRO

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Mol	Chain	Res	Type
1	A	2059	PRO
1	A	2230	VAL
1	A	2324	GLY
1	A	3919	GLY
1	B	381	VAL
1	B	495	VAL
1	B	2230	VAL
1	B	2569	SER
1	B	3919	GLY
1	A	1247	PRO
1	A	1729	PHE
1	B	174	VAL
1	B	544	ILE
1	B	884	VAL
1	B	905	ILE
1	B	1637	SER
1	B	2804	ILE
1	A	1468	LEU
1	A	3178	ILE
1	B	256	ILE
1	B	2802	PRO
1	B	2942	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3259/3384 (96%)	3089 (95%)	170 (5%)	29	67
1	B	3259/3384 (96%)	3084 (95%)	175 (5%)	27	66
2	K	-	1 (100%)	0	100	100
2	S	-	1 (100%)	0	100	100
All	All	6520/6768 (96%)	6175 (95%)	345 (5%)	28	67

All (345) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	LEU
1	A	156	PHE
1	A	274	LEU
1	A	277	LEU
1	A	294	PHE
1	A	326	MSE
1	A	342	MSE
1	A	360	SER
1	A	361	ILE
1	A	368	LEU
1	A	392	CYS
1	A	393	LYS
1	A	396	PHE
1	A	405	ASP
1	A	420	VAL
1	A	444	ASP
1	A	445	SER
1	A	446	PHE
1	A	556	SER
1	A	559	SER
1	A	564	LEU
1	A	595	ASP
1	A	603	ILE
1	A	612	LEU
1	A	620	PHE
1	A	625	ASN
1	A	630	CYS
1	A	631	ARG
1	A	754	MSE
1	A	763	THR
1	A	793	LEU
1	A	858	MSE
1	A	866	ILE
1	A	879	MSE
1	A	884	VAL
1	A	891	ARG
1	A	898	PHE
1	A	907	LEU
1	A	924	ARG
1	A	939	MSE
1	A	963	LYS
1	A	965	THR
1	A	966	PHE

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Mol	Chain	Res	Type
1	A	970	LEU
1	A	975	ASP
1	A	983	LEU
1	A	988	VAL
1	A	989	MSE
1	A	993	HIS
1	A	1005	ASP
1	A	1010	LEU
1	A	1014	LEU
1	A	1017	ILE
1	A	1024	THR
1	A	1068	LEU
1	A	1070	PRO
1	A	1105	VAL
1	A	1107	TYR
1	A	1108	MSE
1	A	1121	LEU
1	A	1131	ILE
1	A	1180	GLN
1	A	1288	SER
1	A	1291	LEU
1	A	1347	THR
1	A	1364	CYS
1	A	1372	LEU
1	A	1403	MSE
1	A	1430	GLU
1	A	1444	ASP
1	A	1507	CYS
1	A	1526	GLU
1	A	1583	MSE
1	A	1590	THR
1	A	1592	MSE
1	A	1597	LEU
1	A	1600	MSE
1	A	1640	GLU
1	A	1643	MSE
1	A	1721	HIS
1	A	1737	ASN
1	A	1743	MSE
1	A	1757	MSE
1	A	1758	LEU
1	A	1759	LEU

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Mol	Chain	Res	Type
1	A	1761	LEU
1	A	1812	LEU
1	A	1883	ARG
1	A	1886	LYS
1	A	1919	CYS
1	A	1942	CYS
1	A	1947	CYS
1	A	1950	SER
1	A	1959	LEU
1	A	1986	ARG
1	A	1993	GLU
1	A	1998	MSE
1	A	2012	ARG
1	A	2104	MSE
1	A	2155	GLU
1	A	2189	ILE
1	A	2239	LYS
1	A	2241	LEU
1	A	2245	TRP
1	A	2277	LEU
1	A	2287	PRO
1	A	2307	MSE
1	A	2330	VAL
1	A	2337	LEU
1	A	2338	GLU
1	A	2355	THR
1	A	2362	VAL
1	A	2370	SER
1	A	2402	LEU
1	A	2404	ARG
1	A	2473	MSE
1	A	2555	LEU
1	A	2568	MSE
1	A	2574	ASN
1	A	2788	SER
1	A	2886	GLN
1	A	2890	ILE
1	A	2921	LEU
1	A	2943	PHE
1	A	2991	LYS
1	A	3011	LEU
1	A	3050	LYS

