



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:46 PM UTC

PDB ID : 2A69 / pdb_00002a69
Title : Crystal structure of the T. Thermophilus RNA polymerase holoenzyme in complex with antibiotic rifapentin
Authors : Artsimovitch, I.; Vassilyeva, M.N.; Svetlov, D.; Svetlov, V.; Perederina, A.; Igarashi, N.; Matsugaki, N.; Wakatsuki, S.; Tahirov, T.H.; Vassilyev, D.G.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2005-07-02
Resolution : 2.50 Å(reported)

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

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

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](#) ①) were used in the production of this report:

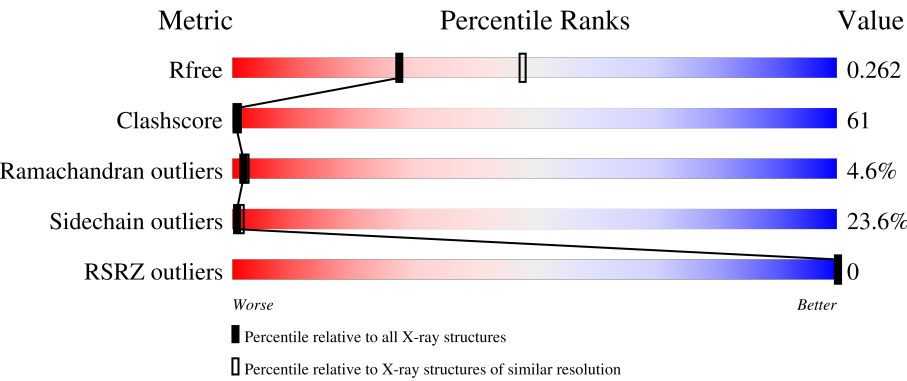
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	16% 44% 10% • 27%
1	B	315	17% 44% 11% • 27%
1	K	315	23% 39% 10% • 27%
1	L	315	19% 41% 11% • 27%
2	C	1119	20% 58% 20% •

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Mol	Chain	Length	Quality of chain
2	M	1119	
3	D	1524	
3	N	1524	
4	E	99	
4	O	99	
5	F	423	
5	P	423	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 60572 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 alpha chain.

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 beta chain.

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 beta' chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1392	Total	C	N	O	S	0	0	0
			10797	6819	1925	2020	33			
3	N	1392	Total	C	N	O	S	0	0	0
			10797	6819	1925	2020	33			

- Molecule 4 is a protein called RNA polymerase omega chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	95	Total	C	N	O	S	0	0	0
			769	488	133	144	4			
4	O	95	Total	C	N	O	S	0	0	0
			769	488	133	144	4			

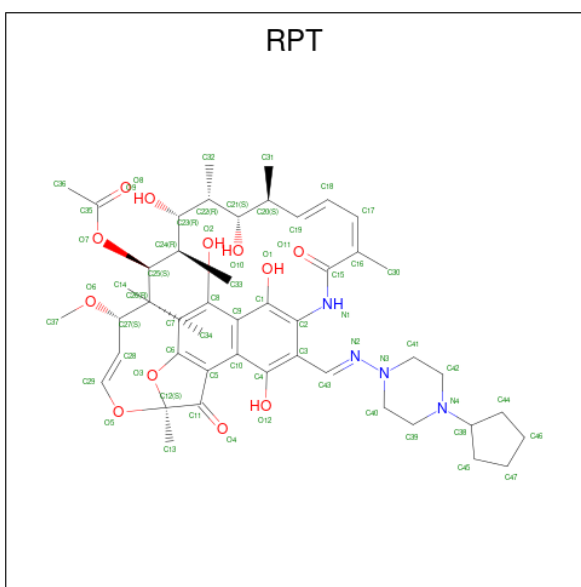
- Molecule 5 is a protein called RNA polymerase sigma factor rpoD.

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 MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	33	Total	Mg	0	0
			33	33		
6	B	21	Total	Mg	0	0
			21	21		
6	C	73	Total	Mg	0	0
			73	73		
6	D	106	Total	Mg	0	0
			106	106		
6	E	5	Total	Mg	0	0
			5	5		
6	F	28	Total	Mg	0	0
			28	28		
6	K	19	Total	Mg	0	0
			19	19		
6	L	17	Total	Mg	0	0
			17	17		
6	M	65	Total	Mg	0	0
			65	65		
6	N	92	Total	Mg	0	0
			92	92		
6	O	8	Total	Mg	0	0
			8	8		
6	P	20	Total	Mg	0	0
			20	20		

- Molecule 7 is RIFAPENTINE (CCD ID: RPT) (formula: C₄₇H₆₄N₄O₁₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	N	O	0	0
			63	47	4	12		
7	M	1	Total	C	N	O	0	0
			63	47	4	12		

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	239	Total	O	0	0
			239	239		
9	B	258	Total	O	0	0
			258	258		
9	C	979	Total	O	0	0
			979	979		
9	D	1252	Total	O	0	0
			1252	1252		
9	E	117	Total	O	0	0
			117	117		

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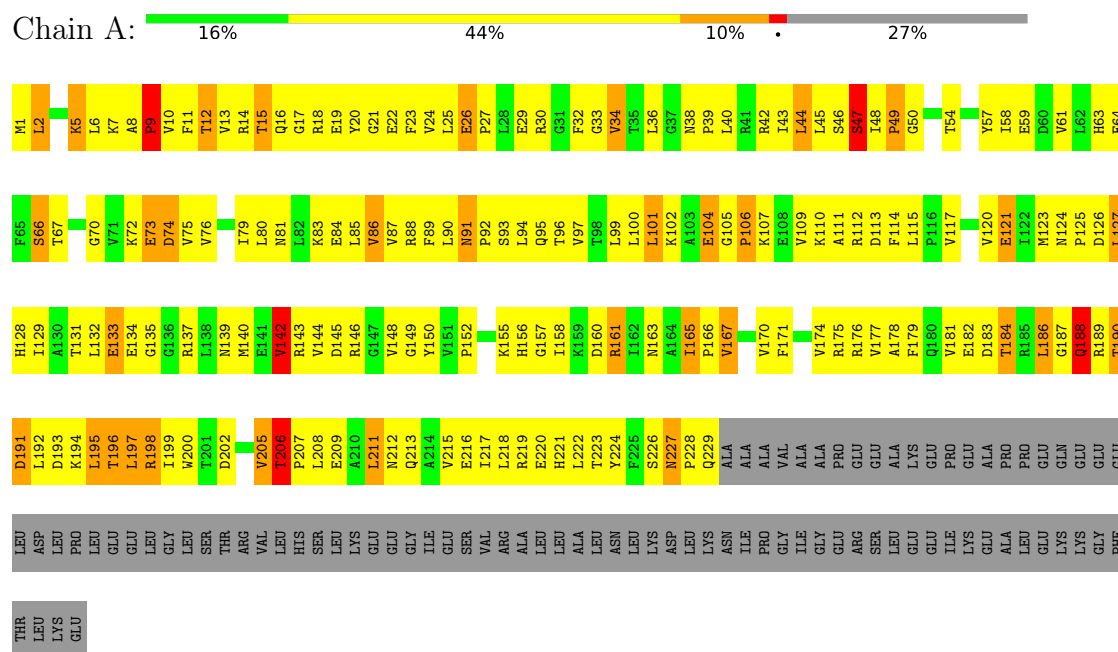
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	F	420	Total 420	O 420	0	0
9	K	183	Total 183	O 183	0	0
9	L	219	Total 219	O 219	0	0
9	M	998	Total 998	O 998	0	0
9	N	1265	Total 1265	O 1265	0	0
9	O	108	Total 108	O 108	0	0
9	P	361	Total 361	O 361	0	0

