



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:25 AM UTC

PDB ID : 3EQL / pdb_00003eqL
Title : Crystal structure of the T. Thermophilus RNA polymerase holoenzyme in complex with antibiotic myxopyronin
Authors : Vassylyev, D.G.; Vassylyeva, M.N.; Artsimovitch, I.
Deposited on : 2008-09-30
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

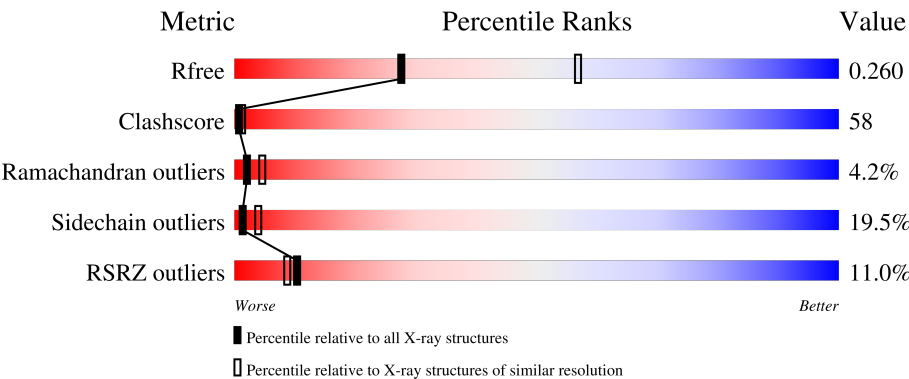
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	315	5% 17%45%10%27%
1	B	315	8% 17%45%10%27%
1	K	315	5% 17%43%12%27%
1	L	315	10% 16%45%10%27%
2	C	1119	13% 24%56%18%

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Mol	Chain	Length	Quality of chain			
2	M	1119	10%23%59%16%			
3	D	1524	9%23%48%14%13%			
3	N	1524	9%24%47%14%13%			
4	E	99	16%20%54%16%6%			
4	O	99	11%22%57%13%			
5	F	423	12%24%44%13%18%			
5	P	423	10%25%44%11%18%			

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 57340 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			
1	B	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			
1	K	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			
1	L	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1119	Total	C	N	O	S	0	0	0
			8829	5581	1577	1647	24			
2	M	1119	Total	C	N	O	S	0	0	0
			8829	5581	1577	1647	24			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1321	Total	C	N	O	S	0	0	0
			10407	6585	1845	1944	33			
3	N	1321	Total	C	N	O	S	0	0	0
			10407	6585	1845	1944	33			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	95	Total	C	N	O	S	0	0	0
			770	491	133	142	4			
4	O	95	Total	C	N	O	S	0	0	0
			770	491	133	142	4			

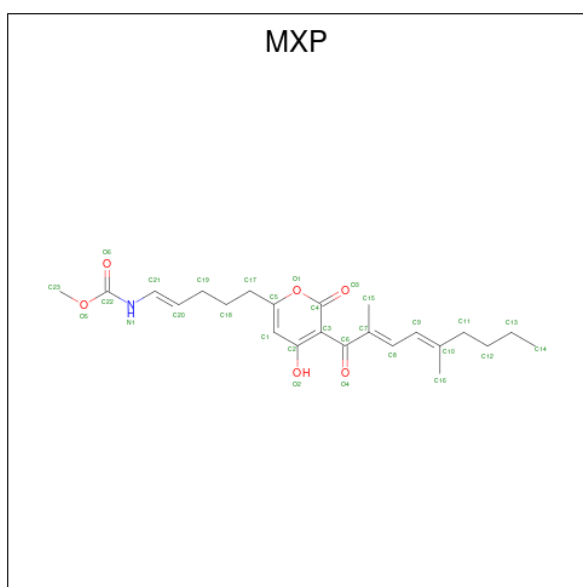
- Molecule 5 is a protein called RNA polymerase sigma factor rpoD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	345	Total	C	N	O	S	0	0	0
			2771	1744	504	519	4			
5	P	345	Total	C	N	O	S	0	0	0
			2771	1744	504	519	4			

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	2	Total	Zn	0	0
			2	2		
6	N	2	Total	Zn	0	0
			2	2		

- Molecule 7 is Myxopyronin B (CCD ID: MXP) (formula: C₂₃H₃₁NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	D	1	Total	C	N	O	0	0
			30	23	1	6		
7	N	1	Total	C	N	O	0	0
			30	23	1	6		

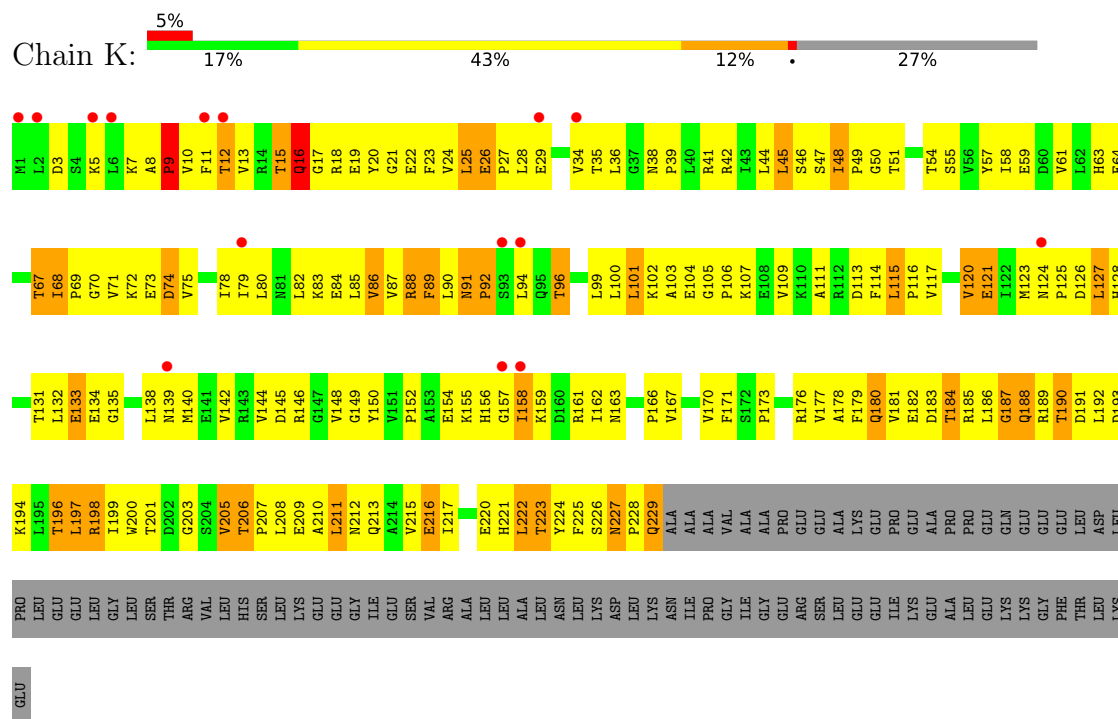
- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	1	Total Mg 1 1	0	0
8	N	1	Total Mg 1 1	0	0

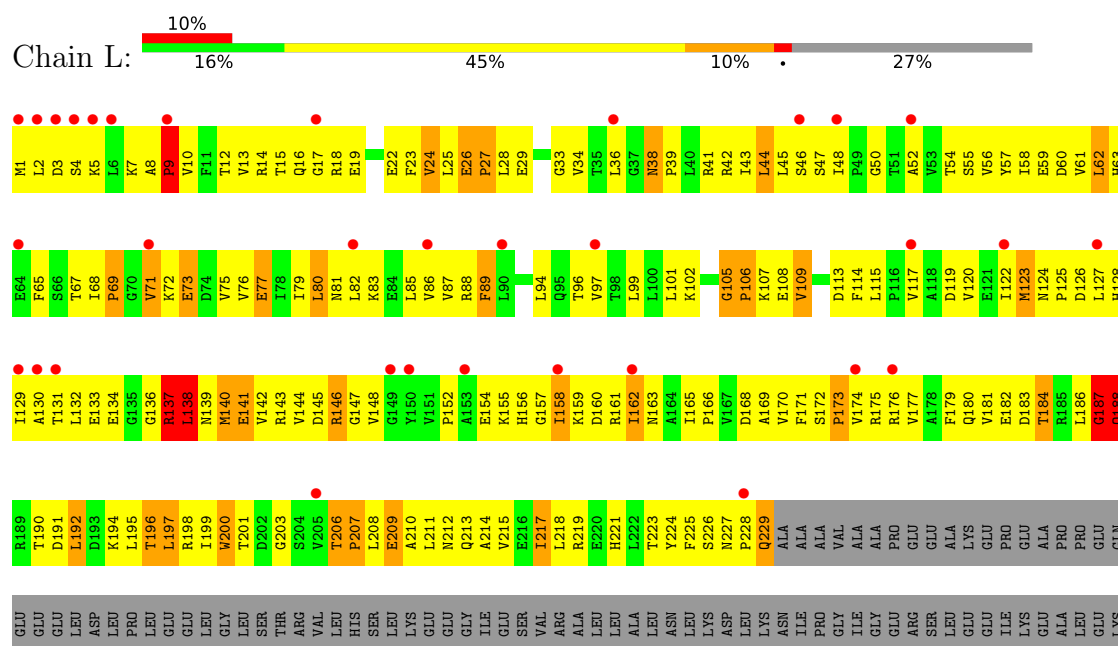
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	141	Total O 141 141	0	0
9	B	149	Total O 149 149	0	0
9	C	704	Total O 704 704	0	0
9	D	927	Total O 927 927	0	0
9	E	82	Total O 82 82	0	0
9	F	305	Total O 305 305	0	0
9	K	152	Total O 152 152	0	0
9	L	148	Total O 148 148	0	0
9	M	680	Total O 680 680	0	0
9	N	864	Total O 864 864	0	0
9	O	84	Total O 84 84	0	0
9	P	260	Total O 260 260	0	0

- Molecule 1: DNA-directed RNA polymerase subunit alpha

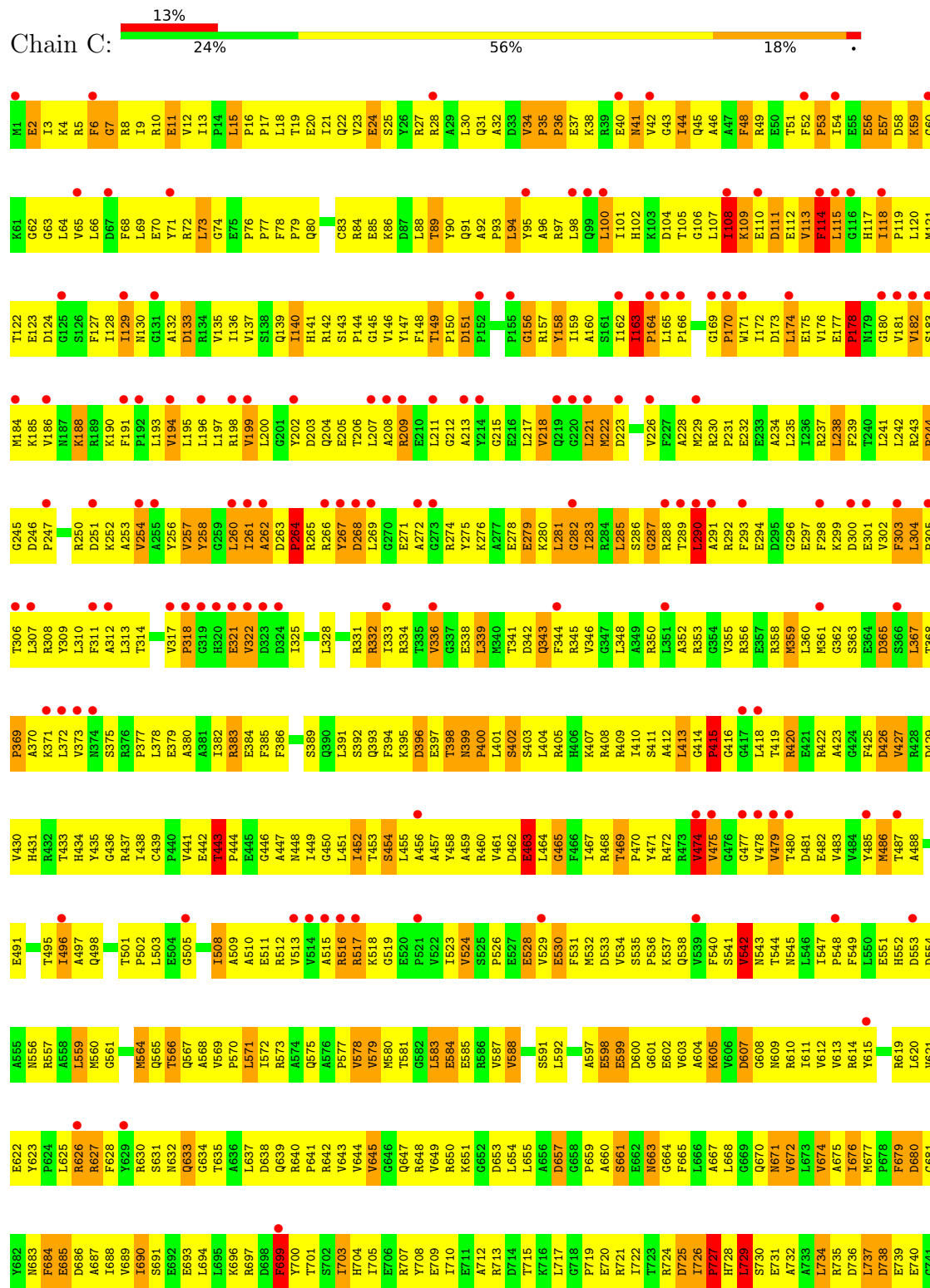


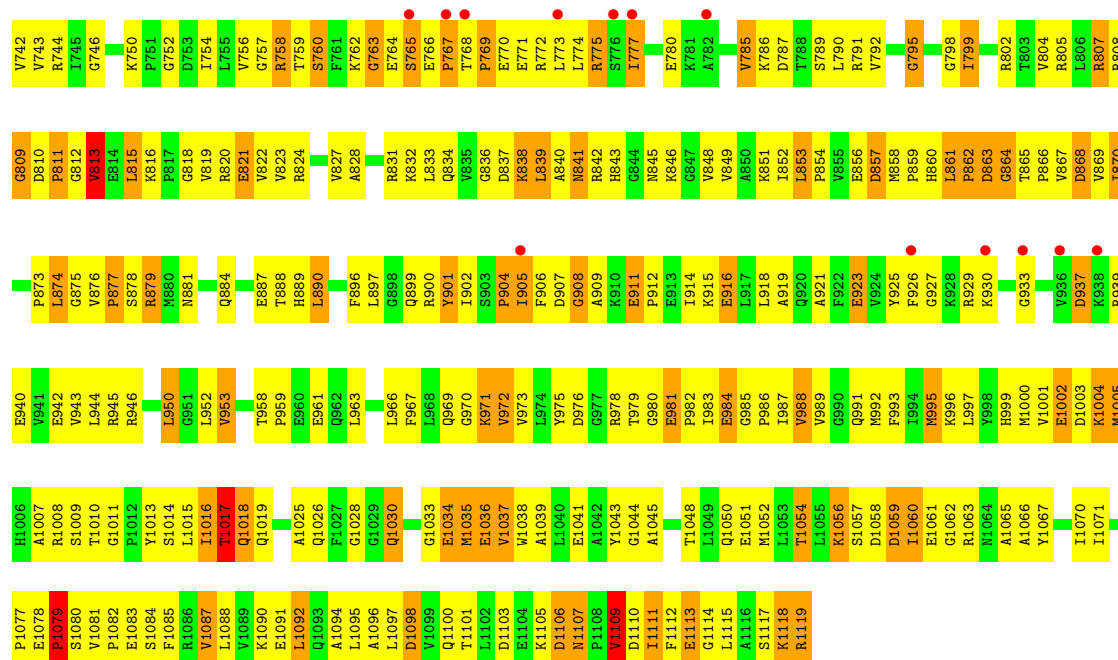
- Molecule 1: DNA-directed RNA polymerase subunit alpha



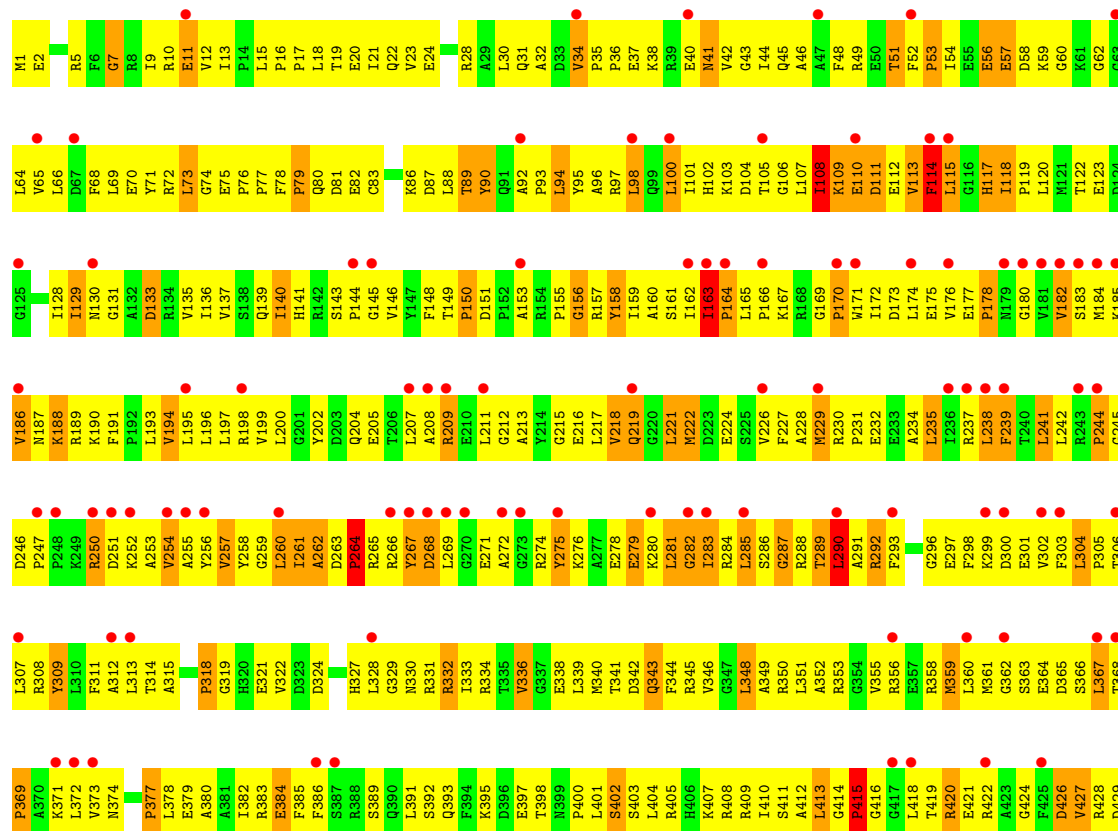
LYS
GLY
PHE
THR
LEU
LVS
GLU

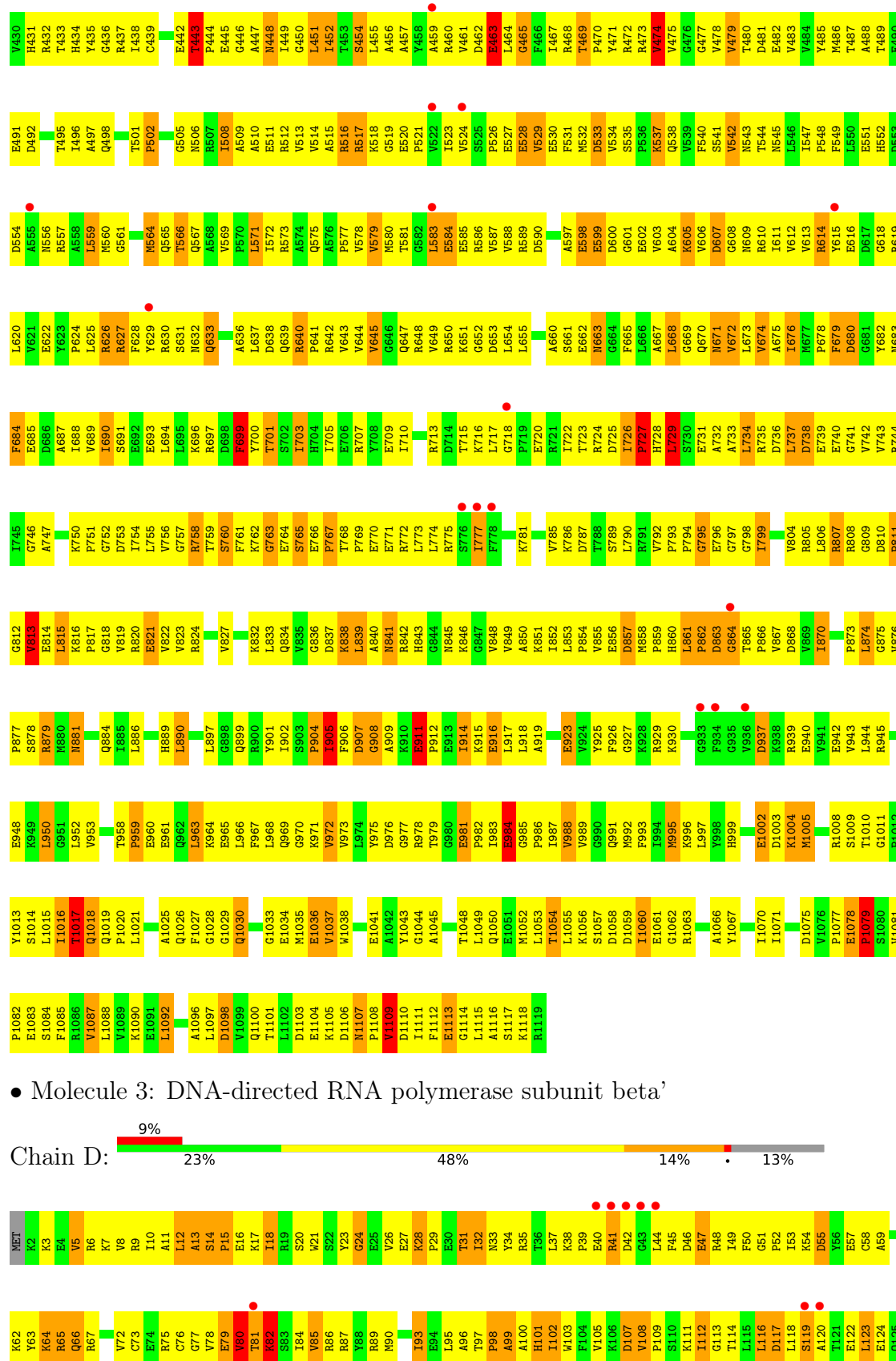
● Molecule 2: DNA-directed RNA polymerase subunit beta



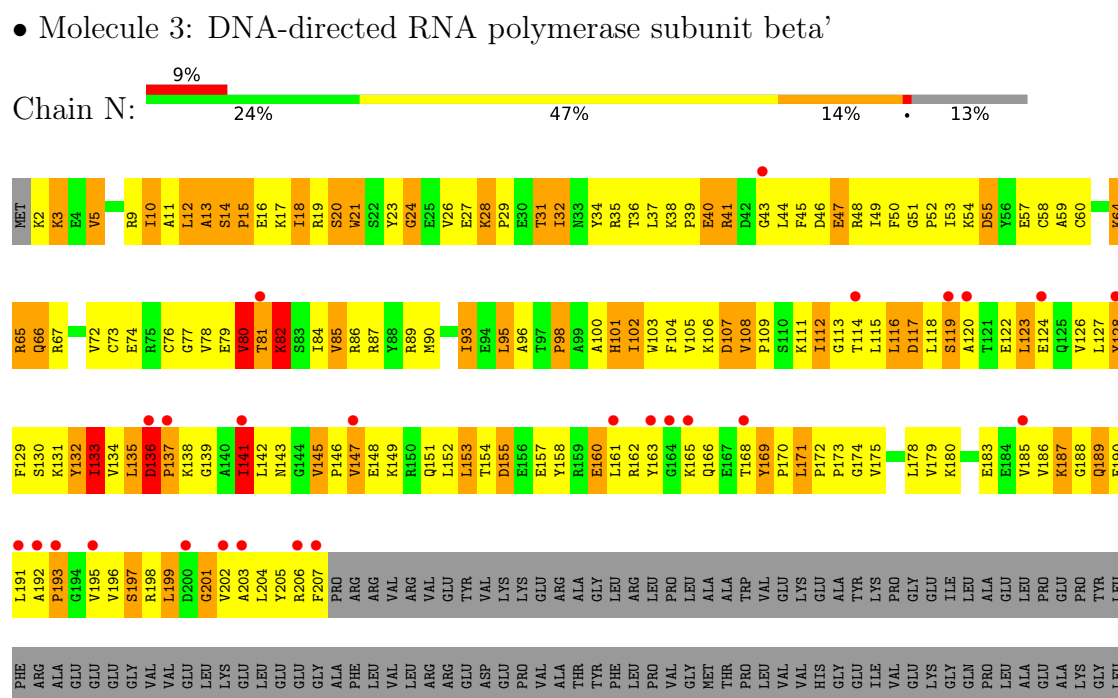
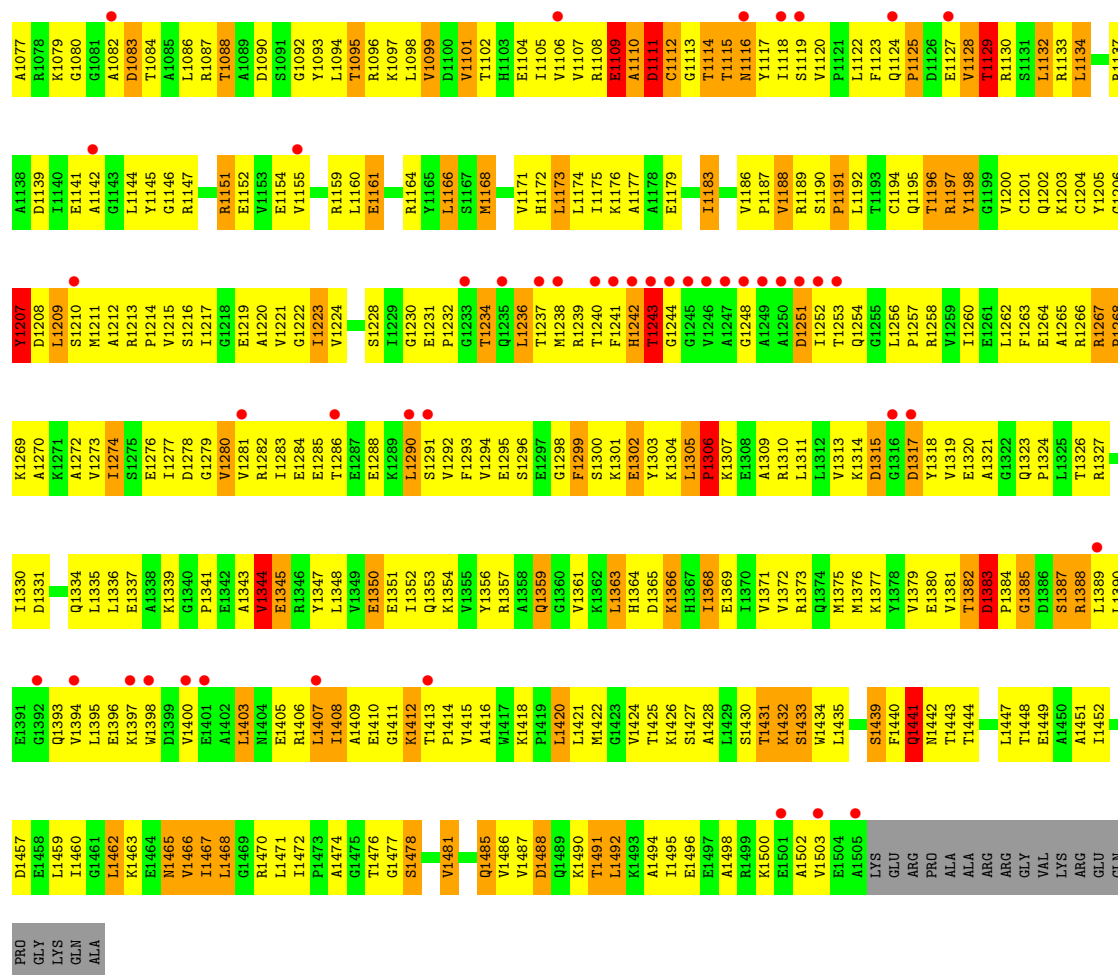


• Molecule 2: DNA-directed RNA polymerase subunit beta

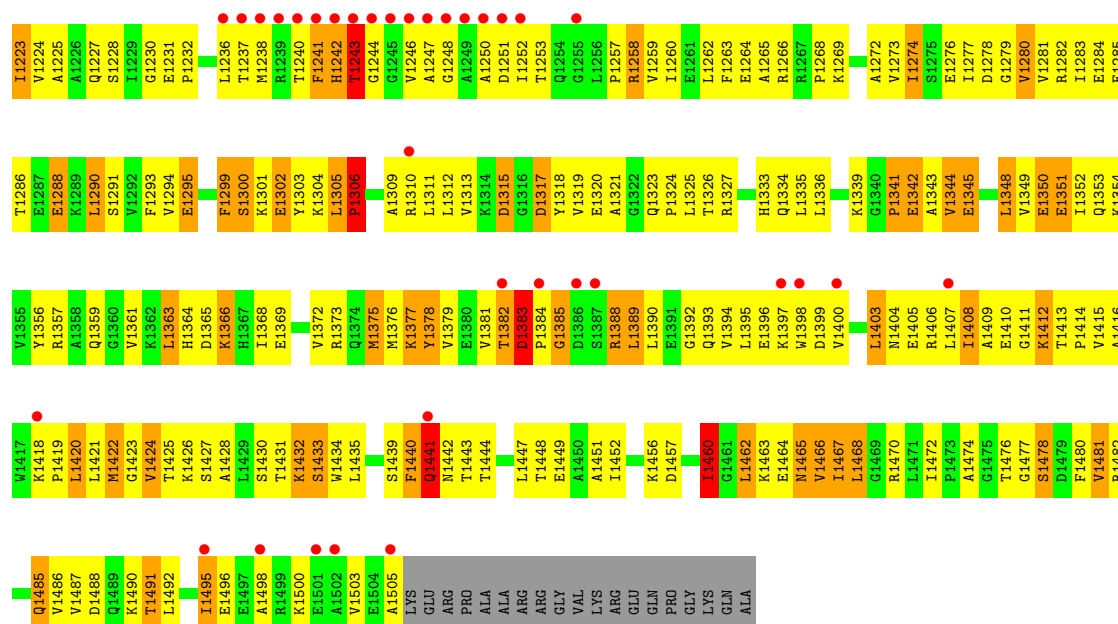




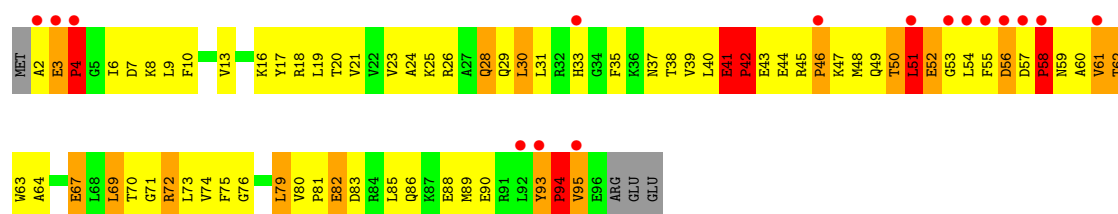
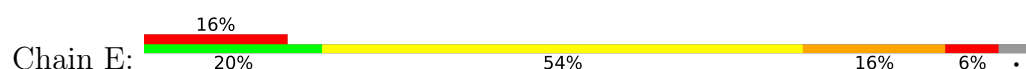
M1010	G938	B872	P809	A746	D885	D624	P563	V499	Y432	ILE	ALA	GLU	K187	V126
M1018	F941	L873	E810	V747	E886	Y625	E564	R500	G433	VAL	LYS	PRO	G186	L127
P1019	S942	E874	E811	H748	W688	S626	E565	A501	R434	ALA	GLY	TYR	Q189	Y128
L1020	T943	L875	A812	T749	W689	G627	E566	D604	V435	ALA	LEU	LEU	L191	P129
Y1021	T944	S876	L813	P750	D690	S629	E567	S505	E436	ILE	ASP	PHE	K130	S130
M1022	S945	G878	A814	P751	A691	W630	E569	G506	V437	ASP	ARG	ARG	A192	K131
M1023	G946	S879	A815	S752	L691	W631	E570	N507	D438	PRO	MET	ALA	P193	Y132
A1024	I947	E880	B816	S753	E692	G632	E571	R508	L439	GLU	PRO	GLU	G194	I133
L1025	T948	L881	E817	F754	E693	W633	E572	N508	V440	GLU	ARG	GLU	V195	V134
S1026	I949	F882	G819	A755	W694	G634	E573	E510	R441	GLU	GLN	GLY	V196	L135
G1027	G950	F883	G819	Q756	I695	G634	E574	W511	R442	VAL	VAL	GLY	S197	D136
A1028	I951	E884	E820	A757	G696	P635	E575	M512	V443	ILE	ARG	VAL	R198	P137
R1029	D952	L885	A822	A759	G698	L637	E576	E513	R445	ALA	ALA	GLU	K199	K138
G1030	V955	E888	L823	R760	V699	K638	A577	L514	V446	GLU	ALA	GLU	G200	G139
M1031	I956	E889	N824	R761	W700	K638	E578	E515	V447	ALA	GLN	LEU	G201	A140
P1032	P957	A890	A825	Q762	L701	H640	E579	E516	E448	GLY	VAL	LYS	V202	T141
Q1033	P957	W890	P826	Q763	L702	H641	E580	A517	S449	GLY	ALA	LEU	A203	N143
L1034	E958	E891	I827	L764	W703	G642	E581	P518	Y450	VAL	ALA	GLU	Y205	G144
I1035	E959	D892	K828	S765	R704	G643	E582	V519	D451	HIS	GLU	GLU	R206	V145
R1036	K960	E893	W829	A766	A705	L644	E583	L520	I452	LEU	GLU	GLY	F207	P146
Q1037	Y963	K894	A830	H767	P706	P645	E584	P521	D453	HIS	GLY	ALA	PRO	Y147
L1038	L1038	W895	G831	Q768	T707	K646	E585	P522	A454	GLY	GLY	PHE	ARG	E148
C1039	L964	A896	R832	L769	L708	R647	E586	D523	R455	THR	LEU	LEU	ARG	K149
G1040	E965	W897	E833	L770	H709	N648	E588	L524	M456	VAL	VAL	VAL	VAL	R150
L1041	D968	E898	T834	S771	R710	A649	E589	R525	G457	TYR	TYR	LEU	ARG	Q151
R1042	L999	L899	S835	P772	L711	E651	E590	P526	A458	LEU	LEU	ARG	VAL	L152
G1043	L972	Q901	W836	G774	G712	L652	E591	V528	I461	THR	THR	ARG	GLU	L153
L1044	L972	G901	R838	G775	T713	S792	E592	V529	Q462	LEU	LEU	ASP	TYR	T154
M1045	E975	L902	L839	E776	Q714	P853	E593	V530	Q463	PHE	ASP	GLY	VAL	D155
K1046	Y980	P905	K840	P777	A715	K654	E594	D531	Q464	LEU	LEU	GLU	LYS	E156
L1047	P1048	Q906	R841	L778	F716	P655	E595	G532	L465	THR	THR	VAL	LYS	E157
S1049	L983	E907	W842	L779	Q717	P656	E596	G533	K466	THR	THR	ALA	ARG	E158
G1050	T984	K908	F843	P781	P719	L658	E597	R534	E471	GLY	GLY	THR	ALA	E159
T1052	D985	L911	A844	S782	L720	K659	E599	F535	A472	PRO	PRO	TYR	GLY	L161
F1053	E987	K912	D847	D784	E722	N661	E601	A536	L473	LYS	ASP	PHE	LEU	R162
P1056	R988	D913	E848	I785	G723	E662	E602	T537	L477	TYR	TYR	PRO	LEU	Y163
V1057	Y989	L914	A849	I786	Q724	E663	E603	S538	L478	ARG	ARG	VAL	PRO	G164
R1058	D990	Y915	L850	L787	S725	K664	E604	D539	E479	VAL	VAL	GLY	PRO	K165
S1059	Q991	L916	L851	G788	I726	G665	E605	L540	E480	GLN	GLN	GLY	LEU	E167
S1060	I992	A852	L851	L789	Q727	I666	E606	L543	M481	PRO	PRO	THR	ALA	E168
F1061	L993	W853	W853	I792	L728	A667	E607	Y544	K482	HIS	HIS	TRP	TRP	Y169
R1062	Q994	L922	E857	V795	P730	V670	E609	R545	H483	MET	MET	VAL	VAL	P170
L1063	L995	G923	W858	R796	L731	K671	E610	R546	P484	ASN	ASN	VAL	GLU	L171
G1064	W996	N924	D859	K797	V732	A673	E611	L547	S485	VAL	VAL	VAL	LYS	P172
L1065	T997	E925	L860	K798	C733	R674	E612	N549	R486	VAL	VAL	GLY	ALA	P173
T1066	E998	K926	Q861	E798	C733	R675	E613	R550	R487	PRO	PRO	GLU	TYR	G174
V1067	T999	T927	D862	K799	F736	R676	E614	N551	R488	GLY	GLY	ILE	LEU	V175
L1068	E1000	A928	W863	R800	A737	M676	E615	L554	R489	VAL	VAL	PRO	PRO	L178
E1069	K1001	R929	E864	G801	A738	L677	E616	R554	R489	GLY	GLY	VAL	GLY	V179
Y1070	K1002	L930	T865	A802	D739	E878	E617	K491	A490	ALA	ALA	LYS	GLY	K180
F1071	V1003	L931	R666	G803	F740	R679	E618	K555	A492	VAL	VAL	GLY	ILE	D181
L1072	L1072	D932	R667	L804	D741	Q680	E619	L558	R493	GLU	GLU	GLN	LEU	G182
S1073	A1006	E868	Y868	E805	G742	R681	E620	A559	K494	ALA	ALA	PRO	ALA	E183
S1074	V1007	F869	R689	F806	D743	D682	E621	Q560	R495	GLY	GLY	LEU	GLU	E184
H1075	H1075	Y936	G870	G870	Q744	L683	E622	G561	K496	ASP	ASP	ALA	LEU	V185
G1076	K1009	Y937	K871	T808	M745	K684	E623	A562	V498	LYS	LYS	GLU	PRO	V186



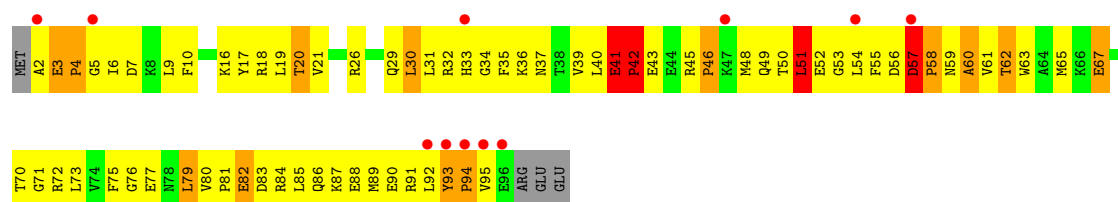
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R1159	D1090	A1028	P957	E891	G819	S753	W888	S626	I566	L503	R434	ASP	ARG
L1160	S1091	R1029	E958	D892	E820	F754	D889	G627	I567	D504	E436	PRO	MET
E1161	G1092	G1030	E959	V895	R821	A755	D	R628	F568	S505	V435	GLU	PRO
L1094	Y1093	N1031	K960	A896	A822	Q756	E693	S629	N569	G506	V437	GLU	ARG
T1095	L1094	P1032	K961	A897	R824	R760	E692	V630	N570	N507	D438	VAL	GLN
R1096	T1095	Q1033	Q962	E896	A825	I761	E694	T631	R571	R508	L439	VAL	GLN
K1097	L1096	Q1034	Y963	E896	R826	L764	E695	V632	R572	P509	V440	ARG	ARG
L1098	L1097	R1036	L964	E965	R827	L765	H696	V633	M573	E510	R441	ALA	ALA
S1167	V1099	Q1037	E965	Q901	K828	A766	V699	P635	L574	M512	M442	ALA	GLN
M1168	D1100	L1038	D968	L902	R829	H767	V700	Q636	E576	M513	V444	VAL	VAL
D1169	V1101	C1039	R969	P905	A830	H767	L701	Q637	E577	I514	R445	GLY	GLU
S1170	T1102	G1040	K970	P905	R831	L770	L702	K638	M578	E515	V446	ALA	ALA
V1171	H1103	L1041	L971	Q906	R832	S771	N703	L639	D579	A516	V447	VAL	GLU
H1172	E1104	R1042	L972	E907	E833	S771	R704	H640	A580	V517	V448	GLU	GLU
L1173	L1105	G1043	L972	Q908	T834	A772	A705	Q641	L581	P518	E448	HIS	GLU
L1174	V1106	L1044	E975	R909	S835	A773	P706	G642	L582	V519	S449	HIS	GLY
L1175	V1107	M1045	G981	S910	R836	S774	T707	G643	D583	L520	D451	THR	THR
K1176	R1108	Q1046	P982	S911	R837	G775	L708	L644	M584	P521	I452	THR	THR
A1177	A1110	P1048	F982	V915	R839	E776	H709	P645	G586	D523	D454	VAL	VAL
E1178	D1111	S1049	T984	Y916	K840	A779	R710	K646	R586	L524	R455	LEU	LEU
A1179	C1112	G1050	T984	Y916	R841	K780	G712	R647	G588	R525	M456	THR	THR
E1182	G1113	D985	D985	Y916	R842	P781	I713	N648	A589	P526	G457	LEU	LEU
I1183	T1114	E987	E987	L920	F843	S782	Q714	E651	P590	M527	A458	PHE	PHE
V1186	T1115	R988	R988	R921	A844	R783	A715	L652	V591	V528	I461	GLU	GLU
P1187	V1117	V989	L922	R922	D847	D784	F716	F653	T592	Q529	I461	GLU	GLU
V1188	Y1118	D990	G923	G923	E848	I785	Q717	K654	N593	V530	Q462	THR	THR
R1189	S1119	R1058	Q991	N924	E848	I786	P718	P655	P594	D531	Q463	THR	THR
V1120	V1120	S1059	L993	E925	A849	L787	V719	F656	G595	G532	L464	GLU	GLU
P1121	P1121	S1060	Q994	K926	L850	G788	L720	L457	S596	G533	L465	PRO	PRO
L1192	L1122	F1061	L995	T927	L851	L789	V721	L658	R594	R534	L473	LYS	LYS
Q1195	F1123	W996	W996	A928	A852	E722	G723	K660	F536	A536	L473	ASP	ASP
T1196	E1063	E1063	T999	R929	R853	I792	G724	K660	P599	T537	L477	TYR	TYR
R1197	G1064	L1065	D932	L931	T857	Q794	S725	K661	R601	S538	L478	VAL	VAL
Y1198	L1000	E1001	D932	D932	V858	V795	I726	K664	S602	D539	E479	GLN	GLN
G1199	E1001	T1066	E1001	A933	D859	R796	Q727	G665	L603	L540	E480	PRO	PRO
V1200	V1003	V1067	V1003	K935	L860	K797	L728	I666	T604	L543	M481	HIS	HIS
C1201	L1068	L1068	L1068	K935	Q861	E798	H729	A667	D605	Y544	K482	MET	MET
Q1202	E1069	E1069	Q1005	Y937	D862	K799	C733	P668	I606	R544	H483	ASN	ASN
K1203	Y1070	Y1070	Q1005	Y937	V863	K800	E734	N669	L607	R545	P484	VAL	VAL
G1204	R1078	R1078	Q1006	Q938	T865	G801	T733	V670	S608	R546	S485	VAL	VAL
Y1205	V1007	V1007	V1007	F939	T865	A802	A735	K671	G609	L547	R486	VAL	VAL
G1206	F1008	F1008	F1008	T940	V866	G803	F736	A672	R610	I548	A487	PRO	PRO
D1208	H1075	H1075	F941	F941	R867	L804	N737	A673	Q611	N549	R488	GLU	GLU
L1209	A1077	A1077	S942	S942	R867	E305	A738	R674	G612	R550	R489	GLY	GLY
S1210	E1141	E1141	T943	T943	E874	R807	D739	R675	R613	N551	A490	ALA	ALA
M1211	L1144	L1144	T944	T944	T875	A807	F740	N676	R614	M552	K491	ARG	ARG
V1215	Y1145	Y1145	I947	I947	S876	T808	D741	L677	R615	L553	A492	VAL	VAL
S1216	G1146	G1080	T948	T948	P877	P809	G742	E678	Q616	L554	R493	GLU	GLU
L1217	R1147	L1020	T949	T949	G878	E810	D743	R679	R617	K555	K494	ALA	ALA
G1218	V1148	Y1021	Y1021	Y1021	R879	E811	Q744	Q680	L618	K556	R495	GLY	GLY
A1219	T1084	V1022	I951	I951	R880	A812	A746	D682	L619	Q560	E497	ASP	ASP
E1219	A1085	A1085	P952	P952	R884	L813	T747	T683	R621	Q561	E498	LYS	LYS
A1220	L1086	L1086	D953	D953	R884	A814	V747	T683	R621	Q562	V498	TLE	TLE
V1221	Q1025	Q1025	A954	A954	E888	A815	H748	D684	R622	A562	V499	VAL	VAL
G1222	E1154	E1154	Y955	Y955	A889	R816	V749	D685	V623	P563	R500	ALA	ALA
						E817		E886	D624	E564	A501	Y432	ALA



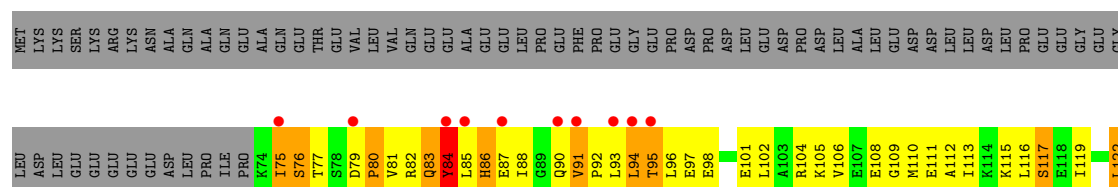
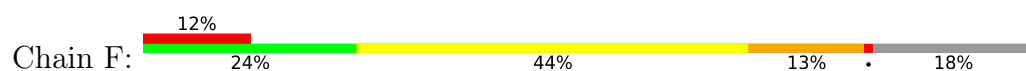
• Molecule 4: DNA-directed RNA polymerase subunit omega

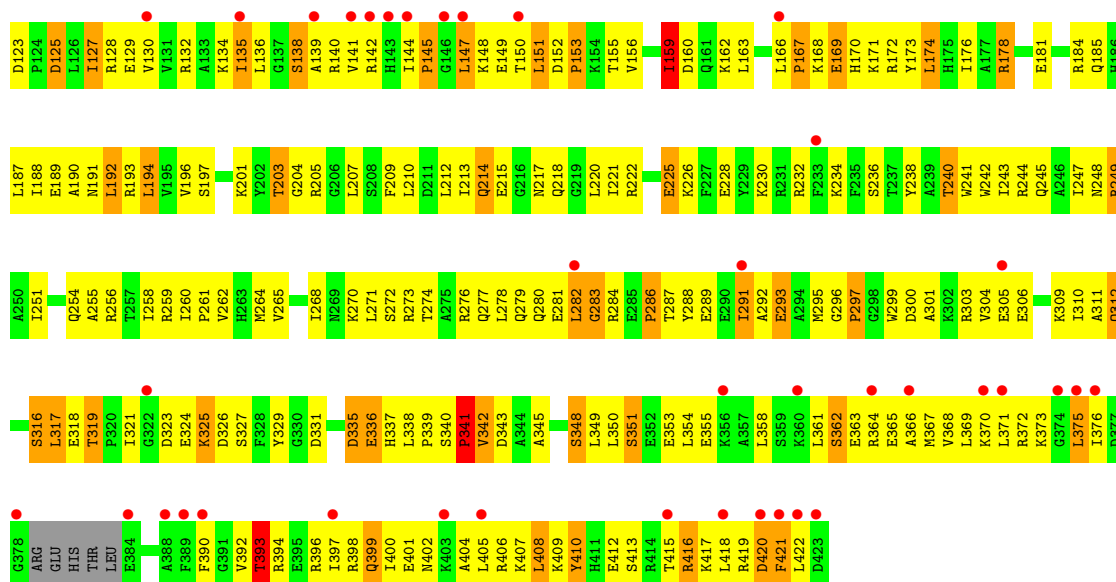


• Molecule 4: DNA-directed RNA polymerase subunit omega

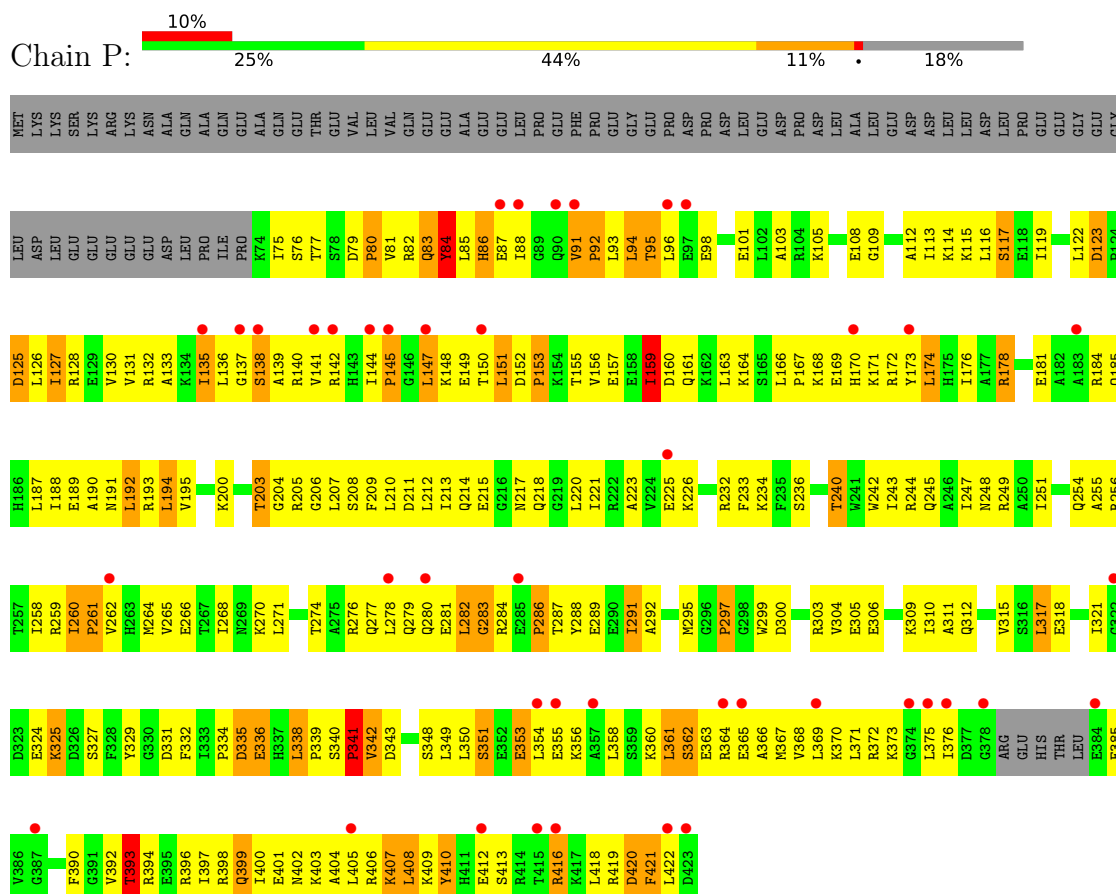


• Molecule 5: RNA polymerase sigma factor rpoD





• Molecule 5: RNA polymerase sigma factor rpoD



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	235.00Å 235.00Å 254.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.70 40.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.7 (40.00-2.70) 90.4 (40.00-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.240 , 0.270 0.237 , 0.260	Depositor DCC
R_{free} test set	18510 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	47.8	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 103.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.166 for -h,-k,l 0.048 for h,-h-k,-l 0.047 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	57340	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	1.04	4/1838 (0.2%)	1.35	14/2498 (0.6%)
1	B	0.96	3/1838 (0.2%)	1.24	15/2498 (0.6%)
1	K	0.98	3/1838 (0.2%)	1.33	17/2498 (0.7%)
1	L	0.93	2/1838 (0.1%)	1.24	14/2498 (0.6%)
2	C	0.88	4/8997 (0.0%)	1.29	68/12164 (0.6%)
2	M	0.87	3/8997 (0.0%)	1.29	72/12164 (0.6%)
3	D	0.91	9/10582 (0.1%)	1.33	87/14294 (0.6%)
3	N	0.91	11/10582 (0.1%)	1.33	91/14294 (0.6%)
4	E	0.97	3/784 (0.4%)	1.70	18/1057 (1.7%)
4	O	0.91	1/784 (0.1%)	1.56	15/1057 (1.4%)
5	F	0.77	3/2812 (0.1%)	1.17	11/3781 (0.3%)
5	P	0.78	2/2812 (0.1%)	1.18	10/3781 (0.3%)
All	All	0.89	48/53702 (0.1%)	1.30	432/72584 (0.6%)

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
3	N	0	1

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	26	GLU	C-O	-19.28	1.03	1.24
1	L	26	GLU	C-O	-18.54	1.04	1.24
1	A	26	GLU	C-O	-17.07	1.02	1.24
1	K	26	GLU	C-O	-16.38	1.03	1.24
2	C	1005	MET	SD-CE	-9.71	1.55	1.79
3	D	18	ILE	CA-CB	7.81	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	26	GLU	CA-C	-6.88	1.45	1.52
3	N	141	ILE	CA-CB	6.46	1.61	1.54
4	E	56	ASP	CA-C	6.25	1.57	1.52
5	F	135	ILE	CA-CB	6.14	1.63	1.54
3	D	1114	THR	CA-CB	6.09	1.60	1.52
3	D	400	VAL	CA-CB	6.04	1.61	1.53
2	M	474	VAL	CA-CB	6.03	1.61	1.54
2	C	163	ILE	CA-CB	6.00	1.60	1.53
4	E	95	VAL	CA-C	-5.96	1.47	1.53
3	N	400	VAL	CA-CB	5.89	1.61	1.53
5	F	319	THR	CA-CB	5.83	1.62	1.53
3	N	527	MET	SD-CE	-5.81	1.65	1.79
5	P	260	ILE	CA-CB	5.80	1.58	1.54
1	L	26	GLU	CA-C	-5.79	1.46	1.52
3	N	1375	MET	SD-CE	-5.78	1.65	1.79
3	D	141	ILE	CA-CB	5.76	1.60	1.54
4	E	41	GLU	CA-C	5.71	1.59	1.52
1	B	98	THR	CA-CB	5.67	1.60	1.53
2	C	474	VAL	CA-CB	5.42	1.60	1.53
5	F	75	ILE	CA-CB	5.42	1.60	1.53
3	D	1045	MET	SD-CE	5.37	1.93	1.79
3	D	147	VAL	CA-CB	5.31	1.60	1.54
3	N	1378	TYR	CA-C	5.31	1.59	1.52
5	P	75	ILE	CA-CB	5.29	1.59	1.53
3	N	13	ALA	CA-CB	-5.29	1.46	1.53
1	A	16	GLN	CB-CG	5.27	1.68	1.52
1	K	16	GLN	CB-CG	5.26	1.68	1.52
3	N	1422	MET	CG-SD	5.24	1.93	1.80
2	C	677	MET	SD-CE	-5.23	1.66	1.79
1	K	27	PRO	CA-C	5.22	1.57	1.52
3	N	999	THR	CA-CB	5.21	1.61	1.53
4	O	41	GLU	CA-C	5.21	1.59	1.52
3	D	1168	MET	SD-CE	-5.20	1.66	1.79
3	N	133	ILE	CA-CB	5.19	1.60	1.53
2	M	676	ILE	CA-CB	5.15	1.61	1.54
3	D	13	ALA	CA-CB	-5.13	1.46	1.53
3	N	1125	PRO	CA-C	5.12	1.59	1.52
2	M	163	ILE	CA-CB	5.11	1.59	1.53
3	D	199	LEU	CA-C	5.09	1.59	1.52
1	A	26	GLU	CA-C	-5.07	1.46	1.52
1	A	158	ILE	CG1-CD1	5.05	1.71	1.51
3	N	1379	VAL	CA-C	5.05	1.58	1.52

All (432) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	94	PRO	CA-N-CD	-18.65	85.89	112.00
3	D	614	PHE	CA-CB-CG	18.16	131.96	113.80
4	E	94	PRO	N-CA-C	15.24	135.26	113.47
1	K	26	GLU	CA-C-O	-13.37	101.84	120.16
1	L	26	GLU	CA-C-O	-12.94	106.95	120.28
1	A	26	GLU	CA-C-O	-12.60	102.90	120.16
4	E	93	TYR	CA-C-N	12.08	131.53	118.97
4	E	93	TYR	C-N-CA	12.08	131.53	118.97
4	O	94	PRO	N-CA-C	11.82	130.37	113.47
1	A	26	GLU	CA-C-N	-11.60	105.96	120.23
1	A	26	GLU	C-N-CA	-11.60	105.96	120.23
1	B	26	GLU	CA-C-O	-11.60	108.33	120.28
1	K	26	GLU	CA-C-N	-10.84	104.52	120.46
1	K	26	GLU	C-N-CA	-10.84	104.52	120.46
3	N	614	PHE	CA-CB-CG	10.82	124.62	113.80
4	O	94	PRO	CA-N-CD	-10.25	97.65	112.00
3	N	611	GLN	OE1-CD-NE2	-10.05	112.55	122.60
3	D	616	GLN	OE1-CD-NE2	-9.84	112.76	122.60
3	N	561	GLY	CA-C-N	-9.80	111.15	122.52
3	N	561	GLY	C-N-CA	-9.80	111.15	122.52
3	D	561	GLY	CA-C-N	-9.61	111.37	122.52
3	D	561	GLY	C-N-CA	-9.61	111.37	122.52
3	N	1411	GLY	N-CA-C	-9.47	90.74	113.18
3	D	1411	GLY	N-CA-C	-9.41	90.88	113.18
1	B	158	ILE	CB-CA-C	-9.38	98.33	111.28
1	L	158	ILE	CB-CA-C	-9.28	98.47	111.28
2	C	264	PRO	CA-C-N	-9.21	108.13	122.59
2	C	264	PRO	C-N-CA	-9.21	108.13	122.59
2	M	264	PRO	CA-C-N	-9.17	108.20	122.59
2	M	264	PRO	C-N-CA	-9.17	108.20	122.59
3	N	616	GLN	OE1-CD-NE2	-9.11	113.49	122.60
2	C	177	GLU	CA-C-N	9.05	131.15	119.84
2	C	177	GLU	C-N-CA	9.05	131.15	119.84
3	N	80	VAL	CA-C-N	9.02	136.82	122.21
3	N	80	VAL	C-N-CA	9.02	136.82	122.21
3	D	611	GLN	OE1-CD-NE2	-8.98	113.62	122.60
2	M	177	GLU	CA-C-N	8.95	131.03	119.84
2	M	177	GLU	C-N-CA	8.95	131.03	119.84
3	D	610	LYS	CA-C-N	-8.79	110.14	123.14
3	D	610	LYS	C-N-CA	-8.79	110.14	123.14
3	N	1109	GLU	CA-C-N	8.75	137.34	121.94
3	N	1109	GLU	C-N-CA	8.75	137.34	121.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	O	93	TYR	CA-C-N	8.62	127.93	118.97
4	O	93	TYR	C-N-CA	8.62	127.93	118.97
4	O	60	ALA	CA-C-N	8.59	132.62	120.42
4	O	60	ALA	C-N-CA	8.59	132.62	120.42
3	N	65	ARG	CA-C-N	8.54	132.66	120.79
3	N	65	ARG	C-N-CA	8.54	132.66	120.79
3	D	1109	GLU	CA-C-N	8.44	136.79	121.85
3	D	1109	GLU	C-N-CA	8.44	136.79	121.85
3	N	611	GLN	CA-C-N	8.33	130.31	121.48
3	N	611	GLN	C-N-CA	8.33	130.31	121.48
3	N	169	TYR	CA-C-N	8.29	128.16	120.21
3	N	169	TYR	C-N-CA	8.29	128.16	120.21
3	D	169	TYR	CA-C-N	8.19	128.08	120.21
3	D	169	TYR	C-N-CA	8.19	128.08	120.21
3	N	1412	LYS	CA-C-N	-8.12	110.07	122.42
3	N	1412	LYS	C-N-CA	-8.12	110.07	122.42
4	E	94	PRO	CB-CA-C	-7.92	100.47	113.06
1	B	138	LEU	CA-CB-CG	7.87	143.84	116.30
3	D	1412	LYS	CA-C-N	-7.82	110.53	122.42
3	D	1412	LYS	C-N-CA	-7.82	110.53	122.42
2	C	58	ASP	CA-C-N	7.82	136.48	121.54
2	C	58	ASP	C-N-CA	7.82	136.48	121.54
2	M	1078	GLU	CA-C-N	7.81	129.60	119.84
2	M	1078	GLU	C-N-CA	7.81	129.60	119.84
2	C	1078	GLU	CA-C-N	7.79	129.58	119.84
2	C	1078	GLU	C-N-CA	7.79	129.58	119.84
3	N	79	GLU	CA-C-N	-7.78	111.07	122.58
3	N	79	GLU	C-N-CA	-7.78	111.07	122.58
3	D	65	ARG	CA-C-N	7.73	131.54	120.79
3	D	65	ARG	C-N-CA	7.73	131.54	120.79
1	L	138	LEU	CA-CB-CG	7.72	143.33	116.30
2	C	763	GLY	CA-C-N	-7.70	109.16	121.86
2	C	763	GLY	C-N-CA	-7.70	109.16	121.86
3	D	79	GLU	CA-C-N	-7.68	111.21	122.58
3	D	79	GLU	C-N-CA	-7.68	111.21	122.58
1	L	26	GLU	O-C-N	-7.66	116.44	121.88
3	D	80	VAL	CA-C-N	7.65	134.60	122.21
3	D	80	VAL	C-N-CA	7.65	134.60	122.21
2	M	58	ASP	CA-C-N	7.63	136.12	121.54
2	M	58	ASP	C-N-CA	7.63	136.12	121.54
5	P	92	PRO	CA-C-N	-7.60	112.04	122.30
5	P	92	PRO	C-N-CA	-7.60	112.04	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	92	PRO	CA-C-N	-7.58	112.06	122.30
5	F	92	PRO	C-N-CA	-7.58	112.06	122.30
2	M	763	GLY	CA-C-N	-7.46	109.55	121.86
2	M	763	GLY	C-N-CA	-7.46	109.55	121.86
2	M	608	GLY	N-CA-C	-7.42	105.60	115.32
2	C	795	GLY	N-CA-C	-7.29	99.58	112.77
2	C	795	GLY	CA-C-N	-7.28	110.71	122.36
2	C	795	GLY	C-N-CA	-7.28	110.71	122.36
3	D	198	ARG	CA-C-N	7.25	135.40	121.54
3	D	198	ARG	C-N-CA	7.25	135.40	121.54
3	N	198	ARG	CA-C-N	7.25	135.39	121.54
3	N	198	ARG	C-N-CA	7.25	135.39	121.54
2	M	795	GLY	N-CA-C	-7.24	99.67	112.77
3	D	93	ILE	CA-C-N	-7.23	112.92	123.05
3	D	93	ILE	C-N-CA	-7.23	112.92	123.05
2	M	463	GLU	CA-C-N	-7.22	112.95	123.05
2	M	463	GLU	C-N-CA	-7.22	112.95	123.05
3	N	508	ARG	CA-C-N	7.17	128.07	120.12
3	N	508	ARG	C-N-CA	7.17	128.07	120.12
3	N	617	ASN	CA-CB-CG	-7.15	105.45	112.60
3	D	616	GLN	CG-CD-NE2	7.12	127.08	116.40
2	C	463	GLU	CA-C-N	-7.11	113.09	123.05
2	C	463	GLU	C-N-CA	-7.11	113.09	123.05
4	E	3	GLU	CA-C-N	7.10	128.72	119.84
4	E	3	GLU	C-N-CA	7.10	128.72	119.84
3	N	1109	GLU	CA-C-O	7.07	128.30	120.94
4	E	95	VAL	CB-CA-C	-7.02	102.82	111.88
3	N	890	VAL	CA-C-N	-6.99	112.14	122.41
3	N	890	VAL	C-N-CA	-6.99	112.14	122.41
3	N	905	PRO	CA-C-N	-6.98	113.15	122.85
3	N	905	PRO	C-N-CA	-6.98	113.15	122.85
3	D	611	GLN	CA-C-N	6.97	128.53	121.35
3	D	611	GLN	C-N-CA	6.97	128.53	121.35
3	D	508	ARG	CA-C-N	6.96	127.84	120.12
3	D	508	ARG	C-N-CA	6.96	127.84	120.12
1	K	188	GLN	CA-CB-CG	-6.96	100.19	114.10
3	D	407	VAL	CB-CA-C	-6.95	102.42	111.25
3	D	1109	GLU	CA-C-O	6.95	128.17	120.94
3	N	1317	ASP	CA-C-N	6.92	131.20	120.75
3	N	1317	ASP	C-N-CA	6.92	131.20	120.75
3	D	890	VAL	CA-C-N	-6.84	112.35	122.41
3	D	890	VAL	C-N-CA	-6.84	112.35	122.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	109	LYS	CA-C-N	-6.84	113.34	122.85
2	M	109	LYS	C-N-CA	-6.84	113.34	122.85
2	M	795	GLY	CA-C-N	-6.84	111.42	122.36
2	M	795	GLY	C-N-CA	-6.84	111.42	122.36
3	N	611	GLN	CG-CD-NE2	6.84	126.65	116.40
3	N	407	VAL	CB-CA-C	-6.80	102.61	111.25
3	N	1124	GLN	CA-C-N	6.79	128.32	119.84
3	N	1124	GLN	C-N-CA	6.79	128.32	119.84
3	D	639	LEU	CA-C-N	6.75	129.65	120.54
3	D	639	LEU	C-N-CA	6.75	129.65	120.54
3	D	905	PRO	CA-C-N	-6.75	113.47	122.85
3	D	905	PRO	C-N-CA	-6.75	113.47	122.85
3	N	93	ILE	CA-C-N	-6.74	113.61	123.05
3	N	93	ILE	C-N-CA	-6.74	113.61	123.05
3	N	526	PRO	CA-C-N	6.73	132.42	122.86
3	N	526	PRO	C-N-CA	6.73	132.42	122.86
3	D	526	PRO	CA-C-N	6.73	132.41	122.86
3	D	526	PRO	C-N-CA	6.73	132.41	122.86
1	B	26	GLU	O-C-N	-6.72	117.11	121.88
4	E	94	PRO	CA-CB-CG	-6.71	91.75	104.50
3	N	610	LYS	CA-C-N	-6.67	111.88	122.76
3	N	610	LYS	C-N-CA	-6.67	111.88	122.76
3	D	1317	ASP	CA-C-N	6.67	130.82	120.75
3	D	1317	ASP	C-N-CA	6.67	130.82	120.75
2	C	109	LYS	CA-C-N	-6.66	113.59	122.85
2	C	109	LYS	C-N-CA	-6.66	113.59	122.85
2	C	1119	ARG	CB-CA-C	6.66	122.75	110.10
4	O	3	GLU	CA-C-N	6.65	128.15	119.84
4	O	3	GLU	C-N-CA	6.65	128.15	119.84
2	M	60	GLY	N-CA-C	-6.64	105.56	111.67
3	D	1209	LEU	CA-C-O	-6.63	113.21	121.50
2	C	726	ILE	CA-C-N	6.58	128.07	119.84
2	C	726	ILE	C-N-CA	6.58	128.07	119.84
2	M	726	ILE	CA-C-N	6.54	128.01	119.84
2	M	726	ILE	C-N-CA	6.54	128.01	119.84
2	M	728	HIS	CA-C-N	-6.53	109.07	121.54
2	M	728	HIS	C-N-CA	-6.53	109.07	121.54
3	D	1207	TYR	CA-CB-CG	6.46	125.53	113.90
5	P	84	TYR	CA-CB-CG	6.39	125.41	113.90
3	N	1209	LEU	CA-C-O	-6.35	113.56	121.50
3	D	564	GLU	CA-CB-CG	-6.32	101.45	114.10
1	B	106	PRO	CA-C-N	-6.30	112.72	122.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	106	PRO	C-N-CA	-6.30	112.72	122.87
2	C	728	HIS	CA-C-N	-6.30	109.51	121.54
2	C	728	HIS	C-N-CA	-6.30	109.51	121.54
3	N	891	GLU	CA-C-N	6.29	133.56	121.54
3	N	891	GLU	C-N-CA	6.29	133.56	121.54
3	D	28	LYS	CA-C-N	6.29	127.70	119.84
3	D	28	LYS	C-N-CA	6.29	127.70	119.84
3	D	891	GLU	CA-C-N	6.28	133.54	121.54
3	D	891	GLU	C-N-CA	6.28	133.54	121.54
3	N	41	ARG	CA-C-N	6.28	133.53	121.54
3	N	41	ARG	C-N-CA	6.28	133.53	121.54
3	N	639	LEU	CA-C-N	6.27	130.23	120.82
3	N	639	LEU	C-N-CA	6.27	130.23	120.82
2	C	728	HIS	CA-C-O	-6.27	112.33	119.41
2	C	1017	THR	CA-C-N	-6.26	112.32	122.34
2	C	1017	THR	C-N-CA	-6.26	112.32	122.34
3	N	1207	TYR	CA-CB-CG	6.24	125.14	113.90
1	A	188	GLN	CA-CB-CG	-6.24	101.63	114.10
3	D	611	GLN	CG-CD-NE2	6.23	125.75	116.40
4	O	41	GLU	CA-C-N	6.19	127.57	119.84
4	O	41	GLU	C-N-CA	6.19	127.57	119.84
2	M	795	GLY	CA-C-O	-6.18	113.13	122.71
4	E	50	THR	CA-C-N	6.17	135.68	121.87
4	E	50	THR	C-N-CA	6.17	135.68	121.87
4	E	51	LEU	CA-C-N	-6.17	112.18	122.17
4	E	51	LEU	C-N-CA	-6.17	112.18	122.17
2	M	728	HIS	CA-C-O	-6.17	112.44	119.41
5	F	283	GLY	N-CA-C	-6.14	106.46	115.30
2	C	727	PRO	CA-C-N	-6.11	111.16	122.09
2	C	727	PRO	C-N-CA	-6.11	111.16	122.09
3	N	613	ARG	N-CA-C	6.10	118.59	109.25
4	O	51	LEU	CA-C-N	-6.10	112.29	122.17
4	O	51	LEU	C-N-CA	-6.10	112.29	122.17
4	O	50	THR	CA-C-N	6.09	135.51	121.87
4	O	50	THR	C-N-CA	6.09	135.51	121.87
3	D	41	ARG	CA-C-N	6.08	133.15	121.54
3	D	41	ARG	C-N-CA	6.08	133.15	121.54
3	D	614	PHE	N-CA-C	-6.08	98.90	108.14
3	D	201	GLY	N-CA-C	6.05	119.43	110.42
2	C	608	GLY	N-CA-C	-6.04	106.12	115.73
3	N	616	GLN	CG-CD-NE2	6.04	125.46	116.40
2	M	287	GLY	N-CA-C	-6.03	98.89	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	107	ASP	CA-C-O	-6.03	113.63	120.32
3	D	517	VAL	N-CA-C	6.03	113.05	107.56
3	N	1351	GLU	CA-CB-CG	-6.03	102.05	114.10
3	D	448	GLU	CA-C-N	-6.01	114.43	122.42
3	D	448	GLU	C-N-CA	-6.01	114.43	122.42
4	E	41	GLU	CA-C-N	6.00	127.34	119.84
4	E	41	GLU	C-N-CA	6.00	127.34	119.84
3	D	831	GLY	N-CA-C	-6.00	98.97	113.18
3	N	831	GLY	N-CA-C	-5.99	98.98	113.18
1	K	26	GLU	O-C-N	-5.99	114.43	121.32
3	N	611	GLN	CB-CA-C	5.97	120.06	111.82
2	C	684	PHE	CA-C-N	-5.96	111.40	122.60
2	C	684	PHE	C-N-CA	-5.96	111.40	122.60
3	D	1344	VAL	CB-CA-C	-5.95	104.35	111.97
3	N	201	GLY	N-CA-C	5.95	119.28	110.42
2	C	287	GLY	N-CA-C	-5.94	99.10	113.18
3	N	28	LYS	CA-C-N	5.94	127.26	119.84
3	N	28	LYS	C-N-CA	5.94	127.26	119.84
2	C	729	LEU	CA-C-N	-5.94	112.49	122.29
2	C	729	LEU	C-N-CA	-5.94	112.49	122.29
3	D	1383	ASP	CA-C-N	5.93	125.90	120.03
3	D	1383	ASP	C-N-CA	5.93	125.90	120.03
2	M	684	PHE	CA-C-N	-5.91	111.19	122.53
2	M	684	PHE	C-N-CA	-5.91	111.19	122.53
2	M	857	ASP	CA-C-N	-5.91	112.47	121.92
2	M	857	ASP	C-N-CA	-5.91	112.47	121.92
1	K	105	GLY	CA-C-N	5.90	127.21	119.84
1	K	105	GLY	C-N-CA	5.90	127.21	119.84
3	N	80	VAL	CA-C-O	5.89	127.53	121.28
2	M	443	THR	CA-C-N	5.88	125.64	119.76
2	M	443	THR	C-N-CA	5.88	125.64	119.76
2	M	114	PHE	N-CA-CB	5.88	118.77	110.24
1	B	67	THR	CA-C-N	-5.87	117.64	123.04
1	B	67	THR	C-N-CA	-5.87	117.64	123.04
5	P	283	GLY	N-CA-C	-5.87	106.84	115.30
2	C	813	VAL	CA-C-N	-5.86	114.85	123.05
2	C	813	VAL	C-N-CA	-5.86	114.85	123.05
3	D	1268	PRO	CA-C-N	-5.85	112.48	120.44
3	D	1268	PRO	C-N-CA	-5.85	112.48	120.44
2	C	60	GLY	N-CA-C	-5.85	106.29	111.67
1	L	188	GLN	CA-CB-CG	5.84	125.78	114.10
3	N	81	THR	CA-C-O	-5.83	114.81	121.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	80	VAL	CA-C-O	5.82	127.45	121.28
1	K	135	GLY	N-CA-C	-5.82	105.31	114.10
1	L	146	ARG	CA-CB-CG	5.79	125.69	114.10
2	C	258	TYR	CA-C-O	5.79	126.33	119.56
2	C	795	GLY	CA-C-O	-5.79	113.74	122.71
1	A	26	GLU	O-C-N	-5.78	114.68	121.32
4	E	94	PRO	N-CD-CG	5.78	111.87	103.20
1	K	68	ILE	CB-CA-C	-5.77	104.15	110.78
1	A	158	ILE	CG1-CB-CG2	-5.76	93.42	110.70
3	N	517	VAL	N-CA-C	5.75	112.80	107.56
2	M	729	LEU	CA-C-N	-5.74	112.83	122.29
2	M	729	LEU	C-N-CA	-5.74	112.83	122.29
1	L	105	GLY	CA-C-N	5.73	127.00	119.84
1	L	105	GLY	C-N-CA	5.73	127.00	119.84
2	M	1017	THR	CA-C-N	-5.73	113.10	122.26
2	M	1017	THR	C-N-CA	-5.73	113.10	122.26
3	N	606	ILE	CB-CA-C	-5.72	104.33	112.22
2	M	813	VAL	CA-C-N	-5.71	115.06	123.05
2	M	813	VAL	C-N-CA	-5.71	115.06	123.05
3	N	1383	ASP	CA-C-N	5.70	125.67	120.03
3	N	1383	ASP	C-N-CA	5.70	125.67	120.03
1	K	158	ILE	CG1-CB-CG2	-5.69	93.63	110.70
3	D	1128	VAL	CA-C-O	-5.69	114.26	121.48
2	C	879	ARG	CA-C-N	-5.67	114.50	123.23
2	C	879	ARG	C-N-CA	-5.67	114.50	123.23
1	A	105	GLY	CA-C-N	5.66	126.92	119.84
1	A	105	GLY	C-N-CA	5.66	126.92	119.84
3	D	1043	GLY	CA-C-N	-5.66	115.25	122.77
3	D	1043	GLY	C-N-CA	-5.66	115.25	122.77
2	C	56	GLU	CA-C-N	-5.66	115.71	122.44
2	C	56	GLU	C-N-CA	-5.66	115.71	122.44
2	C	1109	VAL	CA-C-N	-5.64	114.82	122.77
2	C	1109	VAL	C-N-CA	-5.64	114.82	122.77
3	N	10	ILE	CB-CA-C	-5.63	103.03	110.98
1	K	25	LEU	CA-C-N	-5.63	108.06	121.80
1	K	25	LEU	C-N-CA	-5.63	108.06	121.80
5	P	233	PHE	CA-CB-CG	-5.62	108.18	113.80
3	D	606	ILE	CB-CA-C	-5.62	104.47	112.22
2	M	1109	VAL	CA-C-N	-5.62	114.85	122.77
2	M	1109	VAL	C-N-CA	-5.62	114.85	122.77
2	M	318	PRO	CA-C-N	5.61	131.44	121.05
2	M	318	PRO	C-N-CA	5.61	131.44	121.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	188	GLN	CA-CB-CG	5.61	125.31	114.10
3	D	1408	ILE	CA-C-O	-5.61	115.91	122.13
2	C	318	PRO	CA-C-N	5.60	131.41	121.05
2	C	318	PRO	C-N-CA	5.60	131.41	121.05
3	N	1408	ILE	CA-C-O	-5.60	115.92	122.13
3	D	1467	ILE	CB-CA-C	-5.58	104.73	111.88
2	C	114	PHE	N-CA-CB	5.57	118.32	110.24
2	M	57	GLU	CA-C-N	-5.57	112.97	122.33
2	M	57	GLU	C-N-CA	-5.57	112.97	122.33
2	M	879	ARG	CA-C-N	-5.55	114.68	123.23
2	M	879	ARG	C-N-CA	-5.55	114.68	123.23
1	A	135	GLY	N-CA-C	-5.55	105.72	114.10
3	N	66	GLN	CA-C-O	-5.53	114.99	121.07
3	N	18	ILE	CB-CA-C	-5.51	104.82	111.88
3	N	1467	ILE	CB-CA-C	-5.51	104.64	111.70
1	L	106	PRO	CA-C-N	-5.51	114.00	122.87
1	L	106	PRO	C-N-CA	-5.51	114.00	122.87
3	N	669	ASN	CA-C-N	5.49	127.42	120.72
3	N	669	ASN	C-N-CA	5.49	127.42	120.72
1	K	48	ILE	CA-C-N	5.49	125.69	120.31
1	K	48	ILE	C-N-CA	5.49	125.69	120.31
2	C	640	ARG	CA-C-N	5.48	126.69	119.84
2	C	640	ARG	C-N-CA	5.48	126.69	119.84
5	F	296	GLY	CA-C-N	5.48	126.69	119.84
5	F	296	GLY	C-N-CA	5.48	126.69	119.84
2	M	727	PRO	CA-C-N	-5.48	112.29	122.09
2	M	727	PRO	C-N-CA	-5.48	112.29	122.09
2	C	857	ASP	CA-C-N	-5.47	113.17	121.92
2	C	857	ASP	C-N-CA	-5.47	113.17	121.92
3	D	81	THR	CA-C-O	-5.46	115.22	121.40
5	F	84	TYR	CA-CB-CG	5.43	123.68	113.90
1	B	146	ARG	CA-CB-CG	5.43	124.97	114.10
3	D	132	TYR	CA-C-N	5.42	129.31	121.18
3	D	132	TYR	C-N-CA	5.42	129.31	121.18
3	D	66	GLN	CA-C-O	-5.42	115.11	121.07
3	N	64	LYS	CA-C-N	-5.41	113.35	123.03
3	N	64	LYS	C-N-CA	-5.41	113.35	123.03
3	N	1043	GLY	CA-C-N	-5.38	115.61	122.77
3	N	1043	GLY	C-N-CA	-5.38	115.61	122.77
2	M	469	THR	N-CA-C	5.38	112.97	108.13
3	N	564	GLU	CA-CB-CG	-5.37	103.36	114.10
2	C	1057	SER	CA-C-N	-5.36	113.83	122.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1057	SER	C-N-CA	-5.36	113.83	122.24
3	N	21	TRP	CA-CB-CG	5.35	123.76	113.60
2	M	519	GLY	CA-C-N	-5.34	115.41	122.56
2	M	519	GLY	C-N-CA	-5.34	115.41	122.56
2	C	399	ASN	CA-C-N	5.33	126.50	119.84
2	C	399	ASN	C-N-CA	5.33	126.50	119.84
3	D	615	ARG	N-CA-C	-5.33	99.45	110.80
3	D	613	ARG	N-CA-C	5.32	116.92	108.67
2	C	318	PRO	N-CA-C	-5.30	106.49	113.65
3	N	1242	HIS	CA-C-N	5.30	131.66	121.54
3	N	1242	HIS	C-N-CA	5.30	131.66	121.54
3	D	1110	ALA	CA-C-O	-5.29	115.06	120.99
2	C	57	GLU	CA-C-N	-5.29	113.45	122.33
2	C	57	GLU	C-N-CA	-5.29	113.45	122.33
1	A	137	ARG	CA-CB-CG	-5.28	103.53	114.10
3	N	1128	VAL	CA-C-O	-5.28	114.77	121.48
1	B	105	GLY	CA-C-N	5.28	126.44	119.84
1	B	105	GLY	C-N-CA	5.28	126.44	119.84
2	M	163	ILE	N-CA-C	5.27	113.24	107.60
3	N	1460	ILE	CB-CA-C	-5.27	101.95	110.28
3	N	863	VAL	CB-CA-C	-5.27	105.54	111.23
2	M	1029	GLY	N-CA-C	5.27	119.28	112.54
5	F	214	GLN	CA-C-N	-5.27	112.31	120.31
5	F	214	GLN	C-N-CA	-5.27	112.31	120.31
1	K	91	ASN	N-CA-C	5.26	112.96	108.22
3	D	1101	VAL	CB-CA-C	-5.26	105.31	111.94
1	K	17	GLY	N-CA-C	-5.26	102.56	111.08
2	M	1057	SER	CA-C-N	-5.25	114.00	122.24
2	M	1057	SER	C-N-CA	-5.25	114.00	122.24
3	D	863	VAL	CB-CA-C	-5.24	104.59	111.25
1	K	16	GLN	CB-CG-CD	5.24	121.50	112.60
1	A	25	LEU	CA-C-N	-5.23	109.03	121.80
1	A	25	LEU	C-N-CA	-5.23	109.03	121.80
2	M	1027	PHE	N-CA-C	5.23	117.89	111.82
5	F	159	ILE	CB-CA-C	-5.23	105.17	112.02
3	N	1306	PRO	CA-C-N	5.22	128.66	120.82
3	N	1306	PRO	C-N-CA	5.22	128.66	120.82
2	M	110	GLU	CA-CB-CG	-5.22	103.66	114.10
3	D	107	ASP	CA-C-O	-5.22	114.53	120.32
3	D	1242	HIS	CA-C-N	5.22	131.51	121.54
3	D	1242	HIS	C-N-CA	5.22	131.51	121.54
3	D	18	ILE	CB-CA-C	-5.22	105.29	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	135	GLY	N-CA-C	-5.22	106.22	114.10
1	B	187	GLY	CA-C-N	5.21	127.71	120.63
1	B	187	GLY	C-N-CA	5.21	127.71	120.63
2	M	56	GLU	CA-C-N	-5.20	116.26	122.44
2	M	56	GLU	C-N-CA	-5.20	116.26	122.44
2	M	230	ARG	CA-C-N	5.17	126.30	119.84
2	M	230	ARG	C-N-CA	5.17	126.30	119.84
5	P	259	ARG	CA-C-N	5.17	127.35	122.85
5	P	259	ARG	C-N-CA	5.17	127.35	122.85
5	P	75	ILE	CA-C-N	5.16	131.39	121.54
5	P	75	ILE	C-N-CA	5.16	131.39	121.54
1	L	137	ARG	CB-CG-CD	5.14	123.13	111.30
3	N	1092	GLY	N-CA-C	-5.14	106.15	113.86
3	D	64	LYS	CA-C-N	-5.13	113.84	123.03
3	D	64	LYS	C-N-CA	-5.13	113.84	123.03
2	C	519	GLY	CA-C-N	-5.11	115.71	122.56
2	C	519	GLY	C-N-CA	-5.11	115.71	122.56
2	M	110	GLU	CA-C-N	5.11	131.31	121.54
2	M	110	GLU	C-N-CA	5.11	131.31	121.54
1	A	26	GLU	N-CA-C	5.11	121.11	109.81
4	E	93	TYR	O-C-N	5.11	126.79	121.02
5	P	159	ILE	CB-CA-C	-5.11	105.33	112.02
2	M	108	ILE	CB-CA-C	-5.10	105.11	111.08
2	M	977	GLY	N-CA-C	-5.10	107.82	113.79
2	M	640	ARG	CA-C-N	5.10	126.21	119.84
2	M	640	ARG	C-N-CA	5.10	126.21	119.84
2	C	443	THR	CA-C-N	5.09	125.88	120.13
2	C	443	THR	C-N-CA	5.09	125.88	120.13
5	F	75	ILE	CA-C-N	5.08	131.24	121.54
5	F	75	ILE	C-N-CA	5.08	131.24	121.54
1	L	187	GLY	CA-C-N	5.08	127.54	120.63
1	L	187	GLY	C-N-CA	5.08	127.54	120.63
3	N	634	GLY	CA-C-N	5.08	126.19	119.84
3	N	634	GLY	C-N-CA	5.08	126.19	119.84
4	O	92	LEU	N-CA-C	5.08	119.19	112.89
2	C	108	ILE	CB-CA-C	-5.08	105.14	111.08
2	C	542	VAL	CB-CA-C	-5.08	105.47	111.81
1	A	42	ARG	NE-CZ-NH1	-5.07	116.43	121.50
2	C	1056	LYS	CA-C-N	-5.06	111.87	121.54
2	C	1056	LYS	C-N-CA	-5.06	111.87	121.54
1	L	17	GLY	N-CA-C	-5.05	103.40	110.63
3	D	561	GLY	CA-C-O	-5.05	116.08	122.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	283	ILE	CA-C-N	-5.05	114.75	122.62
2	C	283	ILE	C-N-CA	-5.05	114.75	122.62
2	M	1078	GLU	CB-CA-C	5.04	116.64	109.38
3	N	1108	ARG	CA-C-N	-5.04	113.73	122.84
3	N	1108	ARG	C-N-CA	-5.04	113.73	122.84
4	E	52	GLU	CA-CB-CG	-5.03	104.03	114.10
2	M	318	PRO	N-CA-C	-5.03	106.86	113.65
3	N	1109	GLU	N-CA-C	5.03	114.47	107.73
2	M	283	ILE	CA-C-N	-5.01	114.80	122.62
2	M	283	ILE	C-N-CA	-5.01	114.80	122.62
3	D	99	ALA	CA-C-N	-5.01	114.41	122.82
3	D	99	ALA	C-N-CA	-5.01	114.41	122.82

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	N	132	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1806	0	1861	190	0
1	B	1806	0	1861	205	0
1	K	1806	0	1861	218	0
1	L	1806	0	1861	206	0
2	C	8829	0	8933	1170	0
2	M	8829	0	8933	1097	0
3	D	10407	0	10633	1335	0
3	N	10407	0	10633	1328	0
4	E	770	0	784	124	0
4	O	770	0	784	115	0
5	F	2771	0	2844	323	0
5	P	2771	0	2844	320	0
6	D	2	0	0	0	0
6	N	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	30	0	31	18	0
7	N	30	0	31	18	0
8	D	1	0	0	0	0
8	N	1	0	0	0	0
9	A	141	0	0	28	0
9	B	149	0	0	31	0
9	C	704	0	0	217	0
9	D	927	0	0	239	0
9	E	82	0	0	29	0
9	F	305	0	0	77	0
9	K	152	0	0	41	0
9	L	148	0	0	36	0
9	M	680	0	0	181	0
9	N	864	0	0	241	0
9	O	84	0	0	26	0
9	P	260	0	0	71	0
All	All	57340	0	53894	6228	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 58.