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Mol	Chain	Res	Type
1	A	3051	LEU
1	A	3084	GLN
1	A	3145	ILE
1	A	3173	MSE
1	A	3256	MSE
1	A	3278	GLN
1	A	3283	LEU
1	A	3326	GLN
1	A	3416	LEU
1	A	3451	LEU
1	A	3481	SER
1	A	3509	ASP
1	A	3518	VAL
1	A	3575	LEU
1	A	3636	PHE
1	A	3641	ASP
1	A	3670	MSE
1	A	3687	MSE
1	A	3706	ASP
1	A	3729	MSE
1	A	3771	MSE
1	A	3781	CYS
1	A	3810	VAL
1	A	3811	THR
1	A	3813	LYS
1	A	3824	GLU
1	A	3831	ASP
1	A	3846	MSE
1	A	3883	LEU
1	A	3893	SER
1	A	3895	GLU
1	A	3926	ASN
1	A	3928	PHE
1	A	3929	MSE
1	A	3944	HIS
1	A	3959	MSE
1	A	3963	LEU
1	A	3964	THR
1	A	3967	PHE
1	A	4066	LEU
1	A	4078	VAL
1	A	4104	VAL

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Mol	Chain	Res	Type
1	A	4128	MSE
1	B	42	CYS
1	B	111	CYS
1	B	143	LEU
1	B	145	ASP
1	B	156	PHE
1	B	274	LEU
1	B	298	LEU
1	B	322	GLN
1	B	360	SER
1	B	361	ILE
1	B	368	LEU
1	B	389	ILE
1	B	393	LYS
1	B	395	MSE
1	B	396	PHE
1	B	405	ASP
1	B	408	TYR
1	B	410	MSE
1	B	420	VAL
1	B	444	ASP
1	B	446	PHE
1	B	487	LEU
1	B	491	CYS
1	B	559	SER
1	B	564	LEU
1	B	603	ILE
1	B	612	LEU
1	B	620	PHE
1	B	633	ILE
1	B	653	LEU
1	B	666	PHE
1	B	733	LEU
1	B	741	ILE
1	B	763	THR
1	B	793	LEU
1	B	865	GLN
1	B	898	PHE
1	B	901	MSE
1	B	924	ARG
1	B	963	LYS
1	B	965	THR

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Mol	Chain	Res	Type
1	B	966	PHE
1	B	970	LEU
1	B	989	MSE
1	B	993	HIS
1	B	1000	LYS
1	B	1005	ASP
1	B	1009	LEU
1	B	1010	LEU
1	B	1017	ILE
1	B	1024	THR
1	B	1036	PHE
1	B	1070	PRO
1	B	1108	MSE
1	B	1121	LEU
1	B	1131	ILE
1	B	1287	GLN
1	B	1347	THR
1	B	1354	GLU
1	B	1372	LEU
1	B	1392	MSE
1	B	1399	CYS
1	B	1430	GLU
1	B	1471	GLN
1	B	1507	CYS
1	B	1583	MSE
1	B	1590	THR
1	B	1597	LEU
1	B	1602	ASP
1	B	1639	LEU
1	B	1725	GLN
1	B	1733	THR
1	B	1743	MSE
1	B	1758	LEU
1	B	1759	LEU
1	B	1761	LEU
1	B	1802	TYR
1	B	1812	LEU
1	B	1819	PHE
1	B	1858	LEU
1	B	1909	ASN
1	B	1927	MSE
1	B	1930	GLU

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Mol	Chain	Res	Type
1	B	1942	CYS
1	B	1950	SER
1	B	1959	LEU
1	B	1973	LYS
1	B	1974	ASN
1	B	1976	LEU
1	B	1986	ARG
1	B	1993	GLU
1	B	1998	MSE
1	B	1999	GLU
1	B	2012	ARG
1	B	2023	SER
1	B	2104	MSE
1	B	2126	MSE
1	B	2155	GLU
1	B	2239	LYS
1	B	2245	TRP
1	B	2265	PRO
1	B	2277	LEU
1	B	2287	PRO
1	B	2325	LEU
1	B	2330	VAL
1	B	2338	GLU
1	B	2355	THR
1	B	2362	VAL
1	B	2370	SER
1	B	2374	LEU
1	B	2402	LEU
1	B	2481	HIS
1	B	2555	LEU
1	B	2559	THR
1	B	2576	MSE
1	B	2776	ARG
1	B	2788	SER
1	B	2820	MSE
1	B	2865	HIS
1	B	2886	GLN
1	B	2890	ILE
1	B	2921	LEU
1	B	2929	LEU
1	B	2943	PHE
1	B	2991	LYS