3 Residue-property plots

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

• Molecule 1: DNA-directed RNA polymerase alpha chain



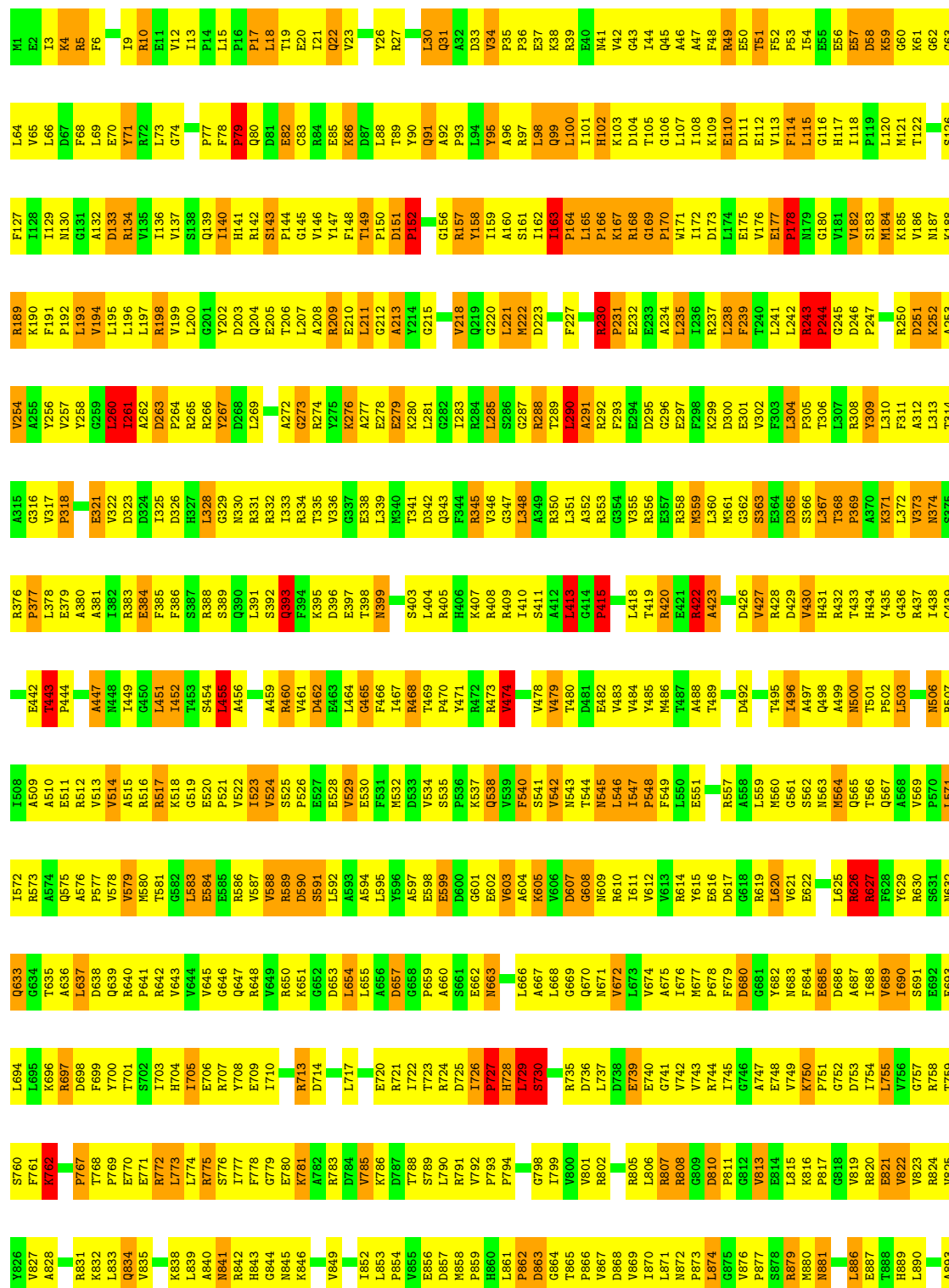


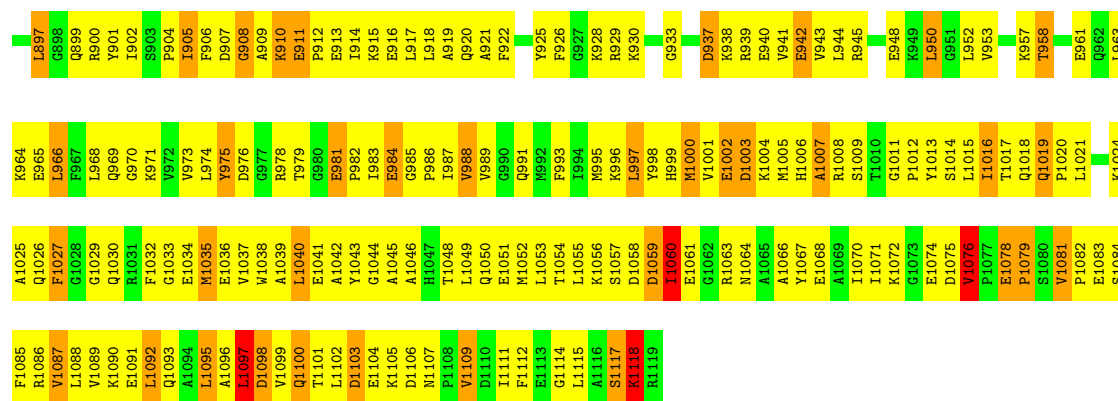
H1006	R945	P877	P811	A747	V686	R626	S562	N500	P430	R376	G316	V254	R189	V65
A1007	E948	S878	G812	E746	A687	R627	N563	T501	V441	P377	V317	A255	K190	L66
R1008	R879	R879	R813	V749	I688	F628	M564	P502	E442	L378	P318	Y256	P191	D67
S1009	K949	K880	S1009	K750	V689	F629	Q565	L503	T443	E379	G319	P128	P192	F68
T1010	L950	N881	T1010	P751	I690	R630	T566	E504	P444	A381	H320	Y258	L193	L69
G1011	G951	L882	G1011	G752	S691	S631	G567	G505	E445	A390	E321	G259	V194	E70
P1012	L952	G983	G818	G753	E692	N632	A568	N506	G446	I382	V322	L260	L195	Y71
Y1013	R993	Q884	R619	I754	E693	Q633	V569	R507	A447	R383	D323	L261	L196	R72
S1014	L885	L885	R820	L765	L694	G634	P570	P508	N448	E384	D324	A262	L197	L73
L1015	L886	E821	E821	V756	L695	T635	L571	A509	I449	F385	I325	P264	R198	G74
G1016	G956	L886	L886	G757	L696	A636	I572	A510	G450	F386	D326	P264	V199	E75
T1017	K957	L887	R825	R758	R697	L637	A574	E511	L451	S387	H327	R265	L200	P76
Q1018	L890	L890	R826	I759	D698	G638	A574	R512	L452	R388	L328	R266	G201	P77
Q1019	P959	G891	R827	S760	F699	Q639	Q575	V513	T453	S389	G329	Y267	Y202	F76
P1020	E960	L892	A828	F761	T701	R640	A576	V514	S454	G390	N390	D288	D203	P79
L1021	A893	K830	K830	K762	S702	R642	V578	A515	L455	L391	R332	G270	Q204	Q80
G1022	G962	R831	R831	P767	I703	V643	V579	S517	A456	S392	I333	E271	T206	D81
Q1026	K964	R896	R832	T768	H704	V644	M580	K518	Y458	F394	R334	A272	L207	E82
F1027	E965	G896	L833	P769	I705	V645	L583	S519	A459	K395	T335	G273	A208	C83
G1029	F967	Q899	Q834	E770	E706	G646	E584	E520	R466	D396	V336	R274	R209	R84
Q1030	L968	R900	R835	E771	R707	G647	E584	P521	V461	E397	G337	Y275	E210	D87
Q1033	Q969	I902	D837	R772	Y708	R648	E585	V522	D462	T388	E338	K276	L211	L88
E1034	G970	S903	R838	L773	E709	V649	R586	I523	E463	N399	L339	G212	G212	T89
M1035	K971	P904	L839	L774	I710	R650	V587	V524	L484	P400	M340	E279	A213	Y90
E1036	V972	I905	R840	R775	E711	K651	V588	S525	G485	K280	T341	K280	Y214	Q91
Y1037	F906	R906	R841	A712	A712	G652	R589	E527	F466	L281	D342	L281	G215	A92
Y1038	D907	I914	R842	R776	R713	D653	D590	P534	I467	L404	Q343	G282	P218	P93
Y1039	G908	R843	R843	F778	D714	L654	S591	S535	R488	R405	F344	I283	L94	L94
D976	A908	G843	G843	T715	L655	L655	L592	P536	T469	R456	R345	Y158	Y95	Y95
G977	K910	R845	R845	K781	K716	A656	A593	E530	P470	K407	V346	L285	L221	A96
R978	E911	R846	R846	K782	L717	D657	A594	F581	Y471	R408	G347	S286	M222	R97
Y979	P912	R849	R849	R783	E720	P659	L595	M532	R472	R409	L348	G287	D223	L98
E981	I914	Y849	Y849	D784	R721	A660	A597	V534	V474	L410	R350	T289	V226	L99
A1046	K915	T852	T852	K786	I722	S661	E598	S535	V475	A412	L351	I280	F227	I101
H1047	E916	L853	L853	D787	T723	E662	E599	P536	G476	L413	A352	A291	F227	H102
T1048	L917	P854	P854	I786	R724	G664	D600	K537	G477	C414	R353	R292	M229	K103
L1049	R984	R855	R855	I788	D725	F685	E602	Q538	V479	P415	G354	F293	R230	D104
Q1050	P986	E856	E856	L790	I726	L666	V603	S541	T480	L418	R356	E297	P231	T105
E1051	I987	D857	D857	R791	P727	A667	A604	V542	D481	T419	E357	E297	E232	G106
M1052	V988	R858	R858	V792	L729	L668	K605	N543	E482	R420	M359	F298	A234	L107
L1053	V924	P859	P859	P793	E730	G669	V606	T544	V483	E421	L360	K299	L235	I108
T1054	Y925	H860	H860	P794	E731	Q670	D607	E551	V484	R422	L360	D300	I236	E110
K1055	F926	L861	L861	G795	A732	N671	G608	T547	Y485	A423	R361	E301	R237	E111
S1057	G927	P862	P862	E796	A733	V672	N609	P648	M486	G424	G362	V302	L238	D111
D1058	F993	D863	D863	G797	L734	L673	R610	F549	T487	F425	S363	F303	L239	E112
M955	I994	G864	G864	G798	R735	V674	T611	L550	A488	D426	E364	L304	F239	V113
D1059	M995	T865	T865	I799	D736	A675	V612	E551	T489	V427	D365	P305	L241	F114
E1061	F934	Y866	Y866	V800	L737	L676	V613	H552	E490	H431	S386	T306	L242	L115
G1062	L987	Y867	Y867	R801	D738	R677	R614	D553	E491	R432	L367	R243	L242	G116
R1063	G999	D868	D868	R802	E739	P678	V615	D554	D492	R432	T368	R308	R243	H117
N1064	D937	R803	R803	F679	E740	F679	E616	A555	R493	T433	P369	Y309	G245	I118
A1065	M1000	V804	V804	G741	G741	D680	N556	N556	Y494	H434	A370	L310	G246	P119
A1066	V1001	R805	R805	V742	G742	G681	B557	B557	T495	V435	K371	F311	D246	M121
Y1067	E1002	R808	R808	V743	V743	V682	V621	A558	I496	G436	L372	A312	R250	T122
E1068	K1004	G809	G809	R744	R744	N683	E622	L559	A497	R437	V373	L313	D251	K185
A1069	M1005	L944	L944	D810	G746	E685	L625	G561	A499	C439	S375	T314	K252	E123