All (6228) 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)
3:D:610:LYS:HD3	7:D:1527:MXP:C15	1.49	1.41
3:N:610:LYS:HD3	7:N:1527:MXP:C15	1.55	1.37
3:N:136:ASP:HB3	3:N:137:PRO:HD3	1.27	1.15
3:D:136:ASP:HB3	3:D:137:PRO:HD3	1.27	1.13
2:M:877:PRO:HG2	3:N:1023:MET:HE2	1.30	1.12
3:D:610:LYS:HD3	7:D:1527:MXP:H15B	1.19	1.10
1:L:109:VAL:HG21	1:L:138:LEU:HD11	1.33	1.08
3:N:610:LYS:HD3	7:N:1527:MXP:H15	1.08	1.06
1:A:42:ARG:HH12	1:B:34:VAL:HB	1.00	1.06
1:B:109:VAL:HG21	1:B:138:LEU:HD11	1.35	1.06
3:D:611:GLN:HE22	3:D:1463:LYS:HE2	1.20	1.05
3:N:613:ARG:HG3	3:N:1441:GLN:HB2	1.39	1.04
3:N:101:HIS:HD1	3:N:103:TRP:HB2	1.21	1.04
2:C:395:LYS:HE2	2:C:403:SER:HB2	1.34	1.04
3:N:180:LYS:HG2	3:N:183:GLU:HB2	1.35	1.04
3:D:180:LYS:HG2	3:D:183:GLU:HB2	1.37	1.03
2:C:795:GLY:HA3	2:C:1004:LYS:HE2	1.41	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:187:LYS:HE2	3:D:199:LEU:HB3	1.42	1.02
3:D:1335:LEU:HD23	3:D:1344:VAL:HA	1.41	1.02
3:N:610:LYS:CD	7:N:1527:MXP:C15	2.37	1.02
1:K:67:THR:HG21	2:M:609:ASN:HD21	1.24	1.02
2:M:150:PRO:HA	2:M:158:TYR:HB3	1.40	1.01
3:N:100:ALA:HB2	3:N:513:ILE:HD13	1.41	1.01
2:C:1054:THR:HG21	2:C:1079:PRO:HB3	1.42	1.01
3:D:610:LYS:CD	7:D:1527:MXP:C15	2.38	1.01
1:A:7:LYS:HE2	1:A:186:LEU:HD11	1.42	1.01
4:E:94:PRO:HD3	9:E:180:HOH:O	1.60	1.00
1:K:7:LYS:HE2	1:K:186:LEU:HD11	1.40	1.00
3:N:1209:LEU:HD21	4:O:16:LYS:HD2	1.38	1.00
2:C:877:PRO:HG2	3:D:1023:MET:HE2	1.44	1.00
3:N:1160:LEU:HD11	3:N:1174:LEU:HD21	1.45	0.98
2:C:150:PRO:HA	2:C:158:TYR:HB3	1.42	0.98
3:D:907:GLU:HA	9:D:2416:HOH:O	1.65	0.97
3:N:148:GLU:HB3	3:N:151:GLN:HB2	1.43	0.97
2:C:2:GLU:HG3	2:C:899:GLN:HB3	1.46	0.97
3:D:1101:VAL:HG21	3:D:1424:VAL:HG22	1.44	0.96
1:A:152:PRO:HA	9:A:351:HOH:O	1.66	0.95
3:N:957:PRO:HG2	3:N:1007:VAL:HA	1.49	0.95
2:M:169:GLY:HA2	2:M:263:ASP:HB3	1.45	0.95
3:N:610:LYS:CD	7:N:1527:MXP:H15	1.96	0.95
3:N:527:MET:HE2	5:P:258:ILE:HD11	1.45	0.95
1:K:42:ARG:HH12	1:L:34:VAL:HB	1.31	0.95
3:N:1405:GLU:O	3:N:1410:GLU:HA	1.67	0.95
3:D:148:GLU:HB3	3:D:151:GLN:HB2	1.49	0.94
3:N:1465:ASN:HD21	3:N:1470:ARG:HD3	1.33	0.94
3:D:1393:GLN:HB2	3:D:1398:TRP:HE1	1.32	0.94
1:A:42:ARG:NH1	1:B:34:VAL:HB	1.82	0.94
3:D:581:LEU:HD12	3:D:603:LEU:HD11	1.50	0.94
2:C:12:VAL:HG21	2:C:472:ARG:HD3	1.48	0.94
5:P:268:ILE:HA	5:P:271:LEU:HD12	1.49	0.94
1:A:42:ARG:HH12	1:B:34:VAL:CB	1.80	0.93
1:L:152:PRO:HD2	1:L:155:LYS:HD3	1.46	0.93
3:D:18:ILE:HG23	3:D:518:PRO:HG3	1.50	0.93
2:C:862:PRO:HA	2:C:975:TYR:HE1	1.32	0.93
2:C:890:LEU:HA	2:C:914:ILE:HD11	1.50	0.93
5:P:361:LEU:HD22	5:P:366:ALA:HB2	1.48	0.93
2:C:66:LEU:HD22	2:C:372:LEU:HD23	1.52	0.92
2:M:62:GLY:HA2	2:M:359:MET:HE1	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:957:PRO:HG2	3:D:1007:VAL:HA	1.52	0.92
2:M:757:GLY:HA2	2:M:789:SER:HB3	1.52	0.92
3:D:1194:CYS:HB2	9:D:1762:HOH:O	1.70	0.92
2:M:890:LEU:HA	2:M:914:ILE:HD11	1.52	0.92
3:D:610:LYS:HD3	7:D:1527:MXP:H15	1.52	0.92
2:M:1054:THR:HG23	2:M:1082:PRO:HG3	1.48	0.92
5:F:268:ILE:HA	5:F:271:LEU:HD12	1.51	0.91
3:N:581:LEU:HD12	3:N:603:LEU:HD11	1.51	0.91
3:D:611:GLN:HE22	3:D:1463:LYS:CE	1.84	0.91
2:M:437:ARG:CZ	2:M:488:ALA:HA	2.01	0.91
3:D:508:ARG:HG2	3:D:509:PRO:HD2	1.52	0.91
2:M:66:LEU:HD22	2:M:372:LEU:HD23	1.53	0.91
3:D:100:ALA:HB2	3:D:513:ILE:HD13	1.50	0.91
3:D:611:GLN:NE2	3:D:1463:LYS:HE2	1.84	0.91
3:N:675:ARG:HH12	5:P:421:PHE:HD2	1.15	0.91
2:M:409:ARG:HA	2:M:454:SER:HA	1.53	0.91
3:D:1405:GLU:O	3:D:1410:GLU:HA	1.71	0.90
2:C:41:ASN:HD22	2:C:41:ASN:H	1.16	0.90
2:M:862:PRO:HA	2:M:975:TYR:HE1	1.34	0.90
2:C:1114:GLY:H	2:C:1115:LEU:HD12	1.35	0.90
1:K:190:THR:HA	9:K:1309:HOH:O	1.70	0.90
3:D:520:LEU:HD12	3:D:521:PRO:HD2	1.53	0.90
3:D:406:ASP:HB3	5:F:168:LYS:HE2	1.54	0.89
3:D:87:ARG:HA	9:D:1713:HOH:O	1.71	0.89
3:D:527:MET:HE2	5:F:258:ILE:HD11	1.55	0.89
1:B:152:PRO:HD2	1:B:155:LYS:HD3	1.54	0.89
3:N:18:ILE:HG23	3:N:518:PRO:HG3	1.54	0.89
1:A:24:VAL:HG22	1:A:196:THR:HB	1.54	0.88
3:D:204:LEU:HA	3:D:441:ARG:HH22	1.36	0.88
2:M:874:LEU:HD21	3:N:787:LEU:HD22	1.53	0.88
3:N:508:ARG:HG2	3:N:509:PRO:HD2	1.54	0.88
5:P:128:ARG:O	5:P:132:ARG:HG3	1.72	0.88
1:B:87:VAL:HG21	1:B:144:VAL:HG11	1.56	0.88
3:D:1383:ASP:HB2	3:D:1416:ALA:HB3	1.54	0.88
2:C:367:LEU:HA	2:C:371:LYS:HG3	1.53	0.88
2:C:1087:VAL:CG1	3:D:610:LYS:NZ	2.36	0.88
3:N:400:VAL:HG22	3:N:443:VAL:HG21	1.54	0.88
2:C:1054:THR:HG22	2:C:1059:ASP:HB2	1.52	0.88
5:P:205:ARG:HD2	5:P:251:ILE:HD13	1.56	0.88
2:C:191:PHE:HZ	2:C:196:LEU:HB2	1.37	0.88
3:N:165:LYS:HB2	3:N:397:LYS:HB3	1.56	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:431:HIS:HB3	2:C:434:HIS:HD2	1.39	0.88
2:C:952:LEU:HD12	2:C:969:GLN:HE22	1.35	0.88
2:C:1008:ARG:HH11	2:C:1028:GLY:HA2	1.39	0.88
5:F:128:ARG:O	5:F:132:ARG:HG3	1.74	0.88
1:L:184:THR:HG23	1:L:192:LEU:HB3	1.55	0.87
2:M:41:ASN:HD22	2:M:41:ASN:H	1.17	0.87
1:B:86:VAL:HG12	1:B:124:ASN:HD22	1.39	0.87
2:C:671:ASN:N	2:C:671:ASN:HD22	1.70	0.87
4:O:41:GLU:HA	4:O:45:ARG:HD3	1.57	0.87
5:F:271:LEU:HG	5:F:295:MET:HE1	1.56	0.87
3:N:131:LYS:HG2	3:N:568:ARG:HG2	1.56	0.87
1:L:194:LYS:HG2	9:L:1676:HOH:O	1.74	0.87
2:M:367:LEU:HA	2:M:371:LYS:HG3	1.57	0.87
3:N:1406:ARG:HA	3:N:1410:GLU:HG2	1.56	0.87
3:N:1393:GLN:HB2	3:N:1398:TRP:HE1	1.40	0.87
5:P:358:LEU:HD21	5:P:367:MET:HE3	1.55	0.87
1:L:86:VAL:HG12	1:L:124:ASN:HD22	1.39	0.86
1:L:132:LEU:HG	1:L:136:GLY:HA3	1.57	0.86
3:N:59:ALA:HB3	3:N:76:CYS:SG	2.14	0.86
3:N:494:LYS:HA	9:N:1731:HOH:O	1.73	0.86
3:N:116:LEU:HD21	3:N:464:LEU:HB3	1.56	0.86
1:A:20:TYR:HD2	1:A:21:GLY:N	1.72	0.86
2:C:121:MET:HA	9:C:1509:HOH:O	1.73	0.86
2:M:140:ILE:HD11	2:M:412:ALA:HA	1.56	0.86
2:M:762:LYS:HB2	2:M:786:LYS:HD2	1.55	0.86
2:M:597:ALA:HB2	2:M:655:LEU:HD21	1.56	0.86
1:L:94:LEU:HD21	1:L:119:ASP:HB2	1.55	0.86
3:N:1383:ASP:HB2	3:N:1416:ALA:HB3	1.56	0.86
1:K:222:LEU:HD21	1:L:218:LEU:HD23	1.58	0.86
3:N:489:ARG:HH22	3:N:1389:LEU:HD21	1.40	0.85
3:N:1232:PRO:HB3	3:N:1361:VAL:HG21	1.58	0.85
1:B:94:LEU:HD21	1:B:119:ASP:HB2	1.56	0.85
2:M:1054:THR:HG22	2:M:1059:ASP:HB2	1.58	0.85
3:N:187:LYS:HE2	3:N:199:LEU:HB3	1.56	0.85
3:N:201:GLY:HA2	3:N:396:VAL:O	1.74	0.85
5:P:291:ILE:HG21	5:P:304:VAL:HG11	1.57	0.85
3:D:201:GLY:HA2	3:D:396:VAL:O	1.76	0.85
3:D:400:VAL:HG22	3:D:443:VAL:HG21	1.57	0.85
5:F:205:ARG:HD2	5:F:251:ILE:HD13	1.56	0.85
3:N:204:LEU:HA	3:N:441:ARG:HH22	1.40	0.85
4:E:41:GLU:HA	4:E:45:ARG:HD3	1.56	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:302:VAL:HG12	9:M:1862:HOH:O	1.75	0.85
5:P:166:LEU:HB3	5:P:170:HIS:HB2	1.57	0.85
1:B:184:THR:HG23	1:B:192:LEU:HB3	1.57	0.85
2:C:1084:SER:HB2	7:D:1527:MXP:O4	1.76	0.85
3:D:561:GLY:HA3	5:F:184:ARG:HH12	1.42	0.85
3:D:1160:LEU:HD11	3:D:1174:LEU:HD21	1.57	0.85
2:M:710:ILE:HB	2:M:790:LEU:HD13	1.59	0.85
1:A:103:ALA:HB1	1:A:107:LYS:HE2	1.57	0.84
3:N:908:LYS:HB3	3:N:1027:GLY:HA3	1.58	0.84
1:B:58:ILE:HG22	1:B:137:ARG:HH21	1.41	0.84
3:D:59:ALA:HB3	3:D:76:CYS:SG	2.17	0.84
3:N:617:ASN:OD1	3:N:617:ASN:N	2.09	0.84
5:F:166:LEU:HB3	5:F:170:HIS:HB2	1.59	0.84
3:D:558:LEU:HD13	5:F:145:PRO:HB3	1.58	0.84
3:D:1232:PRO:HB3	3:D:1361:VAL:HG21	1.59	0.84
3:D:101:HIS:HD1	3:D:103:TRP:HB2	1.42	0.84
3:D:611:GLN:OE1	7:D:1527:MXP:H16B	1.78	0.84
4:O:95:VAL:HG13	9:O:1302:HOH:O	1.75	0.84
3:D:119:SER:HB2	3:D:123:LEU:HB2	1.59	0.84
4:E:25:LYS:HE2	9:E:136:HOH:O	1.78	0.83
2:M:733:ALA:HB2	3:N:679:ARG:NH2	1.93	0.83
1:B:158:ILE:HD11	1:B:166:PRO:HA	1.59	0.83
1:L:158:ILE:HD11	1:L:166:PRO:HA	1.60	0.83
3:D:1465:ASN:HD21	3:D:1470:ARG:HD3	1.43	0.83
2:C:62:GLY:HA2	2:C:359:MET:HE1	1.59	0.83
2:C:461:VAL:HG13	2:C:465:GLY:HA2	1.58	0.83
4:O:54:LEU:HG	4:O:58:PRO:HG2	1.61	0.83
1:A:35:THR:HG21	1:B:43:ILE:HD11	1.58	0.83
2:C:1009:SER:HB2	3:D:651:GLU:O	1.78	0.83
2:M:18:LEU:HD23	2:M:404:LEU:HD21	1.59	0.83
2:M:1114:GLY:H	2:M:1115:LEU:HD12	1.42	0.83
3:N:108:VAL:HB	3:N:109:PRO:HD3	1.60	0.83
1:K:42:ARG:HH21	2:M:857:ASP:HB3	1.44	0.83
3:D:1466:VAL:HG23	3:D:1472:ILE:HD11	1.60	0.83
2:M:952:LEU:HD12	2:M:969:GLN:HE22	1.41	0.83
3:N:611:GLN:HG2	3:N:619:LEU:CD1	2.09	0.82
1:B:132:LEU:HD13	1:B:138:LEU:HD12	1.61	0.82
5:F:291:ILE:HG21	5:F:304:VAL:HG11	1.59	0.82
2:C:148:PHE:HZ	2:C:281:LEU:HD13	1.43	0.82
1:L:87:VAL:HG21	1:L:144:VAL:HG11	1.59	0.82
3:N:520:LEU:HD12	3:N:521:PRO:HD2	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:615:ARG:HH21	3:N:1089:ALA:HB2	1.44	0.82
2:C:409:ARG:HA	2:C:454:SER:HA	1.61	0.82
2:C:114:PHE:H	2:C:114:PHE:HD1	1.25	0.82
3:D:1406:ARG:HA	3:D:1410:GLU:HG2	1.61	0.82
3:D:1141:GLU:HG2	3:D:1168:MET:HE1	1.60	0.82
3:N:32:ILE:HA	9:N:1836:HOH:O	1.79	0.82
2:C:1044:GLY:HA3	4:E:17:TYR:HE1	1.45	0.82
3:D:614:PHE:CD1	3:D:617:ASN:HA	2.14	0.82
3:N:465:LEU:HD21	9:N:1664:HOH:O	1.80	0.82
2:M:571:LEU:HD21	2:M:700:TYR:HA	1.60	0.82
3:N:152:LEU:HD23	3:N:152:LEU:H	1.43	0.82
3:N:1057:VAL:HG13	3:N:1069:GLU:HB3	1.60	0.82
2:C:750:LYS:HG3	3:D:681:ARG:HH21	1.45	0.82
2:M:603:VAL:HG21	2:M:643:VAL:HG11	1.60	0.82
2:M:643:VAL:HG23	9:M:1789:HOH:O	1.80	0.82
2:C:874:LEU:HD21	3:D:787:LEU:HD22	1.61	0.81
3:N:119:SER:HB2	3:N:123:LEU:HB2	1.58	0.81
2:M:1054:THR:HG21	2:M:1079:PRO:HB3	1.62	0.81
3:N:1466:VAL:HG23	3:N:1472:ILE:HD11	1.60	0.81
3:D:798:GLU:HB2	3:D:828:LYS:HE3	1.62	0.81
2:M:114:PHE:HD1	2:M:114:PHE:H	1.23	0.81
3:N:1115:THR:HB	9:N:1624:HOH:O	1.80	0.81
3:D:136:ASP:HB3	3:D:137:PRO:CD	2.10	0.81
3:N:136:ASP:HB3	3:N:137:PRO:CD	2.10	0.81
2:M:513:VAL:HB	9:M:1622:HOH:O	1.80	0.81
4:O:10:PHE:HE2	4:O:16:LYS:HG3	1.45	0.81
3:N:795:VAL:HG11	3:N:863:VAL:HG13	1.61	0.81
5:P:117:SER:HA	9:P:595:HOH:O	1.81	0.81
1:B:132:LEU:HG	1:B:136:GLY:HA3	1.60	0.80
2:C:169:GLY:HA2	2:C:263:ASP:HB3	1.63	0.80
2:C:860:HIS:HB2	9:C:1269:HOH:O	1.81	0.80
3:D:633:VAL:HG22	3:D:635:PRO:HD3	1.62	0.80
3:N:610:LYS:HD3	7:N:1527:MXP:H15B	1.58	0.80
3:N:843:PHE:HE1	3:N:864:VAL:HG11	1.44	0.80
2:C:436:GLY:O	2:C:459:ALA:HB2	1.81	0.80
3:D:592:THR:H	3:D:600:LEU:HD21	1.46	0.80
5:F:350:LEU:HD12	5:F:422:LEU:HD12	1.63	0.80
2:C:413:LEU:H	2:C:413:LEU:HD12	1.45	0.80
1:L:4:SER:HA	1:L:7:LYS:HE2	1.63	0.80
2:M:675:ALA:HA	2:M:989:VAL:HG12	1.63	0.80
3:N:699:VAL:H	3:N:756:GLN:NE2	1.80	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1161:GLU:HG3	3:D:1164:ARG:HB2	1.64	0.80
2:M:599:GLU:HG3	2:M:600:ASP:H	1.46	0.80
2:M:786:LYS:HA	9:M:1657:HOH:O	1.80	0.80
3:N:1277:ILE:HD12	3:N:1301:LYS:HB2	1.63	0.80
3:N:135:LEU:HD11	9:N:2226:HOH:O	1.82	0.80
2:M:675:ALA:HB2	2:M:867:VAL:HG11	1.62	0.80
2:M:943:VAL:HG23	2:M:985:GLY:H	1.46	0.80
5:P:139:ALA:HA	5:P:152:ASP:CG	2.06	0.80
2:M:611:ILE:HD11	2:M:641:PRO:HG3	1.64	0.80
3:D:1220:ALA:HB1	3:D:1223:ILE:HD13	1.63	0.80
3:D:1223:ILE:H	3:D:1223:ILE:HD12	1.47	0.80
1:K:100:LEU:HB2	1:K:115:LEU:HD11	1.64	0.80
1:K:185:ARG:HA	9:K:1309:HOH:O	1.82	0.80
2:C:76:PRO:HB3	9:C:1229:HOH:O	1.83	0.79
3:D:890:VAL:HG11	3:D:922:LEU:HD13	1.64	0.79
3:D:1393:GLN:HB2	3:D:1398:TRP:NE1	1.96	0.79
1:K:87:VAL:HG21	1:K:144:VAL:HG11	1.64	0.79
1:L:55:SER:HB3	1:L:143:ARG:HB3	1.64	0.79
2:C:54:ILE:HD11	2:C:356:ARG:HG2	1.63	0.79
1:K:20:TYR:HD2	1:K:21:GLY:N	1.80	0.79
2:M:260:LEU:HB2	2:M:291:ALA:HB1	1.62	0.79
3:N:1095:THR:HG23	3:N:1230:GLY:HA3	1.62	0.79
5:P:132:ARG:HG2	5:P:181:GLU:OE1	1.81	0.79
3:N:613:ARG:NH2	3:N:1097:LYS:HE2	1.97	0.79
1:B:4:SER:HA	1:B:7:LYS:HE2	1.64	0.79
2:C:143:SER:HB2	2:C:276:LYS:HZ1	1.48	0.79
2:C:199:VAL:HG21	9:C:1705:HOH:O	1.82	0.79
2:M:1008:ARG:HH11	2:M:1028:GLY:HA2	1.47	0.79
3:N:90:MET:HE2	3:N:521:PRO:HD3	1.64	0.79
1:A:87:VAL:HG21	1:A:144:VAL:HG11	1.63	0.79
4:E:94:PRO:CD	9:E:180:HOH:O	2.25	0.79
2:M:578:VAL:HG11	2:M:991:GLN:HB3	1.62	0.79
3:D:119:SER:H	3:D:123:LEU:HD22	1.46	0.79
9:M:1937:HOH:O	3:N:1068:LEU:HD11	1.82	0.79
3:N:783:ARG:NH1	3:N:1029:ARG:HG3	1.96	0.79
3:D:924:MET:HE1	3:D:1211:MET:HE3	1.64	0.79
3:D:1095:THR:HG23	3:D:1230:GLY:HA3	1.64	0.79
2:M:774:LEU:HA	2:M:777:ILE:HD12	1.64	0.79
1:A:222:LEU:HD23	1:B:215:VAL:HB	1.64	0.79
2:C:512:ARG:HD3	2:C:523:ILE:HD11	1.65	0.79
2:C:1087:VAL:CG1	3:D:610:LYS:HZ3	1.96	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:162:ARG:HB3	9:D:2186:HOH:O	1.81	0.79
5:F:293:GLU:HB3	9:F:578:HOH:O	1.82	0.79
2:C:457:ALA:HB3	2:C:538:GLN:HA	1.65	0.78
2:C:675:ALA:HB2	2:C:867:VAL:HG11	1.64	0.78
4:E:54:LEU:HG	4:E:58:PRO:HG2	1.65	0.78
2:M:148:PHE:HZ	2:M:281:LEU:HD13	1.47	0.78
2:M:630:ARG:NH1	2:M:707:ARG:H	1.81	0.78
3:N:546:ARG:O	3:N:550:ARG:HG2	1.81	0.78
1:K:150:TYR:CE1	2:M:696:LYS:HA	2.19	0.78
1:K:206:THR:HG22	1:K:209:GLU:HG3	1.64	0.78
3:N:798:GLU:HB2	3:N:828:LYS:HE3	1.65	0.78
3:N:1273:VAL:HG22	3:N:1326:THR:OG1	1.84	0.78
2:C:256:TYR:CE1	2:C:293:PHE:HB2	2.18	0.78
2:C:474:VAL:HG11	2:C:529:VAL:HG12	1.64	0.78
2:M:571:LEU:HD21	2:M:700:TYR:HD2	1.47	0.78
3:N:493:ARG:HD2	3:N:1390:LEU:O	1.83	0.78
3:N:592:THR:H	3:N:600:LEU:HD21	1.47	0.78
4:O:46:PRO:HB3	4:O:54:LEU:HD22	1.64	0.78
2:M:413:LEU:H	2:M:413:LEU:HD12	1.48	0.78
3:N:630:VAL:HA	3:N:744:GLN:HG2	1.64	0.78
3:D:908:LYS:HB3	3:D:1027:GLY:HA3	1.64	0.78
3:D:1277:ILE:HD12	3:D:1301:LYS:HB2	1.65	0.78
5:F:85:LEU:HA	5:F:88:ILE:HD12	1.66	0.78
1:L:58:ILE:HG22	1:L:137:ARG:HH21	1.48	0.78
3:N:55:ASP:HB3	9:N:1551:HOH:O	1.84	0.78
1:A:88:ARG:HA	9:A:344:HOH:O	1.82	0.78
2:C:578:VAL:HG23	2:C:579:VAL:HG12	1.64	0.78
3:D:1198:TYR:HA	9:D:2099:HOH:O	1.83	0.78
2:M:862:PRO:HA	2:M:975:TYR:CE1	2.19	0.78
2:C:100:LEU:HD23	2:C:368:THR:HA	1.66	0.78
4:E:31:LEU:HD21	4:E:60:ALA:HB2	1.65	0.78
5:P:130:VAL:HG21	5:P:159:ILE:HG21	1.65	0.78
1:B:41:ARG:HG3	1:B:177:VAL:HG21	1.64	0.78
1:B:221:HIS:HA	1:B:224:TYR:HD2	1.46	0.78
2:C:178:PRO:HA	9:C:1213:HOH:O	1.82	0.78
2:C:470:PRO:HB2	2:C:534:VAL:HG21	1.65	0.78
3:N:572:ARG:HH12	5:P:79:ASP:CG	1.92	0.78
3:N:1312:LEU:HB2	9:N:2368:HOH:O	1.84	0.78
2:C:312:ALA:HB1	2:C:318:PRO:HG2	1.65	0.77
2:M:12:VAL:HG12	2:M:534:VAL:HG13	1.64	0.77
3:N:1291:SER:HB2	3:N:1293:PHE:HE1	1.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:PHE:HB2	9:B:398:HOH:O	1.84	0.77
3:D:610:LYS:CD	7:D:1527:MXP:H15B	2.06	0.77
3:N:116:LEU:HD22	3:N:118:LEU:HD11	1.67	0.77
2:C:1083:GLU:HG2	9:D:1751:HOH:O	1.82	0.77
2:M:797:GLY:HA2	9:M:1828:HOH:O	1.83	0.77
1:A:186:LEU:HB2	1:A:192:LEU:HD11	1.67	0.77
3:D:116:LEU:HD21	3:D:464:LEU:HB3	1.66	0.77
3:D:615:ARG:O	3:D:617:ASN:N	2.17	0.77
1:A:9:PRO:HB2	1:B:224:TYR:HB3	1.67	0.77
3:D:403:PHE:HD1	3:D:405:ASP:O	1.67	0.77
2:C:157:ARG:HD2	2:C:314:THR:HG22	1.67	0.77
2:C:163:ILE:HB	2:C:171:TRP:CH2	2.18	0.77
2:C:597:ALA:HB2	2:C:655:LEU:HD21	1.64	0.77
2:M:115:LEU:HD22	2:M:373:VAL:HG11	1.64	0.77
2:M:565:GLN:HG2	2:M:995:MET:HE1	1.67	0.77
3:N:32:ILE:HG22	5:P:258:ILE:HD12	1.66	0.77
2:C:766:GLU:HG2	2:C:772:ARG:HH12	1.50	0.77
3:D:400:VAL:CG2	3:D:443:VAL:HG21	2.15	0.77
2:M:87:ASP:HA	9:M:1651:HOH:O	1.83	0.77
2:M:512:ARG:HD3	2:M:523:ILE:HD11	1.65	0.77
3:D:1495:ILE:HG12	4:E:80:VAL:HG11	1.66	0.77
5:F:132:ARG:HG2	5:F:181:GLU:OE1	1.85	0.77
2:M:1115:LEU:HD23	3:N:85:VAL:HG13	1.65	0.77
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.67	0.77
3:D:1389:LEU:HD12	3:D:1390:LEU:H	1.49	0.77
2:M:431:HIS:HB3	2:M:434:HIS:HD2	1.48	0.77
3:N:1223:ILE:H	3:N:1223:ILE:HD12	1.49	0.77
5:P:142:ARG:HD2	9:P:502:HOH:O	1.85	0.77
5:P:144:ILE:HB	5:P:145:PRO:HD3	1.67	0.77
2:C:760:SER:HA	9:C:1430:HOH:O	1.85	0.76
3:D:135:LEU:HD23	9:D:1592:HOH:O	1.86	0.76
2:M:1019:GLN:HE22	3:N:621:LYS:HA	1.49	0.76
3:D:108:VAL:HB	3:D:109:PRO:HD3	1.66	0.76
3:D:630:VAL:HA	3:D:744:GLN:HG2	1.65	0.76
3:D:1112:CYS:HB2	3:D:1195:GLN:HG2	1.67	0.76
3:N:654:LYS:HB3	3:N:655:PRO:HD3	1.66	0.76
3:D:478:LEU:HD21	3:D:500:ARG:NH2	2.01	0.76
3:D:1191:PRO:HA	9:D:1762:HOH:O	1.86	0.76
2:C:468:ARG:HB2	2:C:486:MET:O	1.85	0.76
2:C:1103:ASP:OD1	3:D:3:LYS:HB2	1.85	0.76
3:D:1057:VAL:HG13	3:D:1069:GLU:HB3	1.65	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:60:ASP:HB2	1:L:137:ARG:CZ	2.16	0.76
3:N:611:GLN:HG2	3:N:619:LEU:HG	1.66	0.76
3:N:863:VAL:HG23	9:N:1635:HOH:O	1.85	0.76
3:D:152:LEU:HD23	3:D:152:LEU:H	1.50	0.76
3:D:1262:LEU:HD23	3:D:1352:ILE:HG13	1.66	0.76
5:F:260:ILE:HG23	5:F:264:MET:HB2	1.66	0.76
3:N:1040:GLY:O	3:N:1060:SER:HB3	1.85	0.76
2:M:914:ILE:HB	9:M:1825:HOH:O	1.85	0.76
2:C:862:PRO:HA	2:C:975:TYR:CE1	2.17	0.76
1:K:117:VAL:HB	1:K:120:VAL:HG12	1.66	0.76
3:N:489:ARG:NH2	3:N:1389:LEU:HD21	2.00	0.76
3:N:1041:LEU:HD12	3:N:1058:ARG:HA	1.68	0.76
3:D:544:TYR:O	3:D:548:ILE:HG12	1.85	0.76
5:F:144:ILE:HB	5:F:145:PRO:HD3	1.68	0.76
3:N:850:LEU:H	3:N:850:LEU:HD12	1.48	0.76
5:F:139:ALA:HA	5:F:152:ASP:CG	2.11	0.76
1:K:103:ALA:HB1	1:K:107:LYS:HE2	1.67	0.76
3:N:1422:MET:HE2	3:N:1427:SER:HA	1.68	0.76
2:C:108:ILE:HB	2:C:368:THR:OG1	1.86	0.76
2:C:260:LEU:HB2	2:C:291:ALA:HB1	1.66	0.76
2:C:905:ILE:HD12	2:C:905:ILE:H	1.50	0.76
3:D:28:LYS:HG3	3:D:41:ARG:HH11	1.50	0.76
3:D:1205:TYR:CD2	3:D:1215:VAL:HG21	2.21	0.76
3:N:608:SER:HA	3:N:1443:THR:HG21	1.66	0.76
3:N:1094:LEU:O	3:N:1098:LEU:HD13	1.86	0.76
3:N:1495:ILE:HG12	4:O:80:VAL:HG11	1.66	0.76
4:O:31:LEU:HD21	4:O:60:ALA:HB2	1.67	0.76
5:F:155:THR:O	5:F:159:ILE:HG12	1.86	0.75
2:M:199:VAL:HG13	2:M:235:LEU:HG	1.66	0.75
3:N:400:VAL:CG2	3:N:443:VAL:HG21	2.17	0.75
3:N:637:LEU:HD21	3:N:642:CYS:HA	1.67	0.75
3:N:1062:ARG:HB2	9:N:1637:HOH:O	1.84	0.75
3:D:13:ALA:HA	9:D:1541:HOH:O	1.86	0.75
3:D:804:LEU:HB2	3:D:830:ALA:O	1.86	0.75
2:M:983:ILE:HG21	2:M:987:ILE:HD11	1.68	0.75
3:N:101:HIS:ND1	3:N:103:TRP:HB2	1.99	0.75
2:C:1081:VAL:HG21	2:C:1111:ILE:HG22	1.67	0.75
2:C:232:GLU:HA	2:C:235:LEU:HD12	1.67	0.75
2:M:163:ILE:HB	2:M:171:TRP:CH2	2.22	0.75
3:N:611:GLN:CD	3:N:619:LEU:HD21	2.12	0.75
3:N:661:MET:HE3	3:N:673:ALA:HB1	1.66	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:54:ILE:HG21	9:C:1578:HOH:O	1.86	0.75
2:M:534:VAL:HB	9:M:1660:HOH:O	1.87	0.75
2:M:18:LEU:HB2	2:M:590:ASP:HB3	1.69	0.75
3:N:100:ALA:HB2	3:N:513:ILE:CD1	2.16	0.75
5:P:155:THR:O	5:P:159:ILE:HG12	1.86	0.75
1:A:224:TYR:HB3	1:B:9:PRO:HB2	1.66	0.75
2:C:197:LEU:HD22	2:C:202:TYR:HD2	1.51	0.75
3:D:1040:GLY:O	3:D:1060:SER:HB3	1.86	0.75
2:M:129:ILE:HG12	2:M:386:PHE:HB3	1.68	0.75
2:M:671:ASN:HD22	2:M:671:ASN:N	1.83	0.75
2:M:691:SER:HB2	2:M:858:MET:SD	2.26	0.75
5:P:271:LEU:HG	5:P:295:MET:HE1	1.68	0.75
1:B:55:SER:HB3	1:B:143:ARG:HB3	1.68	0.75
3:D:508:ARG:HB3	9:D:1761:HOH:O	1.86	0.75
3:D:614:PHE:C	3:D:615:ARG:O	2.26	0.75
3:D:850:LEU:HD12	3:D:850:LEU:H	1.49	0.75
5:F:87:GLU:O	5:F:91:VAL:HG23	1.85	0.75
2:C:325:ILE:HG23	9:C:1315:HOH:O	1.86	0.75
2:M:1090:LYS:HD2	3:N:90:MET:HE3	1.69	0.75
3:N:611:GLN:HE22	7:N:1527:MXP:H16B	1.50	0.75
5:P:132:ARG:O	5:P:136:LEU:HG	1.87	0.75
1:B:34:VAL:HG22	1:B:181:VAL:HG21	1.68	0.74
4:E:45:ARG:HE	4:E:55:PHE:HD2	1.33	0.74
3:N:611:GLN:HG2	3:N:619:LEU:CG	2.17	0.74
3:D:458:ALA:HB1	3:D:513:ILE:HD12	1.67	0.74
5:F:130:VAL:HG21	5:F:159:ILE:HG21	1.68	0.74
3:N:171:LEU:HG	9:N:1934:HOH:O	1.86	0.74
3:N:1101:VAL:HG22	3:N:1428:ALA:HB2	1.70	0.74
3:N:1420:LEU:HD12	3:N:1421:LEU:H	1.51	0.74
2:C:979:THR:HG23	2:C:981:GLU:H	1.52	0.74
3:D:1045:MET:HB2	3:D:1072:ILE:HG22	1.70	0.74
2:C:101:ILE:HG23	2:C:107:LEU:HD22	1.69	0.74
3:N:890:VAL:HG11	3:N:922:LEU:HD13	1.70	0.74
2:C:1056:LYS:O	3:D:624:ASP:HB2	1.87	0.74
3:D:586:ARG:NH1	3:D:1444:THR:HG21	2.02	0.74
5:F:274:THR:O	5:F:278:LEU:HG	1.88	0.74
1:K:221:HIS:HA	1:K:224:TYR:CD2	2.22	0.74
3:N:1264:GLU:HG3	3:N:1424:VAL:HG12	1.69	0.74
1:A:206:THR:HG22	1:A:209:GLU:HG3	1.69	0.74
1:K:226:SER:O	1:K:228:PRO:HD3	1.88	0.74
3:N:1147:ARG:HB3	3:N:1188:VAL:HG21	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1273:VAL:HG22	3:D:1326:THR:OG1	1.88	0.74
1:L:221:HIS:HA	1:L:224:TYR:HD2	1.51	0.74
2:M:139:GLN:OE1	2:M:415:PRO:HD2	1.88	0.74
3:N:458:ALA:HB1	3:N:513:ILE:HD12	1.68	0.74
3:N:1324:PRO:HA	9:N:1761:HOH:O	1.87	0.74
3:D:171:LEU:HB2	3:D:391:ALA:O	1.86	0.74
9:M:2128:HOH:O	3:N:1047:LYS:HE2	1.86	0.74
5:P:101:GLU:HB3	5:P:105:LYS:HE3	1.69	0.74
2:M:431:HIS:HB3	2:M:434:HIS:CD2	2.23	0.74
3:N:489:ARG:HG3	3:N:1388:ARG:HH22	1.53	0.74
1:B:201:THR:HG22	1:B:203:GLY:H	1.53	0.73
2:C:683:ASN:HA	2:C:687:ALA:HB3	1.70	0.73
9:C:1263:HOH:O	5:F:331:ASP:HA	1.88	0.73
3:N:206:ARG:HH12	5:P:98:GLU:HA	1.50	0.73
1:K:42:ARG:HH21	2:M:857:ASP:CB	2.00	0.73
2:M:256:TYR:CE1	2:M:293:PHE:HB2	2.23	0.73
3:N:1209:LEU:HD23	3:N:1211:MET:SD	2.28	0.73
1:B:176:ARG:HH21	3:D:850:LEU:HD13	1.53	0.73
2:C:222:MET:HB3	9:C:1633:HOH:O	1.88	0.73
2:C:1014:SER:HB3	2:C:1017:THR:O	1.88	0.73
3:N:37:LEU:HB3	9:N:1894:HOH:O	1.88	0.73
2:C:191:PHE:CZ	2:C:196:LEU:HB2	2.22	0.73
3:D:569:ASN:HB3	5:F:214:GLN:NE2	2.03	0.73
5:F:400:ILE:HG22	9:F:568:HOH:O	1.88	0.73
3:D:677:LEU:HD11	9:D:2185:HOH:O	1.88	0.73
4:E:46:PRO:HB3	4:E:54:LEU:HD22	1.71	0.73
1:K:22:GLU:HB3	9:K:1055:HOH:O	1.88	0.73
2:M:143:SER:HB2	2:M:276:LYS:HZ3	1.53	0.73
3:N:171:LEU:HB2	3:N:391:ALA:O	1.87	0.73
3:N:804:LEU:HB2	3:N:830:ALA:O	1.87	0.73
2:C:818:GLY:HA2	5:F:309:LYS:HZ3	1.53	0.73
2:C:1008:ARG:HD2	2:C:1028:GLY:H	1.53	0.73
5:F:394:ARG:CZ	5:F:398:ARG:HB2	2.19	0.73
2:M:169:GLY:HA2	2:M:263:ASP:CB	2.19	0.73
2:C:654:LEU:HD11	2:C:663:ASN:ND2	2.03	0.73
3:D:477:LEU:HD11	3:D:495:ARG:HD3	1.69	0.73
1:L:213:GLN:O	1:L:217:ILE:HD12	1.88	0.73
1:B:60:ASP:HB2	1:B:137:ARG:CZ	2.19	0.73
2:C:109:LYS:HE2	2:C:111:ASP:OD1	1.88	0.73
5:P:112:ALA:HA	5:P:173:TYR:HD2	1.54	0.73
1:A:226:SER:O	1:A:228:PRO:HD3	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:431:HIS:HB3	2:C:434:HIS:CD2	2.22	0.73
2:C:603:VAL:HG21	2:C:643:VAL:HG11	1.69	0.73
2:M:431:HIS:CD2	2:M:433:THR:H	2.07	0.73
5:P:132:ARG:HG2	5:P:181:GLU:CD	2.14	0.73
1:A:49:PRO:HB3	1:A:148:VAL:HG22	1.71	0.73
1:B:58:ILE:HG22	1:B:137:ARG:NH2	2.03	0.73
1:B:138:LEU:HD23	1:B:140:MET:SD	2.28	0.73
3:D:453:ASP:HB2	9:D:1592:HOH:O	1.87	0.73
2:M:232:GLU:HA	2:M:235:LEU:HD12	1.70	0.73
3:N:536:ALA:HA	5:P:315:VAL:O	1.88	0.73
2:C:42:VAL:HG12	2:C:43:GLY:H	1.54	0.72
2:C:943:VAL:HG23	2:C:985:GLY:H	1.54	0.72
2:C:1010:THR:HG21	5:F:341:PRO:HB2	1.69	0.72
3:D:80:VAL:HG23	9:D:1536:HOH:O	1.87	0.72
2:M:140:ILE:HA	2:M:332:ARG:O	1.88	0.72
2:M:256:TYR:HE1	2:M:293:PHE:HB2	1.52	0.72
1:B:36:LEU:O	1:B:39:PRO:HD2	1.90	0.72
2:M:738:ASP:HB2	2:M:744:ARG:HB3	1.70	0.72
5:P:260:ILE:HG23	5:P:264:MET:HB2	1.69	0.72
2:C:140:ILE:HD11	2:C:412:ALA:HA	1.71	0.72
2:C:1087:VAL:HG13	3:D:610:LYS:HZ1	1.54	0.72
3:D:705:ALA:HB3	3:D:706:PRO:HD3	1.70	0.72
5:F:394:ARG:HA	5:F:397:ILE:HD12	1.69	0.72
1:K:67:THR:CG2	2:M:609:ASN:HD21	1.98	0.72
1:L:80:LEU:HD12	9:L:3794:HOH:O	1.88	0.72
2:C:115:LEU:HD22	2:C:373:VAL:HG11	1.70	0.72
2:C:276:LYS:HB3	9:C:1337:HOH:O	1.87	0.72
2:M:139:GLN:NE2	2:M:418:LEU:HD22	2.04	0.72
2:M:437:ARG:NH2	2:M:488:ALA:HA	2.05	0.72
2:M:471:TYR:CD1	2:M:486:MET:HE2	2.25	0.72
2:M:549:PHE:HB3	2:M:552:HIS:HD2	1.54	0.72
5:P:260:ILE:HD11	5:P:310:ILE:HG22	1.71	0.72
1:A:150:TYR:HE2	1:A:152:PRO:HG3	1.54	0.72
2:C:274:ARG:HD2	2:C:285:LEU:O	1.90	0.72
2:C:768:THR:HB	2:C:771:GLU:HB3	1.71	0.72
2:C:904:PRO:HD2	2:C:908:GLY:HA2	1.72	0.72
3:D:400:VAL:HG12	9:D:2306:HOH:O	1.87	0.72
3:D:806:PHE:CE1	3:D:813:LEU:HB3	2.25	0.72
2:M:191:PHE:HZ	2:M:196:LEU:HB2	1.53	0.72
2:M:958:THR:HA	9:M:1887:HOH:O	1.89	0.72
3:N:570:GLU:N	5:P:214:GLN:HE22	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:808:THR:HB	3:N:809:PRO:HD3	1.70	0.72
2:C:352:ALA:O	2:C:356:ARG:HG3	1.89	0.72
2:C:1044:GLY:HA3	4:E:17:TYR:CE1	2.24	0.72
2:M:1115:LEU:HB3	3:N:85:VAL:HG13	1.71	0.72
3:N:1393:GLN:HB2	3:N:1398:TRP:NE1	2.04	0.72
5:P:92:PRO:HB3	9:P:672:HOH:O	1.88	0.72
2:C:305:PRO:HA	2:C:308:ARG:HB2	1.70	0.72
1:A:10:VAL:HG12	1:A:12:THR:HG22	1.70	0.72
2:C:952:LEU:HD12	2:C:969:GLN:NE2	2.04	0.72
3:D:810:GLU:O	3:D:813:LEU:HG	1.88	0.72
3:N:1152:GLU:CD	3:N:1159:ARG:HH12	1.97	0.72
2:C:603:VAL:HG12	9:C:1531:HOH:O	1.90	0.72
3:D:546:ARG:O	3:D:550:ARG:HG2	1.90	0.72
1:L:123:MET:C	1:L:125:PRO:HD3	2.15	0.72
2:M:683:ASN:HA	2:M:687:ALA:HB3	1.71	0.72
1:B:97:VAL:HG11	1:B:120:VAL:HG21	1.72	0.71
3:D:206:ARG:HH12	5:F:98:GLU:CA	2.03	0.71
3:D:1377:LYS:HA	9:D:2039:HOH:O	1.89	0.71
5:F:218:GLN:HA	5:F:221:ILE:HD12	1.69	0.71
2:M:305:PRO:HA	2:M:308:ARG:HB2	1.70	0.71
2:M:535:SER:HB2	2:M:537:LYS:HE3	1.72	0.71
5:P:132:ARG:HD2	9:P:505:HOH:O	1.89	0.71
2:C:630:ARG:HA	9:C:1414:HOH:O	1.90	0.71
2:C:654:LEU:HD11	2:C:663:ASN:HD22	1.56	0.71
1:K:18:ARG:HD2	1:K:123:MET:HE1	1.72	0.71
1:K:28:LEU:HD12	9:K:2517:HOH:O	1.88	0.71
2:M:31:GLN:HB3	2:M:71:TYR:OH	1.90	0.71
2:M:408:ARG:HH21	2:M:542:VAL:HG22	1.55	0.71
3:N:406:ASP:HB3	5:P:168:LYS:HE2	1.70	0.71
4:O:45:ARG:HG2	9:O:1147:HOH:O	1.90	0.71
2:C:147:TYR:HE2	2:C:280:LYS:HZ3	1.37	0.71
3:D:1239:ARG:HG3	9:D:2068:HOH:O	1.91	0.71
3:N:705:ALA:HB3	3:N:706:PRO:HD3	1.73	0.71
5:P:204:GLY:HA3	9:P:572:HOH:O	1.89	0.71
1:K:150:TYR:HE1	2:M:696:LYS:HA	1.54	0.71
2:M:461:VAL:HG13	2:M:465:GLY:HA2	1.71	0.71
2:M:569:VAL:HG12	2:M:996:LYS:O	1.89	0.71
3:N:1210:SER:HA	9:N:1732:HOH:O	1.90	0.71
1:B:61:VAL:HG23	1:B:137:ARG:HH22	1.56	0.71
2:C:713:ARG:NH2	3:D:531:ASP:HB3	2.06	0.71
5:F:88:ILE:HG21	5:F:193:ARG:HD3	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:83:LYS:HE2	1:L:168:ASP:HB2	1.71	0.71
1:A:221:HIS:HA	1:A:224:TYR:HD2	1.55	0.71
2:C:685:GLU:N	9:C:1222:HOH:O	2.23	0.71
2:M:298:PHE:HA	9:M:2058:HOH:O	1.90	0.71
2:C:724:ARG:HG2	2:C:734:LEU:HD23	1.73	0.71
2:C:738:ASP:HB2	2:C:744:ARG:HB3	1.71	0.71
3:N:86:ARG:O	3:N:522:PRO:HD2	1.91	0.71
2:C:157:ARG:HA	9:C:1318:HOH:O	1.90	0.71
2:C:671:ASN:HD22	2:C:671:ASN:H	1.36	0.71
2:C:139:GLN:HE22	2:C:415:PRO:HD2	1.56	0.71
3:D:105:VAL:HG21	3:D:128:TYR:HE2	1.55	0.71
3:D:894:LYS:HA	9:D:1776:HOH:O	1.91	0.71
5:F:151:LEU:O	5:F:155:THR:HB	1.90	0.71
2:M:420:ARG:HB2	9:M:1926:HOH:O	1.90	0.71
2:M:1021:LEU:HD21	5:P:332:PHE:O	1.91	0.71
3:N:611:GLN:O	3:N:1439:SER:O	2.09	0.71
3:D:574:LEU:O	3:D:578:VAL:HG23	1.90	0.71
2:M:428:ARG:HE	2:M:451:LEU:HD21	1.54	0.71
2:M:551:GLU:HG3	2:M:552:HIS:CD2	2.25	0.71
3:N:15:PRO:HB3	9:N:1827:HOH:O	1.90	0.71
3:N:574:LEU:O	3:N:578:VAL:HG23	1.91	0.71
1:A:35:THR:HG21	1:B:43:ILE:CD1	2.21	0.70
2:C:83:CYS:HA	2:C:88:LEU:HB3	1.73	0.70
3:D:131:LYS:HG2	3:D:568:ARG:HG2	1.72	0.70
1:L:56:VAL:HG13	1:L:142:VAL:HG12	1.73	0.70
2:M:514:VAL:HB	9:M:2025:HOH:O	1.91	0.70
3:N:1472:ILE:HG22	3:N:1474:ALA:H	1.56	0.70
1:A:20:TYR:CE2	1:A:22:GLU:HG3	2.26	0.70
2:M:904:PRO:HD2	2:M:908:GLY:HA2	1.72	0.70
2:C:76:PRO:HB2	9:C:1121:HOH:O	1.91	0.70
3:D:185:VAL:HG22	3:D:191:LEU:HD21	1.71	0.70
2:M:12:VAL:HG21	2:M:472:ARG:HD3	1.74	0.70
2:M:716:LYS:HB2	9:M:2121:HOH:O	1.91	0.70
3:N:1161:GLU:HG3	3:N:1164:ARG:HB2	1.73	0.70
1:B:55:SER:CB	1:B:158:ILE:HD13	2.21	0.70
2:C:163:ILE:HD13	9:C:1347:HOH:O	1.90	0.70
3:D:696:HIS:HB2	4:E:48:MET:HE3	1.73	0.70
5:F:361:LEU:HD12	5:F:408:LEU:HD11	1.74	0.70
1:L:197:LEU:HD21	1:L:199:ILE:HD11	1.73	0.70
2:M:789:SER:HB2	9:M:1726:HOH:O	1.90	0.70
3:N:1215:VAL:HG13	9:N:1985:HOH:O	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:399:ASN:O	2:C:402:SER:HB2	1.92	0.70
2:M:889:HIS:HE1	3:N:951:ILE:H	1.37	0.70
2:M:890:LEU:HD12	2:M:914:ILE:HD13	1.71	0.70
3:N:1077:ALA:HA	9:N:1738:HOH:O	1.90	0.70
3:N:1481:VAL:HG11	4:O:18:ARG:HA	1.74	0.70
1:A:107:LYS:HG2	9:A:404:HOH:O	1.91	0.70
1:L:132:LEU:HD13	1:L:138:LEU:HD12	1.74	0.70
2:M:45:GLN:HA	9:M:1991:HOH:O	1.89	0.70
2:M:157:ARG:HD2	2:M:314:THR:HG22	1.72	0.70
3:N:785:ILE:HD13	3:N:935:LYS:HA	1.74	0.70
3:N:1205:TYR:CD2	3:N:1215:VAL:HG21	2.25	0.70
1:A:117:VAL:HB	1:A:120:VAL:HG12	1.72	0.70
1:B:85:LEU:HD12	1:B:124:ASN:HB3	1.72	0.70
2:C:156:GLY:HA3	9:C:1282:HOH:O	1.90	0.70
2:C:611:ILE:HD11	2:C:641:PRO:HG3	1.72	0.70
3:D:206:ARG:HH12	5:F:98:GLU:N	1.90	0.70
3:D:1422:MET:HE2	3:D:1427:SER:HA	1.74	0.70
2:M:83:CYS:HA	2:M:88:LEU:HB3	1.73	0.70
3:N:433:GLY:HA3	3:N:447:VAL:O	1.90	0.70
3:N:493:ARG:HH11	3:N:1390:LEU:C	1.99	0.70
2:C:3:ILE:HA	2:C:900:ARG:O	1.91	0.70
2:C:838:LYS:HE3	2:C:846:LYS:HE2	1.71	0.70
3:D:433:GLY:HA3	3:D:447:VAL:O	1.90	0.70
3:D:1101:VAL:HA	3:D:1428:ALA:HB2	1.72	0.70
1:K:186:LEU:HB2	1:K:192:LEU:HD11	1.73	0.70
2:M:163:ILE:HG13	2:M:163:ILE:O	1.91	0.70
2:M:855:VAL:HG12	9:M:1977:HOH:O	1.90	0.70
3:N:1147:ARG:HB3	3:N:1188:VAL:CG2	2.21	0.70
1:B:59:GLU:HG3	1:B:139:ASN:HD22	1.57	0.70
2:C:276:LYS:HD2	9:C:1736:HOH:O	1.90	0.70
2:C:676:ILE:HG23	2:C:676:ILE:O	1.91	0.70
3:D:105:VAL:HG21	3:D:128:TYR:CE2	2.27	0.70
3:D:1114:THR:H	3:D:1195:GLN:HE21	1.39	0.70
4:E:10:PHE:HE2	4:E:16:LYS:HG3	1.55	0.70
1:L:55:SER:CB	1:L:158:ILE:HD13	2.21	0.70
1:L:201:THR:HG22	1:L:203:GLY:H	1.55	0.70
2:M:191:PHE:HB2	2:M:241:LEU:HD13	1.74	0.70
2:M:1009:SER:HB2	3:N:651:GLU:O	1.91	0.70
1:A:221:HIS:HA	1:A:224:TYR:CD2	2.27	0.70
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.74	0.70
3:D:759:ALA:HA	3:D:763:MET:HE2	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1356:TYR:CD2	3:D:1363:LEU:HD23	2.27	0.70
1:L:148:VAL:HG22	9:L:3229:HOH:O	1.92	0.70
2:M:312:ALA:HB1	2:M:318:PRO:HG2	1.73	0.70
2:M:436:GLY:HA2	2:M:538:GLN:O	1.92	0.70
3:N:584:ASN:ND2	3:N:590:PRO:HD2	2.06	0.70
3:N:810:GLU:O	3:N:813:LEU:HG	1.92	0.70
3:N:1498:ALA:HB2	4:O:88:GLU:OE1	1.92	0.70
5:P:394:ARG:CZ	5:P:398:ARG:HB2	2.21	0.70
1:B:158:ILE:HD11	1:B:166:PRO:CA	2.22	0.69
2:C:139:GLN:NE2	2:C:415:PRO:HD2	2.07	0.69
3:D:73:CYS:HB3	3:D:76:CYS:O	1.92	0.69
3:D:1279:GLY:O	3:D:1318:TYR:HA	1.91	0.69
2:M:511:GLU:O	2:M:526:PRO:HD3	1.92	0.69
3:N:481:MET:HG3	3:N:1388:ARG:CZ	2.22	0.69
4:O:45:ARG:HD2	9:O:1011:HOH:O	1.92	0.69
2:C:572:ILE:HG13	9:C:1310:HOH:O	1.92	0.69
2:M:219:GLN:HG3	9:M:1965:HOH:O	1.90	0.69
3:D:607:LEU:O	3:D:610:LYS:HB2	1.92	0.69
1:K:50:GLY:HA3	1:K:173:PRO:HG3	1.74	0.69
2:M:578:VAL:HG23	2:M:579:VAL:HG12	1.73	0.69
3:N:10:ILE:HG13	3:N:1434:TRP:CZ2	2.27	0.69
3:N:680:GLN:HB2	9:N:2087:HOH:O	1.92	0.69
9:N:2060:HOH:O	5:P:147:LEU:HD21	1.91	0.69
4:O:45:ARG:HB2	4:O:46:PRO:HD2	1.74	0.69
1:B:221:HIS:HA	1:B:224:TYR:CD2	2.26	0.69
2:C:307:LEU:HG	2:C:311:PHE:HE2	1.57	0.69
3:D:611:GLN:HB2	7:D:1527:MXP:H11A	1.73	0.69
3:D:1243:THR:OG1	3:D:1253:THR:HB	1.92	0.69
5:F:279:GLN:HA	9:F:487:HOH:O	1.91	0.69
5:F:358:LEU:HD21	5:F:370:LYS:HZ2	1.57	0.69
1:K:24:VAL:HG22	1:K:196:THR:HB	1.74	0.69
1:K:184:THR:HG23	1:K:192:LEU:HB2	1.74	0.69
3:N:705:ALA:CB	3:N:706:PRO:HD3	2.22	0.69
5:P:367:MET:HB2	9:P:493:HOH:O	1.92	0.69
2:C:276:LYS:O	2:C:280:LYS:HB2	1.93	0.69
3:D:795:VAL:HG11	3:D:863:VAL:HG13	1.73	0.69
1:K:7:LYS:NZ	1:K:186:LEU:HD21	2.07	0.69
3:N:1274:ILE:HD11	3:N:1334:GLN:NE2	2.08	0.69
1:A:58:ILE:HG21	1:A:68:ILE:HD11	1.75	0.69
1:B:158:ILE:HG22	1:B:160:ASP:H	1.56	0.69
2:C:139:GLN:OE1	2:C:415:PRO:HD2	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:436:GLY:HA2	2:C:538:GLN:O	1.92	0.69
2:C:603:VAL:HG13	9:C:1654:HOH:O	1.93	0.69
2:C:732:ALA:HB3	9:C:1588:HOH:O	1.93	0.69
3:N:1086:LEU:HB2	9:N:2385:HOH:O	1.91	0.69
4:E:47:LYS:HA	9:E:150:HOH:O	1.93	0.69
5:F:171:LYS:HD3	9:F:640:HOH:O	1.91	0.69
1:K:183:ASP:HB3	9:K:3288:HOH:O	1.93	0.69
2:M:143:SER:HB2	2:M:276:LYS:NZ	2.07	0.69
2:M:838:LYS:HE3	2:M:846:LYS:HE2	1.72	0.69
3:N:1001:GLU:HG2	9:N:2222:HOH:O	1.93	0.69
5:P:160:ASP:HA	5:P:163:LEU:HD12	1.73	0.69
5:P:166:LEU:O	5:P:171:LYS:HB2	1.93	0.69
2:C:909:ALA:HB1	9:C:1225:HOH:O	1.92	0.69
3:D:654:LYS:HB3	3:D:655:PRO:HD3	1.73	0.69
5:F:392:VAL:HG12	9:F:496:HOH:O	1.92	0.69
1:K:9:PRO:HD2	1:L:224:TYR:CD1	2.27	0.69
2:M:141:HIS:HB3	2:M:418:LEU:HG	1.75	0.69
2:M:311:PHE:HB3	9:M:1792:HOH:O	1.92	0.69
2:M:352:ALA:O	2:M:356:ARG:HG3	1.93	0.69
2:M:468:ARG:HB2	2:M:486:MET:O	1.92	0.69
2:M:905:ILE:H	2:M:905:ILE:HD12	1.57	0.69
3:N:149:LYS:HG3	9:N:2241:HOH:O	1.91	0.69
3:N:675:ARG:NH1	5:P:421:PHE:HD2	1.90	0.69
3:N:877:PRO:O	3:N:880:ILE:HG22	1.93	0.69
3:N:1095:THR:O	3:N:1099:VAL:HG23	1.91	0.69
5:P:85:LEU:HA	5:P:88:ILE:HD12	1.74	0.69
1:A:58:ILE:HB	1:A:61:VAL:HB	1.75	0.69
2:C:86:LYS:HD3	2:C:813:VAL:HG12	1.74	0.69
2:C:218:VAL:HG22	2:C:221:LEU:HD23	1.75	0.69
2:C:541:SER:HB2	9:C:1523:HOH:O	1.93	0.69
3:D:799:LYS:H	3:D:826:PRO:HG2	1.58	0.69
4:E:33:HIS:HB2	4:E:37:ASN:HD21	1.58	0.69
2:M:139:GLN:HE22	2:M:415:PRO:HG2	1.56	0.69
2:M:343:GLN:HG2	2:M:385:PHE:HB2	1.75	0.69
2:M:521:PRO:HG3	3:N:1068:LEU:HD23	1.75	0.69
2:M:751:PRO:HG3	2:M:795:GLY:O	1.92	0.69
3:N:484:PRO:HB3	9:N:1630:HOH:O	1.91	0.69
1:A:97:VAL:HG23	9:A:349:HOH:O	1.92	0.69
2:C:176:VAL:HG12	2:C:182:VAL:HG13	1.73	0.69
2:C:396:ASP:HA	2:C:633:GLN:NE2	2.08	0.69
3:D:584:ASN:ND2	3:D:590:PRO:HD2	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:28:ARG:NH1	2:M:463:GLU:HG2	2.07	0.69
3:N:124:GLU:O	3:N:128:TYR:HB2	1.93	0.69
1:A:111:ALA:HB2	1:A:127:LEU:HG	1.75	0.68
2:C:634:GLY:HA3	9:C:1157:HOH:O	1.92	0.68
3:D:206:ARG:HH12	5:F:98:GLU:HA	1.57	0.68
1:K:69:PRO:HB3	9:M:1747:HOH:O	1.93	0.68
3:N:36:THR:HA	9:N:2104:HOH:O	1.93	0.68
3:N:1354:LYS:HA	9:N:1826:HOH:O	1.92	0.68
4:O:46:PRO:HD2	9:O:1011:HOH:O	1.92	0.68
1:B:58:ILE:HB	1:B:61:VAL:HB	1.73	0.68
2:C:399:ASN:HB3	2:C:568:ALA:O	1.93	0.68
3:D:29:PRO:HG2	3:D:549:ASN:ND2	2.07	0.68
3:D:483:HIS:HB2	3:D:484:PRO:HD3	1.75	0.68
4:E:17:TYR:O	4:E:21:VAL:HG23	1.92	0.68
2:M:575:GLN:OE1	2:M:670:GLN:HB3	1.93	0.68
2:M:838:LYS:HE3	2:M:997:LEU:HD12	1.75	0.68
3:N:428:LYS:HD3	9:N:2334:HOH:O	1.93	0.68
3:N:646:LYS:HE2	3:N:722:GLU:HG2	1.75	0.68
3:N:1146:GLY:HA3	3:N:1207:TYR:HB2	1.74	0.68
3:N:1162:GLU:HB3	9:N:1922:HOH:O	1.92	0.68
3:N:1264:GLU:CD	3:N:1425:THR:HB	2.19	0.68
5:P:87:GLU:O	5:P:91:VAL:HG23	1.92	0.68
3:D:1472:ILE:HG22	3:D:1474:ALA:H	1.58	0.68
1:L:101:LEU:HG	9:L:2708:HOH:O	1.91	0.68
3:N:555:LYS:HB3	9:N:1956:HOH:O	1.93	0.68
3:N:1112:CYS:HB2	3:N:1195:GLN:HG2	1.75	0.68
3:N:1317:ASP:HB2	9:N:1639:HOH:O	1.93	0.68
4:O:45:ARG:HE	4:O:55:PHE:HD2	1.40	0.68
1:B:52:ALA:HB2	1:B:170:VAL:O	1.93	0.68
2:C:73:LEU:HD22	2:C:118:ILE:HD11	1.75	0.68
1:L:97:VAL:HG11	1:L:120:VAL:HG21	1.73	0.68
2:M:69:LEU:HB2	2:M:97:ARG:HB2	1.76	0.68
3:N:403:PHE:HD1	3:N:405:ASP:O	1.76	0.68
3:N:523:ASP:HB3	9:N:1572:HOH:O	1.93	0.68
2:C:256:TYR:HE1	2:C:293:PHE:HB2	1.57	0.68
2:C:811:PRO:HB2	2:C:813:VAL:HG13	1.74	0.68
5:F:88:ILE:HD13	5:F:193:ARG:HD2	1.75	0.68
2:M:750:LYS:HD3	9:N:2087:HOH:O	1.93	0.68
3:N:119:SER:H	3:N:123:LEU:HD22	1.56	0.68
1:B:109:VAL:HG21	1:B:138:LEU:CD1	2.19	0.68
2:C:619:ARG:HG2	9:C:1584:HOH:O	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1107:ASN:HB3	9:C:1226:HOH:O	1.94	0.68
3:D:565:ILE:HD12	5:F:192:LEU:HD13	1.75	0.68
5:P:248:ASN:HA	5:P:251:ILE:HD12	1.74	0.68
1:B:213:GLN:O	1:B:217:ILE:HD12	1.94	0.68
2:C:299:LYS:HB3	9:C:1267:HOH:O	1.94	0.68
3:D:704:ARG:HG2	3:D:705:ALA:H	1.57	0.68
5:F:147:LEU:HB2	9:F:2238:HOH:O	1.94	0.68
3:N:46:ASP:OD2	3:N:48:ARG:HG2	1.94	0.68
3:N:607:LEU:O	3:N:610:LYS:HB2	1.93	0.68
3:N:610:LYS:HB3	9:N:1557:HOH:O	1.94	0.68
5:P:77:THR:O	5:P:81:VAL:HG23	1.93	0.68
2:C:554:ASP:OD2	2:C:556:ASN:HB3	1.91	0.68
3:D:153:LEU:HD11	3:D:158:TYR:N	2.09	0.68
3:D:1239:ARG:HB2	9:D:2065:HOH:O	1.94	0.68
5:F:129:GLU:HG2	9:F:492:HOH:O	1.93	0.68
1:L:158:ILE:HG13	1:L:166:PRO:HB3	1.76	0.68
2:M:108:ILE:HB	2:M:368:THR:OG1	1.94	0.68
2:M:571:LEU:HD21	2:M:700:TYR:CD2	2.29	0.68
3:N:614:PHE:C	3:N:615:ARG:O	2.33	0.68
3:N:672:ALA:HB1	9:N:1656:HOH:O	1.93	0.68
1:A:100:LEU:HB2	1:A:115:LEU:HD11	1.76	0.68
1:A:136:GLY:HA3	9:A:320:HOH:O	1.93	0.68
2:C:145:GLY:O	2:C:163:ILE:HG23	1.93	0.68
3:D:162:ARG:HA	3:D:449:SER:CB	2.24	0.68
1:K:133:GLU:HG2	1:K:134:GLU:N	2.07	0.68
1:L:128:HIS:HB2	9:L:3368:HOH:O	1.93	0.68
2:M:148:PHE:CZ	2:M:281:LEU:HD13	2.29	0.68
3:N:535:PHE:O	5:P:315:VAL:N	2.26	0.68
5:P:133:ALA:HA	9:P:567:HOH:O	1.92	0.68
5:P:218:GLN:HA	5:P:221:ILE:HD12	1.75	0.68
2:C:578:VAL:HG13	2:C:671:ASN:OD1	1.93	0.68
2:C:599:GLU:HG3	2:C:600:ASP:H	1.59	0.68
2:C:815:LEU:HD13	9:C:1286:HOH:O	1.94	0.68
2:C:874:LEU:HD12	3:D:784:ASP:OD2	1.94	0.68
2:C:915:LYS:HE3	9:C:1136:HOH:O	1.94	0.68
2:C:1096:ALA:O	3:D:13:ALA:HB2	1.94	0.68
3:D:723:GLY:HA3	9:D:1680:HOH:O	1.94	0.68
5:F:160:ASP:HA	5:F:163:LEU:HD12	1.75	0.68
2:M:492:ASP:HA	9:M:1901:HOH:O	1.92	0.68
3:N:108:VAL:HG21	9:N:2073:HOH:O	1.94	0.68
5:P:368:VAL:HG22	9:P:506:HOH:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ARG:HB2	1:A:200:TRP:CZ3	2.29	0.67
1:B:158:ILE:HG13	1:B:166:PRO:HB3	1.76	0.67
2:C:333:ILE:HD13	2:C:467:ILE:HG13	1.76	0.67
3:D:586:ARG:HH12	3:D:1444:THR:HG21	1.58	0.67
2:M:145:GLY:O	2:M:163:ILE:HG23	1.94	0.67
3:N:1430:SER:HA	9:N:2035:HOH:O	1.92	0.67
2:C:339:LEU:HD11	9:C:1322:HOH:O	1.94	0.67
3:D:805:GLU:HG3	9:D:1779:HOH:O	1.93	0.67
3:D:1146:GLY:HA3	3:D:1207:TYR:HB2	1.76	0.67
2:M:93:PRO:HG3	2:M:117:HIS:CE1	2.29	0.67
2:M:292:ARG:HB3	9:M:2058:HOH:O	1.93	0.67
3:N:611:GLN:NE2	7:N:1527:MXP:H16B	2.09	0.67
3:N:1476:THR:HG23	4:O:21:VAL:HG22	1.75	0.67
4:O:9:LEU:HB3	4:O:19:LEU:HD21	1.76	0.67
4:O:88:GLU:HG3	9:O:2559:HOH:O	1.93	0.67
1:A:103:ALA:CB	1:A:107:LYS:HE2	2.24	0.67
2:C:914:ILE:HB	9:C:1225:HOH:O	1.93	0.67
2:C:983:ILE:HG21	2:C:987:ILE:HD11	1.75	0.67
1:L:180:GLN:HB3	9:L:1094:HOH:O	1.95	0.67
2:M:283:ILE:HD11	9:M:2124:HOH:O	1.95	0.67
2:M:445:GLU:HG2	9:M:1876:HOH:O	1.94	0.67
2:M:660:ALA:HB1	2:M:667:ALA:O	1.93	0.67
2:M:793:PRO:HD2	9:M:2061:HOH:O	1.93	0.67
2:M:966:LEU:HD11	2:M:986:PRO:HG2	1.74	0.67
3:N:130:SER:HB3	3:N:132:TYR:CE1	2.30	0.67
3:N:483:HIS:HB2	3:N:484:PRO:HD3	1.77	0.67
3:N:658:LEU:O	3:N:661:MET:HB2	1.94	0.67
3:N:1243:THR:OG1	3:N:1253:THR:HB	1.94	0.67
5:F:408:LEU:O	5:F:412:GLU:HG2	1.95	0.67
1:K:10:VAL:HG12	1:K:12:THR:HG22	1.77	0.67
2:M:979:THR:HG23	2:M:981:GLU:H	1.59	0.67
3:N:28:LYS:HG3	3:N:41:ARG:HH11	1.59	0.67
3:N:956:ILE:HG12	3:N:1039:CYS:O	1.95	0.67
2:M:318:PRO:HA	9:M:1903:HOH:O	1.94	0.67
3:N:544:TYR:O	3:N:548:ILE:HG12	1.93	0.67
4:O:48:MET:O	4:O:52:GLU:HA	1.94	0.67
5:P:408:LEU:O	5:P:412:GLU:HG2	1.93	0.67
5:F:361:LEU:HD23	5:F:362:SER:H	1.58	0.67
2:M:724:ARG:HG2	2:M:734:LEU:HD23	1.77	0.67
3:N:141:ILE:CG2	3:N:450:TYR:H	2.08	0.67
3:N:185:VAL:HG23	3:N:202:VAL:C	2.18	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:268:ILE:HD13	5:P:311:ALA:HB2	1.77	0.67
2:C:551:GLU:HG3	2:C:552:HIS:CD2	2.30	0.67
2:C:944:LEU:HD21	2:C:963:LEU:HD23	1.77	0.67
3:D:809:PRO:HB2	3:D:812:ALA:HB2	1.76	0.67
3:D:906:GLN:HB3	3:D:911:LEU:CD1	2.24	0.67
3:D:1041:LEU:HD12	3:D:1058:ARG:HA	1.77	0.67
1:L:61:VAL:HG23	1:L:137:ARG:HH22	1.59	0.67
3:N:764:LEU:HD23	3:N:767:HIS:ND1	2.10	0.67
3:N:1277:ILE:HA	9:N:1570:HOH:O	1.95	0.67
1:B:38:ASN:HB3	1:B:39:PRO:HD3	1.77	0.67
2:C:328:LEU:HD13	2:C:433:THR:HB	1.76	0.67
2:C:464:LEU:HG	9:C:1551:HOH:O	1.94	0.67
2:C:889:HIS:CD2	2:C:970:GLY:HA3	2.30	0.67
3:D:617:ASN:HB2	3:D:618:LEU:HD12	1.77	0.67
3:D:1432:LYS:HG2	9:D:1537:HOH:O	1.93	0.67
2:M:722:ILE:HG21	2:M:821:GLU:OE1	1.94	0.67
3:N:65:ARG:CG	3:N:66:GLN:H	2.07	0.67
3:N:508:ARG:HB3	9:N:1796:HOH:O	1.95	0.67
3:N:804:LEU:HD23	3:N:804:LEU:H	1.60	0.67
3:N:1220:ALA:HB1	3:N:1223:ILE:HD13	1.77	0.67
3:N:1279:GLY:O	3:N:1318:TYR:HA	1.94	0.67
1:A:48:ILE:HG22	1:A:173:PRO:HD2	1.75	0.67
1:B:60:ASP:H	1:B:137:ARG:NH2	1.92	0.67
2:C:244:PRO:HG2	2:C:246:ASP:OD2	1.95	0.67
3:D:637:LEU:HD21	3:D:642:CYS:HA	1.75	0.67
3:D:658:LEU:O	3:D:661:MET:HB2	1.95	0.67
5:F:191:ASN:HB3	5:F:220:LEU:HD11	1.76	0.67
1:K:123:MET:O	1:K:125:PRO:HD3	1.95	0.67
3:N:996:TRP:HA	3:N:999:THR:HG22	1.77	0.67
3:D:16:GLU:HA	9:D:2072:HOH:O	1.95	0.67
3:D:613:ARG:HB2	9:D:1834:HOH:O	1.95	0.67
3:D:785:ILE:HD13	3:D:935:LYS:HA	1.75	0.67
3:D:1481:VAL:HG11	4:E:18:ARG:HA	1.77	0.67
5:F:110:MET:HB2	9:F:483:HOH:O	1.94	0.67
1:K:46:SER:HB3	2:M:856:GLU:HG2	1.76	0.67
2:M:156:GLY:HA3	9:M:2199:HOH:O	1.95	0.67
2:M:770:GLU:HG2	9:M:2011:HOH:O	1.94	0.67
2:M:805:ARG:HG3	2:M:823:VAL:HG22	1.77	0.67
3:N:178:LEU:HD12	9:N:2234:HOH:O	1.94	0.67
3:N:556:LYS:HB3	5:P:218:GLN:HE22	1.59	0.67
5:P:295:MET:HG2	5:P:299:TRP:CD2	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:136:ILE:HG21	2:C:336:VAL:HG13	1.77	0.66
3:D:808:THR:HB	3:D:809:PRO:HD3	1.76	0.66
3:D:1094:LEU:O	3:D:1098:LEU:HD13	1.95	0.66
2:M:204:GLN:NE2	2:M:222:MET:HA	2.10	0.66
2:M:1108:PRO:HD3	9:M:2055:HOH:O	1.95	0.66
1:B:169:ALA:HB1	1:B:171:PHE:CD2	2.30	0.66
2:C:310:LEU:HD12	9:C:1562:HOH:O	1.94	0.66
2:C:397:GLU:HB2	9:C:1153:HOH:O	1.94	0.66
2:C:859:PRO:O	2:C:867:VAL:HG22	1.95	0.66
3:D:1410:GLU:OE2	3:D:1414:PRO:HG3	1.95	0.66
2:M:64:LEU:HD13	2:M:359:MET:HG3	1.76	0.66
2:M:1096:ALA:HB1	9:N:1592:HOH:O	1.94	0.66
3:N:188:GLY:N	3:N:199:LEU:HD23	2.11	0.66
3:N:1321:ALA:O	3:N:1339:LYS:HE3	1.96	0.66
3:D:107:ASP:O	3:D:108:VAL:C	2.37	0.66
3:D:609:GLY:O	3:D:617:ASN:ND2	2.28	0.66
3:D:705:ALA:CB	3:D:706:PRO:HD3	2.25	0.66
3:D:965:GLU:HB2	9:D:1794:HOH:O	1.96	0.66
4:E:48:MET:O	4:E:52:GLU:HA	1.96	0.66
2:M:909:ALA:HB1	9:M:1825:HOH:O	1.94	0.66
2:M:952:LEU:HD12	2:M:969:GLN:NE2	2.08	0.66
2:M:1096:ALA:O	3:N:13:ALA:HB2	1.95	0.66
1:B:78:ILE:HA	9:B:438:HOH:O	1.95	0.66
3:D:116:LEU:HD22	3:D:118:LEU:HD11	1.76	0.66
3:D:661:MET:HE3	3:D:673:ALA:HB1	1.77	0.66
3:D:805:GLU:HG2	9:D:1726:HOH:O	1.95	0.66
3:D:843:PHE:HE1	3:D:864:VAL:HG11	1.60	0.66
2:M:1:MET:HE2	9:M:2228:HOH:O	1.94	0.66
3:N:185:VAL:HG22	3:N:191:LEU:HD21	1.76	0.66
5:P:303:ARG:HB2	9:P:433:HOH:O	1.94	0.66
2:C:431:HIS:CD2	2:C:433:THR:H	2.13	0.66
2:C:693:GLU:HA	2:C:696:LYS:HG3	1.76	0.66
3:D:817:GLU:O	3:D:821:VAL:HG23	1.94	0.66
3:D:1147:ARG:HB3	3:D:1188:VAL:CG2	2.25	0.66
5:F:336:GLU:HA	9:F:469:HOH:O	1.94	0.66
3:N:82:LYS:HE2	9:N:1551:HOH:O	1.95	0.66
3:N:569:ASN:OD1	5:P:80:PRO:HB3	1.96	0.66
5:P:234:LYS:HG2	9:P:475:HOH:O	1.95	0.66
1:A:180:GLN:HB3	9:A:352:HOH:O	1.95	0.66
1:B:18:ARG:O	1:B:207:PRO:HD3	1.96	0.66
1:B:173:PRO:HG3	9:B:480:HOH:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:ILE:HD11	1:B:211:LEU:HD13	1.76	0.66
2:C:671:ASN:N	2:C:671:ASN:ND2	2.40	0.66
3:D:1166:LEU:HD12	3:D:1171:VAL:HG22	1.78	0.66
1:L:76:VAL:HG23	9:L:1317:HOH:O	1.95	0.66
2:M:21:ILE:H	2:M:21:ILE:HD12	1.60	0.66
2:M:1033:GLY:O	2:M:1036:GLU:HG2	1.96	0.66
2:M:1083:GLU:HG2	9:M:1724:HOH:O	1.96	0.66
3:N:126:VAL:HG21	9:N:2194:HOH:O	1.94	0.66
3:N:161:LEU:O	3:N:449:SER:HB3	1.95	0.66
5:P:335:ASP:OD1	5:P:338:LEU:HB2	1.95	0.66
2:C:15:LEU:CD2	2:C:583:LEU:HD11	2.26	0.66
2:C:498:GLN:O	2:C:501:THR:HG23	1.96	0.66
3:D:100:ALA:HB2	3:D:513:ILE:CD1	2.24	0.66
3:D:1498:ALA:HB2	4:E:88:GLU:OE1	1.96	0.66
4:E:6:ILE:HA	4:E:9:LEU:HD12	1.77	0.66
2:M:42:VAL:HG12	2:M:43:GLY:H	1.59	0.66
2:M:768:THR:HB	2:M:771:GLU:HB3	1.77	0.66
3:N:58:CYS:HA	3:N:78:VAL:HG11	1.77	0.66
3:N:133:ILE:HD11	3:N:155:ASP:OD1	1.96	0.66
3:N:924:MET:O	3:N:927:THR:HB	1.96	0.66
3:N:996:TRP:CD2	3:N:1056:PRO:HG2	2.31	0.66
3:N:1101:VAL:HG21	3:N:1424:VAL:HG22	1.77	0.66
2:C:141:HIS:HB3	2:C:418:LEU:HG	1.77	0.66
2:C:198:ARG:NE	2:C:228:ALA:HA	2.11	0.66
2:C:713:ARG:HH22	3:D:531:ASP:HB3	1.60	0.66
2:C:1005:MET:HE1	3:D:648:MET:HB2	1.78	0.66
2:C:1018:GLN:OE1	2:C:1060:ILE:HD11	1.95	0.66
2:C:1019:GLN:HE22	3:D:621:LYS:HA	1.61	0.66
3:D:1310:ARG:HG3	3:D:1327:ARG:HB3	1.78	0.66
5:F:260:ILE:HD11	5:F:310:ILE:HG22	1.77	0.66
2:M:781:LYS:HG3	9:M:1700:HOH:O	1.95	0.66
3:N:633:VAL:HG22	3:N:635:PRO:HD3	1.76	0.66
3:N:704:ARG:HG2	3:N:705:ALA:H	1.59	0.66
3:N:1087:ARG:HB3	9:N:1678:HOH:O	1.95	0.66
2:C:864:GLY:O	2:C:866:PRO:HD3	1.96	0.66
2:M:350:ARG:HA	2:M:353:ARG:HD2	1.78	0.66
2:M:627:ARG:HA	9:M:1936:HOH:O	1.95	0.66
2:M:976:ASP:CB	2:M:979:THR:HG22	2.25	0.66
2:M:1014:SER:HB3	2:M:1017:THR:O	1.96	0.66
3:N:806:PHE:CE1	3:N:813:LEU:HB3	2.30	0.66
4:O:17:TYR:O	4:O:21:VAL:HG23	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:289:THR:HB	9:C:1392:HOH:O	1.96	0.66
2:C:471:TYR:CD1	2:C:486:MET:HE2	2.30	0.66
3:D:679:ARG:HB2	3:D:682:ASP:OD2	1.95	0.66
3:D:1044:LEU:HD23	9:D:1976:HOH:O	1.95	0.66
5:F:321:ILE:HB	5:F:327:SER:OG	1.96	0.66
1:K:206:THR:HG22	1:K:209:GLU:H	1.61	0.66
3:N:1258:ARG:CZ	3:N:1262:LEU:HD11	2.26	0.66
5:P:292:ALA:HB1	5:P:299:TRP:O	1.96	0.66
2:C:439:CYS:HB3	9:C:1185:HOH:O	1.96	0.65
2:C:1015:LEU:HD11	9:F:451:HOH:O	1.95	0.65
1:L:158:ILE:HG22	1:L:160:ASP:H	1.60	0.65
2:M:197:LEU:HD22	2:M:202:TYR:HD2	1.61	0.65
2:M:304:LEU:HD23	2:M:305:PRO:HD3	1.78	0.65
5:P:295:MET:HG2	5:P:299:TRP:CE2	2.31	0.65
5:P:407:LYS:HG2	9:P:600:HOH:O	1.95	0.65
3:D:403:PHE:CE1	3:D:407:VAL:HG23	2.31	0.65
5:F:273:ARG:HD3	9:F:735:HOH:O	1.96	0.65
2:M:312:ALA:HA	9:M:1882:HOH:O	1.96	0.65
3:N:139:GLY:HA3	9:N:2226:HOH:O	1.95	0.65
2:C:805:ARG:HG3	2:C:823:VAL:HG22	1.78	0.65
3:D:1102:THR:HG22	3:D:1222:GLY:HA2	1.78	0.65
5:F:415:THR:HG21	9:F:598:HOH:O	1.95	0.65
2:M:368:THR:HB	2:M:369:PRO:HD3	1.77	0.65
2:M:1081:VAL:HG21	2:M:1111:ILE:HG22	1.78	0.65
3:N:154:THR:HG23	3:N:157:GLU:H	1.60	0.65
3:N:1035:ILE:HA	3:N:1038:LEU:CD1	2.26	0.65
5:P:151:LEU:O	5:P:155:THR:HB	1.96	0.65
5:P:261:PRO:HB3	9:P:570:HOH:O	1.94	0.65
3:D:128:TYR:HE1	3:D:461:ILE:HG13	1.61	0.65
3:D:611:GLN:NE2	3:D:1463:LYS:CE	2.53	0.65
3:D:1211:MET:HB3	9:D:2053:HOH:O	1.95	0.65
5:F:125:ASP:HA	9:F:652:HOH:O	1.97	0.65
1:L:58:ILE:HB	1:L:61:VAL:HB	1.77	0.65
1:L:206:THR:HG22	1:L:209:GLU:HB2	1.78	0.65
2:M:150:PRO:CA	2:M:158:TYR:HB3	2.22	0.65
2:M:528:GLU:HB3	9:M:1626:HOH:O	1.97	0.65
3:N:59:ALA:HB1	9:N:1806:HOH:O	1.96	0.65
3:N:65:ARG:HG3	3:N:66:GLN:H	1.62	0.65
3:N:644:LEU:HD12	3:N:645:PRO:HD2	1.78	0.65
2:C:237:ARG:HD2	9:C:1406:HOH:O	1.97	0.65
3:D:611:GLN:HE21	3:D:1439:SER:HB3	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.78	0.65
3:D:1502:ALA:HB1	9:D:2407:HOH:O	1.95	0.65
1:L:158:ILE:HD11	1:L:166:PRO:CA	2.25	0.65
1:L:176:ARG:HD3	3:N:884:ARG:NH2	2.11	0.65
2:M:571:LEU:CD2	2:M:700:TYR:HA	2.26	0.65
3:N:1301:LYS:HG2	9:N:2327:HOH:O	1.95	0.65
1:B:59:GLU:HG3	1:B:139:ASN:ND2	2.12	0.65
2:C:292:ARG:HD2	2:C:299:LYS:HG2	1.78	0.65
2:C:511:GLU:O	2:C:526:PRO:HD3	1.95	0.65
2:C:1030:GLN:NE2	3:D:628:ARG:HB3	2.11	0.65
2:C:1098:ASP:HB2	3:D:21:TRP:HZ2	1.60	0.65
3:D:583:ASP:OD2	3:D:604:THR:HG21	1.96	0.65
3:D:1109:GLU:OE1	3:D:1201:CYS:HB2	1.95	0.65
5:F:132:ARG:HG2	5:F:181:GLU:CD	2.22	0.65
1:L:46:SER:O	1:L:148:VAL:HB	1.96	0.65
2:M:52:PHE:CD2	2:M:68:PHE:HB2	2.31	0.65
2:M:422:ARG:HA	9:M:1913:HOH:O	1.97	0.65
2:M:471:TYR:CE2	2:M:496:ILE:HG21	2.31	0.65
3:N:107:ASP:O	3:N:108:VAL:C	2.39	0.65
3:N:1109:GLU:OE1	3:N:1201:CYS:HB2	1.96	0.65
5:P:392:VAL:HG21	9:P:614:HOH:O	1.97	0.65
1:A:206:THR:CG2	1:A:209:GLU:H	2.10	0.65
2:C:1087:VAL:CG1	3:D:610:LYS:HZ1	2.08	0.65
2:C:1118:LYS:HG3	9:C:1317:HOH:O	1.95	0.65
3:D:1095:THR:O	3:D:1099:VAL:HG23	1.96	0.65
1:K:9:PRO:HB2	1:L:224:TYR:HB3	1.77	0.65
1:L:12:THR:HB	9:L:1867:HOH:O	1.96	0.65
1:L:109:VAL:HG12	9:L:1850:HOH:O	1.96	0.65
2:M:289:THR:HB	9:M:1685:HOH:O	1.97	0.65
2:M:724:ARG:O	2:M:734:LEU:HD21	1.97	0.65
3:N:105:VAL:HG21	3:N:128:TYR:CE2	2.30	0.65
3:N:1046:GLN:HA	3:N:1052:THR:HA	1.79	0.65
1:B:179:PHE:HB2	1:B:195:LEU:HD11	1.77	0.65
2:C:442:GLU:HG2	2:C:454:SER:OG	1.96	0.65
2:C:1103:ASP:HB2	2:C:1107:ASN:O	1.96	0.65
3:D:493:ARG:NH1	3:D:1390:LEU:HB3	2.12	0.65
3:D:833:GLU:HG2	9:D:1935:HOH:O	1.97	0.65
1:K:16:GLN:HB3	9:K:1964:HOH:O	1.97	0.65
2:M:101:ILE:HG23	2:M:107:LEU:HD22	1.77	0.65
3:N:134:VAL:HG12	3:N:152:LEU:HB3	1.77	0.65
3:N:614:PHE:HD1	3:N:615:ARG:N	1.94	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:664:LYS:HE2	9:N:2324:HOH:O	1.96	0.65
2:C:610:ARG:HB2	9:C:1140:HOH:O	1.97	0.65
3:D:161:LEU:HD22	3:D:452:ILE:HG21	1.79	0.65
3:D:957:PRO:CG	3:D:1007:VAL:HA	2.25	0.65
3:D:1264:GLU:HG2	3:D:1425:THR:HG22	1.78	0.65
1:L:221:HIS:HA	1:L:224:TYR:CD2	2.31	0.65
2:M:607:ASP:HB3	2:M:609:ASN:H	1.62	0.65
2:M:755:LEU:HB2	9:M:1781:HOH:O	1.97	0.65
3:N:508:ARG:CG	3:N:509:PRO:HD2	2.26	0.65
3:N:760:ARG:HH21	4:O:61:VAL:HG12	1.62	0.65
5:P:274:THR:O	5:P:278:LEU:HG	1.97	0.65
5:P:291:ILE:HG23	5:P:304:VAL:HG21	1.78	0.65
1:B:2:LEU:HD12	1:B:3:ASP:N	2.11	0.65
2:C:141:HIS:HB3	2:C:418:LEU:CG	2.27	0.65
2:C:627:ARG:HG3	2:C:628:PHE:H	1.61	0.65
3:D:1441:GLN:HB3	9:D:1557:HOH:O	1.97	0.65
5:F:166:LEU:O	5:F:171:LYS:HB2	1.96	0.65
2:M:916:GLU:HG2	9:M:2028:HOH:O	1.96	0.65
3:N:1166:LEU:HD12	3:N:1171:VAL:HG22	1.79	0.65
2:C:905:ILE:HB	9:C:1738:HOH:O	1.96	0.64
3:D:812:ALA:HB1	9:D:1779:HOH:O	1.98	0.64
3:D:906:GLN:HB3	3:D:911:LEU:HD11	1.78	0.64
5:F:187:LEU:HD23	5:F:187:LEU:O	1.97	0.64
1:K:38:ASN:HB3	1:K:39:PRO:HD3	1.77	0.64
1:L:54:THR:HG22	9:L:3428:HOH:O	1.96	0.64
1:L:61:VAL:N	1:L:137:ARG:HH22	1.95	0.64
2:M:838:LYS:HB2	2:M:848:VAL:HG22	1.78	0.64
3:N:611:GLN:HG2	3:N:619:LEU:HD11	1.77	0.64
3:D:1209:LEU:HD23	3:D:1211:MET:SD	2.37	0.64
2:M:54:ILE:HD11	2:M:356:ARG:HG2	1.79	0.64
2:M:73:LEU:HD22	2:M:118:ILE:HD11	1.79	0.64
2:M:429:ASP:HB3	9:M:2136:HOH:O	1.96	0.64
3:N:445:ARG:HB3	9:N:2112:HOH:O	1.98	0.64
3:N:817:GLU:O	3:N:821:VAL:HG23	1.96	0.64
1:A:13:VAL:HG12	1:A:15:THR:HG22	1.78	0.64
1:A:20:TYR:HB3	9:A:413:HOH:O	1.97	0.64
1:A:123:MET:C	1:A:125:PRO:HD3	2.22	0.64
1:B:123:MET:C	1:B:125:PRO:HD3	2.22	0.64
3:D:534:ARG:HG2	9:F:611:HOH:O	1.97	0.64
3:D:1237:THR:HG22	9:D:2068:HOH:O	1.98	0.64
5:F:401:GLU:O	5:F:405:LEU:HB2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:13:VAL:HG12	1:K:15:THR:HG22	1.80	0.64
1:L:38:ASN:HB3	1:L:39:PRO:HD3	1.78	0.64
2:M:100:LEU:HD23	2:M:368:THR:HA	1.78	0.64
2:M:811:PRO:HB2	2:M:813:VAL:HG13	1.78	0.64
3:N:131:LYS:CG	3:N:568:ARG:HG2	2.26	0.64
3:N:141:ILE:HD12	9:N:2046:HOH:O	1.97	0.64
3:N:175:VAL:HG11	3:N:193:PRO:HB2	1.80	0.64
3:N:722:GLU:HA	9:N:1930:HOH:O	1.97	0.64
1:B:124:ASN:OD1	1:B:127:LEU:HB2	1.97	0.64
1:B:226:SER:O	1:B:228:PRO:HD3	1.97	0.64
2:C:645:VAL:HA	9:C:1531:HOH:O	1.96	0.64
2:C:976:ASP:CB	2:C:979:THR:HG22	2.27	0.64
3:D:55:ASP:HB3	3:D:82:LYS:HE2	1.79	0.64
3:D:149:LYS:HA	9:D:1632:HOH:O	1.98	0.64
3:D:1046:GLN:HA	3:D:1052:THR:HA	1.80	0.64
5:F:349:LEU:HB2	9:F:433:HOH:O	1.98	0.64
2:M:263:ASP:HB2	2:M:264:PRO:HD3	1.78	0.64
2:M:877:PRO:CG	3:N:1023:MET:HE2	2.19	0.64
3:N:1013:GLU:HB3	9:N:2351:HOH:O	1.97	0.64
2:C:691:SER:HB2	2:C:858:MET:SD	2.38	0.64
2:C:890:LEU:HD23	9:C:1640:HOH:O	1.97	0.64
3:D:124:GLU:O	3:D:128:TYR:HB2	1.97	0.64
1:K:41:ARG:HH22	2:M:866:PRO:HG3	1.63	0.64
1:L:9:PRO:HD3	9:L:1857:HOH:O	1.98	0.64
1:L:52:ALA:HB1	9:L:1023:HOH:O	1.98	0.64
1:L:109:VAL:HG21	1:L:138:LEU:CD1	2.18	0.64
2:M:170:PRO:HG2	2:M:258:TYR:CD2	2.32	0.64
2:M:176:VAL:HG12	2:M:182:VAL:HG13	1.78	0.64
2:M:549:PHE:CE2	2:M:886:LEU:HB3	2.32	0.64
3:N:565:ILE:HB	5:P:84:TYR:HD2	1.63	0.64
3:N:702:LEU:HD13	3:N:716:PHE:CD1	2.33	0.64
3:N:799:LYS:HB3	3:N:826:PRO:HG2	1.77	0.64
3:N:1209:LEU:HD12	3:N:1219:GLU:OE1	1.97	0.64
4:O:54:LEU:HG	4:O:58:PRO:CG	2.26	0.64
5:P:112:ALA:O	5:P:116:LEU:HG	1.98	0.64
5:P:315:VAL:HA	9:P:479:HOH:O	1.97	0.64
1:B:71:VAL:HG22	1:B:132:LEU:HD12	1.80	0.64
2:C:57:GLU:HB2	9:C:1254:HOH:O	1.97	0.64
2:C:79:PRO:HA	9:C:1251:HOH:O	1.97	0.64
2:C:84:ARG:HH21	2:C:128:ILE:HD11	1.63	0.64
2:C:140:ILE:CD1	2:C:412:ALA:HA	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:265:ARG:HG2	2:C:266:ARG:N	2.11	0.64
3:D:583:ASP:HB2	3:D:604:THR:OG1	1.97	0.64
3:D:1035:ILE:HA	3:D:1038:LEU:HD12	1.80	0.64
2:M:720:GLU:HA	2:M:759:THR:O	1.98	0.64
3:N:426:LYS:HD2	9:N:2209:HOH:O	1.96	0.64
3:N:512:MET:HE2	9:N:1664:HOH:O	1.98	0.64
4:O:67:GLU:OE1	4:O:73:LEU:HD11	1.97	0.64
2:C:200:LEU:HD13	2:C:300:ASP:CG	2.23	0.64
2:C:218:VAL:HG22	2:C:221:LEU:CD2	2.28	0.64
2:C:549:PHE:HB3	2:C:552:HIS:HD2	1.63	0.64
2:C:573:ARG:HB2	9:C:1310:HOH:O	1.97	0.64
2:C:671:ASN:H	2:C:671:ASN:ND2	1.94	0.64
3:D:188:GLY:N	3:D:199:LEU:HD23	2.13	0.64
3:D:564:GLU:HA	3:D:567:ILE:HD13	1.80	0.64
3:D:614:PHE:CZ	5:F:326:ASP:HB3	2.33	0.64
3:D:891:GLU:HG2	9:D:2400:HOH:O	1.96	0.64
5:F:327:SER:HA	9:F:456:HOH:O	1.96	0.64
2:M:545:ASN:OD1	2:M:905:ILE:HG12	1.96	0.64
2:M:603:VAL:HG22	2:M:613:VAL:HG12	1.79	0.64
4:O:88:GLU:HB3	9:O:2455:HOH:O	1.97	0.64
2:C:41:ASN:HD22	2:C:41:ASN:N	1.91	0.64
2:C:69:LEU:HB2	2:C:97:ARG:HB2	1.80	0.64
3:D:175:VAL:HG11	3:D:193:PRO:HB2	1.80	0.64
3:D:1141:GLU:CG	3:D:1168:MET:HE1	2.27	0.64
5:F:112:ALA:HA	5:F:173:TYR:HD2	1.63	0.64
2:M:118:ILE:HB	9:M:2032:HOH:O	1.98	0.64
2:M:200:LEU:HD13	2:M:300:ASP:CG	2.23	0.64
2:M:331:ARG:CZ	2:M:427:VAL:HG12	2.28	0.64
3:N:148:GLU:HG2	3:N:151:GLN:NE2	2.11	0.64
3:N:546:ARG:HA	9:N:1614:HOH:O	1.98	0.64
3:N:679:ARG:HB2	3:N:682:ASP:OD2	1.98	0.64
3:N:1065:LEU:HG	3:N:1070:TYR:HD2	1.63	0.64
2:C:150:PRO:CA	2:C:158:TYR:HB3	2.23	0.64
2:C:314:THR:HG23	9:C:1562:HOH:O	1.98	0.64
2:C:773:LEU:HB2	9:C:1139:HOH:O	1.96	0.64
3:D:148:GLU:HG2	3:D:151:GLN:NE2	2.12	0.64
1:K:197:LEU:HD23	1:K:197:LEU:H	1.62	0.64
1:K:201:THR:HG22	1:K:203:GLY:H	1.63	0.64
2:M:877:PRO:HG2	3:N:1023:MET:CE	2.18	0.64
3:N:153:LEU:HD11	3:N:158:TYR:N	2.13	0.64
3:N:595:GLY:HA2	9:N:2178:HOH:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:144:PRO:O	2:C:276:LYS:HD3	1.96	0.64
2:C:472:ARG:HB3	2:C:480:THR:O	1.97	0.64
3:D:154:THR:HG23	3:D:157:GLU:H	1.63	0.64
3:D:1434:TRP:CZ3	3:D:1457:ASP:HB2	2.33	0.64
1:K:117:VAL:HB	1:K:120:VAL:CG1	2.27	0.64
1:L:61:VAL:HG23	1:L:137:ARG:NH2	2.13	0.64
2:M:19:THR:O	2:M:23:VAL:HG23	1.97	0.64
3:N:615:ARG:HB3	9:N:2387:HOH:O	1.97	0.64
3:N:1023:MET:HB2	3:N:1029:ARG:O	1.98	0.64
4:O:59:ASN:HB3	4:O:62:THR:OG1	1.98	0.64
2:C:129:ILE:HG12	2:C:386:PHE:HB3	1.80	0.63
3:D:1147:ARG:HB3	3:D:1188:VAL:HG21	1.80	0.63
1:K:99:LEU:HB3	1:K:114:PHE:CD2	2.33	0.63
3:N:189:GLN:HG3	3:N:190:GLU:N	2.13	0.63
3:N:610:LYS:O	3:N:611:GLN:HG3	1.98	0.63
2:C:439:CYS:SG	2:C:441:VAL:HB	2.39	0.63
2:C:1014:SER:O	2:C:1018:GLN:HG3	1.97	0.63
3:D:52:PRO:HB2	3:D:80:VAL:HG13	1.79	0.63
3:D:558:LEU:HD13	5:F:145:PRO:CB	2.28	0.63
1:K:150:TYR:HE2	1:K:152:PRO:HG3	1.62	0.63
3:N:569:ASN:HD21	5:P:210:LEU:HD22	1.62	0.63
1:B:61:VAL:N	1:B:137:ARG:HH22	1.96	0.63
2:C:200:LEU:HB2	9:C:1462:HOH:O	1.97	0.63
9:K:1622:HOH:O	2:M:640:ARG:HB2	1.98	0.63
5:P:166:LEU:HD11	9:P:491:HOH:O	1.98	0.63
3:D:764:LEU:HD23	3:D:767:HIS:CE1	2.33	0.63
1:K:120:VAL:HG13	9:K:2485:HOH:O	1.99	0.63
2:M:693:GLU:HA	2:M:696:LYS:HG3	1.80	0.63
2:M:1016:ILE:HG23	3:N:526:PRO:HG2	1.79	0.63
2:M:1098:ASP:HB2	3:N:21:TRP:HZ2	1.63	0.63
3:N:72:VAL:HG23	3:N:78:VAL:H	1.63	0.63
3:N:147:VAL:HA	9:N:1777:HOH:O	1.98	0.63
2:C:18:LEU:HD21	2:C:542:VAL:HG11	1.80	0.63
3:D:1397:LYS:HE3	9:D:2203:HOH:O	1.98	0.63
3:D:1439:SER:HB3	3:D:1463:LYS:HE2	1.79	0.63
1:K:177:VAL:HG12	9:K:1774:HOH:O	1.99	0.63
1:L:41:ARG:HG3	1:L:177:VAL:HG21	1.80	0.63
2:M:437:ARG:HG2	2:M:467:ILE:O	1.97	0.63
2:M:474:VAL:HG11	2:M:529:VAL:HG12	1.79	0.63
2:M:944:LEU:HD21	2:M:963:LEU:HD23	1.80	0.63
2:M:968:LEU:HB3	9:M:2164:HOH:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:169:TYR:CG	3:N:195:VAL:HG11	2.34	0.63
3:N:720:LEU:H	3:N:720:LEU:HD12	1.63	0.63
5:P:372:ARG:N	5:P:372:ARG:HD2	2.12	0.63
1:A:20:TYR:HE2	1:A:22:GLU:HG3	1.62	0.63
1:A:191:ASP:O	1:A:192:LEU:HD23	1.99	0.63
2:C:243:ARG:HG2	9:C:1218:HOH:O	1.99	0.63
2:C:358:ARG:HB3	2:C:371:LYS:O	1.98	0.63
3:D:562:ALA:HB1	3:D:567:ILE:HD11	1.80	0.63
3:D:614:PHE:HZ	5:F:326:ASP:HB3	1.63	0.63
3:D:785:ILE:HG22	3:D:789:LEU:HD12	1.80	0.63
3:D:1266:ARG:O	3:D:1268:PRO:HD3	1.98	0.63
5:F:115:LYS:HD2	5:F:173:TYR:CE2	2.33	0.63
5:F:132:ARG:O	5:F:136:LEU:HG	1.99	0.63
1:L:138:LEU:HD23	1:L:140:MET:SD	2.37	0.63
2:M:307:LEU:HG	2:M:311:PHE:HE2	1.62	0.63
3:N:890:VAL:HG13	3:N:926:LYS:HG2	1.80	0.63
4:O:34:GLY:HA2	9:O:3283:HOH:O	1.98	0.63
1:A:109:VAL:HG23	1:A:132:LEU:HD13	1.80	0.63
2:C:304:LEU:HD23	2:C:305:PRO:HD3	1.80	0.63
3:D:799:LYS:N	3:D:826:PRO:HG2	2.12	0.63
1:L:72:LYS:HD2	9:L:2772:HOH:O	1.98	0.63
2:M:397:GLU:HB2	9:M:1672:HOH:O	1.97	0.63
2:M:820:ARG:HG3	9:M:1785:HOH:O	1.99	0.63
3:N:161:LEU:HD22	3:N:452:ILE:HG21	1.79	0.63
3:N:478:LEU:HD21	3:N:500:ARG:NH2	2.13	0.63
3:N:925:GLU:HB3	4:O:2:ALA:HB3	1.79	0.63
4:O:60:ALA:O	4:O:63:TRP:HB2	1.97	0.63
2:C:139:GLN:CD	2:C:415:PRO:HD2	2.24	0.63
2:C:185:LYS:HE2	2:C:190:LYS:HE2	1.80	0.63
2:C:660:ALA:HB1	2:C:667:ALA:O	1.98	0.63
3:D:65:ARG:HG3	3:D:66:GLN:H	1.64	0.63
3:D:1046:GLN:HG3	9:D:1606:HOH:O	1.98	0.63
3:D:1432:LYS:HG3	3:D:1433:SER:H	1.64	0.63
3:D:1465:ASN:ND2	3:D:1470:ARG:HD3	2.12	0.63
4:E:54:LEU:HG	4:E:58:PRO:CG	2.27	0.63
1:L:182:GLU:O	1:L:194:LYS:HB3	1.98	0.63
3:N:610:LYS:HG2	7:N:1527:MXP:H15A	1.80	0.63
5:P:401:GLU:O	5:P:405:LEU:HB2	1.99	0.63
1:B:61:VAL:HG23	1:B:137:ARG:NH2	2.13	0.63
2:C:599:GLU:HB2	9:C:1216:HOH:O	1.99	0.63
2:C:659:PRO:HD3	9:C:1639:HOH:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1152:GLU:CD	3:D:1159:ARG:HH12	2.06	0.63
5:F:88:ILE:HB	5:F:193:ARG:HH11	1.63	0.63
2:M:139:GLN:CD	2:M:415:PRO:HD2	2.24	0.63
2:M:265:ARG:HG2	2:M:266:ARG:N	2.14	0.63
3:N:403:PHE:CE1	3:N:407:VAL:HG23	2.34	0.63
3:N:906:GLN:HB3	3:N:911:LEU:CD1	2.29	0.63
3:N:961:LYS:HA	9:N:2211:HOH:O	1.99	0.63
3:N:1272:ALA:HA	3:N:1326:THR:HB	1.81	0.63
3:N:1356:TYR:CD2	3:N:1363:LEU:HD23	2.33	0.63
1:A:91:ASN:OD1	1:A:92:PRO:HD2	1.98	0.62
2:C:142:ARG:HH21	2:C:325:ILE:CD1	2.12	0.62
3:D:1109:GLU:HG2	3:D:1201:CYS:HA	1.81	0.62
5:F:372:ARG:HD2	5:F:372:ARG:N	2.14	0.62
2:M:790:LEU:HG	9:M:1781:HOH:O	1.99	0.62
2:M:1103:ASP:HB2	2:M:1107:ASN:O	1.99	0.62
5:P:356:LYS:HB2	9:P:473:HOH:O	1.99	0.62
1:A:18:ARG:O	1:A:207:PRO:HD3	1.98	0.62
1:B:182:GLU:O	1:B:194:LYS:HB3	1.98	0.62
2:C:343:GLN:HG2	2:C:385:PHE:HB2	1.81	0.62
2:C:367:LEU:O	2:C:372:LEU:HD13	1.99	0.62
3:D:55:ASP:HB3	9:D:1577:HOH:O	1.99	0.62
3:D:179:VAL:HG13	3:D:183:GLU:HB3	1.81	0.62
3:D:996:TRP:CE2	3:D:1056:PRO:HG2	2.34	0.62
3:D:1037:GLN:HG2	3:D:1042:ARG:HB3	1.81	0.62
3:D:1488:ASP:HA	9:E:110:HOH:O	1.99	0.62
1:L:55:SER:OG	1:L:158:ILE:HD13	2.00	0.62
2:M:276:LYS:O	2:M:280:LYS:HB2	1.99	0.62
2:M:1067:TYR:HE1	3:N:655:PRO:HG3	1.62	0.62
3:N:188:GLY:HA2	9:N:1751:HOH:O	1.98	0.62
3:N:1109:GLU:HG2	3:N:1201:CYS:HA	1.81	0.62
4:O:37:ASN:HA	4:O:93:TYR:CE2	2.34	0.62
5:P:152:ASP:HA	9:P:502:HOH:O	1.98	0.62
2:C:162:ILE:O	2:C:164:PRO:HD3	1.99	0.62
2:C:1109:VAL:HG11	3:D:5:VAL:HG13	1.79	0.62
3:D:58:CYS:HA	3:D:78:VAL:HG11	1.80	0.62
3:D:185:VAL:HG23	3:D:202:VAL:C	2.24	0.62
4:E:45:ARG:HB2	4:E:46:PRO:HD2	1.80	0.62
4:E:95:VAL:O	4:E:95:VAL:HG12	1.99	0.62
2:M:166:PRO:HD3	2:M:265:ARG:HG3	1.79	0.62
2:M:709:GLU:HG3	2:M:824:ARG:HG2	1.82	0.62
3:N:538:SER:HB3	9:P:565:HOH:O	1.97	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:860:LEU:HD22	3:N:878:GLY:HA2	1.81	0.62
3:N:1262:LEU:HD23	3:N:1352:ILE:CG1	2.29	0.62
4:O:83:ASP:O	4:O:86:GLN:HG2	1.99	0.62
2:C:165:LEU:O	2:C:265:ARG:HD2	1.99	0.62
2:C:1005:MET:O	2:C:1005:MET:HG3	1.99	0.62
1:L:18:ARG:O	1:L:207:PRO:HD3	1.99	0.62
1:L:52:ALA:HB2	1:L:170:VAL:O	1.99	0.62
1:L:59:GLU:HG3	1:L:139:ASN:ND2	2.14	0.62
3:N:40:GLU:N	9:N:1836:HOH:O	2.31	0.62
3:N:643:GLY:HA3	3:N:727:GLN:HB2	1.80	0.62
3:N:1290:LEU:CD2	3:N:1291:SER:H	2.12	0.62
2:C:263:ASP:HB2	2:C:264:PRO:HD3	1.81	0.62
2:C:395:LYS:HE2	2:C:403:SER:CB	2.20	0.62
2:C:838:LYS:CE	2:C:846:LYS:HE2	2.29	0.62
2:C:1001:VAL:HG13	9:C:1323:HOH:O	1.98	0.62
3:D:47:GLU:HG2	3:D:53:ILE:HG22	1.80	0.62
3:D:165:LYS:HB2	3:D:397:LYS:HB3	1.81	0.62
3:D:187:LYS:HG3	3:D:199:LEU:HD22	1.81	0.62
3:D:865:THR:HG22	9:D:1855:HOH:O	1.99	0.62
5:F:119:ILE:HD13	5:F:170:HIS:ND1	2.15	0.62
2:M:110:GLU:CB	2:M:369:PRO:HG3	2.30	0.62
2:M:741:GLY:HA3	9:M:1665:HOH:O	1.99	0.62
3:N:12:LEU:HD11	3:N:512:MET:HG2	1.80	0.62
3:N:52:PRO:HG3	3:N:78:VAL:HG13	1.81	0.62
3:N:510:GLU:HB3	9:N:2186:HOH:O	1.99	0.62
3:N:583:ASP:OD2	3:N:604:THR:HG21	1.99	0.62
5:P:375:LEU:HG	5:P:376:ILE:HG13	1.82	0.62
1:B:79:ILE:HD12	9:B:474:HOH:O	1.98	0.62
2:C:971:LYS:HA	2:C:988:VAL:HA	1.82	0.62
3:D:834:THR:HB	3:D:838:ARG:HB2	1.81	0.62
3:D:860:LEU:HA	3:D:877:PRO:HB2	1.82	0.62
2:M:333:ILE:HD13	2:M:467:ILE:HG13	1.81	0.62
2:M:472:ARG:HB3	2:M:480:THR:O	2.00	0.62
2:M:480:THR:HG22	2:M:481:ASP:H	1.64	0.62
2:M:1005:MET:HE1	3:N:648:MET:HB2	1.82	0.62
3:N:775:GLY:HA2	9:N:2264:HOH:O	2.00	0.62
3:N:864:VAL:HG12	3:N:865:THR:H	1.65	0.62
3:N:1189:ARG:HH11	3:N:1203:LYS:HB2	1.64	0.62
5:P:172:ARG:O	5:P:176:ILE:HD13	1.99	0.62
3:D:493:ARG:HH11	3:D:1390:LEU:HB3	1.63	0.62
3:D:877:PRO:O	3:D:880:ILE:HG22	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1114:THR:CG2	3:D:1195:GLN:HB3	2.29	0.62
3:D:1231:GLU:HB3	3:D:1232:PRO:HD3	1.82	0.62
3:D:1356:TYR:HD2	3:D:1363:LEU:HD23	1.65	0.62
3:D:1467:ILE:HG23	7:D:1527:MXP:H16A	1.81	0.62
1:K:48:ILE:HG22	1:K:173:PRO:HD2	1.80	0.62
1:L:223:THR:HG22	9:L:4161:HOH:O	1.98	0.62
2:M:80:GLN:O	2:M:83:CYS:HB2	1.99	0.62
2:M:146:VAL:HG11	2:M:306:THR:HG22	1.81	0.62
2:M:431:HIS:HD2	2:M:433:THR:H	1.45	0.62
2:M:1002:GLU:HG2	2:M:1003:ASP:N	2.14	0.62
2:C:244:PRO:HG3	9:C:1642:HOH:O	1.98	0.62
3:D:491:LYS:HD3	9:D:1938:HOH:O	1.99	0.62
3:D:1109:GLU:CD	3:D:1202:GLN:H	2.07	0.62
3:D:1321:ALA:O	3:D:1339:LYS:HE3	2.00	0.62
9:D:1795:HOH:O	4:E:50:THR:HB	2.00	0.62
3:N:723:GLY:HA3	9:N:1625:HOH:O	2.00	0.62
3:N:957:PRO:CG	3:N:1007:VAL:HA	2.27	0.62
4:O:30:LEU:O	4:O:35:PHE:HA	1.99	0.62
1:B:206:THR:HG22	1:B:209:GLU:HB2	1.81	0.62
3:D:49:ILE:HG21	9:D:2241:HOH:O	2.00	0.62
3:D:1056:PRO:HD3	9:D:1650:HOH:O	1.99	0.62
3:D:1111:ASP:HB3	3:D:1203:LYS:HG3	1.82	0.62
5:F:396:ARG:HB2	9:F:496:HOH:O	1.98	0.62
2:M:86:LYS:CD	2:M:813:VAL:HG12	2.30	0.62
2:M:498:GLN:O	2:M:501:THR:HG23	2.00	0.62
2:M:557:ARG:NH1	2:M:879:ARG:HG2	2.15	0.62
2:M:559:LEU:HD23	2:M:560:MET:N	2.14	0.62
2:M:567:GLN:HB2	2:M:997:LEU:HD22	1.80	0.62
2:M:676:ILE:O	2:M:676:ILE:HG23	1.99	0.62
2:M:715:THR:HG22	2:M:717:LEU:HG	1.82	0.62
2:M:722:ILE:CD1	2:M:823:VAL:HG21	2.29	0.62
3:N:1192:LEU:HD13	3:N:1345:GLU:HG2	1.81	0.62
2:C:274:ARG:HG2	9:C:1142:HOH:O	1.99	0.62
2:C:307:LEU:HG	2:C:311:PHE:CE2	2.35	0.62
3:D:428:LYS:HE2	9:D:1881:HOH:O	2.00	0.62
3:N:394:LEU:HD21	9:N:2081:HOH:O	2.00	0.62
3:N:1013:GLU:HB2	9:N:1747:HOH:O	2.00	0.62
3:N:1258:ARG:NH2	3:N:1262:LEU:HD11	2.15	0.62
3:N:1293:PHE:CZ	3:N:1302:GLU:HB3	2.34	0.62
1:B:83:LYS:HE2	1:B:168:ASP:HB2	1.81	0.61
2:C:137:VAL:HG22	2:C:391:LEU:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:141:HIS:CB	2:C:418:LEU:HG	2.29	0.61
2:C:420:ARG:HA	9:C:1293:HOH:O	1.98	0.61
2:C:495:THR:H	2:C:530:GLU:CD	2.08	0.61
2:C:738:ASP:CB	2:C:744:ARG:HB3	2.29	0.61
2:C:902:ILE:O	2:C:904:PRO:HD3	2.00	0.61
3:D:1269:LYS:HD3	9:D:2029:HOH:O	1.99	0.61
3:D:1291:SER:HB2	3:D:1293:PHE:HE1	1.65	0.61
1:L:128:HIS:HE1	1:L:131:THR:HG23	1.64	0.61
1:L:169:ALA:HB1	1:L:171:PHE:CD2	2.35	0.61
3:N:80:VAL:HA	9:N:2248:HOH:O	1.99	0.61
3:N:683:ILE:HG22	9:N:1566:HOH:O	2.00	0.61
3:N:702:LEU:HB3	3:N:745:MET:HE2	1.82	0.61
3:N:717:GLN:HG2	9:N:1629:HOH:O	2.00	0.61
3:N:1295:GLU:HB3	3:N:1300:SER:CB	2.30	0.61
2:C:31:GLN:HB3	2:C:71:TYR:OH	2.00	0.61
2:C:63:GLY:HA3	9:C:1168:HOH:O	1.98	0.61
2:C:528:GLU:HG2	9:C:1477:HOH:O	1.99	0.61
3:D:400:VAL:HG22	3:D:443:VAL:CG2	2.29	0.61
3:D:613:ARG:HG3	3:D:1441:GLN:HB2	1.82	0.61
3:D:955:VAL:HA	9:D:2261:HOH:O	1.98	0.61
4:E:30:LEU:O	4:E:35:PHE:HA	2.00	0.61
2:M:864:GLY:O	2:M:866:PRO:HD3	2.00	0.61
3:N:491:LYS:HD3	9:N:2284:HOH:O	1.98	0.61
3:N:611:GLN:CG	3:N:619:LEU:HG	2.29	0.61
3:N:1036:ARG:HH21	3:N:1042:ARG:HA	1.64	0.61
3:N:1274:ILE:HA	9:N:1761:HOH:O	2.00	0.61
3:N:1304:LYS:HA	9:N:1838:HOH:O	1.99	0.61
4:O:86:GLN:O	4:O:90:GLU:HG3	2.00	0.61
5:P:88:ILE:HG21	5:P:193:ARG:HD3	1.83	0.61
2:C:151:ASP:OD2	2:C:159:ILE:HG23	2.00	0.61
2:C:512:ARG:HB2	9:C:1201:HOH:O	2.00	0.61
3:D:50:PHE:CB	3:D:522:PRO:HG2	2.29	0.61
2:M:274:ARG:HD2	2:M:285:LEU:O	1.99	0.61
2:M:838:LYS:CE	2:M:846:LYS:HE2	2.29	0.61
2:M:926:PHE:CE1	2:M:929:ARG:HD3	2.35	0.61
5:P:284:ARG:HD2	9:P:504:HOH:O	1.99	0.61
2:C:305:PRO:HA	2:C:308:ARG:HD2	1.82	0.61
3:D:1097:LYS:HE3	9:D:2031:HOH:O	2.01	0.61
3:D:1430:SER:HA	9:D:1920:HOH:O	1.99	0.61
1:K:67:THR:HG21	2:M:609:ASN:ND2	2.07	0.61
1:K:109:VAL:HG23	1:K:132:LEU:HD13	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:144:PRO:HA	2:M:163:ILE:HG13	1.82	0.61
2:M:239:PHE:HB3	9:M:1968:HOH:O	2.00	0.61
3:N:702:LEU:HD13	3:N:716:PHE:HD1	1.64	0.61
3:N:1042:ARG:O	3:N:1057:VAL:HB	2.00	0.61
9:N:1961:HOH:O	5:P:168:LYS:HG2	2.01	0.61
9:N:2314:HOH:O	5:P:376:ILE:HD11	1.99	0.61
1:A:125:PRO:HD2	9:A:394:HOH:O	2.00	0.61
1:A:184:THR:HG23	1:A:192:LEU:HB2	1.82	0.61
2:C:143:SER:HB2	2:C:276:LYS:NZ	2.14	0.61
2:C:399:ASN:ND2	2:C:568:ALA:HB3	2.15	0.61
2:C:625:LEU:HB3	2:C:639:GLN:HB2	1.82	0.61
2:C:1002:GLU:HG2	2:C:1003:ASP:N	2.14	0.61
2:C:1056:LYS:NZ	3:D:749:VAL:O	2.33	0.61
3:D:847:ASP:O	3:D:851:LEU:HG	2.01	0.61
9:D:1675:HOH:O	5:F:337:HIS:HB3	2.01	0.61
5:F:230:LYS:HD3	9:F:439:HOH:O	1.99	0.61
5:F:361:LEU:HD23	5:F:362:SER:N	2.15	0.61
2:M:267:TYR:HB2	2:M:272:ALA:HB1	1.82	0.61
2:M:358:ARG:HB3	2:M:371:LYS:O	1.99	0.61
2:M:367:LEU:O	2:M:372:LEU:HD13	2.01	0.61
3:N:996:TRP:CE3	3:N:999:THR:HG21	2.35	0.61
3:N:1102:THR:HG22	3:N:1222:GLY:HA2	1.82	0.61
3:N:1173:LEU:HD23	3:N:1174:LEU:HD23	1.83	0.61
3:N:1389:LEU:HD12	3:N:1390:LEU:H	1.65	0.61
1:B:108:GLU:HB2	9:B:409:HOH:O	2.00	0.61
2:C:6:PHE:CG	2:C:909:ALA:HA	2.35	0.61
2:C:123:GLU:HB2	9:C:1197:HOH:O	2.00	0.61
2:C:675:ALA:HA	2:C:989:VAL:HG12	1.83	0.61
2:C:1007:ALA:HB2	3:D:648:MET:HG3	1.82	0.61
2:C:1066:ALA:O	2:C:1070:ILE:HG13	1.99	0.61
3:D:119:SER:HB2	3:D:123:LEU:HD13	1.81	0.61
2:M:15:LEU:H	2:M:15:LEU:HD12	1.66	0.61
2:M:57:GLU:HG3	9:M:1902:HOH:O	1.99	0.61
2:M:176:VAL:HG12	2:M:182:VAL:CG1	2.31	0.61
3:N:52:PRO:HG2	3:N:80:VAL:HG13	1.81	0.61
3:N:119:SER:HB2	3:N:123:LEU:HD13	1.81	0.61
3:N:400:VAL:HG13	3:N:402:PRO:HD3	1.83	0.61
3:N:1377:LYS:HG3	3:N:1394:VAL:HG13	1.81	0.61
2:C:64:LEU:HD13	2:C:359:MET:HG3	1.82	0.61
2:C:333:ILE:CD1	2:C:467:ILE:HG13	2.30	0.61
3:D:204:LEU:HG	3:D:441:ARG:HH12	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:637:LEU:HD11	3:D:642:CYS:N	2.15	0.61
3:D:715:ALA:HB3	3:D:764:LEU:HA	1.82	0.61
5:F:335:ASP:OD1	5:F:338:LEU:HB2	2.01	0.61
3:N:128:TYR:HE1	3:N:461:ILE:HG13	1.65	0.61
3:N:187:LYS:HG3	3:N:199:LEU:HD22	1.83	0.61
3:N:674:ARG:HD3	9:N:1957:HOH:O	2.01	0.61
5:P:203:THR:HG22	5:P:204:GLY:N	2.16	0.61
1:A:150:TYR:CE2	1:A:152:PRO:HG3	2.35	0.61
2:C:176:VAL:C	2:C:178:PRO:HD3	2.25	0.61
2:C:455:LEU:HD12	2:C:456:ALA:O	2.00	0.61
3:D:65:ARG:CG	3:D:66:GLN:H	2.13	0.61
3:D:1384:PRO:HG3	3:D:1389:LEU:HA	1.83	0.61
1:K:20:TYR:HD2	1:K:21:GLY:H	1.49	0.61
1:L:83:LYS:HA	9:L:2646:HOH:O	2.00	0.61
1:L:143:ARG:HD2	1:L:160:ASP:OD2	2.00	0.61
3:N:500:ARG:HD2	9:N:2131:HOH:O	2.00	0.61
3:N:661:MET:HE3	3:N:673:ALA:CB	2.31	0.61
3:N:799:LYS:H	3:N:826:PRO:HG2	1.66	0.61
1:A:20:TYR:CD2	1:A:21:GLY:N	2.63	0.61
2:C:775:ARG:HG3	9:C:1214:HOH:O	1.99	0.61
2:C:919:ALA:HA	9:C:1166:HOH:O	2.00	0.61
3:D:169:TYR:CG	3:D:195:VAL:HG11	2.36	0.61
3:D:206:ARG:HH11	5:F:97:GLU:HB3	1.65	0.61
3:D:486:ARG:HD3	3:D:489:ARG:HD3	1.81	0.61
1:K:91:ASN:CG	1:K:92:PRO:HD2	2.26	0.61
1:L:57:TYR:HE1	1:L:163:ASN:HB2	1.65	0.61
1:L:176:ARG:HH21	3:N:850:LEU:HD13	1.65	0.61
2:M:307:LEU:HG	2:M:311:PHE:CE2	2.36	0.61
3:N:31:THR:HG23	3:N:45:PHE:CE2	2.35	0.61
3:N:824:ASN:HB2	9:N:1978:HOH:O	2.01	0.61
3:N:1420:LEU:HD12	3:N:1421:LEU:N	2.14	0.61
2:C:73:LEU:HD23	2:C:94:LEU:HB2	1.83	0.61
2:C:325:ILE:HG12	9:C:1558:HOH:O	2.00	0.61
2:C:1065:ALA:HB1	2:C:1077:PRO:HG2	1.83	0.61
2:C:1067:TYR:O	2:C:1071:ILE:HG12	2.01	0.61
3:D:400:VAL:HG13	3:D:402:PRO:HD3	1.83	0.61
3:D:633:VAL:HG22	3:D:635:PRO:CD	2.30	0.61
3:D:850:LEU:HD12	3:D:850:LEU:N	2.15	0.61
3:D:1127:GLU:HB2	9:D:1604:HOH:O	2.00	0.61
3:D:1394:VAL:HG11	9:D:2203:HOH:O	2.00	0.61
2:M:41:ASN:H	2:M:41:ASN:ND2	1.94	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:860:LEU:HA	3:N:877:PRO:HB2	1.82	0.61
1:B:90:LEU:HD23	9:B:496:HOH:O	1.99	0.60
2:C:926:PHE:CE1	2:C:929:ARG:HD3	2.36	0.60
2:C:969:GLN:HA	9:D:1915:HOH:O	2.00	0.60
3:D:10:ILE:HG13	3:D:1434:TRP:CZ2	2.35	0.60
3:D:130:SER:HB3	3:D:132:TYR:CE1	2.36	0.60
3:D:471:GLU:HG3	9:D:1589:HOH:O	2.01	0.60
3:D:631:ILE:HG12	3:D:743:ASP:O	2.00	0.60
3:D:1393:GLN:CB	3:D:1398:TRP:HE1	2.10	0.60
3:D:1462:LEU:HD22	3:D:1472:ILE:HG23	1.83	0.60
1:K:206:THR:CG2	1:K:209:GLU:H	2.14	0.60
1:K:221:HIS:HA	1:K:224:TYR:HD2	1.64	0.60
3:N:204:LEU:HD21	3:N:445:ARG:HH12	1.65	0.60
2:C:331:ARG:HB2	9:C:1737:HOH:O	1.99	0.60
2:C:1067:TYR:HE1	3:D:655:PRO:HG3	1.65	0.60
2:C:1118:LYS:HG2	3:D:23:TYR:CE1	2.36	0.60
1:L:2:LEU:HD12	1:L:3:ASP:N	2.16	0.60
3:N:131:LYS:HE3	3:N:568:ARG:CB	2.31	0.60
3:N:809:PRO:HB2	3:N:812:ALA:HB2	1.82	0.60
3:N:1291:SER:HB2	3:N:1293:PHE:CE1	2.35	0.60
5:P:95:THR:HG21	9:P:531:HOH:O	2.01	0.60
5:P:247:ILE:HG22	5:P:251:ILE:HD11	1.82	0.60
1:B:106:PRO:HG3	1:B:134:GLU:HG2	1.82	0.60
1:B:206:THR:HG22	1:B:209:GLU:H	1.66	0.60
2:C:193:LEU:HD21	9:C:1526:HOH:O	2.02	0.60
3:D:507:ASN:HA	9:D:2352:HOH:O	2.01	0.60
3:D:728:LEU:HD22	3:D:745:MET:SD	2.42	0.60
1:K:42:ARG:NH2	2:M:857:ASP:HB3	2.15	0.60
1:K:157:GLY:HA3	9:K:2579:HOH:O	2.01	0.60
2:M:341:THR:O	2:M:345:ARG:HG3	2.00	0.60
3:N:27:GLU:HB2	9:N:2072:HOH:O	2.00	0.60
3:N:509:PRO:HB2	9:N:1664:HOH:O	2.00	0.60
3:N:1434:TRP:CZ3	3:N:1457:ASP:HB2	2.36	0.60
1:B:123:MET:HE1	9:B:512:HOH:O	2.00	0.60
3:D:86:ARG:O	3:D:522:PRO:HD2	2.01	0.60
3:D:559:ALA:HA	9:F:646:HOH:O	2.01	0.60
3:D:829:VAL:H	3:D:835:SER:HB2	1.66	0.60
3:D:860:LEU:HD22	3:D:878:GLY:HA2	1.84	0.60
3:D:1045:MET:HE2	3:D:1073:SER:HB3	1.84	0.60
3:D:1299:PHE:HB2	9:D:2455:HOH:O	2.00	0.60
1:K:213:GLN:O	1:K:217:ILE:HG13	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:811:PRO:HG2	9:M:1891:HOH:O	2.00	0.60
3:N:52:PRO:CG	3:N:78:VAL:HG13	2.31	0.60
3:N:95:LEU:HA	3:N:551:ASN:ND2	2.16	0.60
3:N:566:ILE:HG23	5:P:217:ASN:HD22	1.66	0.60
2:C:720:GLU:HA	2:C:759:THR:O	2.02	0.60
2:C:1101:THR:HB	3:D:5:VAL:HG13	1.83	0.60
3:D:29:PRO:HB3	3:D:545:ARG:HG2	1.84	0.60
3:D:517:VAL:HG11	3:D:581:LEU:HD21	1.83	0.60
3:D:569:ASN:HB3	5:F:214:GLN:HE21	1.65	0.60
1:K:123:MET:HE2	1:K:203:GLY:O	2.01	0.60
2:M:554:ASP:OD2	2:M:556:ASN:HB3	2.01	0.60
2:M:747:ALA:O	2:M:799:ILE:HA	2.01	0.60
2:M:971:LYS:HA	2:M:988:VAL:HA	1.84	0.60