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Mol	Chain	Res	Type
1	B	3044	MSE
1	B	3050	LYS
1	B	3051	LEU
1	B	3058	ASP
1	B	3118	ASP
1	B	3120	LEU
1	B	3133	GLN
1	B	3145	ILE
1	B	3155	VAL
1	B	3238	MSE
1	B	3242	MSE
1	B	3258	LEU
1	B	3282	ARG
1	B	3283	LEU
1	B	3311	ASN
1	B	3397	GLN
1	B	3403	CYS
1	B	3416	LEU
1	B	3450	MSE
1	B	3451	LEU
1	B	3467	ARG
1	B	3509	ASP
1	B	3518	VAL
1	B	3636	PHE
1	B	3641	ASP
1	B	3763	ARG
1	B	3782	SER
1	B	3796	MSE
1	B	3810	VAL
1	B	3813	LYS
1	B	3820	MSE
1	B	3835	PRO
1	B	3846	MSE
1	B	3856	MSE
1	B	3858	MSE
1	B	3883	LEU
1	B	3895	GLU
1	B	3904	PHE
1	B	3926	ASN
1	B	3944	HIS
1	B	3959	MSE
1	B	3963	LEU

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Mol	Chain	Res	Type
1	B	3970	LEU
1	B	4016	PHE
1	B	4020	MSE
1	B	4029	GLN
1	B	4066	LEU
1	B	4090	ARG
1	B	4104	VAL
1	B	4119	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	233	ASN
1	A	334	HIS
1	A	508	HIS
1	A	783	HIS
1	A	1069	HIS
1	A	1083	ASN
1	A	1146	ASN
1	A	1385	ASN
1	A	1418	HIS
1	A	1457	GLN
1	A	1459	HIS
1	A	1476	HIS
1	A	1574	ASN
1	A	1687	HIS
1	A	1725	GLN
1	A	1754	GLN
1	A	1890	HIS
1	A	2170	GLN
1	A	2177	ASN
1	A	2183	HIS
1	A	2234	ASN
1	A	2426	HIS
1	A	2518	GLN
1	A	3003	ASN
1	A	3081	HIS
1	A	3122	HIS
1	A	3251	ASN
1	A	3291	GLN
1	A	3319	ASN
1	A	3501	HIS

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Mol	Chain	Res	Type
1	A	3524	ASN
1	A	3762	GLN
1	A	3927	ASN
1	A	3951	GLN
1	A	4068	HIS
1	B	390	GLN
1	B	409	GLN
1	B	437	HIS
1	B	442	GLN
1	B	508	HIS
1	B	593	ASN
1	B	990	GLN
1	B	993	HIS
1	B	1055	ASN
1	B	1238	GLN
1	B	1350	ASN
1	B	1476	HIS
1	B	1574	ASN
1	B	1687	HIS
1	B	1866	GLN
1	B	1890	HIS
1	B	1897	ASN
1	B	1974	ASN
1	B	2077	HIS
1	B	2177	ASN
1	B	2348	GLN
1	B	2365	ASN
1	B	2481	HIS
1	B	2518	GLN
1	B	3251	ASN
1	B	3459	ASN
1	B	3494	GLN
1	B	3524	ASN
1	B	3772	ASN
1	B	3908	HIS
1	B	3926	ASN
1	B	4018	GLN
1	B	4110	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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
1	B	1
1	A	1
2	K	1
2	S	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	K	133:UNK	C	201:UNK	N	46.74
1	S	133:UNK	C	201:UNK	N	41.40
1	B	3794:VAL	C	3795:PRO	N	1.18
1	A	1069:HIS	C	1070:PRO	N	1.15