● Molecule 2: DNA-directed RNA polymerase beta chain

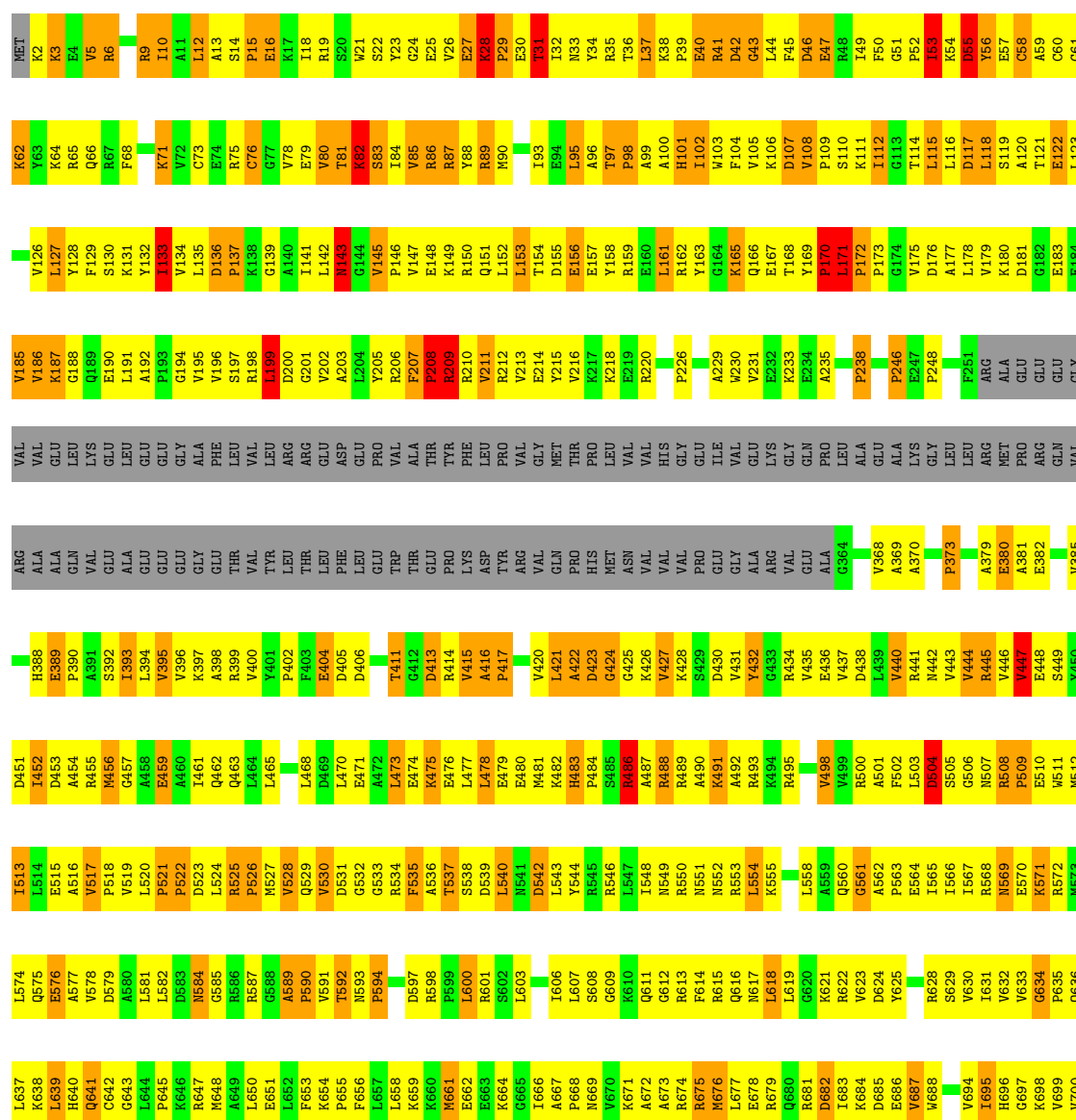
Chain M: 23% 56% 18%





• Molecule 3: DNA-directed RNA polymerase beta' chain

Chain D: 21% 51% 17% 9%



Q1033	D968	S835	P772	T707	K646	A580	V517	M456	I393	GLU	E190	L127	R65
Q1034	R369	V836	A773	L708	R647	L581	P518	E459	L394	GLU	L191	Y128	Q66
I1035	R970	R837	S774	H709	M648	L582	V519	E460	V395	GLY	A192	F129	R67
R1036	L971	R838	G775	R710	G775	D583	L520	I461	V396	ALA	P193	S130	F68
Q1037	L972	G776	E776	L711	E651	N584	P521	Q462	K397	PHE	K131	K131	
L1038	Q973	F843	P777	G712	E652	G885	P522	Q463	A398	LEU	V195	V132	K71
Q1039	Q906	A844	L778	I713	F653	R586	D523	Q464	V399	VAL	V196	I133	V72
G1040	E907			Q714	K654	R588	L524	L464	V400	LEU	S197	V134	E73
L1041	D847	D847	P781	A715	P655	G888	R525	L465	Y401	ARG	L198	L135	C74
R1042	E848	E848	S782	A716	K656	A589	P526	L466	L199	THR	L199	D136	R75
Q1043	L911	A849	R783	Q717	F657	P590	M527	K466	P402	ARG	D200	P137	C76
L1044	R979	L850	D784	P718	L658	V528	L468	L468	F403	GLU	P137	D136	
M1045	L851	L851	I785	V719	K659	V591	Q529	L469	E404	ASP	G139	K138	G77
Q1046	A852	A852	I786	L720	K660	N593	Q530	D469	E408	GLU	V202	G139	V78
K1047	V853	V853	L787	L721	M661	N594	V530	L470	E408	PRO	A203	A140	E79
L1048	V854	V854	E722	V721	M662	P594	G533	E471	T411	VAL	A204	I141	V80
S1049	R855	R855	G723	G723	E662	R598	G534	A472	G412	THR	L204	I141	T81
G1050	L856	L856	V790	I726	K664	R598	F535	L473	D413	ALA	Y205	L142	R82
E1051	I857	I857	I791	Q727	G665	R601	F536	E474	G414	THR	R206	N143	S83
T1052	V858	V858	I792	Q727	I866	S802	T537	K475	R414	PHE	F207	G144	I84
P1053	R921	R921	T793	L728	A667	L603	S538	E476	V415	LEU	P208	V145	V85
	L922	L860	Q794	H729	P668	T804	D539	L477	A416	VAL	R209	P146	R86
V1057	G923	Q861	V795	P730	N669	D805	L540	L478	P417	GLY	R210	V147	R87
S1058	M924	Q861	R796	L731	I606	I606	N541	E479	G418	VAL	R211	E148	V88
E1059	V863	V863	K797	L732	V670	L607	N541	E480	D419	GLN	R212	G148	
S1060	V864	V864	E798	C733	K671	S608	D542	M481	V420	THR	E214	Q151	R89
F1061	T865	T865	K799	E734	A672	G609	L543	K482	L421	PRO	Y215	L152	M90
L1062	V866	V866	A735	E734	A673	G609	R546	H483	A422	LEU	V216	L153	G91
E1063	R867	R867	R674	R674	R674	G609	R546	H483	A422	VAL	K217	T154	H92
Q1064	R868	R868	R675	R675	R675	Q611	L547	L477	D423	ASN	V216	T154	I93
L1065	M669	M669	E676	E676	E676	Q611	L547	S486	G424	VAL	E156	E156	E94
T1066	G870	G870	L677	L677	L677	Q616	I548	R486	G425	VAL	E157	E157	L95
V1067	K871	K871	E678	E678	E678	N617	N550	A487	K426	VAL	R159	V158	A96
L1068	R872	R872	D739	D739	D739	N617	R550	R488	V427	PRO	L223	R159	T97
E1069	L873	L873	D743	D743	D743	L618	R551	R489	K428	ILE	P226	E160	P98
Y1070	P809	P809	M745	M745	M745	L619	N551	A490	S429	GLY	P226	L161	A99
S1073	T874	T874	E810	E810	E810	G820	L554	A492	D430	ALA	V231	R162	H101
H1075	S876	S876	E811	E811	E811	V623	K555	K494	Y432	LYS	V231	K165	I102
Q1076	S877	S877	A812	A812	A812	D624	L557	R496	G433	GLY	A235	Q166	I103
A1077	G878	G878	L813	L813	L813	Y625	L558	L496	R434	PRO	Y236	Q166	F104
K1078	R879	R879	A814	A814	A814	S626	A559	E497	V435	LEU	K237	T168	V105
F1079	I880	I880	E814	E814	E814	G627	Q560	V498	V437	ALA	P238	Y169	K106
	L881	L881	E817	E817	E817	R628	G561	V499	D438	ALA	P246	P170	D107
	F882	F882	R818	R818	R818	S629	A562	R500	L439	LYS	E247	P171	V108
	A883	A883	G819	G819	G819	V630	P563	A501	L439	LYS	P248	P172	P109
	R884	R884	E820	E820	E820	I631	E564	V502	V440	GLY	P248	G174	S110
	I885	I885	V821	V821	V821	V632	I565	F502	R441	LEU	P248	G174	K111
	V886	V886	A822	A822	A822	V633	I567	D504	N442	LEU	P248	G174	I112
	E887	E887	L823	L823	L823	G634	R568	S505	V444	ARG	P248	G174	L115
	A888	A888	N824	N824	N824	P635	N569	S505	V444	ARG	P248	G174	L116
	V889	V889	A825	A825	A825	Q636	E570	G506	R445	PRO	P248	G174	D117
	E890	E890	P826	P826	P826	K637	K572	N507	V446	ARG	P248	G174	L118
	R891	R891	Q827	Q827	Q827	L637	R571	E508	E448	GLN	P248	G174	S119
	D892	D892	L828	L828	L828	G638	M573	P509	E448	VAL	P248	G174	A120
	G893	G893	K828	K828	K828	L639	M573	E510	S449	ARG	P248	G174	VAL
	V894	V894	V763	V763	V763	G639	M573	E510	S449	ARG	P248	G174	VAL
	A895	A895	H764	H764	H764	H640	L574	M511	Y450	ALA	P248	G174	T121
	E896	E896	L702	L702	L702	G641	L574	M511	Y450	ALA	P248	G174	E183
	R897	R897	R703	R703	R703	C642	E576	I513	I452	GLN	P248	G174	E184
	A898	A898	R704	R704	R704	G643	E576	I513	I452	GLN	P248	G174	V185
	E899	E899	A705	A705	A705	L644	E578	E515	D453	VAL	P248	G174	L123
	L899	L899	T771	T771	T771	P645	D579	A516	A454	GLU	P248	G174	E124
										ALA	P248	G174	Q125
										ALA	P248	G174	V126

4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	239.50Å 239.50Å 253.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.50 25.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.50) 92.6 (25.00-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.50Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.230 , 0.267 0.227 , 0.262	Depositor DCC
R_{free} test set	29710 reflections (5.75%)	wwPDB-VP
Wilson B-factor (Å ²)	47.8	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 77.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.499 for -h,-k,l 0.076 for h,-h-k,-l 0.076 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	60572	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% 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: ZN, MG, RPT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.90	5/1838 (0.3%)	1.22	9/2498 (0.4%)
1	B	0.77	0/1838	1.08	7/2498 (0.3%)
1	K	0.80	2/1838 (0.1%)	1.17	10/2498 (0.4%)
1	L	0.79	3/1838 (0.2%)	1.10	9/2498 (0.4%)
2	C	0.88	5/8997 (0.1%)	1.28	76/12164 (0.6%)
2	M	0.86	5/8997 (0.1%)	1.26	71/12164 (0.6%)
3	D	0.94	12/10975 (0.1%)	1.33	102/14836 (0.7%)
3	N	0.91	13/10975 (0.1%)	1.31	88/14836 (0.6%)
4	E	0.96	1/783 (0.1%)	1.37	9/1054 (0.9%)
4	O	0.90	0/783	1.38	8/1054 (0.8%)
5	F	0.79	2/2812 (0.1%)	1.21	15/3781 (0.4%)
5	P	0.76	1/2812 (0.0%)	1.18	13/3781 (0.3%)
All	All	0.88	49/54486 (0.1%)	1.27	417/73662 (0.6%)

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	48	ILE	C-N	9.99	1.45	1.33
1	L	172	SER	N-CA	-7.66	1.35	1.46
3	D	82	LYS	CA-C	7.45	1.62	1.52
3	D	53	ILE	CA-CB	7.41	1.63	1.54
3	N	126	VAL	CA-CB	7.40	1.62	1.54
3	D	498	VAL	CA-CB	6.95	1.62	1.54
3	D	1376	MET	SD-CE	-6.91	1.62	1.79
3	D	1114	THR	CA-CB	6.81	1.61	1.52
3	N	1114	THR	CA-CB	6.74	1.61	1.52
3	D	1375	MET	SD-CE	-6.64	1.62	1.79
3	N	13	ALA	CA-CB	-6.38	1.45	1.53
2	C	163	ILE	CA-CB	6.37	1.62	1.54
3	N	1375	MET	SD-CE	-6.37	1.63	1.79
3	D	207	PHE	CA-C	6.35	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	172	SER	CA-C	-6.35	1.45	1.52
2	C	191	PHE	C-N	6.32	1.41	1.33
2	C	393	GLN	CD-OE1	6.29	1.35	1.23
3	N	1023	MET	SD-CE	-6.28	1.63	1.79
3	N	83	SER	N-CA	-6.23	1.38	1.46
2	C	474	VAL	CA-CB	6.20	1.62	1.54
3	N	207	PHE	CA-C	6.09	1.60	1.52
2	M	1060	ILE	CA-CB	6.08	1.60	1.54
2	C	1060	ILE	CA-CB	5.87	1.60	1.54
3	N	82	LYS	CA-C	-5.86	1.45	1.52
1	A	48	ILE	CA-C	5.86	1.59	1.52
4	E	22	VAL	CA-CB	5.85	1.60	1.54
3	N	83	SER	CA-C	-5.74	1.45	1.52
1	A	142	VAL	CA-CB	5.52	1.60	1.53
2	M	163	ILE	CA-CB	5.48	1.61	1.54
3	D	83	SER	N-CA	5.42	1.53	1.46
3	N	1091	SER	N-CA	5.39	1.53	1.46
1	A	49	PRO	N-CA	5.39	1.52	1.46
3	D	447	VAL	CA-CB	5.34	1.61	1.54
1	K	48	ILE	C-N	5.27	1.39	1.33
3	N	100	ALA	CA-CB	-5.25	1.43	1.53
3	N	1090	ASP	CA-C	5.23	1.59	1.52
1	K	142	VAL	CA-CB	5.22	1.60	1.53
1	A	206	THR	CA-CB	5.20	1.61	1.53
5	P	135	ILE	CA-CB	5.19	1.60	1.54
1	L	171	PHE	C-N	-5.18	1.27	1.33
3	D	836	VAL	CA-CB	5.16	1.61	1.54
2	M	474	VAL	CA-CB	5.16	1.61	1.54
2	M	393	GLN	CD-NE2	-5.15	1.22	1.33
3	D	172	PRO	CA-C	5.12	1.56	1.52
3	N	1378	TYR	CA-C	5.11	1.58	1.52
5	F	329	TYR	CA-C	5.08	1.59	1.52
3	D	53	ILE	CA-C	5.07	1.59	1.53
5	F	190	ALA	CA-CB	-5.06	1.45	1.53
2	M	535	SER	CA-C	5.03	1.59	1.52