3:N:80:VAL:HG12	3:N:81:THR:O	2.02	0.60
3:N:799:LYS:N	3:N:826:PRO:HG2	2.16	0.60
5:P:209:PHE:CE2	5:P:213:ILE:HD11	2.37	0.60
1:A:38:ASN:HB3	1:A:39:PRO:HD3	1.83	0.60
2:C:93:PRO:HG3	2:C:117:HIS:CE1	2.37	0.60
2:C:132:ALA:HB1	2:C:632:ASN:ND2	2.16	0.60
2:C:571:LEU:HD21	2:C:700:TYR:HA	1.82	0.60
5:F:369:LEU:HB2	9:F:426:HOH:O	2.02	0.60
9:K:3509:HOH:O	1:L:155:LYS:HE2	2.00	0.60
2:M:265:ARG:HB3	2:M:267:TYR:CD2	2.36	0.60
2:M:518:LYS:HA	9:M:1901:HOH:O	2.02	0.60
2:M:890:LEU:CA	2:M:914:ILE:HD11	2.31	0.60
3:N:1109:GLU:HG2	3:N:1202:GLN:H	1.66	0.60
4:O:54:LEU:CD2	4:O:63:TRP:HE1	2.14	0.60
5:P:325:LYS:HB2	9:P:652:HOH:O	2.01	0.60
2:C:52:PHE:CD2	2:C:68:PHE:HB2	2.37	0.60
2:C:169:GLY:HA3	9:C:1253:HOH:O	2.01	0.60
2:C:559:LEU:HD23	2:C:560:MET:N	2.17	0.60
3:D:519:VAL:HG13	3:D:544:TYR:CZ	2.36	0.60
3:D:984:THR:HG22	3:D:987:GLU:H	1.66	0.60
5:F:132:ARG:HD2	9:F:492:HOH:O	2.02	0.60
5:F:375:LEU:HG	5:F:376:ILE:HG13	1.83	0.60
1:L:5:LYS:O	1:L:8:ALA:HB2	2.01	0.60
2:M:218:VAL:HA	2:M:221:LEU:HD23	1.84	0.60
2:M:218:VAL:HG22	2:M:221:LEU:HD23	1.84	0.60
2:M:1104:GLU:HG3	9:M:1982:HOH:O	2.01	0.60
3:N:142:LEU:HD11	9:N:2326:HOH:O	2.01	0.60
3:N:439:LEU:HB3	9:N:2015:HOH:O	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:583:ASP:OD1	3:N:586:ARG:HG3	2.01	0.60
3:N:647:ARG:HB3	9:N:2056:HOH:O	1.99	0.60
5:P:88:ILE:HD13	5:P:193:ARG:HB2	1.82	0.60
1:B:175:ARG:O	1:B:176:ARG:HG3	2.01	0.60
2:C:712:ALA:O	2:C:820:ARG:CB	2.50	0.60
2:C:818:GLY:N	5:F:309:LYS:HE2	2.17	0.60
3:D:1123:PHE:HA	3:D:1133:ARG:O	2.01	0.60
5:F:151:LEU:HB3	9:F:614:HOH:O	2.00	0.60
1:L:7:LYS:HG3	1:L:7:LYS:O	2.02	0.60
3:N:477:LEU:HD11	3:N:495:ARG:HD3	1.84	0.60
3:N:961:LYS:HB3	9:N:2007:HOH:O	2.00	0.60
1:A:127:LEU:C	1:A:127:LEU:HD12	2.27	0.60
1:B:132:LEU:HD21	1:B:136:GLY:O	2.01	0.60
2:C:260:LEU:HA	2:C:291:ALA:CB	2.31	0.60
2:C:591:SER:HA	9:C:1421:HOH:O	2.02	0.60
2:C:816:LYS:HB2	2:C:819:VAL:HG21	1.84	0.60
2:C:1017:THR:HG23	9:C:1263:HOH:O	2.00	0.60
3:D:400:VAL:C	3:D:402:PRO:HD3	2.26	0.60
3:D:408:GLU:HA	5:F:171:LYS:NZ	2.16	0.60
1:K:7:LYS:HZ1	1:K:186:LEU:HD21	1.67	0.60
1:K:18:ARG:NH1	1:K:88:ARG:HD3	2.16	0.60
1:K:18:ARG:NH1	1:K:123:MET:HE1	2.17	0.60
2:M:9:ILE:O	2:M:9:ILE:HG13	2.02	0.60
3:N:73:CYS:HB3	3:N:76:CYS:O	2.02	0.60
3:N:141:ILE:HG22	3:N:450:TYR:H	1.66	0.60
3:N:161:LEU:O	3:N:161:LEU:HD23	2.02	0.60
3:N:1114:THR:CG2	3:N:1195:GLN:HB3	2.31	0.60
2:C:137:VAL:HG23	2:C:391:LEU:HG	1.83	0.60
2:C:1008:ARG:HD2	2:C:1028:GLY:N	2.17	0.60
3:D:776:GLU:HB3	3:D:912:LYS:HE2	1.84	0.60
3:D:1125:PRO:HB2	9:D:2360:HOH:O	2.01	0.60
3:D:1295:GLU:HB3	3:D:1300:SER:CB	2.32	0.60
3:D:1326:THR:HG23	9:D:2026:HOH:O	2.01	0.60
1:L:217:ILE:O	1:L:221:HIS:ND1	2.33	0.60
2:M:710:ILE:HD11	2:M:758:ARG:HD3	1.84	0.60
2:M:833:LEU:HD12	2:M:834:GLN:H	1.67	0.60
2:M:874:LEU:HD12	3:N:784:ASP:OD2	2.02	0.60
3:N:10:ILE:HG13	3:N:1434:TRP:CE2	2.37	0.60
3:N:130:SER:O	3:N:568:ARG:NH2	2.35	0.60
3:N:1114:THR:H	3:N:1195:GLN:HE21	1.50	0.60
4:O:9:LEU:HD22	4:O:19:LEU:HD11	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:61:VAL:O	4:O:65:MET:HG3	2.02	0.60
2:C:244:PRO:HD2	2:C:245:GLY:H	1.65	0.59
2:C:431:HIS:H	2:C:434:HIS:CD2	2.20	0.59
3:D:438:ASP:HB3	9:D:1574:HOH:O	2.02	0.59
3:D:519:VAL:HG13	3:D:544:TYR:CE1	2.37	0.59
3:D:1117:TYR:HB3	9:D:2262:HOH:O	2.02	0.59
1:K:191:ASP:O	1:K:192:LEU:HD23	2.01	0.59
2:M:139:GLN:NE2	2:M:415:PRO:HD2	2.17	0.59
2:M:1018:GLN:OE1	2:M:1060:ILE:HD11	2.02	0.59
2:M:1066:ALA:O	2:M:1070:ILE:HG13	2.02	0.59
3:N:204:LEU:HB2	3:N:394:LEU:HG	1.83	0.59
5:P:93:LEU:HG	5:P:190:ALA:CB	2.32	0.59
2:C:139:GLN:HE22	2:C:415:PRO:CD	2.15	0.59
2:C:712:ALA:O	2:C:820:ARG:HB2	2.02	0.59
2:C:933:GLY:HA2	9:C:1525:HOH:O	2.02	0.59
3:D:37:LEU:HD13	3:D:535:PHE:HZ	1.68	0.59
3:D:133:ILE:HG21	9:D:1764:HOH:O	2.02	0.59
3:D:409:VAL:CG1	3:D:435:VAL:HG11	2.31	0.59
3:D:786:ILE:HD13	3:D:1027:GLY:HA3	1.83	0.59
5:F:372:ARG:HG3	9:F:595:HOH:O	2.01	0.59
1:K:198:ARG:HG2	9:K:1904:HOH:O	2.01	0.59
1:L:59:GLU:HG3	1:L:139:ASN:HD22	1.67	0.59
2:M:584:GLU:CD	2:M:584:GLU:H	2.10	0.59
3:N:169:TYR:O	3:N:392:SER:HB2	2.01	0.59
3:N:550:ARG:HH11	3:N:573:MET:HB3	1.67	0.59
3:N:675:ARG:HG2	3:N:678:GLU:OE2	2.02	0.59
3:N:774:SER:C	3:N:776:GLU:H	2.10	0.59
3:N:865:THR:HG22	9:N:1713:HOH:O	2.03	0.59
1:A:117:VAL:HB	1:A:120:VAL:CG1	2.31	0.59
1:B:89:PHE:HB3	1:B:94:LEU:HD22	1.84	0.59
2:C:471:TYR:CE2	2:C:496:ILE:HG21	2.36	0.59
3:D:47:GLU:HG2	9:D:1900:HOH:O	2.02	0.59
3:D:133:ILE:HG22	3:D:455:ARG:N	2.17	0.59
3:D:617:ASN:N	3:D:617:ASN:OD1	2.36	0.59
3:D:704:ARG:HD2	3:D:738:ALA:HB2	1.84	0.59
4:E:47:LYS:HE2	9:E:154:HOH:O	2.03	0.59
2:M:833:LEU:HD12	2:M:834:GLN:N	2.17	0.59
2:M:1085:PHE:CD2	3:N:1468:LEU:HA	2.36	0.59
3:N:50:PHE:HB3	3:N:522:PRO:HG2	1.83	0.59
3:N:95:LEU:HA	3:N:551:ASN:HD21	1.66	0.59
3:N:565:ILE:HD12	5:P:192:LEU:HD13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:704:ARG:HD2	3:N:738:ALA:HB2	1.83	0.59
3:N:770:LEU:HB3	9:N:1689:HOH:O	2.01	0.59
3:N:1087:ARG:HG2	3:N:1238:MET:HB3	1.83	0.59
3:N:1264:GLU:O	3:N:1266:ARG:HG3	2.02	0.59
1:B:169:ALA:HB1	1:B:171:PHE:CE2	2.37	0.59
3:D:486:ARG:HD2	9:D:1689:HOH:O	2.03	0.59
3:D:644:LEU:HD12	3:D:645:PRO:HD2	1.83	0.59
3:D:804:LEU:HD23	3:D:804:LEU:H	1.68	0.59
3:D:980:MET:HG3	9:D:1653:HOH:O	2.01	0.59
3:D:1023:MET:HB2	3:D:1029:ARG:O	2.03	0.59
3:D:1272:ALA:HA	3:D:1326:THR:HB	1.83	0.59
5:F:295:MET:HG2	5:F:299:TRP:CE2	2.37	0.59
1:K:50:GLY:O	1:K:146:ARG:HA	2.02	0.59
1:K:88:ARG:HG2	1:K:121:GLU:HG2	1.84	0.59
1:L:226:SER:O	1:L:228:PRO:HD3	2.02	0.59
2:M:328:LEU:HD22	2:M:437:ARG:HB3	1.83	0.59
2:M:468:ARG:HD3	9:M:2184:HOH:O	2.01	0.59
2:M:1038:TRP:HA	2:M:1041:GLU:HB2	1.84	0.59
3:N:165:LYS:HG3	3:N:397:LYS:HD3	1.84	0.59
3:N:734:GLU:HB2	9:N:1648:HOH:O	2.01	0.59
4:O:33:HIS:HB2	4:O:37:ASN:HD21	1.66	0.59
2:C:510:ALA:HB3	2:C:513:VAL:CG2	2.32	0.59
2:C:966:LEU:HD21	2:C:986:PRO:HG3	1.85	0.59
3:D:192:ALA:HB1	9:D:2083:HOH:O	2.02	0.59
3:D:1088:THR:HG21	9:D:1813:HOH:O	2.02	0.59
1:K:89:PHE:HB3	1:K:94:LEU:HD22	1.84	0.59
1:L:52:ALA:HB2	1:L:170:VAL:C	2.28	0.59
2:M:208:ALA:O	2:M:218:VAL:HG21	2.02	0.59
2:M:305:PRO:HA	2:M:308:ARG:HD2	1.84	0.59
3:N:570:GLU:HB2	5:P:214:GLN:OE1	2.02	0.59
3:N:1342:GLU:HG3	9:N:1945:HOH:O	2.03	0.59
3:N:1357:ARG:HB2	9:N:1826:HOH:O	2.01	0.59
1:A:123:MET:O	1:A:125:PRO:HD3	2.03	0.59
1:B:40:LEU:HD21	1:B:215:VAL:HG12	1.84	0.59
2:C:580:MET:HB3	2:C:584:GLU:CD	2.28	0.59
2:C:984:GLU:HG3	3:D:944:THR:O	2.02	0.59
3:D:169:TYR:O	3:D:392:SER:HB2	2.02	0.59
3:D:926:LYS:HE2	9:D:1617:HOH:O	2.01	0.59
4:E:9:LEU:HB3	4:E:19:LEU:HD21	1.85	0.59
5:F:220:LEU:HD12	5:F:243:ILE:HD11	1.83	0.59
5:F:256:ARG:HD3	9:F:585:HOH:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:268:ILE:HD13	5:F:311:ALA:HB2	1.83	0.59
2:M:404:LEU:HA	2:M:407:LYS:HD2	1.84	0.59
2:M:750:LYS:HB3	9:N:2087:HOH:O	2.02	0.59
3:N:133:ILE:HG22	3:N:455:ARG:N	2.18	0.59
3:N:434:ARG:HG2	9:N:2229:HOH:O	2.03	0.59
3:N:560:GLN:OE1	5:P:218:GLN:HG3	2.01	0.59
3:N:562:ALA:HB1	3:N:567:ILE:HD11	1.85	0.59
3:N:1117:TYR:HB3	9:N:1591:HOH:O	2.03	0.59
3:N:1403:LEU:HD23	9:N:1794:HOH:O	2.02	0.59
5:P:361:LEU:CD2	5:P:366:ALA:HB2	2.27	0.59
2:C:230:ARG:HG3	9:C:1406:HOH:O	2.01	0.59
2:C:260:LEU:HD21	9:C:1182:HOH:O	2.02	0.59
2:C:346:VAL:O	2:C:350:ARG:HG3	2.03	0.59
2:C:987:ILE:HG23	3:D:948:THR:HG21	1.84	0.59
3:D:31:THR:HG23	3:D:45:PHE:CE2	2.37	0.59
3:D:90:MET:HE2	3:D:521:PRO:HD3	1.85	0.59
3:D:490:ALA:HA	9:D:1529:HOH:O	2.03	0.59
4:E:41:GLU:N	4:E:42:PRO:HD2	2.17	0.59
2:M:92:ALA:HB2	2:M:120:LEU:HD11	1.83	0.59
2:M:208:ALA:HB1	2:M:218:VAL:HG13	1.84	0.59
2:M:482:GLU:HB3	9:M:2150:HOH:O	2.02	0.59
2:M:560:MET:O	2:M:564:MET:HE3	2.03	0.59
2:M:627:ARG:HG3	2:M:628:PHE:H	1.68	0.59
2:M:738:ASP:CB	2:M:744:ARG:HB3	2.31	0.59
2:M:816:LYS:HB2	2:M:819:VAL:HG21	1.84	0.59
2:M:1034:GLU:HA	2:M:1037:VAL:HG23	1.83	0.59
5:P:113:ILE:HG23	5:P:127:ILE:HB	1.85	0.59
5:P:400:ILE:HD11	9:P:513:HOH:O	2.02	0.59
1:A:26:GLU:HG3	1:A:27:PRO:HD3	1.85	0.59
2:C:19:THR:O	2:C:23:VAL:HG23	2.02	0.59
2:C:69:LEU:HD12	2:C:97:ARG:HB3	1.85	0.59
2:C:773:LEU:O	2:C:777:ILE:HG13	2.03	0.59
3:D:47:GLU:HA	3:D:51:GLY:O	2.03	0.59
3:D:711:LEU:C	3:D:713:ILE:H	2.11	0.59
3:D:824:ASN:HB3	9:D:2122:HOH:O	2.01	0.59
4:E:7:ASP:HB2	9:E:100:HOH:O	2.03	0.59
5:F:369:LEU:O	5:F:373:LYS:HB2	2.02	0.59
5:F:400:ILE:HD11	9:F:643:HOH:O	2.03	0.59
2:M:191:PHE:CZ	2:M:196:LEU:HB2	2.35	0.59
2:M:579:VAL:HB	2:M:890:LEU:CD2	2.33	0.59
3:N:404:GLU:HB2	9:N:1640:HOH:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:610:LYS:C	3:N:611:GLN:HG3	2.28	0.59
2:C:185:LYS:HE2	2:C:190:LYS:HG2	1.84	0.59
2:C:408:ARG:HH21	2:C:542:VAL:HG22	1.66	0.59
2:C:564:MET:HG3	2:C:997:LEU:HD11	1.84	0.59
2:C:841:ASN:HD21	2:C:845:ASN:H	1.50	0.59
2:C:1115:LEU:HB3	3:D:85:VAL:HG13	1.85	0.59
3:D:646:LYS:HE2	3:D:722:GLU:HG2	1.84	0.59
3:D:1102:THR:HG22	3:D:1222:GLY:CA	2.32	0.59
1:L:182:GLU:HB2	9:L:2617:HOH:O	2.01	0.59
2:M:585:GLU:HB3	9:M:1636:HOH:O	2.01	0.59
2:M:1053:LEU:HB3	9:N:2033:HOH:O	2.03	0.59
3:N:847:ASP:O	3:N:851:LEU:HG	2.02	0.59
3:N:897:TRP:CH2	3:N:902:LEU:HD21	2.38	0.59
3:N:1108:ARG:NH2	3:N:1198:TYR:HB2	2.16	0.59
3:N:1299:PHE:HB2	9:N:1861:HOH:O	2.02	0.59
3:N:1351:GLU:HG2	9:N:1724:HOH:O	2.02	0.59
5:P:130:VAL:HA	5:P:142:ARG:NH2	2.17	0.59
2:C:36:PRO:HG3	2:C:71:TYR:CE2	2.38	0.59
2:C:163:ILE:O	2:C:163:ILE:HG13	2.01	0.59
2:C:362:GLY:HA3	2:C:367:LEU:CD2	2.33	0.59
2:C:410:ILE:HD11	2:C:455:LEU:HB3	1.84	0.59
2:C:705:ILE:HG12	2:C:828:ALA:HB2	1.85	0.59
3:D:187:LYS:CE	3:D:199:LEU:HB3	2.27	0.59
3:D:448:GLU:HG2	3:D:448:GLU:O	2.02	0.59
5:F:361:LEU:HD22	5:F:366:ALA:HB2	1.85	0.59
1:K:158:ILE:H	1:K:166:PRO:HG3	1.68	0.59
1:L:101:LEU:HD11	9:L:1850:HOH:O	2.03	0.59
3:N:489:ARG:HH21	3:N:1389:LEU:HD11	1.67	0.59
5:P:406:ARG:O	5:P:409:LYS:HG2	2.02	0.59
1:A:161:ARG:NH1	1:A:161:ARG:HB2	2.18	0.58
2:C:294:GLU:HB3	9:C:1227:HOH:O	2.03	0.58
2:C:402:SER:OG	2:C:566:THR:HG22	2.02	0.58
2:C:437:ARG:CZ	2:C:488:ALA:HA	2.33	0.58
3:D:99:ALA:HB1	3:D:575:GLN:CD	2.28	0.58
3:D:153:LEU:CD1	3:D:157:GLU:HB2	2.33	0.58
3:D:481:MET:HG3	3:D:1388:ARG:CZ	2.32	0.58
3:D:498:VAL:HG23	3:D:499:VAL:N	2.18	0.58
3:D:592:THR:N	3:D:600:LEU:HD21	2.15	0.58
3:D:1243:THR:HB	3:D:1253:THR:HG22	1.85	0.58
3:D:1311:LEU:HD22	9:D:1836:HOH:O	2.03	0.58
4:E:83:ASP:O	4:E:86:GLN:HG2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:185:LYS:HE2	2:M:190:LYS:HE2	1.84	0.58
2:M:218:VAL:HG22	2:M:221:LEU:CD2	2.32	0.58
2:M:292:ARG:HG2	9:M:1952:HOH:O	2.01	0.58
2:M:1056:LYS:NZ	3:N:749:VAL:O	2.35	0.58
3:N:84:ILE:HG13	3:N:85:VAL:N	2.18	0.58
3:N:117:ASP:HB2	3:N:495:ARG:NH2	2.17	0.58
3:N:584:ASN:CG	3:N:590:PRO:HD2	2.27	0.58
3:N:715:ALA:HB3	3:N:764:LEU:HA	1.84	0.58
5:P:140:ARG:HG3	5:P:141:VAL:H	1.68	0.58
5:P:361:LEU:HD13	5:P:366:ALA:CB	2.33	0.58
1:A:36:LEU:O	1:A:39:PRO:HD2	2.02	0.58
2:C:877:PRO:HG2	3:D:1023:MET:CE	2.27	0.58
3:D:799:LYS:HB3	3:D:826:PRO:HG2	1.84	0.58
3:D:1109:GLU:HG2	3:D:1202:GLN:H	1.66	0.58
3:D:1177:ALA:HB3	3:D:1183:ILE:HD11	1.85	0.58
5:F:270:LYS:HG3	9:F:511:HOH:O	2.02	0.58
2:M:140:ILE:CD1	2:M:412:ALA:HA	2.32	0.58
2:M:194:VAL:HG21	2:M:221:LEU:O	2.02	0.58
2:M:300:ASP:HA	9:M:2239:HOH:O	2.03	0.58
2:M:710:ILE:HD12	2:M:790:LEU:HB2	1.85	0.58
2:M:1005:MET:CE	3:N:648:MET:HB2	2.33	0.58
3:N:206:ARG:HH12	5:P:98:GLU:CA	2.15	0.58
3:N:634:GLY:O	3:N:637:LEU:HB3	2.03	0.58
3:N:640:HIS:HE1	4:O:3:GLU:HG2	1.68	0.58
3:N:767:HIS:CD2	4:O:6:ILE:HG12	2.37	0.58
3:N:957:PRO:HG2	3:N:1007:VAL:CA	2.29	0.58
3:N:1114:THR:H	3:N:1195:GLN:NE2	2.01	0.58
1:A:39:PRO:CG	1:B:39:PRO:HG3	2.33	0.58
2:C:80:GLN:O	2:C:83:CYS:HB2	2.03	0.58
2:C:208:ALA:O	2:C:218:VAL:HG21	2.02	0.58
2:C:838:LYS:HE3	2:C:997:LEU:HD12	1.86	0.58
3:D:481:MET:HG2	3:D:482:LYS:N	2.18	0.58
3:D:992:ILE:O	3:D:995:LEU:HB3	2.03	0.58
4:E:69:LEU:HB3	9:E:140:HOH:O	2.02	0.58
5:F:207:LEU:HB3	5:F:212:LEU:HG	1.84	0.58
1:K:18:ARG:HH11	1:K:123:MET:HE1	1.66	0.58
1:L:99:LEU:HG	9:L:1066:HOH:O	2.03	0.58
2:M:212:GLY:HA3	2:M:218:VAL:HG23	1.85	0.58
2:M:654:LEU:HD11	2:M:663:ASN:ND2	2.18	0.58
2:M:694:LEU:HD11	2:M:868:ASP:HB3	1.85	0.58
2:M:838:LYS:NZ	2:M:846:LYS:HE2	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:859:PRO:O	2:M:867:VAL:HG22	2.03	0.58
3:N:169:TYR:CB	3:N:195:VAL:HG11	2.33	0.58
3:N:610:LYS:O	3:N:611:GLN:CG	2.50	0.58
1:B:46:SER:O	1:B:148:VAL:HB	2.03	0.58
2:C:110:GLU:CB	2:C:369:PRO:HG3	2.33	0.58
2:C:641:PRO:O	2:C:642:ARG:HD2	2.02	0.58
2:C:730:SER:HB2	9:C:1128:HOH:O	2.02	0.58
3:D:52:PRO:HG3	3:D:78:VAL:HG13	1.85	0.58
3:D:560:GLN:HB2	9:D:1923:HOH:O	2.03	0.58
2:M:137:VAL:HG23	2:M:391:LEU:HG	1.85	0.58
5:P:282:LEU:HD22	9:P:504:HOH:O	2.03	0.58
2:C:150:PRO:HD3	9:C:1150:HOH:O	2.04	0.58
2:C:328:LEU:HB2	2:C:433:THR:HG21	1.84	0.58
3:D:523:ASP:N	9:D:1713:HOH:O	2.30	0.58
3:D:957:PRO:HG2	3:D:1007:VAL:CA	2.30	0.58
3:D:1145:TYR:HE2	3:D:1168:MET:HB2	1.69	0.58
4:E:59:ASN:HB3	4:E:62:THR:OG1	2.03	0.58
1:K:123:MET:C	1:K:125:PRO:HD3	2.29	0.58
1:L:188:GLN:HG3	3:N:685:ASP:OD2	2.03	0.58
2:M:15:LEU:HD22	2:M:583:LEU:HD21	1.85	0.58
2:M:742:VAL:HG12	2:M:743:VAL:N	2.19	0.58
3:N:783:ARG:CZ	3:N:1029:ARG:HG3	2.32	0.58
3:N:813:LEU:O	3:N:817:GLU:HB2	2.03	0.58
1:A:218:LEU:O	1:A:222:LEU:HD12	2.04	0.58
2:C:64:LEU:HB2	2:C:359:MET:HE3	1.86	0.58
2:C:429:ASP:HB3	9:C:1177:HOH:O	2.04	0.58
2:C:911:GLU:O	2:C:914:ILE:HG22	2.03	0.58
2:C:980:GLY:HA2	9:C:1431:HOH:O	2.03	0.58
5:F:323:ASP:HA	9:F:481:HOH:O	2.02	0.58
2:M:257:VAL:HG12	2:M:263:ASP:OD1	2.04	0.58
2:M:723:THR:HG21	9:M:1850:HOH:O	2.03	0.58
3:N:481:MET:SD	3:N:1388:ARG:HD2	2.44	0.58
3:N:829:VAL:H	3:N:835:SER:HB2	1.69	0.58
3:N:965:GLU:HA	3:N:968:ASP:HB2	1.84	0.58
3:N:1018:ASN:HB3	3:N:1021:TYR:HB3	1.85	0.58
2:C:265:ARG:HG2	2:C:267:TYR:H	1.68	0.58
2:C:736:ASP:C	2:C:738:ASP:H	2.12	0.58
2:C:1034:GLU:HA	2:C:1037:VAL:HG23	1.84	0.58
3:D:586:ARG:CZ	3:D:1444:THR:HG21	2.34	0.58
3:D:710:ARG:HH21	3:D:1210:SER:HB2	1.69	0.58
3:D:792:ILE:O	3:D:878:GLY:HA3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1026:SER:HA	9:D:2416:HOH:O	2.02	0.58
3:D:1063:GLU:HB3	9:D:1948:HOH:O	2.03	0.58
3:D:1422:MET:CE	3:D:1427:SER:HA	2.34	0.58
5:F:292:ALA:HB1	5:F:299:TRP:O	2.03	0.58
2:M:151:ASP:OD2	2:M:159:ILE:HG23	2.03	0.58
2:M:1037:VAL:HG13	2:M:1049:LEU:HD11	1.86	0.58
3:N:116:LEU:HD21	3:N:464:LEU:CB	2.31	0.58
3:N:699:VAL:HG21	3:N:760:ARG:HB3	1.86	0.58
3:N:787:LEU:HD21	3:N:947:ILE:CD1	2.33	0.58
3:N:984:THR:HG22	3:N:987:GLU:H	1.68	0.58
3:N:1035:ILE:HA	3:N:1038:LEU:HD12	1.84	0.58
3:N:1145:TYR:HE2	3:N:1168:MET:HB2	1.67	0.58
1:B:108:GLU:HB3	9:B:522:HOH:O	2.02	0.58
2:C:56:GLU:OE1	2:C:64:LEU:HD22	2.03	0.58
2:C:86:LYS:CD	2:C:813:VAL:HG12	2.33	0.58
2:C:137:VAL:O	2:C:391:LEU:HD21	2.04	0.58
2:C:208:ALA:HB1	2:C:218:VAL:HG13	1.85	0.58
2:C:267:TYR:HB2	2:C:272:ALA:HB1	1.84	0.58
5:F:77:THR:O	5:F:81:VAL:HG23	2.03	0.58
5:F:406:ARG:HA	5:F:409:LYS:HG2	1.85	0.58
1:K:96:THR:HG21	9:K:4199:HOH:O	2.03	0.58
2:M:101:ILE:HD11	9:M:1739:HOH:O	2.04	0.58
2:M:583:LEU:O	2:M:587:VAL:HG23	2.04	0.58
3:N:631:ILE:HG21	3:N:745:MET:SD	2.43	0.58
3:N:1102:THR:HG22	3:N:1222:GLY:CA	2.34	0.58
1:B:57:TYR:HE1	1:B:163:ASN:HB2	1.69	0.58
1:B:105:GLY:O	1:B:132:LEU:HB3	2.04	0.58
2:C:9:ILE:HG13	2:C:9:ILE:O	2.04	0.58
3:D:686:GLU:HA	3:D:689:ASP:OD2	2.04	0.58
3:D:1114:THR:H	3:D:1195:GLN:NE2	2.01	0.58
3:D:1357:ARG:HG2	9:D:2067:HOH:O	2.04	0.58
5:F:95:THR:HG23	9:F:465:HOH:O	2.02	0.58
1:K:182:GLU:O	1:K:194:LYS:HB3	2.04	0.58
2:M:260:LEU:HA	2:M:291:ALA:CB	2.34	0.58
2:M:902:ILE:O	2:M:904:PRO:HD3	2.03	0.58
2:M:1056:LYS:O	3:N:624:ASP:HB2	2.04	0.58
2:M:1111:ILE:HG13	2:M:1112:PHE:H	1.69	0.58
1:A:133:GLU:HB3	9:C:1680:HOH:O	2.02	0.58
2:C:72:ARG:HB2	9:C:1804:HOH:O	2.04	0.58
2:C:182:VAL:HB	2:C:193:LEU:HD13	1.85	0.58
3:D:171:LEU:HD21	9:D:2083:HOH:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:633:VAL:HB	3:D:740:PHE:CE1	2.39	0.58
5:F:79:ASP:OD2	5:F:80:PRO:HD3	2.04	0.58
2:M:77:PRO:HD3	2:M:93:PRO:HD3	1.85	0.58
3:N:1286:THR:HG22	9:N:1537:HOH:O	2.02	0.58
4:O:31:LEU:HD23	4:O:35:PHE:HE1	1.68	0.58
2:C:52:PHE:CG	2:C:68:PHE:HB2	2.39	0.57
2:C:102:HIS:HB2	2:C:106:GLY:O	2.04	0.57
2:C:184:MET:SD	2:C:303:PHE:HE2	2.27	0.57
2:C:242:LEU:HD23	9:C:1218:HOH:O	2.03	0.57
2:C:404:LEU:O	2:C:407:LYS:HB2	2.04	0.57
2:C:705:ILE:HA	2:C:827:VAL:O	2.04	0.57
3:D:81:THR:HB	3:D:85:VAL:CG2	2.34	0.57
3:D:561:GLY:HA3	5:F:184:ARG:NH1	2.17	0.57
3:D:615:ARG:O	3:D:616:GLN:C	2.44	0.57
3:D:813:LEU:O	3:D:817:GLU:HB2	2.04	0.57
3:D:1290:LEU:CD2	3:D:1291:SER:H	2.17	0.57
2:M:420:ARG:NH1	2:M:422:ARG:HH21	2.02	0.57
2:M:768:THR:HG21	9:P:562:HOH:O	2.04	0.57
3:N:400:VAL:C	3:N:402:PRO:HD3	2.28	0.57
3:N:572:ARG:HH21	5:P:83:GLN:HE21	1.50	0.57
2:C:165:LEU:HD12	2:C:166:PRO:HA	1.84	0.57
3:D:15:PRO:HG3	9:D:1709:HOH:O	2.04	0.57
3:D:204:LEU:HB2	3:D:394:LEU:HG	1.84	0.57
3:D:1045:MET:HG3	3:D:1073:SER:HA	1.86	0.57
3:D:1090:ASP:CG	3:D:1238:MET:HE1	2.29	0.57
2:M:697:ARG:HD2	2:M:699:PHE:CD1	2.39	0.57
2:M:733:ALA:HB2	3:N:679:ARG:HH21	1.69	0.57
3:N:415:VAL:HG13	3:N:419:ASP:HB2	1.86	0.57
3:N:525:ARG:N	3:N:526:PRO:HD3	2.18	0.57
3:N:1209:LEU:HD23	3:N:1211:MET:CG	2.34	0.57
5:P:365:GLU:OE1	5:P:400:ILE:HD12	2.04	0.57
1:A:224:TYR:CD1	1:B:9:PRO:HD2	2.39	0.57
1:B:206:THR:CG2	1:B:209:GLU:H	2.17	0.57
2:C:676:ILE:CG2	2:C:988:VAL:HG22	2.33	0.57
2:C:715:THR:HG22	2:C:717:LEU:HG	1.86	0.57
3:D:582:LEU:HA	3:D:603:LEU:HD12	1.87	0.57
3:D:996:TRP:CE3	3:D:999:THR:HG21	2.39	0.57
3:D:1112:CYS:HB2	3:D:1195:GLN:CG	2.33	0.57
3:D:1232:PRO:HB3	3:D:1361:VAL:CG2	2.34	0.57
3:D:1282:ARG:HA	3:D:1315:ASP:OD1	2.03	0.57
1:K:58:ILE:HB	1:K:61:VAL:HB	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:62:LEU:HD12	1:L:62:LEU:H	1.69	0.57
1:L:99:LEU:HD21	1:L:122:ILE:HD11	1.86	0.57
1:L:101:LEU:HD12	1:L:114:PHE:N	2.18	0.57
2:M:144:PRO:O	2:M:276:LYS:HD3	2.04	0.57
3:N:152:LEU:HD23	3:N:152:LEU:N	2.18	0.57
3:N:493:ARG:HB2	3:N:1388:ARG:CZ	2.34	0.57
3:N:1293:PHE:CE2	3:N:1302:GLU:HB3	2.39	0.57
5:P:130:VAL:HG11	5:P:159:ILE:HB	1.86	0.57
1:A:186:LEU:CB	1:A:192:LEU:HD11	2.34	0.57
1:B:55:SER:OG	1:B:158:ILE:HD13	2.05	0.57
1:B:209:GLU:HB3	9:B:448:HOH:O	2.04	0.57
2:C:94:LEU:HD12	9:C:1545:HOH:O	2.04	0.57
1:K:9:PRO:HB3	1:K:25:LEU:HG	1.86	0.57
1:K:42:ARG:HH12	1:L:34:VAL:CB	2.13	0.57
2:M:136:ILE:HG22	2:M:336:VAL:HG22	1.86	0.57
2:M:139:GLN:O	2:M:333:ILE:HA	2.04	0.57
2:M:334:ARG:NH1	2:M:415:PRO:HG2	2.19	0.57
3:N:18:ILE:HD12	3:N:518:PRO:CG	2.34	0.57
3:N:1115:THR:HG22	9:N:1591:HOH:O	2.04	0.57
1:A:227:ASN:ND2	1:A:227:ASN:H	2.03	0.57
2:C:100:LEU:HD12	2:C:101:ILE:O	2.05	0.57
2:C:166:PRO:HD3	2:C:265:ARG:CG	2.34	0.57
2:C:611:ILE:HG22	2:C:613:VAL:HG13	1.86	0.57
9:C:1139:HOH:O	5:F:373:LYS:HB3	2.03	0.57
3:D:81:THR:O	3:D:82:LYS:O	2.21	0.57
3:D:189:GLN:HG3	3:D:190:GLU:N	2.20	0.57
3:D:195:VAL:HG13	9:D:2268:HOH:O	2.04	0.57
3:D:434:ARG:HB2	3:D:447:VAL:CG2	2.35	0.57
4:E:63:TRP:O	4:E:67:GLU:HG3	2.05	0.57
1:K:16:GLN:HG2	1:K:16:GLN:O	2.05	0.57
1:K:18:ARG:O	1:K:207:PRO:HD3	2.05	0.57
1:L:132:LEU:HD21	1:L:136:GLY:O	2.04	0.57
2:M:56:GLU:OE1	2:M:64:LEU:HD22	2.05	0.57
2:M:480:THR:HB	9:M:2150:HOH:O	2.03	0.57
3:N:480:GLU:HG3	3:N:480:GLU:O	2.04	0.57
3:N:614:PHE:CD1	3:N:615:ARG:N	2.72	0.57
3:N:1109:GLU:CD	3:N:1202:GLN:H	2.12	0.57
4:O:41:GLU:N	4:O:42:PRO:HD2	2.20	0.57
1:B:143:ARG:HD2	1:B:160:ASP:OD2	2.04	0.57
2:C:15:LEU:HD22	2:C:583:LEU:HD11	1.85	0.57
2:C:142:ARG:HD3	9:C:1347:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:480:THR:HG22	2:C:481:ASP:N	2.19	0.57
3:D:576:GLU:HB2	9:D:1696:HOH:O	2.03	0.57
3:D:610:LYS:CD	7:D:1527:MXP:H15A	2.34	0.57
3:D:1179:GLU:HA	9:D:2069:HOH:O	2.05	0.57
5:F:278:LEU:HB2	5:F:286:PRO:HG2	1.85	0.57
2:M:41:ASN:HD22	2:M:41:ASN:N	1.89	0.57
2:M:176:VAL:C	2:M:178:PRO:HD3	2.29	0.57
2:M:420:ARG:HG3	2:M:422:ARG:HG2	1.87	0.57
2:M:959:PRO:HD3	9:M:1887:HOH:O	2.04	0.57
3:N:455:ARG:HD2	9:N:2063:HOH:O	2.05	0.57
3:N:827:ILE:HB	9:N:2048:HOH:O	2.04	0.57
3:N:850:LEU:HD12	3:N:850:LEU:N	2.15	0.57
5:P:147:LEU:HB3	9:P:604:HOH:O	2.04	0.57
5:P:394:ARG:HA	5:P:397:ILE:HD12	1.87	0.57
2:C:21:ILE:H	2:C:21:ILE:HD12	1.70	0.57
2:C:430:VAL:HG11	3:D:1074:SER:OG	2.04	0.57
2:C:705:ILE:HB	9:C:1287:HOH:O	2.04	0.57
2:C:897:LEU:HD23	2:C:899:GLN:NE2	2.19	0.57
3:D:82:LYS:HE2	9:D:1577:HOH:O	2.05	0.57
2:M:1002:GLU:HG3	3:N:744:GLN:NE2	2.20	0.57
3:N:1037:GLN:HG2	3:N:1042:ARG:HB3	1.85	0.57
3:N:1189:ARG:NH1	3:N:1203:LYS:HB2	2.20	0.57
2:C:238:LEU:HD12	9:C:1705:HOH:O	2.05	0.57
2:C:724:ARG:O	2:C:734:LEU:HD21	2.05	0.57
2:C:774:LEU:HA	2:C:777:ILE:HD12	1.87	0.57
2:C:1008:ARG:NH1	2:C:1028:GLY:HA2	2.15	0.57
5:F:113:ILE:HG23	5:F:127:ILE:HB	1.87	0.57
1:K:178:ALA:HB2	2:M:864:GLY:H	1.69	0.57
1:L:39:PRO:O	1:L:43:ILE:HG12	2.05	0.57
2:M:189:ARG:HD2	9:M:2270:HOH:O	2.04	0.57
3:N:992:ILE:O	3:N:995:LEU:HB3	2.05	0.57
2:C:206:THR:HG21	9:C:1559:HOH:O	2.04	0.57
2:C:322:VAL:HG21	9:C:1390:HOH:O	2.04	0.57
2:C:341:THR:HG21	9:C:1365:HOH:O	2.05	0.57
2:C:615:TYR:HB2	9:C:1584:HOH:O	2.05	0.57
3:D:546:ARG:HA	9:D:1595:HOH:O	2.05	0.57
3:D:820:GLU:HG3	3:D:836:VAL:CG1	2.34	0.57
3:D:820:GLU:HG3	3:D:836:VAL:HG11	1.86	0.57
3:D:956:ILE:HG12	3:D:1039:CYS:O	2.05	0.57
3:D:1376:MET:HG2	3:D:1421:LEU:HD12	1.86	0.57
2:M:395:LYS:HE2	2:M:403:SER:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:876:VAL:HA	9:M:1870:HOH:O	2.03	0.57
2:M:939:ARG:HD3	2:M:975:TYR:CE2	2.40	0.57
3:N:77:GLY:O	3:N:78:VAL:HG23	2.05	0.57
3:N:834:THR:HB	3:N:838:ARG:HB2	1.86	0.57
4:O:54:LEU:O	4:O:54:LEU:HD23	2.05	0.57
5:P:138:SER:O	5:P:141:VAL:HG12	2.03	0.57
1:B:101:LEU:HD11	1:B:113:ASP:HB2	1.87	0.57
2:C:477:GLY:O	2:C:508:ILE:HG12	2.05	0.57
2:C:838:LYS:NZ	2:C:846:LYS:HE2	2.20	0.57
2:C:877:PRO:CG	3:D:1023:MET:HE2	2.27	0.57
3:D:774:SER:C	3:D:776:GLU:H	2.13	0.57
3:D:1443:THR:HG22	9:D:1543:HOH:O	2.03	0.57
1:K:18:ARG:HD2	1:K:123:MET:CE	2.35	0.57
1:K:91:ASN:OD1	1:K:92:PRO:HD2	2.05	0.57
1:K:227:ASN:H	1:K:227:ASN:ND2	2.02	0.57
1:L:44:LEU:HD21	1:L:199:ILE:HD13	1.85	0.57
3:N:171:LEU:HD13	9:N:1797:HOH:O	2.05	0.57
3:N:409:VAL:CG1	3:N:435:VAL:HG11	2.33	0.57
3:N:1295:GLU:HB3	3:N:1300:SER:HB3	1.87	0.57
3:N:1390:LEU:HB2	9:N:1897:HOH:O	2.05	0.57
4:O:33:HIS:CE1	4:O:89:MET:HG2	2.39	0.57
5:P:361:LEU:HD13	5:P:366:ALA:HB2	1.86	0.57
5:P:393:THR:O	5:P:397:ILE:HG13	2.05	0.57
1:A:34:VAL:HB	1:B:42:ARG:HH21	1.69	0.56
1:A:178:ALA:HB1	9:C:1688:HOH:O	2.05	0.56
1:B:201:THR:HG21	1:B:205:VAL:O	2.05	0.56
2:C:207:LEU:HD22	2:C:221:LEU:HD22	1.87	0.56
2:C:457:ALA:N	2:C:540:PHE:O	2.36	0.56
2:C:857:ASP:HB2	2:C:978:ARG:HB3	1.85	0.56
2:C:1038:TRP:HA	2:C:1041:GLU:HB2	1.87	0.56
9:C:1255:HOH:O	5:F:354:LEU:HD11	2.04	0.56
3:D:32:ILE:HG22	5:F:258:ILE:HD12	1.87	0.56
3:D:101:HIS:ND1	3:D:103:TRP:HB2	2.16	0.56
3:D:1090:ASP:HA	3:D:1093:TYR:HB2	1.87	0.56
3:D:1258:ARG:CZ	3:D:1262:LEU:HD11	2.36	0.56
2:M:144:PRO:HA	2:M:163:ILE:CG1	2.35	0.56
2:M:404:LEU:O	2:M:407:LYS:HB2	2.05	0.56
2:M:665:PHE:HB2	9:M:1978:HOH:O	2.04	0.56
2:M:1105:LYS:HG3	9:M:1731:HOH:O	2.04	0.56
3:N:957:PRO:HG3	3:N:1010:ASN:HD22	1.70	0.56
3:N:1231:GLU:HB3	3:N:1232:PRO:HD3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1384:PRO:HG3	3:N:1389:LEU:HA	1.86	0.56
3:N:1462:LEU:HD22	3:N:1472:ILE:HG23	1.87	0.56
1:A:149:GLY:O	1:A:171:PHE:HB2	2.06	0.56
1:A:158:ILE:H	1:A:166:PRO:HG3	1.70	0.56
1:A:206:THR:HG22	1:A:209:GLU:H	1.69	0.56
2:C:252:LYS:HE2	9:C:1771:HOH:O	2.04	0.56
2:C:713:ARG:HH12	3:D:531:ASP:CG	2.14	0.56
2:C:766:GLU:HG2	2:C:772:ARG:NH1	2.19	0.56
2:C:1115:LEU:HD23	3:D:85:VAL:HA	1.85	0.56
3:D:428:LYS:HD3	9:D:1840:HOH:O	2.05	0.56
3:D:894:LYS:HB3	9:D:2117:HOH:O	2.05	0.56
3:D:1410:GLU:HG3	9:D:1966:HOH:O	2.04	0.56
1:K:103:ALA:CB	1:K:107:LYS:HE2	2.35	0.56
1:K:224:TYR:HB3	1:L:9:PRO:HB2	1.87	0.56
1:L:57:TYR:O	1:L:140:MET:HA	2.05	0.56
1:L:123:MET:O	1:L:125:PRO:HD3	2.05	0.56
2:M:102:HIS:HB2	2:M:106:GLY:O	2.05	0.56
2:M:110:GLU:H	2:M:368:THR:HG21	1.69	0.56
2:M:141:HIS:HB3	2:M:418:LEU:CG	2.35	0.56
2:M:722:ILE:HG23	2:M:722:ILE:O	2.04	0.56
3:N:2:LYS:HD3	9:N:2388:HOH:O	2.04	0.56
3:N:106:LYS:HB3	9:N:2026:HOH:O	2.05	0.56
3:N:1087:ARG:HG2	3:N:1238:MET:CB	2.34	0.56
3:N:1288:GLU:HA	9:N:1542:HOH:O	2.04	0.56
4:O:45:ARG:NH2	4:O:55:PHE:HB3	2.20	0.56
1:A:88:ARG:NH2	1:A:90:LEU:HD21	2.20	0.56
1:A:198:ARG:HB2	1:A:200:TRP:CH2	2.41	0.56
2:C:8:ARG:HB3	9:C:1721:HOH:O	2.05	0.56
2:C:435:TYR:C	2:C:437:ARG:H	2.13	0.56
2:C:1018:GLN:NE2	3:D:87:ARG:HH12	2.03	0.56
2:C:1097:LEU:HD12	2:C:1097:LEU:N	2.20	0.56
3:D:81:THR:HG22	3:D:82:LYS:N	2.21	0.56
3:D:165:LYS:HA	9:D:2176:HOH:O	2.05	0.56
3:D:169:TYR:CE1	3:D:197:SER:HB2	2.40	0.56
3:D:611:GLN:NE2	3:D:1439:SER:HB3	2.20	0.56
3:D:661:MET:HE3	3:D:673:ALA:CB	2.35	0.56
3:D:697:GLY:C	9:D:1581:HOH:O	2.48	0.56
3:D:1007:VAL:HG23	3:D:1008:PHE:N	2.21	0.56
4:E:45:ARG:NH2	4:E:55:PHE:HB3	2.20	0.56
4:E:54:LEU:CD2	4:E:63:TRP:HE1	2.18	0.56
5:F:88:ILE:HG12	5:F:193:ARG:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:203:THR:HG22	5:F:204:GLY:N	2.20	0.56
1:K:5:LYS:O	1:K:8:ALA:HB2	2.05	0.56
1:K:127:LEU:C	1:K:127:LEU:HD12	2.30	0.56
1:K:161:ARG:NH1	1:K:161:ARG:HB2	2.19	0.56
1:L:34:VAL:HG22	1:L:181:VAL:HG21	1.85	0.56
1:L:36:LEU:O	1:L:39:PRO:HD2	2.04	0.56
1:L:71:VAL:HG22	1:L:132:LEU:HD12	1.87	0.56
1:L:169:ALA:HB1	1:L:171:PHE:CE2	2.40	0.56
2:M:52:PHE:CG	2:M:68:PHE:HB2	2.40	0.56
2:M:328:LEU:HD23	2:M:467:ILE:HB	1.87	0.56
2:M:378:LEU:HG	2:M:382:ILE:HD11	1.87	0.56
2:M:480:THR:HG22	2:M:481:ASP:N	2.19	0.56
2:M:631:SER:HB3	2:M:637:LEU:HD21	1.87	0.56
2:M:733:ALA:HB2	3:N:679:ARG:HH22	1.66	0.56
2:M:863:ASP:O	2:M:865:THR:N	2.37	0.56
2:M:1015:LEU:HD12	9:P:651:HOH:O	2.04	0.56
3:N:114:THR:O	3:N:495:ARG:HG3	2.06	0.56
3:N:799:LYS:HB3	3:N:826:PRO:CG	2.34	0.56
3:N:1169:ASP:HA	9:N:1842:HOH:O	2.04	0.56
3:N:1232:PRO:HB3	3:N:1361:VAL:CG2	2.33	0.56
3:N:1356:TYR:HD2	3:N:1363:LEU:HD23	1.69	0.56
3:N:1388:ARG:HG3	3:N:1389:LEU:N	2.19	0.56
1:B:132:LEU:CD1	1:B:138:LEU:HD12	2.35	0.56
2:C:770:GLU:CG	3:D:65:ARG:HH12	2.17	0.56
3:D:394:LEU:HD21	9:D:1995:HOH:O	2.06	0.56
3:D:640:HIS:HB2	9:E:156:HOH:O	2.05	0.56
2:M:292:ARG:HD2	2:M:299:LYS:HG2	1.86	0.56
2:M:565:GLN:OE1	2:M:842:ARG:HG2	2.05	0.56
2:M:662:GLU:HB3	9:M:1978:HOH:O	2.05	0.56
3:N:113:GLY:HA3	3:N:120:ALA:HA	1.88	0.56
3:N:560:GLN:HG2	5:P:221:ILE:HG21	1.86	0.56
1:A:66:SER:O	1:A:75:VAL:HG23	2.05	0.56
2:C:350:ARG:HA	2:C:353:ARG:HD2	1.87	0.56
2:C:413:LEU:HB3	9:C:1518:HOH:O	2.05	0.56
2:C:838:LYS:HB2	2:C:848:VAL:HG22	1.86	0.56
2:C:979:THR:HG23	2:C:981:GLU:N	2.18	0.56
3:D:55:ASP:O	3:D:80:VAL:HG11	2.06	0.56
3:D:1092:GLY:HA3	9:D:2012:HOH:O	2.05	0.56
3:D:1389:LEU:HD12	3:D:1390:LEU:N	2.19	0.56
5:F:140:ARG:HG3	5:F:141:VAL:H	1.69	0.56
1:K:34:VAL:HG13	2:M:939:ARG:HH21	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:58:ILE:HG22	1:L:137:ARG:NH2	2.17	0.56
2:M:69:LEU:HD12	2:M:97:ARG:HB3	1.86	0.56
2:M:114:PHE:CE2	5:P:283:GLY:HA3	2.40	0.56
2:M:418:LEU:N	2:M:418:LEU:HD12	2.20	0.56
2:M:464:LEU:HD12	2:M:465:GLY:H	1.70	0.56
2:M:611:ILE:HG22	2:M:613:VAL:HG13	1.88	0.56
3:N:45:PHE:HD1	3:N:86:ARG:HH22	1.52	0.56
3:N:102:ILE:HD12	3:N:579:ASP:HB3	1.86	0.56
3:N:119:SER:HB2	3:N:123:LEU:CB	2.34	0.56
3:N:143:ASN:HD21	3:N:145:VAL:HG12	1.70	0.56
3:N:592:THR:N	3:N:600:LEU:HD21	2.18	0.56
3:N:814:ALA:O	3:N:818:ARG:HG3	2.05	0.56
3:N:1243:THR:HG22	3:N:1244:GLY:H	1.71	0.56
5:P:295:MET:HE3	5:P:299:TRP:CZ3	2.41	0.56
1:A:198:ARG:C	1:A:199:ILE:HD12	2.29	0.56
1:B:2:LEU:HD12	1:B:3:ASP:HB2	1.86	0.56
1:B:15:THR:HB	9:B:419:HOH:O	2.05	0.56
2:C:470:PRO:HD3	2:C:485:TYR:CE2	2.41	0.56
2:C:785:VAL:HG21	9:C:1244:HOH:O	2.05	0.56
3:D:169:TYR:CB	3:D:195:VAL:HG11	2.34	0.56
3:D:842:VAL:HG23	9:D:1531:HOH:O	2.06	0.56
3:D:996:TRP:HE3	3:D:999:THR:HG21	1.70	0.56
3:D:1495:ILE:HG12	4:E:80:VAL:CG1	2.35	0.56
5:F:291:ILE:HG23	5:F:304:VAL:HG21	1.87	0.56
1:K:69:PRO:C	1:K:71:VAL:H	2.13	0.56
2:M:141:HIS:HB2	9:M:2163:HOH:O	2.06	0.56
2:M:369:PRO:HD2	9:M:1905:HOH:O	2.06	0.56
2:M:408:ARG:HH21	2:M:542:VAL:CG2	2.17	0.56
2:M:510:ALA:HB3	2:M:513:VAL:CG2	2.36	0.56
2:M:510:ALA:HB3	2:M:513:VAL:HG23	1.88	0.56
2:M:660:ALA:HB3	9:M:1638:HOH:O	2.06	0.56
3:N:39:PRO:HB3	3:N:45:PHE:C	2.31	0.56
3:N:72:VAL:HG13	9:N:1744:HOH:O	2.05	0.56
3:N:485:SER:O	3:N:489:ARG:HB3	2.05	0.56
3:N:564:GLU:HA	3:N:567:ILE:HD13	1.88	0.56
3:N:637:LEU:HD11	3:N:642:CYS:N	2.21	0.56
3:N:711:LEU:C	3:N:713:ILE:H	2.12	0.56
3:N:1113:GLY:N	3:N:1195:GLN:HE22	2.03	0.56
5:P:113:ILE:HA	5:P:116:LEU:HD12	1.88	0.56
1:B:115:LEU:HD23	9:B:435:HOH:O	2.04	0.56
2:C:28:ARG:NH1	2:C:463:GLU:HG2	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:80:GLN:HB2	9:C:1803:HOH:O	2.04	0.56
2:C:176:VAL:HG12	2:C:182:VAL:CG1	2.36	0.56
2:C:607:ASP:HB3	2:C:609:ASN:H	1.70	0.56
3:D:1336:LEU:HA	3:D:1344:VAL:HG22	1.87	0.56
2:M:15:LEU:HD21	2:M:583:LEU:HD11	1.88	0.56
2:M:34:VAL:HG21	2:M:38:LYS:HD3	1.87	0.56
2:M:97:ARG:HG3	9:M:2157:HOH:O	2.05	0.56
2:M:857:ASP:HB2	2:M:978:ARG:HB3	1.87	0.56
3:N:602:SER:O	3:N:606:ILE:HG13	2.06	0.56
3:N:800:LYS:HE2	3:N:804:LEU:HD13	1.88	0.56
3:N:1007:VAL:HG23	3:N:1008:PHE:N	2.21	0.56
3:N:1495:ILE:HG12	4:O:80:VAL:CG1	2.35	0.56
5:P:108:GLU:HG3	5:P:176:ILE:HG21	1.88	0.56
5:P:138:SER:HB2	5:P:140:ARG:HG2	1.88	0.56
9:A:318:HOH:O	2:C:627:ARG:HA	2.05	0.56
2:C:1101:THR:HB	3:D:5:VAL:CG1	2.35	0.56
3:D:485:SER:O	3:D:489:ARG:HB3	2.06	0.56
5:F:101:GLU:HB3	5:F:105:LYS:HE3	1.87	0.56
5:F:225:GLU:HB3	9:F:605:HOH:O	2.06	0.56
1:K:20:TYR:CE2	1:K:22:GLU:HG3	2.41	0.56
2:M:167:LYS:HB2	9:M:1774:HOH:O	2.06	0.56
3:N:111:LYS:HZ3	3:N:1452:ILE:HG21	1.69	0.56
3:N:443:VAL:HG22	3:N:444:VAL:N	2.20	0.56
3:N:1047:LYS:HA	3:N:1053:PHE:CE1	2.41	0.56
3:N:1091:SER:HA	9:N:1706:HOH:O	2.06	0.56
4:O:84:ARG:HG3	9:O:2468:HOH:O	2.06	0.56
1:A:133:GLU:HG2	1:A:134:GLU:N	2.20	0.56
2:C:165:LEU:HD13	9:C:1292:HOH:O	2.05	0.56
2:C:580:MET:SD	2:C:584:GLU:HG3	2.46	0.56
2:C:750:LYS:HD2	3:D:681:ARG:HE	1.70	0.56
3:D:403:PHE:CD1	3:D:405:ASP:O	2.53	0.56
4:E:33:HIS:HB2	4:E:37:ASN:ND2	2.21	0.56
1:K:72:LYS:HE2	9:M:2012:HOH:O	2.05	0.56
2:M:193:LEU:HD11	9:M:1951:HOH:O	2.04	0.56
2:M:625:LEU:HB3	2:M:639:GLN:HB2	1.86	0.56
2:M:1115:LEU:HB3	3:N:85:VAL:CG1	2.35	0.56
3:N:1492:LEU:HD23	9:N:2099:HOH:O	2.04	0.56
4:O:95:VAL:HG22	9:O:1302:HOH:O	2.06	0.56
5:P:193:ARG:HD2	9:P:514:HOH:O	2.05	0.56
5:P:375:LEU:HD23	9:P:476:HOH:O	2.05	0.56
1:A:138:LEU:HD21	9:A:355:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:LYS:O	1:B:7:LYS:HG3	2.05	0.56
2:C:365:ASP:HB3	9:C:1410:HOH:O	2.06	0.56
2:C:729:LEU:HD22	9:D:1907:HOH:O	2.06	0.56
3:D:126:VAL:O	3:D:132:TYR:HD1	1.89	0.56
3:D:925:GLU:HB3	4:E:2:ALA:HB3	1.88	0.56
3:D:1113:GLY:N	3:D:1195:GLN:NE2	2.53	0.56
3:D:1204:CYS:HB3	9:D:1762:HOH:O	2.06	0.56
1:K:88:ARG:HG3	1:K:88:ARG:O	2.06	0.56
2:M:158:TYR:CE1	2:M:313:LEU:HG	2.40	0.56
2:M:235:LEU:HD11	9:M:2260:HOH:O	2.06	0.56
2:M:328:LEU:CD2	2:M:437:ARG:HB3	2.36	0.56
2:M:626:ARG:HB2	2:M:639:GLN:HE21	1.70	0.56
2:M:670:GLN:HE22	2:M:699:PHE:CA	2.19	0.56
2:M:1109:VAL:HG11	3:N:5:VAL:HG22	1.87	0.56
3:N:118:LEU:O	3:N:120:ALA:N	2.39	0.56
3:N:486:ARG:HD3	3:N:489:ARG:HD3	1.87	0.56
3:N:1466:VAL:HG23	3:N:1472:ILE:CD1	2.35	0.56
1:B:99:LEU:HD13	9:B:416:HOH:O	2.06	0.55
1:B:158:ILE:HG22	1:B:159:LYS:N	2.20	0.55
2:C:630:ARG:HG3	9:C:1287:HOH:O	2.07	0.55
3:D:80:VAL:N	9:D:1536:HOH:O	2.40	0.55
3:D:806:PHE:HE1	3:D:813:LEU:HB3	1.70	0.55
3:D:1035:ILE:HA	3:D:1038:LEU:CD1	2.36	0.55
3:D:1087:ARG:HD3	3:D:1236:LEU:O	2.06	0.55
5:F:416:ARG:HD3	5:F:419:ARG:HD3	1.89	0.55
1:K:88:ARG:NH2	1:K:90:LEU:HD21	2.21	0.55
1:L:85:LEU:HD13	1:L:127:LEU:HD23	1.88	0.55
1:L:206:THR:HG22	1:L:209:GLU:H	1.71	0.55
2:M:12:VAL:CG1	2:M:534:VAL:HG13	2.35	0.55
2:M:100:LEU:HD12	2:M:101:ILE:O	2.06	0.55
2:M:172:ILE:HA	2:M:185:LYS:O	2.07	0.55
2:M:208:ALA:HB1	2:M:218:VAL:CG1	2.36	0.55
3:N:421:LEU:HG	3:N:429:SER:HB3	1.88	0.55
3:N:592:THR:HG23	9:N:1987:HOH:O	2.06	0.55
4:O:54:LEU:HA	4:O:58:PRO:HG2	1.88	0.55
5:P:95:THR:HB	9:P:638:HOH:O	2.05	0.55
2:C:34:VAL:HG21	2:C:38:LYS:HD3	1.88	0.55
2:C:416:GLY:HA3	9:C:1419:HOH:O	2.06	0.55
2:C:605:LYS:HG3	2:C:612:VAL:HB	1.88	0.55
2:C:657:ASP:OD1	2:C:661:SER:HB2	2.06	0.55
2:C:670:GLN:O	2:C:672:VAL:HG12	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:408:GLU:HB3	9:D:2146:HOH:O	2.05	0.55
3:D:1305:LEU:HD13	9:D:1836:HOH:O	2.06	0.55
3:D:1486:VAL:HG12	4:E:73:LEU:HD22	1.89	0.55
4:E:76:GLY:HA3	4:E:79:LEU:HD12	1.88	0.55
5:F:234:LYS:HG3	5:F:236:SER:H	1.71	0.55
2:M:473:ARG:HB3	9:M:2150:HOH:O	2.05	0.55
2:M:598:GLU:O	2:M:651:LYS:HG3	2.06	0.55
2:M:987:ILE:HG23	3:N:948:THR:HG21	1.87	0.55
2:M:1008:ARG:NH1	2:M:1028:GLY:HA2	2.17	0.55
3:N:561:GLY:HA3	5:P:184:ARG:HH12	1.71	0.55
5:P:261:PRO:O	5:P:265:VAL:HG23	2.07	0.55
1:B:111:ALA:HB2	9:B:460:HOH:O	2.05	0.55
2:C:22:GLN:HE22	2:C:135:VAL:HG12	1.71	0.55
2:C:144:PRO:HA	2:C:163:ILE:CG1	2.37	0.55
2:C:149:THR:HA	9:C:1150:HOH:O	2.05	0.55
2:C:172:ILE:HA	2:C:185:LYS:O	2.07	0.55
2:C:197:LEU:HD22	2:C:202:TYR:CD2	2.38	0.55
2:C:1105:LYS:O	2:C:1107:ASN:N	2.38	0.55
3:D:133:ILE:HG22	3:D:455:ARG:C	2.31	0.55
3:D:421:LEU:HG	3:D:429:SER:HB3	1.87	0.55
3:D:537:THR:C	5:F:317:LEU:HB2	2.32	0.55
3:D:646:LYS:HD3	9:D:1609:HOH:O	2.06	0.55
9:D:1806:HOH:O	5:F:309:LYS:HB3	2.07	0.55
1:K:184:THR:HG23	1:K:192:LEU:HD12	1.87	0.55
1:L:58:ILE:HD13	1:L:140:MET:HB3	1.88	0.55
2:M:654:LEU:HD11	2:M:663:ASN:HD22	1.70	0.55
2:M:770:GLU:HG3	3:N:65:ARG:HH12	1.70	0.55
3:N:19:ARG:NH2	9:N:1827:HOH:O	2.40	0.55
3:N:1463:LYS:O	3:N:1467:ILE:HG13	2.06	0.55
1:B:59:GLU:HG2	9:B:405:HOH:O	2.05	0.55
1:B:212:ASN:O	1:B:215:VAL:HG22	2.05	0.55
2:C:139:GLN:HG2	2:C:140:ILE:H	1.71	0.55
2:C:208:ALA:HB1	2:C:218:VAL:CG1	2.36	0.55
2:C:583:LEU:O	2:C:587:VAL:HG23	2.06	0.55
2:C:1019:GLN:NE2	3:D:621:LYS:HA	2.20	0.55
2:C:1094:ALA:HB1	3:D:603:LEU:HD22	1.88	0.55
3:D:82:LYS:HG2	9:D:1675:HOH:O	2.06	0.55
4:E:86:GLN:O	4:E:90:GLU:HG3	2.06	0.55
5:F:138:SER:O	5:F:141:VAL:HG12	2.07	0.55
1:L:199:ILE:HD11	1:L:211:LEU:HD13	1.89	0.55
2:M:80:GLN:HB2	9:M:1668:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:261:ILE:HG21	9:M:2030:HOH:O	2.05	0.55
2:M:410:ILE:HD12	2:M:410:ILE:N	2.22	0.55
2:M:578:VAL:HG11	2:M:991:GLN:CB	2.35	0.55
2:M:589:ARG:HD2	9:M:1929:HOH:O	2.05	0.55
2:M:641:PRO:O	2:M:642:ARG:HD2	2.07	0.55
2:M:726:ILE:HG22	2:M:726:ILE:O	2.06	0.55
3:N:111:LYS:HE3	3:N:1449:GLU:HG2	1.88	0.55
3:N:128:TYR:HB3	3:N:129:PHE:HD1	1.71	0.55
3:N:703:ASN:HB2	3:N:713:ILE:HG12	1.89	0.55
3:N:1243:THR:HB	3:N:1253:THR:HG22	1.87	0.55
3:N:1281:VAL:HG23	3:N:1317:ASP:O	2.07	0.55
5:P:317:LEU:O	5:P:329:TYR:HB3	2.07	0.55
1:B:65:PHE:HB2	9:B:397:HOH:O	2.05	0.55
2:C:36:PRO:HB3	9:C:1632:HOH:O	2.06	0.55
2:C:770:GLU:HG3	3:D:65:ARG:HH12	1.70	0.55
3:D:16:GLU:HG3	9:D:1656:HOH:O	2.06	0.55
3:D:1398:TRP:HB2	9:D:2042:HOH:O	2.07	0.55
1:K:16:GLN:O	1:K:16:GLN:CG	2.55	0.55
2:M:73:LEU:HD23	2:M:94:LEU:HB2	1.88	0.55
2:M:701:THR:HG23	2:M:832:LYS:HA	1.88	0.55
2:M:877:PRO:HG3	3:N:1020:LEU:HD12	1.89	0.55
3:N:615:ARG:O	3:N:616:GLN:C	2.46	0.55
3:N:741:ASP:OD2	3:N:741:ASP:N	2.33	0.55
3:N:829:VAL:HG11	9:N:1877:HOH:O	2.07	0.55
3:N:1066:THR:HG22	3:N:1069:GLU:HG3	1.86	0.55
2:C:199:VAL:HG13	2:C:235:LEU:HG	1.89	0.55
2:C:318:PRO:HD2	9:C:1596:HOH:O	2.07	0.55
3:D:187:LYS:HG3	3:D:199:LEU:HB3	1.89	0.55
3:D:1095:THR:CG2	3:D:1230:GLY:HA3	2.36	0.55
5:F:373:LYS:HG3	9:F:450:HOH:O	2.06	0.55
1:K:74:ASP:O	1:K:78:ILE:HG13	2.06	0.55
1:K:198:ARG:HB2	1:K:200:TRP:CZ3	2.42	0.55
2:M:53:PRO:HD3	9:M:1709:HOH:O	2.06	0.55
2:M:128:ILE:HG22	9:M:1824:HOH:O	2.06	0.55
2:M:139:GLN:HE22	2:M:415:PRO:CG	2.19	0.55
2:M:736:ASP:C	2:M:738:ASP:H	2.13	0.55
2:M:918:LEU:HD23	2:M:967:PHE:O	2.07	0.55
3:N:586:ARG:HB2	9:N:1869:HOH:O	2.06	0.55
4:O:29:GLN:NE2	4:O:89:MET:HE3	2.22	0.55
2:C:9:ILE:HG12	2:C:907:ASP:OD2	2.07	0.55
2:C:172:ILE:H	2:C:172:ILE:HD12	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:362:GLY:HA3	2:C:367:LEU:HD23	1.89	0.55
2:C:889:HIS:HE1	3:D:951:ILE:H	1.54	0.55
3:D:924:MET:O	3:D:927:THR:HB	2.06	0.55
3:D:1277:ILE:HD11	3:D:1301:LYS:HD2	1.89	0.55
4:E:29:GLN:NE2	4:E:89:MET:HE3	2.22	0.55
5:F:256:ARG:HB2	9:F:658:HOH:O	2.07	0.55
1:K:94:LEU:HD13	9:K:1900:HOH:O	2.06	0.55
1:K:176:ARG:O	1:K:200:TRP:HE3	1.88	0.55
2:M:114:PHE:CD1	2:M:114:PHE:N	2.73	0.55
2:M:195:LEU:HD12	2:M:234:ALA:HB1	1.89	0.55
2:M:346:VAL:O	2:M:350:ARG:HG3	2.07	0.55
2:M:557:ARG:HD2	2:M:879:ARG:HG2	1.89	0.55
2:M:580:MET:O	2:M:902:ILE:HA	2.07	0.55
2:M:937:ASP:OD2	2:M:939:ARG:HD2	2.06	0.55
2:M:1010:THR:HG21	5:P:341:PRO:HB2	1.89	0.55
3:N:906:GLN:HB3	3:N:911:LEU:HD11	1.87	0.55
3:N:1312:LEU:HD22	9:N:2126:HOH:O	2.06	0.55
3:N:1432:LYS:HG3	3:N:1433:SER:H	1.72	0.55
3:D:111:LYS:HE2	3:D:498:VAL:HG12	1.88	0.55
3:D:482:LYS:HD2	9:D:2211:HOH:O	2.07	0.55
3:D:634:GLY:O	3:D:637:LEU:HB3	2.05	0.55
3:D:760:ARG:HD2	4:E:3:GLU:OE2	2.06	0.55
3:D:1311:LEU:HD23	3:D:1311:LEU:H	1.71	0.55
3:D:1397:LYS:HG2	9:D:1681:HOH:O	2.06	0.55
2:M:49:ARG:HA	9:M:1709:HOH:O	2.07	0.55
2:M:86:LYS:HD3	2:M:813:VAL:HG12	1.89	0.55
2:M:368:THR:HG22	9:M:2230:HOH:O	2.05	0.55
2:M:966:LEU:HD21	2:M:986:PRO:HG3	1.88	0.55
3:N:126:VAL:O	3:N:132:TYR:HD1	1.90	0.55
3:N:126:VAL:HG11	3:N:152:LEU:HD12	1.88	0.55
3:N:646:LYS:HD3	9:N:2006:HOH:O	2.06	0.55
3:N:843:PHE:CD2	3:N:849:ALA:HA	2.42	0.55
3:N:843:PHE:CE1	3:N:864:VAL:HG11	2.32	0.55
3:N:1177:ALA:HB3	3:N:1183:ILE:HD11	1.88	0.55
3:N:1220:ALA:O	3:N:1224:VAL:HG23	2.07	0.55
3:N:1281:VAL:HG21	3:N:1313:VAL:CG2	2.37	0.55
3:N:1396:GLU:O	3:N:1400:VAL:HG23	2.07	0.55
1:A:99:LEU:HB3	1:A:114:PHE:CD2	2.41	0.55
2:C:2:GLU:HG3	2:C:899:GLN:CB	2.29	0.55
2:C:551:GLU:OE1	2:C:906:PHE:HA	2.07	0.55
2:C:567:GLN:HB2	2:C:997:LEU:HD22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:575:GLN:OE1	2:C:670:GLN:HB3	2.07	0.55
2:C:737:LEU:HD12	2:C:754:ILE:HB	1.88	0.55
2:C:1054:THR:CG2	2:C:1079:PRO:HB3	2.28	0.55
3:D:714:GLN:OE1	3:D:765:SER:HB2	2.07	0.55
3:D:890:VAL:HA	9:D:1617:HOH:O	2.07	0.55
3:D:1147:ARG:O	3:D:1166:LEU:HD23	2.06	0.55
3:D:1293:PHE:CE2	3:D:1302:GLU:HB3	2.42	0.55
5:F:172:ARG:O	5:F:176:ILE:HD13	2.07	0.55
1:L:179:PHE:HB2	1:L:195:LEU:HD11	1.88	0.55
2:M:137:VAL:CG2	2:M:391:LEU:HG	2.36	0.55
2:M:985:GLY:C	9:N:1555:HOH:O	2.49	0.55
3:N:481:MET:HG3	3:N:1388:ARG:NH1	2.22	0.55
3:N:561:GLY:HA3	5:P:184:ARG:NH2	2.22	0.55
3:N:561:GLY:HA3	5:P:184:ARG:HH22	1.71	0.55
3:N:576:GLU:HB2	9:N:1886:HOH:O	2.06	0.55
3:N:989:TYR:CZ	3:N:993:LEU:HD11	2.42	0.55
3:N:1408:ILE:O	3:N:1409:ALA:C	2.47	0.55
1:A:132:LEU:HD21	1:A:138:LEU:HB2	1.89	0.55
2:C:56:GLU:OE2	2:C:356:ARG:HG2	2.07	0.55
2:C:57:GLU:O	2:C:62:GLY:HA3	2.06	0.55
2:C:553:ASP:OD1	2:C:843:HIS:ND1	2.40	0.55
2:C:670:GLN:HE22	2:C:699:PHE:CA	2.20	0.55
3:D:1090:ASP:HA	3:D:1093:TYR:CB	2.36	0.55
3:D:1431:THR:HB	9:D:1537:HOH:O	2.06	0.55
4:E:39:VAL:CG2	4:E:72:ARG:HD2	2.36	0.55
5:F:393:THR:HG22	9:F:485:HOH:O	2.07	0.55
2:M:632:ASN:N	9:M:1672:HOH:O	2.39	0.55
2:M:770:GLU:HA	9:M:1880:HOH:O	2.06	0.55
2:M:1060:ILE:CG2	2:M:1061:GLU:N	2.69	0.55
3:N:561:GLY:HA3	5:P:184:ARG:NH1	2.22	0.55
3:N:1225:ALA:HB2	9:N:1769:HOH:O	2.06	0.55
5:P:292:ALA:HB2	9:P:522:HOH:O	2.05	0.55
1:B:33:GLY:O	1:B:195:LEU:HD22	2.06	0.54
2:C:6:PHE:HB2	2:C:908:GLY:C	2.32	0.54
2:C:54:ILE:HD11	2:C:356:ARG:CG	2.35	0.54
2:C:136:ILE:HG22	2:C:336:VAL:HG22	1.89	0.54
2:C:194:VAL:HG21	2:C:221:LEU:O	2.07	0.54
2:C:260:LEU:HG	2:C:261:ILE:HG13	1.89	0.54
3:D:80:VAL:HG12	3:D:81:THR:O	2.06	0.54
3:D:149:LYS:HD2	9:D:1914:HOH:O	2.07	0.54
3:D:583:ASP:OD1	3:D:586:ARG:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1101:VAL:CG2	3:D:1424:VAL:HG22	2.29	0.54
3:D:1336:LEU:HB2	3:D:1344:VAL:HG21	1.89	0.54
3:D:1382:THR:HG23	9:D:1608:HOH:O	2.07	0.54
3:D:1413:THR:HG23	9:D:1816:HOH:O	2.07	0.54
5:F:152:ASP:HB3	5:F:153:PRO:HD3	1.87	0.54
1:K:24:VAL:HG23	9:K:1055:HOH:O	2.06	0.54
1:L:105:GLY:O	1:L:132:LEU:HB3	2.07	0.54
1:L:175:ARG:O	1:L:176:ARG:HG3	2.07	0.54
2:M:254:VAL:O	2:M:257:VAL:HG23	2.07	0.54
2:M:413:LEU:H	2:M:413:LEU:CD1	2.13	0.54
2:M:455:LEU:HD12	2:M:456:ALA:O	2.07	0.54
2:M:1075:ASP:HA	9:M:2290:HOH:O	2.06	0.54
2:M:1084:SER:HB2	7:N:1527:MXP:O4	2.07	0.54
3:N:1083:ASP:O	3:N:1087:ARG:HG3	2.07	0.54
3:N:1147:ARG:O	3:N:1166:LEU:HD23	2.08	0.54
3:N:1467:ILE:HG23	7:N:1527:MXP:H16A	1.89	0.54
1:A:88:ARG:HG2	1:A:121:GLU:HG2	1.89	0.54
2:C:41:ASN:O	2:C:46:ALA:HB2	2.08	0.54
2:C:510:ALA:HB3	2:C:513:VAL:HG23	1.89	0.54
2:C:805:ARG:HD2	9:C:1160:HOH:O	2.07	0.54
2:C:818:GLY:HA2	5:F:309:LYS:NZ	2.20	0.54
2:C:1056:LYS:HB3	3:D:623:VAL:HG13	1.89	0.54
3:D:611:GLN:OE1	7:D:1527:MXP:C16	2.53	0.54
3:D:675:ARG:HH12	5:F:421:PHE:HD2	1.55	0.54
3:D:786:ILE:HD13	3:D:908:LYS:HB3	1.87	0.54
5:F:84:TYR:O	5:F:88:ILE:HD12	2.07	0.54
5:F:94:LEU:HD23	9:F:642:HOH:O	2.07	0.54
1:L:69:PRO:C	1:L:71:VAL:H	2.13	0.54
1:L:85:LEU:HD12	1:L:124:ASN:HB3	1.89	0.54
2:M:197:LEU:HD12	2:M:207:LEU:HD11	1.89	0.54
2:M:580:MET:HB3	2:M:584:GLU:CD	2.32	0.54
3:N:77:GLY:HA3	9:N:2213:HOH:O	2.07	0.54
3:N:679:ARG:HB3	9:N:2172:HOH:O	2.06	0.54
3:N:996:TRP:CE2	3:N:1056:PRO:HG2	2.42	0.54
3:N:1144:LEU:HB3	3:N:1166:LEU:HD11	1.89	0.54
4:O:17:TYR:CD2	4:O:17:TYR:N	2.74	0.54
5:P:278:LEU:HB2	5:P:286:PRO:HG2	1.88	0.54
1:A:20:TYR:HD2	1:A:21:GLY:H	1.53	0.54
1:A:57:TYR:CE2	1:A:59:GLU:HA	2.42	0.54
1:A:213:GLN:O	1:A:217:ILE:HG13	2.07	0.54
1:B:56:VAL:HG13	1:B:142:VAL:HG12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:LYS:HG3	1:B:108:GLU:N	2.22	0.54
2:C:272:ALA:HB1	9:C:1127:HOH:O	2.06	0.54
2:C:724:ARG:HE	2:C:734:LEU:HD23	1.72	0.54
2:C:816:LYS:HE2	2:C:819:VAL:HG21	1.89	0.54
3:D:165:LYS:HG3	3:D:397:LYS:HD3	1.90	0.54
3:D:533:GLY:HA3	9:D:1806:HOH:O	2.07	0.54
3:D:568:ARG:O	3:D:572:ARG:HG3	2.06	0.54
3:D:675:ARG:HG2	3:D:678:GLU:OE2	2.06	0.54
3:D:1286:THR:HG22	9:D:1533:HOH:O	2.07	0.54
5:F:254:GLN:HA	9:F:443:HOH:O	2.08	0.54
1:L:106:PRO:HG3	1:L:134:GLU:HG2	1.88	0.54
1:L:158:ILE:HG22	1:L:159:LYS:N	2.21	0.54
2:M:276:LYS:HG2	2:M:280:LYS:HZ2	1.73	0.54
2:M:1084:SER:O	2:M:1087:VAL:HG12	2.08	0.54
3:N:98:PRO:HG3	3:N:515:GLU:HB3	1.89	0.54
3:N:583:ASP:HB2	3:N:604:THR:OG1	2.07	0.54
3:N:820:GLU:HG3	3:N:836:VAL:CG1	2.36	0.54
3:N:1087:ARG:HD3	3:N:1237:THR:HA	1.90	0.54
3:N:1351:GLU:HG3	3:N:1354:LYS:HD2	1.90	0.54
5:P:205:ARG:HD3	5:P:251:ILE:HG21	1.89	0.54
5:P:358:LEU:O	5:P:358:LEU:HG	2.06	0.54
1:A:91:ASN:CG	1:A:92:PRO:HD2	2.32	0.54
1:A:132:LEU:N	1:A:132:LEU:HD12	2.23	0.54
1:B:175:ARG:HA	9:B:492:HOH:O	2.08	0.54
1:B:211:LEU:O	1:B:214:ALA:HB3	2.07	0.54
2:C:84:ARG:NH2	2:C:128:ILE:HD11	2.23	0.54
2:C:120:LEU:HD23	9:C:1499:HOH:O	2.06	0.54
2:C:577:PRO:HG3	2:C:993:PHE:CE2	2.43	0.54
2:C:710:ILE:HD11	2:C:758:ARG:HD3	1.88	0.54
3:D:39:PRO:HB3	3:D:45:PHE:C	2.33	0.54
3:D:49:ILE:HB	3:D:50:PHE:CD1	2.42	0.54
3:D:570:GLU:N	5:F:214:GLN:HE22	2.05	0.54
3:D:1042:ARG:O	3:D:1057:VAL:HB	2.08	0.54
3:D:1293:PHE:CZ	3:D:1302:GLU:HB3	2.43	0.54
3:D:1381:VAL:HB	3:D:1389:LEU:O	2.08	0.54
5:F:305:GLU:O	5:F:309:LYS:HG3	2.07	0.54
2:M:565:GLN:HG2	2:M:995:MET:CE	2.37	0.54
2:M:889:HIS:CD2	2:M:970:GLY:HA3	2.43	0.54
3:N:32:ILE:HD11	9:N:1596:HOH:O	2.06	0.54
3:N:566:ILE:HG12	5:P:192:LEU:HD21	1.88	0.54
3:N:1009:LYS:HE2	9:N:1963:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1041:LEU:CD1	3:N:1058:ARG:HA	2.36	0.54
3:N:1262:LEU:HD23	3:N:1352:ILE:HG13	1.90	0.54
3:N:1472:ILE:O	3:N:1477:GLY:HA3	2.08	0.54
5:P:88:ILE:HB	9:P:514:HOH:O	2.06	0.54
1:A:184:THR:HG23	1:A:192:LEU:HD12	1.89	0.54
2:C:17:PRO:HB2	9:C:1289:HOH:O	2.07	0.54
2:C:165:LEU:HD12	2:C:166:PRO:C	2.32	0.54
2:C:292:ARG:NH1	2:C:299:LYS:HD3	2.22	0.54
3:D:41:ARG:HD2	9:D:2449:HOH:O	2.07	0.54
3:D:72:VAL:HG23	3:D:78:VAL:H	1.71	0.54
3:D:118:LEU:O	3:D:120:ALA:N	2.41	0.54
3:D:957:PRO:CD	3:D:1007:VAL:HG12	2.37	0.54
3:D:1045:MET:HG3	3:D:1073:SER:OG	2.07	0.54
3:D:1112:CYS:HA	9:D:2179:HOH:O	2.08	0.54
3:D:1142:ALA:HB3	9:D:2234:HOH:O	2.06	0.54
5:F:88:ILE:CB	5:F:193:ARG:HH11	2.20	0.54
1:K:18:ARG:HH11	1:K:123:MET:CE	2.21	0.54
2:M:137:VAL:HG22	2:M:391:LEU:O	2.08	0.54
2:M:362:GLY:HA3	2:M:367:LEU:CD2	2.37	0.54
2:M:679:PHE:C	3:N:943:THR:HG22	2.33	0.54
3:N:764:LEU:HD23	3:N:767:HIS:CE1	2.42	0.54
3:N:799:LYS:O	3:N:826:PRO:HD2	2.08	0.54
3:N:1080:GLY:O	3:N:1084:THR:HG23	2.07	0.54
1:B:122:ILE:HG23	9:B:527:HOH:O	2.08	0.54
1:B:123:MET:O	1:B:125:PRO:HD3	2.08	0.54
2:C:398:THR:O	2:C:570:PRO:HD3	2.08	0.54
2:C:420:ARG:CZ	2:C:422:ARG:HH21	2.20	0.54
2:C:481:ASP:O	2:C:483:VAL:HG23	2.06	0.54
2:C:584:GLU:CD	2:C:584:GLU:H	2.14	0.54
2:C:725:ASP:HA	9:C:1479:HOH:O	2.08	0.54
3:D:478:LEU:HD21	3:D:500:ARG:HH21	1.71	0.54
3:D:534:ARG:HE	5:F:312:GLN:HE22	1.56	0.54
1:K:86:VAL:HG13	1:K:124:ASN:HB2	1.89	0.54
2:M:157:ARG:NH1	2:M:314:THR:HB	2.22	0.54
2:M:252:LYS:HD3	2:M:296:GLY:HA2	1.89	0.54
2:M:671:ASN:N	2:M:671:ASN:ND2	2.48	0.54
2:M:1049:LEU:O	2:M:1053:LEU:HG	2.07	0.54
3:N:172:PRO:HA	9:N:2177:HOH:O	2.06	0.54
3:N:493:ARG:HB2	3:N:1388:ARG:NE	2.23	0.54
2:C:191:PHE:HD2	2:C:195:LEU:HD23	1.72	0.54
2:C:359:MET:HE2	9:C:1464:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:502:PRO:HB2	2:C:509:ALA:HB3	1.90	0.54
3:D:117:ASP:HB2	3:D:495:ARG:NH2	2.23	0.54
3:D:1109:GLU:CG	3:D:1202:GLN:H	2.21	0.54
3:D:1466:VAL:HG23	3:D:1472:ILE:CD1	2.33	0.54
1:K:111:ALA:HB2	1:K:127:LEU:HG	1.90	0.54
1:K:193:ASP:HA	9:K:2597:HOH:O	2.07	0.54
1:L:206:THR:CG2	1:L:209:GLU:H	2.21	0.54
2:M:185:LYS:HB3	2:M:188:LYS:O	2.07	0.54
2:M:281:LEU:CD1	2:M:306:THR:HA	2.38	0.54
2:M:669:GLY:HA3	2:M:995:MET:HA	1.90	0.54
3:N:573:MET:HE3	5:P:210:LEU:HB3	1.90	0.54
3:N:1005:GLN:HB2	9:N:1763:HOH:O	2.07	0.54
3:N:1104:GLU:O	3:N:1106:VAL:HG23	2.08	0.54
3:N:1290:LEU:HD22	3:N:1291:SER:H	1.73	0.54
3:N:1422:MET:CE	3:N:1427:SER:HA	2.36	0.54
1:A:101:LEU:HD12	1:A:114:PHE:CD1	2.43	0.54
2:C:334:ARG:NH2	2:C:418:LEU:HD11	2.23	0.54
2:C:740:GLU:HB3	9:C:1664:HOH:O	2.08	0.54
3:D:1206:GLY:HA3	3:D:1366:LYS:HZ1	1.72	0.54
1:K:173:PRO:O	1:K:201:THR:HG23	2.08	0.54
2:M:129:ILE:CG1	2:M:386:PHE:HB3	2.35	0.54
2:M:139:GLN:CD	2:M:418:LEU:HD22	2.33	0.54
2:M:250:ARG:HG3	9:M:2168:HOH:O	2.06	0.54
2:M:338:GLU:HA	2:M:341:THR:HG22	1.89	0.54
2:M:420:ARG:CZ	2:M:422:ARG:HH21	2.20	0.54
2:M:841:ASN:HD21	2:M:845:ASN:H	1.56	0.54
2:M:1034:GLU:OE2	3:N:616:GLN:HG2	2.08	0.54
3:N:127:LEU:HD11	3:N:461:ILE:HD11	1.89	0.54
3:N:187:LYS:HG3	3:N:199:LEU:HB3	1.89	0.54
3:N:477:LEU:HD23	9:N:1890:HOH:O	2.07	0.54
4:O:46:PRO:CB	4:O:54:LEU:HD22	2.35	0.54
4:O:70:THR:HG21	4:O:72:ARG:NE	2.23	0.54
5:P:142:ARG:CZ	5:P:156:VAL:HG22	2.38	0.54
5:P:207:LEU:HB3	5:P:212:LEU:HG	1.90	0.54
1:B:185:ARG:HD2	9:D:1847:HOH:O	2.08	0.54
2:C:51:THR:HB	2:C:348:LEU:HD23	1.89	0.54
2:C:77:PRO:HD3	2:C:93:PRO:HD3	1.89	0.54
2:C:130:ASN:HA	9:C:1363:HOH:O	2.07	0.54
2:C:438:ILE:HD11	2:C:467:ILE:HD12	1.89	0.54
2:C:774:LEU:HB2	9:C:1255:HOH:O	2.07	0.54
2:C:1115:LEU:HD12	2:C:1115:LEU:N	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:24:GLY:HA2	9:D:2024:HOH:O	2.07	0.54
3:D:119:SER:H	3:D:123:LEU:CD2	2.17	0.54
3:D:148:GLU:HG2	3:D:151:GLN:HE21	1.73	0.54
3:D:1113:GLY:HA2	9:D:1697:HOH:O	2.07	0.54
3:D:1137:ARG:O	3:D:1141:GLU:HG3	2.08	0.54
4:E:35:PHE:HZ	4:E:60:ALA:HA	1.73	0.54
5:F:94:LEU:HB2	5:F:98:GLU:OE2	2.08	0.54
1:K:184:THR:HG23	1:K:192:LEU:CB	2.36	0.54
1:L:173:PRO:O	1:L:201:THR:HG23	2.07	0.54
2:M:229:MET:HG3	9:M:1707:HOH:O	2.07	0.54
2:M:1008:ARG:HH11	2:M:1028:GLY:CA	2.20	0.54
3:N:187:LYS:CE	3:N:199:LEU:HB3	2.34	0.54
3:N:800:LYS:HD3	9:N:1722:HOH:O	2.08	0.54
3:N:891:GLU:HB2	9:N:2068:HOH:O	2.07	0.54
3:N:1128:VAL:O	3:N:1129:THR:C	2.49	0.54
3:N:1389:LEU:HD22	9:N:1771:HOH:O	2.08	0.54
4:O:6:ILE:HA	4:O:9:LEU:HD12	1.89	0.54
1:B:73:GLU:CD	1:B:130:ALA:HA	2.32	0.54
1:B:83:LYS:O	1:B:170:VAL:HG21	2.08	0.54
2:C:602:GLU:HA	2:C:647:GLN:O	2.07	0.54
2:C:650:ARG:HG3	9:C:1791:HOH:O	2.08	0.54
2:C:863:ASP:O	2:C:865:THR:N	2.41	0.54
3:D:52:PRO:HG2	3:D:79:GLU:O	2.08	0.54
3:D:169:TYR:HB3	3:D:195:VAL:HG11	1.89	0.54
3:D:584:ASN:CG	3:D:590:PRO:HD2	2.33	0.54
3:D:1176:LYS:O	3:D:1179:GLU:HB2	2.08	0.54
3:D:1369:GLU:O	3:D:1372:VAL:HG12	2.08	0.54
5:F:301:ALA:HB2	9:F:602:HOH:O	2.08	0.54
1:K:23:PHE:HE1	1:K:208:LEU:HD13	1.73	0.54
2:M:137:VAL:O	2:M:391:LEU:HD21	2.08	0.54
2:M:182:VAL:HG11	9:M:2050:HOH:O	2.08	0.54
2:M:216:GLU:HB3	9:M:1627:HOH:O	2.08	0.54
2:M:481:ASP:O	2:M:483:VAL:HG23	2.07	0.54
3:N:1277:ILE:HD11	3:N:1301:LYS:HD2	1.89	0.54
2:C:860:HIS:HE1	9:C:1431:HOH:O	1.91	0.53
2:C:1111:ILE:HG13	2:C:1112:PHE:H	1.73	0.53
3:D:550:ARG:HH11	3:D:573:MET:HB3	1.73	0.53
3:D:699:VAL:HG12	3:D:717:GLN:HA	1.88	0.53
3:D:820:GLU:HG2	3:D:825:ALA:O	2.08	0.53
3:D:1213:ARG:HG3	9:D:2053:HOH:O	2.06	0.53
3:D:1485:GLN:O	4:E:75:PHE:HA	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:399:GLN:HG3	9:F:571:HOH:O	2.08	0.53
1:L:57:TYR:CE1	1:L:163:ASN:HB2	2.43	0.53
2:M:191:PHE:HD2	2:M:195:LEU:HD23	1.72	0.53
2:M:315:ALA:HB3	9:M:1882:HOH:O	2.08	0.53
2:M:352:ALA:HA	2:M:355:VAL:HG12	1.89	0.53
2:M:435:TYR:C	2:M:437:ARG:H	2.15	0.53
2:M:689:VAL:HB	2:M:870:ILE:HG13	1.89	0.53
2:M:874:LEU:HA	3:N:1023:MET:HE1	1.90	0.53
3:N:81:THR:O	3:N:82:LYS:O	2.26	0.53
1:B:106:PRO:HG2	9:B:483:HOH:O	2.07	0.53
3:D:131:LYS:HD2	5:F:83:GLN:NE2	2.23	0.53
3:D:139:GLY:O	3:D:147:VAL:HB	2.08	0.53
3:D:161:LEU:O	3:D:161:LEU:HD23	2.08	0.53
3:D:1476:THR:HG23	4:E:21:VAL:HG22	1.90	0.53
4:E:49:GLN:HG2	9:E:108:HOH:O	2.09	0.53
1:L:14:ARG:HA	9:L:3344:HOH:O	2.07	0.53
1:L:68:ILE:HG23	1:L:137:ARG:NH1	2.24	0.53
1:L:212:ASN:O	1:L:215:VAL:HG22	2.07	0.53
2:M:41:ASN:O	2:M:46:ALA:HB2	2.09	0.53
2:M:89:THR:HA	2:M:129:ILE:O	2.08	0.53
2:M:411:SER:HA	2:M:452:ILE:HA	1.90	0.53
2:M:685:GLU:CG	3:N:783:ARG:HD2	2.38	0.53
2:M:911:GLU:O	2:M:914:ILE:HG22	2.08	0.53
3:N:610:LYS:CG	7:N:1527:MXP:C15	2.85	0.53
3:N:820:GLU:HB2	3:N:836:VAL:HG11	1.90	0.53
3:N:983:LEU:HD13	3:N:991:GLN:OE1	2.08	0.53
3:N:1049:SER:OG	3:N:1051:GLU:HG3	2.08	0.53
3:N:1381:VAL:HB	3:N:1389:LEU:O	2.07	0.53
5:P:234:LYS:HG3	5:P:236:SER:H	1.74	0.53
1:B:44:LEU:HD21	1:B:199:ILE:HD13	1.89	0.53
2:C:254:VAL:O	2:C:257:VAL:HG23	2.09	0.53
3:D:57:GLU:HG3	3:D:64:LYS:HG2	1.91	0.53
3:D:454:ALA:HB3	9:D:2225:HOH:O	2.08	0.53
3:D:764:LEU:HD23	3:D:767:HIS:ND1	2.24	0.53
3:D:787:LEU:HD21	3:D:947:ILE:HD13	1.90	0.53
3:D:959:GLU:O	3:D:963:TYR:HD1	1.91	0.53
3:D:1273:VAL:HG13	9:D:2190:HOH:O	2.08	0.53
4:E:19:LEU:HB3	9:E:116:HOH:O	2.08	0.53
5:F:95:THR:HG22	5:F:96:LEU:HD23	1.90	0.53
1:K:126:ASP:HB2	9:K:1975:HOH:O	2.06	0.53
1:L:83:LYS:O	1:L:170:VAL:HG21	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:86:VAL:HG12	1:L:124:ASN:ND2	2.16	0.53
2:M:599:GLU:HG3	2:M:600:ASP:N	2.18	0.53
2:M:673:LEU:HD22	2:M:867:VAL:HA	1.90	0.53
2:M:690:ILE:CG2	2:M:852:ILE:HG13	2.38	0.53
2:M:766:GLU:HG2	2:M:772:ARG:HH12	1.73	0.53
2:M:1103:ASP:OD1	3:N:3:LYS:HB2	2.09	0.53
3:N:407:VAL:HG13	3:N:421:LEU:O	2.09	0.53
3:N:1209:LEU:HD23	3:N:1211:MET:HG3	1.90	0.53
3:N:1278:ASP:HA	3:N:1319:VAL:O	2.08	0.53
3:N:1395:LEU:HD21	9:N:1988:HOH:O	2.08	0.53
3:D:408:GLU:O	3:D:408:GLU:HG2	2.07	0.53
3:D:614:PHE:O	3:D:615:ARG:C	2.51	0.53
3:D:662:GLU:HB2	9:D:1987:HOH:O	2.09	0.53
3:D:1080:GLY:O	3:D:1084:THR:HG23	2.08	0.53
3:D:1258:ARG:HG3	3:D:1262:LEU:HD13	1.89	0.53
3:D:1264:GLU:O	3:D:1266:ARG:HG3	2.07	0.53
4:E:29:GLN:HB2	4:E:33:HIS:CD2	2.43	0.53
5:F:162:LYS:HE2	9:F:641:HOH:O	2.08	0.53
5:F:345:ALA:HB1	9:F:710:HOH:O	2.08	0.53
5:F:358:LEU:CD2	5:F:370:LYS:HZ2	2.20	0.53
1:K:63:HIS:HB3	2:M:746:GLY:HA2	1.89	0.53
2:M:52:PHE:O	2:M:54:ILE:N	2.41	0.53
2:M:182:VAL:CG1	2:M:193:LEU:HD13	2.38	0.53
2:M:227:PHE:HA	2:M:237:ARG:NH1	2.23	0.53
2:M:571:LEU:HD23	2:M:699:PHE:O	2.09	0.53
2:M:604:ALA:HB3	2:M:612:VAL:O	2.08	0.53
2:M:611:ILE:CD1	2:M:625:LEU:HD11	2.38	0.53
2:M:632:ASN:HB2	9:M:1672:HOH:O	2.09	0.53
3:N:17:LYS:HA	3:N:20:SER:HB3	1.91	0.53
3:N:612:GLY:HA2	3:N:1441:GLN:HA	1.90	0.53
3:N:1144:LEU:HA	3:N:1147:ARG:HG3	1.90	0.53
3:N:1466:VAL:HG11	7:N:1527:MXP:H20	1.90	0.53
5:P:130:VAL:HA	5:P:142:ARG:HH21	1.73	0.53
2:C:4:LYS:O	2:C:901:TYR:HB3	2.08	0.53
2:C:378:LEU:HG	2:C:382:ILE:HD11	1.90	0.53
2:C:385:PHE:O	2:C:389:SER:HB3	2.08	0.53
2:C:765:SER:O	2:C:767:PRO:HD3	2.09	0.53
2:C:897:LEU:HB3	2:C:899:GLN:HE21	1.73	0.53
2:C:1087:VAL:HG12	3:D:610:LYS:HZ3	1.74	0.53
3:D:800:LYS:CE	3:D:804:LEU:HD13	2.39	0.53
3:D:1105:ILE:HD13	9:D:2099:HOH:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1175:ILE:O	3:D:1179:GLU:HG3	2.08	0.53
3:D:1390:LEU:HA	9:D:2323:HOH:O	2.08	0.53
5:F:108:GLU:HG3	5:F:176:ILE:HG21	1.91	0.53
5:F:130:VAL:HG11	5:F:159:ILE:HB	1.90	0.53
2:M:328:LEU:HD21	2:M:438:ILE:HD11	1.90	0.53
2:M:806:LEU:HD22	9:M:1891:HOH:O	2.07	0.53
3:N:448:GLU:O	3:N:448:GLU:HG2	2.08	0.53
3:N:524:LEU:C	3:N:526:PRO:HD3	2.33	0.53
3:N:1047:LYS:HB3	3:N:1048:PRO:CD	2.38	0.53
3:N:1486:VAL:HG12	4:O:73:LEU:HD22	1.90	0.53
1:B:140:MET:HB2	9:B:514:HOH:O	2.08	0.53
2:C:185:LYS:HB3	2:C:188:LYS:O	2.07	0.53
2:C:267:TYR:CD1	2:C:272:ALA:HB1	2.43	0.53
2:C:496:ILE:O	2:C:515:ALA:HB1	2.09	0.53
2:C:1008:ARG:HH11	2:C:1028:GLY:CA	2.18	0.53
3:D:493:ARG:HA	3:D:1388:ARG:NH1	2.24	0.53
3:D:799:LYS:HB3	3:D:826:PRO:CG	2.37	0.53
3:D:1485:GLN:NE2	4:E:80:VAL:H	2.07	0.53
5:F:415:THR:HB	9:F:522:HOH:O	2.09	0.53
1:K:20:TYR:CD2	1:K:21:GLY:N	2.69	0.53
1:K:45:LEU:HD21	9:K:2558:HOH:O	2.08	0.53
3:N:55:ASP:O	3:N:80:VAL:HG11	2.08	0.53
3:N:138:LYS:HD3	9:N:1530:HOH:O	2.08	0.53
3:N:169:TYR:CE1	3:N:197:SER:HB2	2.44	0.53
3:N:792:ILE:O	3:N:878:GLY:HA3	2.09	0.53
3:N:860:LEU:HD23	3:N:877:PRO:HB2	1.91	0.53
3:N:1236:LEU:HA	3:N:1359:GLN:NE2	2.24	0.53
4:O:39:VAL:CG2	4:O:72:ARG:HD2	2.39	0.53
5:P:94:LEU:HD23	9:P:638:HOH:O	2.09	0.53
2:C:403:SER:O	2:C:407:LYS:HG3	2.09	0.53
2:C:1054:THR:HG22	2:C:1059:ASP:CB	2.33	0.53
9:C:1255:HOH:O	5:F:354:LEU:HD21	2.08	0.53
3:D:113:GLY:HA3	3:D:120:ALA:HA	1.91	0.53
3:D:493:ARG:HB2	3:D:1388:ARG:CZ	2.39	0.53
3:D:591:VAL:HB	9:D:1809:HOH:O	2.08	0.53
3:D:996:TRP:HA	3:D:999:THR:HG22	1.89	0.53
3:D:1113:GLY:N	3:D:1195:GLN:HE22	2.07	0.53
3:D:1195:GLN:HG3	3:D:1196:THR:N	2.22	0.53
3:D:1274:ILE:HD12	9:D:1674:HOH:O	2.08	0.53
3:D:1274:ILE:HD11	3:D:1334:GLN:NE2	2.24	0.53
1:L:60:ASP:H	1:L:137:ARG:NH2	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:328:LEU:HD21	2:M:438:ILE:CD1	2.38	0.53
2:M:410:ILE:HD12	2:M:410:ILE:H	1.73	0.53
2:M:874:LEU:HD23	3:N:1023:MET:CE	2.37	0.53
2:M:915:LYS:HB3	9:M:2164:HOH:O	2.09	0.53
3:N:46:ASP:HB3	3:N:49:ILE:HG13	1.89	0.53
3:N:55:ASP:HB3	3:N:82:LYS:HE2	1.90	0.53
3:N:160:GLU:HG2	9:N:2310:HOH:O	2.09	0.53
3:N:785:ILE:HG22	3:N:789:LEU:HD12	1.91	0.53
3:N:860:LEU:O	3:N:877:PRO:HD2	2.07	0.53
3:N:908:LYS:CB	3:N:1027:GLY:HA3	2.33	0.53
3:N:996:TRP:HE3	3:N:999:THR:HG21	1.73	0.53
3:N:1087:ARG:HD3	3:N:1238:MET:N	2.23	0.53
3:N:1323:GLN:HG3	3:N:1324:PRO:HD2	1.90	0.53
4:O:29:GLN:HB2	4:O:33:HIS:CD2	2.43	0.53
5:P:368:VAL:O	5:P:372:ARG:HB2	2.09	0.53
2:C:496:ILE:H	2:C:496:ILE:HD12	1.74	0.53
2:C:690:ILE:CG2	2:C:852:ILE:HG13	2.39	0.53
2:C:816:LYS:HB2	2:C:819:VAL:CG2	2.39	0.53
3:D:34:TYR:O	3:D:35:ARG:C	2.51	0.53
3:D:52:PRO:CB	3:D:80:VAL:HG13	2.39	0.53
3:D:631:ILE:HG21	3:D:745:MET:SD	2.49	0.53
4:E:31:LEU:HD23	4:E:35:PHE:HE1	1.73	0.53
2:M:54:ILE:O	2:M:54:ILE:HG23	2.09	0.53
3:N:503:LEU:HD22	9:N:2051:HOH:O	2.09	0.53
3:N:550:ARG:NH1	3:N:573:MET:HB3	2.24	0.53
3:N:692:GLU:HG3	3:N:720:LEU:HD13	1.91	0.53
3:N:786:ILE:HD13	3:N:908:LYS:HB3	1.89	0.53
3:N:1066:THR:HA	9:N:1984:HOH:O	2.09	0.53
3:N:1377:LYS:O	3:N:1395:LEU:N	2.37	0.53
2:C:535:SER:HB2	2:C:537:LYS:HG3	1.91	0.53
2:C:984:GLU:OE1	3:D:945:SER:HA	2.09	0.53
3:D:53:ILE:HG22	9:D:1900:HOH:O	2.08	0.53
3:D:1220:ALA:HB1	3:D:1223:ILE:CD1	2.36	0.53
3:D:1492:LEU:HD12	9:D:2354:HOH:O	2.09	0.53
5:F:321:ILE:O	5:F:327:SER:HB3	2.08	0.53
1:K:133:GLU:HG2	1:K:134:GLU:H	1.72	0.53
1:L:65:PHE:HB2	9:L:1134:HOH:O	2.08	0.53
2:M:64:LEU:HD11	2:M:100:LEU:HD13	1.90	0.53
2:M:162:ILE:O	2:M:164:PRO:HD3	2.09	0.53
2:M:607:ASP:HB2	2:M:610:ARG:HG3	1.91	0.53
2:M:737:LEU:HD12	2:M:754:ILE:HB	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:753:ASP:O	2:M:792:VAL:HG23	2.09	0.53
3:N:407:VAL:HG13	3:N:422:ALA:HB2	1.91	0.53
3:N:591:VAL:HG11	3:N:597:ASP:HA	1.91	0.53
3:N:1462:LEU:N	3:N:1462:LEU:HD23	2.23	0.53
2:C:495:THR:HB	2:C:530:GLU:HG3	1.91	0.53
2:C:1101:THR:OG1	2:C:1109:VAL:HG12	2.09	0.53
3:D:760:ARG:NH2	4:E:62:THR:N	2.57	0.53
3:D:1310:ARG:NE	3:D:1327:ARG:HB3	2.24	0.53
3:D:1330:ILE:HB	3:D:1347:TYR:CZ	2.43	0.53
1:K:23:PHE:O	1:K:196:THR:HA	2.09	0.53
1:L:80:LEU:HG	3:N:844:ALA:HB2	1.91	0.53
2:M:109:LYS:HE2	2:M:111:ASP:OD1	2.09	0.53
2:M:290:LEU:HD11	9:M:1886:HOH:O	2.09	0.53
2:M:413:LEU:HD12	2:M:413:LEU:N	2.21	0.53
2:M:549:PHE:HB3	2:M:552:HIS:CD2	2.42	0.53
3:N:81:THR:HG23	9:N:1885:HOH:O	2.09	0.53
3:N:1175:ILE:O	3:N:1179:GLU:HG3	2.09	0.53
5:P:127:ILE:HD11	9:P:595:HOH:O	2.08	0.53
1:A:181:VAL:HG11	9:A:337:HOH:O	2.10	0.52
1:B:57:TYR:CE1	1:B:163:ASN:HB2	2.44	0.52
1:B:58:ILE:HD13	1:B:140:MET:HB3	1.91	0.52
1:B:218:LEU:O	1:B:222:LEU:HG	2.08	0.52
2:C:52:PHE:O	2:C:54:ILE:N	2.42	0.52
2:C:110:GLU:H	2:C:368:THR:HG21	1.74	0.52
2:C:162:ILE:HD11	2:C:306:THR:HG21	1.90	0.52
3:D:407:VAL:HG13	3:D:421:LEU:O	2.09	0.52
3:D:570:GLU:HB2	5:F:214:GLN:OE1	2.08	0.52
4:E:8:LYS:HG3	9:E:100:HOH:O	2.09	0.52
5:F:282:LEU:HD13	9:F:621:HOH:O	2.08	0.52
2:M:197:LEU:HB3	2:M:202:TYR:HB2	1.90	0.52
2:M:1115:LEU:HD12	2:M:1115:LEU:N	2.23	0.52
3:N:49:ILE:HB	3:N:50:PHE:CD1	2.44	0.52
3:N:104:PHE:CD2	3:N:1448:THR:HG23	2.44	0.52
3:N:567:ILE:N	3:N:567:ILE:HD12	2.24	0.52
3:N:826:PRO:HB3	9:N:1811:HOH:O	2.08	0.52
3:N:984:THR:HG21	9:N:1536:HOH:O	2.09	0.52
3:N:1176:LYS:O	3:N:1179:GLU:HB2	2.09	0.52
3:N:1243:THR:HG1	3:N:1253:THR:HB	1.73	0.52
4:O:33:HIS:HB2	4:O:37:ASN:ND2	2.24	0.52
5:P:369:LEU:O	5:P:373:LYS:HB2	2.09	0.52
1:A:211:LEU:O	1:A:214:ALA:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:PHE:CE2	1:B:199:ILE:HD12	2.44	0.52
1:B:197:LEU:HD21	1:B:199:ILE:HD11	1.91	0.52
2:C:166:PRO:HD3	2:C:265:ARG:HB2	1.91	0.52
2:C:260:LEU:HA	2:C:291:ALA:HB2	1.90	0.52
2:C:603:VAL:HG22	2:C:613:VAL:HG12	1.90	0.52
2:C:739:GLU:HA	9:C:1304:HOH:O	2.09	0.52
2:C:772:ARG:HB3	9:F:459:HOH:O	2.09	0.52
3:D:62:LYS:HD2	9:D:1735:HOH:O	2.08	0.52
3:D:102:ILE:HG13	9:D:1613:HOH:O	2.09	0.52
5:F:102:LEU:O	5:F:106:VAL:HG23	2.09	0.52
2:M:577:PRO:HG3	2:M:993:PHE:CE2	2.43	0.52
2:M:602:GLU:HA	2:M:647:GLN:O	2.09	0.52
2:M:1005:MET:HG3	2:M:1005:MET:O	2.09	0.52
3:N:32:ILE:O	5:P:258:ILE:HG23	2.09	0.52
3:N:104:PHE:HE2	3:N:1448:THR:HA	1.73	0.52
3:N:141:ILE:HG13	3:N:142:LEU:N	2.24	0.52
3:N:611:GLN:OE1	3:N:619:LEU:HD21	2.09	0.52
3:N:892:ASP:OD2	3:N:895:VAL:HG21	2.09	0.52
3:N:1114:THR:HG23	3:N:1114:THR:O	2.09	0.52
3:N:1141:GLU:CG	3:N:1168:MET:HE1	2.40	0.52
4:O:85:LEU:HD21	4:O:89:MET:HE2	1.91	0.52
5:P:220:LEU:HD12	5:P:243:ILE:HD11	1.92	0.52
2:C:6:PHE:CD1	2:C:6:PHE:N	2.77	0.52
2:C:129:ILE:HG22	2:C:130:ASN:ND2	2.24	0.52
2:C:368:THR:HB	2:C:369:PRO:HD3	1.90	0.52
2:C:404:LEU:HA	2:C:407:LYS:HD2	1.91	0.52
3:D:1128:VAL:O	3:D:1129:THR:C	2.51	0.52
5:F:371:LEU:HB2	5:F:372:ARG:HH11	1.74	0.52
5:F:393:THR:O	5:F:397:ILE:HG13	2.09	0.52
1:K:149:GLY:O	1:K:171:PHE:HB2	2.10	0.52
1:K:189:ARG:HD2	1:K:191:ASP:OD1	2.09	0.52
2:M:470:PRO:HB2	2:M:534:VAL:HG21	1.90	0.52
2:M:626:ARG:H	2:M:639:GLN:NE2	2.06	0.52
3:N:153:LEU:CD1	3:N:157:GLU:HB2	2.39	0.52
3:N:163:TYR:HB3	9:N:2151:HOH:O	2.10	0.52
3:N:179:VAL:HG13	3:N:183:GLU:HB3	1.92	0.52
3:N:408:GLU:HA	5:P:171:LYS:NZ	2.23	0.52
3:N:498:VAL:HG23	3:N:499:VAL:N	2.24	0.52
3:N:584:ASN:HD21	3:N:590:PRO:HD2	1.72	0.52
3:N:1305:LEU:HD22	3:N:1309:ALA:HB1	1.91	0.52
5:P:392:VAL:HG11	5:P:396:ARG:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:265:ARG:HB3	2:C:267:TYR:CD2	2.45	0.52
2:C:442:GLU:HB3	9:C:1185:HOH:O	2.08	0.52
2:C:643:VAL:HB	9:C:1145:HOH:O	2.09	0.52
3:D:114:THR:O	3:D:495:ARG:HG3	2.09	0.52
3:D:591:VAL:HG11	3:D:597:ASP:HA	1.92	0.52
3:D:710:ARG:HH21	3:D:1210:SER:CB	2.22	0.52
3:D:892:ASP:OD2	3:D:895:VAL:HG21	2.09	0.52
3:D:965:GLU:HA	3:D:968:ASP:HB2	1.91	0.52
3:D:1243:THR:HG1	3:D:1253:THR:HB	1.72	0.52
1:L:45:LEU:HD21	1:L:177:VAL:HG13	1.91	0.52
2:M:289:THR:HG22	2:M:290:LEU:HD23	1.92	0.52
2:M:605:LYS:HG3	2:M:612:VAL:HB	1.92	0.52
3:N:408:GLU:HB3	9:N:1846:HOH:O	2.09	0.52
3:N:534:ARG:HG3	5:P:312:GLN:NE2	2.24	0.52
3:N:633:VAL:C	3:N:635:PRO:HD3	2.35	0.52
3:N:661:MET:O	3:N:664:LYS:O	2.26	0.52
3:N:1076:GLY:O	3:N:1079:LYS:HG2	2.09	0.52
3:N:1110:ALA:O	3:N:1111:ASP:C	2.49	0.52
3:N:1182:GLU:HG3	9:N:1552:HOH:O	2.08	0.52
3:N:1205:TYR:HE1	3:N:1221:VAL:HG13	1.73	0.52
5:P:115:LYS:O	5:P:119:ILE:HG13	2.08	0.52
5:P:141:VAL:O	5:P:145:PRO:HD2	2.09	0.52
1:B:69:PRO:C	1:B:71:VAL:H	2.18	0.52
1:B:198:ARG:HD2	9:B:489:HOH:O	2.09	0.52
2:C:142:ARG:HH21	2:C:325:ILE:HD11	1.72	0.52
2:C:208:ALA:HA	2:C:218:VAL:HG22	1.91	0.52
2:C:212:GLY:HA3	2:C:218:VAL:HG23	1.90	0.52
2:C:252:LYS:HD3	2:C:296:GLY:HA2	1.91	0.52
2:C:302:VAL:O	2:C:306:THR:HG23	2.09	0.52
2:C:480:THR:HG22	2:C:482:GLU:H	1.74	0.52
3:D:403:PHE:CZ	3:D:407:VAL:HG23	2.44	0.52
3:D:720:LEU:H	3:D:720:LEU:HD12	1.73	0.52
3:D:853:VAL:HA	3:D:858:VAL:O	2.10	0.52
3:D:1189:ARG:NH1	3:D:1203:LYS:HB2	2.24	0.52
3:D:1284:GLU:HG3	9:D:1992:HOH:O	2.10	0.52
4:E:54:LEU:HD23	4:E:54:LEU:O	2.09	0.52
5:F:181:GLU:O	5:F:184:ARG:HB3	2.10	0.52
5:F:187:LEU:HD23	5:F:187:LEU:C	2.34	0.52
5:F:338:LEU:HD12	9:F:562:HOH:O	2.09	0.52
1:K:206:THR:HG22	1:K:209:GLU:CG	2.36	0.52
1:L:101:LEU:HD11	1:L:113:ASP:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:131:GLY:N	9:M:1824:HOH:O	2.43	0.52
2:M:139:GLN:HE22	2:M:415:PRO:HD2	1.74	0.52
2:M:765:SER:O	2:M:767:PRO:HD3	2.10	0.52
3:N:169:TYR:HB3	3:N:195:VAL:HG11	1.91	0.52
3:N:633:VAL:HG22	3:N:635:PRO:CD	2.39	0.52
3:N:1109:GLU:CG	3:N:1202:GLN:H	2.22	0.52
3:N:1277:ILE:CD1	3:N:1301:LYS:HB2	2.38	0.52
4:O:63:TRP:O	4:O:67:GLU:HG3	2.09	0.52
5:P:152:ASP:HB3	5:P:153:PRO:HD3	1.92	0.52
5:P:306:GLU:HG3	9:P:674:HOH:O	2.10	0.52
5:P:363:GLU:HA	5:P:367:MET:HG3	1.91	0.52
1:B:62:LEU:H	1:B:62:LEU:HD12	1.74	0.52
1:B:71:VAL:HG22	1:B:132:LEU:CD1	2.39	0.52
1:B:156:HIS:CG	1:B:157:GLY:H	2.27	0.52
2:C:145:GLY:H	2:C:163:ILE:HG12	1.72	0.52
2:C:603:VAL:HG21	2:C:643:VAL:CG1	2.40	0.52
3:D:116:LEU:HD21	3:D:464:LEU:CB	2.38	0.52
3:D:447:VAL:HA	9:D:2047:HOH:O	2.09	0.52
3:D:567:ILE:HD12	3:D:567:ILE:N	2.24	0.52
3:D:715:ALA:O	3:D:764:LEU:HD12	2.08	0.52
3:D:809:PRO:HB2	3:D:812:ALA:CB	2.40	0.52
3:D:1363:LEU:HD12	3:D:1364:HIS:O	2.10	0.52
3:D:1394:VAL:HG21	9:D:2203:HOH:O	2.08	0.52
3:D:1503:VAL:HG13	9:D:1882:HOH:O	2.09	0.52
4:E:94:PRO:HA	9:E:126:HOH:O	2.08	0.52
1:K:90:LEU:HD11	9:K:1139:HOH:O	2.09	0.52
2:M:670:GLN:HE22	2:M:699:PHE:C	2.18	0.52
2:M:670:GLN:O	2:M:672:VAL:HG12	2.10	0.52
3:N:52:PRO:HB2	3:N:80:VAL:HG13	1.92	0.52
3:N:400:VAL:HG22	3:N:443:VAL:CG2	2.31	0.52
3:N:473:LEU:HD21	3:N:495:ARG:CZ	2.40	0.52
3:N:504:ASP:HB3	9:N:2286:HOH:O	2.08	0.52
3:N:710:ARG:NH2	3:N:1210:SER:OG	2.43	0.52
3:N:875:THR:HG22	3:N:879:ARG:HB2	1.92	0.52
3:N:1041:LEU:HD12	3:N:1058:ARG:CA	2.38	0.52
3:N:1097:LYS:O	3:N:1101:VAL:HG23	2.09	0.52
5:P:393:THR:HG22	5:P:394:ARG:H	1.75	0.52
2:C:64:LEU:HD22	2:C:359:MET:HG3	1.91	0.52
2:C:195:LEU:HD12	2:C:234:ALA:HB1	1.91	0.52
2:C:408:ARG:HH21	2:C:542:VAL:CG2	2.23	0.52
2:C:697:ARG:HD2	2:C:699:PHE:CD1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:865:THR:C	9:C:1269:HOH:O	2.52	0.52
2:C:1059:ASP:OD1	2:C:1080:SER:HB3	2.10	0.52
9:C:1344:HOH:O	3:D:603:LEU:HB3	2.09	0.52
3:D:481:MET:HE3	3:D:1389:LEU:HG	1.92	0.52
3:D:916:TYR:CE2	3:D:920:LEU:HD13	2.45	0.52
3:D:1408:ILE:O	3:D:1409:ALA:C	2.49	0.52
1:L:195:LEU:C	9:L:1676:HOH:O	2.53	0.52
2:M:926:PHE:O	2:M:930:LYS:HG3	2.10	0.52
3:N:34:TYR:O	3:N:35:ARG:C	2.52	0.52
3:N:637:LEU:CD1	3:N:641:GLN:HB2	2.40	0.52
3:N:1019:PRO:O	3:N:1023:MET:HG2	2.10	0.52
3:N:1272:ALA:CA	3:N:1326:THR:HB	2.40	0.52
5:P:181:GLU:O	5:P:184:ARG:HB3	2.10	0.52
5:P:288:TYR:HA	5:P:291:ILE:HG22	1.91	0.52
1:A:59:GLU:HG3	1:A:139:ASN:CG	2.35	0.52
1:B:5:LYS:O	1:B:8:ALA:HB2	2.09	0.52
2:C:196:LEU:O	2:C:199:VAL:HB	2.10	0.52
2:C:209:ARG:O	2:C:213:ALA:HB2	2.10	0.52
2:C:338:GLU:O	2:C:341:THR:HG22	2.10	0.52
2:C:367:LEU:HD13	9:C:1770:HOH:O	2.10	0.52
2:C:722:ILE:HG13	2:C:757:GLY:O	2.10	0.52
2:C:878:SER:HB3	3:D:1029:ARG:HH11	1.74	0.52
2:C:966:LEU:HD11	2:C:986:PRO:HG2	1.91	0.52
2:C:1087:VAL:HG13	3:D:610:LYS:NZ	2.13	0.52
3:D:524:LEU:C	3:D:526:PRO:HD3	2.35	0.52
3:D:989:TYR:CZ	3:D:993:LEU:HD11	2.45	0.52
3:D:1101:VAL:HG21	3:D:1424:VAL:CG2	2.31	0.52
3:D:1321:ALA:O	3:D:1339:LYS:HG3	2.10	0.52
4:E:54:LEU:HD23	4:E:58:PRO:HD2	1.91	0.52
5:F:151:LEU:HD21	9:F:675:HOH:O	2.08	0.52
2:M:79:PRO:HA	9:M:2242:HOH:O	2.09	0.52
2:M:165:LEU:O	2:M:265:ARG:HD2	2.10	0.52
2:M:166:PRO:HD3	2:M:265:ARG:CG	2.39	0.52
2:M:208:ALA:HA	2:M:218:VAL:HG22	1.91	0.52
2:M:332:ARG:HH21	2:M:338:GLU:CD	2.17	0.52
2:M:402:SER:OG	2:M:566:THR:HG22	2.09	0.52
2:M:773:LEU:O	2:M:777:ILE:HG13	2.10	0.52
3:N:408:GLU:HG2	3:N:408:GLU:O	2.10	0.52
3:N:947:ILE:O	3:N:947:ILE:HD12	2.09	0.52
3:N:1283:ILE:HG22	3:N:1284:GLU:N	2.24	0.52
5:P:191:ASN:HB3	5:P:220:LEU:HD11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:SER:CB	1:A:158:ILE:HG21	2.40	0.52
1:A:107:LYS:HE3	1:A:113:ASP:OD2	2.10	0.52
1:B:19:GLU:O	1:B:200:TRP:HA	2.10	0.52
2:C:170:PRO:HD3	2:C:263:ASP:HB3	1.92	0.52
2:C:281:LEU:CD1	2:C:306:THR:HA	2.40	0.52
2:C:971:LYS:HE2	9:C:1494:HOH:O	2.09	0.52
3:D:77:GLY:O	3:D:78:VAL:HG23	2.10	0.52
3:D:551:ASN:O	3:D:555:LYS:HG3	2.09	0.52
3:D:863:VAL:HG12	9:D:1596:HOH:O	2.10	0.52
3:D:1324:PRO:HG3	3:D:1330:ILE:HD11	1.91	0.52
3:D:1462:LEU:N	3:D:1462:LEU:HD23	2.24	0.52
5:F:88:ILE:CD1	5:F:193:ARG:HB2	2.40	0.52
2:M:54:ILE:HG22	2:M:66:LEU:HB3	1.92	0.52
2:M:385:PHE:O	2:M:389:SER:HB3	2.10	0.52
2:M:770:GLU:CG	3:N:65:ARG:HH12	2.23	0.52
2:M:807:ARG:HD3	9:M:1889:HOH:O	2.09	0.52
2:M:911:GLU:O	2:M:915:LYS:HG2	2.10	0.52
2:M:926:PHE:CD1	2:M:929:ARG:HD3	2.44	0.52
3:N:50:PHE:CB	3:N:522:PRO:HG2	2.40	0.52
3:N:1487:VAL:HG13	3:N:1491:THR:HB	1.91	0.52
5:P:279:GLN:HA	9:P:477:HOH:O	2.10	0.52
1:A:44:LEU:HB3	1:A:177:VAL:HG21	1.91	0.52
1:A:128:HIS:CE1	1:A:131:THR:HG23	2.45	0.52
2:C:70:GLU:HB3	9:C:1236:HOH:O	2.09	0.52
2:C:207:LEU:HD22	2:C:221:LEU:CD2	2.39	0.52
2:C:352:ALA:HA	2:C:355:VAL:HG12	1.91	0.52
3:D:162:ARG:HA	3:D:449:SER:HB3	1.91	0.52
3:D:567:ILE:HD12	3:D:567:ILE:H	1.75	0.52
3:D:675:ARG:O	3:D:678:GLU:HG2	2.10	0.52
3:D:864:VAL:HG12	3:D:865:THR:H	1.73	0.52
3:D:1481:VAL:CG1	4:E:18:ARG:HG3	2.40	0.52
4:E:54:LEU:HA	4:E:58:PRO:HG2	1.91	0.52
5:F:163:LEU:HB3	5:F:174:LEU:HD13	1.92	0.52
1:K:146:ARG:HD2	9:K:2782:HOH:O	2.10	0.52
2:M:42:VAL:HG12	2:M:43:GLY:N	2.25	0.52
2:M:197:LEU:HD22	2:M:202:TYR:CD2	2.43	0.52
2:M:676:ILE:O	3:N:948:THR:HB	2.09	0.52
2:M:816:LYS:HE2	2:M:819:VAL:HG21	1.92	0.52
3:N:631:ILE:HG12	3:N:743:ASP:O	2.10	0.52
3:N:988:ARG:O	3:N:992:ILE:HG13	2.10	0.52
1:A:5:LYS:O	1:A:8:ALA:HB2	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:59:LYS:HB2	9:C:1378:HOH:O	2.08	0.51
2:C:815:LEU:HG	2:C:819:VAL:CG1	2.40	0.51
2:C:918:LEU:HD23	2:C:967:PHE:O	2.09	0.51
2:C:976:ASP:HB3	2:C:979:THR:HG22	1.92	0.51
2:C:1060:ILE:CG2	2:C:1061:GLU:N	2.72	0.51
3:D:105:VAL:HG13	3:D:124:GLU:OE1	2.10	0.51
3:D:1059:SER:OG	3:D:1065:LEU:HA	2.11	0.51
3:D:1280:VAL:O	3:D:1294:VAL:HA	2.10	0.51
3:D:1494:ALA:HB1	9:E:137:HOH:O	2.10	0.51
5:F:88:ILE:CG1	5:F:193:ARG:HB2	2.41	0.51
5:F:226:LYS:HD2	5:F:242:TRP:CZ2	2.45	0.51
1:K:57:TYR:O	1:K:140:MET:HA	2.10	0.51
1:L:9:PRO:HB3	1:L:25:LEU:HG	1.93	0.51
1:L:117:VAL:HA	9:L:1875:HOH:O	2.10	0.51
1:L:156:HIS:CG	1:L:157:GLY:H	2.28	0.51
2:M:816:LYS:HB2	2:M:819:VAL:CG2	2.39	0.51
3:N:527:MET:HE3	3:N:535:PHE:CD2	2.45	0.51
3:N:534:ARG:HG3	5:P:312:GLN:HE22	1.74	0.51
3:N:551:ASN:O	3:N:555:LYS:HG3	2.10	0.51
3:N:957:PRO:HD2	3:N:1007:VAL:HG12	1.91	0.51
3:N:1485:GLN:NE2	4:O:80:VAL:H	2.08	0.51
4:O:51:LEU:HB2	9:O:1054:HOH:O	2.09	0.51
5:P:336:GLU:HG3	9:P:629:HOH:O	2.09	0.51
3:D:126:VAL:HG11	3:D:152:LEU:HD12	1.92	0.51
3:D:127:LEU:HD11	3:D:461:ILE:HD11	1.92	0.51
3:D:840:LYS:HB3	3:D:841:TYR:CD2	2.46	0.51
3:D:1118:ILE:HG23	9:D:1773:HOH:O	2.09	0.51
3:D:1385:GLY:CA	3:D:1413:THR:HG21	2.39	0.51
9:D:2077:HOH:O	5:F:349:LEU:HD22	2.10	0.51
5:F:278:LEU:CB	5:F:286:PRO:HG2	2.40	0.51
9:K:1749:HOH:O	2:M:929:ARG:HG3	2.08	0.51
1:L:25:LEU:HD23	1:L:28:LEU:HD11	1.91	0.51
2:M:260:LEU:HD22	9:M:2052:HOH:O	2.10	0.51
2:M:464:LEU:HD12	2:M:465:GLY:N	2.25	0.51
2:M:498:GLN:HE21	2:M:498:GLN:HA	1.74	0.51
3:N:192:ALA:HB2	3:N:393:ILE:HD11	1.92	0.51
3:N:428:LYS:HE2	9:N:1658:HOH:O	2.11	0.51
3:N:833:GLU:HG2	9:N:2184:HOH:O	2.08	0.51
5:P:189:GLU:HA	5:P:192:LEU:HD12	1.90	0.51
1:A:42:ARG:HH21	2:C:857:ASP:HB3	1.75	0.51
2:C:2:GLU:CG	2:C:899:GLN:HB3	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:141:HIS:O	2:C:331:ARG:HA	2.10	0.51
2:C:631:SER:HB3	2:C:637:LEU:HD21	1.92	0.51
2:C:1025:ALA:C	2:C:1026:GLN:HG3	2.35	0.51
3:D:10:ILE:HD11	3:D:1434:TRP:NE1	2.24	0.51
3:D:187:LYS:HG3	3:D:199:LEU:CD2	2.40	0.51
3:D:527:MET:CE	5:F:258:ILE:HD11	2.33	0.51
3:D:1205:TYR:HE1	3:D:1221:VAL:HG13	1.75	0.51
5:F:130:VAL:HA	5:F:142:ARG:NH2	2.26	0.51
5:F:361:LEU:HD21	5:F:404:ALA:HB1	1.92	0.51
1:L:57:TYR:CZ	1:L:161:ARG:HD3	2.45	0.51
1:L:196:THR:HG22	9:L:1676:HOH:O	2.10	0.51
2:M:489:THR:HG21	9:M:2237:HOH:O	2.09	0.51
3:N:31:THR:HG23	3:N:45:PHE:HE2	1.75	0.51
3:N:133:ILE:HG22	3:N:455:ARG:C	2.35	0.51
3:N:398:ALA:HB1	3:N:446:VAL:O	2.10	0.51
3:N:861:GLN:HG2	9:N:2139:HOH:O	2.09	0.51
3:N:1342:GLU:HB3	9:N:2128:HOH:O	2.10	0.51