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	3551/4128 (86%)	0.24	229 (6%) 23 16	83, 248, 332, 443	0
1	B	3551/4128 (86%)	0.30	236 (6%) 22 15	117, 251, 358, 507	0
2	K	0/194	-	-	-	-
2	S	0/194	-	-	-	-
All	All	7102/8644 (82%)	0.27	465 (6%) 22 16	83, 249, 343, 507	0

All (465) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	122	LYS	12.9
1	B	31	GLY	9.7
1	B	1355	GLY	9.6
1	A	126	PRO	9.1
1	A	123	CYS	8.7
1	B	586	GLN	8.5
1	A	1290	LEU	8.4
1	B	145	ASP	8.2
1	A	1763	THR	8.1
1	A	1286	ALA	8.0
1	A	121	ALA	7.6
1	B	3026	ASP	7.6
1	B	30	ALA	7.4
1	A	1289	SER	7.2
1	A	1287	GLN	7.1
1	A	1523	GLY	7.0
1	B	3023	ASN	6.8
1	A	1285	GLU	6.7
1	B	3033	GLU	6.7
1	B	3358	ARG	6.6
1	B	215	PRO	6.6
1	B	24	ARG	6.4

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Mol	Chain	Res	Type	RSRZ
1	B	1357	LYS	6.4
1	B	25	CYS	6.3
1	A	215	PRO	6.3
1	B	3025	PRO	6.3
1	A	2910	VAL	6.2
1	B	153	PHE	6.2
1	A	590	GLU	6.1
1	B	22	ALA	6.1
1	A	589	GLY	6.1
1	A	2906	PRO	5.9
1	B	3029	LYS	5.8
1	A	953	GLN	5.8
1	A	1761	LEU	5.8
1	A	124	LYS	5.7
1	A	2898	LEU	5.7
1	A	2905	LEU	5.6
1	B	3027	LEU	5.6
1	A	2202	PRO	5.5
1	A	125	ILE	5.5
1	B	3028	ASN	5.5
1	B	2263	LYS	5.3
1	A	3029	LYS	5.2
1	B	3515	GLN	5.2
1	B	32	HIS	5.1
1	B	100	ILE	5.1
1	B	26	GLY	5.0
1	A	503	SER	5.0
1	B	2900	LEU	5.0
1	A	2250	SER	4.9
1	A	3403	CYS	4.9
1	A	2897	LEU	4.8
1	A	2113	GLY	4.8
1	B	280	SER	4.8
1	A	2900	LEU	4.8
1	B	3153	SER	4.8
1	B	23	ASP	4.8
1	B	2430	GLU	4.7
1	B	257	ARG	4.7
1	A	950	GLU	4.7
1	B	10	CYS	4.6
1	A	237	SER	4.6
1	B	253	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	127	ALA	4.6
1	A	1288	SER	4.5
1	B	1286	ALA	4.5
1	A	3152	SER	4.5
1	B	125	ILE	4.4
1	B	1044	ILE	4.4
1	B	3024	PRO	4.4
1	B	3675	LYS	4.4
1	B	72	SER	4.4
1	A	128	LEU	4.4
1	B	3359	ILE	4.4
1	A	2821	ASP	4.3
1	B	582	THR	4.3
1	A	1589	ASN	4.3
1	A	670	LEU	4.3
1	A	3311	ASN	4.3
1	B	3976	GLU	4.3
1	A	3357	ARG	4.3
1	B	1763	THR	4.2
1	B	495	VAL	4.2
1	A	3402	SER	4.2
1	B	3528	ALA	4.2
1	A	2985	GLU	4.2
1	A	951	GLY	4.2
1	B	123	CYS	4.2
1	B	3623	PRO	4.2
1	A	280	SER	4.2
1	B	27	ALA	4.1
1	B	3406	ALA	4.1
1	A	2183	HIS	4.1
1	B	3020	ASP	4.1
1	A	3510	GLN	4.1
1	B	3152	SER	4.0
1	A	2203	THR	4.0
1	B	1761	LEU	4.0
1	B	126	PRO	4.0
1	B	216	LYS	4.0
1	A	2868	LEU	4.0
1	B	3074	GLN	3.9