All (417) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	207	PHE	CA-C-N	16.48	140.44	119.84
3	D	207	PHE	C-N-CA	16.48	140.44	119.84
3	N	207	PHE	CA-C-N	16.42	140.37	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	207	PHE	C-N-CA	16.42	140.37	119.84
3	N	508	ARG	CA-C-N	15.57	139.30	119.84
3	N	508	ARG	C-N-CA	15.57	139.30	119.84
2	M	177	GLU	CA-C-N	15.40	139.09	119.84
2	M	177	GLU	C-N-CA	15.40	139.09	119.84
2	C	177	GLU	CA-C-N	14.81	138.36	119.84
2	C	177	GLU	C-N-CA	14.81	138.36	119.84
3	D	508	ARG	CA-C-N	14.74	138.27	119.84
3	D	508	ARG	C-N-CA	14.74	138.27	119.84
1	A	48	ILE	CA-C-N	12.82	136.66	120.51
1	A	48	ILE	C-N-CA	12.82	136.66	120.51
2	M	443	THR	CA-C-N	10.37	132.80	119.84
2	M	443	THR	C-N-CA	10.37	132.80	119.84
2	C	6	PHE	N-CA-C	10.31	123.98	111.40
2	C	726	ILE	CA-C-N	10.10	132.47	119.84
2	C	726	ILE	C-N-CA	10.10	132.47	119.84
1	K	48	ILE	CA-C-N	10.09	130.20	120.31
1	K	48	ILE	C-N-CA	10.09	130.20	120.31
4	O	49	GLN	N-CA-C	10.02	124.81	112.59
2	C	443	THR	CA-C-N	9.99	131.57	119.98
2	C	443	THR	C-N-CA	9.99	131.57	119.98
2	M	728	HIS	N-CA-C	9.90	125.48	113.41
2	C	230	ARG	CA-C-N	9.80	132.09	119.84
2	C	230	ARG	C-N-CA	9.80	132.09	119.84
5	F	91	VAL	CA-C-N	-9.70	110.42	120.03
5	F	91	VAL	C-N-CA	-9.70	110.42	120.03
1	A	105	GLY	CA-C-N	9.65	131.90	119.84
1	A	105	GLY	C-N-CA	9.65	131.90	119.84
2	M	6	PHE	N-CA-C	9.62	123.65	111.24
5	P	296	GLY	CA-C-N	9.62	131.86	119.84
5	P	296	GLY	C-N-CA	9.62	131.86	119.84
5	F	296	GLY	CA-C-N	9.61	131.85	119.84
5	F	296	GLY	C-N-CA	9.61	131.85	119.84
1	B	105	GLY	CA-C-N	9.61	131.85	119.84
1	B	105	GLY	C-N-CA	9.61	131.85	119.84
3	N	171	LEU	CA-C-N	9.58	130.25	120.38
3	N	171	LEU	C-N-CA	9.58	130.25	120.38
2	M	726	ILE	CA-C-N	9.38	131.57	119.84
2	M	726	ILE	C-N-CA	9.38	131.57	119.84
3	N	705	ALA	CA-C-N	-9.34	106.74	120.46
3	N	705	ALA	C-N-CA	-9.34	106.74	120.46
2	C	728	HIS	N-CA-C	9.33	124.79	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	91	VAL	CA-C-N	-9.29	110.83	120.03
5	P	91	VAL	C-N-CA	-9.29	110.83	120.03
1	K	105	GLY	CA-C-N	9.27	131.42	119.84
1	K	105	GLY	C-N-CA	9.27	131.42	119.84
3	N	80	VAL	CA-C-N	9.27	136.59	121.58
3	N	80	VAL	C-N-CA	9.27	136.59	121.58
3	D	705	ALA	CA-C-N	-9.25	106.86	120.46
3	D	705	ALA	C-N-CA	-9.25	106.86	120.46
3	N	1209	LEU	N-CA-C	-9.24	95.43	109.94
1	L	105	GLY	CA-C-N	9.22	131.37	119.84
1	L	105	GLY	C-N-CA	9.22	131.37	119.84
2	M	260	LEU	N-CA-C	9.20	123.10	111.24
3	D	171	LEU	CA-C-N	9.19	129.85	120.38
3	D	171	LEU	C-N-CA	9.19	129.85	120.38
4	E	49	GLN	N-CA-C	9.18	123.79	112.59
3	N	1383	ASP	CA-C-N	9.10	129.04	120.03
3	N	1383	ASP	C-N-CA	9.10	129.04	120.03
3	D	1209	LEU	N-CA-C	-9.10	95.66	109.94
2	M	230	ARG	CA-C-N	9.08	131.19	119.84
2	M	230	ARG	C-N-CA	9.08	131.19	119.84
3	D	1383	ASP	CA-C-N	9.06	129.00	120.03
3	D	1383	ASP	C-N-CA	9.06	129.00	120.03
3	D	517	VAL	N-CA-C	9.04	115.79	107.56
3	N	186	VAL	N-CA-C	8.99	119.81	111.45
3	D	172	PRO	CA-C-N	8.94	131.02	119.84
3	D	172	PRO	C-N-CA	8.94	131.02	119.84
3	D	634	GLY	CA-C-N	8.91	130.98	119.84
3	D	634	GLY	C-N-CA	8.91	130.98	119.84
3	N	517	VAL	N-CA-C	8.86	115.63	107.56
3	D	186	VAL	N-CA-C	8.75	119.58	111.45
3	N	561	GLY	CA-C-N	-8.65	111.83	122.64
3	N	561	GLY	C-N-CA	-8.65	111.83	122.64
3	N	172	PRO	CA-C-N	8.62	130.62	119.84
3	N	172	PRO	C-N-CA	8.62	130.62	119.84
5	F	76	SER	N-CA-C	8.53	120.57	111.28
1	L	171	PHE	CA-C-N	-8.50	108.53	122.65
1	L	171	PHE	C-N-CA	-8.50	108.53	122.65
3	D	80	VAL	CA-C-N	8.50	137.77	121.54
3	D	80	VAL	C-N-CA	8.50	137.77	121.54
2	M	729	LEU	N-CA-C	8.49	124.30	114.62
3	D	1127	GLU	N-CA-C	-8.41	100.10	111.96
5	P	76	SER	N-CA-C	8.32	120.35	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	634	GLY	CA-C-N	8.30	130.21	119.84
3	N	634	GLY	C-N-CA	8.30	130.21	119.84
3	N	1127	GLU	N-CA-C	-8.29	100.27	111.96
2	C	1078	GLU	CA-C-N	8.28	130.19	119.84
2	C	1078	GLU	C-N-CA	8.28	130.19	119.84
2	M	243	ARG	CA-C-N	8.15	130.03	119.84
2	M	243	ARG	C-N-CA	8.15	130.03	119.84
3	N	187	LYS	N-CA-C	8.11	119.75	111.07
3	D	199	LEU	N-CA-C	8.10	122.97	112.12
2	C	191	PHE	CA-C-N	7.99	128.46	119.83
2	C	191	PHE	C-N-CA	7.99	128.46	119.83
2	C	535	SER	N-CA-C	7.94	115.27	108.13
3	N	380	GLU	N-CA-C	-7.92	96.01	109.24
2	C	729	LEU	N-CA-C	7.90	123.63	114.62
3	N	199	LEU	N-CA-C	7.88	122.69	112.12
2	M	317	VAL	CA-C-N	-7.81	110.91	119.19
2	M	317	VAL	C-N-CA	-7.81	110.91	119.19
1	A	48	ILE	N-CA-C	7.79	117.52	108.96
2	M	1078	GLU	CA-C-N	7.70	129.46	119.84
2	M	1078	GLU	C-N-CA	7.70	129.46	119.84
2	C	260	LEU	N-CA-C	7.70	123.33	111.56
3	D	380	GLU	N-CA-C	-7.69	96.39	109.24
3	D	187	LYS	N-CA-C	7.67	119.27	111.07
3	N	82	LYS	CA-C-N	-7.65	106.93	121.54
3	N	82	LYS	C-N-CA	-7.65	106.93	121.54
3	N	1124	GLN	CA-C-N	7.64	129.38	119.84
3	N	1124	GLN	C-N-CA	7.64	129.38	119.84
3	N	805	GLU	N-CA-C	7.63	121.06	112.97
3	N	198	ARG	CA-C-N	-7.60	110.47	122.17
3	N	198	ARG	C-N-CA	-7.60	110.47	122.17
3	D	198	ARG	N-CA-C	7.59	122.74	113.17
3	N	209	ARG	N-CA-C	7.55	126.89	110.80
3	D	423	ASP	N-CA-C	7.53	123.80	111.37
3	N	423	ASP	N-CA-C	7.53	123.79	111.37
2	C	317	VAL	CA-C-N	-7.49	111.25	119.19
2	C	317	VAL	C-N-CA	-7.49	111.25	119.19
3	N	198	ARG	N-CA-C	7.49	122.60	113.17
3	D	80	VAL	N-CA-C	7.43	121.24	108.90
2	M	39	ARG	N-CA-C	7.42	119.45	111.36
2	C	243	ARG	CA-C-N	7.33	129.01	119.84
2	C	243	ARG	C-N-CA	7.33	129.01	119.84
2	C	39	ARG	N-CA-C	7.31	119.24	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	80	VAL	N-CA-C	7.31	121.00	108.95
3	D	1110	ALA	N-CA-C	-7.17	98.11	109.23
3	D	198	ARG	CA-C-N	-7.13	111.19	122.17
3	D	198	ARG	C-N-CA	-7.13	111.19	122.17
2	C	169	GLY	CA-C-N	7.13	128.75	119.84
2	C	169	GLY	C-N-CA	7.13	128.75	119.84
2	C	1027	PHE	N-CA-C	7.12	121.07	112.38
2	M	762	LYS	N-CA-C	7.11	119.69	111.02
2	C	547	ILE	CA-C-N	7.02	128.62	119.84
2	C	547	ILE	C-N-CA	7.02	128.62	119.84
3	D	209	ARG	N-CA-C	6.95	125.59	110.80
3	D	589	ALA	CA-C-N	6.90	126.89	119.78
3	D	589	ALA	C-N-CA	6.90	126.89	119.78
2	C	373	VAL	N-CA-C	6.90	117.83	108.17
2	M	1027	PHE	N-CA-C	6.88	119.63	111.71
3	N	1110	ALA	N-CA-C	-6.88	98.57	109.23
2	M	591	SER	N-CA-C	-6.88	101.66	110.53
5	F	283	GLY	N-CA-C	-6.86	106.24	115.36
2	C	591	SER	N-CA-C	-6.83	101.72	110.53
2	C	263	ASP	CA-C-N	-6.80	112.76	119.90
2	C	263	ASP	C-N-CA	-6.80	112.76	119.90
5	P	283	GLY	N-CA-C	-6.79	106.33	115.36
2	M	365	ASP	N-CA-C	6.78	118.67	111.28
2	C	762	LYS	N-CA-C	6.77	119.28	111.02
3	D	1285	GLU	N-CA-C	6.75	121.84	112.45
3	D	248	PRO	N-CA-CB	6.74	109.60	103.20
2	M	58	ASP	CA-C-N	6.73	134.39	121.54
2	M	58	ASP	C-N-CA	6.73	134.39	121.54
2	C	365	ASP	N-CA-C	6.72	118.61	111.28
3	D	798	GLU	N-CA-C	6.72	121.34	112.13
3	D	53	ILE	N-CA-CB	-6.70	104.55	112.39
4	E	41	GLU	N-CA-C	6.70	121.32	112.35
2	C	58	ASP	CA-C-N	6.61	134.16	121.54
2	C	58	ASP	C-N-CA	6.61	134.16	121.54
3	D	1116	ASN	N-CA-C	-6.59	98.15	108.90
2	M	169	GLY	CA-C-N	6.57	128.05	119.84
2	M	169	GLY	C-N-CA	6.57	128.05	119.84
3	D	1109	GLU	N-CA-C	6.56	117.24	108.38
3	N	798	GLU	N-CA-C	6.54	120.96	111.02
2	M	165	LEU	C-N-CD	-6.53	106.22	120.60
2	M	151	ASP	CA-C-N	6.52	127.99	119.84
2	M	151	ASP	C-N-CA	6.52	127.99	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1440	PHE	N-CA-C	6.50	119.33	111.40
2	C	151	ASP	CA-C-N	6.50	127.96	119.84
2	C	151	ASP	C-N-CA	6.50	127.96	119.84
3	N	143	ASN	N-CA-C	-6.49	105.67	113.97
2	M	318	PRO	N-CA-C	-6.48	105.08	113.57
2	M	373	VAL	N-CA-C	6.48	117.25	108.17
3	N	1109	GLU	N-CA-C	6.46	117.10	108.38
2	M	1057	SER	CA-C-N	-6.43	112.14	122.24
2	M	1057	SER	C-N-CA	-6.43	112.14	122.24
3	N	108	VAL	CA-C-N	-6.42	111.81	119.84
3	N	108	VAL	C-N-CA	-6.42	111.81	119.84
3	N	1213	ARG	CA-C-N	-6.42	112.92	120.11
3	N	1213	ARG	C-N-CA	-6.42	112.92	120.11
3	D	238	PRO	N-CA-CB	6.40	109.97	103.25
4	O	41	GLU	N-CA-C	6.39	120.92	112.35
2	C	9	ILE	N-CA-C	-6.39	98.31	107.77
3	N	589	ALA	CA-C-N	6.36	126.27	119.85
3	N	589	ALA	C-N-CA	6.36	126.27	119.85
1	A	47	SER	N-CA-C	6.34	119.14	111.40
3	D	593	ASN	CA-C-N	6.33	127.75	119.84
3	D	593	ASN	C-N-CA	6.33	127.75	119.84
2	C	318	PRO	N-CA-C	-6.31	105.30	113.57
3	D	79	GLU	CA-C-N	-6.31	113.73	122.69
3	D	79	GLU	C-N-CA	-6.31	113.73	122.69
2	C	879	ARG	CA-C-N	-6.30	114.58	123.03
2	C	879	ARG	C-N-CA	-6.30	114.58	123.03
3	D	28	LYS	CA-C-N	6.30	127.72	119.84
3	D	28	LYS	C-N-CA	6.30	127.72	119.84
2	C	1057	SER	CA-C-N	-6.30	112.34	122.24
2	C	1057	SER	C-N-CA	-6.30	112.34	122.24
2	M	547	ILE	CA-C-N	6.29	127.71	119.84
2	M	547	ILE	C-N-CA	6.29	127.71	119.84
3	D	1344	VAL	CB-CA-C	-6.29	103.66	111.70
1	K	91	ASN	CA-C-N	6.26	127.66	119.84
1	K	91	ASN	C-N-CA	6.26	127.66	119.84
2	C	58	ASP	N-CA-C	6.22	119.70	108.69
3	N	593	ASN	CA-C-N	6.22	127.61	119.84