2:C:211:LEU:HD11	2:C:308:ARG:HA	1.93	0.51
2:C:512:ARG:HB3	2:C:523:ILE:HD11	1.92	0.51
2:C:633:GLN:HG3	9:C:1153:HOH:O	2.09	0.51
2:C:810:ASP:N	2:C:811:PRO:HD3	2.25	0.51
2:C:987:ILE:HG12	3:D:948:THR:HG21	1.91	0.51
2:C:1030:GLN:CD	3:D:628:ARG:HB3	2.35	0.51
3:D:10:ILE:HG13	3:D:1434:TRP:CE2	2.45	0.51
3:D:18:ILE:HD12	3:D:518:PRO:CG	2.40	0.51
3:D:398:ALA:HB1	3:D:446:VAL:O	2.10	0.51
3:D:879:ARG:HD3	3:D:902:LEU:O	2.10	0.51
3:D:1115:THR:HG21	9:D:2063:HOH:O	2.10	0.51
3:D:1306:PRO:HG3	9:D:1723:HOH:O	2.10	0.51
3:D:1341:PRO:O	3:D:1345:GLU:HB2	2.10	0.51
4:E:33:HIS:CB	4:E:37:ASN:HD21	2.21	0.51
4:E:60:ALA:O	4:E:63:TRP:HB2	2.10	0.51
2:M:141:HIS:CB	2:M:418:LEU:HG	2.40	0.51
2:M:191:PHE:CZ	2:M:238:LEU:HD11	2.45	0.51
2:M:218:VAL:HG12	9:M:1965:HOH:O	2.11	0.51
2:M:264:PRO:HB2	9:M:1685:HOH:O	2.11	0.51
2:M:561:GLY:HA3	2:M:842:ARG:O	2.11	0.51
2:M:565:GLN:HA	2:M:995:MET:HE1	1.92	0.51
2:M:897:LEU:HB3	2:M:899:GLN:HE21	1.76	0.51
3:N:111:LYS:HE2	3:N:498:VAL:HG12	1.92	0.51
3:N:1264:GLU:HG2	3:N:1425:THR:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1485:GLN:O	4:O:75:PHE:HA	2.11	0.51
5:P:416:ARG:HD3	5:P:419:ARG:HD3	1.92	0.51
1:A:19:GLU:O	1:A:200:TRP:HA	2.10	0.51
1:A:182:GLU:HG2	9:A:412:HOH:O	2.11	0.51
2:C:114:PHE:CD1	2:C:114:PHE:N	2.77	0.51
2:C:257:VAL:HG21	9:C:1517:HOH:O	2.11	0.51
2:C:278:GLU:HB2	9:C:1544:HOH:O	2.10	0.51
2:C:420:ARG:NH1	2:C:422:ARG:HH21	2.08	0.51
2:C:874:LEU:HD23	3:D:1023:MET:CE	2.41	0.51
2:C:876:VAL:O	2:C:879:ARG:O	2.29	0.51
2:C:1105:LYS:O	2:C:1105:LYS:HG3	2.10	0.51
2:C:1109:VAL:HG21	3:D:3:LYS:O	2.11	0.51
3:D:26:VAL:HG23	9:D:2241:HOH:O	2.10	0.51
3:D:137:PRO:N	9:D:1592:HOH:O	2.43	0.51
3:D:436:GLU:HB2	9:D:2406:HOH:O	2.10	0.51
3:D:480:GLU:HG3	3:D:480:GLU:O	2.10	0.51
3:D:1258:ARG:NH2	3:D:1262:LEU:HD11	2.26	0.51
3:D:1277:ILE:CD1	3:D:1301:LYS:HB2	2.40	0.51
5:F:410:TYR:O	5:F:413:SER:HB2	2.11	0.51
1:L:133:GLU:O	1:L:134:GLU:HG2	2.10	0.51
2:M:313:LEU:HD12	2:M:313:LEU:O	2.10	0.51
2:M:349:ALA:HB3	9:M:1970:HOH:O	2.10	0.51
2:M:398:THR:N	2:M:633:GLN:OE1	2.43	0.51
2:M:606:VAL:CG2	2:M:645:VAL:HG22	2.40	0.51
2:M:685:GLU:HG3	3:N:783:ARG:HD2	1.92	0.51
3:N:65:ARG:CG	3:N:66:GLN:N	2.73	0.51
3:N:145:VAL:HG13	3:N:146:PRO:N	2.26	0.51
3:N:1145:TYR:CE2	3:N:1168:MET:HB2	2.44	0.51
4:O:33:HIS:CB	4:O:37:ASN:HD21	2.24	0.51
5:P:350:LEU:HD12	5:P:422:LEU:HD12	1.92	0.51
2:C:334:ARG:HB2	9:C:1322:HOH:O	2.09	0.51
2:C:551:GLU:HB3	2:C:906:PHE:CD2	2.46	0.51
2:C:911:GLU:O	2:C:915:LYS:HG2	2.11	0.51
3:D:97:THR:HB	9:D:1781:HOH:O	2.10	0.51
3:D:586:ARG:NH2	3:D:1444:THR:HG21	2.26	0.51
3:D:637:LEU:CD1	3:D:641:GLN:HB2	2.41	0.51
3:D:799:LYS:O	3:D:826:PRO:HD2	2.09	0.51
3:D:1372:VAL:HG13	3:D:1373:ARG:N	2.26	0.51
5:F:273:ARG:HG2	9:F:688:HOH:O	2.10	0.51
1:K:19:GLU:HB3	9:K:2538:HOH:O	2.09	0.51
1:K:49:PRO:HB3	1:K:148:VAL:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:23:PHE:O	1:L:196:THR:HA	2.10	0.51
2:M:244:PRO:HD2	2:M:245:GLY:H	1.75	0.51
2:M:264:PRO:HB3	2:M:289:THR:HG21	1.93	0.51
2:M:411:SER:OG	2:M:452:ILE:HG23	2.11	0.51
2:M:477:GLY:O	2:M:508:ILE:HG12	2.11	0.51
2:M:838:LYS:HZ2	2:M:846:LYS:HE2	1.76	0.51
2:M:976:ASP:HB3	2:M:979:THR:HG22	1.92	0.51
3:N:34:TYR:OH	5:P:261:PRO:HD2	2.10	0.51
3:N:204:LEU:HD21	3:N:445:ARG:NH1	2.26	0.51
3:N:613:ARG:CZ	3:N:1097:LYS:HE2	2.40	0.51
3:N:1113:GLY:N	3:N:1195:GLN:NE2	2.58	0.51
5:P:370:LYS:HD3	5:P:371:LEU:HG	1.93	0.51
2:C:165:LEU:HA	2:C:166:PRO:O	2.10	0.51
2:C:264:PRO:HB3	2:C:289:THR:HG21	1.91	0.51
2:C:551:GLU:OE2	2:C:552:HIS:NE2	2.43	0.51
3:D:52:PRO:HD2	9:D:1552:HOH:O	2.10	0.51
3:D:443:VAL:HG22	3:D:444:VAL:N	2.26	0.51
3:D:820:GLU:HA	3:D:825:ALA:O	2.10	0.51
3:D:1382:THR:HG21	3:D:1418:LYS:NZ	2.25	0.51
3:D:1441:GLN:HG3	3:D:1442:ASN:N	2.25	0.51
5:F:153:PRO:HD2	9:F:614:HOH:O	2.09	0.51
1:K:11:PHE:HB2	9:K:1022:HOH:O	2.10	0.51
1:K:70:GLY:N	2:M:607:ASP:OD1	2.38	0.51
2:M:516:ARG:HD2	9:M:1937:HOH:O	2.10	0.51
2:M:676:ILE:CG2	2:M:988:VAL:HG22	2.40	0.51
2:M:881:ASN:HD22	2:M:881:ASN:H	1.59	0.51
2:M:1058:ASP:HB2	3:N:621:LYS:HE2	1.93	0.51
3:N:26:VAL:HG11	3:N:44:LEU:HD23	1.91	0.51
3:N:141:ILE:HG21	3:N:449:SER:HA	1.92	0.51
3:N:658:LEU:HD11	3:N:674:ARG:HH11	1.76	0.51
3:N:754:PHE:HE2	3:N:1476:THR:HG21	1.76	0.51
3:N:986:ARG:HG3	9:N:1540:HOH:O	2.11	0.51
3:N:996:TRP:O	3:N:999:THR:HG22	2.11	0.51
3:N:1382:THR:HG21	3:N:1418:LYS:HE3	1.92	0.51
1:A:1:MET:HB3	9:A:440:HOH:O	2.10	0.51
1:A:49:PRO:O	1:A:173:PRO:HG2	2.10	0.51
2:C:334:ARG:NH1	2:C:415:PRO:HG2	2.25	0.51
3:D:687:VAL:HG13	9:D:2185:HOH:O	2.11	0.51
3:D:1101:VAL:CA	3:D:1428:ALA:HB2	2.40	0.51
3:D:1120:VAL:HB	3:D:1144:LEU:HD21	1.92	0.51
3:D:1243:THR:HG22	3:D:1244:GLY:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1305:LEU:HD22	3:D:1309:ALA:HB1	1.92	0.51
4:E:17:TYR:N	4:E:17:TYR:CD2	2.78	0.51
5:F:339:PRO:HB3	5:F:343:ASP:HB2	1.92	0.51
1:K:180:GLN:HE22	2:M:929:ARG:HH21	1.59	0.51
2:M:98:LEU:HG	9:M:1826:HOH:O	2.10	0.51
2:M:208:ALA:HA	2:M:221:LEU:HD21	1.93	0.51
2:M:244:PRO:HG2	2:M:246:ASP:OD2	2.09	0.51
2:M:260:LEU:HA	2:M:291:ALA:HB2	1.91	0.51
2:M:333:ILE:HB	9:M:1750:HOH:O	2.10	0.51
2:M:1105:LYS:O	2:M:1107:ASN:N	2.44	0.51
3:N:14:SER:O	3:N:17:LYS:N	2.44	0.51
3:N:434:ARG:HB2	3:N:447:VAL:CG2	2.41	0.51
3:N:563:PRO:HG2	3:N:566:ILE:HD12	1.93	0.51
3:N:866:VAL:HG12	3:N:867:ARG:N	2.25	0.51
3:N:957:PRO:CD	3:N:1007:VAL:HG12	2.40	0.51
3:N:1250:ALA:HB2	9:N:1888:HOH:O	2.09	0.51
7:N:1527:MXP:H11A	9:N:1557:HOH:O	2.11	0.51
4:O:41:GLU:N	4:O:42:PRO:CD	2.74	0.51
5:P:103:ALA:HB3	9:P:455:HOH:O	2.11	0.51
2:C:6:PHE:CB	2:C:909:ALA:HA	2.40	0.51
2:C:129:ILE:CG1	2:C:386:PHE:HB3	2.41	0.51
2:C:275:TYR:HB2	9:C:1736:HOH:O	2.10	0.51
2:C:305:PRO:CA	2:C:308:ARG:HB2	2.41	0.51
2:C:676:ILE:O	2:C:676:ILE:CG2	2.56	0.51
2:C:742:VAL:HG12	2:C:743:VAL:N	2.26	0.51
3:D:46:ASP:OD2	3:D:48:ARG:HG2	2.11	0.51
3:D:50:PHE:HB3	3:D:522:PRO:HG2	1.91	0.51
3:D:661:MET:O	3:D:664:LYS:O	2.28	0.51
3:D:1278:ASP:HA	3:D:1319:VAL:O	2.11	0.51
4:E:41:GLU:N	4:E:42:PRO:CD	2.72	0.51
5:F:260:ILE:CG2	5:F:264:MET:HB2	2.40	0.51
1:K:25:LEU:HB2	9:K:1260:HOH:O	2.11	0.51
1:L:128:HIS:CE1	1:L:131:THR:HG23	2.46	0.51
2:M:267:TYR:HD1	9:M:2269:HOH:O	1.94	0.51
2:M:644:VAL:HG22	2:M:647:GLN:OE1	2.11	0.51
3:N:399:ARG:HD2	9:N:1669:HOH:O	2.09	0.51
3:N:569:ASN:HB3	5:P:214:GLN:NE2	2.25	0.51
5:P:163:LEU:HD22	5:P:174:LEU:HD12	1.91	0.51
1:A:9:PRO:HD2	1:B:224:TYR:CE1	2.46	0.51
1:B:68:ILE:HG23	1:B:137:ARG:NH1	2.25	0.51
2:C:18:LEU:HD21	2:C:542:VAL:CG1	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:498:GLN:HA	2:C:498:GLN:NE2	2.26	0.51
2:C:929:ARG:HH12	2:C:940:GLU:CD	2.19	0.51
2:C:952:LEU:HD22	9:C:1205:HOH:O	2.10	0.51
3:D:134:VAL:HG12	3:D:152:LEU:HB3	1.93	0.51
3:D:141:ILE:CG2	3:D:450:TYR:H	2.24	0.51
3:D:162:ARG:HD2	3:D:434:ARG:CZ	2.41	0.51
3:D:407:VAL:HG13	3:D:422:ALA:HB2	1.92	0.51
3:D:581:LEU:O	3:D:603:LEU:HG	2.11	0.51
3:D:761:ILE:HG21	9:E:116:HOH:O	2.11	0.51
3:D:1145:TYR:CE2	3:D:1168:MET:HB2	2.45	0.51
3:D:1393:GLN:HB2	3:D:1398:TRP:CE2	2.46	0.51
1:K:89:PHE:HB3	1:K:94:LEU:CD2	2.40	0.51
1:L:50:GLY:HA3	1:L:171:PHE:O	2.11	0.51
2:M:437:ARG:HH22	2:M:491:GLU:CB	2.24	0.51
2:M:603:VAL:HG21	2:M:643:VAL:CG1	2.35	0.51
2:M:979:THR:HG23	2:M:981:GLU:N	2.24	0.51
3:N:137:PRO:HD2	3:N:453:ASP:CG	2.36	0.51
3:N:569:ASN:HD21	5:P:210:LEU:CD2	2.22	0.51
3:N:615:ARG:O	3:N:617:ASN:N	2.44	0.51
3:N:820:GLU:HA	3:N:825:ALA:O	2.11	0.51
3:N:1280:VAL:O	3:N:1294:VAL:HA	2.11	0.51
9:N:2109:HOH:O	5:P:164:LYS:HE3	2.10	0.51
1:A:16:GLN:HG2	1:A:16:GLN:O	2.10	0.50
1:A:57:TYR:O	1:A:140:MET:HA	2.11	0.50
1:A:216:GLU:HG2	9:A:422:HOH:O	2.10	0.50
2:C:42:VAL:HG23	9:C:1299:HOH:O	2.10	0.50
2:C:861:LEU:HD21	2:C:925:TYR:HE2	1.76	0.50
2:C:890:LEU:HD12	2:C:914:ILE:HD13	1.93	0.50
2:C:942:GLU:O	2:C:945:ARG:HB3	2.11	0.50
3:D:6:ARG:HD3	9:D:1692:HOH:O	2.11	0.50
3:D:448:GLU:HA	9:D:2218:HOH:O	2.11	0.50
3:D:1147:ARG:HD2	3:D:1188:VAL:HG21	1.92	0.50
4:E:26:ARG:HH11	4:E:29:GLN:CD	2.18	0.50
5:F:209:PHE:CE2	5:F:213:ILE:HD11	2.45	0.50
1:L:73:GLU:CD	1:L:130:ALA:HA	2.34	0.50
2:M:68:PHE:HE1	2:M:96:ALA:HB1	1.76	0.50
2:M:139:GLN:HE21	2:M:334:ARG:HD2	1.77	0.50
2:M:157:ARG:NH2	2:M:314:THR:O	2.44	0.50
2:M:275:TYR:HD2	9:M:1681:HOH:O	1.94	0.50
2:M:289:THR:O	2:M:291:ALA:N	2.44	0.50
2:M:352:ALA:C	2:M:355:VAL:HG12	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:358:ARG:HD3	2:M:371:LYS:O	2.11	0.50
2:M:463:GLU:HB3	9:M:1990:HOH:O	2.09	0.50
2:M:502:PRO:HB2	2:M:509:ALA:HB3	1.93	0.50
2:M:755:LEU:HD12	9:M:1781:HOH:O	2.10	0.50
3:N:137:PRO:HD2	3:N:453:ASP:OD2	2.11	0.50
3:N:955:VAL:O	3:N:1039:CYS:HB3	2.11	0.50
5:P:372:ARG:HD3	9:P:506:HOH:O	2.11	0.50
2:C:290:LEU:HB3	2:C:302:VAL:CG1	2.41	0.50
3:D:421:LEU:CG	3:D:429:SER:HB3	2.42	0.50
3:D:627:GLY:O	3:D:747:VAL:HG12	2.12	0.50
3:D:1018:ASN:HB3	3:D:1021:TYR:HB3	1.92	0.50
3:D:1110:ALA:O	3:D:1111:ASP:C	2.52	0.50
4:E:45:ARG:HH21	4:E:55:PHE:HB3	1.75	0.50
5:F:88:ILE:HD13	5:F:193:ARG:HB2	1.93	0.50
5:F:287:THR:HG23	5:F:289:GLU:HB3	1.92	0.50
1:K:179:PHE:HZ	2:M:939:ARG:HH22	1.57	0.50
1:L:15:THR:C	1:L:16:GLN:HG2	2.35	0.50
2:M:573:ARG:HH12	2:M:697:ARG:HB3	1.75	0.50
2:M:671:ASN:ND2	2:M:671:ASN:H	2.08	0.50
2:M:710:ILE:CD1	2:M:790:LEU:HB2	2.41	0.50
2:M:930:LYS:HA	9:M:1678:HOH:O	2.11	0.50
3:N:9:ARG:HE	3:N:11:ALA:HB2	1.75	0.50
1:A:50:GLY:O	1:A:146:ARG:HA	2.11	0.50
2:C:41:ASN:H	2:C:41:ASN:ND2	1.97	0.50
2:C:181:VAL:HG11	9:C:1754:HOH:O	2.10	0.50
2:C:185:LYS:CE	2:C:190:LYS:HE2	2.40	0.50
2:C:480:THR:HG22	2:C:481:ASP:H	1.76	0.50
2:C:756:VAL:HG21	2:C:823:VAL:HG11	1.92	0.50
2:C:1051:GLU:HG2	2:C:1056:LYS:HD2	1.93	0.50
2:C:1115:LEU:HD23	3:D:85:VAL:HG13	1.94	0.50
3:D:800:LYS:NZ	3:D:804:LEU:HD13	2.26	0.50
5:F:361:LEU:HD13	5:F:366:ALA:CB	2.42	0.50
2:M:136:ILE:CG2	2:M:336:VAL:HG22	2.41	0.50
2:M:143:SER:C	2:M:163:ILE:HD11	2.37	0.50
2:M:253:ALA:O	2:M:256:TYR:HB2	2.11	0.50
2:M:274:ARG:HG2	9:M:1662:HOH:O	2.10	0.50
2:M:334:ARG:NH2	2:M:418:LEU:HD11	2.26	0.50
2:M:470:PRO:HD3	2:M:485:TYR:CE2	2.46	0.50
3:N:52:PRO:CG	3:N:80:VAL:HG13	2.41	0.50
3:N:414:ARG:HB3	9:N:2299:HOH:O	2.11	0.50
3:N:1299:PHE:N	3:N:1299:PHE:CD2	2.79	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1495:ILE:HA	4:O:88:GLU:OE2	2.11	0.50
4:O:49:GLN:HB3	9:O:1772:HOH:O	2.11	0.50
1:A:69:PRO:C	1:A:71:VAL:H	2.18	0.50
1:A:183:ASP:HB3	9:A:322:HOH:O	2.11	0.50
2:C:42:VAL:HG12	2:C:43:GLY:N	2.23	0.50
2:C:578:VAL:HG11	2:C:991:GLN:HB3	1.93	0.50
2:C:759:THR:HB	2:C:785:VAL:CG2	2.41	0.50
2:C:841:ASN:C	2:C:841:ASN:HD22	2.19	0.50
3:D:543:LEU:HB2	9:D:1714:HOH:O	2.10	0.50
3:D:1276:GLU:HG3	3:D:1303:TYR:OH	2.12	0.50
3:D:1466:VAL:CG2	3:D:1472:ILE:HD11	2.36	0.50
3:D:1495:ILE:HD12	4:E:88:GLU:OE2	2.11	0.50
5:F:85:LEU:HD11	9:F:543:HOH:O	2.11	0.50
5:F:141:VAL:O	5:F:145:PRO:HD2	2.12	0.50
5:F:363:GLU:HA	5:F:367:MET:HG3	1.93	0.50
1:K:9:PRO:HB3	1:K:25:LEU:CD2	2.41	0.50
2:M:274:ARG:HG2	2:M:274:ARG:O	2.10	0.50
2:M:837:ASP:O	2:M:848:VAL:HG13	2.11	0.50
2:M:877:PRO:HG3	3:N:1020:LEU:CD1	2.41	0.50
2:M:1019:GLN:NE2	3:N:621:LYS:HA	2.22	0.50
3:N:102:ILE:HD12	3:N:579:ASP:CG	2.36	0.50
3:N:561:GLY:CA	5:P:184:ARG:HH12	2.23	0.50
3:N:1189:ARG:HD3	9:N:1595:HOH:O	2.10	0.50
1:B:15:THR:C	1:B:16:GLN:HG2	2.35	0.50
2:C:73:LEU:HD23	2:C:94:LEU:HD13	1.93	0.50
2:C:93:PRO:HG3	2:C:117:HIS:HE1	1.76	0.50
2:C:604:ALA:HB3	2:C:612:VAL:O	2.12	0.50
3:D:145:VAL:HG22	3:D:146:PRO:CD	2.41	0.50
3:D:610:LYS:CG	7:D:1527:MXP:C15	2.90	0.50
3:D:1192:LEU:HD13	3:D:1345:GLU:HG2	1.94	0.50
3:D:1223:ILE:H	3:D:1223:ILE:CD1	2.22	0.50
4:E:9:LEU:HD22	4:E:19:LEU:HD11	1.94	0.50
5:F:288:TYR:HA	5:F:291:ILE:HG22	1.92	0.50
2:M:78:PHE:CG	2:M:88:LEU:HD21	2.46	0.50
2:M:96:ALA:HB3	9:M:1826:HOH:O	2.10	0.50
2:M:186:VAL:HG23	2:M:187:ASN:H	1.75	0.50
2:M:227:PHE:HA	2:M:237:ARG:HH12	1.75	0.50
2:M:290:LEU:HD23	2:M:290:LEU:H	1.76	0.50
2:M:545:ASN:O	2:M:581:THR:HG21	2.11	0.50
3:N:34:TYR:OH	5:P:264:MET:HG3	2.11	0.50
3:N:627:GLY:O	3:N:747:VAL:HG12	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:728:LEU:HD22	3:N:745:MET:SD	2.52	0.50
3:N:970:LYS:HD3	9:N:2041:HOH:O	2.12	0.50
3:N:1128:VAL:HG13	9:N:2137:HOH:O	2.12	0.50
3:N:1481:VAL:HG13	4:O:18:ARG:HG3	1.93	0.50
5:P:214:GLN:O	5:P:217:ASN:HB2	2.12	0.50
1:A:150:TYR:CE1	2:C:696:LYS:HA	2.47	0.50
2:C:897:LEU:HB3	2:C:899:GLN:HG2	1.93	0.50
3:D:11:ALA:HB1	3:D:507:ASN:OD1	2.12	0.50
3:D:66:GLN:O	3:D:67:ARG:C	2.53	0.50
3:D:641:GLN:HG2	9:D:1610:HOH:O	2.10	0.50
4:E:64:ALA:HA	4:E:67:GLU:OE1	2.12	0.50
5:F:88:ILE:CG2	5:F:193:ARG:HH11	2.24	0.50
1:K:19:GLU:O	1:K:200:TRP:HA	2.12	0.50
2:M:110:GLU:HB3	9:M:2230:HOH:O	2.10	0.50
2:M:153:ALA:O	2:M:155:PRO:HD3	2.12	0.50
2:M:269:LEU:HB3	9:M:2007:HOH:O	2.11	0.50
2:M:496:ILE:H	2:M:496:ILE:HD12	1.77	0.50
2:M:517:ARG:HB2	9:M:2072:HOH:O	2.12	0.50
2:M:762:LYS:HG2	2:M:763:GLY:H	1.76	0.50
2:M:795:GLY:HA3	2:M:1004:LYS:HE2	1.93	0.50
3:N:403:PHE:HE2	3:N:443:VAL:N	2.10	0.50
3:N:567:ILE:HD12	3:N:567:ILE:H	1.77	0.50
3:N:699:VAL:HG12	3:N:717:GLN:HA	1.93	0.50
3:N:1128:VAL:HG11	9:N:1633:HOH:O	2.10	0.50
4:O:53:GLY:C	4:O:55:PHE:N	2.67	0.50
5:P:392:VAL:HG11	5:P:396:ARG:CD	2.41	0.50
1:A:106:PRO:HG3	1:A:134:GLU:HG3	1.93	0.50
2:C:64:LEU:HD13	2:C:359:MET:CG	2.41	0.50
2:C:197:LEU:HB3	2:C:202:TYR:HB2	1.92	0.50
2:C:244:PRO:CD	2:C:245:GLY:H	2.24	0.50
2:C:689:VAL:HB	2:C:870:ILE:HG13	1.93	0.50
2:C:808:ARG:HA	2:C:815:LEU:HD22	1.92	0.50
2:C:811:PRO:HD2	2:C:813:VAL:HG22	1.93	0.50
2:C:1004:LYS:HA	9:C:1776:HOH:O	2.11	0.50
3:D:418:GLY:N	3:D:429:SER:O	2.35	0.50
3:D:630:VAL:CA	3:D:744:GLN:HG2	2.38	0.50
3:D:753:SER:HB3	9:E:134:HOH:O	2.11	0.50
3:D:800:LYS:HE2	3:D:804:LEU:HD13	1.94	0.50
3:D:862:ASP:O	3:D:876:SER:HB2	2.12	0.50
3:D:1216:SER:HB3	9:D:2106:HOH:O	2.11	0.50
4:E:38:THR:HG22	9:E:103:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:196:VAL:HG13	5:F:213:ILE:HD11	1.94	0.50
5:F:282:LEU:HD12	9:F:487:HOH:O	2.11	0.50
1:K:186:LEU:CB	1:K:192:LEU:HD11	2.40	0.50
1:L:4:SER:HA	1:L:7:LYS:HG2	1.93	0.50
1:L:19:GLU:O	1:L:200:TRP:HA	2.12	0.50
2:M:878:SER:HB3	3:N:1029:ARG:HH11	1.75	0.50
3:N:630:VAL:CA	3:N:744:GLN:HG2	2.39	0.50
3:N:716:PHE:CE2	3:N:765:SER:HB3	2.47	0.50
3:N:806:PHE:HE1	3:N:813:LEU:HB3	1.74	0.50
3:N:1310:ARG:HG3	3:N:1327:ARG:HB3	1.94	0.50
5:P:163:LEU:HB3	5:P:174:LEU:HD13	1.93	0.50
2:C:650:ARG:HB2	2:C:653:ASP:HB2	1.93	0.50
2:C:1090:LYS:HD2	3:D:90:MET:HE3	1.94	0.50
2:C:1096:ALA:O	3:D:13:ALA:CB	2.60	0.50
3:D:999:THR:O	3:D:1003:VAL:HG13	2.12	0.50
3:D:1281:VAL:HG21	3:D:1313:VAL:CG2	2.42	0.50
3:D:1295:GLU:HB3	3:D:1300:SER:OG	2.12	0.50
5:F:406:ARG:O	5:F:409:LYS:HG2	2.12	0.50
1:K:216:GLU:O	1:K:220:GLU:HG3	2.11	0.50
2:M:57:GLU:O	2:M:62:GLY:HA3	2.11	0.50
2:M:145:GLY:H	2:M:163:ILE:HG12	1.76	0.50
2:M:359:MET:HE3	9:M:2193:HOH:O	2.12	0.50
2:M:618:GLY:HA2	9:M:1827:HOH:O	2.10	0.50
2:M:876:VAL:O	2:M:879:ARG:O	2.29	0.50
4:O:89:MET:HA	9:O:1936:HOH:O	2.12	0.50
1:A:73:GLU:HG3	9:A:363:HOH:O	2.11	0.50
1:A:85:LEU:HB2	1:A:127:LEU:HD21	1.94	0.50
2:C:32:ALA:HB2	2:C:73:LEU:HD11	1.93	0.50
2:C:70:GLU:HA	9:C:1632:HOH:O	2.12	0.50
2:C:262:ALA:O	2:C:264:PRO:O	2.30	0.50
2:C:605:LYS:HB2	9:C:1120:HOH:O	2.11	0.50
2:C:1034:GLU:CA	2:C:1037:VAL:HG23	2.42	0.50
3:D:520:LEU:O	3:D:525:ARG:NH1	2.45	0.50
3:D:614:PHE:HB3	3:D:617:ASN:HB3	1.94	0.50
3:D:1214:PRO:HB2	9:D:2327:HOH:O	2.11	0.50
4:E:40:LEU:HD22	9:E:124:HOH:O	2.11	0.50
4:E:45:ARG:HB2	4:E:46:PRO:CD	2.42	0.50
4:E:70:THR:HG22	4:E:71:GLY:N	2.27	0.50
5:F:167:PRO:HB2	5:F:169:GLU:OE1	2.12	0.50
1:K:34:VAL:HG22	2:M:939:ARG:NH2	2.27	0.50
1:K:211:LEU:HD12	1:K:211:LEU:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:713:ARG:NH2	3:N:531:ASP:HB3	2.27	0.50
2:M:729:LEU:HD13	3:N:675:ARG:CZ	2.42	0.50
2:M:1116:ALA:HA	9:M:2070:HOH:O	2.12	0.50
3:N:19:ARG:HG2	9:N:2118:HOH:O	2.11	0.50
3:N:129:PHE:O	3:N:572:ARG:HG2	2.11	0.50
3:N:131:LYS:HE3	3:N:568:ARG:HB2	1.94	0.50
3:N:394:LEU:HD11	9:N:1920:HOH:O	2.11	0.50
3:N:1209:LEU:HD13	9:N:1985:HOH:O	2.12	0.50
3:N:1310:ARG:NE	3:N:1327:ARG:HB3	2.27	0.50
5:P:278:LEU:CB	5:P:286:PRO:HG2	2.42	0.50
5:P:358:LEU:HD13	5:P:370:LYS:CG	2.42	0.50
2:C:461:VAL:HG12	2:C:462:ASP:O	2.12	0.49
2:C:739:GLU:CD	2:C:742:VAL:HB	2.37	0.49
3:D:617:ASN:C	3:D:618:LEU:HD12	2.37	0.49
3:D:1147:ARG:HB3	3:D:1188:VAL:HG23	1.93	0.49
3:D:1383:ASP:HB2	3:D:1416:ALA:CB	2.34	0.49
4:E:74:VAL:HA	9:E:163:HOH:O	2.12	0.49
5:F:113:ILE:HG23	5:F:127:ILE:CG2	2.42	0.49
5:F:189:GLU:HA	5:F:192:LEU:HD12	1.94	0.49
1:L:211:LEU:O	1:L:214:ALA:HB3	2.12	0.49
2:M:36:PRO:HG2	2:M:70:GLU:HB3	1.94	0.49
2:M:196:LEU:O	2:M:199:VAL:HB	2.12	0.49
2:M:498:GLN:HB2	9:M:2088:HOH:O	2.11	0.49
2:M:538:GLN:CD	9:M:1660:HOH:O	2.54	0.49
2:M:1034:GLU:CA	2:M:1037:VAL:HG23	2.42	0.49
3:N:148:GLU:HG2	3:N:151:GLN:HE21	1.77	0.49
3:N:409:VAL:HB	3:N:421:LEU:HA	1.93	0.49
3:N:516:ALA:O	3:N:518:PRO:HD3	2.12	0.49
3:N:675:ARG:O	3:N:678:GLU:HG2	2.12	0.49
3:N:1003:VAL:O	3:N:1006:ALA:HB3	2.12	0.49
3:N:1353:GLN:NE2	3:N:1363:LEU:O	2.43	0.49
3:N:1389:LEU:HD12	3:N:1390:LEU:HG	1.94	0.49
5:P:115:LYS:HD2	5:P:173:TYR:CE2	2.47	0.49
5:P:187:LEU:O	5:P:187:LEU:HD23	2.11	0.49
1:B:25:LEU:HD23	1:B:28:LEU:HD11	1.94	0.49
1:B:85:LEU:HG	9:B:527:HOH:O	2.10	0.49
2:C:252:LYS:HB3	2:C:298:PHE:HZ	1.77	0.49
2:C:358:ARG:HG3	9:C:1597:HOH:O	2.11	0.49
2:C:523:ILE:HG22	9:C:1356:HOH:O	2.12	0.49
2:C:626:ARG:HB2	2:C:639:GLN:HE21	1.77	0.49
2:C:684:PHE:HE2	3:D:733:CYS:SG	2.35	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:789:SER:O	2:C:791:ARG:HG3	2.12	0.49
2:C:1087:VAL:HG12	3:D:610:LYS:NZ	2.27	0.49
3:D:17:LYS:HB2	9:D:1656:HOH:O	2.12	0.49
3:D:119:SER:HB2	3:D:123:LEU:CB	2.36	0.49
5:F:151:LEU:HD22	9:F:737:HOH:O	2.12	0.49
1:K:57:TYR:CE2	1:K:59:GLU:HA	2.46	0.49
2:M:305:PRO:CA	2:M:308:ARG:HB2	2.42	0.49
2:M:403:SER:O	2:M:407:LYS:HG3	2.12	0.49
2:M:1059:ASP:CG	2:M:1062:GLY:HA3	2.37	0.49
1:A:189:ARG:HG3	9:A:334:HOH:O	2.12	0.49
2:C:435:TYR:OH	2:C:498:GLN:NE2	2.44	0.49
2:C:607:ASP:HB2	2:C:610:ARG:HG3	1.95	0.49
2:C:670:GLN:HE22	2:C:699:PHE:C	2.21	0.49
2:C:722:ILE:HG21	2:C:821:GLU:OE1	2.12	0.49
2:C:926:PHE:CD1	2:C:929:ARG:HD3	2.46	0.49
3:D:27:GLU:HA	9:D:2102:HOH:O	2.11	0.49
3:D:65:ARG:HB2	5:F:375:LEU:O	2.11	0.49
3:D:465:LEU:HD22	3:D:509:PRO:O	2.12	0.49
3:D:540:LEU:HA	3:D:543:LEU:HD12	1.94	0.49
3:D:633:VAL:O	3:D:633:VAL:HG13	2.11	0.49
3:D:656:PHE:HB3	3:D:694:VAL:HG11	1.93	0.49
3:D:984:THR:CG2	3:D:987:GLU:H	2.25	0.49
3:D:1281:VAL:HG23	3:D:1317:ASP:O	2.12	0.49
3:D:1291:SER:HB2	3:D:1293:PHE:CE1	2.45	0.49
3:D:1307:LYS:HE3	9:D:2288:HOH:O	2.12	0.49
3:D:1388:ARG:HG3	3:D:1389:LEU:N	2.26	0.49
3:D:1420:LEU:HD12	3:D:1421:LEU:N	2.26	0.49
5:F:259:ARG:HA	9:F:658:HOH:O	2.12	0.49
1:K:134:GLU:HG2	9:K:1422:HOH:O	2.11	0.49
1:L:12:THR:OG1	1:L:24:VAL:HB	2.12	0.49
2:M:191:PHE:CD2	2:M:195:LEU:HD23	2.48	0.49
2:M:302:VAL:O	2:M:306:THR:HG23	2.11	0.49
2:M:338:GLU:O	2:M:341:THR:HG22	2.12	0.49
2:M:629:TYR:HB3	9:M:1712:HOH:O	2.11	0.49
2:M:897:LEU:HB3	2:M:899:GLN:HG2	1.94	0.49
2:M:1115:LEU:CD2	3:N:85:VAL:HG13	2.40	0.49
3:N:862:ASP:O	3:N:877:PRO:HD3	2.13	0.49
3:N:928:ALA:O	3:N:931:LEU:HB2	2.12	0.49
4:O:72:ARG:HB2	9:O:4461:HOH:O	2.12	0.49
5:P:299:TRP:CE3	5:P:303:ARG:HD3	2.46	0.49
5:P:361:LEU:HD21	5:P:404:ALA:HB1	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:9:ILE:HG12	2:C:907:ASP:CG	2.38	0.49
2:C:21:ILE:O	2:C:25:SER:HB2	2.13	0.49
2:C:163:ILE:HG21	9:C:1347:HOH:O	2.11	0.49
2:C:625:LEU:O	2:C:627:ARG:N	2.46	0.49
2:C:775:ARG:HG2	9:C:1674:HOH:O	2.12	0.49
2:C:810:ASP:N	2:C:811:PRO:CD	2.75	0.49
3:D:14:SER:O	3:D:17:LYS:N	2.46	0.49
3:D:145:VAL:HG13	3:D:146:PRO:N	2.28	0.49
3:D:787:LEU:HD21	3:D:947:ILE:CD1	2.43	0.49
3:D:957:PRO:HG3	3:D:1010:ASN:HD22	1.77	0.49
3:D:1209:LEU:HD21	4:E:16:LYS:HD2	1.94	0.49
3:D:1396:GLU:O	3:D:1400:VAL:HG23	2.12	0.49
1:K:198:ARG:C	1:K:199:ILE:HD12	2.37	0.49
2:M:443:THR:CG2	2:M:449:ILE:HG13	2.42	0.49
2:M:810:ASP:N	2:M:811:PRO:CD	2.75	0.49
2:M:854:PRO:C	2:M:856:GLU:N	2.70	0.49
2:M:1060:ILE:HB	9:M:1724:HOH:O	2.12	0.49
3:N:141:ILE:HG23	3:N:161:LEU:HD21	1.95	0.49
3:N:502:PHE:CE1	3:N:509:PRO:HB3	2.46	0.49
3:N:527:MET:HE3	3:N:535:PHE:HB3	1.94	0.49
3:N:820:GLU:HG2	3:N:825:ALA:O	2.13	0.49
3:N:1066:THR:CG2	3:N:1069:GLU:HG3	2.42	0.49
3:N:1262:LEU:HD23	3:N:1352:ILE:HG12	1.93	0.49
3:N:1372:VAL:HA	3:N:1375:MET:SD	2.53	0.49
5:P:185:GLN:O	5:P:189:GLU:HG3	2.12	0.49
5:P:369:LEU:HD11	5:P:401:GLU:HB2	1.94	0.49
1:B:86:VAL:HG12	1:B:124:ASN:ND2	2.18	0.49
1:B:149:GLY:O	1:B:171:PHE:HB2	2.13	0.49
2:C:85:GLU:OE2	2:C:802:ARG:NH2	2.45	0.49
3:D:481:MET:HG3	3:D:1388:ARG:NH2	2.27	0.49
3:D:527:MET:HB3	9:D:1582:HOH:O	2.11	0.49
3:D:1159:ARG:HB3	3:D:1159:ARG:CZ	2.43	0.49
3:D:1463:LYS:HB2	7:D:1527:MXP:H23B	1.95	0.49
5:F:364:ARG:HD2	9:F:435:HOH:O	2.12	0.49
2:M:678:PRO:O	3:N:943:THR:HA	2.11	0.49
2:M:818:GLY:N	5:P:309:LYS:HE2	2.26	0.49
3:N:149:LYS:HA	9:N:2241:HOH:O	2.12	0.49
3:N:207:PHE:HA	9:N:1567:HOH:O	2.12	0.49
3:N:827:ILE:O	3:N:837:GLY:HA3	2.13	0.49
3:N:895:VAL:O	3:N:899:LEU:HG	2.12	0.49
5:P:299:TRP:HE3	9:P:492:HOH:O	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:GLU:HG2	1:A:134:GLU:H	1.77	0.49
2:C:113:VAL:HB	2:C:115:LEU:HD23	1.95	0.49
2:C:1004:LYS:HG3	9:C:1776:HOH:O	2.12	0.49
3:D:409:VAL:HB	3:D:421:LEU:HA	1.94	0.49
3:D:674:ARG:HD3	9:D:1564:HOH:O	2.11	0.49
3:D:767:HIS:CD2	4:E:6:ILE:HG12	2.47	0.49
3:D:1283:ILE:HB	3:D:1315:ASP:OD2	2.13	0.49
1:L:158:ILE:HG12	9:L:3428:HOH:O	2.13	0.49
2:M:5:ARG:HB3	2:M:902:ILE:HB	1.93	0.49
2:M:101:ILE:HG23	2:M:107:LEU:CD2	2.41	0.49
2:M:209:ARG:O	2:M:213:ALA:HB2	2.12	0.49
2:M:364:GLU:O	2:M:367:LEU:HD21	2.12	0.49
2:M:442:GLU:HG2	2:M:454:SER:OG	2.12	0.49
3:N:185:VAL:HG22	3:N:203:ALA:HB2	1.95	0.49
3:N:736:PHE:O	3:N:738:ALA:N	2.46	0.49
3:N:1393:GLN:CB	3:N:1398:TRP:HE1	2.20	0.49
3:N:1435:LEU:HA	9:N:1677:HOH:O	2.13	0.49
5:P:209:PHE:O	5:P:213:ILE:HG13	2.12	0.49
5:P:358:LEU:HD22	5:P:370:LYS:HE3	1.94	0.49
1:A:176:ARG:O	1:A:200:TRP:HE3	1.96	0.49
2:C:44:ILE:HG23	2:C:344:PHE:CE1	2.48	0.49
2:C:191:PHE:CD2	2:C:195:LEU:HD23	2.47	0.49
2:C:622:GLU:HB3	9:C:1635:HOH:O	2.12	0.49
2:C:681:GLY:O	3:D:633:VAL:HG21	2.12	0.49
2:C:722:ILE:O	2:C:722:ILE:HG23	2.13	0.49
2:C:815:LEU:HD23	2:C:819:VAL:O	2.12	0.49
2:C:816:LYS:O	2:C:819:VAL:HB	2.12	0.49
3:D:53:ILE:HG23	3:D:54:LYS:H	1.78	0.49
3:D:521:PRO:O	3:D:525:ARG:HG2	2.13	0.49
3:D:530:VAL:HG13	9:D:2079:HOH:O	2.12	0.49
3:D:664:LYS:HA	9:D:1859:HOH:O	2.12	0.49
3:D:988:ARG:O	3:D:992:ILE:HG13	2.13	0.49
3:D:1114:THR:HG23	3:D:1116:ASN:HD21	1.78	0.49
3:D:1177:ALA:CB	3:D:1183:ILE:HD11	2.42	0.49
3:D:1189:ARG:HH11	3:D:1203:LYS:HB2	1.77	0.49
3:D:1272:ALA:CA	3:D:1326:THR:HB	2.41	0.49
5:F:295:MET:HG2	5:F:299:TRP:CD2	2.47	0.49
1:L:2:LEU:HD12	1:L:3:ASP:HB2	1.95	0.49
2:M:93:PRO:HG3	2:M:117:HIS:HE1	1.76	0.49
2:M:136:ILE:HG21	2:M:336:VAL:HG13	1.93	0.49
2:M:185:LYS:HE2	2:M:190:LYS:HG2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:358:ARG:HA	2:M:361:MET:HB2	1.95	0.49
2:M:923:GLU:O	2:M:927:GLY:HA3	2.12	0.49
2:M:1109:VAL:HA	3:N:3:LYS:HE3	1.93	0.49
3:N:28:LYS:CG	3:N:41:ARG:HH11	2.25	0.49
3:N:443:VAL:HG22	3:N:444:VAL:H	1.77	0.49
3:N:1066:THR:HG22	3:N:1069:GLU:CG	2.42	0.49
3:N:1246:VAL:HG13	3:N:1269:LYS:NZ	2.28	0.49
5:P:287:THR:HG23	5:P:289:GLU:HB3	1.93	0.49
2:C:332:ARG:CZ	2:C:464:LEU:HD11	2.43	0.49
2:C:420:ARG:HG3	2:C:422:ARG:HG2	1.95	0.49
2:C:762:LYS:C	2:C:763:GLY:O	2.52	0.49
9:C:1813:HOH:O	3:D:532:GLY:HA3	2.13	0.49
3:D:99:ALA:HB1	3:D:575:GLN:OE1	2.11	0.49
3:D:122:GLU:O	3:D:126:VAL:HG23	2.13	0.49
3:D:507:ASN:HB2	9:D:1793:HOH:O	2.12	0.49
3:D:728:LEU:HD13	3:D:745:MET:HE1	1.94	0.49
3:D:937:TYR:O	3:D:941:PHE:HD1	1.95	0.49
3:D:1382:THR:HG21	3:D:1418:LYS:HE3	1.95	0.49
4:E:23:VAL:HG12	4:E:61:VAL:HG13	1.95	0.49
5:F:81:VAL:O	5:F:85:LEU:HB2	2.12	0.49
5:F:94:LEU:HB2	5:F:98:GLU:CD	2.37	0.49
2:M:139:GLN:HE22	2:M:415:PRO:CD	2.26	0.49
2:M:331:ARG:NH1	2:M:427:VAL:HG12	2.27	0.49
2:M:352:ALA:HA	2:M:355:VAL:CG1	2.43	0.49
2:M:506:ASN:HB2	9:M:1906:HOH:O	2.12	0.49
2:M:967:PHE:CD1	2:M:972:VAL:HG12	2.47	0.49
3:N:128:TYR:CE1	3:N:461:ILE:HG13	2.47	0.49
3:N:1161:GLU:HG3	3:N:1164:ARG:CB	2.41	0.49
3:N:1363:LEU:HD12	3:N:1364:HIS:O	2.12	0.49
5:P:226:LYS:HD2	5:P:242:TRP:CZ2	2.48	0.49
1:B:88:ARG:HB2	1:B:123:MET:HE2	1.95	0.49
2:C:341:THR:O	2:C:345:ARG:HG3	2.12	0.49
2:C:418:LEU:N	2:C:418:LEU:HD12	2.28	0.49
2:C:1098:ASP:HB2	3:D:21:TRP:CZ2	2.46	0.49
2:C:1115:LEU:HD23	3:D:85:VAL:CA	2.43	0.49
3:D:32:ILE:HD12	3:D:527:MET:HG2	1.94	0.49
3:D:572:ARG:NH2	5:F:83:GLN:HE21	2.10	0.49
3:D:1051:GLU:HA	9:D:1601:HOH:O	2.12	0.49
3:D:1161:GLU:HG3	3:D:1164:ARG:CB	2.39	0.49
3:D:1379:VAL:HG11	3:D:1395:LEU:HD12	1.95	0.49
4:E:40:LEU:C	4:E:42:PRO:HD2	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:442:GLU:O	2:M:442:GLU:HG3	2.11	0.49
2:M:1096:ALA:O	3:N:13:ALA:CB	2.61	0.49
3:N:34:TYR:HE2	5:P:260:ILE:HA	1.77	0.49
3:N:66:GLN:O	3:N:67:ARG:C	2.55	0.49
3:N:141:ILE:HG21	3:N:450:TYR:H	1.78	0.49
3:N:418:GLY:N	3:N:429:SER:O	2.34	0.49
3:N:528:VAL:O	3:N:535:PHE:HA	2.13	0.49
3:N:964:LEU:HD22	9:N:2037:HOH:O	2.13	0.49
5:P:191:ASN:OD1	5:P:194:LEU:HD13	2.13	0.49
1:B:45:LEU:HB2	9:B:399:HOH:O	2.12	0.49
1:B:101:LEU:HD12	1:B:114:PHE:N	2.28	0.49
2:C:143:SER:CB	2:C:276:LYS:HZ1	2.23	0.49
2:C:148:PHE:CZ	2:C:281:LEU:HD13	2.35	0.49
2:C:358:ARG:HA	2:C:361:MET:HB2	1.93	0.49
2:C:367:LEU:HA	2:C:371:LYS:CG	2.35	0.49
2:C:890:LEU:CA	2:C:914:ILE:HD11	2.33	0.49
9:C:1162:HOH:O	3:D:943:THR:HG21	2.13	0.49
3:D:99:ALA:HA	3:D:575:GLN:HE22	1.77	0.49
3:D:116:LEU:HB3	3:D:118:LEU:HG	1.94	0.49
3:D:127:LEU:HD12	3:D:128:TYR:N	2.28	0.49
3:D:696:HIS:HB2	4:E:48:MET:CE	2.42	0.49
3:D:897:TRP:CH2	3:D:902:LEU:HD21	2.47	0.49
3:D:1101:VAL:HG22	3:D:1428:ALA:HB2	1.94	0.49
3:D:1481:VAL:HG13	4:E:18:ARG:HG3	1.93	0.49
5:F:112:ALA:O	5:F:116:LEU:HG	2.13	0.49
5:F:300:ASP:CG	5:F:301:ALA:N	2.71	0.49
2:M:254:VAL:HG13	2:M:258:TYR:HE1	1.77	0.49
2:M:564:MET:HG3	2:M:997:LEU:HD11	1.94	0.49
2:M:770:GLU:O	2:M:773:LEU:HB3	2.13	0.49
2:M:987:ILE:HA	3:N:948:THR:HG21	1.95	0.49
3:N:709:HIS:CD2	3:N:711:LEU:HB2	2.48	0.49
3:N:804:LEU:HB3	9:N:1996:HOH:O	2.11	0.49
3:N:1242:HIS:HE1	3:N:1266:ARG:HB3	1.78	0.49
5:P:116:LEU:HB2	5:P:127:ILE:HD12	1.95	0.49
5:P:135:ILE:O	5:P:135:ILE:HD13	2.13	0.49
2:C:17:PRO:HG2	9:C:1758:HOH:O	2.12	0.48
2:C:121:MET:HG3	9:C:1509:HOH:O	2.11	0.48
2:C:208:ALA:HA	2:C:221:LEU:HD21	1.94	0.48
2:C:379:GLU:O	2:C:383:ARG:HB3	2.13	0.48
2:C:976:ASP:HB2	2:C:979:THR:HG22	1.94	0.48
2:C:1033:GLY:O	2:C:1036:GLU:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:186:VAL:HB	3:D:189:GLN:HB2	1.95	0.48
3:D:610:LYS:CG	7:D:1527:MXP:H15A	2.42	0.48
3:D:660:LYS:HE3	3:D:663:GLU:CD	2.38	0.48
3:D:834:THR:HA	9:D:2405:HOH:O	2.13	0.48
3:D:1049:SER:OG	3:D:1051:GLU:HG3	2.13	0.48
3:D:1114:THR:HG23	3:D:1114:THR:O	2.13	0.48
3:D:1310:ARG:CZ	3:D:1327:ARG:HD3	2.43	0.48
4:E:28:GLN:HG3	9:E:134:HOH:O	2.12	0.48
1:K:7:LYS:HE2	1:K:186:LEU:CD1	2.29	0.48
2:M:64:LEU:HD13	2:M:359:MET:CG	2.42	0.48
2:M:242:LEU:HD22	9:M:1924:HOH:O	2.11	0.48
2:M:858:MET:HB2	2:M:859:PRO:CD	2.43	0.48
2:M:1101:THR:HB	3:N:5:VAL:HG13	1.94	0.48
3:N:39:PRO:HB3	3:N:45:PHE:O	2.13	0.48
3:N:118:LEU:O	3:N:119:SER:C	2.56	0.48
3:N:984:THR:CG2	3:N:987:GLU:H	2.25	0.48
3:N:1116:ASN:N	3:N:1116:ASN:ND2	2.60	0.48
3:N:1128:VAL:HG12	9:N:1593:HOH:O	2.13	0.48
3:N:1141:GLU:HG2	3:N:1168:MET:HE1	1.94	0.48
5:P:220:LEU:HB2	5:P:243:ILE:HD11	1.95	0.48
1:A:9:PRO:HB3	1:A:25:LEU:HG	1.94	0.48
1:A:189:ARG:HD2	1:A:191:ASP:OD1	2.12	0.48
2:C:18:LEU:HD23	2:C:404:LEU:HD21	1.95	0.48
2:C:139:GLN:NE2	2:C:418:LEU:HD22	2.28	0.48
2:C:367:LEU:O	2:C:371:LYS:HB2	2.13	0.48
3:D:14:SER:HB2	9:D:1656:HOH:O	2.13	0.48
3:D:128:TYR:CE1	3:D:461:ILE:HG13	2.45	0.48
3:D:741:ASP:OD2	3:D:741:ASP:N	2.41	0.48
9:D:1893:HOH:O	4:E:85:LEU:HG	2.13	0.48
5:F:277:GLN:O	5:F:280:GLN:HB3	2.13	0.48
1:K:55:SER:CB	1:K:158:ILE:HG21	2.43	0.48
1:K:150:TYR:CE2	1:K:152:PRO:HG3	2.44	0.48
2:M:200:LEU:HD13	2:M:300:ASP:OD2	2.12	0.48
2:M:439:CYS:SG	2:M:540:PHE:HB3	2.53	0.48
2:M:461:VAL:HG12	2:M:462:ASP:O	2.13	0.48
2:M:636:ALA:HB2	2:M:703:ILE:HG22	1.95	0.48
2:M:671:ASN:ND2	2:M:993:PHE:HD2	2.10	0.48
3:N:112:ILE:HD12	3:N:461:ILE:HG21	1.94	0.48
3:N:180:LYS:HG3	3:N:183:GLU:H	1.77	0.48
3:N:417:PRO:HD2	3:N:432:TYR:CE1	2.48	0.48
3:N:610:LYS:HG2	7:N:1527:MXP:C15	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:754:PHE:CE2	3:N:1476:THR:HG21	2.49	0.48
5:P:371:LEU:HD12	9:P:669:HOH:O	2.11	0.48
1:A:5:LYS:HB2	9:A:440:HOH:O	2.12	0.48
1:A:201:THR:HG22	1:A:203:GLY:H	1.78	0.48
2:C:15:LEU:HD21	2:C:583:LEU:HD11	1.93	0.48
2:C:198:ARG:HD2	2:C:228:ALA:CB	2.44	0.48
2:C:212:GLY:C	2:C:215:GLY:H	2.21	0.48
2:C:468:ARG:NE	2:C:485:TYR:HB3	2.27	0.48
2:C:644:VAL:HG22	2:C:647:GLN:OE1	2.14	0.48
2:C:888:THR:HG22	9:C:1474:HOH:O	2.13	0.48
2:C:1054:THR:HG23	2:C:1082:PRO:HG3	1.93	0.48
3:D:190:GLU:HB2	9:D:1738:HOH:O	2.14	0.48
3:D:760:ARG:HH22	4:E:62:THR:CA	2.26	0.48
3:D:881:LEU:O	3:D:885:ILE:HG13	2.13	0.48
5:F:109:GLY:O	5:F:113:ILE:HG13	2.13	0.48
5:F:247:ILE:HG22	5:F:251:ILE:HD11	1.95	0.48
5:F:312:GLN:HB2	9:F:706:HOH:O	2.12	0.48
1:K:34:VAL:HG22	2:M:939:ARG:HH21	1.79	0.48
2:M:139:GLN:HG2	2:M:140:ILE:H	1.77	0.48
2:M:601:GLY:HA2	2:M:616:GLU:HG3	1.95	0.48
3:N:161:LEU:O	3:N:449:SER:CB	2.59	0.48
3:N:638:LYS:C	3:N:729:HIS:HD2	2.21	0.48
3:N:1123:PHE:CE1	3:N:1134:LEU:HD12	2.48	0.48
5:P:93:LEU:HG	5:P:190:ALA:HB1	1.96	0.48
5:P:306:GLU:O	5:P:310:ILE:HG13	2.13	0.48
1:B:12:THR:OG1	1:B:24:VAL:HB	2.14	0.48
1:B:58:ILE:HG21	1:B:68:ILE:HD13	1.96	0.48
2:C:183:SER:CB	2:C:190:LYS:HD3	2.43	0.48
2:C:290:LEU:HB3	2:C:302:VAL:HG11	1.94	0.48
2:C:472:ARG:O	2:C:531:PHE:HD2	1.96	0.48
2:C:627:ARG:O	2:C:638:ASP:HA	2.13	0.48
2:C:663:ASN:C	2:C:665:PHE:H	2.22	0.48
2:C:809:GLY:HA2	9:C:1126:HOH:O	2.12	0.48
3:D:491:LYS:HE2	9:D:1851:HOH:O	2.12	0.48
5:F:369:LEU:HD11	5:F:401:GLU:HB2	1.94	0.48
1:L:22:GLU:HG2	1:L:198:ARG:HG2	1.94	0.48
2:M:101:ILE:HG22	2:M:102:HIS:N	2.28	0.48
2:M:258:TYR:HB3	9:M:1886:HOH:O	2.13	0.48
2:M:412:ALA:HB1	2:M:419:THR:CG2	2.43	0.48
2:M:1014:SER:O	2:M:1018:GLN:HG3	2.14	0.48
3:N:9:ARG:HH22	3:N:507:ASN:HD21	1.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:534:ARG:HG2	9:P:456:HOH:O	2.13	0.48
3:N:553:ARG:HH12	5:P:211:ASP:HA	1.78	0.48
3:N:572:ARG:NH1	5:P:79:ASP:OD1	2.39	0.48
3:N:1312:LEU:HD12	9:N:2368:HOH:O	2.12	0.48
5:P:339:PRO:HB3	5:P:343:ASP:HB2	1.94	0.48
1:B:107:LYS:HG3	1:B:108:GLU:H	1.78	0.48
2:C:140:ILE:HA	2:C:332:ARG:O	2.14	0.48
2:C:281:LEU:HD12	2:C:305:PRO:O	2.13	0.48
2:C:352:ALA:C	2:C:355:VAL:HG12	2.39	0.48
2:C:405:ARG:HA	9:C:1409:HOH:O	2.12	0.48
2:C:462:ASP:HB3	2:C:468:ARG:HD3	1.96	0.48
2:C:575:GLN:C	2:C:667:ALA:HB1	2.38	0.48
2:C:831:ARG:HD2	9:C:1303:HOH:O	2.14	0.48
2:C:1115:LEU:CB	3:D:85:VAL:HG13	2.43	0.48
3:D:32:ILE:HG12	9:D:1967:HOH:O	2.13	0.48
3:D:760:ARG:HB2	4:E:3:GLU:OE2	2.14	0.48
3:D:805:GLU:OE1	3:D:809:PRO:HG2	2.14	0.48
3:D:829:VAL:H	3:D:835:SER:CB	2.26	0.48
3:D:840:LYS:HB3	3:D:841:TYR:CE2	2.48	0.48
3:D:938:GLY:O	3:D:942:SER:HB3	2.14	0.48
3:D:1209:LEU:C	3:D:1211:MET:N	2.71	0.48
5:F:369:LEU:HA	9:F:450:HOH:O	2.13	0.48
2:M:165:LEU:HB2	9:M:2226:HOH:O	2.14	0.48
2:M:212:GLY:HA3	2:M:218:VAL:CG2	2.44	0.48
2:M:305:PRO:HA	2:M:308:ARG:CD	2.44	0.48
2:M:380:ALA:O	2:M:384:GLU:HB2	2.14	0.48
2:M:968:LEU:HD22	9:M:2164:HOH:O	2.13	0.48
3:N:57:GLU:HG3	3:N:64:LYS:HG2	1.95	0.48
3:N:1198:TYR:HE2	9:N:2318:HOH:O	1.96	0.48
3:N:1264:GLU:OE2	3:N:1425:THR:HB	2.14	0.48
3:N:1325:LEU:C	9:N:2368:HOH:O	2.57	0.48
5:P:80:PRO:HA	5:P:83:GLN:HB2	1.95	0.48
5:P:136:LEU:HD23	5:P:181:GLU:OE2	2.13	0.48
1:A:16:GLN:O	1:A:16:GLN:CG	2.62	0.48
1:A:64:GLU:HG3	1:A:165:ILE:HD12	1.96	0.48
1:A:112:ARG:HA	9:A:397:HOH:O	2.13	0.48
1:A:158:ILE:C	1:A:159:LYS:HG3	2.38	0.48
1:B:101:LEU:HB2	1:B:114:PHE:CD2	2.48	0.48
2:C:672:VAL:CG2	2:C:868:ASP:HB2	2.44	0.48
2:C:1065:ALA:CB	2:C:1077:PRO:HG2	2.43	0.48
3:D:12:LEU:HD13	3:D:511:TRP:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:126:VAL:HG12	3:D:132:TYR:HB2	1.96	0.48
3:D:162:ARG:HH11	3:D:434:ARG:HH22	1.62	0.48
3:D:670:VAL:O	3:D:674:ARG:HG3	2.14	0.48
3:D:760:ARG:HH22	4:E:62:THR:N	2.11	0.48
3:D:947:ILE:HD12	3:D:947:ILE:O	2.14	0.48
3:D:1104:GLU:O	3:D:1106:VAL:HG23	2.14	0.48
3:D:1209:LEU:HD12	3:D:1219:GLU:OE1	2.14	0.48
3:D:1258:ARG:NH2	3:D:1351:GLU:OE2	2.46	0.48
3:D:1290:LEU:HD22	3:D:1291:SER:H	1.79	0.48
4:E:4:PRO:HB2	9:E:109:HOH:O	2.13	0.48
5:F:80:PRO:HA	5:F:83:GLN:HB2	1.94	0.48
5:F:82:ARG:HD3	9:F:608:HOH:O	2.14	0.48
5:F:134:LYS:HB2	5:F:178:ARG:NH2	2.28	0.48
2:M:462:ASP:O	2:M:463:GLU:C	2.57	0.48
2:M:544:THR:O	2:M:547:ILE:HG13	2.14	0.48
2:M:679:PHE:O	2:M:680:ASP:C	2.56	0.48
2:M:958:THR:HG23	2:M:961:GLU:H	1.79	0.48
3:N:409:VAL:O	3:N:437:VAL:HG21	2.13	0.48
3:N:417:PRO:HD2	3:N:432:TYR:CD1	2.48	0.48
3:N:443:VAL:HG11	3:N:445:ARG:HE	1.79	0.48
3:N:853:VAL:HA	3:N:858:VAL:O	2.14	0.48
3:N:1147:ARG:HD2	3:N:1188:VAL:HG21	1.95	0.48
3:N:1282:ARG:HA	3:N:1315:ASP:OD1	2.14	0.48
3:N:1310:ARG:HE	3:N:1327:ARG:HB3	1.78	0.48
3:N:1351:GLU:HA	3:N:1354:LYS:HG3	1.95	0.48
1:A:23:PHE:O	1:A:196:THR:HA	2.13	0.48
1:A:222:LEU:HD11	1:B:218:LEU:HD23	1.95	0.48
1:B:156:HIS:CG	1:B:157:GLY:N	2.82	0.48
2:C:120:LEU:HA	9:C:1499:HOH:O	2.12	0.48
2:C:412:ALA:HB1	2:C:419:THR:CG2	2.44	0.48
3:D:409:VAL:HG12	3:D:435:VAL:HG11	1.94	0.48
3:D:486:ARG:HB2	9:D:2292:HOH:O	2.12	0.48
3:D:565:ILE:HD12	5:F:192:LEU:CD1	2.42	0.48
3:D:1041:LEU:CD1	3:D:1058:ARG:HA	2.42	0.48
1:K:197:LEU:HD23	1:K:197:LEU:N	2.29	0.48
1:K:206:THR:CG2	1:K:209:GLU:HG3	2.39	0.48
2:M:565:GLN:CG	2:M:995:MET:HE1	2.40	0.48
2:M:682:TYR:CE1	2:M:851:LYS:HD2	2.49	0.48
3:N:521:PRO:O	3:N:525:ARG:HG2	2.13	0.48
3:N:1197:ARG:N	9:N:1577:HOH:O	2.46	0.48
1:B:7:LYS:HG3	9:B:434:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:211:LEU:CD1	2:C:308:ARG:HA	2.44	0.48
2:C:305:PRO:HA	2:C:308:ARG:CD	2.42	0.48
2:C:719:PRO:HB3	2:C:820:ARG:CZ	2.43	0.48
2:C:724:ARG:HG2	2:C:734:LEU:CD2	2.43	0.48
2:C:971:LYS:HB3	2:C:987:ILE:C	2.39	0.48
3:D:45:PHE:HB3	3:D:86:ARG:NH2	2.29	0.48
3:D:204:LEU:O	3:D:393:ILE:HA	2.13	0.48
3:D:466:LYS:NZ	9:D:1668:HOH:O	2.47	0.48
3:D:705:ALA:HB3	3:D:706:PRO:CD	2.43	0.48
3:D:767:HIS:O	3:D:924:MET:HE2	2.14	0.48
4:E:73:LEU:N	9:E:131:HOH:O	2.46	0.48
5:F:172:ARG:NH1	9:F:462:HOH:O	2.45	0.48
1:L:129:ILE:HG21	1:L:140:MET:HE1	1.96	0.48
2:M:431:HIS:H	2:M:434:HIS:CD2	2.30	0.48
2:M:625:LEU:O	2:M:627:ARG:N	2.47	0.48
2:M:687:ALA:C	2:M:688:ILE:HD12	2.38	0.48
2:M:1056:LYS:HB3	3:N:623:VAL:HG13	1.94	0.48
2:M:1088:LEU:HG	2:M:1092:LEU:HD12	1.95	0.48
3:N:615:ARG:HH21	3:N:1089:ALA:CB	2.20	0.48
3:N:820:GLU:HG3	3:N:836:VAL:HG11	1.95	0.48
3:N:1047:LYS:HB3	3:N:1048:PRO:HD2	1.94	0.48
3:N:1110:ALA:O	3:N:1112:CYS:N	2.46	0.48
3:N:1240:THR:O	3:N:1257:PRO:HB3	2.14	0.48
1:A:7:LYS:NZ	1:A:186:LEU:HD21	2.29	0.48
1:A:206:THR:HG22	1:A:209:GLU:CG	2.40	0.48
2:C:11:GLU:HB2	9:C:1190:HOH:O	2.14	0.48
2:C:139:GLN:OE1	2:C:414:GLY:HA3	2.14	0.48
2:C:165:LEU:HD12	2:C:166:PRO:CA	2.43	0.48
2:C:611:ILE:CD1	2:C:625:LEU:HD11	2.44	0.48
2:C:676:ILE:HG22	2:C:988:VAL:HG22	1.96	0.48
2:C:851:LYS:HG3	9:C:1250:HOH:O	2.12	0.48
3:D:12:LEU:HD23	3:D:13:ALA:H	1.79	0.48
3:D:633:VAL:C	3:D:635:PRO:HD3	2.39	0.48
3:D:693:GLU:O	4:E:48:MET:HE1	2.13	0.48
3:D:702:LEU:HD13	3:D:716:PHE:HD1	1.79	0.48
9:D:2077:HOH:O	5:F:349:LEU:HD13	2.13	0.48
5:F:79:ASP:CG	5:F:80:PRO:HD3	2.39	0.48
5:F:358:LEU:HD13	5:F:370:LYS:HG3	1.96	0.48
1:K:9:PRO:HB3	1:K:25:LEU:HD21	1.96	0.48
1:K:101:LEU:HD12	1:K:114:PHE:CD1	2.49	0.48
1:L:50:GLY:O	1:L:146:ARG:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:123:MET:HE1	9:L:1342:HOH:O	2.13	0.48
1:L:207:PRO:HD2	9:L:3232:HOH:O	2.13	0.48
3:N:73:CYS:SG	3:N:74:GLU:N	2.86	0.48
3:N:81:THR:HG22	3:N:82:LYS:N	2.29	0.48
3:N:421:LEU:CG	3:N:429:SER:HB3	2.43	0.48
3:N:676:MET:HE3	9:N:1656:HOH:O	2.14	0.48
3:N:1321:ALA:O	3:N:1339:LYS:HG3	2.13	0.48
4:O:54:LEU:HD23	4:O:58:PRO:HD2	1.96	0.48
5:P:292:ALA:O	5:P:299:TRP:HB2	2.14	0.48
1:B:39:PRO:O	1:B:43:ILE:HG12	2.14	0.48
2:C:19:THR:O	2:C:19:THR:HG22	2.14	0.48
2:C:289:THR:O	2:C:291:ALA:N	2.46	0.48
2:C:410:ILE:H	2:C:410:ILE:HD12	1.78	0.48
2:C:410:ILE:HD12	2:C:410:ILE:N	2.29	0.48
2:C:762:LYS:HG3	2:C:786:LYS:HD2	1.95	0.48
2:C:879:ARG:HB3	9:C:1196:HOH:O	2.14	0.48
3:D:550:ARG:NH1	3:D:573:MET:HB3	2.29	0.48
3:D:561:GLY:CA	5:F:184:ARG:HH12	2.21	0.48
3:D:1238:MET:HG3	3:D:1257:PRO:HG3	1.95	0.48
5:F:128:ARG:HB2	9:F:652:HOH:O	2.14	0.48
2:M:369:PRO:HG2	9:M:2247:HOH:O	2.14	0.48
2:M:496:ILE:O	2:M:515:ALA:HB1	2.14	0.48
2:M:644:VAL:HG22	9:M:2151:HOH:O	2.13	0.48
2:M:762:LYS:C	2:M:763:GLY:O	2.53	0.48
2:M:1098:ASP:HB2	3:N:21:TRP:CZ2	2.47	0.48
3:N:47:GLU:HA	3:N:51:GLY:O	2.13	0.48
3:N:116:LEU:HB3	3:N:118:LEU:HG	1.96	0.48
3:N:126:VAL:O	3:N:132:TYR:CD1	2.67	0.48
3:N:127:LEU:HD12	3:N:128:TYR:N	2.29	0.48
3:N:407:VAL:HA	3:N:422:ALA:CB	2.44	0.48
3:N:465:LEU:HB3	9:N:2360:HOH:O	2.14	0.48
3:N:540:LEU:HD21	3:N:603:LEU:HD23	1.95	0.48
3:N:1177:ALA:CB	3:N:1183:ILE:HD11	2.44	0.48
3:N:1384:PRO:O	3:N:1413:THR:HG21	2.13	0.48
4:O:31:LEU:HD23	4:O:35:PHE:CE1	2.48	0.48
5:P:240:THR:O	5:P:244:ARG:HG3	2.13	0.48
1:B:50:GLY:O	1:B:146:ARG:HA	2.14	0.47
2:C:43:GLY:HA2	2:C:341:THR:OG1	2.13	0.47
2:C:544:THR:O	2:C:547:ILE:HG13	2.13	0.47
2:C:556:ASN:HA	9:C:1448:HOH:O	2.12	0.47
2:C:571:LEU:CD2	2:C:700:TYR:HA	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:679:PHE:CE1	2:C:870:ILE:HD13	2.49	0.47
2:C:843:HIS:CD2	2:C:884:GLN:HA	2.49	0.47
2:C:896:PHE:CD2	2:C:925:TYR:HB2	2.49	0.47
2:C:926:PHE:O	2:C:930:LYS:HG3	2.12	0.47
2:C:930:LYS:HD3	9:C:1707:HOH:O	2.14	0.47
3:D:133:ILE:HG22	3:D:455:ARG:CA	2.43	0.47
3:D:666:ILE:H	3:D:666:ILE:HG13	1.55	0.47
3:D:1323:GLN:HG3	3:D:1324:PRO:HD2	1.95	0.47
4:E:53:GLY:C	4:E:55:PHE:N	2.70	0.47
1:K:155:LYS:HD3	9:K:3774:HOH:O	2.14	0.47
1:K:180:GLN:NE2	2:M:929:ARG:HH21	2.11	0.47
2:M:252:LYS:NZ	2:M:296:GLY:HA3	2.29	0.47
2:M:614:ARG:HD3	9:M:2272:HOH:O	2.14	0.47
2:M:650:ARG:HB2	2:M:653:ASP:HB2	1.94	0.47
2:M:879:ARG:HD2	2:M:879:ARG:H	1.79	0.47
3:N:87:ARG:HA	3:N:523:ASP:HB2	1.96	0.47
3:N:147:VAL:HG21	9:N:2101:HOH:O	2.13	0.47
3:N:916:TYR:CE2	3:N:920:LEU:HD13	2.49	0.47
3:N:1000:THR:HG23	3:N:1001:GLU:N	2.29	0.47
5:P:139:ALA:HB1	9:P:558:HOH:O	2.13	0.47
1:A:49:PRO:CB	1:A:148:VAL:HG22	2.42	0.47
2:C:101:ILE:HG22	2:C:102:HIS:N	2.28	0.47
2:C:218:VAL:HA	2:C:221:LEU:HD23	1.95	0.47
2:C:333:ILE:N	2:C:333:ILE:HD12	2.28	0.47
2:C:378:LEU:HG	2:C:382:ILE:CD1	2.44	0.47
2:C:704:HIS:O	2:C:828:ALA:HA	2.14	0.47
3:D:62:LYS:HB2	9:D:1735:HOH:O	2.14	0.47
3:D:1109:GLU:CD	3:D:1202:GLN:HB2	2.39	0.47
3:D:1262:LEU:HD23	3:D:1352:ILE:CG1	2.38	0.47
3:D:1337:GLU:HB2	9:D:1785:HOH:O	2.14	0.47
4:E:94:PRO:CG	9:E:180:HOH:O	2.56	0.47
5:F:138:SER:H	5:F:140:ARG:HE	1.62	0.47
1:K:101:LEU:HG	1:K:113:ASP:C	2.40	0.47
2:M:72:ARG:HB2	9:M:1985:HOH:O	2.13	0.47
2:M:176:VAL:O	2:M:178:PRO:HD3	2.13	0.47
2:M:1002:GLU:HG3	3:N:744:GLN:HE22	1.79	0.47
3:N:131:LYS:HD2	5:P:83:GLN:CD	2.39	0.47
3:N:133:ILE:HG22	3:N:455:ARG:CA	2.44	0.47
3:N:603:LEU:HA	3:N:606:ILE:HD12	1.96	0.47
3:N:1467:ILE:HG12	7:N:1527:MXP:H16A	1.96	0.47
5:P:119:ILE:HD13	5:P:170:HIS:ND1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:277:GLN:O	5:P:280:GLN:HB3	2.13	0.47
1:A:18:ARG:HH11	1:A:123:MET:HE1	1.79	0.47
1:B:120:VAL:HG11	9:B:416:HOH:O	2.15	0.47
2:C:115:LEU:HD22	2:C:373:VAL:CG1	2.41	0.47
2:C:207:LEU:O	2:C:211:LEU:HB3	2.14	0.47
2:C:281:LEU:O	2:C:282:GLY:O	2.32	0.47
2:C:837:ASP:O	2:C:848:VAL:HG13	2.14	0.47
2:C:1106:ASP:OD1	3:D:7:LYS:HD2	2.14	0.47
3:D:403:PHE:HE2	3:D:443:VAL:N	2.12	0.47
3:D:528:VAL:HG12	3:D:529:GLN:N	2.29	0.47
3:D:583:ASP:OD1	3:D:583:ASP:C	2.57	0.47
3:D:1087:ARG:NH1	3:D:1234:THR:O	2.47	0.47
3:D:1463:LYS:O	3:D:1467:ILE:HG13	2.13	0.47
3:D:1476:THR:CG2	4:E:21:VAL:HG22	2.44	0.47
4:E:4:PRO:HG2	9:E:175:HOH:O	2.12	0.47
4:E:82:GLU:HG3	4:E:83:ASP:H	1.78	0.47
1:K:9:PRO:HB3	1:K:25:LEU:CG	2.44	0.47
1:K:70:GLY:H	2:M:607:ASP:CG	2.19	0.47
2:M:262:ALA:O	2:M:264:PRO:O	2.32	0.47
2:M:501:THR:OG1	2:M:532:MET:HE1	2.15	0.47
3:N:1090:ASP:OD1	3:N:1241:PHE:CZ	2.68	0.47
3:N:1129:THR:HG23	3:N:1130:ARG:H	1.78	0.47
3:N:1238:MET:HG3	3:N:1257:PRO:HG3	1.96	0.47
3:N:1481:VAL:CG1	4:O:18:ARG:HG3	2.44	0.47
4:O:87:LYS:HD3	9:O:2559:HOH:O	2.15	0.47
5:P:321:ILE:O	5:P:327:SER:HB3	2.13	0.47
1:B:87:VAL:CG2	1:B:144:VAL:HG11	2.36	0.47
2:C:772:ARG:HD3	9:F:459:HOH:O	2.15	0.47
2:C:923:GLU:O	2:C:927:GLY:HA3	2.15	0.47
3:D:87:ARG:HB2	3:D:523:ASP:HB2	1.96	0.47
3:D:432:TYR:O	3:D:448:GLU:HA	2.15	0.47
3:D:895:VAL:O	3:D:899:LEU:HG	2.14	0.47
3:D:1372:VAL:O	3:D:1375:MET:HB2	2.13	0.47
4:E:67:GLU:OE1	4:E:73:LEU:HD11	2.15	0.47
2:M:410:ILE:HD11	2:M:455:LEU:HB3	1.96	0.47
2:M:668:LEU:O	2:M:993:PHE:CZ	2.67	0.47
2:M:975:TYR:HA	2:M:982:PRO:HA	1.95	0.47
9:M:1815:HOH:O	3:N:1456:LYS:HD3	2.13	0.47
3:N:81:THR:HB	3:N:85:VAL:CG2	2.43	0.47
3:N:87:ARG:HD2	9:N:1572:HOH:O	2.14	0.47
3:N:162:ARG:HA	3:N:449:SER:CB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:787:LEU:HD21	3:N:947:ILE:HD11	1.96	0.47
3:N:807:ALA:HB2	9:N:1559:HOH:O	2.15	0.47
3:N:957:PRO:HB3	3:N:959:GLU:HG3	1.95	0.47
3:N:1440:PHE:CD2	3:N:1440:PHE:N	2.82	0.47
1:A:184:THR:HG23	1:A:192:LEU:CB	2.42	0.47
1:B:102:LYS:HA	1:B:138:LEU:O	2.15	0.47
2:C:21:ILE:HG12	2:C:455:LEU:HD21	1.96	0.47
2:C:157:ARG:N	9:C:1172:HOH:O	2.46	0.47
2:C:1058:ASP:OD1	2:C:1084:SER:HB3	2.14	0.47
2:C:1082:PRO:C	2:C:1084:SER:N	2.71	0.47
3:D:109:PRO:HB2	9:D:2000:HOH:O	2.13	0.47
3:D:119:SER:CB	3:D:123:LEU:HD13	2.44	0.47
3:D:589:ALA:HA	9:D:1703:HOH:O	2.12	0.47
3:D:1478:SER:HG	3:D:1481:VAL:H	1.62	0.47
3:D:1500:LYS:HE3	9:D:2173:HOH:O	2.13	0.47
5:F:365:GLU:HG2	5:F:397:ILE:HA	1.96	0.47
2:M:160:ALA:O	2:M:173:ASP:HA	2.14	0.47
2:M:164:PRO:HB3	9:M:1703:HOH:O	2.14	0.47
2:M:378:LEU:HG	2:M:382:ILE:CD1	2.44	0.47
2:M:446:GLY:O	2:M:447:ALA:C	2.57	0.47
2:M:817:PRO:HG3	5:P:288:TYR:OH	2.14	0.47
2:M:965:GLU:HG3	9:M:2274:HOH:O	2.15	0.47
9:M:2079:HOH:O	3:N:606:ILE:HG21	2.15	0.47
3:N:100:ALA:CB	3:N:513:ILE:HD13	2.29	0.47
3:N:611:GLN:CG	3:N:619:LEU:HD11	2.42	0.47
3:N:679:ARG:HB2	3:N:682:ASP:CG	2.39	0.47
3:N:752:SER:HB2	9:N:1905:HOH:O	2.14	0.47
3:N:795:VAL:HA	3:N:861:GLN:O	2.15	0.47
3:N:1236:LEU:HD11	3:N:1356:TYR:CE1	2.48	0.47
3:N:1448:THR:O	3:N:1451:ALA:HB3	2.14	0.47
5:P:353:GLU:HG2	9:P:485:HOH:O	2.13	0.47
1:A:5:LYS:HD2	9:A:440:HOH:O	2.14	0.47
1:B:27:PRO:HB3	1:B:192:LEU:CD2	2.45	0.47
2:C:129:ILE:HG22	2:C:130:ASN:N	2.29	0.47
2:C:313:LEU:HA	9:C:1596:HOH:O	2.15	0.47
2:C:422:ARG:HG3	2:C:423:ALA:H	1.78	0.47
2:C:479:VAL:HG21	2:C:503:LEU:HD11	1.96	0.47
2:C:726:ILE:O	2:C:726:ILE:HG22	2.14	0.47
3:D:17:LYS:HA	3:D:20:SER:HB3	1.95	0.47
3:D:75:ARG:HB2	9:D:1539:HOH:O	2.15	0.47
3:D:80:VAL:HG12	3:D:81:THR:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:133:ILE:H	3:D:133:ILE:HG12	1.35	0.47
3:D:180:LYS:HG3	3:D:183:GLU:H	1.79	0.47
3:D:1109:GLU:HG2	3:D:1202:GLN:N	2.29	0.47
5:F:350:LEU:O	5:F:354:LEU:HB2	2.14	0.47
2:M:328:LEU:HD22	2:M:437:ARG:CB	2.44	0.47
2:M:421:GLU:O	2:M:421:GLU:HG2	2.15	0.47
2:M:497:ALA:HA	2:M:515:ALA:HA	1.96	0.47
2:M:564:MET:HE2	2:M:846:LYS:HE3	1.96	0.47
3:N:137:PRO:HD2	3:N:453:ASP:CB	2.45	0.47
3:N:486:ARG:HH12	3:N:1389:LEU:HD11	1.78	0.47
3:N:844:ALA:O	3:N:867:ARG:HB3	2.14	0.47
3:N:900:ILE:O	3:N:900:ILE:HG13	2.15	0.47
5:P:280:GLN:O	5:P:280:GLN:HG2	2.14	0.47
1:A:133:GLU:N	9:A:320:HOH:O	2.46	0.47
1:A:162:ILE:HG13	1:A:163:ASN:N	2.28	0.47
1:A:182:GLU:O	1:A:194:LYS:HB3	2.14	0.47
1:B:185:ARG:HB3	9:D:1701:HOH:O	2.14	0.47
2:C:5:ARG:HB3	2:C:902:ILE:HB	1.97	0.47
2:C:129:ILE:HG23	9:C:1478:HOH:O	2.14	0.47
2:C:165:LEU:HG	2:C:265:ARG:HH12	1.79	0.47
2:C:279:GLU:HG3	2:C:280:LYS:N	2.30	0.47
2:C:289:THR:HG22	2:C:290:LEU:HD23	1.97	0.47
2:C:462:ASP:O	2:C:463:GLU:C	2.56	0.47
2:C:726:ILE:HG22	9:C:1346:HOH:O	2.14	0.47
2:C:875:GLY:HA2	2:C:879:ARG:NH1	2.30	0.47
2:C:958:THR:HG23	2:C:961:GLU:H	1.78	0.47
3:D:18:ILE:HG21	3:D:516:ALA:O	2.14	0.47
3:D:397:LYS:CE	3:D:448:GLU:HB3	2.45	0.47
3:D:455:ARG:HH11	3:D:463:GLN:HG3	1.78	0.47
3:D:520:LEU:HD23	3:D:540:LEU:CD2	2.45	0.47
3:D:637:LEU:HD11	3:D:642:CYS:CA	2.45	0.47
3:D:1066:THR:HG22	3:D:1069:GLU:HG3	1.96	0.47
3:D:1168:MET:HE3	3:D:1172:HIS:CD2	2.49	0.47
3:D:1236:LEU:HA	3:D:1359:GLN:NE2	2.30	0.47
3:D:1403:LEU:HD12	9:D:1814:HOH:O	2.15	0.47
5:F:140:ARG:HG3	5:F:141:VAL:N	2.29	0.47
1:K:209:GLU:O	1:K:213:GLN:HG3	2.15	0.47
2:M:165:LEU:HD12	2:M:166:PRO:C	2.40	0.47
2:M:165:LEU:HD12	2:M:166:PRO:HA	1.95	0.47
2:M:175:GLU:HB3	2:M:183:SER:OG	2.14	0.47
2:M:212:GLY:C	2:M:215:GLY:H	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:267:TYR:HB2	2:M:272:ALA:CB	2.44	0.47
2:M:286:SER:C	2:M:287:GLY:O	2.57	0.47
2:M:362:GLY:HA3	2:M:367:LEU:HD23	1.95	0.47
2:M:448:ASN:HB3	2:M:452:ILE:HD11	1.97	0.47
2:M:472:ARG:O	2:M:531:PHE:HD2	1.97	0.47
2:M:495:THR:H	2:M:530:GLU:CD	2.22	0.47
2:M:839:LEU:HD21	2:M:849:VAL:CG2	2.45	0.47
2:M:1015:LEU:N	9:M:1708:HOH:O	2.47	0.47
2:M:1050:GLN:NE2	9:M:2160:HOH:O	2.48	0.47
2:M:1067:TYR:O	2:M:1071:ILE:HG12	2.14	0.47
3:N:84:ILE:O	3:N:87:ARG:HB3	2.15	0.47
3:N:171:LEU:HD22	3:N:175:VAL:HB	1.96	0.47
3:N:540:LEU:HA	3:N:543:LEU:HD12	1.97	0.47
3:N:543:LEU:HA	3:N:546:ARG:HG3	1.96	0.47
3:N:685:ASP:HB3	9:N:1697:HOH:O	2.14	0.47
3:N:827:ILE:HG23	3:N:837:GLY:HA2	1.97	0.47
3:N:1045:MET:HG3	3:N:1073:SER:HA	1.97	0.47
3:N:1111:ASP:HB3	3:N:1203:LYS:HG3	1.96	0.47
3:N:1394:VAL:HG21	9:N:1598:HOH:O	2.14	0.47
3:N:1490:LYS:HB2	9:O:3444:HOH:O	2.14	0.47
4:O:39:VAL:HG21	4:O:72:ARG:HD2	1.97	0.47
4:O:53:GLY:C	4:O:55:PHE:H	2.22	0.47
5:P:81:VAL:O	5:P:85:LEU:HB2	2.14	0.47
5:P:109:GLY:O	5:P:113:ILE:HG13	2.15	0.47
5:P:160:ASP:OD1	5:P:178:ARG:NH2	2.48	0.47
5:P:361:LEU:HD23	5:P:362:SER:N	2.29	0.47
2:C:290:LEU:HD23	2:C:290:LEU:H	1.78	0.47
2:C:446:GLY:O	2:C:447:ALA:C	2.58	0.47
2:C:535:SER:CB	2:C:537:LYS:HG3	2.45	0.47
2:C:627:ARG:HG3	2:C:628:PHE:N	2.29	0.47
3:D:118:LEU:O	3:D:119:SER:C	2.58	0.47
3:D:205:TYR:HB2	3:D:393:ILE:HG12	1.95	0.47
3:D:443:VAL:HG11	3:D:445:ARG:HE	1.80	0.47
3:D:525:ARG:N	3:D:526:PRO:HD3	2.29	0.47
3:D:827:ILE:O	3:D:837:GLY:HA3	2.15	0.47
3:D:907:GLU:O	3:D:911:LEU:HD13	2.15	0.47
3:D:1003:VAL:O	3:D:1006:ALA:HB3	2.15	0.47
3:D:1212:ALA:HB3	9:D:1618:HOH:O	2.15	0.47
4:E:85:LEU:HD23	4:E:85:LEU:C	2.39	0.47
5:F:261:PRO:O	5:F:265:VAL:HG23	2.14	0.47
2:M:405:ARG:CZ	9:M:1857:HOH:O	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:798:GLY:H	2:M:827:VAL:CG1	2.27	0.47
2:M:1034:GLU:O	2:M:1037:VAL:N	2.48	0.47
2:M:1082:PRO:C	2:M:1084:SER:N	2.71	0.47
3:N:582:LEU:HA	3:N:603:LEU:HD12	1.96	0.47
3:N:874:GLU:HG3	9:N:1713:HOH:O	2.14	0.47
3:N:933:ALA:O	3:N:937:TYR:HD1	1.98	0.47
3:N:1341:PRO:O	3:N:1343:ALA:N	2.48	0.47
5:P:234:LYS:HE2	9:P:430:HOH:O	2.14	0.47
5:P:358:LEU:HD22	5:P:370:LYS:CE	2.45	0.47
1:A:89:PHE:HB3	1:A:94:LEU:HD22	1.97	0.47
1:B:165:ILE:HG22	9:B:502:HOH:O	2.14	0.47
2:C:274:ARG:HG2	2:C:274:ARG:O	2.15	0.47
2:C:301:GLU:O	2:C:305:PRO:HG2	2.15	0.47
2:C:497:ALA:HA	2:C:515:ALA:HA	1.96	0.47
3:D:65:ARG:CG	3:D:66:GLN:N	2.77	0.47
3:D:421:LEU:HB2	3:D:427:VAL:HG12	1.95	0.47
3:D:844:ALA:O	3:D:867:ARG:HB3	2.15	0.47
3:D:983:LEU:HD13	3:D:991:GLN:OE1	2.15	0.47
5:F:309:LYS:O	5:F:312:GLN:HB2	2.15	0.47
2:M:113:VAL:O	2:M:115:LEU:HD23	2.15	0.47
2:M:551:GLU:O	3:N:1065:LEU:HB3	2.15	0.47
2:M:983:ILE:HG23	3:N:944:THR:O	2.15	0.47
3:N:18:ILE:HD12	3:N:518:PRO:HD3	1.97	0.47
3:N:85:VAL:HG12	3:N:89:ARG:NE	2.30	0.47
3:N:204:LEU:HG	3:N:441:ARG:HH12	1.80	0.47
3:N:593:ASN:HD21	5:P:206:GLY:HA2	1.80	0.47
5:P:95:THR:HG22	5:P:96:LEU:HD23	1.97	0.47
5:P:410:TYR:O	5:P:413:SER:HB2	2.15	0.47
1:B:46:SER:HB2	9:B:503:HOH:O	2.14	0.47
1:B:141:GLU:HG3	9:B:405:HOH:O	2.14	0.47
2:C:176:VAL:O	2:C:178:PRO:HD3	2.15	0.47
2:C:732:ALA:O	2:C:735:ARG:HG3	2.15	0.47
2:C:854:PRO:C	2:C:856:GLU:N	2.72	0.47
2:C:1035:MET:HG2	3:D:707:THR:O	2.14	0.47
2:C:1071:ILE:O	3:D:659:LYS:HB2	2.15	0.47
3:D:407:VAL:HA	3:D:422:ALA:CB	2.45	0.47
3:D:699:VAL:HG21	3:D:760:ARG:HB3	1.97	0.47
3:D:810:GLU:HG2	9:D:2253:HOH:O	2.14	0.47
3:D:843:PHE:CD2	3:D:849:ALA:HA	2.49	0.47
3:D:1051:GLU:HG3	3:D:1051:GLU:H	1.46	0.47
3:D:1240:THR:O	3:D:1257:PRO:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:45:LEU:HD23	9:K:1231:HOH:O	2.14	0.47
1:K:89:PHE:HD1	1:K:120:VAL:HG23	1.80	0.47
2:M:172:ILE:H	2:M:172:ILE:HD12	1.78	0.47
2:M:224:GLU:HG3	9:M:2180:HOH:O	2.14	0.47
2:M:1060:ILE:HG22	2:M:1061:GLU:H	1.78	0.47
5:P:371:LEU:HD22	5:P:375:LEU:HD22	1.95	0.47
5:P:372:ARG:HB3	9:P:615:HOH:O	2.14	0.47
2:C:36:PRO:HB2	2:C:70:GLU:HG2	1.97	0.46
2:C:54:ILE:HG22	2:C:66:LEU:HB3	1.96	0.46
2:C:122:THR:HG22	2:C:123:GLU:N	2.31	0.46
2:C:166:PRO:HD3	2:C:265:ARG:HG3	1.97	0.46
2:C:183:SER:HB3	2:C:190:LYS:HD3	1.97	0.46
2:C:1115:LEU:HB3	3:D:85:VAL:CG1	2.44	0.46
3:D:39:PRO:HD2	3:D:47:GLU:OE1	2.15	0.46
3:D:204:LEU:HG	3:D:441:ARG:NH1	2.30	0.46
3:D:481:MET:HB2	3:D:1388:ARG:NH1	2.30	0.46
3:D:1106:VAL:HG12	3:D:1107:VAL:N	2.30	0.46
4:E:42:PRO:HD3	9:E:101:HOH:O	2.16	0.46
5:F:292:ALA:O	5:F:299:TRP:HB2	2.15	0.46
1:K:106:PRO:HG3	1:K:134:GLU:CG	2.45	0.46
1:K:158:ILE:C	1:K:159:LYS:HG3	2.40	0.46
1:L:162:ILE:HA	9:L:1885:HOH:O	2.15	0.46
2:M:379:GLU:O	2:M:383:ARG:HB3	2.15	0.46
2:M:439:CYS:SG	2:M:541:SER:N	2.87	0.46
2:M:627:ARG:O	2:M:638:ASP:HA	2.15	0.46
2:M:751:PRO:HG3	2:M:796:GLU:HG2	1.98	0.46
2:M:815:LEU:HD23	2:M:819:VAL:O	2.15	0.46
2:M:851:LYS:NZ	9:M:2027:HOH:O	2.48	0.46
3:N:153:LEU:HD12	3:N:157:GLU:HB2	1.97	0.46
3:N:421:LEU:HB2	3:N:427:VAL:HG12	1.96	0.46
3:N:1112:CYS:HB2	3:N:1195:GLN:CG	2.45	0.46
4:O:45:ARG:HB3	9:O:1014:HOH:O	2.14	0.46
4:O:70:THR:HG21	4:O:72:ARG:HE	1.80	0.46
5:P:288:TYR:HA	5:P:291:ILE:CG2	2.45	0.46
1:A:227:ASN:H	1:A:227:ASN:HD22	1.61	0.46
1:B:158:ILE:HD11	1:B:165:ILE:C	2.40	0.46
1:B:217:ILE:O	1:B:221:HIS:ND1	2.43	0.46
2:C:204:GLN:NE2	2:C:222:MET:HA	2.29	0.46
2:C:267:TYR:HB2	2:C:272:ALA:CB	2.45	0.46
2:C:328:LEU:CD1	2:C:433:THR:HB	2.44	0.46
2:C:557:ARG:NE	2:C:560:MET:SD	2.88	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:672:VAL:HG23	2:C:868:ASP:HB2	1.96	0.46
2:C:1050:GLN:HG2	2:C:1079:PRO:HG2	1.97	0.46
3:D:39:PRO:HB3	3:D:45:PHE:O	2.15	0.46
3:D:204:LEU:HA	3:D:441:ARG:NH2	2.18	0.46
3:D:204:LEU:HD21	3:D:445:ARG:NH1	2.30	0.46
3:D:422:ALA:O	3:D:427:VAL:HB	2.16	0.46
3:D:543:LEU:HA	3:D:546:ARG:HG3	1.96	0.46
3:D:702:LEU:HD13	3:D:716:PHE:CD1	2.50	0.46
3:D:863:VAL:HA	9:D:1596:HOH:O	2.14	0.46
3:D:1097:LYS:O	3:D:1101:VAL:HG23	2.16	0.46
5:F:396:ARG:HA	5:F:399:GLN:HB2	1.97	0.46
2:M:18:LEU:HB2	2:M:590:ASP:CB	2.44	0.46
2:M:400:PRO:HG2	9:M:1638:HOH:O	2.15	0.46
2:M:648:ARG:O	2:M:648:ARG:HG3	2.14	0.46
3:N:850:LEU:O	3:N:853:VAL:HB	2.14	0.46
3:N:1108:ARG:NE	3:N:1198:TYR:O	2.47	0.46
4:O:59:ASN:N	9:O:4171:HOH:O	2.48	0.46
5:P:398:ARG:HG3	5:P:402:ASN:ND2	2.29	0.46
2:C:648:ARG:HG3	2:C:648:ARG:O	2.14	0.46
3:D:26:VAL:HG11	3:D:44:LEU:HD23	1.96	0.46
3:D:112:ILE:HD12	3:D:461:ILE:HG21	1.96	0.46
3:D:537:THR:O	5:F:317:LEU:HB2	2.15	0.46
3:D:730:PRO:HA	3:D:733:CYS:SG	2.55	0.46
3:D:795:VAL:HG22	3:D:876:SER:HB3	1.96	0.46
3:D:1037:GLN:OE1	3:D:1042:ARG:HD3	2.15	0.46
5:F:319:THR:O	5:F:321:ILE:HG12	2.15	0.46
2:M:1078:GLU:HA	2:M:1079:PRO:HD3	1.86	0.46
3:N:187:LYS:HG3	3:N:199:LEU:CD2	2.44	0.46
3:N:1217:ILE:HD12	3:N:1480:PHE:CE2	2.51	0.46
3:N:1283:ILE:HD12	3:N:1315:ASP:CG	2.40	0.46
4:O:33:HIS:CD2	4:O:89:MET:HG2	2.49	0.46
4:O:40:LEU:C	4:O:42:PRO:HD2	2.41	0.46
1:A:65:PHE:CE1	2:C:799:ILE:HD11	2.51	0.46
1:A:161:ARG:HB2	1:A:161:ARG:HH11	1.79	0.46
1:B:23:PHE:O	1:B:196:THR:HA	2.14	0.46
2:C:64:LEU:HB2	2:C:359:MET:CE	2.45	0.46
2:C:139:GLN:HA	2:C:411:SER:O	2.15	0.46
2:C:147:TYR:HE1	9:C:1347:HOH:O	1.98	0.46
2:C:160:ALA:O	2:C:173:ASP:HA	2.15	0.46
2:C:271:GLU:HA	2:C:275:TYR:CD1	2.51	0.46
2:C:328:LEU:HB2	2:C:433:THR:CG2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:677:LEU:HD21	9:D:2185:HOH:O	2.14	0.46
3:D:928:ALA:O	3:D:931:LEU:HB2	2.16	0.46
3:D:951:ILE:CD1	3:D:1062:ARG:HG3	2.45	0.46
3:D:1382:THR:OG1	3:D:1418:LYS:HE3	2.16	0.46
1:K:42:ARG:HE	2:M:857:ASP:HB3	1.79	0.46
1:L:102:LYS:HA	1:L:138:LEU:O	2.16	0.46
1:L:200:TRP:HZ3	9:N:2120:HOH:O	1.98	0.46
2:M:426:ASP:OD1	2:M:427:VAL:HG22	2.14	0.46
2:M:459:ALA:HB1	2:M:467:ILE:CG2	2.46	0.46
2:M:760:SER:O	2:M:786:LYS:N	2.40	0.46
3:N:562:ALA:HB1	3:N:567:ILE:CD1	2.45	0.46
3:N:705:ALA:HB3	3:N:706:PRO:CD	2.45	0.46
3:N:705:ALA:HB2	9:N:1965:HOH:O	2.16	0.46
3:N:924:MET:HE1	3:N:1211:MET:HE3	1.96	0.46
3:N:1135:ARG:HH21	3:N:1350:GLU:CD	2.23	0.46
3:N:1281:VAL:HG21	3:N:1313:VAL:HG21	1.96	0.46
3:N:1476:THR:CG2	4:O:21:VAL:HG22	2.42	0.46
5:P:123:ASP:HB2	5:P:126:LEU:HD13	1.96	0.46
5:P:420:ASP:O	5:P:422:LEU:HD23	2.16	0.46
1:B:85:LEU:HD13	1:B:127:LEU:HD23	1.98	0.46
1:B:128:HIS:HE1	1:B:131:THR:HG23	1.81	0.46
2:C:31:GLN:NE2	2:C:71:TYR:OH	2.49	0.46
2:C:89:THR:HA	2:C:129:ILE:O	2.15	0.46
2:C:588:VAL:HG21	9:C:1718:HOH:O	2.15	0.46
2:C:798:GLY:H	2:C:827:VAL:CG1	2.29	0.46
3:D:23:TYR:O	3:D:49:ILE:HG23	2.16	0.46
3:D:131:LYS:HD2	5:F:83:GLN:CD	2.40	0.46
3:D:795:VAL:HG12	3:D:796:ARG:N	2.31	0.46
3:D:860:LEU:O	3:D:877:PRO:HD2	2.14	0.46
3:D:952:ASP:HA	3:D:1062:ARG:NH2	2.31	0.46
5:F:116:LEU:CB	5:F:127:ILE:HD12	2.46	0.46
5:F:151:LEU:HD11	9:F:626:HOH:O	2.14	0.46
5:F:171:LYS:HA	9:F:473:HOH:O	2.16	0.46
1:K:58:ILE:HG21	1:K:68:ILE:HD11	1.97	0.46
1:L:89:PHE:HB3	1:L:94:LEU:HD22	1.98	0.46
2:M:468:ARG:HB3	2:M:487:THR:HA	1.97	0.46
2:M:718:GLY:HA3	2:M:761:PHE:CE1	2.51	0.46
2:M:843:HIS:CD2	2:M:884:GLN:HA	2.50	0.46
2:M:1077:PRO:HG3	9:M:2203:HOH:O	2.15	0.46
3:N:18:ILE:HD12	3:N:518:PRO:CD	2.45	0.46
3:N:403:PHE:CD1	3:N:405:ASP:O	2.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:82:GLU:HG3	4:O:83:ASP:H	1.80	0.46
5:P:209:PHE:HE2	5:P:213:ILE:HD11	1.79	0.46
1:B:57:TYR:O	1:B:140:MET:HA	2.15	0.46
1:B:60:ASP:HB2	1:B:137:ARG:NH1	2.31	0.46
2:C:6:PHE:CD1	2:C:909:ALA:HB2	2.50	0.46
2:C:575:GLN:O	2:C:667:ALA:HB1	2.15	0.46
2:C:939:ARG:HD3	2:C:975:TYR:CE2	2.51	0.46
2:C:975:TYR:HA	2:C:982:PRO:HA	1.97	0.46
3:D:191:LEU:HD13	3:D:393:ILE:HG21	1.97	0.46
3:D:421:LEU:HD11	3:D:446:VAL:CG2	2.45	0.46
3:D:455:ARG:NH1	3:D:463:GLN:HG3	2.31	0.46
3:D:1076:GLY:O	3:D:1079:LYS:HG2	2.16	0.46
4:E:13:VAL:HG23	9:E:151:HOH:O	2.14	0.46
1:K:35:THR:HG21	1:L:43:ILE:HD11	1.98	0.46
1:K:132:LEU:HD12	1:K:132:LEU:N	2.30	0.46
1:L:69:PRO:O	1:L:71:VAL:HG23	2.15	0.46
2:M:491:GLU:OE1	2:M:516:ARG:NH2	2.48	0.46
2:M:810:ASP:N	2:M:811:PRO:HD3	2.30	0.46
3:N:145:VAL:HG22	3:N:146:PRO:CD	2.46	0.46
3:N:1115:THR:HG21	3:N:1151:ARG:HH21	1.80	0.46
3:N:1195:GLN:CG	3:N:1196:THR:N	2.78	0.46
3:N:1266:ARG:O	3:N:1268:PRO:HD3	2.15	0.46
5:P:396:ARG:HA	5:P:399:GLN:HB2	1.98	0.46
1:B:176:ARG:NH2	3:D:847:ASP:HA	2.31	0.46
1:B:179:PHE:HZ	9:B:437:HOH:O	1.99	0.46
2:C:89:THR:HB	2:C:129:ILE:O	2.16	0.46
2:C:140:ILE:HD13	2:C:331:ARG:HH21	1.80	0.46
2:C:396:ASP:HA	2:C:633:GLN:CD	2.40	0.46
2:C:674:VAL:HB	2:C:869:VAL:HG13	1.98	0.46
2:C:875:GLY:HA2	2:C:879:ARG:HH11	1.80	0.46
3:D:53:ILE:HG23	3:D:54:LYS:N	2.30	0.46
3:D:73:CYS:HB2	9:D:2023:HOH:O	2.14	0.46
3:D:421:LEU:HD11	3:D:446:VAL:HG21	1.97	0.46
3:D:443:VAL:HG22	3:D:444:VAL:H	1.81	0.46
3:D:1377:LYS:NZ	9:D:1537:HOH:O	2.45	0.46
3:D:1389:LEU:HD12	3:D:1390:LEU:HG	1.98	0.46
3:D:1472:ILE:O	3:D:1477:GLY:HA3	2.14	0.46
1:L:27:PRO:HB3	1:L:192:LEU:HD22	1.98	0.46
2:M:333:ILE:HD12	2:M:333:ILE:N	2.30	0.46
3:N:119:SER:HB3	9:N:1620:HOH:O	2.15	0.46
3:N:407:VAL:HG22	3:N:422:ALA:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:522:PRO:HA	3:N:525:ARG:NH1	2.31	0.46
3:N:644:LEU:HD23	3:N:718:PRO:HB3	1.98	0.46
3:N:937:TYR:O	3:N:941:PHE:HD1	1.99	0.46
3:N:1311:LEU:HD23	3:N:1311:LEU:H	1.81	0.46
3:N:1382:THR:HG21	3:N:1418:LYS:NZ	2.31	0.46
3:N:1410:GLU:OE2	3:N:1414:PRO:HG3	2.16	0.46
1:B:22:GLU:HG2	1:B:198:ARG:HG2	1.97	0.46
1:B:205:VAL:HB	9:B:448:HOH:O	2.15	0.46
2:C:101:ILE:HG23	2:C:107:LEU:CD2	2.43	0.46
2:C:799:ILE:HD13	2:C:799:ILE:N	2.30	0.46
3:D:131:LYS:HG3	3:D:572:ARG:HH21	1.81	0.46
3:D:409:VAL:O	3:D:437:VAL:HG21	2.16	0.46
3:D:498:VAL:CG2	3:D:499:VAL:N	2.79	0.46
3:D:562:ALA:HB1	3:D:567:ILE:CD1	2.45	0.46
3:D:643:GLY:CA	3:D:727:GLN:HB2	2.46	0.46
3:D:693:GLU:HG3	4:E:48:MET:CE	2.46	0.46
3:D:783:ARG:NH1	3:D:1029:ARG:HG3	2.30	0.46
3:D:800:LYS:HE3	3:D:830:ALA:HB3	1.98	0.46
3:D:1209:LEU:HD12	3:D:1219:GLU:CD	2.41	0.46
3:D:1335:LEU:CD2	3:D:1344:VAL:HA	2.29	0.46
5:F:241:TRP:HB2	9:F:438:HOH:O	2.15	0.46
5:F:398:ARG:HG3	5:F:402:ASN:ND2	2.31	0.46
2:M:82:GLU:OE2	2:M:86:LYS:HE3	2.16	0.46
2:M:122:THR:HG22	2:M:123:GLU:N	2.30	0.46
2:M:361:MET:HE2	9:M:2183:HOH:O	2.15	0.46
2:M:518:LYS:HG3	9:M:1841:HOH:O	2.16	0.46
2:M:663:ASN:C	2:M:665:PHE:H	2.24	0.46
2:M:988:VAL:HG11	3:N:949:ILE:O	2.16	0.46
2:M:1097:LEU:HD21	3:N:103:TRP:HZ3	1.81	0.46
3:N:795:VAL:HG22	3:N:876:SER:HB3	1.97	0.46
3:N:1344:VAL:HG12	3:N:1348:LEU:HD22	1.97	0.46
3:N:1385:GLY:CA	3:N:1413:THR:HG21	2.46	0.46
3:N:1426:LYS:HA	9:N:1705:HOH:O	2.15	0.46
1:A:9:PRO:HD2	1:B:224:TYR:CD1	2.51	0.46
2:C:437:ARG:NH2	2:C:488:ALA:HA	2.31	0.46
2:C:1002:GLU:O	2:C:1003:ASP:C	2.58	0.46
2:C:1067:TYR:CE1	3:D:655:PRO:HG3	2.49	0.46
2:C:1087:VAL:HG11	3:D:610:LYS:HZ3	1.78	0.46
3:D:48:ARG:NH2	9:D:1710:HOH:O	2.48	0.46
3:D:408:GLU:HA	5:F:171:LYS:HZ1	1.81	0.46
3:D:525:ARG:HA	3:D:538:SER:OG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:596:SER:C	3:D:598:ARG:H	2.24	0.46
3:D:866:VAL:HG12	3:D:867:ARG:N	2.30	0.46
3:D:1083:ASP:O	3:D:1087:ARG:HG3	2.15	0.46
5:F:214:GLN:O	5:F:217:ASN:HB2	2.16	0.46
1:K:36:LEU:O	1:K:39:PRO:HD2	2.16	0.46
2:M:9:ILE:HG12	2:M:907:ASP:OD2	2.15	0.46
2:M:103:LYS:HB3	9:M:2059:HOH:O	2.15	0.46
2:M:115:LEU:HD22	2:M:373:VAL:CG1	2.41	0.46
2:M:211:LEU:HD11	2:M:308:ARG:HA	1.98	0.46
2:M:540:PHE:HE1	2:M:906:PHE:HE1	1.64	0.46
2:M:612:VAL:HG22	2:M:622:GLU:HA	1.97	0.46
3:N:560:GLN:O	5:P:184:ARG:NH2	2.48	0.46
3:N:775:GLY:C	9:N:1689:HOH:O	2.58	0.46
3:N:1197:ARG:HG3	3:N:1198:TYR:H	1.80	0.46
3:N:1209:LEU:C	3:N:1211:MET:N	2.72	0.46
5:P:113:ILE:HG23	5:P:127:ILE:CG2	2.46	0.46
5:P:266:GLU:O	5:P:270:LYS:HG3	2.16	0.46
5:P:358:LEU:HD13	5:P:370:LYS:HG3	1.97	0.46
5:P:400:ILE:HA	9:P:540:HOH:O	2.15	0.46
5:P:406:ARG:HA	5:P:409:LYS:HG2	1.97	0.46
1:A:46:SER:HB3	2:C:856:GLU:CD	2.41	0.46
1:A:198:ARG:HD2	1:A:200:TRP:CH2	2.51	0.46
1:A:212:ASN:O	1:A:215:VAL:HG22	2.16	0.46
2:C:199:VAL:HG13	2:C:235:LEU:CD2	2.46	0.46
2:C:292:ARG:HH11	2:C:299:LYS:HD3	1.81	0.46
2:C:564:MET:SD	2:C:846:LYS:HE3	2.55	0.46
3:D:27:GLU:O	3:D:28:LYS:HG2	2.16	0.46
3:D:45:PHE:HD1	3:D:86:ARG:HH22	1.64	0.46
3:D:539:ASP:OD2	5:F:318:GLU:HB2	2.15	0.46
3:D:704:ARG:CG	3:D:705:ALA:H	2.24	0.46
3:D:911:LEU:O	3:D:915:VAL:HG23	2.15	0.46
3:D:1295:GLU:HB3	3:D:1300:SER:HB3	1.97	0.46
3:D:1326:THR:HG22	3:D:1327:ARG:N	2.31	0.46
3:D:1485:GLN:HE21	4:E:80:VAL:H	1.63	0.46
5:F:176:ILE:HA	9:F:463:HOH:O	2.16	0.46
5:F:368:VAL:O	5:F:372:ARG:HB2	2.16	0.46
1:K:46:SER:HB3	2:M:856:GLU:CG	2.45	0.46
1:K:51:THR:HA	1:K:145:ASP:O	2.16	0.46
2:M:110:GLU:HB2	2:M:369:PRO:HG3	1.97	0.46
2:M:976:ASP:HB2	2:M:979:THR:HG22	1.96	0.46
2:M:1097:LEU:N	2:M:1097:LEU:HD12	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:1109:VAL:HG11	3:N:5:VAL:HG13	1.97	0.46
2:M:1115:LEU:CB	3:N:85:VAL:HG13	2.42	0.46
3:N:18:ILE:HG21	3:N:516:ALA:O	2.15	0.46
3:N:131:LYS:HD2	5:P:83:GLN:OE1	2.15	0.46
3:N:884:ARG:O	3:N:888:GLU:HB2	2.16	0.46
3:N:1223:ILE:O	3:N:1224:VAL:C	2.59	0.46
5:P:88:ILE:HD13	5:P:193:ARG:CB	2.46	0.46
5:P:138:SER:H	5:P:140:ARG:HE	1.64	0.46
1:B:9:PRO:HD3	9:B:452:HOH:O	2.17	0.45
2:C:6:PHE:HB2	2:C:908:GLY:O	2.16	0.45
2:C:86:LYS:HD2	9:C:1425:HOH:O	2.16	0.45
2:C:286:SER:C	2:C:287:GLY:O	2.56	0.45
2:C:411:SER:OG	2:C:452:ILE:HG23	2.16	0.45
2:C:437:ARG:HG2	2:C:467:ILE:HG22	1.97	0.45
2:C:791:ARG:HD3	9:C:1572:HOH:O	2.15	0.45
3:D:803:GLY:CA	9:D:1726:HOH:O	2.64	0.45
3:D:1144:LEU:HB3	3:D:1166:LEU:HD11	1.97	0.45
3:D:1267:ARG:O	3:D:1267:ARG:HG2	2.16	0.45
5:F:148:LYS:HE3	9:F:489:HOH:O	2.16	0.45
1:L:124:ASN:OD1	1:L:127:LEU:HB2	2.17	0.45
2:M:9:ILE:HD11	2:M:537:LYS:CE	2.45	0.45
2:M:217:LEU:HB2	2:M:311:PHE:CE1	2.50	0.45
2:M:265:ARG:NH2	9:M:2236:HOH:O	2.48	0.45
2:M:612:VAL:HG22	2:M:622:GLU:HG3	1.99	0.45
2:M:675:ALA:CA	2:M:989:VAL:HG12	2.41	0.45
2:M:1114:GLY:HA2	9:M:1820:HOH:O	2.15	0.45
3:N:10:ILE:HD11	3:N:1434:TRP:NE1	2.31	0.45
3:N:573:MET:SD	5:P:210:LEU:HB3	2.56	0.45
3:N:625:TYR:O	3:N:749:VAL:HG23	2.16	0.45
3:N:711:LEU:C	3:N:713:ILE:N	2.74	0.45
3:N:1258:ARG:NE	3:N:1262:LEU:HD11	2.31	0.45
3:N:1283:ILE:CG2	3:N:1290:LEU:HD21	2.46	0.45
4:O:45:ARG:HB2	4:O:46:PRO:CD	2.45	0.45
4:O:70:THR:HG22	4:O:71:GLY:N	2.31	0.45
4:O:87:LYS:HB3	9:O:2559:HOH:O	2.15	0.45
2:C:18:LEU:CD2	2:C:542:VAL:HG11	2.45	0.45
2:C:137:VAL:CG2	2:C:391:LEU:HG	2.46	0.45
2:C:146:VAL:HG22	2:C:162:ILE:HG23	1.97	0.45
2:C:425:PHE:O	2:C:429:ASP:OD2	2.35	0.45
2:C:536:PRO:HB2	9:C:1738:HOH:O	2.16	0.45
2:C:679:PHE:O	2:C:680:ASP:C	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:916:GLU:O	2:C:919:ALA:HB3	2.17	0.45
2:C:1044:GLY:CA	4:E:17:TYR:HE1	2.21	0.45
3:D:195:VAL:HG12	3:D:196:VAL:N	2.31	0.45
3:D:736:PHE:O	3:D:738:ALA:N	2.50	0.45
3:D:907:GLU:HG2	3:D:908:LYS:H	1.81	0.45
3:D:1031:ASN:O	3:D:1034:GLN:HB2	2.16	0.45
4:E:53:GLY:C	4:E:55:PHE:H	2.24	0.45
5:F:80:PRO:O	5:F:83:GLN:HB2	2.16	0.45
5:F:94:LEU:HD12	5:F:98:GLU:OE2	2.16	0.45
5:F:288:TYR:HA	5:F:291:ILE:CG2	2.46	0.45
1:K:55:SER:HB2	1:K:158:ILE:HG21	1.98	0.45
1:K:158:ILE:HD12	1:K:158:ILE:HG23	1.88	0.45
1:K:162:ILE:HG13	1:K:163:ASN:N	2.32	0.45
2:M:49:ARG:HG2	2:M:266:ARG:HH12	1.82	0.45
2:M:165:LEU:HA	2:M:166:PRO:O	2.15	0.45
2:M:367:LEU:O	2:M:371:LYS:HB2	2.17	0.45
2:M:914:ILE:HD12	2:M:914:ILE:HA	1.75	0.45
3:N:23:TYR:O	3:N:24:GLY:O	2.35	0.45
3:N:204:LEU:O	3:N:393:ILE:HA	2.15	0.45
3:N:570:GLU:CA	5:P:214:GLN:HE22	2.29	0.45
3:N:1203:LYS:HG2	9:N:1955:HOH:O	2.15	0.45
3:N:1264:GLU:HG2	3:N:1425:THR:H	1.81	0.45
5:P:142:ARG:NH1	5:P:150:THR:OG1	2.49	0.45
5:P:157:GLU:HG2	9:P:498:HOH:O	2.16	0.45
1:A:158:ILE:HG22	1:A:160:ASP:H	1.81	0.45
2:C:271:GLU:HA	2:C:275:TYR:HD1	1.81	0.45
2:C:460:ARG:NE	2:C:485:TYR:CZ	2.84	0.45
2:C:551:GLU:HA	2:C:906:PHE:CE2	2.51	0.45
2:C:612:VAL:HG22	2:C:622:GLU:HA	1.99	0.45
2:C:905:ILE:H	2:C:905:ILE:CD1	2.13	0.45
2:C:1002:GLU:HA	9:C:1756:HOH:O	2.15	0.45
3:D:421:LEU:HB3	3:D:444:VAL:HG11	1.98	0.45
3:D:667:ALA:HB2	3:D:676:MET:SD	2.56	0.45
3:D:699:VAL:H	3:D:756:GLN:NE2	2.15	0.45
3:D:710:ARG:NH2	3:D:1210:SER:HB2	2.31	0.45
3:D:754:PHE:HA	4:E:24:ALA:HB1	1.98	0.45
3:D:814:ALA:O	3:D:818:ARG:HG3	2.17	0.45
3:D:1116:ASN:N	3:D:1116:ASN:ND2	2.63	0.45
3:D:1350:GLU:OE2	3:D:1357:ARG:NH1	2.48	0.45
5:F:82:ARG:O	5:F:86:HIS:HB2	2.15	0.45
2:M:19:THR:O	2:M:19:THR:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:51:THR:HB	2:M:348:LEU:HD23	1.98	0.45
2:M:1044:GLY:HA3	4:O:17:TYR:HE1	1.80	0.45
3:N:102:ILE:HD12	3:N:579:ASP:CB	2.45	0.45
3:N:157:GLU:HA	3:N:160:GLU:OE1	2.16	0.45
3:N:455:ARG:NH2	9:N:2369:HOH:O	2.49	0.45
3:N:584:ASN:HD21	3:N:590:PRO:CD	2.29	0.45
3:N:684:LYS:HD2	9:N:2165:HOH:O	2.16	0.45
3:N:999:THR:O	3:N:1003:VAL:HG13	2.16	0.45
3:N:1378:TYR:HA	3:N:1394:VAL:HA	1.98	0.45
4:O:16:LYS:HB2	9:O:3818:HOH:O	2.14	0.45
5:P:300:ASP:HB3	9:P:433:HOH:O	2.16	0.45
5:P:419:ARG:O	5:P:421:PHE:N	2.49	0.45
1:B:169:ALA:HB1	1:B:171:PHE:HD2	1.80	0.45
2:C:64:LEU:HB2	2:C:359:MET:SD	2.56	0.45
2:C:110:GLU:HB2	2:C:369:PRO:HG3	1.98	0.45
2:C:114:PHE:CE2	5:F:283:GLY:HA3	2.51	0.45
2:C:212:GLY:HA3	2:C:218:VAL:CG2	2.45	0.45
2:C:352:ALA:HA	2:C:355:VAL:CG1	2.46	0.45
3:D:9:ARG:HA	3:D:1434:TRP:CH2	2.50	0.45
3:D:87:ARG:HA	3:D:523:ASP:HB2	1.98	0.45
3:D:473:LEU:HD21	3:D:495:ARG:CZ	2.46	0.45
3:D:684:LYS:HD3	3:D:686:GLU:OE1	2.17	0.45
3:D:760:ARG:HD2	4:E:3:GLU:CD	2.41	0.45
3:D:1299:PHE:CD2	3:D:1299:PHE:N	2.84	0.45
3:D:1447:LEU:O	3:D:1448:THR:C	2.60	0.45
3:D:1492:LEU:HA	9:D:2354:HOH:O	2.16	0.45
4:E:44:GLU:HG2	9:E:142:HOH:O	2.16	0.45
5:F:336:GLU:N	9:F:562:HOH:O	2.48	0.45
5:F:371:LEU:HB2	5:F:372:ARG:NH1	2.32	0.45
5:F:392:VAL:HG11	5:F:396:ARG:CD	2.46	0.45
1:L:101:LEU:HD12	1:L:113:ASP:C	2.40	0.45
1:L:156:HIS:CG	1:L:157:GLY:N	2.84	0.45
1:L:165:ILE:O	1:L:165:ILE:HG13	2.16	0.45
2:M:285:LEU:HD22	9:M:1655:HOH:O	2.15	0.45
2:M:329:GLY:HA3	2:M:489:THR:HG23	1.98	0.45
2:M:418:LEU:N	2:M:418:LEU:CD1	2.80	0.45
2:M:752:GLY:H	2:M:792:VAL:HB	1.82	0.45
2:M:929:ARG:HH22	2:M:940:GLU:CD	2.24	0.45
3:N:93:ILE:HD13	3:N:548:ILE:HD11	1.98	0.45
3:N:104:PHE:CE2	3:N:1448:THR:HG23	2.51	0.45
3:N:1369:GLU:O	3:N:1372:VAL:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1505:ALA:HB1	9:N:2193:HOH:O	2.17	0.45
4:O:75:PHE:HE1	9:O:3411:HOH:O	1.98	0.45
4:O:76:GLY:HA3	4:O:79:LEU:HD12	1.98	0.45
2:C:54:ILE:HG23	2:C:54:ILE:O	2.16	0.45
2:C:265:ARG:HD3	2:C:267:TYR:HB3	1.99	0.45
2:C:443:THR:HA	2:C:444:PRO:HD3	1.79	0.45
2:C:474:VAL:HA	2:C:478:VAL:O	2.17	0.45
2:C:565:GLN:OE1	2:C:842:ARG:HG2	2.17	0.45
2:C:1060:ILE:HG22	2:C:1061:GLU:H	1.81	0.45
3:D:72:VAL:CG2	3:D:78:VAL:H	2.29	0.45
3:D:540:LEU:HD21	3:D:603:LEU:HD23	1.98	0.45
3:D:563:PRO:HG2	5:F:188:ILE:HG21	1.99	0.45
3:D:760:ARG:HD2	4:E:3:GLU:OE1	2.17	0.45
3:D:1000:THR:HG23	3:D:1001:GLU:N	2.31	0.45
3:D:1047:LYS:HG2	3:D:1053:PHE:CE2	2.51	0.45
4:E:31:LEU:HD23	4:E:35:PHE:CE1	2.52	0.45
5:F:340:SER:O	5:F:342:VAL:N	2.50	0.45
5:F:394:ARG:NE	5:F:398:ARG:HB2	2.31	0.45
1:L:223:THR:C	1:L:225:PHE:H	2.25	0.45
2:M:118:ILE:O	2:M:118:ILE:HD12	2.16	0.45
2:M:400:PRO:O	2:M:401:LEU:C	2.58	0.45
2:M:807:ARG:HA	2:M:821:GLU:HB2	1.99	0.45
2:M:929:ARG:HH12	2:M:940:GLU:CD	2.24	0.45
3:N:45:PHE:HD1	3:N:86:ARG:NH2	2.15	0.45
3:N:126:VAL:CG1	3:N:132:TYR:HB2	2.47	0.45
3:N:596:SER:C	3:N:598:ARG:H	2.24	0.45
3:N:675:ARG:HH22	5:P:421:PHE:HE2	1.63	0.45
3:N:700:VAL:HG22	3:N:718:PRO:HG3	1.98	0.45
3:N:779:ALA:HA	9:N:1773:HOH:O	2.16	0.45
3:N:796:ARG:NH1	3:N:861:GLN:HE21	2.14	0.45
3:N:939:PHE:O	3:N:943:THR:HG23	2.17	0.45
3:N:1109:GLU:CD	3:N:1202:GLN:HB2	2.42	0.45
3:N:1299:PHE:N	3:N:1299:PHE:HD2	2.15	0.45
3:N:1420:LEU:HD23	9:N:1853:HOH:O	2.15	0.45
5:P:91:VAL:HG21	9:P:550:HOH:O	2.17	0.45
5:P:360:LYS:HG2	9:P:511:HOH:O	2.17	0.45
1:A:28:LEU:HD23	1:A:28:LEU:HA	1.75	0.45
1:A:151:VAL:H	1:A:169:ALA:HB3	1.81	0.45
2:C:68:PHE:HE1	2:C:96:ALA:HB1	1.82	0.45
2:C:418:LEU:N	2:C:418:LEU:CD1	2.79	0.45
2:C:598:GLU:HG3	2:C:623:TYR:OH	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:95:LEU:HD23	3:D:574:LEU:HD11	1.98	0.45
3:D:638:LYS:C	3:D:729:HIS:HD2	2.25	0.45
3:D:892:ASP:O	3:D:895:VAL:N	2.49	0.45
2:M:279:GLU:HG3	2:M:280:LYS:N	2.29	0.45
2:M:455:LEU:HD12	2:M:456:ALA:N	2.32	0.45
2:M:838:LYS:HZ2	2:M:846:LYS:CE	2.30	0.45
3:N:28:LYS:HG3	3:N:41:ARG:CD	2.47	0.45
3:N:403:PHE:CE2	3:N:443:VAL:N	2.85	0.45
3:N:409:VAL:HG12	3:N:435:VAL:HG11	1.98	0.45
3:N:456:MET:HE1	9:N:1992:HOH:O	2.16	0.45
3:N:560:GLN:NE2	5:P:221:ILE:HB	2.31	0.45
3:N:704:ARG:CG	3:N:705:ALA:H	2.27	0.45
3:N:728:LEU:HD12	9:N:1892:HOH:O	2.17	0.45
3:N:861:GLN:HG2	3:N:861:GLN:H	1.55	0.45
3:N:1084:THR:HG21	9:N:2214:HOH:O	2.16	0.45
3:N:1384:PRO:C	3:N:1413:THR:HG21	2.42	0.45
4:O:85:LEU:HD23	4:O:85:LEU:C	2.42	0.45
5:P:351:SER:O	5:P:355:GLU:HB2	2.15	0.45
5:P:361:LEU:HD21	5:P:404:ALA:CB	2.46	0.45
1:A:58:ILE:HG21	1:A:68:ILE:CD1	2.45	0.45
1:B:61:VAL:H	1:B:137:ARG:HH22	1.65	0.45
2:C:342:ASP:O	2:C:346:VAL:HG23	2.16	0.45
2:C:400:PRO:O	2:C:401:LEU:C	2.58	0.45
2:C:469:THR:OG1	2:C:470:PRO:HD2	2.16	0.45
2:C:837:ASP:OD1	2:C:999:HIS:NE2	2.49	0.45
2:C:876:VAL:HB	2:C:877:PRO:HD3	1.98	0.45
2:C:1009:SER:CB	3:D:651:GLU:HG2	2.47	0.45
3:D:584:ASN:HD21	3:D:590:PRO:HB2	1.82	0.45
3:D:640:HIS:HE1	4:E:3:GLU:HG2	1.80	0.45
3:D:1108:ARG:HB2	9:D:2164:HOH:O	2.15	0.45
3:D:1173:LEU:HD23	3:D:1174:LEU:HD23	1.98	0.45
3:D:1242:HIS:NE2	3:D:1266:ARG:HD3	2.31	0.45
3:D:1285:GLU:O	3:D:1285:GLU:HG2	2.17	0.45
3:D:1487:VAL:HG13	3:D:1491:THR:HB	1.97	0.45
5:F:284:ARG:HB2	9:F:621:HOH:O	2.17	0.45
5:F:393:THR:HG22	5:F:394:ARG:H	1.82	0.45
2:M:92:ALA:HB2	2:M:120:LEU:CD1	2.45	0.45
2:M:551:GLU:HB3	2:M:906:PHE:CD2	2.51	0.45
3:N:16:GLU:HG3	9:N:1701:HOH:O	2.16	0.45
3:N:105:VAL:HG21	3:N:128:TYR:HE2	1.75	0.45
3:N:486:ARG:HG2	9:N:1964:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:569:ASN:ND2	5:P:210:LEU:HD22	2.29	0.45
3:N:586:ARG:HG2	9:N:2201:HOH:O	2.16	0.45
3:N:770:LEU:HB2	3:N:1210:SER:O	2.17	0.45
3:N:838:ARG:HB3	9:N:2366:HOH:O	2.17	0.45
3:N:1335:LEU:O	3:N:1335:LEU:HG	2.16	0.45
3:N:1350:GLU:O	3:N:1350:GLU:HG3	2.16	0.45
9:N:1980:HOH:O	5:P:210:LEU:HD12	2.17	0.45
5:P:125:ASP:HA	9:P:579:HOH:O	2.16	0.45
2:C:266:ARG:HA	2:C:288:ARG:HD3	1.97	0.45
2:C:471:TYR:CD2	2:C:496:ILE:HG21	2.51	0.45
2:C:475:VAL:O	2:C:475:VAL:HG12	2.17	0.45
2:C:810:ASP:H	2:C:811:PRO:HD3	1.81	0.45
2:C:971:LYS:HG2	9:C:1494:HOH:O	2.17	0.45
2:C:1059:ASP:CG	2:C:1062:GLY:HA3	2.42	0.45
3:D:137:PRO:HD2	3:D:453:ASP:CB	2.46	0.45
3:D:1047:LYS:HB3	3:D:1048:PRO:CD	2.46	0.45
4:E:37:ASN:HA	4:E:93:TYR:CE2	2.52	0.45
5:F:361:LEU:HD13	5:F:366:ALA:HB2	1.98	0.45
2:M:18:LEU:HD13	2:M:590:ASP:OD2	2.16	0.45
2:M:694:LEU:CD1	2:M:868:ASP:HB3	2.47	0.45
2:M:715:THR:CG2	2:M:717:LEU:HG	2.45	0.45
2:M:1048:THR:O	2:M:1052:MET:HG2	2.17	0.45
3:N:44:LEU:HB3	3:N:525:ARG:HH21	1.82	0.45
3:N:119:SER:CB	3:N:123:LEU:HD13	2.46	0.45
3:N:809:PRO:HB2	3:N:812:ALA:CB	2.45	0.45
3:N:896:ALA:O	3:N:900:ILE:HG23	2.17	0.45
3:N:1095:THR:O	3:N:1096:ARG:C	2.60	0.45
3:N:1107:VAL:HA	3:N:1200:VAL:O	2.17	0.45