1	A	3272	TRP	3.9
1	A	1284	THR	3.9
1	A	3308	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	216	LYS	3.9
1	A	897	PRO	3.9
1	A	2782	ASP	3.9
1	A	3478	GLU	3.8
1	B	122	LYS	3.8
1	B	2116	ASP	3.8
1	A	3269	ARG	3.8
1	A	171	LEU	3.8
1	B	3499	ILE	3.8
1	B	1354	GLU	3.8
1	A	1357	LYS	3.8
1	A	1489	LYS	3.7
1	B	631	ARG	3.7
1	A	129	ASP	3.7
1	A	3509	ASP	3.7
1	A	671	SER	3.7
1	A	956	PRO	3.7
1	B	279	ALA	3.7
1	A	2984	GLY	3.7
1	A	952	GLY	3.6
1	B	1287	GLN	3.6
1	B	1856	THR	3.6
1	A	588	VAL	3.6
1	B	2942	ILE	3.6
1	B	1043	GLN	3.6
1	A	2978	LYS	3.6
1	A	3358	ARG	3.6
1	A	2986	PRO	3.6
1	A	506	GLU	3.6
1	B	3936	GLY	3.6
1	A	2201	THR	3.5
1	B	2067	ARG	3.5
1	A	1586	SER	3.5
1	B	1290	LEU	3.5
1	A	591	GLN	3.5
1	A	1673	THR	3.5
1	B	3676	PRO	3.5
1	A	2527	HIS	3.5
1	B	2090	ARG	3.5
1	B	154	SER	3.5
1	B	4039	TYR	3.5
1	A	3317	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	4082	ARG	3.4
1	A	1526	GLU	3.4
1	B	542	ASP	3.4
1	B	157	TYR	3.4
1	B	1356	TRP	3.4
1	A	2308	SER	3.4
1	A	3196	LYS	3.4
1	B	3035	PHE	3.4
1	B	668	LYS	3.4
1	A	153	PHE	3.4
1	B	116	THR	3.3
1	B	3624	GLY	3.3
1	A	2068	ARG	3.3
1	B	628	GLU	3.3
1	A	252	VAL	3.3
1	B	1437	TYR	3.3
1	B	213	ARG	3.2
1	B	3056	GLU	3.2
1	A	2197	THR	3.2
1	A	120	ALA	3.2
1	B	3405	PRO	3.2
1	B	1671	VAL	3.2
1	B	71	LYS	3.2
1	A	2988	GLU	3.2
1	A	604	PRO	3.2
1	A	892	LEU	3.2
1	A	3199	PRO	3.1
1	A	3515	GLN	3.1
1	A	3700	GLU	3.1
1	B	2981	TRP	3.1
1	A	1522	GLY	3.1
1	A	3149	GLY	3.1
1	A	3150	ASN	3.1
1	A	2444	PRO	3.1
1	A	2980	ASP	3.1
1	B	585	ILE	3.1
1	B	4081	ALA	3.1
1	B	265	TYR	3.1
1	A	2867	ALA	3.0
1	A	1435	ASN	3.0
1	A	1604	SER	3.0
1	A	214	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	157	TYR	3.0
1	A	896	VAL	3.0
1	B	627	VAL	3.0
1	A	739	ASN	3.0
1	A	513	GLU	3.0
1	A	2267	SER	3.0
1	B	3355	LYS	3.0
1	A	505	SER	3.0
1	B	14	ARG	3.0
1	A	2899	ARG	3.0
1	A	3026	ASP	3.0
1	A	3098	ARG	3.0
1	B	3510	GLN	2.9
1	B	2078	ASP	2.9
1	A	213	ARG	2.9
1	A	3102	TYR	2.9
1	B	34	LEU	2.9
1	B	190	ILE	2.9
1	B	2464	HIS	2.9
1	A	1436	LEU	2.9
1	B	92	PHE	2.9
1	B	2175	GLU	2.9
1	B	124	LYS	2.9
1	B	262	LEU	2.9
1	B	3540	TYR	2.9
1	B	2533	SER	2.9
1	A	2975	ALA	2.9
1	B	2980	ASP	2.9
1	B	1284	THR	2.9
1	B	35	ILE	2.9
1	B	3879	PRO	2.9
1	A	3404	GLY	2.9
1	A	1558	TYR	2.9
1	A	1488	TYR	2.8