3	N	593	ASN	C-N-CA	6.22	127.61	119.84
4	E	51	LEU	N-CA-C	-6.19	100.07	108.24
2	C	535	SER	CA-C-N	-6.14	112.16	119.84
2	C	535	SER	C-N-CA	-6.14	112.16	119.84
3	D	208	PRO	CA-C-N	6.14	133.27	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	208	PRO	C-N-CA	6.14	133.27	121.54
3	D	143	ASN	N-CA-C	-6.14	106.11	113.97
2	M	263	ASP	CA-C-N	-6.13	113.46	119.90
2	M	263	ASP	C-N-CA	-6.13	113.46	119.90
5	F	287	THR	N-CA-C	-6.10	102.48	110.53
5	F	285	GLU	CA-C-N	6.09	127.45	119.84
5	F	285	GLU	C-N-CA	6.09	127.45	119.84
2	C	1118	LYS	N-CA-C	6.07	119.72	109.76
4	E	41	GLU	CA-C-N	6.07	127.42	119.84
4	E	41	GLU	C-N-CA	6.07	127.42	119.84
2	C	399	ASN	CA-C-N	6.04	127.38	119.84
2	C	399	ASN	C-N-CA	6.04	127.38	119.84
3	D	811	GLU	N-CA-C	-6.00	105.96	113.28
4	O	51	LEU	N-CA-C	-5.99	100.33	108.24
5	F	203	THR	N-CA-C	5.98	117.67	111.03
3	D	915	VAL	CB-CA-C	-5.97	104.05	111.70
3	D	1125	PRO	CA-C-N	-5.96	114.37	122.95
3	D	1125	PRO	C-N-CA	-5.96	114.37	122.95
2	M	58	ASP	N-CA-C	5.96	119.23	108.69
3	D	1109	GLU	CA-C-N	5.96	132.12	122.29
3	D	1109	GLU	C-N-CA	5.96	132.12	122.29
2	C	165	LEU	CA-C-N	5.94	141.26	127.00
2	C	165	LEU	C-N-CA	5.94	141.26	127.00
2	C	330	ASN	N-CA-C	-5.93	106.68	114.04
2	M	213	ALA	N-CA-C	-5.93	104.82	111.28
3	N	1109	GLU	CA-C-N	5.92	132.07	122.29
3	N	1109	GLU	C-N-CA	5.92	132.07	122.29
3	D	1190	SER	CA-C-N	5.91	125.79	119.28
3	D	1190	SER	C-N-CA	5.91	125.79	119.28
3	D	749	VAL	N-CA-C	5.89	114.62	107.61
3	N	238	PRO	N-CA-CB	5.88	109.43	103.25
3	D	406	ASP	N-CA-C	5.88	119.52	112.93
3	N	248	PRO	N-CA-CB	5.88	109.35	102.76
3	D	226	PRO	N-CA-CB	5.85	109.04	103.19
3	D	1331	ASP	CA-C-N	5.85	125.32	119.24
3	D	1331	ASP	C-N-CA	5.85	125.32	119.24
2	C	938	LYS	N-CA-C	-5.85	105.04	111.82
2	M	938	LYS	N-CA-C	-5.84	105.05	111.82
3	D	208	PRO	CA-N-CD	-5.82	103.86	112.00
2	M	1118	LYS	N-CA-C	5.82	119.30	109.76
2	C	318	PRO	CA-C-N	5.81	131.94	120.84
2	C	318	PRO	C-N-CA	5.81	131.94	120.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	879	ARG	CA-C-N	-5.81	115.24	123.03
2	M	879	ARG	C-N-CA	-5.81	115.24	123.03
5	F	330	GLY	N-CA-C	5.81	122.52	115.31
3	D	10	ILE	CB-CA-C	-5.81	103.71	110.91
1	K	47	SER	N-CA-C	5.80	118.48	111.40
4	E	57	ASP	CA-C-N	-5.79	112.60	119.84
4	E	57	ASP	C-N-CA	-5.79	112.60	119.84
3	D	1126	ASP	N-CA-C	5.78	119.78	107.70
1	B	91	ASN	CA-C-N	5.77	127.06	119.84
1	B	91	ASN	C-N-CA	5.77	127.06	119.84
2	M	318	PRO	CA-C-N	5.76	131.84	120.84
2	M	318	PRO	C-N-CA	5.76	131.84	120.84
2	M	443	THR	N-CA-C	5.75	116.21	109.60
3	N	226	PRO	N-CA-CB	5.75	108.94	103.19
3	N	1285	GLU	N-CA-C	5.75	120.43	112.90
1	B	171	PHE	N-CA-C	5.74	119.60	110.70
5	P	287	THR	N-CA-C	-5.74	102.95	110.53
5	P	285	GLU	CA-C-N	5.73	127.00	119.84
5	P	285	GLU	C-N-CA	5.73	127.00	119.84
2	C	506	ASN	N-CA-C	-5.71	106.36	113.38
5	F	340	SER	CA-C-N	5.70	126.97	119.84
5	F	340	SER	C-N-CA	5.70	126.97	119.84
3	N	811	GLU	N-CA-C	-5.70	105.83	112.89
3	N	28	LYS	CA-C-N	5.66	126.91	119.84
3	N	28	LYS	C-N-CA	5.66	126.91	119.84
3	N	1440	PHE	N-CA-C	5.65	118.29	111.40
3	D	1469	GLY	N-CA-C	-5.64	106.40	115.08
1	L	91	ASN	CA-C-N	5.63	126.88	119.84
1	L	91	ASN	C-N-CA	5.63	126.88	119.84
4	O	41	GLU	CA-C-N	5.63	126.88	119.84
4	O	41	GLU	C-N-CA	5.63	126.88	119.84
3	N	1469	GLY	N-CA-C	-5.61	106.44	115.08
1	L	2	LEU	N-CA-C	5.61	119.90	112.72
3	D	1043	GLY	CA-C-N	-5.60	114.88	122.77
3	D	1043	GLY	C-N-CA	-5.60	114.88	122.77
2	M	165	LEU	CA-C-N	5.60	140.43	127.00
2	M	165	LEU	C-N-CA	5.60	140.43	127.00
2	C	291	ALA	N-CA-C	5.58	118.55	109.06
2	C	213	ALA	N-CA-C	-5.57	105.21	111.28
2	C	442	GLU	N-CA-C	5.56	117.34	111.28
3	D	1066	THR	CA-C-N	5.54	127.75	120.60
3	D	1066	THR	C-N-CA	5.54	127.75	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	592	THR	N-CA-C	-5.53	102.70	110.50
3	N	441	ARG	N-CA-C	-5.50	102.37	110.52
3	D	373	PRO	N-CA-CB	5.49	109.02	103.25
2	M	506	ASN	N-CA-C	-5.49	106.63	113.38
2	C	685	GLU	N-CA-C	-5.49	105.38	112.68
5	P	340	SER	CA-C-N	5.47	126.68	119.84
5	P	340	SER	C-N-CA	5.47	126.68	119.84
1	L	226	SER	N-CA-C	5.47	118.30	111.24
3	N	208	PRO	CA-N-CD	-5.47	104.34	112.00
3	D	1317	ASP	CA-C-N	5.47	129.00	120.75
3	D	1317	ASP	C-N-CA	5.47	129.00	120.75
2	C	730	SER	N-CA-C	5.46	117.37	109.07
3	N	81	THR	N-CA-C	-5.46	98.92	107.93
1	B	2	LEU	N-CA-C	5.44	119.68	112.72
2	C	261	ILE	N-CA-C	5.44	120.65	109.34
3	D	108	VAL	CA-C-N	-5.42	113.06	119.84
3	D	108	VAL	C-N-CA	-5.42	113.06	119.84
2	M	291	ALA	N-CA-C	5.40	118.24	109.06
3	N	1476	THR	N-CA-C	-5.38	105.98	112.54
3	D	592	THR	N-CA-C	-5.38	102.92	110.50
3	N	379	ALA	N-CA-C	-5.37	104.46	111.02
1	A	91	ASN	CA-C-N	5.37	126.55	119.84
1	A	91	ASN	C-N-CA	5.37	126.55	119.84
3	D	824	ASN	N-CA-C	5.37	117.95	111.40
2	M	261	ILE	N-CA-C	5.37	120.50	109.34
3	D	1476	THR	N-CA-C	-5.33	106.03	112.54
3	D	486	ARG	N-CA-C	5.33	118.88	112.38
3	D	379	ALA	N-CA-C	-5.32	104.53	111.02
5	F	313	GLU	CA-C-N	-5.31	113.20	119.84
5	F	313	GLU	C-N-CA	-5.31	113.20	119.84
1	A	2	LEU	N-CA-C	5.31	119.52	112.72
3	N	1116	ASN	N-CA-C	-5.31	99.75	108.41
2	M	730	SER	N-CA-C	5.30	117.13	109.07
3	N	208	PRO	CA-C-N	5.30	131.67	121.54
3	N	208	PRO	C-N-CA	5.30	131.67	121.54
3	D	1251	ASP	N-CA-C	5.30	119.67	112.04
2	C	253	ALA	N-CA-C	5.29	116.90	111.03
3	D	199	LEU	CA-CB-CG	-5.27	97.84	116.30
3	N	824	ASN	N-CA-C	5.27	117.83	111.40
1	K	48	ILE	N-CA-C	5.26	114.70	108.96
2	C	243	ARG	N-CA-C	5.26	121.42	109.81
4	E	50	THR	CA-C-N	5.25	131.57	122.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	50	THR	C-N-CA	5.25	131.57	122.32
3	N	1317	ASP	CA-C-N	5.24	128.66	120.75
3	N	1317	ASP	C-N-CA	5.24	128.66	120.75
2	C	679	PHE	CA-C-O	-5.24	115.22	120.77
2	C	1056	LYS	CA-C-N	-5.24	111.63	121.63
2	C	1056	LYS	C-N-CA	-5.24	111.63	121.63
2	C	315	ALA	N-CA-C	5.23	118.97	112.59
2	C	761	PHE	CA-C-N	5.23	128.06	120.79
2	C	761	PHE	C-N-CA	5.23	128.06	120.79
3	D	133	ILE	N-CA-C	5.23	116.33	109.58
2	M	728	HIS	CA-C-O	-5.23	113.50	119.41
3	N	373	PRO	N-CA-CB	5.22	108.73	103.25
1	K	2	LEU	N-CA-C	5.21	119.39	112.72
3	D	561	GLY	N-CA-C	-5.21	103.30	111.00
2	C	165	LEU	C-N-CD	-5.20	109.16	120.60
3	N	1128	VAL	N-CA-C	-5.20	100.40	107.99
2	M	244	PRO	CA-N-CD	-5.19	104.73	112.00
2	M	1019	GLN	CA-C-N	5.19	126.33	119.84
2	M	1019	GLN	C-N-CA	5.19	126.33	119.84
3	D	81	THR	N-CA-C	-5.19	99.75	110.80
2	M	685	GLU	N-CA-C	-5.18	105.78	112.68
2	M	243	ARG	N-CA-C	5.17	121.25	109.81
2	C	768	THR	CA-C-N	5.17	124.35	118.97
2	C	768	THR	C-N-CA	5.17	124.35	118.97
5	P	313	GLU	CA-C-N	-5.16	113.39	119.84
5	P	313	GLU	C-N-CA	-5.16	113.39	119.84
3	N	79	GLU	CA-C-N	-5.16	114.53	122.68
3	N	79	GLU	C-N-CA	-5.16	114.53	122.68
2	M	810	ASP	CA-C-N	5.15	126.28	119.84
2	M	810	ASP	C-N-CA	5.15	126.28	119.84
3	N	132	TYR	CA-CB-CG	-5.15	104.64	113.90
3	N	749	VAL	N-CA-C	5.15	113.73	107.61
3	D	54	LYS	N-CA-C	5.13	117.71	108.48
3	N	509	PRO	CA-N-CD	-5.12	104.83	112.00
2	M	1109	VAL	CA-C-N	-5.12	115.55	122.77
2	M	1109	VAL	C-N-CA	-5.12	115.55	122.77
3	D	246	PRO	N-CA-CB	5.12	108.62	103.25
3	D	1044	LEU	N-CA-C	5.11	116.72	108.34
3	N	422	ALA	CA-C-N	5.10	128.47	120.82
3	N	422	ALA	C-N-CA	5.10	128.47	120.82
2	M	243	ARG	C-N-CD	-5.10	104.10	125.00
3	D	422	ALA	CA-C-N	5.10	128.46	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	422	ALA	C-N-CA	5.10	128.46	120.82
1	L	47	SER	N-CA-C	5.09	117.61	111.40
3	N	380	GLU	CA-C-O	-5.09	114.81	120.66
3	N	525	ARG	CA-C-N	5.09	126.20	119.84
3	N	525	ARG	C-N-CA	5.09	126.20	119.84
3	D	107	ASP	CA-C-O	-5.09	116.02	121.56
1	B	47	SER	N-CA-C	5.08	117.60	111.40
3	N	246	PRO	N-CA-CB	5.08	108.58	103.25
3	D	1281	VAL	N-CA-C	5.07	116.82	108.97
3	N	1251	ASP	N-CA-C	5.07	119.33	112.04
4	O	50	THR	CA-C-N	5.07	131.24	122.32
4	O	50	THR	C-N-CA	5.07	131.24	122.32
3	D	1128	VAL	N-CA-C	-5.06	100.60	107.99
2	C	398	THR	N-CA-C	-5.06	106.94	113.01
3	D	1344	VAL	N-CA-CB	5.06	115.93	110.62
3	D	1389	LEU	CA-CB-CG	5.05	133.99	116.30
4	O	40	LEU	N-CA-C	5.05	116.92	110.61
2	C	414	GLY	CA-C-N	5.04	126.14	119.84
2	C	414	GLY	C-N-CA	5.04	126.14	119.84
3	D	1472	ILE	N-CA-C	5.04	113.71	109.02
1	K	211	LEU	CA-CB-CG	5.04	133.95	116.30
3	N	10	ILE	CB-CA-C	-5.04	104.30	111.21
3	N	133	ILE	N-CA-C	5.04	116.08	109.58
3	N	247	GLU	N-CA-C	5.04	120.95	109.81
3	D	201	GLY	N-CA-C	-5.04	101.24	113.18
2	M	761	PHE	CA-C-N	5.03	127.78	120.79
2	M	761	PHE	C-N-CA	5.03	127.78	120.79
2	M	57	GLU	CA-C-N	-5.03	113.89	122.33
2	M	57	GLU	C-N-CA	-5.03	113.89	122.33
3	D	80	VAL	O-C-N	5.02	128.69	123.02
3	D	380	GLU	CA-C-O	-5.01	114.89	120.66
2	M	727	PRO	CA-C-N	-5.01	113.11	122.09
2	M	727	PRO	C-N-CA	-5.01	113.11	122.09
2	M	608	GLY	N-CA-C	-5.01	107.05	115.62
3	D	525	ARG	CA-C-N	5.00	126.10	119.84
3	D	525	ARG	C-N-CA	5.00	126.10	119.84