1:A:64:GLU:O	1:A:64:GLU:HG2	2.14	0.45
1:A:158:ILE:HG22	1:A:159:LYS:N	2.32	0.45
2:C:13:ILE:HG12	2:C:534:VAL:HG13	1.98	0.45
2:C:36:PRO:HG2	2:C:70:GLU:HB3	1.97	0.45
2:C:185:LYS:NZ	2:C:190:LYS:HE2	2.32	0.45
2:C:267:TYR:O	2:C:268:ASP:C	2.60	0.45
2:C:841:ASN:HD21	2:C:845:ASN:N	2.15	0.45
2:C:926:PHE:HE1	2:C:929:ARG:NH1	2.15	0.45
2:C:1118:LYS:C	2:C:1119:ARG:OXT	2.60	0.45
3:D:72:VAL:HG23	3:D:78:VAL:N	2.32	0.45
3:D:850:LEU:O	3:D:853:VAL:HB	2.16	0.45
3:D:1124:GLN:HA	3:D:1125:PRO:HD3	1.79	0.45
4:E:46:PRO:CB	4:E:54:LEU:HD22	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:248:ASN:HA	5:F:251:ILE:HD12	1.98	0.45
2:M:9:ILE:HD11	2:M:537:LYS:HE2	1.98	0.45
2:M:537:LYS:H	2:M:537:LYS:HG2	1.44	0.45
2:M:987:ILE:HG22	2:M:988:VAL:O	2.17	0.45
3:N:28:LYS:HA	3:N:29:PRO:HD3	1.72	0.45
3:N:863:VAL:HG11	9:N:2345:HOH:O	2.17	0.45
3:N:1045:MET:HG3	3:N:1073:SER:OG	2.17	0.45
3:N:1120:VAL:HB	3:N:1144:LEU:HD21	1.99	0.45
5:P:132:ARG:HB3	5:P:136:LEU:HD21	1.99	0.45
1:B:55:SER:HB2	1:B:158:ILE:HD13	1.96	0.45
2:C:338:GLU:HA	2:C:341:THR:HG22	1.99	0.45
2:C:358:ARG:HD3	2:C:371:LYS:O	2.17	0.45
2:C:889:HIS:HD2	2:C:970:GLY:HA3	1.81	0.45
2:C:939:ARG:HB3	2:C:982:PRO:HG3	1.98	0.45
2:C:1109:VAL:CG1	3:D:5:VAL:HG13	2.46	0.45
3:D:31:THR:HG23	3:D:45:PHE:HE2	1.80	0.45
3:D:76:CYS:N	9:D:1539:HOH:O	2.49	0.45
3:D:608:SER:C	3:D:610:LYS:N	2.72	0.45
3:D:637:LEU:HD12	3:D:641:GLN:HB2	1.99	0.45
3:D:1087:ARG:CD	3:D:1236:LEU:O	2.65	0.45
3:D:1254:GLN:HB2	9:D:1984:HOH:O	2.17	0.45
3:D:1368:ILE:H	3:D:1368:ILE:HG13	1.57	0.45
3:D:1448:THR:O	3:D:1451:ALA:HB3	2.16	0.45
3:D:1476:THR:C	3:D:1478:SER:H	2.24	0.45
2:M:90:TYR:HE1	9:M:2242:HOH:O	2.00	0.45
2:M:165:LEU:O	2:M:265:ARG:HB2	2.17	0.45
2:M:572:ILE:HD11	2:M:701:THR:HB	1.99	0.45
2:M:673:LEU:CD2	2:M:867:VAL:HG12	2.46	0.45
3:N:50:PHE:HB3	3:N:522:PRO:CG	2.46	0.45
3:N:54:LYS:O	3:N:55:ASP:O	2.34	0.45
3:N:103:TRP:NE1	3:N:1444:THR:HG23	2.31	0.45
3:N:142:LEU:C	3:N:142:LEU:HD12	2.42	0.45
3:N:477:LEU:HD22	3:N:492:ALA:HB1	1.99	0.45
3:N:500:ARG:HH11	3:N:500:ARG:HG3	1.82	0.45
3:N:656:PHE:HB3	3:N:694:VAL:HG11	1.98	0.45
3:N:1372:VAL:HG13	3:N:1373:ARG:N	2.32	0.45
3:N:1376:MET:HG2	3:N:1421:LEU:HD12	1.98	0.45
1:B:129:ILE:HG21	1:B:140:MET:HE1	1.98	0.44
2:C:102:HIS:CE1	2:C:365:ASP:HA	2.52	0.44
2:C:221:LEU:HD11	9:C:1633:HOH:O	2.17	0.44
2:C:410:ILE:CD1	2:C:455:LEU:HB3	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:750:LYS:HG3	3:D:681:ARG:NH2	2.24	0.44
3:D:169:TYR:HA	3:D:170:PRO:HD3	1.82	0.44
3:D:514:LEU:HA	9:D:1709:HOH:O	2.15	0.44
3:D:609:GLY:O	3:D:610:LYS:O	2.35	0.44
3:D:820:GLU:HB2	3:D:836:VAL:HG11	1.99	0.44
3:D:1465:ASN:HD22	3:D:1465:ASN:HA	1.50	0.44
5:F:420:ASP:O	5:F:422:LEU:HD23	2.16	0.44
2:M:281:LEU:O	2:M:282:GLY:O	2.35	0.44
2:M:690:ILE:HG12	2:M:694:LEU:HD12	1.99	0.44
2:M:863:ASP:OD1	2:M:865:THR:HG22	2.16	0.44
2:M:988:VAL:HG13	3:N:948:THR:OG1	2.17	0.44
2:M:1058:ASP:OD1	2:M:1084:SER:HB3	2.16	0.44
2:M:1115:LEU:HD12	2:M:1115:LEU:H	1.81	0.44
3:N:486:ARG:N	9:N:1964:HOH:O	2.49	0.44
3:N:644:LEU:HD12	3:N:645:PRO:CD	2.46	0.44
3:N:860:LEU:HB2	9:N:2139:HOH:O	2.17	0.44
4:O:32:ARG:HD2	9:O:4200:HOH:O	2.16	0.44
5:P:195:VAL:HG11	5:P:217:ASN:OD1	2.17	0.44
5:P:340:SER:OG	5:P:342:VAL:HG23	2.17	0.44
2:C:158:TYR:CE1	2:C:313:LEU:HG	2.52	0.44
2:C:598:GLU:O	2:C:651:LYS:HG3	2.16	0.44
3:D:625:TYR:O	3:D:749:VAL:HG23	2.16	0.44
3:D:810:GLU:HA	3:D:813:LEU:HD23	1.98	0.44
3:D:960:LYS:HG2	3:D:964:LEU:HD12	1.99	0.44
3:D:1161:GLU:CG	3:D:1164:ARG:HD2	2.46	0.44
5:F:191:ASN:OD1	5:F:194:LEU:HD13	2.17	0.44
5:F:256:ARG:HH12	5:F:311:ALA:HA	1.82	0.44
1:L:228:PRO:O	1:L:229:GLN:HG3	2.17	0.44
2:M:355:VAL:CG2	2:M:372:LEU:HG	2.48	0.44
2:M:861:LEU:HD21	2:M:925:TYR:HE2	1.81	0.44
3:N:72:VAL:HG23	3:N:78:VAL:N	2.30	0.44
3:N:81:THR:O	3:N:82:LYS:C	2.61	0.44
3:N:169:TYR:HA	3:N:170:PRO:HD3	1.83	0.44
3:N:455:ARG:HA	9:N:2093:HOH:O	2.17	0.44
3:N:611:GLN:OE1	3:N:619:LEU:HD11	2.17	0.44
3:N:614:PHE:O	3:N:615:ARG:C	2.56	0.44
3:N:708:LEU:HD23	3:N:708:LEU:HA	1.80	0.44
3:N:1010:ASN:HA	9:N:1747:HOH:O	2.17	0.44
3:N:1109:GLU:HG2	3:N:1202:GLN:N	2.30	0.44
3:N:1447:LEU:O	3:N:1448:THR:C	2.60	0.44
5:P:187:LEU:HD23	5:P:187:LEU:C	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:226:LYS:HD2	5:P:242:TRP:HZ2	1.82	0.44
1:A:86:VAL:CG1	1:A:124:ASN:HB2	2.48	0.44
2:C:208:ALA:CA	2:C:221:LEU:HD21	2.48	0.44
2:C:258:TYR:HB3	9:C:1773:HOH:O	2.17	0.44
2:C:265:ARG:CG	2:C:266:ARG:N	2.80	0.44
2:C:380:ALA:O	2:C:384:GLU:HB2	2.18	0.44
2:C:402:SER:OG	2:C:566:THR:O	2.36	0.44
2:C:565:GLN:HG2	2:C:995:MET:HE1	1.99	0.44
2:C:601:GLY:O	2:C:649:VAL:HG22	2.18	0.44
2:C:684:PHE:HD2	3:D:740:PHE:HE1	1.65	0.44
2:C:690:ILE:HG12	2:C:694:LEU:HD12	1.99	0.44
2:C:1058:ASP:HB2	3:D:621:LYS:HE2	1.99	0.44
3:D:28:LYS:CG	3:D:41:ARG:HH11	2.24	0.44
3:D:136:ASP:CB	3:D:137:PRO:HD3	2.20	0.44
3:D:560:GLN:OE1	5:F:218:GLN:HG3	2.18	0.44
3:D:814:ALA:HB2	9:D:1889:HOH:O	2.18	0.44
3:D:1310:ARG:HE	3:D:1327:ARG:HB3	1.80	0.44
4:E:49:GLN:C	4:E:51:LEU:N	2.73	0.44
1:L:152:PRO:HG2	3:N:857:ILE:HD12	2.00	0.44
2:M:12:VAL:HG13	2:M:13:ILE:HG23	1.98	0.44
2:M:36:PRO:HG3	2:M:71:TYR:CE2	2.53	0.44
2:M:78:PHE:HB3	2:M:79:PRO:HD2	1.99	0.44
2:M:729:LEU:HD13	3:N:675:ARG:NH2	2.33	0.44
2:M:850:ALA:HA	3:N:632:VAL:CG1	2.47	0.44
2:M:926:PHE:CE2	2:M:960:GLU:HG3	2.52	0.44
2:M:1021:LEU:HD13	5:P:331:ASP:O	2.18	0.44
3:N:596:SER:C	3:N:598:ARG:N	2.76	0.44
3:N:666:ILE:H	3:N:666:ILE:HG13	1.61	0.44
3:N:806:PHE:O	3:N:807:ALA:C	2.60	0.44
3:N:826:PRO:HD2	3:N:829:VAL:HG22	1.99	0.44
3:N:1159:ARG:CZ	3:N:1159:ARG:HB3	2.47	0.44
3:N:1326:THR:HG22	3:N:1327:ARG:N	2.33	0.44
5:P:318:GLU:HG2	9:P:448:HOH:O	2.16	0.44
1:B:10:VAL:HG12	1:B:12:THR:HG23	1.98	0.44
2:C:113:VAL:O	2:C:115:LEU:HD23	2.17	0.44
2:C:529:VAL:HG21	9:C:1134:HOH:O	2.18	0.44
2:C:598:GLU:HG2	9:C:1352:HOH:O	2.18	0.44
2:C:674:VAL:HB	2:C:869:VAL:CG1	2.47	0.44
2:C:759:THR:HB	2:C:785:VAL:HG21	1.99	0.44
2:C:863:ASP:OD1	2:C:865:THR:HG22	2.16	0.44
3:D:63:TYR:HB2	9:D:2023:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:85:VAL:HG11	3:D:89:ARG:CZ	2.48	0.44
3:D:614:PHE:CB	3:D:617:ASN:HB3	2.47	0.44
3:D:624:ASP:HB3	3:D:625:TYR:CD1	2.53	0.44
3:D:1376:MET:HA	9:D:2082:HOH:O	2.17	0.44
3:D:1380:GLU:HB2	3:D:1420:LEU:CD2	2.47	0.44
1:K:227:ASN:H	1:K:227:ASN:HD22	1.65	0.44
1:K:229:GLN:HE21	1:K:229:GLN:HB2	1.56	0.44
1:L:45:LEU:HD21	1:L:177:VAL:HG22	1.99	0.44
1:L:45:LEU:HD11	1:L:177:VAL:CG2	2.48	0.44
2:M:114:PHE:CD2	5:P:283:GLY:HA3	2.52	0.44
2:M:211:LEU:CD1	2:M:308:ARG:HA	2.47	0.44
2:M:810:ASP:H	2:M:811:PRO:HD3	1.82	0.44
2:M:862:PRO:HD3	2:M:973:VAL:O	2.18	0.44
2:M:968:LEU:CB	9:M:2164:HOH:O	2.58	0.44
2:M:1030:GLN:NE2	3:N:628:ARG:HB3	2.32	0.44
3:N:165:LYS:HE2	9:N:2305:HOH:O	2.17	0.44
3:N:420:VAL:HG13	9:N:2303:HOH:O	2.17	0.44
3:N:1182:GLU:HB3	9:N:2331:HOH:O	2.17	0.44
4:O:45:ARG:HH21	4:O:55:PHE:HB3	1.80	0.44
5:P:276:ARG:HA	9:P:451:HOH:O	2.17	0.44
1:A:88:ARG:O	1:A:88:ARG:HG3	2.16	0.44
1:A:127:LEU:HD11	1:A:129:ILE:CD1	2.47	0.44
1:B:23:PHE:HE2	1:B:199:ILE:HD12	1.81	0.44
1:B:27:PRO:HB3	1:B:192:LEU:HD22	1.99	0.44
2:C:139:GLN:HG2	2:C:140:ILE:N	2.33	0.44
2:C:260:LEU:C	2:C:260:LEU:HD12	2.43	0.44
2:C:278:GLU:HG3	2:C:283:ILE:HG23	2.00	0.44
2:C:443:THR:CG2	2:C:449:ILE:HG13	2.48	0.44
2:C:468:ARG:HB2	2:C:486:MET:C	2.42	0.44
2:C:474:VAL:HG13	2:C:529:VAL:O	2.17	0.44
2:C:1043:TYR:HE1	3:D:710:ARG:O	2.00	0.44
3:D:28:LYS:HA	3:D:29:PRO:HD3	1.69	0.44
3:D:880:ILE:O	3:D:883:ALA:HB3	2.17	0.44
5:F:351:SER:O	5:F:355:GLU:HB2	2.17	0.44
1:K:132:LEU:HD21	1:K:138:LEU:HB2	2.00	0.44
1:K:212:ASN:O	1:K:215:VAL:HG22	2.18	0.44
1:L:191:ASP:O	1:L:192:LEU:HG	2.18	0.44
2:M:227:PHE:HD2	2:M:237:ARG:CZ	2.30	0.44
2:M:247:PRO:HB2	9:M:2082:HOH:O	2.16	0.44
2:M:474:VAL:HA	2:M:478:VAL:O	2.17	0.44
3:N:204:LEU:HA	3:N:441:ARG:NH2	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:204:LEU:O	3:N:393:ILE:HG23	2.17	0.44
3:N:421:LEU:HD11	3:N:446:VAL:CG2	2.48	0.44
3:N:953:ASP:O	3:N:955:VAL:HG23	2.17	0.44
3:N:1002:LYS:HA	9:N:1776:HOH:O	2.17	0.44
3:N:1217:ILE:H	3:N:1217:ILE:HG13	1.68	0.44
3:N:1326:THR:HG22	3:N:1327:ARG:H	1.81	0.44
3:N:1426:LYS:HG2	9:N:1735:HOH:O	2.18	0.44
1:A:39:PRO:HG3	1:B:39:PRO:CG	2.44	0.44
1:A:229:GLN:HE21	1:A:229:GLN:HB2	1.57	0.44
1:B:59:GLU:HG3	1:B:139:ASN:HB3	2.00	0.44
2:C:48:PHE:CE1	2:C:348:LEU:HD11	2.53	0.44
2:C:217:LEU:HB2	2:C:311:PHE:CE1	2.53	0.44
2:C:564:MET:HE2	2:C:846:LYS:HE3	2.00	0.44
2:C:873:PRO:HB3	3:D:949:ILE:HG12	2.00	0.44
2:C:1000:MET:HE1	9:C:1188:HOH:O	2.17	0.44
3:D:629:SER:C	3:D:744:GLN:HG2	2.43	0.44
3:D:631:ILE:O	3:D:632:VAL:HG23	2.18	0.44
3:D:1155:VAL:CG1	3:D:1177:ALA:HB1	2.47	0.44
4:E:85:LEU:HD23	4:E:86:GLN:N	2.32	0.44
4:E:85:LEU:HD21	4:E:89:MET:HE2	1.99	0.44
4:E:88:GLU:HB3	9:E:137:HOH:O	2.18	0.44
5:F:240:THR:O	5:F:244:ARG:HG3	2.18	0.44
5:F:299:TRP:CE3	5:F:303:ARG:HD3	2.52	0.44
5:F:419:ARG:O	5:F:421:PHE:N	2.50	0.44
1:K:92:PRO:HB3	9:K:3732:HOH:O	2.17	0.44
1:L:158:ILE:HD11	1:L:165:ILE:C	2.42	0.44
2:M:118:ILE:HA	2:M:119:PRO:HD3	1.88	0.44
2:M:263:ASP:C	2:M:264:PRO:O	2.58	0.44
2:M:264:PRO:HA	9:M:1703:HOH:O	2.17	0.44
2:M:281:LEU:HD12	2:M:305:PRO:O	2.17	0.44
2:M:319:GLY:HA2	9:M:1910:HOH:O	2.18	0.44
2:M:405:ARG:NH1	2:M:566:THR:HG21	2.32	0.44
2:M:1010:THR:HG22	2:M:1011:GLY:N	2.32	0.44
2:M:1105:LYS:HB3	9:M:1845:HOH:O	2.16	0.44
3:N:122:GLU:O	3:N:126:VAL:HG23	2.18	0.44
3:N:817:GLU:CD	3:N:839:LEU:HD23	2.42	0.44
3:N:1167:SER:O	3:N:1171:VAL:HG23	2.18	0.44
3:N:1247:ALA:HB3	9:N:1888:HOH:O	2.16	0.44
3:N:1412:LYS:O	3:N:1414:PRO:HD3	2.18	0.44
5:P:141:VAL:HG22	9:P:496:HOH:O	2.18	0.44
2:C:92:ALA:HB2	2:C:120:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:265:ARG:HG2	2:C:267:TYR:N	2.31	0.44
2:C:267:TYR:H	2:C:267:TYR:HD2	1.64	0.44
2:C:278:GLU:HA	2:C:283:ILE:HA	2.00	0.44
2:C:398:THR:O	2:C:635:THR:HG21	2.17	0.44
2:C:588:VAL:HG21	2:C:664:GLY:O	2.18	0.44
3:D:52:PRO:CG	3:D:78:VAL:HG13	2.47	0.44
3:D:596:SER:C	3:D:598:ARG:N	2.76	0.44
3:D:786:ILE:O	3:D:787:LEU:C	2.60	0.44
3:D:1326:THR:HA	9:D:2026:HOH:O	2.17	0.44
1:K:8:ALA:HB2	9:K:1466:HOH:O	2.18	0.44
1:K:64:GLU:O	1:K:64:GLU:HG2	2.17	0.44
2:M:207:LEU:HD22	2:M:221:LEU:HD22	1.99	0.44
2:M:340:MET:SD	2:M:344:PHE:HB2	2.58	0.44
2:M:573:ARG:HB3	2:M:670:GLN:OE1	2.17	0.44
2:M:599:GLU:HB2	9:M:1699:HOH:O	2.18	0.44
2:M:732:ALA:O	2:M:735:ARG:HG3	2.18	0.44
2:M:751:PRO:CG	2:M:796:GLU:HG2	2.48	0.44
2:M:873:PRO:HB3	3:N:949:ILE:HG12	1.99	0.44
2:M:1034:GLU:O	2:M:1037:VAL:HG23	2.17	0.44
3:N:52:PRO:CB	3:N:80:VAL:HG13	2.47	0.44
3:N:172:PRO:O	3:N:174:GLY:N	2.51	0.44
3:N:421:LEU:HB3	3:N:444:VAL:HG11	2.00	0.44
3:N:643:GLY:CA	3:N:727:GLN:HB2	2.47	0.44
3:N:699:VAL:H	3:N:756:GLN:HE21	1.59	0.44
3:N:795:VAL:HG12	3:N:796:ARG:N	2.32	0.44
3:N:799:LYS:HE2	3:N:801:GLY:HA3	2.00	0.44
4:O:33:HIS:HB3	9:O:1494:HOH:O	2.18	0.44
5:P:385:GLU:O	5:P:397:ILE:HD13	2.18	0.44
1:A:33:GLY:O	1:A:195:LEU:HD22	2.18	0.44
1:A:67:THR:HG23	1:A:67:THR:O	2.17	0.44
1:A:106:PRO:HG3	1:A:133:GLU:O	2.17	0.44
1:B:158:ILE:HD11	1:B:166:PRO:N	2.33	0.44
2:C:146:VAL:N	9:C:1337:HOH:O	2.50	0.44
2:C:191:PHE:CZ	2:C:238:LEU:HD11	2.52	0.44
2:C:435:TYR:C	2:C:437:ARG:N	2.75	0.44
2:C:1118:LYS:O	2:C:1119:ARG:OXT	2.36	0.44
3:D:204:LEU:HD11	3:D:445:ARG:HH12	1.81	0.44
3:D:508:ARG:CG	3:D:509:PRO:HD2	2.36	0.44
3:D:798:GLU:HB2	3:D:828:LYS:CE	2.40	0.44
3:D:1074:SER:O	3:D:1077:ALA:HB3	2.18	0.44
3:D:1123:PHE:HB3	3:D:1132:LEU:HG	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:271:LEU:HG	5:F:295:MET:CE	2.37	0.44
5:F:392:VAL:HG11	5:F:396:ARG:HD2	2.00	0.44
1:L:80:LEU:HD23	3:N:867:ARG:HD2	1.99	0.44
2:M:64:LEU:HB2	2:M:359:MET:SD	2.57	0.44
2:M:176:VAL:HB	9:M:2210:HOH:O	2.18	0.44
2:M:207:LEU:O	2:M:211:LEU:HB3	2.18	0.44
2:M:324:ASP:CG	2:M:431:HIS:HE1	2.26	0.44
2:M:564:MET:SD	2:M:846:LYS:HE3	2.58	0.44
2:M:854:PRO:C	2:M:856:GLU:H	2.25	0.44
2:M:942:GLU:O	2:M:945:ARG:HB3	2.17	0.44
3:N:36:THR:O	3:N:38:LYS:N	2.51	0.44
3:N:44:LEU:O	3:N:50:PHE:CE1	2.70	0.44
3:N:528:VAL:HG12	3:N:529:GLN:N	2.33	0.44
3:N:701:LEU:C	3:N:702:LEU:HD12	2.43	0.44
3:N:774:SER:C	3:N:776:GLU:N	2.75	0.44
4:O:29:GLN:HE21	4:O:89:MET:HE3	1.83	0.44
4:O:49:GLN:C	4:O:51:LEU:N	2.74	0.44
5:P:205:ARG:CD	5:P:251:ILE:HG21	2.48	0.44
5:P:226:LYS:HE3	9:P:445:HOH:O	2.18	0.44
2:C:146:VAL:HG11	2:C:306:THR:HG22	1.99	0.44
2:C:264:PRO:HB3	2:C:289:THR:CB	2.47	0.44
2:C:545:ASN:O	2:C:581:THR:HG21	2.17	0.44
2:C:687:ALA:C	2:C:688:ILE:HD12	2.43	0.44
2:C:1052:MET:SD	3:D:623:VAL:HG21	2.57	0.44
3:D:162:ARG:HA	3:D:449:SER:OG	2.17	0.44
3:D:554:LEU:HD23	3:D:570:GLU:HG2	2.00	0.44
3:D:569:ASN:HD21	5:F:210:LEU:HD22	1.82	0.44
3:D:937:TYR:HD2	3:D:941:PHE:HE1	1.66	0.44
3:D:1008:PHE:HB3	9:D:1941:HOH:O	2.17	0.44
3:D:1211:MET:C	9:D:1554:HOH:O	2.61	0.44
3:D:1276:GLU:OE2	3:D:1303:TYR:HE2	2.00	0.44
5:F:151:LEU:HD23	9:F:489:HOH:O	2.17	0.44
5:F:306:GLU:HG3	9:F:582:HOH:O	2.18	0.44
1:L:101:LEU:CD1	9:L:1850:HOH:O	2.64	0.44
2:M:7:GLY:O	2:M:907:ASP:OD1	2.36	0.44
2:M:64:LEU:CD1	2:M:100:LEU:HD13	2.48	0.44
2:M:198:ARG:NE	2:M:228:ALA:HA	2.33	0.44
2:M:207:LEU:HD13	2:M:221:LEU:HD13	2.00	0.44
2:M:564:MET:SD	2:M:846:LYS:HG3	2.58	0.44
3:N:155:ASP:HA	3:N:158:TYR:HB3	2.00	0.44
3:N:195:VAL:HG12	3:N:196:VAL:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:987:GLU:HA	9:N:2147:HOH:O	2.18	0.44
3:N:996:TRP:HA	3:N:999:THR:CG2	2.46	0.44
4:O:57:ASP:N	4:O:58:PRO:HD3	2.32	0.44
5:P:140:ARG:HG3	5:P:141:VAL:N	2.33	0.44
5:P:396:ARG:HG2	9:P:513:HOH:O	2.18	0.44
1:A:42:ARG:HH12	1:B:34:VAL:CG1	2.28	0.43
2:C:73:LEU:CD2	2:C:94:LEU:HB2	2.47	0.43
2:C:257:VAL:HG12	2:C:263:ASP:OD1	2.17	0.43
2:C:516:ARG:N	9:C:1381:HOH:O	2.50	0.43
2:C:813:VAL:HB	9:C:1471:HOH:O	2.18	0.43
2:C:929:ARG:HH22	2:C:940:GLU:CD	2.26	0.43
2:C:979:THR:HG23	2:C:981:GLU:HB2	2.00	0.43
3:D:158:TYR:CE1	3:D:454:ALA:HB3	2.53	0.43
3:D:481:MET:CE	3:D:1389:LEU:HG	2.48	0.43
3:D:951:ILE:HD12	3:D:1062:ARG:HG3	1.99	0.43
3:D:1251:ASP:O	3:D:1270:ALA:HB3	2.18	0.43
3:D:1331:ASP:OD2	3:D:1331:ASP:C	2.60	0.43
3:D:1393:GLN:HG3	3:D:1398:TRP:HZ2	1.83	0.43
4:E:47:LYS:C	4:E:54:LEU:HB2	2.43	0.43
5:F:115:LYS:HD2	5:F:173:TYR:HE2	1.82	0.43
5:F:185:GLN:O	5:F:189:GLU:HG3	2.17	0.43
5:F:205:ARG:HD3	5:F:251:ILE:HG21	2.00	0.43
1:K:224:TYR:CD1	1:L:9:PRO:HD2	2.53	0.43
1:L:7:LYS:HE3	9:L:1689:HOH:O	2.18	0.43
1:L:125:PRO:HD2	9:L:3251:HOH:O	2.18	0.43
2:M:757:GLY:HA2	2:M:789:SER:CB	2.35	0.43
3:N:15:PRO:HG3	9:N:2008:HOH:O	2.17	0.43
3:N:37:LEU:HD13	3:N:535:PHE:HZ	1.83	0.43
3:N:93:ILE:CD1	3:N:548:ILE:HD11	2.48	0.43
3:N:615:ARG:NH2	3:N:1089:ALA:HB2	2.23	0.43
3:N:800:LYS:CE	3:N:804:LEU:HD13	2.48	0.43
3:N:1025:GLN:HE21	3:N:1025:GLN:HB3	1.62	0.43
4:O:67:GLU:HG3	4:O:67:GLU:H	1.68	0.43
5:P:82:ARG:O	5:P:86:HIS:HB2	2.18	0.43
5:P:101:GLU:O	5:P:105:LYS:HG3	2.17	0.43
5:P:403:LYS:HB2	9:P:540:HOH:O	2.17	0.43
1:A:218:LEU:HD23	1:B:222:LEU:HD21	1.99	0.43
2:C:20:GLU:HB2	9:C:1289:HOH:O	2.18	0.43
2:C:32:ALA:HB2	2:C:73:LEU:CD1	2.47	0.43
2:C:191:PHE:CE2	2:C:238:LEU:HD11	2.54	0.43
2:C:292:ARG:HD2	2:C:299:LYS:CG	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:454:SER:HB3	9:C:1409:HOH:O	2.18	0.43
2:C:501:THR:OG1	2:C:532:MET:HE1	2.19	0.43
2:C:564:MET:CE	2:C:846:LYS:HE3	2.49	0.43
2:C:599:GLU:CG	2:C:600:ASP:H	2.29	0.43
2:C:720:GLU:HA	9:C:1430:HOH:O	2.18	0.43
2:C:958:THR:HG23	2:C:961:GLU:HB2	2.00	0.43
2:C:1088:LEU:HG	2:C:1092:LEU:HD12	2.00	0.43
3:D:31:THR:HG22	3:D:32:ILE:HB	2.00	0.43
3:D:143:ASN:HD21	3:D:145:VAL:HG12	1.81	0.43
3:D:1147:ARG:HD2	3:D:1188:VAL:CG2	2.48	0.43
3:D:1220:ALA:O	3:D:1224:VAL:HG23	2.18	0.43
5:F:152:ASP:HB3	9:F:665:HOH:O	2.17	0.43
1:K:61:VAL:HG11	1:K:75:VAL:HG21	1.99	0.43
1:K:91:ASN:N	9:K:1900:HOH:O	2.51	0.43
1:L:33:GLY:O	1:L:195:LEU:HD22	2.19	0.43
2:M:11:GLU:HB3	9:M:2054:HOH:O	2.18	0.43
2:M:18:LEU:C	2:M:20:GLU:H	2.26	0.43
2:M:133:ASP:N	2:M:133:ASP:OD2	2.51	0.43
2:M:610:ARG:NE	9:M:1664:HOH:O	2.49	0.43
3:N:131:LYS:HE3	3:N:568:ARG:HB3	1.99	0.43
3:N:761:ILE:CD1	4:O:20:THR:HA	2.49	0.43
3:N:938:GLY:O	3:N:942:SER:HB3	2.18	0.43
3:N:1068:LEU:O	3:N:1069:GLU:C	2.59	0.43
4:O:57:ASP:H	4:O:58:PRO:HD3	1.83	0.43
5:P:271:LEU:HD23	5:P:291:ILE:HD11	2.00	0.43
1:A:158:ILE:HD13	1:A:158:ILE:HA	1.88	0.43
2:C:208:ALA:HA	2:C:218:VAL:CG2	2.48	0.43
2:C:230:ARG:HG2	9:C:1514:HOH:O	2.17	0.43
2:C:345:ARG:HD2	9:C:1463:HOH:O	2.18	0.43
2:C:561:GLY:HA3	2:C:842:ARG:O	2.19	0.43
2:C:569:VAL:HG12	2:C:996:LYS:O	2.18	0.43
2:C:601:GLY:HA3	2:C:615:TYR:HA	2.01	0.43
2:C:670:GLN:HE22	2:C:699:PHE:HA	1.81	0.43
2:C:911:GLU:HG2	2:C:915:LYS:NZ	2.33	0.43
2:C:1033:GLY:H	2:C:1036:GLU:HG3	1.83	0.43
3:D:610:LYS:HG2	7:D:1527:MXP:H15A	1.99	0.43
3:D:678:GLU:HB2	9:D:1759:HOH:O	2.18	0.43
3:D:704:ARG:HG2	3:D:705:ALA:N	2.30	0.43
3:D:844:ALA:HB3	3:D:848:GLU:OE2	2.19	0.43
3:D:848:GLU:N	9:D:1677:HOH:O	2.51	0.43
3:D:888:GLU:HB3	9:D:1740:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1047:LYS:HB3	3:D:1048:PRO:HD2	2.00	0.43
3:D:1095:THR:HG22	9:D:1551:HOH:O	2.16	0.43
3:D:1110:ALA:O	3:D:1112:CYS:N	2.50	0.43
5:F:93:LEU:HD23	5:F:93:LEU:HA	1.81	0.43
1:K:102:LYS:HA	1:K:138:LEU:O	2.18	0.43
1:K:138:LEU:HA	9:K:2460:HOH:O	2.19	0.43
9:K:1685:HOH:O	1:L:219:ARG:HD2	2.18	0.43
2:M:208:ALA:CA	2:M:221:LEU:HD21	2.47	0.43
2:M:267:TYR:O	2:M:268:ASP:C	2.61	0.43
2:M:278:GLU:HG3	2:M:283:ILE:HA	1.99	0.43
2:M:422:ARG:HG2	9:M:1926:HOH:O	2.18	0.43
2:M:537:LYS:HD3	2:M:905:ILE:HD11	2.01	0.43
2:M:1063:ARG:O	2:M:1066:ALA:HB3	2.18	0.43
3:N:527:MET:HE3	3:N:535:PHE:HD2	1.83	0.43
3:N:661:MET:HE2	3:N:677:LEU:HD11	2.00	0.43
3:N:961:LYS:HE3	9:N:2153:HOH:O	2.17	0.43
3:N:1066:THR:O	3:N:1070:TYR:HB2	2.18	0.43
9:N:2374:HOH:O	4:O:51:LEU:HD23	2.18	0.43
1:A:186:LEU:HD23	1:A:186:LEU:C	2.43	0.43
1:A:227:ASN:HD22	1:A:227:ASN:N	2.15	0.43
2:C:22:GLN:HE22	2:C:135:VAL:CG1	2.30	0.43
2:C:49:ARG:HG2	2:C:266:ARG:HH12	1.83	0.43
2:C:263:ASP:CB	2:C:264:PRO:HD3	2.48	0.43
2:C:313:LEU:HD13	2:C:321:GLU:HB2	1.99	0.43
2:C:413:LEU:HD12	2:C:413:LEU:N	2.24	0.43
2:C:517:ARG:HB2	9:C:1698:HOH:O	2.17	0.43
2:C:610:ARG:NE	9:C:1120:HOH:O	2.52	0.43
2:C:690:ILE:HD12	2:C:833:LEU:HD21	2.01	0.43
2:C:896:PHE:CE2	2:C:925:TYR:HB2	2.53	0.43
2:C:1009:SER:HB2	3:D:651:GLU:HG2	2.01	0.43
3:D:84:ILE:HG13	3:D:85:VAL:N	2.34	0.43
3:D:86:ARG:HB3	3:D:523:ASP:OD2	2.18	0.43
3:D:420:VAL:HA	9:D:2307:HOH:O	2.19	0.43
3:D:584:ASN:HD21	3:D:590:PRO:HD2	1.81	0.43
3:D:649:ALA:HB3	3:D:691:LEU:HD21	1.98	0.43
3:D:688:TRP:HA	3:D:688:TRP:CE3	2.53	0.43
3:D:1281:VAL:HG21	3:D:1313:VAL:HG21	1.99	0.43
3:D:1304:LYS:HB3	9:D:1723:HOH:O	2.18	0.43
3:D:1354:LYS:HE2	9:D:2358:HOH:O	2.19	0.43
3:D:1395:LEU:HD23	3:D:1396:GLU:N	2.33	0.43
3:D:1426:LYS:HD2	9:D:2086:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1451:ALA:O	3:D:1452:ILE:C	2.62	0.43
5:F:418:LEU:HD12	5:F:418:LEU:N	2.33	0.43
1:L:55:SER:HB2	1:L:158:ILE:HD13	1.96	0.43
1:L:115:LEU:HD12	1:L:115:LEU:O	2.18	0.43
2:M:65:VAL:HB	2:M:101:ILE:HB	2.00	0.43
2:M:199:VAL:HG13	2:M:235:LEU:CG	2.42	0.43
2:M:260:LEU:C	2:M:260:LEU:HD12	2.43	0.43
2:M:575:GLN:C	2:M:667:ALA:HB1	2.43	0.43
2:M:876:VAL:HB	2:M:877:PRO:HD3	2.01	0.43
2:M:881:ASN:N	2:M:881:ASN:ND2	2.66	0.43
2:M:964:LYS:O	2:M:968:LEU:HG	2.18	0.43
2:M:1013:TYR:OH	3:N:624:ASP:OD2	2.33	0.43
3:N:9:ARG:HA	3:N:1434:TRP:CH2	2.52	0.43
3:N:539:ASP:CG	3:N:598:ARG:HH22	2.26	0.43
3:N:637:LEU:HD11	3:N:641:GLN:HB2	2.00	0.43
3:N:1004:THR:HG21	9:N:2039:HOH:O	2.17	0.43
3:N:1031:ASN:O	3:N:1035:ILE:HG12	2.18	0.43
3:N:1147:ARG:HB3	3:N:1188:VAL:HG23	1.99	0.43
5:P:137:GLY:HA2	9:P:480:HOH:O	2.19	0.43
5:P:163:LEU:HD22	5:P:174:LEU:HB2	2.01	0.43
1:A:63:HIS:HB3	2:C:746:GLY:HA2	1.99	0.43
1:A:131:THR:C	1:A:132:LEU:HD12	2.44	0.43
1:B:72:LYS:HB3	1:B:131:THR:OG1	2.19	0.43
2:C:110:GLU:CD	2:C:369:PRO:HG3	2.44	0.43
2:C:139:GLN:N	9:C:1322:HOH:O	2.52	0.43
2:C:207:LEU:HD13	2:C:221:LEU:CD1	2.48	0.43
2:C:679:PHE:CE1	2:C:859:PRO:HD3	2.53	0.43
2:C:798:GLY:H	2:C:827:VAL:HG11	1.82	0.43
2:C:987:ILE:HG12	3:D:948:THR:CG2	2.48	0.43
3:D:111:LYS:NZ	3:D:1449:GLU:HG2	2.34	0.43
3:D:126:VAL:O	3:D:132:TYR:CD1	2.70	0.43
3:D:128:TYR:HB3	3:D:129:PHE:HD1	1.84	0.43
3:D:843:PHE:CE1	3:D:864:VAL:HG11	2.47	0.43
3:D:871:LYS:O	3:D:873:LEU:HG	2.18	0.43
3:D:875:THR:HG22	3:D:879:ARG:HB2	1.99	0.43
3:D:1186:VAL:HA	3:D:1187:PRO:HD3	1.90	0.43
3:D:1195:GLN:CG	3:D:1196:THR:N	2.81	0.43
3:D:1197:ARG:HG3	3:D:1198:TYR:H	1.82	0.43
3:D:1221:VAL:O	3:D:1222:GLY:C	2.61	0.43
5:F:209:PHE:O	5:F:213:ILE:HG13	2.18	0.43
1:K:123:MET:HB3	9:K:2581:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:182:VAL:HB	2:M:193:LEU:HD13	2.00	0.43
2:M:260:LEU:HG	2:M:261:ILE:HG13	2.00	0.43
2:M:437:ARG:HH22	2:M:491:GLU:HB2	1.82	0.43
2:M:1002:GLU:O	2:M:1003:ASP:C	2.61	0.43
3:N:45:PHE:HB3	3:N:86:ARG:NH2	2.33	0.43
3:N:206:ARG:HG2	9:N:2269:HOH:O	2.18	0.43
3:N:561:GLY:HA3	5:P:184:ARG:CZ	2.48	0.43
3:N:593:ASN:O	3:N:594:PRO:C	2.62	0.43
3:N:715:ALA:O	3:N:764:LEU:HD12	2.17	0.43
3:N:853:VAL:HG22	3:N:858:VAL:HG23	2.00	0.43
3:N:879:ARG:HD3	3:N:902:LEU:O	2.17	0.43
3:N:1171:VAL:O	3:N:1171:VAL:HG12	2.18	0.43
3:N:1451:ALA:O	3:N:1452:ILE:C	2.62	0.43
5:P:375:LEU:HB3	9:P:476:HOH:O	2.18	0.43
1:A:67:THR:HG21	2:C:609:ASN:HD21	1.82	0.43
1:B:52:ALA:HB2	1:B:170:VAL:C	2.42	0.43
2:C:64:LEU:HD11	2:C:100:LEU:HD13	2.00	0.43
2:C:78:PHE:HB2	2:C:88:LEU:HD21	2.01	0.43
2:C:232:GLU:O	2:C:235:LEU:HB2	2.18	0.43
2:C:263:ASP:C	2:C:264:PRO:O	2.59	0.43
2:C:280:LYS:HB3	9:C:1547:HOH:O	2.18	0.43
2:C:396:ASP:O	2:C:402:SER:HB3	2.18	0.43
2:C:572:ILE:CG2	2:C:703:ILE:HD13	2.48	0.43
3:D:192:ALA:HB2	3:D:393:ILE:CD1	2.48	0.43
3:D:400:VAL:HG21	9:D:2433:HOH:O	2.19	0.43
3:D:417:PRO:HD2	3:D:432:TYR:CE1	2.54	0.43
3:D:614:PHE:O	3:D:615:ARG:O	2.36	0.43
3:D:1112:CYS:CB	3:D:1195:GLN:HG2	2.42	0.43
3:D:1139:ASP:O	3:D:1142:ALA:HB3	2.18	0.43
5:F:196:VAL:HG13	5:F:213:ILE:CD1	2.48	0.43
5:F:226:LYS:HB2	5:F:238:TYR:OH	2.19	0.43
5:F:271:LEU:HD23	5:F:291:ILE:HD11	2.00	0.43
5:F:338:LEU:HA	5:F:339:PRO:HD3	1.85	0.43
5:F:412:GLU:OE1	5:F:418:LEU:HD13	2.19	0.43
5:F:415:THR:HG22	5:F:417:LYS:HG3	2.00	0.43
1:L:44:LEU:CD2	1:L:199:ILE:HD13	2.48	0.43
1:L:107:LYS:HG3	1:L:108:GLU:N	2.34	0.43
2:M:244:PRO:CD	2:M:245:GLY:H	2.31	0.43
2:M:288:ARG:HB3	9:M:1852:HOH:O	2.17	0.43
2:M:816:LYS:O	2:M:819:VAL:HB	2.18	0.43
2:M:897:LEU:HD23	2:M:899:GLN:NE2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:969:GLN:HE21	2:M:969:GLN:HB3	1.71	0.43
3:N:403:PHE:CZ	3:N:407:VAL:HG23	2.53	0.43
3:N:611:GLN:NE2	7:N:1527:MXP:C16	2.80	0.43
3:N:1068:LEU:C	3:N:1070:TYR:N	2.75	0.43
3:N:1285:GLU:O	3:N:1285:GLU:HG2	2.19	0.43
3:N:1393:GLN:HB2	3:N:1398:TRP:CE2	2.53	0.43
5:P:215:GLU:OE2	5:P:254:GLN:NE2	2.49	0.43
2:C:511:GLU:HG3	9:C:1690:HOH:O	2.17	0.43
2:C:762:LYS:HB2	2:C:786:LYS:HD2	2.01	0.43
3:D:142:LEU:C	3:D:142:LEU:HD12	2.44	0.43
3:D:724:GLN:N	9:D:1680:HOH:O	2.46	0.43
3:D:799:LYS:O	3:D:829:VAL:HG13	2.19	0.43
3:D:835:SER:C	3:D:837:GLY:N	2.76	0.43
3:D:1036:ARG:HH21	3:D:1042:ARG:HA	1.84	0.43
3:D:1065:LEU:CD1	3:D:1069:GLU:HB2	2.48	0.43
3:D:1115:THR:HG21	3:D:1151:ARG:HH21	1.83	0.43
3:D:1119:SER:HA	3:D:1186:VAL:O	2.19	0.43
3:D:1209:LEU:O	3:D:1210:SER:C	2.61	0.43
4:E:39:VAL:HG21	4:E:72:ARG:HD2	2.00	0.43
5:F:225:GLU:HG3	5:F:226:LYS:N	2.32	0.43
5:F:348:SER:OG	5:F:349:LEU:N	2.51	0.43
1:L:57:TYR:HB3	1:L:141:GLU:HG3	2.01	0.43
1:L:86:VAL:HG12	1:L:124:ASN:HB2	2.00	0.43
2:M:17:PRO:O	2:M:20:GLU:HB2	2.18	0.43
2:M:232:GLU:O	2:M:235:LEU:HB2	2.18	0.43
2:M:495:THR:HB	2:M:530:GLU:HG3	2.00	0.43
2:M:532:MET:HG3	2:M:533:ASP:N	2.33	0.43
2:M:551:GLU:HB3	2:M:906:PHE:HD2	1.84	0.43
2:M:601:GLY:O	2:M:649:VAL:HG22	2.18	0.43
2:M:1044:GLY:HA3	4:O:17:TYR:CE1	2.53	0.43
3:N:44:LEU:O	3:N:525:ARG:NH2	2.51	0.43
3:N:47:GLU:HG2	3:N:53:ILE:HG22	2.00	0.43
3:N:133:ILE:HG23	3:N:456:MET:SD	2.58	0.43
3:N:448:GLU:HG3	9:N:1563:HOH:O	2.17	0.43
3:N:1035:ILE:CA	3:N:1038:LEU:HD12	2.49	0.43
3:N:1281:VAL:HG21	3:N:1313:VAL:HG22	2.00	0.43
5:P:94:LEU:HB3	9:P:503:HOH:O	2.18	0.43
1:A:25:LEU:HD23	1:A:25:LEU:C	2.43	0.43
1:B:4:SER:HA	1:B:7:LYS:HG2	2.00	0.43
2:C:174:LEU:HB2	2:C:310:LEU:HD22	2.01	0.43
2:C:175:GLU:HB3	2:C:183:SER:OG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:419:THR:N	9:C:1152:HOH:O	2.50	0.43
2:C:937:ASP:OD2	2:C:939:ARG:HD2	2.18	0.43
2:C:1005:MET:HE3	3:D:648:MET:HE3	1.99	0.43
3:D:644:LEU:HD12	3:D:645:PRO:CD	2.48	0.43
3:D:806:PHE:CD1	3:D:813:LEU:HB3	2.53	0.43
3:D:1082:ALA:O	3:D:1086:LEU:HG	2.18	0.43
3:D:1107:VAL:HA	3:D:1200:VAL:O	2.19	0.43
3:D:1154:GLU:HG2	9:D:2105:HOH:O	2.19	0.43
3:D:1166:LEU:HD23	3:D:1166:LEU:H	1.84	0.43
3:D:1495:ILE:HA	4:E:88:GLU:OE2	2.19	0.43
4:E:19:LEU:O	4:E:23:VAL:HG23	2.19	0.43
4:E:54:LEU:HG	4:E:58:PRO:CB	2.49	0.43
1:K:161:ARG:HG2	9:K:1051:HOH:O	2.18	0.43
1:K:176:ARG:HA	9:K:2558:HOH:O	2.18	0.43
1:L:42:ARG:HG2	1:L:42:ARG:HH11	1.83	0.43
1:L:176:ARG:HD3	3:N:884:ARG:CZ	2.48	0.43
2:M:32:ALA:HB2	2:M:73:LEU:HD11	2.00	0.43
2:M:764:GLU:O	2:M:765:SER:C	2.61	0.43
2:M:841:ASN:C	2:M:841:ASN:HD22	2.27	0.43
2:M:1033:GLY:HA3	9:N:1659:HOH:O	2.18	0.43
3:N:489:ARG:HG3	3:N:1388:ARG:NH2	2.27	0.43
3:N:554:LEU:HD23	3:N:570:GLU:HG2	2.01	0.43
3:N:1031:ASN:O	3:N:1034:GLN:HB2	2.19	0.43
3:N:1352:ILE:CG2	3:N:1368:ILE:HD13	2.49	0.43
5:P:356:LYS:O	5:P:360:LYS:HG3	2.19	0.43
1:B:44:LEU:HD11	1:B:199:ILE:HD11	2.00	0.43
2:C:118:ILE:HG22	2:C:382:ILE:HD13	2.00	0.43
2:C:144:PRO:CG	2:C:165:LEU:HB3	2.48	0.43
2:C:455:LEU:HD12	2:C:456:ALA:N	2.34	0.43
2:C:458:TYR:HB2	2:C:538:GLN:HB2	2.01	0.43
2:C:487:THR:HG22	2:C:488:ALA:N	2.34	0.43
2:C:832:LYS:HG2	9:C:1178:HOH:O	2.17	0.43
2:C:1034:GLU:O	2:C:1037:VAL:N	2.52	0.43
2:C:1070:ILE:HG23	3:D:656:PHE:CE2	2.53	0.43
3:D:116:LEU:CD1	3:D:465:LEU:HG	2.49	0.43
3:D:185:VAL:HG22	3:D:203:ALA:HB2	2.00	0.43
3:D:711:LEU:C	3:D:713:ILE:N	2.75	0.43
3:D:829:VAL:O	3:D:831:GLY:N	2.52	0.43
3:D:1041:LEU:HD12	3:D:1058:ARG:CA	2.48	0.43
3:D:1147:ARG:NH1	3:D:1190:SER:HB2	2.34	0.43
7:D:1527:MXP:H15	7:D:1527:MXP:H9	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:361:LEU:HG	5:F:408:LEU:HD21	2.01	0.43
1:K:161:ARG:HB2	1:K:161:ARG:HH11	1.84	0.43
1:L:81:ASN:ND2	1:L:128:HIS:O	2.52	0.43
1:L:186:LEU:O	1:L:187:GLY:C	2.62	0.43
2:M:209:ARG:HB2	9:M:2284:HOH:O	2.19	0.43
2:M:309:TYR:HA	2:M:312:ALA:HB3	2.00	0.43
2:M:342:ASP:O	2:M:346:VAL:HG23	2.18	0.43
2:M:350:ARG:HG2	9:M:1970:HOH:O	2.18	0.43
2:M:432:ARG:HD2	9:M:1743:HOH:O	2.19	0.43
2:M:457:ALA:HB3	2:M:538:GLN:HA	2.00	0.43
2:M:520:GLU:HA	2:M:521:PRO:HD3	1.84	0.43
2:M:540:PHE:CE1	2:M:906:PHE:HE1	2.36	0.43
2:M:620:LEU:HD12	2:M:620:LEU:O	2.19	0.43
2:M:640:ARG:HA	2:M:641:PRO:HD3	1.93	0.43
2:M:836:GLY:HA2	3:N:725:SER:OG	2.19	0.43
2:M:837:ASP:OD1	2:M:999:HIS:NE2	2.51	0.43
3:N:34:TYR:CE1	5:P:264:MET:HE2	2.53	0.43
3:N:126:VAL:HG11	3:N:152:LEU:CD1	2.49	0.43
3:N:191:LEU:HD23	3:N:191:LEU:HA	1.75	0.43
3:N:565:ILE:CD1	5:P:84:TYR:HB3	2.49	0.43
3:N:1243:THR:CB	3:N:1253:THR:HB	2.49	0.43
3:N:1467:ILE:HG13	3:N:1467:ILE:H	1.58	0.43
4:O:41:GLU:HB2	4:O:45:ARG:NH1	2.34	0.43
1:A:95:GLN:HA	9:A:395:HOH:O	2.17	0.43
1:A:220:GLU:HG2	9:A:339:HOH:O	2.18	0.43
2:C:144:PRO:HA	2:C:163:ILE:HG13	2.01	0.43
2:C:267:TYR:N	2:C:267:TYR:HD2	2.16	0.43
2:C:313:LEU:HD13	2:C:321:GLU:O	2.19	0.43
2:C:317:VAL:O	2:C:317:VAL:HG12	2.19	0.43
2:C:464:LEU:HD12	2:C:465:GLY:H	1.83	0.43
3:D:32:ILE:HG22	5:F:258:ILE:CD1	2.47	0.43
3:D:145:VAL:HG22	3:D:146:PRO:HD2	2.01	0.43
3:D:478:LEU:HD21	3:D:500:ARG:HH22	1.83	0.43
3:D:522:PRO:N	9:D:1713:HOH:O	2.51	0.43
3:D:809:PRO:O	3:D:812:ALA:HB3	2.19	0.43
3:D:1045:MET:HG3	3:D:1073:SER:CA	2.46	0.43
3:D:1292:VAL:HB	9:D:2010:HOH:O	2.19	0.43
3:D:1491:THR:HG22	3:D:1495:ILE:HD13	2.01	0.43
5:F:172:ARG:HG3	9:F:453:HOH:O	2.19	0.43
5:F:201:LYS:HE2	9:F:724:HOH:O	2.18	0.43
1:K:78:ILE:HG13	1:K:78:ILE:H	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:106:PRO:HG3	1:K:133:GLU:O	2.19	0.43
1:K:158:ILE:O	1:K:159:LYS:HG3	2.19	0.43
2:M:82:GLU:HG2	2:M:86:LYS:HD2	2.00	0.43
2:M:193:LEU:HD21	9:M:1951:HOH:O	2.18	0.43
2:M:405:ARG:HH11	2:M:566:THR:HG21	1.84	0.43
2:M:905:ILE:HD11	9:M:1895:HOH:O	2.19	0.43
3:N:519:VAL:HG13	3:N:544:TYR:CE1	2.54	0.43
3:N:1383:ASP:HB2	3:N:1416:ALA:CB	2.37	0.43
4:O:91:ARG:CZ	9:O:1090:HOH:O	2.67	0.43
1:B:60:ASP:N	1:B:137:ARG:NH2	2.65	0.42
1:B:208:LEU:HD12	1:B:212:ASN:OD1	2.19	0.42
2:C:203:ASP:OD1	2:C:206:THR:HG22	2.19	0.42
2:C:212:GLY:O	2:C:215:GLY:O	2.37	0.42
2:C:271:GLU:HG2	2:C:275:TYR:HE1	1.84	0.42
2:C:355:VAL:CG2	2:C:372:LEU:HG	2.49	0.42
2:C:408:ARG:NH2	2:C:542:VAL:HG22	2.33	0.42
2:C:431:HIS:HD2	2:C:433:THR:H	1.61	0.42
2:C:585:GLU:HB2	9:C:1331:HOH:O	2.18	0.42
2:C:1085:PHE:CD2	3:D:1468:LEU:HA	2.54	0.42
2:C:1091:GLU:O	2:C:1094:ALA:HB3	2.19	0.42
3:D:732:VAL:HG12	9:D:1673:HOH:O	2.19	0.42
3:D:1109:GLU:HG2	3:D:1201:CYS:CA	2.47	0.42
3:D:1155:VAL:HG11	3:D:1177:ALA:CB	2.49	0.42
3:D:1242:HIS:HE1	3:D:1266:ARG:HB3	1.84	0.42
1:K:128:HIS:CE1	1:K:131:THR:HG23	2.54	0.42
1:K:206:THR:HG22	1:K:209:GLU:CB	2.48	0.42
1:L:13:VAL:HG13	1:L:23:PHE:CD1	2.54	0.42
1:L:88:ARG:HB2	1:L:123:MET:HE2	2.02	0.42
2:M:16:PRO:HB3	2:M:460:ARG:NH1	2.34	0.42
2:M:98:LEU:HB2	9:M:1972:HOH:O	2.17	0.42
2:M:622:GLU:O	2:M:624:PRO:HD3	2.18	0.42
2:M:1013:TYR:O	5:P:334:PRO:HA	2.19	0.42
3:N:18:ILE:HG23	3:N:518:PRO:CG	2.38	0.42
3:N:393:ILE:HG13	9:N:1934:HOH:O	2.19	0.42
3:N:573:MET:CE	5:P:210:LEU:HB3	2.48	0.42
3:N:786:ILE:O	3:N:787:LEU:C	2.62	0.42
3:N:1023:MET:HG2	3:N:1023:MET:H	1.46	0.42
3:N:1114:THR:HG22	3:N:1195:GLN:HB3	1.99	0.42
3:N:1124:GLN:HA	3:N:1125:PRO:HD3	1.72	0.42
3:N:1221:VAL:O	3:N:1222:GLY:C	2.62	0.42
3:N:1481:VAL:O	3:N:1482:ARG:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:41:GLU:CA	4:O:45:ARG:HD3	2.40	0.42
1:A:67:THR:OG1	2:C:609:ASN:ND2	2.52	0.42
1:B:51:THR:HA	1:B:145:ASP:O	2.20	0.42
1:B:91:ASN:O	1:B:94:LEU:HD12	2.18	0.42
2:C:311:PHE:HB3	9:C:1209:HOH:O	2.18	0.42
2:C:1048:THR:O	2:C:1052:MET:HG2	2.19	0.42
2:C:1103:ASP:HB2	9:C:1226:HOH:O	2.19	0.42
3:D:12:LEU:HD11	3:D:512:MET:HG2	2.01	0.42
3:D:560:GLN:HG2	5:F:221:ILE:HG21	2.01	0.42
3:D:602:SER:O	3:D:603:LEU:C	2.62	0.42
3:D:660:LYS:HE2	9:D:1780:HOH:O	2.19	0.42
3:D:795:VAL:CG1	3:D:863:VAL:HG13	2.45	0.42
3:D:853:VAL:HG22	3:D:858:VAL:HG23	2.01	0.42
3:D:996:TRP:O	3:D:999:THR:HG22	2.19	0.42
3:D:1026:SER:C	3:D:1028:ALA:N	2.77	0.42
3:D:1129:THR:HG23	3:D:1130:ARG:H	1.83	0.42
2:M:52:PHE:HB3	2:M:53:PRO:HD3	2.00	0.42
2:M:443:THR:CG2	2:M:450:GLY:H	2.33	0.42
2:M:722:ILE:HG13	2:M:757:GLY:O	2.19	0.42
2:M:724:ARG:HD2	2:M:740:GLU:HG2	2.02	0.42
2:M:943:VAL:HG11	2:M:973:VAL:HG13	2.01	0.42
2:M:952:LEU:CD1	2:M:969:GLN:HE22	2.23	0.42
3:N:168:THR:HA	3:N:394:LEU:HA	2.02	0.42
3:N:455:ARG:HH11	3:N:463:GLN:HG3	1.84	0.42
3:N:537:THR:C	5:P:317:LEU:HB2	2.45	0.42
3:N:633:VAL:HG13	3:N:633:VAL:O	2.18	0.42
3:N:1121:PRO:C	3:N:1122:LEU:HD12	2.44	0.42
3:N:1274:ILE:HD12	3:N:1274:ILE:H	1.82	0.42
3:N:1394:VAL:HB	3:N:1397:LYS:HD2	2.02	0.42
4:O:85:LEU:HD23	4:O:86:GLN:N	2.34	0.42
5:P:172:ARG:NH1	9:P:483:HOH:O	2.50	0.42
5:P:217:ASN:O	5:P:221:ILE:HG13	2.20	0.42
5:P:309:LYS:O	5:P:312:GLN:HB2	2.19	0.42
5:P:321:ILE:HD11	5:P:329:TYR:HB2	2.00	0.42
5:P:418:LEU:O	5:P:419:ARG:C	2.62	0.42
1:A:20:TYR:CD2	1:A:20:TYR:C	2.98	0.42
1:A:101:LEU:HD23	1:A:102:LYS:N	2.34	0.42
1:A:206:THR:HG23	1:A:209:GLU:H	1.84	0.42
2:C:52:PHE:HB3	2:C:53:PRO:HD3	1.99	0.42
2:C:78:PHE:HB3	2:C:79:PRO:HD2	2.00	0.42
2:C:144:PRO:HG2	2:C:165:LEU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:267:TYR:CD2	2:C:267:TYR:N	2.87	0.42
2:C:370:ALA:HB1	9:C:1667:HOH:O	2.18	0.42
2:C:627:ARG:HG2	9:C:1753:HOH:O	2.19	0.42
2:C:674:VAL:HG11	2:C:992:MET:HB3	2.02	0.42
2:C:707:ARG:NH2	2:C:824:ARG:CZ	2.82	0.42
2:C:946:ARG:HD2	2:C:984:GLU:HB3	1.99	0.42
2:C:1030:GLN:OE1	3:D:627:GLY:C	2.62	0.42
2:C:1084:SER:O	2:C:1087:VAL:HG12	2.19	0.42
3:D:15:PRO:HA	3:D:18:ILE:HG12	2.00	0.42
3:D:98:PRO:HG3	3:D:515:GLU:HB3	2.01	0.42
3:D:153:LEU:HD12	3:D:154:THR:N	2.34	0.42
3:D:729:HIS:CE1	3:D:935:LYS:HD3	2.54	0.42
3:D:754:PHE:CG	4:E:24:ALA:HB1	2.55	0.42
3:D:795:VAL:HA	3:D:861:GLN:O	2.19	0.42
3:D:1107:VAL:HG12	3:D:1217:ILE:HA	2.01	0.42
3:D:1428:ALA:O	3:D:1431:THR:CG2	2.66	0.42
5:F:271:LEU:HD22	5:F:304:VAL:HG13	1.99	0.42
1:K:16:GLN:HA	9:K:3198:HOH:O	2.18	0.42
2:M:129:ILE:HG22	2:M:130:ASN:ND2	2.33	0.42
2:M:161:SER:HB3	9:M:2298:HOH:O	2.19	0.42
2:M:173:ASP:O	2:M:184:MET:HA	2.19	0.42
2:M:232:GLU:HG3	2:M:235:LEU:CD1	2.49	0.42
2:M:300:ASP:HA	9:M:1862:HOH:O	2.19	0.42
2:M:412:ALA:HB1	2:M:419:THR:HG23	2.00	0.42
2:M:514:VAL:HG23	9:M:1623:HOH:O	2.18	0.42
2:M:564:MET:CE	2:M:846:LYS:HE3	2.50	0.42
2:M:627:ARG:HG3	2:M:628:PHE:N	2.33	0.42
2:M:674:VAL:HG11	2:M:992:MET:HB3	2.01	0.42
2:M:808:ARG:HA	2:M:815:LEU:HD22	2.00	0.42
2:M:897:LEU:HD23	9:M:1930:HOH:O	2.19	0.42
3:N:399:ARG:NE	9:N:2195:HOH:O	2.52	0.42
3:N:1167:SER:HB3	9:N:1789:HOH:O	2.19	0.42
3:N:1182:GLU:CG	9:N:1552:HOH:O	2.66	0.42
3:N:1216:SER:HB3	4:O:16:LYS:H	1.84	0.42
3:N:1462:LEU:HD22	3:N:1472:ILE:CG2	2.47	0.42
5:P:247:ILE:O	5:P:251:ILE:HG13	2.20	0.42
1:B:24:VAL:HG13	1:B:196:THR:HB	2.01	0.42
1:B:99:LEU:HD21	1:B:122:ILE:HD11	2.00	0.42
2:C:260:LEU:CB	2:C:291:ALA:HB1	2.45	0.42
2:C:549:PHE:HB3	2:C:552:HIS:CD2	2.49	0.42
2:C:764:GLU:O	2:C:765:SER:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:840:ALA:HB2	2:C:846:LYS:HA	2.02	0.42
2:C:897:LEU:HB3	2:C:899:GLN:NE2	2.33	0.42
3:D:133:ILE:HG23	3:D:456:MET:SD	2.60	0.42
3:D:568:ARG:HG3	3:D:572:ARG:HE	1.85	0.42
3:D:806:PHE:O	3:D:807:ALA:C	2.61	0.42
3:D:820:GLU:HB3	3:D:836:VAL:HG21	2.02	0.42
3:D:1019:PRO:O	3:D:1023:MET:HG2	2.19	0.42
3:D:1047:LYS:HA	3:D:1053:PHE:CE1	2.54	0.42
3:D:1108:ARG:NH2	3:D:1198:TYR:HB2	2.34	0.42
3:D:1129:THR:HA	9:D:1695:HOH:O	2.18	0.42
3:D:1144:LEU:HA	3:D:1147:ARG:HG3	2.01	0.42
3:D:1382:THR:HG21	3:D:1418:LYS:CE	2.50	0.42
5:F:363:GLU:CA	5:F:367:MET:HG3	2.49	0.42
2:M:397:GLU:O	2:M:398:THR:C	2.60	0.42
2:M:612:VAL:HG22	2:M:622:GLU:CB	2.48	0.42
2:M:684:PHE:HD2	3:N:740:PHE:HE1	1.67	0.42
2:M:850:ALA:HA	3:N:632:VAL:HG11	2.01	0.42
3:N:9:ARG:HA	3:N:1434:TRP:HH2	1.83	0.42
3:N:139:GLY:O	3:N:147:VAL:HB	2.20	0.42
3:N:434:ARG:H	3:N:447:VAL:HG23	1.84	0.42
3:N:799:LYS:CB	3:N:826:PRO:HG2	2.48	0.42
3:N:834:THR:HA	3:N:838:ARG:HD2	2.01	0.42
3:N:892:ASP:O	3:N:895:VAL:N	2.51	0.42
3:N:1392:GLY:C	3:N:1393:GLN:HG2	2.45	0.42
5:P:286:PRO:HD3	9:P:477:HOH:O	2.19	0.42
5:P:358:LEU:CD2	5:P:370:LYS:HZ1	2.33	0.42
1:A:55:SER:HB2	1:A:158:ILE:HG13	2.01	0.42
1:B:58:ILE:CG2	1:B:137:ARG:NH2	2.80	0.42
1:B:90:LEU:O	1:B:90:LEU:HG	2.19	0.42
1:B:133:GLU:O	1:B:134:GLU:HG2	2.19	0.42
2:C:91:GLN:HA	2:C:119:PRO:HA	2.01	0.42
2:C:173:ASP:O	2:C:184:MET:HA	2.20	0.42
2:C:263:ASP:HB2	2:C:264:PRO:CD	2.48	0.42
2:C:724:ARG:HA	2:C:737:LEU:CD2	2.49	0.42
2:C:769:PRO:HB3	5:F:373:LYS:O	2.19	0.42
2:C:833:LEU:HD12	2:C:834:GLN:N	2.34	0.42
2:C:889:HIS:CD2	9:C:1474:HOH:O	2.72	0.42
2:C:946:ARG:NH1	2:C:984:GLU:CD	2.78	0.42
2:C:950:LEU:HB3	2:C:952:LEU:HD23	2.01	0.42
2:C:1016:ILE:HG23	3:D:526:PRO:HG2	2.01	0.42
2:C:1033:GLY:O	2:C:1037:VAL:HG23	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1109:VAL:HA	3:D:3:LYS:HE3	2.00	0.42
3:D:131:LYS:HG2	3:D:456:MET:HE3	2.01	0.42
3:D:671:LYS:N	9:D:1660:HOH:O	2.38	0.42
3:D:796:ARG:NH1	3:D:861:GLN:HE21	2.17	0.42
3:D:1023:MET:HG2	3:D:1023:MET:H	1.42	0.42
3:D:1311:LEU:HB3	9:D:1836:HOH:O	2.20	0.42
3:D:1314:LYS:HA	9:D:1812:HOH:O	2.19	0.42
3:D:1407:LEU:HD11	9:D:2177:HOH:O	2.19	0.42
3:D:1478:SER:HG	3:D:1481:VAL:HG23	1.84	0.42
5:F:111:GLU:O	5:F:115:LYS:HG3	2.20	0.42
5:F:260:ILE:HD12	9:F:458:HOH:O	2.19	0.42
1:L:63:HIS:HB3	9:L:3750:HOH:O	2.20	0.42
1:L:63:HIS:HD2	9:L:3508:HOH:O	2.03	0.42
2:M:742:VAL:HG12	2:M:743:VAL:H	1.85	0.42
2:M:787:ASP:OD1	2:M:787:ASP:C	2.63	0.42
2:M:814:GLU:HB2	9:M:1921:HOH:O	2.18	0.42
3:N:152:LEU:H	3:N:152:LEU:CD2	2.24	0.42
3:N:407:VAL:HG22	3:N:422:ALA:CB	2.50	0.42
3:N:610:LYS:C	3:N:611:GLN:CG	2.93	0.42
3:N:684:LYS:C	9:N:1566:HOH:O	2.63	0.42
3:N:829:VAL:H	3:N:835:SER:CB	2.32	0.42
3:N:1207:TYR:H	3:N:1366:LYS:HZ1	1.67	0.42
3:N:1209:LEU:O	3:N:1210:SER:C	2.61	0.42
3:N:1223:ILE:HD12	3:N:1223:ILE:N	2.27	0.42
5:P:200:LYS:HD3	9:P:559:HOH:O	2.20	0.42
5:P:416:ARG:HB2	9:P:461:HOH:O	2.18	0.42
1:A:86:VAL:HG13	1:A:124:ASN:HB2	2.01	0.42
2:C:115:LEU:HA	2:C:375:SER:HB3	2.01	0.42
2:C:172:ILE:HG23	2:C:184:MET:HE3	2.01	0.42
2:C:176:VAL:O	2:C:176:VAL:HG23	2.20	0.42
2:C:253:ALA:O	2:C:256:TYR:HB2	2.19	0.42
2:C:878:SER:OG	3:D:1029:ARG:HD3	2.20	0.42
2:C:953:VAL:HG13	2:C:966:LEU:HD13	2.01	0.42
2:C:971:LYS:HB3	2:C:988:VAL:N	2.35	0.42
2:C:1090:LYS:HD2	3:D:90:MET:CE	2.50	0.42
2:C:1118:LYS:HG3	2:C:1118:LYS:H	1.77	0.42
3:D:38:LYS:N	9:D:1967:HOH:O	2.44	0.42
3:D:393:ILE:C	3:D:394:LEU:HD23	2.45	0.42
3:D:774:SER:C	3:D:776:GLU:N	2.77	0.42
3:D:882:PHE:C	3:D:882:PHE:CD2	2.97	0.42
3:D:1231:GLU:CB	3:D:1232:PRO:HD3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1481:VAL:HG13	4:E:18:ARG:HE	1.84	0.42
3:D:1503:VAL:HB	9:D:2384:HOH:O	2.18	0.42
5:F:358:LEU:HD22	5:F:370:LYS:HE3	2.02	0.42
1:K:106:PRO:HG3	1:K:134:GLU:HG2	2.01	0.42
1:K:184:THR:HG23	1:K:192:LEU:CD1	2.49	0.42
1:K:227:ASN:HD22	1:K:227:ASN:N	2.16	0.42
1:L:48:ILE:HD13	1:L:210:ALA:HB1	2.02	0.42
1:L:89:PHE:HE2	1:L:146:ARG:HB3	1.83	0.42
2:M:435:TYR:C	2:M:437:ARG:N	2.77	0.42
2:M:630:ARG:HB2	2:M:705:ILE:HG21	2.02	0.42
2:M:670:GLN:HE22	2:M:699:PHE:HA	1.84	0.42
2:M:798:GLY:H	2:M:827:VAL:HG11	1.83	0.42
3:N:23:TYR:O	3:N:49:ILE:HG23	2.20	0.42
3:N:500:ARG:HG3	3:N:500:ARG:NH1	2.35	0.42
3:N:610:LYS:CD	7:N:1527:MXP:H15B	2.31	0.42
3:N:1290:LEU:HD23	3:N:1291:SER:H	1.82	0.42
3:N:1425:THR:HG23	3:N:1426:LYS:N	2.35	0.42
4:O:35:PHE:HZ	4:O:60:ALA:HA	1.85	0.42
4:O:54:LEU:HD11	9:O:1151:HOH:O	2.20	0.42
1:B:89:PHE:HE2	1:B:146:ARG:HB3	1.84	0.42
1:B:173:PRO:HB3	1:B:204:SER:HB3	2.02	0.42
2:C:136:ILE:CG2	2:C:336:VAL:HG22	2.49	0.42
2:C:264:PRO:HB3	2:C:289:THR:CG2	2.49	0.42
2:C:265:ARG:HB3	2:C:267:TYR:CE2	2.55	0.42
2:C:411:SER:HA	2:C:452:ILE:HA	2.00	0.42
2:C:479:VAL:HG21	2:C:503:LEU:CD1	2.50	0.42
2:C:710:ILE:HB	2:C:790:LEU:HD13	2.00	0.42
2:C:1100:GLN:HE21	2:C:1100:GLN:HB2	1.60	0.42
3:D:131:LYS:HG3	3:D:572:ARG:NH2	2.34	0.42
3:D:141:ILE:HG13	3:D:142:LEU:N	2.31	0.42
3:D:185:VAL:HG21	3:D:191:LEU:HD11	2.01	0.42
3:D:462:GLN:HB2	3:D:513:ILE:HG21	2.02	0.42
3:D:701:LEU:C	3:D:702:LEU:HD12	2.45	0.42
3:D:1095:THR:O	3:D:1096:ARG:C	2.61	0.42
3:D:1382:THR:CG2	3:D:1418:LYS:HE3	2.49	0.42
5:F:152:ASP:O	5:F:156:VAL:HB	2.19	0.42
5:F:249:ARG:HD2	9:F:655:HOH:O	2.19	0.42
1:L:54:THR:HG22	1:L:54:THR:O	2.20	0.42
2:M:146:VAL:HG22	2:M:162:ILE:HG23	2.01	0.42
2:M:254:VAL:HA	2:M:257:VAL:HG23	2.01	0.42
2:M:265:ARG:CG	2:M:266:ARG:N	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:352:ALA:CA	2:M:355:VAL:HG12	2.48	0.42
2:M:916:GLU:O	2:M:919:ALA:HB3	2.19	0.42
2:M:1003:ASP:O	2:M:1005:MET:N	2.53	0.42
3:N:497:GLU:HB2	9:N:1731:HOH:O	2.19	0.42
3:N:670:VAL:O	3:N:674:ARG:HG3	2.19	0.42
3:N:1119:SER:HA	3:N:1186:VAL:O	2.20	0.42
3:N:1242:HIS:CE1	3:N:1266:ARG:HB3	2.54	0.42
3:N:1272:ALA:CB	3:N:1326:THR:HB	2.50	0.42
3:N:1373:ARG:HD3	9:N:1685:HOH:O	2.18	0.42
3:N:1460:ILE:O	3:N:1464:GLU:CD	2.62	0.42
3:N:1466:VAL:CG2	3:N:1472:ILE:HD11	2.39	0.42
5:P:114:LYS:HD2	9:P:618:HOH:O	2.20	0.42
1:A:101:LEU:HD12	1:A:114:PHE:CE1	2.55	0.42
1:A:156:HIS:CD2	1:A:157:GLY:H	2.38	0.42
1:B:28:LEU:HA	9:B:395:HOH:O	2.19	0.42
1:B:86:VAL:HG12	1:B:124:ASN:HB2	2.00	0.42
2:C:671:ASN:ND2	2:C:993:PHE:HD2	2.16	0.42
2:C:715:THR:HG22	2:C:717:LEU:H	1.85	0.42
2:C:1081:VAL:HA	2:C:1082:PRO:HD3	1.86	0.42
2:C:1109:VAL:HG11	3:D:5:VAL:HG22	2.01	0.42
2:C:1115:LEU:HD12	2:C:1115:LEU:H	1.83	0.42
3:D:8:VAL:C	3:D:1434:TRP:HH2	2.28	0.42
3:D:55:ASP:O	3:D:80:VAL:CG1	2.67	0.42
3:D:168:THR:HA	3:D:394:LEU:HA	2.02	0.42
3:D:403:PHE:CE2	3:D:443:VAL:N	2.88	0.42
3:D:612:GLY:H	3:D:617:ASN:HD21	1.68	0.42
3:D:749:VAL:HA	3:D:750:PRO:HD3	1.90	0.42
3:D:862:ASP:O	3:D:877:PRO:HD3	2.20	0.42
3:D:932:ASP:O	3:D:935:LYS:HB3	2.20	0.42
3:D:1495:ILE:O	3:D:1498:ALA:HB3	2.20	0.42
5:F:167:PRO:HD2	5:F:170:HIS:HD2	1.84	0.42
5:F:394:ARG:HB3	9:F:575:HOH:O	2.19	0.42
1:K:186:LEU:O	1:K:187:GLY:C	2.62	0.42
1:L:60:ASP:HB2	1:L:137:ARG:NH1	2.34	0.42
1:L:183:ASP:HA	1:L:192:LEU:O	2.20	0.42
2:M:129:ILE:HG22	2:M:130:ASN:N	2.35	0.42
2:M:171:TRP:HZ3	9:M:2226:HOH:O	2.02	0.42
2:M:267:TYR:CD1	2:M:272:ALA:HB1	2.54	0.42
2:M:443:THR:HG21	2:M:449:ILE:HG13	2.02	0.42
3:N:145:VAL:HG22	3:N:146:PRO:HD2	2.02	0.42
3:N:185:VAL:HG21	3:N:191:LEU:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:667:ALA:HB1	9:N:1656:HOH:O	2.19	0.42
3:N:820:GLU:HB3	3:N:836:VAL:HG21	2.01	0.42
3:N:1074:SER:O	3:N:1077:ALA:HB3	2.20	0.42
3:N:1082:ALA:O	3:N:1086:LEU:HG	2.19	0.42
3:N:1109:GLU:HG2	3:N:1201:CYS:CA	2.48	0.42
4:O:6:ILE:HG23	4:O:7:ASP:N	2.34	0.42
4:O:77:GLU:HG3	9:O:3449:HOH:O	2.20	0.42
5:P:284:ARG:O	5:P:286:PRO:N	2.53	0.42
1:A:79:ILE:O	1:A:83:LYS:HG3	2.19	0.42
1:B:101:LEU:HD12	1:B:113:ASP:C	2.45	0.42
2:C:142:ARG:HG2	9:C:1315:HOH:O	2.20	0.42
2:C:839:LEU:HD21	2:C:849:VAL:CG2	2.50	0.42
2:C:911:GLU:HB3	2:C:912:PRO:HD3	2.02	0.42
2:C:967:PHE:CD1	2:C:972:VAL:HG12	2.55	0.42
2:C:1034:GLU:HA	2:C:1037:VAL:CG2	2.47	0.42
3:D:84:ILE:O	3:D:87:ARG:HB3	2.19	0.42
3:D:133:ILE:HD11	3:D:155:ASP:OD1	2.19	0.42
3:D:141:ILE:HG21	3:D:450:TYR:H	1.85	0.42
3:D:161:LEU:O	3:D:449:SER:OG	2.38	0.42
3:D:544:TYR:N	9:D:1714:HOH:O	2.52	0.42
3:D:684:LYS:C	3:D:686:GLU:H	2.28	0.42
3:D:729:HIS:ND1	3:D:730:PRO:HD2	2.34	0.42
3:D:957:PRO:HD2	3:D:1007:VAL:HG12	2.00	0.42
3:D:1090:ASP:C	3:D:1092:GLY:N	2.77	0.42
3:D:1258:ARG:NE	3:D:1262:LEU:HD11	2.35	0.42
3:D:1311:LEU:H	3:D:1311:LEU:CD2	2.32	0.42
1:K:59:GLU:HG3	1:K:139:ASN:CG	2.44	0.42
1:K:181:VAL:HG12	9:K:2597:HOH:O	2.20	0.42
2:M:178:PRO:HB3	9:M:1853:HOH:O	2.19	0.42
2:M:183:SER:CB	2:M:190:LYS:HD3	2.50	0.42
2:M:259:GLY:O	2:M:290:LEU:O	2.38	0.42
2:M:289:THR:HG22	2:M:290:LEU:H	1.84	0.42
2:M:461:VAL:HG12	9:M:1945:HOH:O	2.19	0.42
2:M:487:THR:HG22	2:M:488:ALA:N	2.35	0.42
2:M:498:GLN:HA	2:M:498:GLN:NE2	2.34	0.42
2:M:580:MET:HB3	2:M:584:GLU:OE1	2.20	0.42
2:M:599:GLU:CG	2:M:600:ASP:N	2.82	0.42
2:M:676:ILE:O	2:M:676:ILE:CG2	2.68	0.42
2:M:722:ILE:HG23	2:M:805:ARG:HH21	1.85	0.42
3:N:48:ARG:HB2	9:N:2213:HOH:O	2.18	0.42
3:N:421:LEU:HD13	3:N:444:VAL:CG1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:500:ARG:O	3:N:504:ASP:HB2	2.20	0.42
3:N:526:PRO:HB2	5:P:317:LEU:HD11	2.02	0.42
3:N:570:GLU:HB2	5:P:214:GLN:CD	2.45	0.42
3:N:633:VAL:HB	3:N:740:PHE:CE1	2.55	0.42
3:N:704:ARG:HB2	3:N:736:PHE:HB3	2.01	0.42
3:N:1153:VAL:HG12	3:N:1155:VAL:CG2	2.50	0.42
3:N:1205:TYR:CE2	3:N:1366:LYS:HD3	2.54	0.42
3:N:1264:GLU:CG	3:N:1425:THR:H	2.32	0.42
3:N:1382:THR:HG21	3:N:1418:LYS:CE	2.50	0.42
1:A:55:SER:HB2	1:A:158:ILE:HG21	2.01	0.42
1:A:143:ARG:HB2	9:A:331:HOH:O	2.19	0.42
2:C:6:PHE:CE1	2:C:909:ALA:HB2	2.54	0.42
2:C:12:VAL:HB	2:C:472:ARG:CZ	2.50	0.42
2:C:139:GLN:HE22	2:C:415:PRO:HG2	1.85	0.42
2:C:247:PRO:HB2	9:C:1179:HOH:O	2.20	0.42
2:C:254:VAL:HA	2:C:257:VAL:HG23	2.02	0.42
2:C:299:LYS:O	2:C:299:LYS:HG3	2.20	0.42
2:C:443:THR:HG23	2:C:449:ILE:HG13	2.02	0.42
2:C:460:ARG:HG2	2:C:485:TYR:CE2	2.55	0.42
2:C:634:GLY:HA2	9:C:1287:HOH:O	2.20	0.42
3:D:42:ASP:HA	3:D:46:ASP:OD1	2.19	0.42
3:D:112:ILE:CD1	3:D:461:ILE:HG21	2.50	0.42
3:D:119:SER:CB	3:D:123:LEU:HB2	2.40	0.42
3:D:126:VAL:CG1	3:D:132:TYR:HB2	2.49	0.42
3:D:897:TRP:HB2	9:D:1776:HOH:O	2.20	0.42
3:D:1066:THR:CG2	3:D:1069:GLU:HG3	2.49	0.42
3:D:1134:LEU:HD22	9:D:1694:HOH:O	2.20	0.42
3:D:1263:PHE:CE2	3:D:1371:VAL:HG11	2.55	0.42
3:D:1467:ILE:HG12	7:D:1527:MXP:H16A	2.02	0.42
4:E:48:MET:N	4:E:54:LEU:HB2	2.34	0.42
5:F:88:ILE:HD13	5:F:193:ARG:CB	2.50	0.42
5:F:88:ILE:HB	5:F:193:ARG:HD2	2.01	0.42
5:F:93:LEU:HG	5:F:190:ALA:HB1	2.02	0.42
5:F:192:LEU:O	5:F:196:VAL:HG23	2.19	0.42
1:K:48:ILE:HG22	1:K:173:PRO:CD	2.49	0.42
1:K:177:VAL:O	2:M:864:GLY:HA3	2.19	0.42
1:L:27:PRO:HB3	1:L:192:LEU:CD2	2.50	0.42
1:L:108:GLU:HG2	9:L:1515:HOH:O	2.19	0.42
1:L:133:GLU:HB3	9:L:1918:HOH:O	2.20	0.42
2:M:146:VAL:HG11	2:M:306:THR:CG2	2.47	0.42
2:M:411:SER:CB	2:M:452:ILE:HG23	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:601:GLY:HA3	2:M:615:TYR:HA	2.02	0.42
2:M:1067:TYR:CE1	3:N:655:PRO:HG3	2.50	0.42
3:N:76:CYS:HA	9:N:1714:HOH:O	2.20	0.42
3:N:563:PRO:HG2	5:P:188:ILE:HG21	2.00	0.42
3:N:684:LYS:C	3:N:686:GLU:H	2.28	0.42
3:N:959:GLU:H	3:N:959:GLU:HG2	1.24	0.42
3:N:959:GLU:O	3:N:963:TYR:HD1	2.03	0.42
3:N:1066:THR:OG1	3:N:1067:VAL:N	2.51	0.42
3:N:1465:ASN:ND2	3:N:1470:ARG:HD3	2.15	0.42
2:C:124:ASP:HB2	2:C:407:LYS:NZ	2.35	0.41
2:C:204:GLN:NE2	9:C:1386:HOH:O	2.53	0.41
2:C:426:ASP:OD1	2:C:427:VAL:HG22	2.19	0.41
2:C:752:GLY:H	2:C:792:VAL:HB	1.85	0.41
2:C:950:LEU:HD12	9:C:1205:HOH:O	2.20	0.41
3:D:587:ARG:O	3:D:588:GLY:O	2.38	0.41
3:D:614:PHE:CG	3:D:617:ASN:HB3	2.55	0.41
3:D:804:LEU:O	3:D:831:GLY:HA2	2.20	0.41
3:D:1065:LEU:HD11	3:D:1070:TYR:N	2.35	0.41
5:F:88:ILE:HD13	5:F:193:ARG:CD	2.47	0.41
1:K:41:ARG:HD2	9:K:1774:HOH:O	2.19	0.41
1:K:54:THR:O	1:K:54:THR:HG22	2.19	0.41
1:K:156:HIS:CD2	1:K:157:GLY:H	2.38	0.41
1:K:223:THR:C	1:K:225:PHE:H	2.28	0.41
2:M:170:PRO:HG2	2:M:258:TYR:HD2	1.82	0.41
2:M:202:TYR:OH	2:M:304:LEU:HD22	2.20	0.41
2:M:301:GLU:O	2:M:305:PRO:HG2	2.20	0.41
2:M:756:VAL:HG12	2:M:757:GLY:N	2.35	0.41
2:M:877:PRO:O	2:M:878:SER:C	2.62	0.41
2:M:983:ILE:O	2:M:984:GLU:C	2.62	0.41
2:M:1043:TYR:HE1	3:N:710:ARG:O	2.03	0.41
3:N:584:ASN:OD1	3:N:590:PRO:HD2	2.20	0.41
3:N:776:GLU:C	9:N:1689:HOH:O	2.63	0.41
3:N:840:LYS:HB3	3:N:841:TYR:CE2	2.55	0.41
3:N:984:THR:HG23	3:N:986:ARG:H	1.85	0.41
3:N:1195:GLN:HG3	3:N:1196:THR:N	2.34	0.41
3:N:1263:PHE:HA	3:N:1375:MET:HE1	2.02	0.41
3:N:1274:ILE:HD11	3:N:1334:GLN:HE21	1.82	0.41
5:P:348:SER:OG	5:P:349:LEU:N	2.53	0.41
1:A:124:ASN:OD1	1:A:127:LEU:HB3	2.18	0.41
2:C:86:LYS:CD	9:C:1425:HOH:O	2.69	0.41
2:C:274:ARG:CZ	2:C:285:LEU:H	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:290:LEU:HD23	2:C:290:LEU:N	2.36	0.41
2:C:328:LEU:HD13	2:C:433:THR:CB	2.47	0.41
2:C:862:PRO:HD3	2:C:973:VAL:O	2.19	0.41
2:C:952:LEU:HD22	2:C:952:LEU:N	2.35	0.41
2:C:969:GLN:HG3	9:C:1350:HOH:O	2.20	0.41
2:C:1039:ALA:HB3	3:D:713:ILE:HD12	2.02	0.41
2:C:1094:ALA:CB	3:D:603:LEU:HD22	2.51	0.41
3:D:172:PRO:O	3:D:174:GLY:N	2.52	0.41
3:D:804:LEU:N	9:D:1726:HOH:O	2.53	0.41
3:D:1134:LEU:HD21	3:D:1175:ILE:HG23	2.01	0.41
3:D:1147:ARG:HH22	3:D:1369:GLU:CD	2.28	0.41
5:F:85:LEU:HA	5:F:88:ILE:CD1	2.44	0.41
5:F:104:ARG:NH1	9:F:673:HOH:O	2.53	0.41
5:F:116:LEU:HB2	5:F:127:ILE:HD12	2.01	0.41
5:F:222:ARG:HG2	9:F:631:HOH:O	2.19	0.41
1:K:124:ASN:OD1	1:K:127:LEU:HB3	2.20	0.41
1:L:44:LEU:HD23	1:L:48:ILE:CD1	2.50	0.41
2:M:22:GLN:OE1	2:M:336:VAL:HG21	2.20	0.41
2:M:260:LEU:CB	2:M:291:ALA:HB1	2.42	0.41
2:M:724:ARG:HA	2:M:737:LEU:CD2	2.50	0.41
2:M:739:GLU:CD	2:M:742:VAL:HB	2.45	0.41
2:M:926:PHE:O	2:M:929:ARG:HB3	2.20	0.41
3:N:122:GLU:N	9:N:1620:HOH:O	2.52	0.41
3:N:186:VAL:HB	3:N:189:GLN:HB2	2.02	0.41
3:N:432:TYR:O	3:N:448:GLU:HA	2.20	0.41
3:N:633:VAL:O	3:N:635:PRO:HD3	2.20	0.41
3:N:1323:GLN:HG3	3:N:1324:PRO:CD	2.50	0.41
3:N:1486:VAL:CG1	4:O:73:LEU:HD22	2.50	0.41
5:P:147:LEU:HD23	5:P:147:LEU:HA	1.80	0.41
5:P:220:LEU:O	5:P:223:ALA:HB3	2.20	0.41
1:A:180:GLN:HB3	1:A:180:GLN:HE21	1.62	0.41
1:A:211:LEU:O	1:A:211:LEU:HD12	2.21	0.41
2:C:118:ILE:CG2	2:C:382:ILE:HD13	2.50	0.41
2:C:394:PHE:HB2	9:C:1403:HOH:O	2.19	0.41
2:C:412:ALA:HB1	2:C:419:THR:HG21	2.01	0.41
2:C:709:GLU:HG3	2:C:824:ARG:CG	2.50	0.41
2:C:853:LEU:HG	9:C:1271:HOH:O	2.20	0.41
2:C:854:PRO:C	2:C:856:GLU:H	2.28	0.41
3:D:103:TRP:HE1	3:D:604:THR:CG2	2.33	0.41
3:D:116:LEU:HD23	3:D:118:LEU:HD21	2.01	0.41
3:D:206:ARG:HH12	5:F:97:GLU:C	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:835:SER:O	3:D:837:GLY:N	2.53	0.41
3:D:874:GLU:HG3	9:D:1855:HOH:O	2.20	0.41
3:D:1065:LEU:C	3:D:1065:LEU:HD12	2.46	0.41
3:D:1283:ILE:HG22	3:D:1284:GLU:N	2.35	0.41
3:D:1350:GLU:O	3:D:1350:GLU:HG3	2.21	0.41
5:F:76:SER:O	5:F:80:PRO:HG2	2.20	0.41
1:K:18:ARG:HH12	1:K:88:ARG:CD	2.33	0.41
1:K:79:ILE:O	1:K:83:LYS:HG3	2.19	0.41
2:M:328:LEU:C	2:M:330:ASN:H	2.26	0.41
2:M:557:ARG:CZ	2:M:879:ARG:HG2	2.50	0.41
3:N:119:SER:CB	3:N:123:LEU:HB2	2.40	0.41
3:N:131:LYS:O	3:N:133:ILE:HD13	2.21	0.41
3:N:405:ASP:HB3	9:N:1860:HOH:O	2.20	0.41
3:N:638:LYS:C	3:N:729:HIS:CD2	2.98	0.41
3:N:688:TRP:HA	3:N:688:TRP:CE3	2.56	0.41
2:C:64:LEU:HG	2:C:65:VAL:N	2.34	0.41
2:C:540:PHE:HE1	2:C:906:PHE:HE1	1.68	0.41
2:C:815:LEU:HD12	9:C:1534:HOH:O	2.20	0.41
3:D:501:ALA:HB2	9:D:2147:HOH:O	2.20	0.41
3:D:560:GLN:O	5:F:132:ARG:NH1	2.47	0.41
3:D:633:VAL:O	3:D:635:PRO:HD3	2.20	0.41
3:D:1057:VAL:HG22	3:D:1069:GLU:HB3	2.02	0.41
3:D:1217:ILE:N	9:D:2106:HOH:O	2.52	0.41
3:D:1490:LYS:HG2	9:D:2098:HOH:O	2.19	0.41
5:F:117:SER:HB3	5:F:122:LEU:O	2.19	0.41
1:K:115:LEU:HA	1:K:116:PRO:HD3	1.90	0.41
1:K:159:LYS:HA	9:K:1082:HOH:O	2.19	0.41
2:M:479:VAL:HG11	2:M:532:MET:HE2	2.02	0.41
2:M:597:ALA:O	2:M:652:GLY:N	2.53	0.41
2:M:875:GLY:HA2	2:M:879:ARG:HH11	1.85	0.41
2:M:1100:GLN:HE21	2:M:1100:GLN:HB2	1.65	0.41
3:N:686:GLU:HA	3:N:689:ASP:OD2	2.21	0.41
3:N:696:HIS:HB3	9:N:1565:HOH:O	2.19	0.41
5:P:172:ARG:HD3	9:P:483:HOH:O	2.21	0.41
5:P:315:VAL:HG11	9:P:467:HOH:O	2.20	0.41
5:P:361:LEU:O	5:P:362:SER:C	2.62	0.41
1:A:11:PHE:CD1	1:B:225:PHE:HA	2.55	0.41
1:A:47:SER:OG	1:B:32:PHE:HZ	2.03	0.41
1:B:23:PHE:CD2	1:B:211:LEU:HD22	2.56	0.41
2:C:127:PHE:O	2:C:133:ASP:HA	2.21	0.41
2:C:1034:GLU:O	2:C:1037:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1082:PRO:C	2:C:1084:SER:H	2.29	0.41
3:D:196:VAL:HG13	9:D:1768:HOH:O	2.20	0.41
3:D:688:TRP:HA	3:D:688:TRP:HE3	1.86	0.41
3:D:693:GLU:HG2	9:D:1780:HOH:O	2.21	0.41
3:D:699:VAL:HG12	3:D:717:GLN:CA	2.51	0.41
3:D:767:HIS:NE2	4:E:6:ILE:HG12	2.36	0.41
3:D:850:LEU:H	3:D:850:LEU:CD1	2.24	0.41
3:D:1112:CYS:HB2	3:D:1195:GLN:CD	2.44	0.41
3:D:1191:PRO:HD3	3:D:1204:CYS:O	2.21	0.41
3:D:1192:LEU:HD22	3:D:1345:GLU:HG2	2.02	0.41
1:L:47:SER:O	1:L:48:ILE:C	2.64	0.41
1:L:77:GLU:O	1:L:77:GLU:HG3	2.15	0.41
1:L:147:GLY:N	1:L:171:PHE:CE1	2.88	0.41
2:M:22:GLN:HE22	2:M:135:VAL:CG1	2.33	0.41
2:M:113:VAL:HB	2:M:115:LEU:HD23	2.02	0.41
2:M:475:VAL:O	2:M:478:VAL:HB	2.20	0.41
3:N:50:PHE:CD2	3:N:522:PRO:HG3	2.56	0.41
3:N:87:ARG:HB2	3:N:523:ASP:HB2	2.03	0.41
3:N:570:GLU:HB2	5:P:214:GLN:NE2	2.35	0.41
3:N:852:ALA:HB1	3:N:857:ILE:HB	2.02	0.41
3:N:1364:HIS:ND1	3:N:1366:LYS:HB2	2.36	0.41
5:P:163:LEU:HD13	5:P:174:LEU:CD1	2.51	0.41
2:C:24:GLU:HG2	2:C:27:ARG:CD	2.50	0.41
2:C:118:ILE:H	2:C:118:ILE:HG13	1.64	0.41
2:C:462:ASP:HB3	2:C:468:ARG:CD	2.50	0.41
2:C:479:VAL:HG13	2:C:508:ILE:HD12	2.03	0.41
2:C:592:LEU:HD23	2:C:592:LEU:HA	1.90	0.41
2:C:620:LEU:HD12	2:C:620:LEU:O	2.21	0.41
2:C:742:VAL:HG21	9:C:1160:HOH:O	2.19	0.41
3:D:29:PRO:HG2	3:D:549:ASN:HD21	1.84	0.41
3:D:204:LEU:HD21	3:D:445:ARG:HH12	1.86	0.41
3:D:766:ALA:O	3:D:769:LEU:HD21	2.19	0.41
3:D:832:ARG:HB2	9:D:1797:HOH:O	2.19	0.41
3:D:888:GLU:O	3:D:889:ALA:C	2.62	0.41
3:D:889:ALA:HB1	3:D:930:LEU:HA	2.02	0.41
3:D:1122:LEU:O	3:D:1134:LEU:HA	2.20	0.41
3:D:1372:VAL:HA	3:D:1375:MET:HE3	2.03	0.41
4:E:41:GLU:HB2	4:E:45:ARG:NH1	2.36	0.41
5:F:75:ILE:HG13	9:F:645:HOH:O	2.20	0.41
5:F:151:LEU:O	5:F:152:ASP:C	2.63	0.41
5:F:196:VAL:HG22	5:F:213:ILE:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:215:GLU:OE2	5:F:254:GLN:NE2	2.50	0.41
1:L:127:LEU:HD12	9:L:1125:HOH:O	2.20	0.41
2:M:292:ARG:NH1	2:M:299:LYS:HD3	2.35	0.41
2:M:327:HIS:O	2:M:330:ASN:HB2	2.21	0.41
2:M:374:ASN:O	2:M:377:PRO:HD2	2.20	0.41
2:M:1025:ALA:C	2:M:1026:GLN:HG3	2.45	0.41
2:M:1034:GLU:HA	2:M:1037:VAL:CG2	2.49	0.41
3:N:570:GLU:HB2	5:P:214:GLN:HE22	1.85	0.41
3:N:637:LEU:HD12	3:N:641:GLN:HB2	2.02	0.41
3:N:806:PHE:O	3:N:808:THR:N	2.53	0.41
3:N:835:SER:C	3:N:837:GLY:N	2.78	0.41
3:N:1276:GLU:OE2	3:N:1303:TYR:HE2	2.04	0.41
3:N:1389:LEU:HD12	3:N:1390:LEU:N	2.32	0.41
5:P:169:GLU:H	5:P:169:GLU:HG3	1.67	0.41
5:P:305:GLU:HG2	5:P:309:LYS:HE3	2.01	0.41
5:P:324:GLU:O	5:P:325:LYS:C	2.64	0.41
9:A:432:HOH:O	2:C:832:LYS:HE3	2.20	0.41
1:B:57:TYR:CE2	1:B:59:GLU:HA	2.55	0.41
1:B:223:THR:C	1:B:225:PHE:H	2.28	0.41
2:C:162:ILE:CD1	2:C:306:THR:HG21	2.50	0.41
2:C:274:ARG:HB2	2:C:285:LEU:HB3	2.02	0.41
2:C:437:ARG:HG2	2:C:467:ILE:O	2.21	0.41
2:C:914:ILE:HA	2:C:914:ILE:HD12	1.74	0.41
2:C:1013:TYR:OH	3:D:624:ASP:OD2	2.37	0.41
9:C:1734:HOH:O	3:D:1471:LEU:HD12	2.20	0.41
3:D:165:LYS:HG2	9:D:1699:HOH:O	2.21	0.41
3:D:601:ARG:HG3	9:D:2091:HOH:O	2.21	0.41
3:D:771:SER:HA	3:D:772:PRO:HD3	1.91	0.41
5:F:321:ILE:HG13	5:F:329:TYR:HA	2.01	0.41
5:F:335:ASP:C	5:F:336:GLU:HG2	2.43	0.41
1:K:101:LEU:HD23	1:K:102:LYS:N	2.35	0.41
1:K:158:ILE:HG22	1:K:159:LYS:N	2.35	0.41
1:L:1:MET:HE2	9:L:1888:HOH:O	2.21	0.41
1:L:172:SER:OG	1:L:174:VAL:HB	2.21	0.41
2:M:22:GLN:HE22	2:M:135:VAL:HG12	1.85	0.41
2:M:264:PRO:HB3	2:M:289:THR:CB	2.50	0.41
2:M:299:LYS:O	2:M:299:LYS:HG3	2.21	0.41
2:M:663:ASN:HD22	2:M:663:ASN:HA	1.52	0.41
2:M:724:ARG:HB2	2:M:740:GLU:HA	2.01	0.41
2:M:968:LEU:HD13	9:M:2164:HOH:O	2.21	0.41
3:N:611:GLN:N	9:N:1557:HOH:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:637:LEU:HD11	3:N:642:CYS:CA	2.51	0.41
3:N:818:ARG:O	3:N:821:VAL:HB	2.20	0.41
3:N:911:LEU:O	3:N:915:VAL:HG23	2.20	0.41
3:N:1007:VAL:CG2	3:N:1008:PHE:N	2.84	0.41
3:N:1333:HIS:O	3:N:1336:LEU:HB3	2.19	0.41
2:C:96:ALA:HB2	9:C:1545:HOH:O	2.20	0.41
2:C:172:ILE:HD12	2:C:172:ILE:N	2.34	0.41
2:C:313:LEU:HD12	2:C:313:LEU:O	2.21	0.41
2:C:414:GLY:O	2:C:416:GLY:N	2.54	0.41
2:C:469:THR:HG23	2:C:471:TYR:CE1	2.56	0.41
2:C:511:GLU:N	9:C:1690:HOH:O	2.53	0.41
2:C:952:LEU:CD1	2:C:969:GLN:HE22	2.19	0.41
2:C:1112:PHE:O	2:C:1113:GLU:C	2.63	0.41
3:D:415:VAL:HG13	3:D:419:ASP:HB2	2.01	0.41
3:D:925:GLU:OE1	4:E:6:ILE:HG22	2.20	0.41
3:D:998:GLU:HB3	9:D:2202:HOH:O	2.20	0.41
3:D:1326:THR:HG22	3:D:1327:ARG:H	1.85	0.41
3:D:1339:LYS:HB3	3:D:1343:ALA:HB2	2.02	0.41
3:D:1459:LEU:HB2	3:D:1470:ARG:NH1	2.35	0.41
4:E:50:THR:HA	9:E:107:HOH:O	2.20	0.41
5:F:280:GLN:NE2	9:F:601:HOH:O	2.54	0.41
5:F:284:ARG:O	5:F:286:PRO:N	2.53	0.41
5:F:324:GLU:O	5:F:325:LYS:C	2.64	0.41
1:K:16:GLN:HB2	9:K:3198:HOH:O	2.20	0.41
1:L:101:LEU:HD12	1:L:114:PHE:CA	2.50	0.41
1:L:117:VAL:HB	1:L:120:VAL:HB	2.03	0.41
1:L:142:VAL:O	1:L:142:VAL:HG23	2.21	0.41
2:M:140:ILE:H	2:M:140:ILE:HD12	1.86	0.41
2:M:278:GLU:HA	2:M:283:ILE:HA	2.03	0.41
2:M:676:ILE:HG21	2:M:988:VAL:HG22	2.01	0.41
2:M:1008:ARG:CZ	2:M:1020:PRO:HB3	2.51	0.41
2:M:1054:THR:HB	2:M:1055:LEU:H	1.61	0.41
2:M:1112:PHE:O	2:M:1113:GLU:C	2.63	0.41
3:N:105:VAL:HG12	3:N:106:LYS:HG3	2.02	0.41
3:N:165:LYS:CG	3:N:397:LYS:HD3	2.50	0.41
3:N:206:ARG:HA	9:N:2058:HOH:O	2.20	0.41
3:N:489:ARG:HD3	9:N:1694:HOH:O	2.20	0.41
3:N:804:LEU:O	3:N:831:GLY:HA2	2.21	0.41
3:N:899:LEU:HD12	3:N:900:ILE:HG23	2.02	0.41
3:N:1051:GLU:HG3	3:N:1051:GLU:H	1.53	0.41
3:N:1147:ARG:NH1	9:N:2122:HOH:O	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1341:PRO:HB2	9:N:1945:HOH:O	2.19	0.41
5:P:350:LEU:O	5:P:354:LEU:HB2	2.21	0.41
5:P:371:LEU:HB2	5:P:372:ARG:HH11	1.86	0.41
1:A:18:ARG:HH12	1:A:88:ARG:HD3	1.86	0.41
1:A:101:LEU:HG	1:A:113:ASP:C	2.46	0.41
1:A:170:VAL:HA	9:A:399:HOH:O	2.21	0.41
1:B:111:ALA:HB3	1:B:124:ASN:O	2.21	0.41
2:C:7:GLY:O	2:C:907:ASP:OD1	2.38	0.41
2:C:35:PRO:HB3	9:C:1537:HOH:O	2.21	0.41
2:C:36:PRO:CB	2:C:70:GLU:HG2	2.51	0.41
2:C:45:GLN:NE2	9:C:1426:HOH:O	2.52	0.41
2:C:149:THR:HA	2:C:150:PRO:HD3	1.92	0.41
2:C:317:VAL:HB	9:C:1324:HOH:O	2.20	0.41
2:C:501:THR:O	2:C:502:PRO:C	2.64	0.41
2:C:612:VAL:HG22	2:C:622:GLU:CB	2.51	0.41
2:C:612:VAL:HG22	2:C:622:GLU:HG3	2.02	0.41
2:C:724:ARG:HB2	2:C:740:GLU:HA	2.02	0.41
2:C:787:ASP:OD1	2:C:787:ASP:C	2.63	0.41
2:C:807:ARG:HA	2:C:821:GLU:HB2	2.02	0.41
2:C:815:LEU:HG	2:C:819:VAL:HG11	2.00	0.41
2:C:818:GLY:N	5:F:309:LYS:CE	2.82	0.41
2:C:969:GLN:HE21	2:C:969:GLN:HB3	1.72	0.41
2:C:1063:ARG:O	2:C:1066:ALA:HB3	2.21	0.41
2:C:1067:TYR:CE1	2:C:1071:ILE:HD11	2.56	0.41
3:D:29:PRO:CB	3:D:545:ARG:HG2	2.49	0.41
3:D:33:ASN:HB3	9:D:2304:HOH:O	2.21	0.41
3:D:44:LEU:HD21	3:D:544:TYR:HB3	2.03	0.41
3:D:85:VAL:HG11	3:D:89:ARG:NH2	2.35	0.41
3:D:93:ILE:HD13	3:D:547:LEU:HD23	2.03	0.41
3:D:119:SER:N	3:D:123:LEU:HD22	2.26	0.41
3:D:482:LYS:HB2	9:D:1744:HOH:O	2.20	0.41
3:D:647:ARG:HB2	9:D:1878:HOH:O	2.21	0.41
3:D:704:ARG:HB2	3:D:736:PHE:HB3	2.03	0.41
3:D:899:LEU:HD12	3:D:900:ILE:HG23	2.03	0.41
3:D:1026:SER:C	3:D:1028:ALA:H	2.29	0.41
3:D:1285:GLU:O	3:D:1286:THR:C	2.63	0.41
3:D:1296:SER:C	3:D:1298:GLY:N	2.78	0.41
3:D:1361:VAL:HG23	9:D:1625:HOH:O	2.21	0.41
1:K:48:ILE:HD11	1:K:210:ALA:O	2.21	0.41
1:K:49:PRO:HB3	1:K:148:VAL:CG2	2.51	0.41
1:K:198:ARG:NH2	9:K:1749:HOH:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:75:VAL:O	1:L:79:ILE:HG23	2.20	0.41
2:M:34:VAL:CG2	2:M:38:LYS:HD3	2.49	0.41
2:M:56:GLU:OE2	2:M:356:ARG:HG2	2.20	0.41
2:M:129:ILE:CD1	2:M:386:PHE:HB3	2.51	0.41
2:M:131:GLY:HA2	9:M:1651:HOH:O	2.20	0.41
2:M:190:LYS:H	2:M:190:LYS:HG3	1.56	0.41
2:M:218:VAL:CA	2:M:221:LEU:HD23	2.50	0.41
2:M:255:ALA:HB3	2:M:298:PHE:CZ	2.56	0.41
2:M:280:LYS:HA	9:M:1935:HOH:O	2.20	0.41
2:M:408:ARG:HH11	2:M:408:ARG:HD2	1.74	0.41
2:M:535:SER:HB2	2:M:537:LYS:HG3	2.03	0.41
2:M:817:PRO:C	5:P:309:LYS:HE2	2.46	0.41
2:M:911:GLU:HB3	2:M:912:PRO:HD3	2.03	0.41
2:M:958:THR:HG23	2:M:961:GLU:HB2	2.03	0.41
2:M:971:LYS:HB3	2:M:988:VAL:N	2.36	0.41
3:N:26:VAL:HG13	3:N:43:GLY:C	2.46	0.41
3:N:60:CYS:N	3:N:76:CYS:SG	2.91	0.41
3:N:131:LYS:HE2	3:N:456:MET:CE	2.51	0.41
3:N:192:ALA:HB2	3:N:393:ILE:CD1	2.51	0.41
3:N:398:ALA:HB2	9:N:1561:HOH:O	2.21	0.41
3:N:417:PRO:HG3	3:N:430:ASP:O	2.21	0.41
3:N:562:ALA:HB3	9:P:599:HOH:O	2.20	0.41
3:N:572:ARG:HH11	3:N:572:ARG:HD3	1.63	0.41
3:N:591:VAL:CG1	3:N:597:ASP:HA	2.50	0.41
3:N:611:GLN:CG	3:N:619:LEU:CG	2.91	0.41
3:N:705:ALA:CB	3:N:706:PRO:CD	2.94	0.41
3:N:771:SER:HA	3:N:772:PRO:HD3	1.86	0.41
3:N:889:ALA:HB1	3:N:930:LEU:HA	2.03	0.41
3:N:1000:THR:CG2	3:N:1001:GLU:N	2.84	0.41
3:N:1075:HIS:CE1	9:N:1553:HOH:O	2.74	0.41
3:N:1148:VAL:HG21	3:N:1203:LYS:HA	2.03	0.41
3:N:1155:VAL:CG1	3:N:1177:ALA:HB1	2.50	0.41
3:N:1264:GLU:HA	3:N:1423:GLY:CA	2.51	0.41
3:N:1369:GLU:HA	3:N:1372:VAL:HG12	2.02	0.41
3:N:1441:GLN:N	9:N:1579:HOH:O	2.54	0.41
3:N:1442:ASN:N	9:N:1579:HOH:O	2.53	0.41
4:O:16:LYS:HD3	4:O:17:TYR:CE2	2.56	0.41
4:O:36:LYS:HG2	9:O:3235:HOH:O	2.20	0.41
4:O:54:LEU:HA	4:O:58:PRO:CG	2.50	0.41
5:P:207:LEU:HD23	5:P:207:LEU:HA	1.95	0.41
5:P:277:GLN:HA	9:P:458:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:ILE:CG2	1:B:159:LYS:N	2.83	0.41
1:B:158:ILE:CD1	1:B:165:ILE:C	2.94	0.41
2:C:162:ILE:HD12	2:C:172:ILE:HB	2.03	0.41
2:C:166:PRO:HD3	2:C:265:ARG:CB	2.51	0.41
2:C:663:ASN:HD22	2:C:663:ASN:HA	1.51	0.41
2:C:707:ARG:CZ	2:C:824:ARG:CZ	2.98	0.41
2:C:818:GLY:CA	5:F:309:LYS:HZ3	2.28	0.41
2:C:818:GLY:CA	5:F:309:LYS:NZ	2.83	0.41
2:C:983:ILE:O	2:C:984:GLU:C	2.64	0.41
2:C:1097:LEU:N	2:C:1097:LEU:CD1	2.84	0.41
3:D:155:ASP:HA	3:D:158:TYR:HB3	2.03	0.41
3:D:687:VAL:CG1	9:D:2185:HOH:O	2.67	0.41
3:D:729:HIS:ND1	3:D:730:PRO:CD	2.84	0.41
3:D:1035:ILE:CA	3:D:1038:LEU:HD12	2.50	0.41
3:D:1116:ASN:HB3	9:D:2418:HOH:O	2.20	0.41
3:D:1243:THR:CB	3:D:1253:THR:HB	2.50	0.41
3:D:1384:PRO:HB3	3:D:1387:SER:O	2.20	0.41
1:K:85:LEU:HB2	1:K:127:LEU:HD21	2.03	0.41
1:K:198:ARG:HB2	1:K:200:TRP:CH2	2.55	0.41
1:L:41:ARG:NH1	1:L:177:VAL:HG23	2.36	0.41
2:M:182:VAL:HG12	2:M:193:LEU:HD13	2.02	0.41
2:M:271:GLU:HA	2:M:275:TYR:CD1	2.56	0.41
2:M:474:VAL:HG23	2:M:478:VAL:O	2.21	0.41
2:M:1098:ASP:OD1	2:M:1098:ASP:C	2.64	0.41
3:N:601:ARG:HG2	3:N:605:ASP:OD1	2.21	0.41
3:N:712:GLY:O	3:N:713:ILE:HG13	2.21	0.41
3:N:907:GLU:HG2	3:N:908:LYS:H	1.85	0.41
3:N:937:TYR:HD2	3:N:941:PHE:HE1	1.69	0.41
3:N:1404:ASN:HA	9:N:1794:HOH:O	2.19	0.41
5:P:132:ARG:NH2	5:P:184:ARG:NH1	2.69	0.41
2:C:91:GLN:HG2	2:C:119:PRO:HG3	2.03	0.40
2:C:234:ALA:HA	2:C:237:ARG:HB2	2.02	0.40
2:C:269:LEU:O	2:C:269:LEU:HD23	2.22	0.40
2:C:292:ARG:NH1	9:C:1267:HOH:O	2.54	0.40
2:C:442:GLU:O	2:C:442:GLU:HG3	2.21	0.40
2:C:495:THR:HG21	2:C:524:VAL:HG21	2.02	0.40
2:C:518:LYS:N	9:C:1698:HOH:O	2.52	0.40
2:C:836:GLY:HA3	3:D:724:GLN:OE1	2.20	0.40
2:C:966:LEU:HD21	2:C:986:PRO:CG	2.51	0.40
3:D:674:ARG:HH11	3:D:674:ARG:HG2	1.86	0.40
3:D:684:LYS:HG2	9:D:2411:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:717:GLN:CG	9:D:1581:HOH:O	2.68	0.40
3:D:820:GLU:CB	3:D:836:VAL:HG21	2.51	0.40
3:D:1223:ILE:O	3:D:1224:VAL:C	2.63	0.40
3:D:1412:LYS:O	3:D:1414:PRO:HD3	2.21	0.40
5:F:77:THR:C	5:F:80:PRO:HD2	2.46	0.40
5:F:90:GLN:HE21	5:F:90:GLN:HB3	1.73	0.40
1:K:25:LEU:HD23	1:K:25:LEU:C	2.46	0.40
1:L:71:VAL:HG22	1:L:132:LEU:CD1	2.50	0.40
2:M:242:LEU:HD23	2:M:242:LEU:HA	1.78	0.40
2:M:414:GLY:C	2:M:416:GLY:N	2.78	0.40
2:M:414:GLY:O	2:M:416:GLY:N	2.54	0.40
2:M:437:ARG:NH1	2:M:488:ALA:HA	2.35	0.40
2:M:471:TYR:CD2	2:M:496:ILE:HG21	2.55	0.40
2:M:512:ARG:HB3	2:M:523:ILE:HD11	2.03	0.40
2:M:840:ALA:HB2	2:M:846:LYS:HA	2.02	0.40
2:M:861:LEU:CD2	2:M:925:TYR:HE2	2.33	0.40
3:N:515:GLU:HG3	9:N:1827:HOH:O	2.20	0.40
3:N:516:ALA:HB1	9:N:2118:HOH:O	2.21	0.40
3:N:729:HIS:CE1	3:N:935:LYS:HD3	2.56	0.40
3:N:850:LEU:H	3:N:850:LEU:CD1	2.24	0.40
3:N:1047:LYS:HG2	3:N:1053:PHE:CZ	2.56	0.40
3:N:1223:ILE:O	3:N:1227:GLN:HG3	2.22	0.40
3:N:1396:GLU:O	3:N:1396:GLU:HG2	2.22	0.40
5:P:256:ARG:HA	9:P:486:HOH:O	2.21	0.40
5:P:321:ILE:HB	5:P:327:SER:OG	2.21	0.40
2:C:15:LEU:HA	2:C:16:PRO:HD3	1.95	0.40
2:C:181:VAL:HG12	2:C:182:VAL:N	2.36	0.40
2:C:269:LEU:HD23	2:C:269:LEU:C	2.46	0.40
2:C:305:PRO:C	2:C:308:ARG:HB2	2.47	0.40
2:C:464:LEU:HD12	2:C:465:GLY:N	2.36	0.40
2:C:468:ARG:NH1	9:C:1743:HOH:O	2.54	0.40
2:C:708:TYR:CD1	2:C:708:TYR:N	2.89	0.40
2:C:858:MET:HB2	2:C:859:PRO:CD	2.51	0.40
2:C:958:THR:HA	9:C:1402:HOH:O	2.19	0.40
3:D:152:LEU:HD23	3:D:152:LEU:N	2.27	0.40
3:D:400:VAL:HG13	3:D:402:PRO:CD	2.51	0.40
3:D:610:LYS:HB3	7:D:1527:MXP:H15	2.03	0.40
3:D:709:HIS:CD2	3:D:711:LEU:HB2	2.56	0.40
3:D:840:LYS:NZ	9:D:2398:HOH:O	2.55	0.40
3:D:1007:VAL:CG2	3:D:1008:PHE:N	2.84	0.40
3:D:1114:THR:HG23	3:D:1116:ASN:ND2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1310:ARG:HG3	3:D:1327:ARG:CB	2.48	0.40
3:D:1394:VAL:HG23	9:D:2328:HOH:O	2.21	0.40
5:F:94:LEU:HB2	5:F:98:GLU:CG	2.52	0.40
5:F:270:LYS:N	9:F:511:HOH:O	2.54	0.40
5:F:316:SER:C	5:F:318:GLU:N	2.78	0.40
5:F:358:LEU:HD21	5:F:367:MET:HE3	2.03	0.40
5:F:364:ARG:HH12	5:F:396:ARG:CZ	2.34	0.40
1:K:107:LYS:HE3	1:K:113:ASP:OD2	2.19	0.40
1:K:176:ARG:HG3	1:K:200:TRP:CE3	2.57	0.40
1:K:201:THR:HG21	1:K:205:VAL:O	2.20	0.40
1:L:158:ILE:CG2	1:L:159:LYS:N	2.84	0.40
1:L:197:LEU:HD21	1:L:199:ILE:CD1	2.47	0.40
2:M:75:GLU:HA	2:M:76:PRO:HD3	1.97	0.40
2:M:308:ARG:HG2	9:M:1753:HOH:O	2.21	0.40
2:M:443:THR:HA	2:M:444:PRO:HD3	1.80	0.40
2:M:606:VAL:HG21	2:M:645:VAL:HG22	2.03	0.40
2:M:674:VAL:O	2:M:989:VAL:HA	2.20	0.40
2:M:1060:ILE:O	2:M:1063:ARG:HG2	2.20	0.40
3:N:111:LYS:NZ	3:N:1452:ILE:HG21	2.34	0.40
3:N:489:ARG:NH2	3:N:1389:LEU:HD11	2.32	0.40
3:N:530:VAL:HG23	3:N:534:ARG:O	2.21	0.40
3:N:951:ILE:HD12	3:N:1062:ARG:HG3	2.02	0.40
3:N:1087:ARG:HD3	3:N:1238:MET:H	1.86	0.40
3:N:1161:GLU:H	3:N:1161:GLU:HG2	1.37	0.40
3:N:1376:MET:C	3:N:1378:TYR:H	2.29	0.40
5:P:340:SER:O	5:P:341:PRO:C	2.64	0.40
1:A:191:ASP:O	1:A:191:ASP:CG	2.64	0.40
1:B:61:VAL:N	1:B:137:ARG:NH2	2.67	0.40
2:C:491:GLU:HG2	9:C:1297:HOH:O	2.21	0.40
2:C:721:ARG:NE	9:C:1244:HOH:O	2.55	0.40
2:C:773:LEU:HG	2:C:777:ILE:HD11	2.03	0.40
2:C:865:THR:O	2:C:865:THR:HG23	2.21	0.40
2:C:1010:THR:HG22	2:C:1011:GLY:N	2.36	0.40
3:D:93:ILE:HD13	3:D:548:ILE:HD11	2.03	0.40
3:D:521:PRO:O	3:D:525:ARG:NH1	2.52	0.40
3:D:797:LYS:HA	3:D:828:LYS:HB2	2.04	0.40
3:D:1066:THR:OG1	3:D:1067:VAL:N	2.53	0.40
3:D:1231:GLU:O	3:D:1232:PRO:C	2.64	0.40
3:D:1335:LEU:HD23	3:D:1344:VAL:CA	2.28	0.40
3:D:1353:GLN:OE1	3:D:1365:ASP:OD2	2.39	0.40
3:D:1372:VAL:CG1	3:D:1373:ARG:N	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:205:ARG:NH1	5:F:248:ASN:OD1	2.54	0.40
5:F:272:SER:O	5:F:276:ARG:HG3	2.22	0.40
1:K:28:LEU:HD23	1:K:28:LEU:HA	1.77	0.40
1:L:10:VAL:HG12	1:L:12:THR:HG23	2.02	0.40
2:M:110:GLU:HB3	2:M:369:PRO:HG3	2.02	0.40
2:M:118:ILE:H	2:M:118:ILE:HG13	1.63	0.40
2:M:221:LEU:HG	2:M:222:MET:N	2.37	0.40
2:M:234:ALA:HA	2:M:237:ARG:HB2	2.02	0.40
2:M:420:ARG:H	2:M:420:ARG:HG2	1.44	0.40
2:M:424:GLY:N	9:M:1722:HOH:O	2.54	0.40
2:M:480:THR:CG2	2:M:481:ASP:H	2.34	0.40
2:M:583:LEU:O	2:M:584:GLU:C	2.62	0.40
2:M:586:ARG:NE	2:M:590:ASP:OD2	2.53	0.40
2:M:742:VAL:CG1	2:M:743:VAL:N	2.83	0.40
2:M:950:LEU:HB3	2:M:952:LEU:HD23	2.02	0.40
2:M:1017:THR:OG1	2:M:1019:GLN:HG3	2.22	0.40
3:N:46:ASP:O	3:N:48:ARG:N	2.54	0.40
3:N:497:GLU:CD	9:N:1731:HOH:O	2.64	0.40
3:N:521:PRO:C	3:N:525:ARG:NH1	2.79	0.40
3:N:776:GLU:HB3	3:N:912:LYS:HE2	2.03	0.40
3:N:793:THR:HG22	3:N:879:ARG:HA	2.03	0.40
3:N:862:ASP:O	3:N:876:SER:HB2	2.21	0.40
3:N:932:ASP:O	3:N:935:LYS:HB3	2.22	0.40
3:N:1365:ASP:O	3:N:1366:LYS:C	2.63	0.40
3:N:1366:LYS:O	3:N:1369:GLU:HB2	2.22	0.40
3:N:1435:LEU:HD23	3:N:1467:ILE:HD12	2.02	0.40
3:N:1478:SER:HG	3:N:1480:PHE:HB3	1.87	0.40
4:O:26:ARG:HG2	4:O:67:GLU:OE1	2.22	0.40
1:A:13:VAL:CG1	1:A:15:THR:HG22	2.49	0.40
1:A:95:GLN:HG2	9:A:325:HOH:O	2.21	0.40
1:A:96:THR:N	9:A:349:HOH:O	2.54	0.40
2:C:54:ILE:HD13	9:C:1578:HOH:O	2.21	0.40
2:C:166:PRO:HG2	9:C:1175:HOH:O	2.21	0.40
2:C:378:LEU:O	2:C:382:ILE:HG13	2.22	0.40
2:C:410:ILE:N	2:C:453:THR:O	2.53	0.40
2:C:549:PHE:HE2	2:C:887:GLU:N	2.20	0.40
2:C:686:ASP:N	9:C:1222:HOH:O	2.54	0.40
2:C:897:LEU:CD1	2:C:921:ALA:HA	2.51	0.40
3:D:46:ASP:O	3:D:48:ARG:N	2.54	0.40
3:D:97:THR:O	3:D:98:PRO:O	2.40	0.40
3:D:137:PRO:HD2	3:D:453:ASP:CG	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:500:ARG:O	3:D:504:ASP:HB2	2.21	0.40
3:D:521:PRO:HA	3:D:522:PRO:HD3	1.91	0.40
3:D:778:LEU:HD11	9:D:1940:HOH:O	2.21	0.40
3:D:898:GLU:OE2	3:D:921:ARG:NH1	2.54	0.40
3:D:1106:VAL:HG21	3:D:1474:ALA:HB2	2.03	0.40
3:D:1256:LEU:N	3:D:1257:PRO:CD	2.85	0.40
3:D:1305:LEU:HD22	3:D:1309:ALA:CB	2.52	0.40
5:F:280:GLN:O	5:F:280:GLN:HG2	2.22	0.40
1:K:42:ARG:NH1	1:L:34:VAL:HB	2.14	0.40
1:K:180:GLN:HE21	1:K:180:GLN:HB3	1.65	0.40
2:M:172:ILE:HG22	2:M:173:ASP:N	2.36	0.40
2:M:176:VAL:O	2:M:176:VAL:HG23	2.22	0.40
2:M:284:ARG:HD2	9:M:2219:HOH:O	2.21	0.40
2:M:443:THR:HG21	2:M:450:GLY:H	1.85	0.40
2:M:713:ARG:HB2	2:M:720:GLU:OE1	2.21	0.40
2:M:1008:ARG:HD2	2:M:1028:GLY:H	1.85	0.40
2:M:1019:GLN:O	2:M:1020:PRO:C	2.64	0.40
3:N:565:ILE:HD12	5:P:192:LEU:CD1	2.50	0.40
3:N:610:LYS:CG	7:N:1527:MXP:H15A	2.47	0.40
3:N:935:LYS:HB3	3:N:935:LYS:HE2	1.94	0.40
3:N:982:PHE:HA	9:N:1762:HOH:O	2.21	0.40
3:N:1144:LEU:HD12	3:N:1171:VAL:HG13	2.04	0.40
3:N:1161:GLU:CG	3:N:1164:ARG:HD2	2.52	0.40
3:N:1399:ASP:O	3:N:1403:LEU:HB2	2.21	0.40
5:P:363:GLU:CA	5:P:367:MET:HG3	2.51	0.40
5:P:399:GLN:O	5:P:403:LYS:HB2	2.21	0.40
1:A:42:ARG:HD3	1:B:35:THR:OG1	2.21	0.40
1:A:43:ILE:HG21	1:A:214:ALA:HA	2.04	0.40
1:A:44:LEU:O	1:A:174:VAL:HG21	2.21	0.40
1:B:36:LEU:C	1:B:39:PRO:HD2	2.46	0.40
2:C:207:LEU:HD13	2:C:221:LEU:HD13	2.03	0.40
2:C:861:LEU:CD2	2:C:925:TYR:HE2	2.34	0.40
2:C:1005:MET:HB2	3:D:629:SER:HB2	2.02	0.40
2:C:1097:LEU:HD12	2:C:1097:LEU:H	1.86	0.40
3:D:99:ALA:HA	3:D:575:GLN:NE2	2.37	0.40
3:D:659:LYS:O	3:D:659:LYS:HG2	2.21	0.40
3:D:758:GLU:O	3:D:762:GLN:HG3	2.20	0.40
3:D:1209:LEU:HD23	3:D:1211:MET:CG	2.50	0.40
3:D:1364:HIS:ND1	3:D:1366:LYS:HB2	2.36	0.40
5:F:220:LEU:HB2	5:F:243:ILE:HD11	2.02	0.40
5:F:364:ARG:HD3	9:F:425:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:20:TYR:HE2	1:K:22:GLU:HG3	1.85	0.40
1:K:41:ARG:NH2	2:M:860:HIS:HB3	2.37	0.40
1:L:145:ASP:O	1:L:171:PHE:HE1	2.04	0.40
2:M:73:LEU:HD23	2:M:94:LEU:HD13	2.04	0.40
2:M:174:LEU:CD2	2:M:184:MET:HG3	2.52	0.40
2:M:183:SER:HB3	2:M:190:LYS:HD3	2.03	0.40
2:M:351:LEU:HD11	2:M:373:VAL:HG13	2.03	0.40
2:M:890:LEU:HD12	2:M:914:ILE:CD1	2.46	0.40
3:N:153:LEU:HB3	9:N:1717:HOH:O	2.20	0.40
3:N:199:LEU:H	3:N:199:LEU:HG	1.60	0.40
3:N:397:LYS:HE3	3:N:448:GLU:HB3	2.04	0.40
3:N:447:VAL:HG11	9:N:1573:HOH:O	2.21	0.40
3:N:478:LEU:HD21	3:N:500:ARG:HH21	1.84	0.40
3:N:489:ARG:HG2	3:N:490:ALA:N	2.37	0.40
3:N:733:CYS:HG	3:N:740:PHE:HZ	1.66	0.40
3:N:835:SER:O	3:N:837:GLY:N	2.54	0.40
3:N:1148:VAL:HG13	3:N:1163:GLY:O	2.21	0.40
3:N:1500:LYS:O	3:N:1503:VAL:HG23	2.22	0.40
5:P:295:MET:HB3	5:P:299:TRP:CG	2.57	0.40
5:P:368:VAL:HA	9:P:506:HOH:O	2.21	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	227/315 (72%)	200 (88%)	24 (11%)	3 (1%)	9	25
1	B	227/315 (72%)	195 (86%)	29 (13%)	3 (1%)	9	25
1	K	227/315 (72%)	201 (88%)	22 (10%)	4 (2%)	6	18
1	L	227/315 (72%)	199 (88%)	25 (11%)	3 (1%)	9	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	1117/1119 (100%)	905 (81%)	154 (14%)	58 (5%)	1	3
2	M	1117/1119 (100%)	904 (81%)	153 (14%)	60 (5%)	1	2
3	D	1317/1524 (86%)	1098 (83%)	170 (13%)	49 (4%)	2	6
3	N	1317/1524 (86%)	1089 (83%)	176 (13%)	52 (4%)	2	5
4	E	93/99 (94%)	77 (83%)	12 (13%)	4 (4%)	2	4
4	O	93/99 (94%)	77 (83%)	10 (11%)	6 (6%)	1	1
5	F	341/423 (81%)	285 (84%)	37 (11%)	19 (6%)	1	2
5	P	341/423 (81%)	287 (84%)	36 (11%)	18 (5%)	1	3
All	All	6644/7590 (88%)	5517 (83%)	848 (13%)	279 (4%)	2	4