1	B	3550	LYS	2.8
1	A	1699	PHE	2.8
1	B	3809	THR	2.8
1	A	3153	SER	2.8
1	A	3976	GLU	2.8
1	B	2899	ARG	2.8
1	A	3273	LEU	2.8
1	B	2427	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	3624	GLY	2.8
1	A	2263	LYS	2.8
1	B	950	GLU	2.8
1	A	2907	ALA	2.8
1	B	86	LEU	2.8
1	B	103	TYR	2.8
1	B	3486	GLU	2.8
1	B	3674	SER	2.8
1	A	2208	ASP	2.8
1	B	38	LEU	2.8
1	A	781	ASP	2.7
1	A	355	ASN	2.7
1	B	2905	LEU	2.7
1	A	259	GLN	2.7
1	A	18	THR	2.7
1	B	3514	VAL	2.7
1	B	3841	ASP	2.7
1	B	2930	TYR	2.7
1	B	1822	ARG	2.7
1	B	2898	LEU	2.7
1	B	252	VAL	2.7
1	B	2822	LYS	2.7
1	B	330	ASN	2.7
1	B	3341	LEU	2.7
1	B	908	ASP	2.7
1	B	3830	SER	2.7
1	B	21	ALA	2.7
1	A	890	LYS	2.7
1	A	809	THR	2.7
1	A	2496	GLN	2.7
1	B	3822	GLN	2.7
1	B	2081	LEU	2.7
1	B	1672	PHE	2.7
1	A	3300	VAL	2.7
1	B	115	TYR	2.7
1	A	3828	TYR	2.6
1	B	104	SER	2.6
1	B	2077	HIS	2.6
1	A	81	CYS	2.6
1	A	543	SER	2.6
1	A	2979	GLN	2.6
1	B	472	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	3380	ARG	2.6
1	B	583	LEU	2.6
1	B	1816	ARG	2.6
1	A	3312	VAL	2.6
1	B	2264	ASP	2.6
1	B	2486	ASP	2.6
1	A	782	ARG	2.6
1	B	11	SER	2.6
1	B	1548	GLY	2.6
1	B	2465	PRO	2.6
1	A	3708	ARG	2.6
1	A	2259	LYS	2.6
1	B	1101	PHE	2.6
1	B	3875	GLU	2.6
1	A	2781	PRO	2.6
1	B	4115	ASN	2.6
1	B	3432	SER	2.6
1	A	3405	PRO	2.6
1	B	2390	HIS	2.6
1	A	3052	LEU	2.6
1	B	20	SER	2.6
1	B	2986	PRO	2.5
1	B	2488	GLU	2.5
1	A	1907	GLU	2.5
1	B	3070	HIS	2.5
1	B	28	ALA	2.5
1	B	101	ALA	2.5
1	B	2412	TYR	2.5
1	A	3318	LYS	2.5
1	A	1698	PHE	2.5
1	A	262	LEU	2.5
1	B	877	ASP	2.5
1	B	2084	GLU	2.5
1	A	587	THR	2.5
1	A	3603	LYS	2.5
1	B	2411	LEU	2.5
1	B	82	ARG	2.5
1	B	2821	ASP	2.5
1	A	3633	ILE	2.5
1	A	3252	PHE	2.5
1	B	1799	GLU	2.5
1	A	799	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	117	LYS	2.5
1	B	3828	TYR	2.5
1	B	1255	CYS	2.5
1	A	2869	LEU	2.5
1	B	191	ASN	2.5
1	B	1732	GLY	2.5
1	B	99	LYS	2.5
1	A	3627	ALA	2.4
1	B	494	PRO	2.4
1	B	95	LYS	2.4
1	B	2943	PHE	2.4
1	B	3489	SER	2.4
1	A	3074	GLN	2.4
1	B	1426	GLN	2.4
1	B	59	PHE	2.4
1	B	3105	ASN	2.4
1	A	119	ARG	2.4
1	B	2461	PHE	2.4
1	A	80	GLU	2.4
1	A	3406	ALA	2.4
1	A	514	VAL	2.4
1	B	2904	GLU	2.4
1	B	1589	ASN	2.4
1	A	585	ILE	2.4
1	A	2440	TYR	2.4
1	B	3553	GLU	2.4
1	A	2893	LEU	2.4
1	B	1002	GLU	2.4
1	A	3695	LEU	2.3
1	A	3875	GLU	2.3