There are no chirality outliers.

There are no planarity outliers.

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	238	0
1	B	1806	0	1861	217	0
1	K	1806	0	1861	176	0
1	L	1806	0	1861	186	0
2	C	8829	0	8933	1252	0
2	M	8829	0	8933	1198	0
3	D	10797	0	10873	1532	0
3	N	10797	0	10873	1349	0
4	E	769	0	775	95	0
4	O	769	0	775	99	0
5	F	2771	0	2844	358	0
5	P	2771	0	2844	363	0
6	A	33	0	0	0	0
6	B	21	0	0	0	0
6	C	73	0	0	0	0
6	D	106	0	0	0	0
6	E	5	0	0	0	0
6	F	28	0	0	0	0
6	K	19	0	0	0	0
6	L	17	0	0	0	0
6	M	65	0	0	0	0
6	N	92	0	0	0	0
6	O	8	0	0	0	0
6	P	20	0	0	0	0
7	C	63	0	62	5	0
7	M	63	0	62	7	0
8	D	2	0	0	0	0
8	N	2	0	0	0	0
9	A	239	0	0	50	0
9	B	258	0	0	46	0
9	C	979	0	0	226	0
9	D	1252	0	0	280	0
9	E	117	0	0	28	0
9	F	420	0	0	94	0
9	K	183	0	0	39	0
9	L	219	0	0	46	0
9	M	998	0	0	251	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	N	1265	0	0	253	0
9	O	108	0	0	26	0
9	P	361	0	0	79	0
All	All	60572	0	54418	6667	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 61.