All (279) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	B	29	GLU
2	C	7	GLY
2	C	178	PRO
2	C	231	PRO
2	C	244	PRO
2	C	262	ALA
2	C	290	LEU
2	C	363	SER
2	C	369	PRO
2	C	465	GLY
2	C	517	ARG
2	C	548	PRO
2	C	598	GLU
2	C	627	ARG
2	C	767	PRO
2	C	864	GLY
2	C	908	GLY
2	C	1079	PRO
2	C	1106	ASP
3	D	55	ASP
3	D	82	LYS
3	D	136	ASP
3	D	199	LEU
3	D	610	LYS
3	D	822	ALA

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Mol	Chain	Res	Type
3	D	1129	THR
3	D	1208	ASP
3	D	1243	THR
3	D	1441	GLN
4	E	42	PRO
4	E	58	PRO
5	F	76	SER
5	F	95	THR
5	F	147	LEU
5	F	232	ARG
5	F	325	LYS
5	F	390	PHE
1	K	29	GLU
1	L	29	GLU
2	M	7	GLY
2	M	178	PRO
2	M	231	PRO
2	M	244	PRO
2	M	262	ALA
2	M	290	LEU
2	M	369	PRO
2	M	465	GLY
2	M	548	PRO
2	M	598	GLU
2	M	627	ARG
2	M	767	PRO
2	M	864	GLY
2	M	908	GLY
2	M	1079	PRO
2	M	1106	ASP
3	N	55	ASP
3	N	82	LYS
3	N	136	ASP
3	N	199	LEU
3	N	705	ALA
3	N	822	ALA
3	N	1129	THR
3	N	1208	ASP
3	N	1243	THR
4	O	42	PRO
4	O	58	PRO
5	P	76	SER