1	B	3549	HIS	2.3
1	A	2067	ARG	2.3
1	B	167	PRO	2.3
1	A	593	ASN	2.3
1	B	136	GLN	2.3
1	B	579	LEU	2.3
1	B	1020	PRO	2.3
1	A	2421	VAL	2.3
1	B	3580	ASN	2.3
1	B	4118	GLY	2.3
1	B	3346	ALA	2.3
1	B	2201	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	3488	SER	2.3
1	B	3627	ALA	2.3
1	B	68	PHE	2.3
1	A	3629	ARG	2.3
1	A	580	ASP	2.3
1	A	2093	CYS	2.3
1	B	2491	THR	2.3
1	A	3493	TRP	2.3
1	B	183	GLU	2.3
1	B	132	ILE	2.2
1	A	2939	LEU	2.2
1	B	29	LEU	2.2
1	B	81	CYS	2.2
1	A	3159	ARG	2.2
1	B	146	GLU	2.2
1	A	3058	ASP	2.2
1	A	3879	PRO	2.2
1	B	1818	SER	2.2
1	A	1788	ARG	2.2
1	A	3282	ARG	2.2
1	A	3699	LEU	2.2
1	B	1138	ILE	2.2
1	A	3698	GLU	2.2
1	B	1509	GLN	2.2
1	A	1465	HIS	2.2
1	A	2195	SER	2.2
1	B	1512	SER	2.2
1	A	3604	LYS	2.2
1	A	507	ASP	2.2
1	B	1442	GLN	2.2
1	B	2308	SER	2.2
1	B	516	THR	2.2
1	A	3610	TYR	2.2
1	B	3625	LEU	2.2
1	A	3105	ASN	2.2
1	B	37	GLY	2.2
1	A	3007	GLU	2.2
1	A	3696	ARG	2.2
1	B	3407	ALA	2.2
1	B	63	PHE	2.2
1	B	3622	ALA	2.2
1	A	2464	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	62	ASP	2.2
1	A	130	LEU	2.2
1	A	2903	ALA	2.2
1	B	3199	PRO	2.2
1	B	1350	ASN	2.2
1	A	891	ARG	2.2
1	A	582	THR	2.2
1	B	2176	ASN	2.2
1	A	1277	GLY	2.2
1	B	79	ARG	2.2
1	B	2391	GLY	2.1
1	B	3350	GLU	2.1
1	A	2492	ASP	2.1
1	A	3356	ALA	2.1
1	A	586	GLN	2.1
1	B	867	ASN	2.1
1	B	1031	ARG	2.1
1	A	3849	LYS	2.1
1	A	4092	GLN	2.1
1	A	1557	GLU	2.1
1	A	2114	GLU	2.1
1	A	3326	GLN	2.1
1	B	2184	TYR	2.1
1	A	194	GLU	2.1
1	B	868	LYS	2.1
1	B	3617	LEU	2.1
1	B	3500	SER	2.1
1	A	300	TRP	2.1
1	A	2909	ARG	2.1
1	B	3150	ASN	2.1
1	B	258	PRO	2.1
1	B	493	LYS	2.1
1	A	634	LEU	2.1
1	B	413	PHE	2.1
1	A	2904	GLU	2.1
1	A	2461	PHE	2.1
1	A	3443	PRO	2.1
1	A	1088	GLU	2.1
1	B	4110	GLN	2.1
1	A	356	ASN	2.1
1	B	1436	LEU	2.1
1	A	3479	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	1051	LYS	2.1
1	A	672	ILE	2.1
1	A	2842	ARG	2.0
1	A	512	GLY	2.0
1	A	1506	SER	2.0
1	B	738	HIS	2.0
1	B	3032	SER	2.0
1	A	3290	SER	2.0
1	A	1463	LEU	2.0
1	A	3197	LEU	2.0
1	A	3630	ARG	2.0
1	A	27	ALA	2.0
1	A	3008	TRP	2.0
1	B	676	ASN	2.0
1	A	3546	SER	2.0
1	A	3285	HIS	2.0
1	A	3310	ASN	2.0
1	B	1360	LYS	2.0
1	A	3104	GLN	2.0
1	B	47	SER	2.0
1	A	3393	GLU	2.0
1	A	2309	PHE	2.0
1	A	1760	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.