All (6667) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:GLN:HA	1:A:146:ARG:HH12	1.07	1.11
2:M:952:LEU:HD12	2:M:969:GLN:HE22	1.13	1.11
3:D:1087:ARG:HG2	3:D:1234:THR:HA	1.27	1.07
1:B:152:PRO:HD2	1:B:155:LYS:HD3	1.36	1.05
2:M:605:LYS:HB2	2:M:610:ARG:HH12	1.16	1.05
3:D:1481:VAL:HG11	4:E:18:ARG:HA	1.41	1.03
1:B:86:VAL:HG12	1:B:124:ASN:HD22	1.24	1.02
2:C:274:ARG:HD2	2:C:285:LEU:HD22	1.37	1.02
2:C:775:ARG:HH21	2:C:782:ALA:HB1	1.24	1.02
5:F:94:LEU:HD22	5:F:97:GLU:HG2	1.39	1.01
3:N:783:ARG:HH21	3:N:1029:ARG:HD3	1.26	1.01
2:C:110:GLU:HG2	2:C:369:PRO:HB3	1.42	1.00
3:N:197:SER:HB3	3:N:203:ALA:HB3	1.42	1.00
2:M:110:GLU:HG2	2:M:369:PRO:HG3	1.40	1.00
3:D:197:SER:HB3	3:D:203:ALA:HB3	1.43	1.00
3:N:210:ARG:HH11	3:N:398:ALA:HB3	1.26	0.99
3:N:1144:LEU:HD12	3:N:1171:VAL:HG13	1.43	0.99
3:N:52:PRO:HB2	3:N:80:VAL:HG13	1.45	0.99
3:N:1036:ARG:HH21	3:N:1042:ARG:HA	1.28	0.98
3:D:422:ALA:HB3	3:D:427:VAL:HG22	1.45	0.98
2:C:724:ARG:HG3	2:C:741:GLY:H	1.27	0.97
3:N:422:ALA:HB3	3:N:427:VAL:HG22	1.45	0.97
5:F:268:ILE:HA	5:F:271:LEU:HD12	1.45	0.97
2:M:1114:GLY:H	2:M:1115:LEU:HD12	1.26	0.97
2:M:1092:LEU:HD13	2:M:1099:VAL:HG21	1.47	0.97
1:L:88:ARG:HB3	1:L:88:ARG:HH11	1.29	0.96
3:N:423:ASP:HB2	5:P:178:ARG:HD2	1.45	0.96
3:D:667:ALA:HB2	3:D:676:MET:HE2	1.48	0.95
2:M:905:ILE:H	2:M:905:ILE:HD12	1.31	0.95
2:M:169:GLY:HA2	2:M:263:ASP:HB3	1.48	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:404:LEU:HA	2:M:407:LYS:HD3	1.47	0.95
3:D:214:GLU:HB2	3:D:390:PRO:HD2	1.49	0.95
2:C:846:LYS:HD3	3:D:741:ASP:HB2	1.47	0.94
2:C:413:LEU:HD21	2:C:448:ASN:HD21	1.31	0.94
3:D:118:LEU:HB3	3:D:123:LEU:HD22	1.46	0.94
2:C:1114:GLY:H	2:C:1115:LEU:HD12	1.31	0.94
3:D:119:SER:HB2	3:D:123:LEU:H	1.32	0.94
3:D:1095:THR:HG23	3:D:1230:GLY:HA3	1.46	0.94
1:B:57:TYR:HB3	1:B:141:GLU:HG3	1.49	0.94
2:C:150:PRO:HA	2:C:158:TYR:HB3	1.50	0.94
3:D:191:LEU:HD12	3:D:211:VAL:HG21	1.47	0.94
3:N:1210:SER:HA	9:N:9537:HOH:O	1.68	0.94
2:C:689:VAL:HB	2:C:870:ILE:HG13	1.50	0.94
3:D:1310:ARG:HE	3:D:1327:ARG:HB3	1.33	0.94
2:M:1018:GLN:HE21	2:M:1060:ILE:HD11	1.28	0.94
3:N:637:LEU:HD21	3:N:642:CYS:HA	1.50	0.94
3:N:928:ALA:HA	3:N:931:LEU:HD12	1.50	0.94
5:P:366:ALA:HB3	5:P:367:MET:HE2	1.50	0.94
3:N:1205:TYR:HD2	3:N:1215:VAL:HG21	1.32	0.93
2:C:329:GLY:HA3	2:C:489:THR:HG23	1.47	0.93
2:C:987:ILE:HG23	3:D:948:THR:HG21	1.48	0.93
3:N:1262:LEU:HD21	3:N:1351:GLU:HG3	1.51	0.93
3:N:1481:VAL:HG11	4:O:18:ARG:HA	1.48	0.93
3:D:1468:LEU:HD22	3:D:1470:ARG:HB2	1.51	0.92
5:P:371:LEU:HD22	5:P:375:LEU:HD22	1.52	0.92
1:A:63:HIS:HB3	2:C:746:GLY:HA2	1.50	0.92
2:C:54:ILE:HD11	2:C:356:ARG:HG2	1.52	0.92
3:N:1101:VAL:HG21	3:N:1424:VAL:HG22	1.49	0.91
3:D:87:ARG:HB3	3:D:523:ASP:HB2	1.51	0.91
5:P:163:LEU:HD13	5:P:174:LEU:HD21	1.49	0.91
3:N:572:ARG:HH22	5:P:83:GLN:HG3	1.36	0.91
2:C:328:LEU:HD13	2:C:433:THR:HB	1.51	0.90
3:D:148:GLU:HB3	3:D:151:GLN:HB2	1.53	0.90
2:C:358:ARG:HH22	2:C:374:ASN:HB3	1.36	0.90
1:A:14:ARG:HH21	1:A:22:GLU:HB3	1.35	0.90
4:E:37:ASN:HD22	4:E:89:MET:HE2	1.36	0.90
2:M:791:ARG:HB3	9:M:9759:HOH:O	1.71	0.90
3:D:145:VAL:HG22	3:D:146:PRO:HD2	1.53	0.90
4:E:67:GLU:HB2	4:E:73:LEU:HD11	1.52	0.90
2:M:289:THR:HG22	2:M:290:LEU:HD23	1.54	0.90
2:M:979:THR:HG23	2:M:981:GLU:H	1.37	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:41:ARG:HD3	3:D:42:ASP:H	1.37	0.89
1:L:57:TYR:HB3	1:L:141:GLU:HG3	1.53	0.89
2:C:93:PRO:HA	9:C:9729:HOH:O	1.71	0.89
3:D:871:LYS:HE3	3:D:873:LEU:HD21	1.54	0.89
3:D:1326:THR:HA	9:D:9756:HOH:O	1.71	0.89
2:C:479:VAL:HG21	2:C:503:LEU:HD11	1.55	0.89
2:C:211:LEU:HD11	2:C:308:ARG:HB2	1.54	0.88
3:D:1057:VAL:HG13	3:D:1069:GLU:HB3	1.55	0.88
2:C:860:HIS:HB2	9:C:9519:HOH:O	1.72	0.88
3:D:1096:ARG:HH11	3:D:1096:ARG:HB2	1.36	0.88
2:M:964:LYS:O	2:M:968:LEU:HG	1.72	0.88
5:P:394:ARG:HA	5:P:397:ILE:HD12	1.54	0.88
5:F:88:ILE:HD13	5:F:193:ARG:HB2	1.54	0.88
3:D:520:LEU:HD12	3:D:521:PRO:HD2	1.56	0.88
2:M:92:ALA:HB2	2:M:120:LEU:HD11	1.55	0.88
2:M:146:VAL:HG22	2:M:162:ILE:HA	1.56	0.88
2:C:671:ASN:H	2:C:671:ASN:ND2	1.70	0.88
2:C:979:THR:HG23	2:C:981:GLU:H	1.39	0.88
3:D:572:ARG:HH21	5:F:83:GLN:HE21	1.21	0.88
3:N:133:ILE:HG21	3:N:454:ALA:HB1	1.52	0.88
3:N:661:MET:HE1	3:N:677:LEU:HD11	1.56	0.88
3:D:973:GLN:HA	3:D:976:GLN:HE21	1.34	0.88
3:N:18:ILE:HG23	3:N:518:PRO:HG3	1.56	0.87
3:N:978:TYR:HA	9:N:9888:HOH:O	1.72	0.87
5:P:88:ILE:HD13	5:P:193:ARG:HB2	1.55	0.87
3:D:906:GLN:HB3	3:D:911:LEU:HD11	1.54	0.87
2:C:945:ARG:HB3	2:C:945:ARG:HH11	1.37	0.87
3:N:566:ILE:HD11	5:P:192:LEU:HD21	1.54	0.87
5:F:125:ASP:HA	5:F:128:ARG:NH1	1.90	0.87
2:M:144:PRO:HA	2:M:163:ILE:HG12	1.57	0.87
2:C:724:ARG:HH12	2:C:734:LEU:HD23	1.37	0.87
2:C:671:ASN:HD22	2:C:671:ASN:N	1.71	0.86
1:K:186:LEU:HB2	1:K:192:LEU:HD11	1.55	0.86
5:P:260:ILE:HG23	5:P:264:MET:HB2	1.57	0.86
1:A:95:GLN:HA	1:A:146:ARG:NH1	1.88	0.86
2:C:66:LEU:HD22	2:C:372:LEU:HD23	1.57	0.86
3:D:18:ILE:HG23	3:D:518:PRO:HG3	1.58	0.86
2:C:671:ASN:H	2:C:671:ASN:HD22	0.91	0.86
2:C:1060:ILE:HD12	2:C:1063:ARG:HH12	1.38	0.86
3:D:57:GLU:HG3	3:D:64:LYS:HG2	1.57	0.86
1:L:112:ARG:HB3	1:L:112:ARG:HH11	1.38	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:165:LEU:O	2:M:265:ARG:HB2	1.76	0.86
2:M:129:ILE:HD13	2:M:134:ARG:HB2	1.55	0.85
3:N:119:SER:HB2	3:N:123:LEU:H	1.39	0.85
1:A:67:THR:HA	9:A:9598:HOH:O	1.75	0.85
2:C:579:VAL:HB	2:C:890:LEU:HD22	1.55	0.85
5:F:160:ASP:HA	5:F:163:LEU:HD12	1.58	0.85
1:A:186:LEU:HB2	1:A:192:LEU:HD11	1.58	0.85
1:B:87:VAL:HG21	1:B:144:VAL:HG11	1.57	0.85
3:D:1232:PRO:HB3	3:D:1361:VAL:HG21	1.58	0.85
3:D:560:GLN:HG2	5:F:218:GLN:HE22	1.39	0.85
2:C:135:VAL:HG11	2:C:407:LYS:HA	1.59	0.85
2:M:134:ARG:HH21	2:M:393:GLN:HA	1.41	0.85
5:F:363:GLU:HA	5:F:367:MET:HE3	1.57	0.85
2:C:49:ARG:HH11	2:C:49:ARG:HB2	1.41	0.85
3:N:1314:LYS:HZ2	3:N:1314:LYS:H	1.23	0.84
2:C:874:LEU:HD21	3:D:787:LEU:HD22	1.59	0.84
4:E:85:LEU:HA	9:E:9594:HOH:O	1.77	0.84
2:C:433:THR:HG21	2:C:488:ALA:HB1	1.59	0.84
5:F:101:GLU:HA	9:F:9749:HOH:O	1.76	0.84
5:P:358:LEU:HD13	5:P:370:LYS:HG3	1.57	0.84
5:P:363:GLU:HA	5:P:367:MET:HE3	1.56	0.84
3:N:1380:GLU:HB3	3:N:1418:LYS:HG3	1.59	0.84
2:C:1005:MET:HB3	3:D:724:GLN:HE22	1.43	0.84
3:D:1223:ILE:H	3:D:1223:ILE:HD12	1.42	0.84
3:D:1160:LEU:HD11	3:D:1174:LEU:HD21	1.58	0.84
3:D:1209:LEU:HD21	4:E:16:LYS:NZ	1.92	0.84
3:D:1466:VAL:HG23	3:D:1472:ILE:HD11	1.58	0.84
3:D:44:LEU:HB3	3:D:525:ARG:HH21	1.43	0.84
3:N:565:ILE:H	3:N:565:ILE:HD12	1.41	0.84
2:M:589:ARG:HH11	2:M:589:ARG:HB2	1.42	0.83
2:M:675:ALA:HA	2:M:989:VAL:HG12	1.58	0.83
3:D:86:ARG:O	3:D:522:PRO:HD2	1.77	0.83
2:C:953:VAL:HG13	2:C:966:LEU:HD13	1.59	0.83
2:C:656:ALA:HB3	9:C:2223:HOH:O	1.79	0.83
3:N:168:THR:HG22	3:N:170:PRO:HD2	1.61	0.83
3:N:785:ILE:H	3:N:785:ILE:HD12	1.42	0.83
2:C:232:GLU:HA	2:C:235:LEU:HD12	1.59	0.83
2:C:362:GLY:HA3	2:C:367:LEU:HD23	1.60	0.83
2:C:524:VAL:HG13	2:C:528:GLU:HB2	1.61	0.83
1:A:178:ALA:HB3	1:A:198:ARG:HG3	1.59	0.82
3:D:513:ILE:HG23	9:D:9966:HOH:O	1.77	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1238:MET:HE2	3:N:1257:PRO:HG3	1.61	0.82
2:C:943:VAL:HG23	2:C:985:GLY:H	1.43	0.82
5:F:191:ASN:HA	5:F:194:LEU:HD23	1.59	0.82
2:M:115:LEU:HD22	2:M:373:VAL:HG11	1.60	0.82
2:M:1096:ALA:O	3:N:13:ALA:HB2	1.79	0.82
2:C:47:ALA:HB1	2:C:345:ARG:HB3	1.61	0.82
3:D:209:ARG:HD2	3:D:210:ARG:HG2	1.62	0.82
3:N:214:GLU:HB2	3:N:390:PRO:HD2	1.60	0.82
3:N:704:ARG:HG3	3:N:736:PHE:HB3	1.60	0.82
2:M:51:THR:HG21	9:M:2064:HOH:O	1.80	0.82
3:N:186:VAL:HG21	3:N:213:VAL:HB	1.62	0.82
5:P:160:ASP:HA	5:P:163:LEU:HD12	1.62	0.82
5:P:166:LEU:HB3	5:P:170:HIS:HB2	1.59	0.82
3:N:55:ASP:HA	3:N:82:LYS:HG3	1.61	0.82
3:N:105:VAL:HG21	3:N:128:TYR:HE2	1.43	0.82
3:N:558:LEU:HD13	5:P:145:PRO:HB3	1.60	0.82
3:N:796:ARG:HH11	3:N:861:GLN:HB2	1.44	0.82
5:F:130:VAL:HG21	5:F:159:ILE:HG21	1.59	0.82
2:M:157:ARG:HD2	2:M:314:THR:HG22	1.62	0.82
2:M:447:ALA:HA	3:N:1085:ALA:HB1	1.62	0.81
1:A:87:VAL:HG21	1:A:144:VAL:HG11	1.62	0.81
3:D:699:VAL:H	3:D:756:GLN:NE2	1.77	0.81
3:N:165:LYS:HB3	3:N:395:VAL:HG11	1.60	0.81
1:A:133:GLU:HG2	1:A:134:GLU:H	1.46	0.81
3:D:1465:ASN:HD21	3:D:1470:ARG:HH11	1.25	0.81
5:F:291:ILE:HG21	5:F:304:VAL:HG11	1.62	0.81
1:K:35:THR:HG21	1:L:43:ILE:HD11	1.62	0.81
3:D:671:LYS:HG3	5:F:422:LEU:HA	1.60	0.81
2:M:436:GLY:HA2	2:M:538:GLN:O	1.78	0.81
2:C:672:VAL:HG23	2:C:868:ASP:HB2	1.62	0.81
2:C:457:ALA:HB3	2:C:538:GLN:HA	1.60	0.81
3:D:1101:VAL:HG21	3:D:1424:VAL:HG22	1.60	0.81
1:A:195:LEU:HD11	1:A:197:LEU:HD22	1.61	0.81
3:D:73:CYS:HB3	3:D:76:CYS:O	1.81	0.81
2:M:707:ARG:HH12	2:M:709:GLU:HB2	1.44	0.81
2:C:244:PRO:HD2	2:C:245:GLY:H	1.46	0.81
2:C:512:ARG:HB3	2:C:523:ILE:HD11	1.62	0.81
2:C:949:LYS:HD2	3:D:796:ARG:HH21	1.44	0.81
1:L:22:GLU:HG2	1:L:198:ARG:HG2	1.62	0.81
3:N:1123:PHE:HE2	3:N:1184:GLN:HA	1.46	0.81
3:D:530:VAL:HB	3:D:534:ARG:HB2	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:10:ARG:HA	2:C:10:ARG:HH11	1.45	0.80
2:C:1005:MET:HE1	3:D:648:MET:HB2	1.63	0.80
2:M:462:ASP:HB3	2:M:468:ARG:HD2	1.62	0.80
2:M:904:PRO:HD2	2:M:908:GLY:HA2	1.63	0.80
3:N:148:GLU:HB3	3:N:151:GLN:HB2	1.61	0.80
2:C:675:ALA:HA	2:C:989:VAL:HG12	1.62	0.80
3:D:152:LEU:HD23	3:D:152:LEU:H	1.44	0.80
2:M:227:PHE:HA	2:M:230:ARG:HE	1.46	0.80
3:D:666:ILE:HG22	3:D:676:MET:HE1	1.61	0.80
1:L:185:ARG:HG3	1:L:190:THR:HG22	1.62	0.80
2:M:890:LEU:HD12	2:M:914:ILE:HD13	1.61	0.80
3:N:1352:ILE:O	3:N:1355:VAL:HG23	1.81	0.80
3:D:1359:GLN:HB3	9:D:9531:HOH:O	1.81	0.80
3:D:487:ALA:HB3	9:D:9629:HOH:O	1.81	0.80
3:D:584:ASN:HD22	3:D:585:GLY:N	1.80	0.80
3:D:720:LEU:H	3:D:720:LEU:HD12	1.47	0.80
2:M:83:CYS:HA	2:M:88:LEU:HB3	1.64	0.80
1:A:206:THR:HG22	1:A:209:GLU:HG3	1.63	0.80
3:D:550:ARG:HA	9:D:9572:HOH:O	1.80	0.80
2:M:728:HIS:HB3	2:M:729:LEU:HD12	1.64	0.80