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Mol	Chain	Res	Type
5	P	95	THR
5	P	147	LEU
5	P	232	ARG
5	P	325	LYS
5	P	390	PHE
1	A	187	GLY
1	B	187	GLY
2	C	59	LYS
2	C	156	GLY
2	C	251	ASP
2	C	282	GLY
2	C	626	ARG
2	C	680	ASP
2	C	738	ASP
2	C	777	ILE
2	C	807	ARG
2	C	809	GLY
2	C	811	PRO
2	C	1004	LYS
3	D	24	GLY
3	D	98	PRO
3	D	137	PRO
3	D	504	ASP
3	D	588	GLY
3	D	616	GLN
3	D	705	ALA
3	D	803	GLY
3	D	1064	GLY
3	D	1196	THR
3	D	1265	ALA
4	E	4	PRO
5	F	153	PRO
5	F	255	ALA
5	F	416	ARG
1	K	187	GLY
1	L	187	GLY
2	M	59	LYS
2	M	156	GLY
2	M	251	ASP
2	M	282	GLY
2	M	363	SER
2	M	517	ARG

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Mol	Chain	Res	Type
2	M	626	ARG
2	M	680	ASP
2	M	738	ASP
2	M	777	ILE
2	M	807	ARG
2	M	809	GLY
2	M	811	PRO
2	M	1004	LYS
3	N	24	GLY
3	N	137	PRO
3	N	504	ASP
3	N	588	GLY
3	N	803	GLY
3	N	1064	GLY
3	N	1125	PRO
3	N	1197	ARG
3	N	1265	ALA
3	N	1342	GLU
3	N	1441	GLN
4	O	4	PRO
5	P	153	PRO
5	P	255	ALA
5	P	416	ARG
2	C	40	GLU
2	C	74	GLY
2	C	164	PRO
2	C	727	PRO
2	C	812	GLY
2	C	874	LEU
2	C	911	GLU
3	D	31	THR
3	D	47	GLU
3	D	96	ALA
3	D	119	SER
3	D	592	THR
3	D	594	PRO
3	D	807	ALA
3	D	844	ALA
3	D	1125	PRO
3	D	1197	ARG
3	D	1241	PHE
3	D	1388	ARG

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Mol	Chain	Res	Type
4	E	82	GLU
5	F	167	PRO
5	F	203	THR
5	F	286	PRO
5	F	297	PRO
5	F	341	PRO
5	F	393	THR
2	M	40	GLU
2	M	74	GLY
2	M	164	PRO
2	M	699	PHE
2	M	727	PRO
2	M	911	GLU
2	M	1045	ALA
3	N	31	THR
3	N	96	ALA
3	N	98	PRO
3	N	119	SER
3	N	592	THR
3	N	594	PRO
3	N	807	ALA
3	N	844	ALA
3	N	1111	ASP
3	N	1196	THR
3	N	1241	PHE
3	N	1388	ARG
4	O	82	GLU
5	P	167	PRO
5	P	203	THR
5	P	286	PRO
5	P	297	PRO
5	P	364	ARG
5	P	393	THR
1	A	26	GLU
2	C	111	ASP
2	C	170	PRO
2	C	250	ARG
2	C	699	PHE
2	C	1045	ALA
3	D	484	PRO
3	D	1111	ASP
3	D	1432	LYS

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Mol	Chain	Res	Type
5	F	421	PHE
2	M	111	ASP
2	M	170	PRO
2	M	188	LYS
2	M	250	ARG
2	M	268	ASP
2	M	812	GLY
3	N	484	PRO
3	N	526	PRO
3	N	617	ASN
3	N	892	ASP
3	N	1066	THR
3	N	1341	PRO
3	N	1432	LYS
5	P	421	PHE
2	C	53	PRO
2	C	188	LYS
2	C	268	ASP
2	C	400	PRO
2	C	1113	GLU
3	D	173	PRO
3	D	483	HIS
3	D	522	PRO
3	D	530	VAL
3	D	533	GLY
3	D	808	THR
3	D	892	ASP
3	D	1306	PRO
5	F	138	SER
1	K	26	GLU
2	M	10	ARG
2	M	53	PRO
2	M	90	TYR
2	M	292	ARG
2	M	984	GLU
2	M	1113	GLU
3	N	47	GLU
3	N	173	PRO
3	N	483	HIS
3	N	522	PRO
3	N	766	ALA
3	N	808	THR

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Mol	Chain	Res	Type
3	N	1306	PRO
5	P	341	PRO
2	C	10	ARG
2	C	90	TYR
2	C	180	GLY
2	C	377	PRO
2	C	1059	ASP
5	F	293	GLU
5	F	375	LEU
2	M	180	GLY
2	M	377	PRO
2	M	874	LEU
2	M	1005	MET
3	N	530	VAL
3	N	787	LEU
5	P	138	SER
2	C	336	VAL
3	D	526	PRO
3	D	1385	GLY
3	N	1385	GLY
2	C	264	PRO
2	C	415	PRO
1	K	9	PRO
2	M	261	ILE
2	M	336	VAL
2	M	415	PRO
2	M	505	GLY
3	N	1248	GLY
2	C	261	ILE
2	C	505	GLY
3	D	1248	GLY
1	L	9	PRO
2	M	264	PRO
2	M	529	VAL
3	N	1349	VAL
2	C	450	GLY
3	D	108	VAL
3	D	1267	ARG
2	M	905	ILE
3	N	108	VAL
4	O	5	GLY
4	O	57	ASP

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Mol	Chain	Res	Type
1	B	9	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	202/273 (74%)	159 (79%)	43 (21%)	1	3
1	B	202/273 (74%)	163 (81%)	39 (19%)	1	4
1	K	202/273 (74%)	157 (78%)	45 (22%)	1	3
1	L	202/273 (74%)	162 (80%)	40 (20%)	1	4
2	C	941/941 (100%)	739 (78%)	202 (22%)	1	3
2	M	941/941 (100%)	743 (79%)	198 (21%)	1	3
3	D	1112/1279 (87%)	907 (82%)	205 (18%)	1	4
3	N	1112/1279 (87%)	912 (82%)	200 (18%)	2	5
4	E	84/88 (96%)	64 (76%)	20 (24%)	1	2
4	O	84/88 (96%)	69 (82%)	15 (18%)	2	5
5	F	295/370 (80%)	245 (83%)	50 (17%)	2	6
5	P	295/370 (80%)	245 (83%)	50 (17%)	2	6
All	All	5672/6448 (88%)	4565 (80%)	1107 (20%)	1	4

All (1107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASP
1	A	9	PRO
1	A	12	THR
1	A	15	THR
1	A	16	GLN
1	A	44	LEU
1	A	45	LEU
1	A	47	SER
1	A	67	THR

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Mol	Chain	Res	Type
1	A	73	GLU
1	A	74	ASP
1	A	77	GLU
1	A	84	GLU
1	A	86	VAL
1	A	88	ARG
1	A	89	PHE
1	A	92	PRO
1	A	96	THR
1	A	101	LEU
1	A	104	GLU
1	A	115	LEU
1	A	120	VAL
1	A	121	GLU
1	A	127	LEU
1	A	133	GLU
1	A	142	VAL
1	A	154	GLU
1	A	167	VAL
1	A	170	VAL
1	A	180	GLN
1	A	184	THR
1	A	190	THR
1	A	196	THR
1	A	197	LEU
1	A	198	ARG
1	A	205	VAL
1	A	206	THR
1	A	211	LEU
1	A	216	GLU
1	A	222	LEU
1	A	223	THR
1	A	227	ASN
1	A	229	GLN
1	B	24	VAL
1	B	25	LEU
1	B	26	GLU
1	B	27	PRO
1	B	47	SER
1	B	62	LEU
1	B	67	THR
1	B	69	PRO

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Mol	Chain	Res	Type
1	B	73	GLU
1	B	77	GLU
1	B	80	LEU
1	B	82	LEU
1	B	89	PHE
1	B	96	THR
1	B	112	ARG
1	B	123	MET
1	B	126	ASP
1	B	137	ARG
1	B	140	MET
1	B	141	GLU
1	B	154	GLU
1	B	162	ILE
1	B	170	VAL
1	B	181	VAL
1	B	184	THR
1	B	188	GLN
1	B	190	THR
1	B	192	LEU
1	B	196	THR
1	B	197	LEU
1	B	200	TRP
1	B	206	THR
1	B	208	LEU
1	B	209	GLU
1	B	213	GLN
1	B	217	ILE
1	B	220	GLU
1	B	227	ASN
1	B	229	GLN
2	C	2	GLU
2	C	6	PHE
2	C	11	GLU
2	C	15	LEU
2	C	24	GLU
2	C	30	LEU
2	C	34	VAL
2	C	35	PRO
2	C	36	PRO
2	C	37	GLU
2	C	41	ASN

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Mol	Chain	Res	Type
2	C	44	ILE
2	C	48	PHE
2	C	73	LEU
2	C	89	THR
2	C	94	LEU
2	C	95	TYR
2	C	98	LEU
2	C	100	LEU
2	C	104	ASP
2	C	105	THR
2	C	108	ILE
2	C	112	GLU
2	C	113	VAL
2	C	114	PHE
2	C	115	LEU
2	C	118	ILE
2	C	129	ILE
2	C	133	ASP
2	C	140	ILE
2	C	149	THR
2	C	151	ASP
2	C	158	TYR
2	C	163	ILE
2	C	174	LEU
2	C	178	PRO
2	C	182	VAL
2	C	186	VAL
2	C	194	VAL
2	C	199	VAL
2	C	205	GLU
2	C	209	ARG
2	C	218	VAL
2	C	221	LEU
2	C	222	MET
2	C	223	ASP
2	C	226	VAL
2	C	229	MET
2	C	238	LEU
2	C	239	PHE
2	C	241	LEU
2	C	254	VAL
2	C	257	VAL

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Mol	Chain	Res	Type
2	C	260	LEU
2	C	264	PRO
2	C	267	TYR
2	C	279	GLU
2	C	281	LEU
2	C	285	LEU
2	C	290	LEU
2	C	297	GLU
2	C	303	PHE
2	C	304	LEU
2	C	309	TYR
2	C	321	GLU
2	C	322	VAL
2	C	332	ARG
2	C	339	LEU
2	C	343	GLN
2	C	359	MET
2	C	360	LEU
2	C	365	ASP
2	C	367	LEU
2	C	383	ARG
2	C	392	SER
2	C	393	GLN
2	C	396	ASP
2	C	398	THR
2	C	402	SER
2	C	413	LEU
2	C	415	PRO
2	C	420	ARG
2	C	426	ASP
2	C	427	VAL
2	C	443	THR
2	C	448	ASN
2	C	451	LEU
2	C	452	ILE
2	C	454	SER
2	C	463	GLU
2	C	469	THR
2	C	474	VAL
2	C	475	VAL
2	C	479	VAL
2	C	486	MET

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Mol	Chain	Res	Type
2	C	496	ILE
2	C	508	ILE
2	C	516	ARG
2	C	524	VAL
2	C	528	GLU
2	C	530	GLU
2	C	533	ASP
2	C	542	VAL
2	C	543	ASN
2	C	559	LEU
2	C	564	MET
2	C	566	THR
2	C	571	LEU
2	C	578	VAL
2	C	579	VAL
2	C	583	LEU
2	C	584	GLU
2	C	588	VAL
2	C	599	GLU
2	C	605	LYS
2	C	607	ASP
2	C	614	ARG
2	C	621	VAL
2	C	633	GLN
2	C	645	VAL
2	C	657	ASP
2	C	661	SER
2	C	663	ASN
2	C	668	LEU
2	C	671	ASN
2	C	672	VAL
2	C	674	VAL
2	C	676	ILE
2	C	679	PHE
2	C	685	GLU
2	C	690	ILE
2	C	699	PHE
2	C	701	THR
2	C	703	ILE
2	C	725	ASP
2	C	727	PRO
2	C	729	LEU

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Mol	Chain	Res	Type
2	C	731	GLU
2	C	734	LEU
2	C	737	LEU
2	C	758	ARG
2	C	760	SER
2	C	765	SER
2	C	769	PRO
2	C	775	ARG
2	C	780	GLU
2	C	785	VAL
2	C	799	ILE
2	C	804	VAL
2	C	813	VAL
2	C	815	LEU
2	C	821	GLU
2	C	822	VAL
2	C	838	LYS
2	C	839	LEU
2	C	841	ASN
2	C	853	LEU
2	C	861	LEU
2	C	862	PRO
2	C	863	ASP
2	C	868	ASP
2	C	870	ILE
2	C	877	PRO
2	C	881	ASN
2	C	890	LEU
2	C	901	TYR
2	C	904	PRO
2	C	905	ILE
2	C	916	GLU
2	C	923	GLU
2	C	937	ASP
2	C	950	LEU
2	C	953	VAL
2	C	959	PRO
2	C	971	LYS
2	C	972	VAL
2	C	981	GLU
2	C	984	GLU
2	C	988	VAL

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Mol	Chain	Res	Type
2	C	995	MET
2	C	1002	GLU
2	C	1016	ILE
2	C	1017	THR
2	C	1018	GLN
2	C	1030	GLN
2	C	1034	GLU
2	C	1035	MET
2	C	1036	GLU
2	C	1037	VAL
2	C	1054	THR
2	C	1060	ILE
2	C	1079	PRO
2	C	1087	VAL
2	C	1092	LEU
2	C	1095	LEU
2	C	1098	ASP
2	C	1107	ASN
2	C	1109	VAL
2	C	1110	ASP
2	C	1111	ILE
2	C	1117	SER
2	C	1118	LYS
3	D	5	VAL
3	D	12	LEU
3	D	14	SER
3	D	15	PRO
3	D	32	ILE
3	D	40	GLU
3	D	80	VAL
3	D	82	LYS
3	D	85	VAL
3	D	101	HIS
3	D	102	ILE
3	D	112	ILE
3	D	116	LEU
3	D	117	ASP
3	D	123	LEU
3	D	128	TYR
3	D	133	ILE
3	D	135	LEU
3	D	141	ILE

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Mol	Chain	Res	Type
3	D	145	VAL
3	D	147	VAL
3	D	153	LEU
3	D	155	ASP
3	D	160	GLU
3	D	161	LEU
3	D	166	GLN
3	D	171	LEU
3	D	187	LYS
3	D	189	GLN
3	D	195	VAL
3	D	197	SER
3	D	205	TYR
3	D	394	LEU
3	D	400	VAL
3	D	402	PRO
3	D	405	ASP
3	D	406	ASP
3	D	409	VAL
3	D	417	PRO
3	D	431	VAL
3	D	438	ASP
3	D	456	MET
3	D	461	ILE
3	D	465	LEU
3	D	473	LEU
3	D	489	ARG
3	D	493	ARG
3	D	504	ASP
3	D	513	ILE
3	D	521	PRO
3	D	554	LEU
3	D	565	ILE
3	D	569	ASN
3	D	573	MET
3	D	581	LEU
3	D	591	VAL
3	D	594	PRO
3	D	599	PRO
3	D	605	ASP
3	D	615	ARG
3	D	617	ASN

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Mol	Chain	Res	Type
3	D	619	LEU
3	D	624	ASP
3	D	636	GLN
3	D	641	GLN
3	D	652	LEU
3	D	660	LYS
3	D	666	ILE
3	D	682	ASP
3	D	695	ILE
3	D	704	ARG
3	D	719	VAL
3	D	724	GLN
3	D	726	ILE
3	D	736	PHE
3	D	739	ASP
3	D	741	ASP
3	D	749	VAL
3	D	752	SER
3	D	756	GLN
3	D	781	PRO
3	D	783	ARG
3	D	789	LEU
3	D	792	ILE
3	D	810	GLU
3	D	824	ASN
3	D	832	ARG
3	D	833	GLU
3	D	836	VAL
3	D	839	LEU
3	D	847	ASP
3	D	850	LEU
3	D	861	GLN
3	D	863	VAL
3	D	864	VAL
3	D	865	THR
3	D	876	SER
3	D	880	ILE
3	D	888	GLU
3	D	892	ASP
3	D	899	LEU
3	D	901	GLN
3	D	902	LEU

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Mol	Chain	Res	Type
3	D	914	LEU
3	D	915	VAL
3	D	920	LEU
3	D	942	SER
3	D	944	THR
3	D	948	THR
3	D	951	ILE
3	D	958	GLU
3	D	959	GLU
3	D	964	LEU
3	D	968	ASP
3	D	972	LEU
3	D	975	GLU
3	D	984	THR
3	D	985	ASP
3	D	999	THR
3	D	1001	GLU
3	D	1003	VAL
3	D	1022	VAL
3	D	1023	MET
3	D	1025	GLN
3	D	1032	PRO
3	D	1033	GLN
3	D	1038	LEU
3	D	1041	LEU
3	D	1051	GLU
3	D	1052	THR
3	D	1065	LEU
3	D	1068	LEU
3	D	1074	SER
3	D	1083	ASP
3	D	1088	THR
3	D	1095	THR
3	D	1099	VAL
3	D	1109	GLU
3	D	1111	ASP
3	D	1112	CYS
3	D	1115	THR
3	D	1116	ASN
3	D	1129	THR
3	D	1132	LEU
3	D	1134	LEU

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Mol	Chain	Res	Type
3	D	1151	ARG
3	D	1161	GLU
3	D	1166	LEU
3	D	1173	LEU
3	D	1183	ILE
3	D	1188	VAL
3	D	1191	PRO
3	D	1198	TYR
3	D	1207	TYR
3	D	1223	ILE
3	D	1228	SER
3	D	1234	THR
3	D	1236	LEU
3	D	1243	THR
3	D	1251	ASP
3	D	1252	ILE
3	D	1260	ILE
3	D	1274	ILE
3	D	1280	VAL
3	D	1288	GLU
3	D	1290	LEU
3	D	1299	PHE
3	D	1302	GLU
3	D	1305	LEU
3	D	1306	PRO
3	D	1315	ASP
3	D	1320	GLU
3	D	1344	VAL
3	D	1345	GLU
3	D	1348	LEU
3	D	1350	GLU
3	D	1359	GLN
3	D	1363	LEU
3	D	1366	LYS
3	D	1368	ILE
3	D	1382	THR
3	D	1383	ASP
3	D	1387	SER
3	D	1403	LEU
3	D	1407	LEU
3	D	1415	VAL
3	D	1420	LEU

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Mol	Chain	Res	Type
3	D	1431	THR
3	D	1433	SER
3	D	1435	LEU
3	D	1439	SER
3	D	1440	PHE
3	D	1441	GLN
3	D	1460	ILE
3	D	1462	LEU
3	D	1465	ASN
3	D	1466	VAL
3	D	1468	LEU
3	D	1478	SER
3	D	1481	VAL
3	D	1485	GLN
3	D	1488	ASP
3	D	1491	THR
3	D	1492	LEU
3	D	1496	GLU
4	E	4	PRO
4	E	20	THR
4	E	28	GLN
4	E	30	LEU
4	E	41	GLU
4	E	42	PRO
4	E	43	GLU
4	E	46	PRO
4	E	51	LEU
4	E	56	ASP
4	E	57	ASP
4	E	58	PRO
4	E	61	VAL
4	E	62	THR
4	E	67	GLU
4	E	69	LEU
4	E	72	ARG
4	E	79	LEU
4	E	81	PRO
4	E	94	PRO
5	F	80	PRO
5	F	83	GLN
5	F	84	TYR
5	F	86	HIS

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Mol	Chain	Res	Type
5	F	91	VAL
5	F	94	LEU
5	F	117	SER
5	F	122	LEU
5	F	123	ASP
5	F	125	ASP
5	F	127	ILE
5	F	135	ILE
5	F	145	PRO
5	F	149	GLU
5	F	150	THR
5	F	151	LEU
5	F	159	ILE
5	F	169	GLU
5	F	174	LEU
5	F	178	ARG
5	F	192	LEU
5	F	194	LEU
5	F	197	SER
5	F	225	GLU
5	F	228	GLU
5	F	240	THR
5	F	245	GLN
5	F	249	ARG
5	F	262	VAL
5	F	281	GLU
5	F	282	LEU
5	F	291	ILE
5	F	297	PRO
5	F	312	GLN
5	F	316	SER
5	F	317	LEU
5	F	335	ASP
5	F	336	GLU
5	F	341	PRO
5	F	342	VAL
5	F	348	SER
5	F	351	SER
5	F	353	GLU
5	F	362	SER
5	F	393	THR
5	F	399	GLN

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Mol	Chain	Res	Type
5	F	407	LYS
5	F	408	LEU
5	F	410	TYR
5	F	420	ASP
1	K	3	ASP
1	K	9	PRO
1	K	12	THR
1	K	15	THR
1	K	16	GLN
1	K	44	LEU
1	K	45	LEU
1	K	47	SER
1	K	67	THR
1	K	73	GLU
1	K	74	ASP
1	K	80	LEU
1	K	82	LEU
1	K	84	GLU
1	K	86	VAL
1	K	88	ARG
1	K	89	PHE
1	K	92	PRO
1	K	96	THR
1	K	101	LEU
1	K	104	GLU
1	K	115	LEU
1	K	120	VAL
1	K	121	GLU
1	K	127	LEU
1	K	133	GLU
1	K	142	VAL
1	K	154	GLU
1	K	167	VAL
1	K	170	VAL
1	K	180	GLN
1	K	184	THR
1	K	188	GLN
1	K	190	THR
1	K	196	THR
1	K	197	LEU
1	K	198	ARG
1	K	205	VAL

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Mol	Chain	Res	Type
1	K	206	THR
1	K	211	LEU
1	K	216	GLU
1	K	222	LEU
1	K	223	THR
1	K	227	ASN
1	K	229	GLN
1	L	9	PRO
1	L	24	VAL
1	L	26	GLU
1	L	27	PRO
1	L	38	ASN
1	L	44	LEU
1	L	62	LEU
1	L	67	THR
1	L	69	PRO
1	L	71	VAL
1	L	73	GLU
1	L	77	GLU
1	L	80	LEU
1	L	82	LEU
1	L	89	PHE
1	L	96	THR
1	L	109	VAL
1	L	123	MET
1	L	126	ASP
1	L	137	ARG
1	L	138	LEU
1	L	140	MET
1	L	141	GLU
1	L	154	GLU
1	L	162	ILE
1	L	173	PRO
1	L	184	THR
1	L	188	GLN
1	L	190	THR
1	L	192	LEU
1	L	196	THR
1	L	197	LEU
1	L	200	TRP
1	L	206	THR
1	L	207	PRO

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Mol	Chain	Res	Type
1	L	208	LEU
1	L	209	GLU
1	L	217	ILE
1	L	227	ASN
1	L	229	GLN
2	M	2	GLU
2	M	11	GLU
2	M	24	GLU
2	M	30	LEU
2	M	34	VAL
2	M	35	PRO
2	M	37	GLU
2	M	41	ASN
2	M	44	ILE
2	M	48	PHE
2	M	51	THR
2	M	73	LEU
2	M	79	PRO
2	M	81	ASP
2	M	89	THR
2	M	94	LEU
2	M	95	TYR
2	M	98	LEU
2	M	100	LEU
2	M	104	ASP
2	M	105	THR
2	M	108	ILE
2	M	112	GLU
2	M	113	VAL
2	M	114	PHE
2	M	115	LEU
2	M	117	HIS
2	M	118	ILE
2	M	129	ILE
2	M	133	ASP
2	M	140	ILE
2	M	149	THR
2	M	150	PRO
2	M	158	TYR
2	M	163	ILE
2	M	182	VAL
2	M	186	VAL

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Mol	Chain	Res	Type
2	M	194	VAL
2	M	205	GLU
2	M	209	ARG
2	M	218	VAL
2	M	219	GLN
2	M	221	LEU
2	M	222	MET
2	M	226	VAL
2	M	229	MET
2	M	235	LEU
2	M	238	LEU
2	M	239	PHE
2	M	241	LEU
2	M	254	VAL
2	M	257	VAL
2	M	260	LEU
2	M	264	PRO
2	M	267	TYR
2	M	275	TYR
2	M	279	GLU
2	M	281	LEU
2	M	285	LEU
2	M	289	THR
2	M	290	LEU
2	M	297	GLU
2	M	303	PHE
2	M	304	LEU
2	M	309	TYR
2	M	321	GLU
2	M	322	VAL
2	M	332	ARG
2	M	339	LEU
2	M	343	GLN
2	M	348	LEU
2	M	359	MET
2	M	360	LEU
2	M	365	ASP
2	M	366	SER
2	M	367	LEU
2	M	384	GLU
2	M	392	SER
2	M	393	GLN

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Mol	Chain	Res	Type
2	M	402	SER
2	M	413	LEU
2	M	415	PRO
2	M	420	ARG
2	M	426	ASP
2	M	427	VAL
2	M	443	THR
2	M	448	ASN
2	M	451	LEU
2	M	452	ILE
2	M	454	SER
2	M	463	GLU
2	M	469	THR
2	M	474	VAL
2	M	479	VAL
2	M	502	PRO
2	M	508	ILE
2	M	516	ARG
2	M	524	VAL
2	M	527	GLU
2	M	528	GLU
2	M	533	ASP
2	M	537	LYS
2	M	542	VAL
2	M	543	ASN
2	M	559	LEU
2	M	564	MET
2	M	566	THR
2	M	571	LEU
2	M	579	VAL
2	M	583	LEU
2	M	584	GLU
2	M	588	VAL
2	M	599	GLU
2	M	605	LYS
2	M	607	ASP
2	M	614	ARG
2	M	619	ARG
2	M	633	GLN
2	M	645	VAL
2	M	661	SER
2	M	663	ASN

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Mol	Chain	Res	Type
2	M	668	LEU
2	M	671	ASN
2	M	672	VAL
2	M	674	VAL
2	M	679	PHE
2	M	690	ILE
2	M	699	PHE
2	M	701	THR
2	M	703	ILE
2	M	725	ASP
2	M	727	PRO
2	M	729	LEU
2	M	731	GLU
2	M	734	LEU
2	M	737	LEU
2	M	758	ARG
2	M	760	SER
2	M	765	SER
2	M	769	PRO
2	M	775	ARG
2	M	785	VAL
2	M	794	PRO
2	M	799	ILE
2	M	804	VAL
2	M	813	VAL
2	M	815	LEU
2	M	821	GLU
2	M	822	VAL
2	M	838	LYS
2	M	839	LEU
2	M	841	ASN
2	M	853	LEU
2	M	861	LEU
2	M	862	PRO
2	M	863	ASP
2	M	870	ILE
2	M	881	ASN
2	M	890	LEU
2	M	901	TYR
2	M	904	PRO
2	M	905	ILE
2	M	907	ASP

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Mol	Chain	Res	Type
2	M	911	GLU
2	M	914	ILE
2	M	916	GLU
2	M	917	LEU
2	M	923	GLU
2	M	937	ASP
2	M	948	GLU
2	M	950	LEU
2	M	953	VAL
2	M	959	PRO
2	M	963	LEU
2	M	972	VAL
2	M	981	GLU
2	M	984	GLU
2	M	988	VAL
2	M	995	MET
2	M	1002	GLU
2	M	1016	ILE
2	M	1017	THR
2	M	1018	GLN
2	M	1030	GLN
2	M	1035	MET
2	M	1036	GLU
2	M	1037	VAL
2	M	1054	THR
2	M	1060	ILE
2	M	1079	PRO
2	M	1087	VAL
2	M	1092	LEU
2	M	1098	ASP
2	M	1107	ASN
2	M	1109	VAL
2	M	1110	ASP
2	M	1117	SER
2	M	1118	LYS
3	N	3	LYS
3	N	5	VAL
3	N	12	LEU
3	N	14	SER
3	N	15	PRO
3	N	20	SER
3	N	32	ILE

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Mol	Chain	Res	Type
3	N	40	GLU
3	N	80	VAL
3	N	82	LYS
3	N	85	VAL
3	N	95	LEU
3	N	101	HIS
3	N	102	ILE
3	N	112	ILE
3	N	115	LEU
3	N	116	LEU
3	N	117	ASP
3	N	123	LEU
3	N	128	TYR
3	N	133	ILE
3	N	135	LEU
3	N	136	ASP
3	N	141	ILE
3	N	145	VAL
3	N	147	VAL
3	N	153	LEU
3	N	155	ASP
3	N	160	GLU
3	N	166	GLN
3	N	171	LEU
3	N	187	LYS
3	N	189	GLN
3	N	193	PRO
3	N	197	SER
3	N	205	TYR
3	N	394	LEU
3	N	400	VAL
3	N	402	PRO
3	N	405	ASP
3	N	406	ASP
3	N	409	VAL
3	N	431	VAL
3	N	438	ASP
3	N	440	VAL
3	N	449	SER
3	N	456	MET
3	N	461	ILE
3	N	465	LEU

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Mol	Chain	Res	Type
3	N	473	LEU
3	N	489	ARG
3	N	493	ARG
3	N	504	ASP
3	N	505	SER
3	N	521	PRO
3	N	565	ILE
3	N	569	ASN
3	N	581	LEU
3	N	590	PRO
3	N	591	VAL
3	N	594	PRO
3	N	605	ASP
3	N	614	PHE
3	N	615	ARG
3	N	617	ASN
3	N	619	LEU
3	N	624	ASP
3	N	636	GLN
3	N	639	LEU
3	N	641	GLN
3	N	652	LEU
3	N	660	LYS
3	N	661	MET
3	N	682	ASP
3	N	695	ILE
3	N	704	ARG
3	N	717	GLN
3	N	719	VAL
3	N	724	GLN
3	N	726	ILE
3	N	736	PHE
3	N	739	ASP
3	N	741	ASP
3	N	749	VAL
3	N	781	PRO
3	N	783	ARG
3	N	792	ILE
3	N	810	GLU
3	N	824	ASN
3	N	832	ARG
3	N	833	GLU

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Mol	Chain	Res	Type
3	N	836	VAL
3	N	839	LEU
3	N	847	ASP
3	N	863	VAL
3	N	864	VAL
3	N	865	THR
3	N	880	ILE
3	N	888	GLU
3	N	892	ASP
3	N	899	LEU
3	N	901	GLN
3	N	910	SER
3	N	915	VAL
3	N	942	SER
3	N	944	THR
3	N	948	THR
3	N	951	ILE
3	N	958	GLU
3	N	959	GLU
3	N	968	ASP
3	N	972	LEU
3	N	975	GLU
3	N	987	GLU
3	N	1001	GLU
3	N	1003	VAL
3	N	1022	VAL
3	N	1023	MET
3	N	1025	GLN
3	N	1032	PRO
3	N	1033	GLN
3	N	1038	LEU
3	N	1041	LEU
3	N	1051	GLU
3	N	1052	THR
3	N	1065	LEU
3	N	1068	LEU
3	N	1083	ASP
3	N	1088	THR
3	N	1095	THR
3	N	1099	VAL
3	N	1109	GLU
3	N	1112	CYS

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Mol	Chain	Res	Type
3	N	1115	THR
3	N	1116	ASN
3	N	1129	THR
3	N	1132	LEU
3	N	1133	ARG
3	N	1134	LEU
3	N	1151	ARG
3	N	1161	GLU
3	N	1166	LEU
3	N	1173	LEU
3	N	1183	ILE
3	N	1198	TYR
3	N	1207	TYR
3	N	1210	SER
3	N	1215	VAL
3	N	1223	ILE
3	N	1228	SER
3	N	1243	THR
3	N	1251	ASP
3	N	1252	ILE
3	N	1258	ARG
3	N	1259	VAL
3	N	1260	ILE
3	N	1274	ILE
3	N	1280	VAL
3	N	1288	GLU
3	N	1290	LEU
3	N	1295	GLU
3	N	1299	PHE
3	N	1300	SER
3	N	1302	GLU
3	N	1305	LEU
3	N	1306	PRO
3	N	1315	ASP
3	N	1320	GLU
3	N	1344	VAL
3	N	1345	GLU
3	N	1348	LEU
3	N	1350	GLU
3	N	1363	LEU
3	N	1366	LYS
3	N	1377	LYS

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Mol	Chain	Res	Type
3	N	1382	THR
3	N	1383	ASP
3	N	1389	LEU
3	N	1403	LEU
3	N	1407	LEU
3	N	1415	VAL
3	N	1419	PRO
3	N	1420	LEU
3	N	1424	VAL
3	N	1431	THR
3	N	1433	SER
3	N	1440	PHE
3	N	1441	GLN
3	N	1460	ILE
3	N	1462	LEU
3	N	1465	ASN
3	N	1466	VAL
3	N	1468	LEU
3	N	1478	SER
3	N	1481	VAL
3	N	1485	GLN
3	N	1488	ASP
3	N	1491	THR
3	N	1495	ILE
3	N	1496	GLU
4	O	4	PRO
4	O	20	THR
4	O	30	LEU
4	O	41	GLU
4	O	42	PRO
4	O	43	GLU
4	O	46	PRO
4	O	51	LEU
4	O	56	ASP
4	O	57	ASP
4	O	62	THR
4	O	67	GLU
4	O	79	LEU
4	O	81	PRO
4	O	94	PRO
5	P	80	PRO
5	P	83	GLN

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Mol	Chain	Res	Type
5	P	84	TYR
5	P	86	HIS
5	P	91	VAL
5	P	94	LEU
5	P	117	SER
5	P	122	LEU
5	P	123	ASP
5	P	125	ASP
5	P	127	ILE
5	P	131	VAL
5	P	135	ILE
5	P	145	PRO
5	P	148	LYS
5	P	149	GLU
5	P	151	LEU
5	P	159	ILE
5	P	161	GLN
5	P	174	LEU
5	P	178	ARG
5	P	192	LEU
5	P	194	LEU
5	P	208	SER
5	P	225	GLU
5	P	240	THR
5	P	245	GLN
5	P	249	ARG
5	P	261	PRO
5	P	262	VAL
5	P	281	GLU
5	P	282	LEU
5	P	291	ILE
5	P	297	PRO
5	P	317	LEU
5	P	335	ASP
5	P	336	GLU
5	P	338	LEU
5	P	341	PRO
5	P	342	VAL
5	P	351	SER
5	P	353	GLU
5	P	361	LEU
5	P	362	SER

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Mol	Chain	Res	Type
5	P	393	THR
5	P	399	GLN
5	P	407	LYS
5	P	408	LEU
5	P	410	TYR
5	P	420	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (187) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	81	ASN
1	A	95	GLN
1	A	124	ASN
1	A	139	ASN
1	A	156	HIS
1	A	180	GLN
1	A	221	HIS
1	A	227	ASN
1	A	229	GLN
1	B	38	ASN
1	B	95	GLN
1	B	124	ASN
1	B	128	HIS
1	B	163	ASN
1	B	180	GLN
1	B	213	GLN
1	B	227	ASN
2	C	22	GLN
2	C	31	GLN
2	C	41	ASN
2	C	99	GLN
2	C	117	HIS
2	C	139	GLN
2	C	204	GLN
2	C	320	HIS
2	C	343	GLN
2	C	390	GLN
2	C	393	GLN
2	C	399	ASN
2	C	431	HIS
2	C	434	HIS

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Mol	Chain	Res	Type
2	C	498	GLN
2	C	552	HIS
2	C	609	ASN
2	C	632	ASN
2	C	639	GLN
2	C	663	ASN
2	C	670	GLN
2	C	671	ASN
2	C	834	GLN
2	C	841	ASN
2	C	845	ASN
2	C	881	ASN
2	C	889	HIS
2	C	899	GLN
2	C	969	GLN
2	C	991	GLN
2	C	1018	GLN
2	C	1019	GLN
2	C	1026	GLN
2	C	1047	HIS
2	C	1050	GLN
3	D	33	ASN
3	D	143	ASN
3	D	151	GLN
3	D	166	GLN
3	D	507	ASN
3	D	549	ASN
3	D	611	GLN
3	D	696	HIS
3	D	727	GLN
3	D	756	GLN
3	D	816	HIS
3	D	824	ASN
3	D	861	GLN
3	D	917	GLN
3	D	962	GLN
3	D	994	GLN
3	D	1014	ASN
3	D	1025	GLN
3	D	1116	ASN
3	D	1172	HIS
3	D	1195	GLN

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Mol	Chain	Res	Type
3	D	1202	GLN
3	D	1323	GLN
3	D	1359	GLN
3	D	1441	GLN
3	D	1465	ASN
3	D	1485	GLN
4	E	28	GLN
4	E	37	ASN
4	E	86	GLN
5	F	83	GLN
5	F	86	HIS
5	F	90	GLN
5	F	186	HIS
5	F	245	GLN
5	F	263	HIS
5	F	312	GLN
5	F	337	HIS
5	F	402	ASN
1	K	16	GLN
1	K	81	ASN
1	K	124	ASN
1	K	128	HIS
1	K	139	ASN
1	K	156	HIS
1	K	163	ASN
1	K	180	GLN
1	K	227	ASN
1	K	229	GLN
1	L	38	ASN
1	L	95	GLN
1	L	124	ASN
1	L	128	HIS
1	L	163	ASN
1	L	180	GLN
1	L	213	GLN
1	L	227	ASN
2	M	22	GLN
2	M	31	GLN
2	M	41	ASN
2	M	80	GLN
2	M	102	HIS
2	M	117	HIS

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Mol	Chain	Res	Type
2	M	130	ASN
2	M	139	GLN
2	M	179	ASN
2	M	204	GLN
2	M	219	GLN
2	M	320	HIS
2	M	343	GLN
2	M	374	ASN
2	M	393	GLN
2	M	431	HIS
2	M	434	HIS
2	M	498	GLN
2	M	556	ASN
2	M	565	GLN
2	M	609	ASN
2	M	632	ASN
2	M	639	GLN
2	M	663	ASN
2	M	670	GLN
2	M	671	ASN
2	M	834	GLN
2	M	841	ASN
2	M	881	ASN
2	M	889	HIS
2	M	899	GLN
2	M	969	GLN
2	M	991	GLN
2	M	1019	GLN
3	N	143	ASN
3	N	151	GLN
3	N	166	GLN
3	N	507	ASN
3	N	549	ASN
3	N	593	ASN
3	N	611	GLN
3	N	640	HIS
3	N	696	HIS
3	N	709	HIS
3	N	727	GLN
3	N	744	GLN
3	N	748	HIS
3	N	756	GLN

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Mol	Chain	Res	Type
3	N	768	ASN
3	N	824	ASN
3	N	861	GLN
3	N	1010	ASN
3	N	1014	ASN
3	N	1025	GLN
3	N	1033	GLN
3	N	1046	GLN
3	N	1116	ASN
3	N	1184	GLN
3	N	1195	GLN
3	N	1202	GLN
3	N	1323	GLN
3	N	1359	GLN
3	N	1465	ASN
3	N	1485	GLN
3	N	1489	GLN
4	O	28	GLN
4	O	37	ASN
4	O	86	GLN
5	P	83	GLN
5	P	86	HIS
5	P	90	GLN
5	P	214	GLN
5	P	245	GLN
5	P	279	GLN
5	P	312	GLN
5	P	337	HIS
5	P	402	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MXP	D	1527	-	30,30,30	2.12	12 (40%)	33,38,38	3.48	14 (42%)
7	MXP	N	1527	-	30,30,30	2.35	13 (43%)	33,38,38	3.70	15 (45%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MXP	D	1527	-	-	10/28/28/28	0/1/1/1
7	MXP	N	1527	-	-	10/28/28/28	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	N	1527	MXP	C1-C5	4.35	1.45	1.34
7	N	1527	MXP	C21-C20	4.32	1.38	1.32
7	D	1527	MXP	O6-C22	4.30	1.29	1.21
7	N	1527	MXP	O5-C22	-4.23	1.27	1.34
7	D	1527	MXP	C9-C8	3.98	1.56	1.42
7	D	1527	MXP	C21-C20	3.96	1.38	1.32
7	N	1527	MXP	C9-C8	3.90	1.56	1.42
7	N	1527	MXP	O2-C2	3.71	1.43	1.33
7	N	1527	MXP	O6-C22	3.55	1.28	1.21
7	D	1527	MXP	O5-C22	-3.53	1.28	1.34
7	N	1527	MXP	C8-C7	3.23	1.43	1.34
7	N	1527	MXP	C7-C6	3.20	1.55	1.48
7	D	1527	MXP	O1-C5	3.20	1.43	1.37
7	N	1527	MXP	O1-C5	3.19	1.43	1.37
7	D	1527	MXP	O5-C23	-3.18	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	1527	MXP	C8-C7	2.83	1.42	1.34
7	N	1527	MXP	O5-C23	-2.76	1.39	1.45
7	D	1527	MXP	C1-C5	2.65	1.41	1.34
7	N	1527	MXP	O1-C4	2.46	1.44	1.39
7	D	1527	MXP	C7-C6	2.39	1.53	1.48
7	D	1527	MXP	C3-C6	2.32	1.59	1.46
7	N	1527	MXP	C3-C6	2.18	1.58	1.46
7	D	1527	MXP	C3-C2	2.07	1.45	1.41
7	N	1527	MXP	C9-C10	2.04	1.41	1.35
7	D	1527	MXP	O2-C2	2.04	1.39	1.33

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	1527	MXP	O4-C6-C7	11.57	138.42	120.85
7	D	1527	MXP	O4-C6-C7	10.79	137.24	120.85
7	N	1527	MXP	C9-C8-C7	-8.64	113.82	126.48
7	D	1527	MXP	C9-C8-C7	-7.79	115.06	126.48
7	D	1527	MXP	O1-C5-C17	6.49	119.05	110.54
7	D	1527	MXP	C23-O5-C22	6.25	122.86	115.63
7	N	1527	MXP	C23-O5-C22	6.05	122.63	115.63
7	N	1527	MXP	O1-C5-C17	6.04	118.46	110.54
7	N	1527	MXP	O1-C5-C1	-5.74	117.16	121.99
7	N	1527	MXP	C15-C7-C6	5.53	124.54	115.68
7	N	1527	MXP	O5-C22-N1	5.12	115.04	109.15
7	D	1527	MXP	C15-C7-C6	5.09	123.84	115.68
7	D	1527	MXP	O5-C22-N1	4.73	114.59	109.15
7	D	1527	MXP	O1-C5-C1	-4.22	118.44	121.99
7	N	1527	MXP	O6-C22-N1	-3.82	120.10	125.44
7	D	1527	MXP	O6-C22-N1	-3.70	120.27	125.44
7	N	1527	MXP	O2-C2-C3	-3.04	118.35	121.83
7	N	1527	MXP	C19-C20-C21	-2.84	112.12	122.79
7	D	1527	MXP	O1-C4-C3	2.72	121.19	117.23
7	D	1527	MXP	O3-C4-C3	-2.63	118.99	126.75
7	D	1527	MXP	C19-C20-C21	-2.63	112.93	122.79
7	N	1527	MXP	O1-C4-C3	2.59	121.00	117.23
7	D	1527	MXP	O1-C4-O3	2.53	119.82	115.24
7	D	1527	MXP	C12-C11-C10	2.46	119.46	113.47
7	N	1527	MXP	C12-C11-C10	2.44	119.42	113.47
7	N	1527	MXP	C2-C3-C4	-2.26	116.85	118.39
7	D	1527	MXP	C4-C3-C6	2.19	127.17	117.54
7	N	1527	MXP	C2-C1-C5	2.12	121.80	118.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	1527	MXP	O3-C4-C3	-2.11	120.54	126.75

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	1527	MXP	C3-C6-C7-C15
7	N	1527	MXP	C3-C6-C7-C15
7	D	1527	MXP	C10-C11-C12-C13
7	D	1527	MXP	C18-C17-C5-C1
7	N	1527	MXP	C18-C17-C5-C1
7	N	1527	MXP	C10-C11-C12-C13
7	D	1527	MXP	C18-C17-C5-O1
7	N	1527	MXP	C18-C17-C5-O1
7	N	1527	MXP	C18-C19-C20-C21
7	D	1527	MXP	O4-C6-C7-C8
7	D	1527	MXP	O4-C6-C7-C15
7	N	1527	MXP	O4-C6-C7-C8
7	N	1527	MXP	O4-C6-C7-C15
7	D	1527	MXP	C18-C19-C20-C21
7	D	1527	MXP	C16-C10-C11-C12
7	N	1527	MXP	C16-C10-C11-C12
7	N	1527	MXP	C9-C10-C11-C12
7	D	1527	MXP	C9-C10-C11-C12
7	N	1527	MXP	C5-C17-C18-C19
7	D	1527	MXP	C5-C17-C18-C19

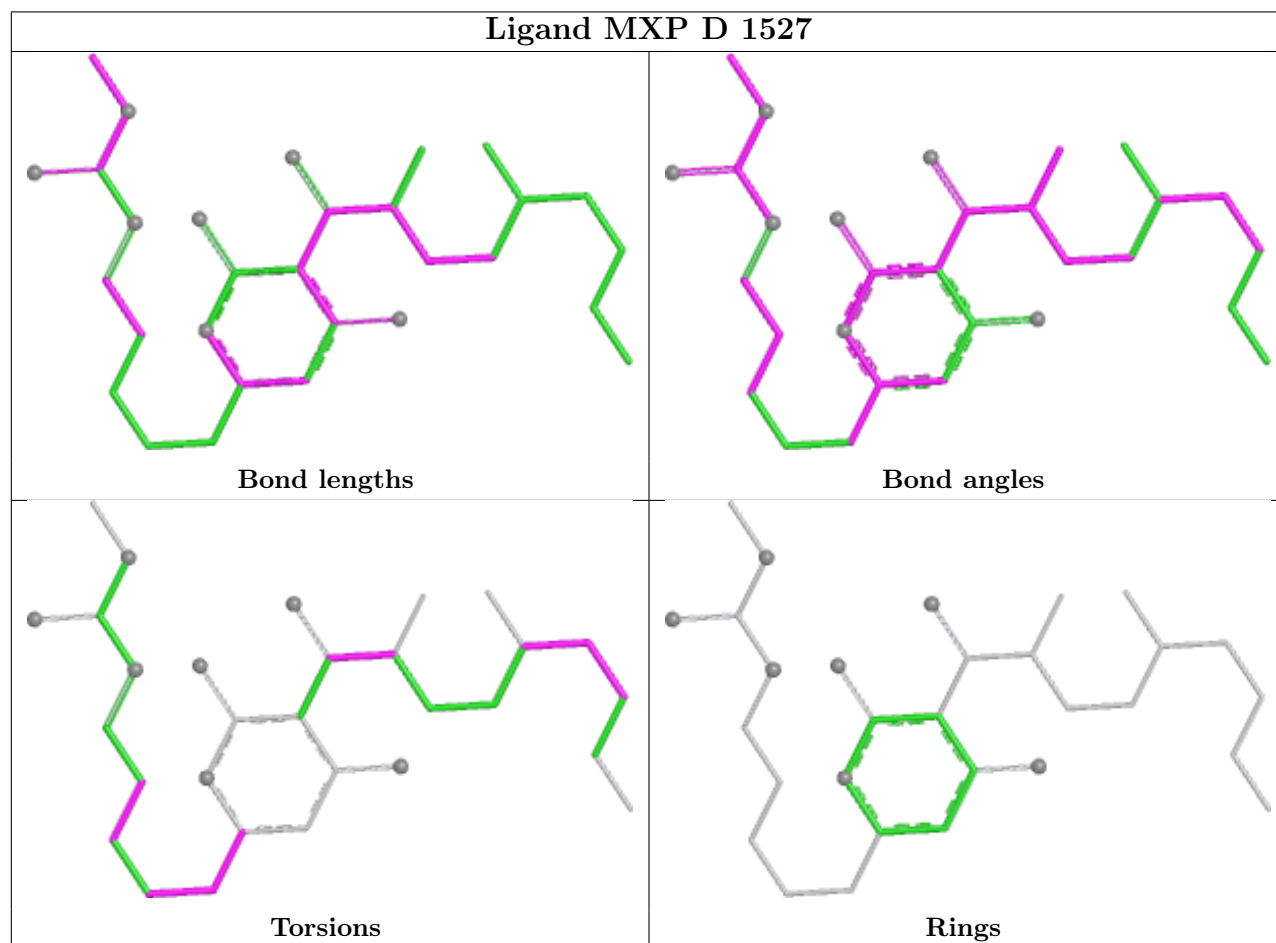
There are no ring outliers.

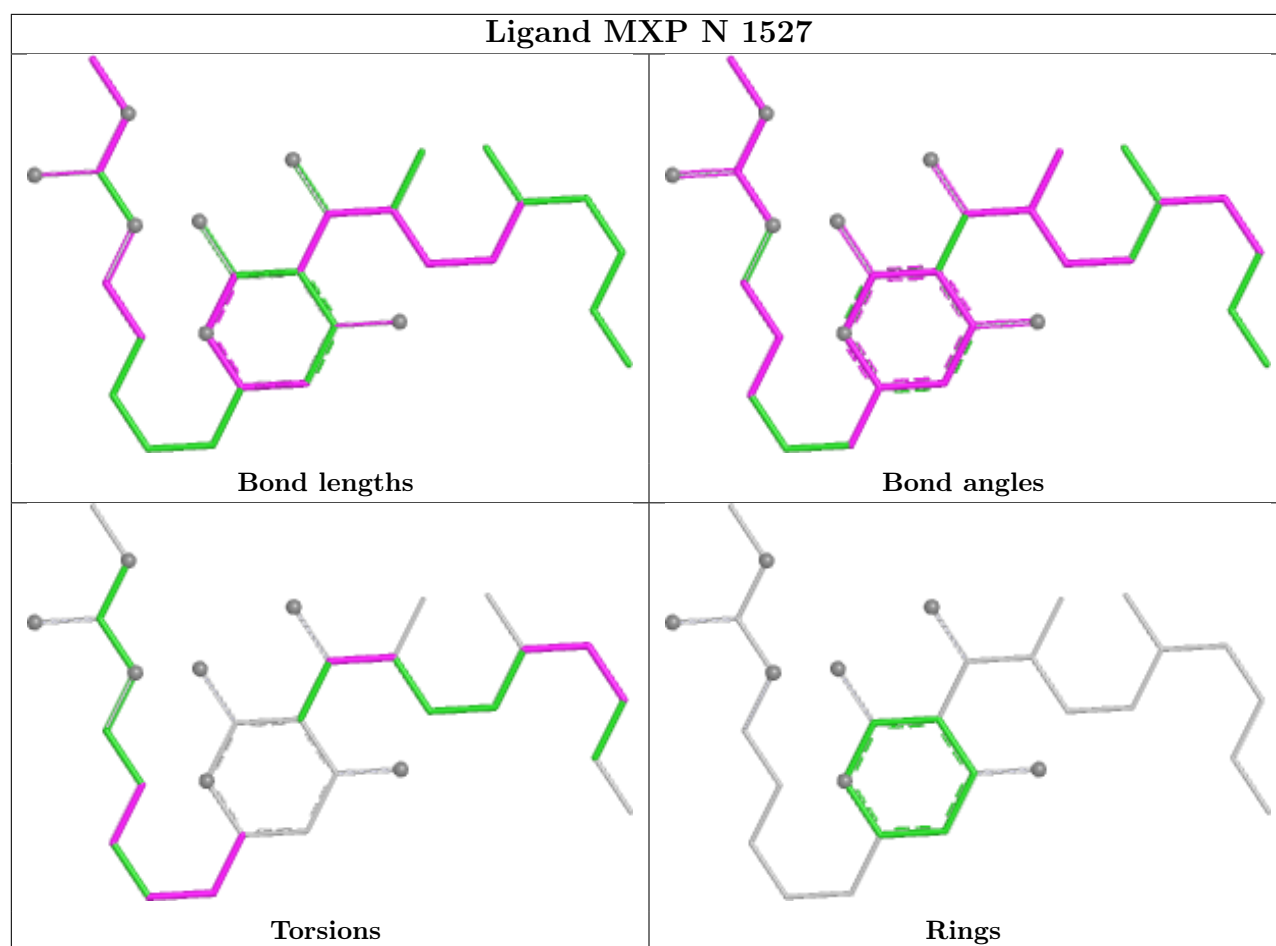
2 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	1527	MXP	18	0
7	N	1527	MXP	18	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	229/315 (72%)	0.67	15 (6%) 24 21	28, 50, 78, 101	0
1	B	229/315 (72%)	0.98	26 (11%) 10 8	36, 71, 86, 104	0
1	K	229/315 (72%)	0.73	15 (6%) 24 21	25, 52, 81, 93	0
1	L	229/315 (72%)	1.08	33 (14%) 6 5	47, 73, 86, 104	0
2	C	1119/1119 (100%)	0.86	145 (12%) 7 6	14, 62, 88, 96	0
2	M	1119/1119 (100%)	0.79	112 (10%) 12 10	11, 60, 86, 101	0
3	D	1321/1524 (86%)	0.75	130 (9%) 13 11	10, 53, 85, 107	0
3	N	1321/1524 (86%)	0.73	139 (10%) 11 9	11, 54, 84, 109	0
4	E	95/99 (95%)	0.98	16 (16%) 4 3	30, 64, 90, 95	0
4	O	95/99 (95%)	0.85	11 (11%) 9 8	29, 61, 83, 100	0
5	F	345/423 (81%)	1.02	49 (14%) 6 5	27, 68, 89, 100	0
5	P	345/423 (81%)	1.01	42 (12%) 8 7	23, 68, 91, 103	0
All	All	6676/7590 (87%)	0.82	733 (10%) 10 9	10, 59, 87, 109	0

All (733) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	1241	PHE	8.4
4	O	95	VAL	7.7
3	D	1248	GLY	7.5
3	N	1240	THR	7.5
3	D	43	GLY	6.7
2	C	186	VAL	6.6
3	N	1243	THR	6.4
4	E	95	VAL	6.4
3	N	839	LEU	6.3
5	F	144	ILE	6.1
2	M	417	GLY	6.0

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Mol	Chain	Res	Type	RSRZ
3	N	802	ALA	5.9
5	P	90	GLN	5.9
3	D	1240	THR	5.7
3	D	1398	TRP	5.7
2	C	182	VAL	5.6
2	M	182	VAL	5.6
5	F	142	ARG	5.5
2	M	186	VAL	5.4
3	N	191	LEU	5.4
3	N	1398	TRP	5.4
2	C	164	PRO	5.3
2	M	418	LEU	5.2
3	D	1246	VAL	5.2
3	N	1252	ILE	5.1
2	M	176	VAL	5.1
3	N	611	GLN	5.1
2	C	307	LEU	5.1
3	D	1245	GLY	5.0
2	C	417	GLY	5.0
5	P	422	LEU	4.9
3	N	450	TYR	4.8
3	N	1248	GLY	4.8
3	D	422	ALA	4.8
3	D	561	GLY	4.7
1	A	157	GLY	4.7
3	D	395	VAL	4.7
5	P	145	PRO	4.7
3	D	611	GLN	4.7
1	A	93	SER	4.6
1	K	6	LEU	4.5
3	N	612	GLY	4.5
3	N	1247	ALA	4.5
3	D	407	VAL	4.5
3	D	1242	HIS	4.5
3	N	816	HIS	4.5
4	E	56	ASP	4.5
5	P	378	GLY	4.5
2	C	372	LEU	4.4
2	C	125	GLY	4.4
2	C	65	VAL	4.4
3	N	1238	MET	4.4
3	D	612	GLY	4.4

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Mol	Chain	Res	Type	RSRZ
3	D	1249	ALA	4.4
4	E	2	ALA	4.4
3	N	412	GLY	4.4
3	D	802	ALA	4.3
2	C	306	THR	4.3
1	K	158	ILE	4.3
3	N	1241	PHE	4.3
2	C	529	VAL	4.3
2	M	372	LEU	4.3
3	N	1242	HIS	4.3
3	N	806	PHE	4.3
2	C	226	VAL	4.3
3	N	119	SER	4.2
3	D	409	VAL	4.2
2	C	170	PRO	4.2
5	F	415	THR	4.1
3	D	1247	ALA	4.1
3	D	1250	ALA	4.1
5	P	142	ARG	4.1
3	N	203	ALA	4.1
3	N	193	PRO	4.0
3	N	853	VAL	4.0
2	C	289	THR	4.0
2	C	517	ARG	4.0
2	M	181	VAL	4.0
5	P	141	VAL	4.0
3	N	1237	THR	4.0
2	C	180	GLY	3.9
3	N	43	GLY	3.9
4	O	57	ASP	3.9
4	E	92	LEU	3.9
2	M	615	TYR	3.9
5	P	147	LEU	3.8
4	O	94	PRO	3.8
3	D	1210	SER	3.8
1	A	158	ILE	3.8
2	C	318	PRO	3.8
3	D	1252	ILE	3.8
3	N	505	SER	3.8
5	F	389	PHE	3.8
2	C	513	VAL	3.8
5	F	139	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
2	C	260	LEU	3.7
1	L	162	ILE	3.7
5	P	376	ILE	3.7
5	P	357	ALA	3.7
3	D	391	ALA	3.7
3	N	1246	VAL	3.7
1	K	2	LEU	3.7
2	C	207	LEU	3.7
2	C	269	LEU	3.7
2	C	418	LEU	3.7
3	N	1239	ARG	3.7
2	C	198	ARG	3.6
3	N	1387	SER	3.6
2	M	268	ASP	3.6
2	M	183	SER	3.6
3	N	411	THR	3.6
2	M	145	GLY	3.6
2	M	273	GLY	3.6
3	D	182	GLY	3.6
3	N	1498	ALA	3.6
4	E	58	PRO	3.6
2	C	777	ILE	3.5
3	D	1237	THR	3.5
5	F	322	GLY	3.5
2	M	629	TYR	3.5
3	D	450	TYR	3.5
2	C	768	THR	3.5
3	D	1243	THR	3.5
2	M	293	PHE	3.5
3	N	128	TYR	3.5
2	M	185	LYS	3.5
2	C	515	ALA	3.5
2	M	144	PRO	3.5
3	N	414	ARG	3.5
1	K	93	SER	3.4
3	N	185	VAL	3.4
2	C	108	ILE	3.4
2	C	333	ILE	3.4
3	D	1413	THR	3.4
5	P	150	THR	3.4
3	N	836	VAL	3.4
4	E	93	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
5	F	422	LEU	3.4
3	N	489	ARG	3.4
3	D	839	LEU	3.4
5	F	282	LEU	3.4
2	C	300	ASP	3.4
3	N	485	SER	3.3
2	C	174	LEU	3.3
3	N	616	GLN	3.3
2	C	184	MET	3.3
2	C	344	PHE	3.3
2	C	629	TYR	3.3
3	N	163	TYR	3.3
2	C	98	LEU	3.3
3	N	509	PRO	3.3
5	F	90	GLN	3.3
2	C	268	ASP	3.3
1	L	2	LEU	3.3
2	C	155	PRO	3.3
3	D	808	THR	3.3
3	N	897	TRP	3.2
3	D	823	LEU	3.2
3	D	858	VAL	3.2
5	F	397	ILE	3.2
2	M	164	PRO	3.2
2	C	208	ALA	3.2
1	B	6	LEU	3.2
3	N	813	LEU	3.2
1	A	105	GLY	3.2
2	C	116	GLY	3.2
2	M	776	SER	3.2
3	D	1233	GLY	3.2
3	D	1316	GLY	3.2
5	P	322	GLY	3.2
3	D	825	ALA	3.2
3	D	163	TYR	3.2
4	O	93	TYR	3.2
3	D	875	THR	3.2
3	D	801	GLY	3.2
3	N	825	ALA	3.2
2	C	479	VAL	3.2
2	M	280	LYS	3.1
2	M	174	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
5	P	96	LEU	3.1
5	F	384	GLU	3.1
1	A	229	GLN	3.1
2	M	255	ALA	3.1
3	D	203	ALA	3.1
2	M	163	ILE	3.1
5	P	384	GLU	3.1
5	P	412	GLU	3.1
1	L	52	ALA	3.1
2	C	213	ALA	3.1
2	C	115	LEU	3.1
3	D	836	VAL	3.1
1	A	1	MET	3.1
3	N	1210	SER	3.1
2	C	214	TYR	3.1
3	D	128	TYR	3.1
1	B	2	LEU	3.1
2	M	307	LEU	3.1
4	E	3	GLU	3.1
5	F	376	ILE	3.1
3	N	488	ARG	3.1
2	C	181	VAL	3.1
3	N	608	SER	3.1
1	L	150	TYR	3.0
3	N	136	ASP	3.0
1	K	5	LYS	3.0
2	C	272	ALA	3.0
2	C	291	ALA	3.0
2	C	312	ALA	3.0
3	N	1197	ARG	3.0
2	C	183	SER	3.0
5	F	147	LEU	3.0
2	C	223	ASP	3.0
4	E	57	ASP	3.0
3	N	501	ALA	3.0
5	P	405	LEU	3.0
3	N	1386	ASP	3.0
5	F	378	GLY	3.0
2	M	114	PHE	3.0
1	L	90	LEU	3.0
3	D	1389	LEU	3.0
5	F	84	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
5	P	280	GLN	3.0
3	N	1251	ASP	3.0
3	N	981	GLY	3.0
1	K	124	ASN	2.9
2	M	256	TYR	2.9
2	M	360	LEU	2.9
2	M	283	ILE	2.9
3	N	875	THR	2.9
5	F	95	THR	2.9
1	B	138	LEU	2.9
2	M	207	LEU	2.9
5	F	143	HIS	2.9
1	L	122	ILE	2.9
5	F	291	ILE	2.9
3	D	803	GLY	2.9
3	N	1249	ALA	2.9
3	D	806	PHE	2.9
3	N	821	VAL	2.9
5	F	356	LYS	2.9
3	N	137	PRO	2.9
3	N	680	GLN	2.9
3	D	141	ILE	2.9
5	F	75	ILE	2.9
2	M	267	TYR	2.9
3	N	1112	CYS	2.9
1	L	131	THR	2.9
2	C	290	LEU	2.9
3	D	1505	ALA	2.9
2	C	373	VAL	2.9
3	N	863	VAL	2.9
3	D	674	ARG	2.8
3	N	615	ARG	2.8
3	N	679	ARG	2.8
3	N	617	ASN	2.8
2	M	299	LYS	2.8
2	M	208	ALA	2.8
5	F	405	LEU	2.8
2	C	114	PHE	2.8
3	D	440	VAL	2.8
4	E	4	PRO	2.8
3	D	680	GLN	2.8
3	D	588	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
3	D	870	GLY	2.8
3	N	533	GLY	2.8
3	N	609	GLY	2.8
2	C	196	LEU	2.8
2	M	260	LEU	2.8
2	M	367	LEU	2.8
2	M	254	VAL	2.8
2	C	521	PRO	2.8
3	D	615	ARG	2.8
2	C	477	GLY	2.8
2	M	313	LEU	2.8
4	E	54	LEU	2.8
5	F	420	ASP	2.8
5	P	278	LEU	2.8
2	M	386	PHE	2.8
1	B	5	LYS	2.8
2	C	374	ASN	2.8
1	A	94	LEU	2.8
2	C	221	LEU	2.8
3	D	191	LEU	2.8
2	M	251	ASP	2.8
2	M	300	ASP	2.8
2	M	229	MET	2.8
3	N	1400	VAL	2.8
4	E	46	PRO	2.7
3	N	538	SER	2.7
2	C	323	ASP	2.7
1	A	30	ARG	2.7
2	M	198	ARG	2.7
2	M	209	ARG	2.7
2	M	302	VAL	2.7
3	D	406	ASP	2.7
3	D	670	VAL	2.7
3	N	207	PHE	2.7
3	N	394	LEU	2.7
3	D	119	SER	2.7
5	F	364	ARG	2.7
2	M	425	PHE	2.7
5	P	423	ASP	2.7
2	C	219	GLN	2.7
2	C	371	LYS	2.7
3	N	695	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	6	LEU	2.7
2	M	98	LEU	2.7
3	D	481	MET	2.7
2	M	373	VAL	2.7
2	M	778	PHE	2.7
3	D	207	PHE	2.7
3	D	411	THR	2.7
1	K	94	LEU	2.7
2	M	238	LEU	2.7
2	M	290	LEU	2.7
3	N	481	MET	2.7
5	F	85	LEU	2.7
2	C	288	ARG	2.7
2	M	180	GLY	2.7
4	O	5	GLY	2.7
3	D	1291	SER	2.7
3	N	1397	LYS	2.7
3	D	1238	MET	2.6
5	F	375	LEU	2.6
3	D	613	ARG	2.6
2	M	864	GLY	2.6
5	F	374	GLY	2.6
2	C	366	SER	2.6
2	C	52	PHE	2.6
2	C	475	VAL	2.6
5	F	150	THR	2.6
2	M	285	LEU	2.6
2	C	266	ARG	2.6
2	M	11	GLU	2.6
3	N	588	GLY	2.6
5	P	285	GLU	2.6
1	B	87	VAL	2.6
3	N	195	VAL	2.6
3	N	81	THR	2.6
2	C	162	ILE	2.6
2	C	211	LEU	2.6
5	P	375	LEU	2.6
2	C	516	ARG	2.6
2	M	40	GLU	2.6
2	C	336	VAL	2.6
2	C	311	PHE	2.6
2	M	153	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	C	99	GLN	2.6
2	M	368	THR	2.6
3	N	141	ILE	2.6
1	A	2	LEU	2.6
5	P	369	LEU	2.6
1	L	5	LYS	2.6
2	C	255	ALA	2.6
5	P	415	THR	2.5
3	D	1118	ILE	2.5
1	B	62	LEU	2.5
2	M	100	LEU	2.5
3	D	394	LEU	2.5
3	N	1236	LEU	2.5
3	D	445	ARG	2.5
3	D	1401	GLU	2.5
1	B	71	VAL	2.5
2	C	194	VAL	2.5
3	N	202	VAL	2.5
2	M	52	PHE	2.5
5	F	366	ALA	2.5
3	N	613	ARG	2.5
2	C	282	GLY	2.5
2	M	63	GLY	2.5
2	C	305	PRO	2.5
3	N	877	PRO	2.5
1	L	97	VAL	2.5
2	C	478	VAL	2.5
3	D	400	VAL	2.5
5	F	233	PHE	2.5
3	D	1397	LYS	2.5
1	B	186	LEU	2.5
2	C	165	LEU	2.5
3	N	161	LEU	2.5
3	N	1407	LEU	2.5
2	C	60	GLY	2.5
1	L	71	VAL	2.5
5	F	390	PHE	2.5
5	P	135	ILE	2.5
2	C	324	ASP	2.5
3	D	816	HIS	2.5
2	C	505	GLY	2.5
2	C	192	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
2	C	615	TYR	2.5
3	N	432	TYR	2.5
5	P	374	GLY	2.5
2	M	936	VAL	2.5
3	D	530	VAL	2.5
1	B	103	ALA	2.5
1	L	130	ALA	2.5
2	C	303	PHE	2.5
2	C	782	ALA	2.5
1	B	68	ILE	2.4
4	O	92	LEU	2.4
5	F	371	LEU	2.4
2	C	553	ASP	2.4
3	D	136	ASP	2.4
3	D	1251	ASP	2.4
3	D	1244	GLY	2.4
2	M	524	VAL	2.4
2	M	934	PHE	2.4
3	D	165	LYS	2.4
3	N	530	VAL	2.4
3	N	799	LYS	2.4
3	N	840	LYS	2.4
3	D	44	LEU	2.4
3	N	618	LEU	2.4
3	N	1495	ILE	2.4
5	F	79	ASP	2.4
5	F	423	ASP	2.4
5	F	305	GLU	2.4
3	D	532	GLY	2.4
3	N	826	PRO	2.4
3	N	1244	GLY	2.4
2	C	202	TYR	2.4
5	P	173	TYR	2.4
2	C	6	PHE	2.4
2	C	262	ALA	2.4
2	C	456	ALA	2.4
3	N	849	ALA	2.4
5	F	388	ALA	2.4
2	C	487	THR	2.4
3	D	1290	LEU	2.4
2	M	387	SER	2.4
3	D	505	SER	2.4

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Mol	Chain	Res	Type	RSRZ
3	D	608	SER	2.4
3	D	404	GLU	2.4
4	O	96	GLU	2.4
2	C	166	PRO	2.4
3	N	165	LYS	2.4
2	M	933	GLY	2.4
3	N	595	GLY	2.4
3	D	1124	GLN	2.4
3	N	445	ARG	2.4
1	B	85	LEU	2.4
2	M	306	THR	2.4
1	K	139	ASN	2.4
2	M	179	ASN	2.4
5	P	87	GLU	2.4
5	P	355	GLU	2.4
1	B	116	PRO	2.4
1	B	147	GLY	2.4
2	M	362	GLY	2.4
1	L	205	VAL	2.4
3	D	1407	LEU	2.3
3	D	857	ILE	2.3
5	P	365	GLU	2.3
3	N	200	ASP	2.3
1	L	176	ARG	2.3
1	B	117	VAL	2.3
2	M	34	VAL	2.3
5	F	141	VAL	2.3
2	M	459	ALA	2.3
3	N	490	ALA	2.3
3	N	822	ALA	2.3
2	M	777	ILE	2.3
2	C	485	TYR	2.3
1	B	12	THR	2.3
3	N	1084	THR	2.3
2	M	130	ASN	2.3
3	N	1501	GLU	2.3
2	C	67	ASP	2.3
2	M	166	PRO	2.3
4	E	53	GLY	2.3
3	D	1155	VAL	2.3
5	P	91	VAL	2.3
2	C	191	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
2	M	211	LEU	2.3
2	M	303	PHE	2.3
3	N	614	PHE	2.3
3	D	1082	ALA	2.3
3	N	1085	ALA	2.3
5	F	135	ILE	2.3
2	C	267	TYR	2.3
2	M	105	THR	2.3
3	N	1382	THR	2.3
1	B	1	MET	2.3
1	L	1	MET	2.3
2	C	321	GLU	2.3
3	D	593	ASN	2.3
2	C	765	SER	2.3
2	C	152	PRO	2.3
2	C	251	ASP	2.3
2	M	67	ASP	2.3
3	D	1317	ASP	2.3
1	A	16	GLN	2.3
2	C	171	TRP	2.3
2	M	171	TRP	2.3
3	D	41	ARG	2.3
3	N	1384	PRO	2.3
2	C	131	GLY	2.3
3	D	1392	GLY	2.3
2	C	42	VAL	2.3
3	N	400	VAL	2.3
2	C	351	LEU	2.3
2	C	773	LEU	2.3
4	O	54	LEU	2.3
2	M	47	ALA	2.3
3	D	562	ALA	2.3
2	M	184	MET	2.3
2	C	776	SER	2.3
2	M	244	PRO	2.3
1	K	157	GLY	2.3
2	C	273	GLY	2.3
1	B	75	VAL	2.3
1	L	6	LEU	2.3
1	L	117	VAL	2.3
3	D	863	VAL	2.3
1	A	32	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
2	M	239	PHE	2.3
2	M	236	ILE	2.2
4	E	33	HIS	2.2
2	M	371	LYS	2.2
5	F	360	LYS	2.2
1	K	29	GLU	2.2
2	C	209	ARG	2.2
3	D	399	ARG	2.2
3	D	484	PRO	2.2
2	C	933	GLY	2.2
2	M	282	GLY	2.2
2	M	583	LEU	2.2
3	D	1394	VAL	2.2
3	D	610	LYS	2.2
3	D	822	ALA	2.2
3	D	1142	ALA	2.2
3	N	120	ALA	2.2
5	P	144	ILE	2.2
2	C	480	THR	2.2
3	D	40	GLU	2.2
5	P	364	ARG	2.2
2	C	548	PRO	2.2
1	B	229	GLN	2.2
3	D	1119	SER	2.2
3	N	164	GLY	2.2
5	P	137	GLY	2.2
2	C	100	LEU	2.2
2	M	269	LEU	2.2
1	L	86	VAL	2.2
2	C	514	VAL	2.2
2	C	229	MET	2.2
2	C	699	PHE	2.2
4	E	55	PHE	2.2
5	F	421	PHE	2.2
5	P	170	HIS	2.2
3	D	398	ALA	2.2
2	C	110	GLU	2.2
2	C	301	GLU	2.2
3	N	1127	GLU	2.2
2	C	28	ARG	2.2
2	M	243	ARG	2.2
2	M	356	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	95	TYR	2.2
2	M	275	TYR	2.2
3	D	868	TYR	2.2
2	M	170	PRO	2.2
2	M	248	PRO	2.2
3	N	1195	GLN	2.2
3	N	1441	GLN	2.2
1	B	187	GLY	2.2
2	M	718	GLY	2.2
3	N	837	GLY	2.2
3	N	1245	GLY	2.2
3	N	1255	GLY	2.2
2	C	1	MET	2.2
3	N	1188	VAL	2.2
1	L	48	ILE	2.2
2	C	905	ILE	2.2
1	B	118	ALA	2.2
1	B	164	ALA	2.2
2	M	92	ALA	2.2
3	N	1250	ALA	2.2
5	P	416	ARG	2.2
5	F	403	LYS	2.2
1	L	127	LEU	2.2
2	M	115	LEU	2.2
2	M	328	LEU	2.2
3	D	869	MET	2.2
1	L	174	VAL	2.2
3	D	566	ILE	2.2
3	N	435	VAL	2.2
4	E	61	VAL	2.2
4	O	33	HIS	2.2
5	F	91	VAL	2.2
5	F	130	VAL	2.2
5	P	138	SER	2.2
2	C	926	PHE	2.2
2	M	272	ALA	2.1
3	D	120	ALA	2.1
3	N	422	ALA	2.1
1	L	64	GLU	2.1
3	D	81	THR	2.1
2	M	247	PRO	2.1
2	C	71	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
5	F	370	LYS	2.1
2	M	195	LEU	2.1
2	C	319	GLY	2.1
2	C	539	VAL	2.1
2	C	936	VAL	2.1
2	M	162	ILE	2.1
2	M	522	VAL	2.1
3	D	444	VAL	2.1
3	D	1106	VAL	2.1
3	D	1503	VAL	2.1
3	N	829	VAL	2.1
5	P	262	VAL	2.1
1	K	11	PHE	2.1
1	L	153	ALA	2.1
2	C	626	ARG	2.1
2	M	266	ARG	2.1
3	D	488	ARG	2.1
3	N	568	ARG	2.1
3	D	1253	THR	2.1
3	D	1286	THR	2.1
3	N	834	THR	2.1
2	M	252	LYS	2.1
1	L	36	LEU	2.1
2	C	361	MET	2.1
5	F	166	LEU	2.1
2	M	270	GLY	2.1
1	A	68	ILE	2.1
1	B	109	VAL	2.1
1	K	34	VAL	2.1
1	K	79	ILE	2.1
2	C	317	VAL	2.1
2	C	322	VAL	2.1
2	C	474	VAL	2.1
2	C	496	ILE	2.1
2	M	226	VAL	2.1
1	A	4	SER	2.1
1	L	4	SER	2.1
1	L	46	SER	2.1
3	D	589	ALA	2.1
3	N	830	ALA	2.1
3	N	1502	ALA	2.1
3	N	1505	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
2	M	422	ARG	2.1
1	K	12	THR	2.1
4	O	47	LYS	2.1
3	N	901	GLN	2.1
1	L	82	LEU	2.1
5	P	354	LEU	2.1
2	C	320	HIS	2.1
1	B	162	ILE	2.1
2	C	118	ILE	2.1
2	C	261	ILE	2.1
2	M	65	VAL	2.1
3	D	185	VAL	2.1
1	B	3	ASP	2.1
2	C	293	PHE	2.1
3	D	42	ASP	2.1
2	M	110	GLU	2.1
2	M	555	ALA	2.1
3	D	410	SER	2.1
3	D	1127	GLU	2.1
3	N	124	GLU	2.1
3	N	192	ALA	2.1
3	N	399	ARG	2.1
2	C	930	LYS	2.1
3	D	671	LYS	2.1
3	N	168	THR	2.1
1	L	9	PRO	2.1
3	D	616	GLN	2.1
4	E	51	LEU	2.1
5	F	418	LEU	2.1
1	L	17	GLY	2.1
5	P	88	ILE	2.1
2	C	254	VAL	2.1
3	D	431	VAL	2.1
3	D	1400	VAL	2.1
1	L	3	ASP	2.0
2	C	298	PHE	2.1
2	M	250	ARG	2.0
3	N	413	ASP	2.0
3	D	1501	GLU	2.0
4	O	2	ALA	2.0
5	F	87	GLU	2.0
1	K	1	MET	2.0

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Mol	Chain	Res	Type	RSRZ
1	L	228	PRO	2.0
2	C	767	PRO	2.0
3	D	509	PRO	2.0
3	D	178	LEU	2.0
3	D	1235	GLN	2.0
5	F	94	LEU	2.0
3	D	1116	ASN	2.0
1	L	149	GLY	2.0
2	C	54	ILE	2.0
2	C	169	GLY	2.0
2	C	220	GLY	2.0
3	D	609	GLY	2.0
3	N	827	ILE	2.0
5	F	146	GLY	2.0
2	C	199	VAL	2.0
3	D	202	VAL	2.0
3	D	396	VAL	2.0
3	N	415	VAL	2.0
2	M	237	ARG	2.0
3	D	534	ARG	2.0
3	N	206	ARG	2.0
3	N	1310	ARG	2.0
2	C	40	GLU	2.0
5	P	97	GLU	2.0
5	P	225	GLU	2.0
2	C	938	LYS	2.0
2	M	312	ALA	2.0
3	N	487	ALA	2.0
3	N	1418	LYS	2.0
5	P	183	ALA	2.0
1	A	226	SER	2.0
3	N	1131	SER	2.0
2	C	247	PRO	2.0
3	D	594	PRO	2.0
3	N	114	THR	2.0
3	N	1114	THR	2.0
1	B	82	LEU	2.0
2	M	219	GLN	2.0
5	F	93	LEU	2.0
1	L	129	ILE	2.0
1	L	158	ILE	2.0
2	C	129	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
2	M	125	GLY	2.0
3	N	803	GLY	2.0
3	N	1092	GLY	2.0
5	P	387	GLY	2.0
1	B	142	VAL	2.0
3	D	1281	VAL	2.0
3	N	147	VAL	2.0
3	N	396	VAL	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

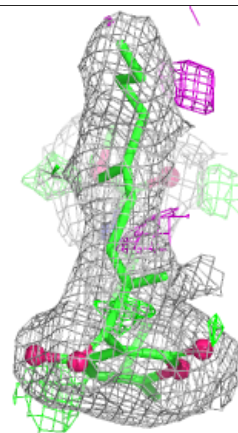
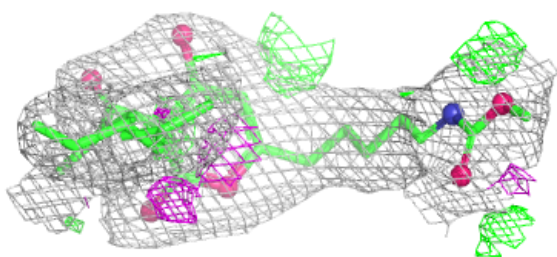
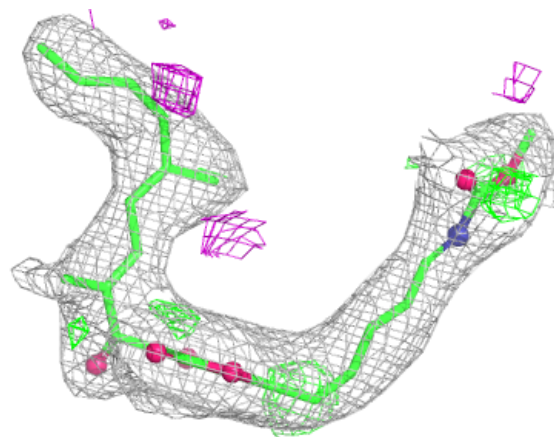
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	MG	N	1528	1/1	0.91	0.17	41,41,41,41	0
7	MXP	N	1527	30/30	0.93	0.12	17,30,38,40	0
7	MXP	D	1527	30/30	0.94	0.11	13,20,27,34	0
8	MG	D	1528	1/1	0.96	0.07	35,35,35,35	0
6	ZN	D	1525	1/1	0.98	0.03	62,62,62,62	0
6	ZN	N	1526	1/1	0.98	0.04	66,66,66,66	0
6	ZN	N	1525	1/1	0.99	0.02	58,58,58,58	0
6	ZN	D	1526	1/1	0.99	0.05	48,48,48,48	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

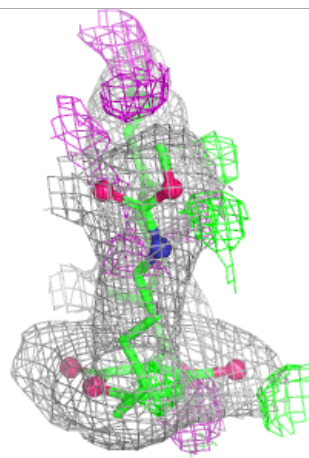
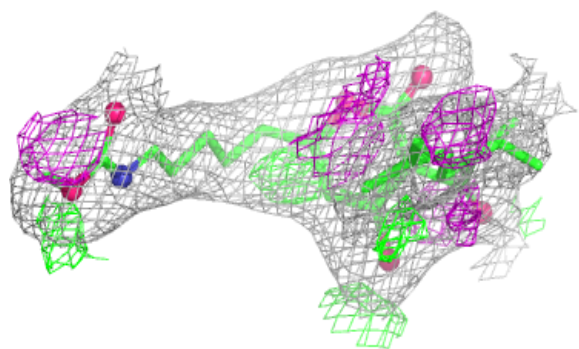
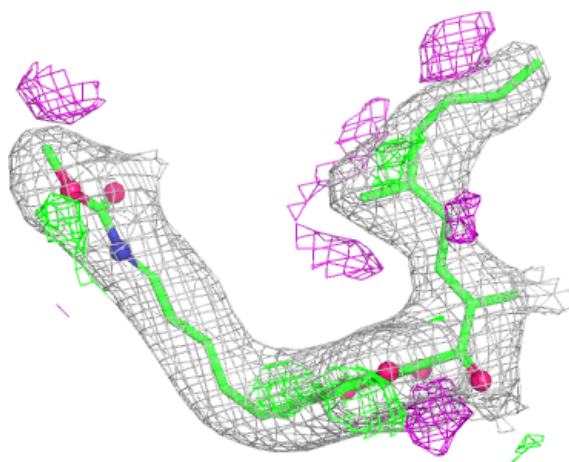
Electron density around MXP N 1527:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MXP D 1527:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.