5:F:394:ARG:HA	5:F:397:ILE:HD12	1.62	0.80
1:K:24:VAL:HG22	1:K:196:THR:HB	1.64	0.80
2:C:62:GLY:HA2	2:C:359:MET:HE1	1.64	0.80
3:D:153:LEU:HD12	3:D:154:THR:N	1.97	0.80
3:D:601:ARG:HD2	5:F:328:PHE:HE1	1.46	0.80
5:P:94:LEU:HB2	5:P:98:GLU:HG3	1.64	0.79
2:C:873:PRO:HG2	3:D:947:ILE:HD12	1.64	0.79
3:D:397:LYS:HG2	9:D:9991:HOH:O	1.82	0.79
1:L:214:ALA:HA	1:L:217:ILE:HD12	1.64	0.79
3:N:86:ARG:O	3:N:522:PRO:HD2	1.81	0.79
2:C:292:ARG:HD2	2:C:299:LYS:HE2	1.64	0.79
5:P:85:LEU:HA	5:P:88:ILE:HD12	1.65	0.79
2:C:36:PRO:HG2	2:C:70:GLU:HB3	1.63	0.79
3:N:1205:TYR:CD2	3:N:1215:VAL:HG21	2.17	0.79
1:B:176:ARG:HH22	3:D:884:ARG:HD3	1.47	0.79
2:C:773:LEU:HB2	5:F:373:LYS:HB3	1.64	0.79
3:D:704:ARG:HE	3:D:705:ALA:H	1.28	0.79
3:D:41:ARG:HH11	3:D:42:ASP:HB2	1.47	0.79
2:C:83:CYS:HA	2:C:88:LEU:HB3	1.64	0.79
1:K:227:ASN:HD22	1:K:227:ASN:H	1.30	0.79
2:M:676:ILE:HD12	2:M:871:LEU:HB2	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1160:LEU:HD11	3:N:1174:LEU:HD21	1.64	0.79
3:D:697:GLY:HA2	9:D:2528:HOH:O	1.83	0.79
3:D:400:VAL:HG21	3:D:441:ARG:HH11	1.49	0.78
3:D:908:LYS:HB3	3:D:1027:GLY:HA3	1.65	0.78
2:M:333:ILE:HB	9:M:9987:HOH:O	1.84	0.78
3:N:1223:ILE:H	3:N:1223:ILE:HD12	1.47	0.78
3:D:9:ARG:HH12	3:D:506:GLY:HA2	1.48	0.78
3:N:26:VAL:HG11	3:N:44:LEU:HD23	1.64	0.78
2:C:690:ILE:HG23	2:C:852:ILE:HG23	1.64	0.78
2:M:326:ASP:HA	2:M:331:ARG:HD3	1.64	0.78
3:N:628:ARG:HD3	3:N:744:GLN:NE2	1.97	0.78
3:N:806:PHE:CE1	3:N:813:LEU:HB3	2.18	0.78
2:C:343:GLN:HG2	2:C:385:PHE:HB2	1.66	0.78
3:D:1045:MET:HG2	3:D:1073:SER:HA	1.65	0.78
3:N:1045:MET:HG2	3:N:1073:SER:HA	1.65	0.78
5:P:268:ILE:HA	5:P:271:LEU:HD12	1.65	0.78
2:C:462:ASP:HB3	2:C:468:ARG:HD2	1.66	0.78
1:K:42:ARG:HH12	2:M:857:ASP:HB3	1.49	0.78
3:D:1258:ARG:CZ	3:D:1262:LEU:HD11	2.13	0.78
1:L:13:VAL:HG11	1:L:208:LEU:HD11	1.65	0.78
2:C:455:LEU:HD12	2:C:459:ALA:HB3	1.66	0.78
3:D:1381:VAL:HB	3:D:1389:LEU:O	1.84	0.78
2:M:329:GLY:HA3	2:M:489:THR:HG23	1.65	0.78
2:M:250:ARG:HG2	2:M:253:ALA:HB3	1.66	0.78
3:D:1109:GLU:HG2	3:D:1201:CYS:HA	1.65	0.78
1:K:123:MET:HG2	9:K:3485:HOH:O	1.82	0.78
2:M:707:ARG:HD2	2:M:824:ARG:HD3	1.65	0.78
2:M:724:ARG:HG3	2:M:741:GLY:H	1.49	0.78
1:B:123:MET:HE3	1:B:204:SER:HA	1.65	0.78
2:C:144:PRO:HA	2:C:163:ILE:HG12	1.64	0.78
3:D:637:LEU:HD21	3:D:642:CYS:HA	1.66	0.77
2:M:833:LEU:HD11	2:M:849:VAL:HG21	1.65	0.77
2:C:41:ASN:HD22	2:C:41:ASN:H	1.29	0.77
5:F:117:SER:HA	9:F:9599:HOH:O	1.84	0.77
2:M:771:GLU:O	2:M:775:ARG:HG2	1.85	0.77
2:M:879:ARG:HH12	3:N:1029:ARG:NH2	1.83	0.77
1:A:198:ARG:HG2	9:A:9490:HOH:O	1.85	0.77
2:M:312:ALA:HB1	2:M:318:PRO:HG2	1.66	0.77
2:M:601:GLY:HA2	2:M:616:GLU:HG2	1.66	0.77
3:N:984:THR:HG22	3:N:987:GLU:HG3	1.66	0.77
1:A:133:GLU:HG2	1:A:134:GLU:N	2.00	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:405:ARG:HH12	2:C:563:ASN:ND2	1.83	0.77
1:K:54:THR:CG2	1:K:158:ILE:HG13	2.15	0.77
2:M:897:LEU:HB3	2:M:899:GLN:HE21	1.50	0.77
3:N:35:ARG:HD2	3:N:36:THR:H	1.47	0.77
3:N:53:ILE:HG23	3:N:54:LYS:H	1.48	0.77
1:A:126:ASP:HB2	9:A:9492:HOH:O	1.85	0.77
3:N:58:CYS:HA	3:N:78:VAL:HG11	1.66	0.77
2:C:1054:THR:HG21	2:C:1079:PRO:HB3	1.66	0.77
5:F:125:ASP:HA	5:F:128:ARG:HH12	1.48	0.77
5:P:132:ARG:HH11	5:P:136:LEU:HD21	1.50	0.77
3:D:1209:LEU:HD21	4:E:16:LYS:HZ2	1.47	0.77
3:N:396:VAL:HG21	3:N:447:VAL:HB	1.67	0.77
3:N:488:ARG:NH1	3:N:488:ARG:HB3	2.00	0.77
3:D:1194:CYS:HB3	3:D:1373:ARG:NH2	1.99	0.77
5:F:411:HIS:HA	5:F:414:ARG:HG3	1.67	0.77
3:N:906:GLN:HB3	3:N:911:LEU:HD11	1.66	0.77
3:N:1123:PHE:CE2	3:N:1184:GLN:HA	2.19	0.77
3:N:1277:ILE:HA	9:N:9881:HOH:O	1.84	0.77
3:D:631:ILE:HG21	3:D:745:MET:HG3	1.66	0.77
5:F:196:VAL:HG22	5:F:213:ILE:HD13	1.66	0.77
2:M:232:GLU:HA	2:M:235:LEU:HD12	1.65	0.77
3:D:1236:LEU:HD11	3:D:1356:TYR:HE1	1.49	0.77
1:K:198:ARG:HD3	1:K:200:TRP:HH2	1.50	0.77
2:M:172:ILE:HG23	2:M:184:MET:HE3	1.65	0.77
3:N:67:ARG:HB2	5:P:375:LEU:HD11	1.66	0.76
3:D:1311:LEU:HA	9:D:9756:HOH:O	1.85	0.76
5:F:136:LEU:HD11	9:F:9565:HOH:O	1.84	0.76
2:C:903:SER:HA	9:C:2024:HOH:O	1.84	0.76
2:C:1098:ASP:HB2	3:D:21:TRP:HZ2	1.48	0.76
3:D:194:GLY:H	3:D:206:ARG:HA	1.50	0.76
1:L:206:THR:HG22	1:L:209:GLU:H	1.49	0.76
2:M:332:ARG:HD3	9:M:9675:HOH:O	1.86	0.76
2:M:997:LEU:HG	9:M:9828:HOH:O	1.83	0.76
3:N:217:LYS:HA	9:N:2156:HOH:O	1.85	0.76
3:N:1147:ARG:HB3	3:N:1188:VAL:HG21	1.65	0.76
1:A:110:LYS:HG3	9:A:9494:HOH:O	1.86	0.76
3:D:133:ILE:HG23	3:D:456:MET:SD	2.26	0.76
1:K:178:ALA:HB3	1:K:198:ARG:HG3	1.66	0.76
1:L:205:VAL:HG23	9:L:3448:HOH:O	1.85	0.76
3:N:141:ILE:HD13	3:N:450:TYR:HB2	1.67	0.76
1:B:206:THR:HG22	1:B:209:GLU:HB2	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:131:VAL:HG12	5:P:181:GLU:HG3	1.68	0.76
3:D:1175:ILE:O	3:D:1179:GLU:HG3	1.86	0.76
5:F:75:ILE:HG22	9:F:9601:HOH:O	1.85	0.76
3:N:658:LEU:HA	3:N:661:MET:HE3	1.68	0.76
3:N:1197:ARG:HG3	3:N:1198:TYR:H	1.49	0.76
2:M:420:ARG:HD2	2:M:420:ARG:H	1.50	0.76
3:N:1109:GLU:HG2	3:N:1201:CYS:HA	1.68	0.76
3:D:904:VAL:HG22	9:D:2047:HOH:O	1.84	0.76
1:L:152:PRO:HD2	1:L:155:LYS:HG3	1.66	0.76
3:N:6:ARG:HB3	3:N:6:ARG:HH11	1.51	0.76
3:N:422:ALA:H	3:N:427:VAL:HG11	1.51	0.76
3:N:1220:ALA:HB1	3:N:1223:ILE:HD13	1.67	0.76
1:L:56:VAL:HG13	1:L:142:VAL:HG12	1.68	0.76
3:N:119:SER:HB2	3:N:123:LEU:HB2	1.66	0.76
3:D:562:ALA:HB1	3:D:567:ILE:HD11	1.65	0.75
5:F:261:PRO:O	5:F:264:MET:HG2	1.86	0.75
2:C:710:ILE:HB	2:C:790:LEU:HD13	1.68	0.75
2:C:904:PRO:HD2	2:C:908:GLY:HA2	1.69	0.75
3:D:956:ILE:HG12	3:D:1039:CYS:O	1.85	0.75
9:M:2201:HOH:O	4:O:31:LEU:HB2	1.86	0.75
5:F:76:SER:O	5:F:80:PRO:HD2	1.86	0.75
2:M:396:ASP:HA	2:M:633:GLN:HE22	1.51	0.75
2:M:952:LEU:HD12	2:M:969:GLN:NE2	1.97	0.75
2:C:157:ARG:HD2	2:C:314:THR:HG22	1.67	0.75
2:C:1056:LYS:HB3	3:D:624:ASP:H	1.52	0.75
5:F:93:LEU:HG	5:F:190:ALA:CB	2.16	0.75
2:M:49:ARG:HA	9:M:9640:HOH:O	1.85	0.75
2:M:691:SER:HB2	2:M:858:MET:SD	2.27	0.75
3:N:192:ALA:O	3:N:195:VAL:HG23	1.85	0.75
2:M:1097:LEU:HD13	2:M:1097:LEU:H	1.51	0.75
3:N:211:VAL:HG22	3:N:393:ILE:HG23	1.67	0.75
3:N:1273:VAL:HG22	3:N:1326:THR:OG1	1.86	0.75
9:C:9697:HOH:O	4:E:28:GLN:HA	1.87	0.75
2:M:517:ARG:HE	2:M:522:VAL:HG11	1.50	0.75
3:D:422:ALA:H	3:D:427:VAL:HG11	1.52	0.75
2:M:598:GLU:O	2:M:651:LYS:HG3	1.87	0.75
3:D:65:ARG:HG3	3:D:66:GLN:H	1.49	0.75
5:F:120:THR:HB	9:F:9599:HOH:O	1.87	0.75
3:N:145:VAL:HG22	3:N:146:PRO:HD2	1.69	0.75
2:C:603:VAL:HG21	2:C:643:VAL:HG11	1.67	0.75
3:D:478:LEU:HD13	3:D:1388:ARG:HH22	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:24:VAL:HG12	9:L:3467:HOH:O	1.86	0.75
2:M:736:ASP:O	2:M:744:ARG:HG2	1.87	0.74
2:M:943:VAL:HG23	2:M:985:GLY:H	1.52	0.74
2:M:1005:MET:HE1	3:N:648:MET:HB2	1.68	0.74
3:D:965:GLU:HG3	3:D:969:ARG:HH21	1.51	0.74
2:M:1038:TRP:HE1	3:N:1463:LYS:NZ	1.85	0.74
1:A:101:LEU:HG	1:A:114:PHE:HA	1.70	0.74
2:C:10:ARG:HA	2:C:10:ARG:NH1	2.03	0.74
2:C:186:VAL:HG23	2:C:187:ASN:H	1.51	0.74
3:D:890:VAL:HA	9:D:9911:HOH:O	1.87	0.74
1:L:156:HIS:ND1	1:L:158:ILE:HG12	2.02	0.74
3:N:468:LEU:HB3	9:N:9663:HOH:O	1.87	0.74
2:C:1056:LYS:HD3	3:D:623:VAL:HG13	1.69	0.74
3:D:1438:ALA:O	3:D:1443:THR:HG22	1.86	0.74
2:C:132:ALA:HB1	2:C:632:ASN:HD21	1.53	0.74
2:C:1054:THR:HG23	2:C:1082:PRO:HG3	1.70	0.74
3:D:55:ASP:HA	3:D:82:LYS:HG3	1.67	0.74
5:F:156:VAL:HA	5:F:159:ILE:HD12	1.68	0.74
5:F:248:ASN:HA	5:F:251:ILE:HD12	1.70	0.74
2:M:579:VAL:HG11	2:M:887:GLU:HG3	1.69	0.74
2:M:1111:ILE:HG13	2:M:1112:PHE:H	1.53	0.74
3:N:1290:LEU:HD23	3:N:1291:SER:H	1.52	0.74
1:K:117:VAL:HB	1:K:120:VAL:HG12	1.68	0.74
1:L:100:LEU:HB2	1:L:115:LEU:HD21	1.69	0.74
1:A:177:VAL:HG12	9:A:9593:HOH:O	1.88	0.74
2:C:144:PRO:HG2	2:C:265:ARG:HH12	1.52	0.74
2:C:282:GLY:HA2	2:C:308:ARG:HH12	1.53	0.74
3:N:136:ASP:HB2	3:N:137:PRO:HD3	1.70	0.74
3:N:1062:ARG:HG3	9:N:9910:HOH:O	1.87	0.74
3:N:1438:ALA:O	3:N:1443:THR:HG22	1.88	0.74
2:C:72:ARG:HG2	9:C:9760:HOH:O	1.86	0.74
2:C:500:ASN:HD21	3:D:1067:VAL:HG23	1.52	0.74
2:C:768:THR:HB	2:C:771:GLU:HB3	1.70	0.74
2:M:64:LEU:HA	9:M:9656:HOH:O	1.86	0.74
3:D:1109:GLU:OE1	3:D:1201:CYS:HB2	1.86	0.74
5:F:163:LEU:HD22	5:F:174:LEU:HG	1.69	0.74
5:P:92:PRO:HA	9:P:4361:HOH:O	1.87	0.74
1:B:20:TYR:HB3	9:B:9501:HOH:O	1.87	0.74
3:D:1087:ARG:HD3	3:D:1090:ASP:HB2	1.70	0.74
5:F:191:ASN:HB2	9:F:9537:HOH:O	1.87	0.74
2:M:786:LYS:HA	9:M:9505:HOH:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:644:LEU:HD12	3:N:645:PRO:HD2	1.70	0.74
3:N:1393:GLN:HB2	3:N:1398:TRP:HE1	1.53	0.74
5:P:142:ARG:HB3	5:P:142:ARG:HH11	1.53	0.74
1:B:16:GLN:HB2	9:B:9501:HOH:O	1.89	0.73
2:C:117:HIS:HA	9:C:9729:HOH:O	1.87	0.73
3:N:569:ASN:HD22	3:N:573:MET:HE1	1.53	0.73
1:A:27:PRO:HG2	1:A:186:LEU:HD22	1.68	0.73
2:C:96:ALA:HA	9:C:9760:HOH:O	1.88	0.73
3:D:97:THR:HG21	3:D:571:LYS:HD3	1.70	0.73
3:D:161:LEU:HD22	3:D:452:ILE:HG21	1.68	0.73
1:K:87:VAL:HG21	1:K:144:VAL:HG11	1.70	0.73
3:D:1264:GLU:OE1	3:D:1425:THR:HB	1.88	0.73
3:N:12:LEU:HD23	3:N:13:ALA:H	1.53	0.73
3:N:194:GLY:H	3:N:206:ARG:HA	1.52	0.73
3:N:972:LEU:HD22	9:N:9844:HOH:O	1.88	0.73
2:C:136:ILE:HG21	2:C:336:VAL:HG13	1.70	0.73
2:C:1055:LEU:HD23	9:C:9632:HOH:O	1.87	0.73
3:D:1273:VAL:HG22	3:D:1326:THR:OG1	1.89	0.73
3:N:422:ALA:HB1	5:P:178:ARG:HH12	1.53	0.73
3:N:850:LEU:H	3:N:850:LEU:HD12	1.53	0.73
5:P:256:ARG:NH1	5:P:313:GLU:HG2	2.03	0.73
2:C:479:VAL:CG2	2:C:503:LEU:HD11	2.19	0.73
3:D:704:ARG:NE	3:D:705:ALA:H	1.86	0.73
3:N:399:ARG:HG3	9:N:2231:HOH:O	1.87	0.73
2:C:1091:GLU:OE1	3:D:613:ARG:HG2	1.87	0.73
3:D:1221:VAL:HG13	9:D:9929:HOH:O	1.88	0.73
3:D:1277:ILE:HD12	3:D:1301:LYS:HB2	1.70	0.73
5:F:366:ALA:HB3	5:F:367:MET:HE2	1.69	0.73
2:M:1016:ILE:HG12	9:P:5990:HOH:O	1.88	0.73
2:C:233:GLU:OE1	2:C:237:ARG:HD3	1.89	0.73
3:D:633:VAL:HG22	3:D:635:PRO:HD3	1.71	0.73
2:M:1051:GLU:HG2	2:M:1056:LYS:HD2	1.70	0.73
3:N:783:ARG:NH2	3:N:1029:ARG:HD3	2.02	0.73
3:N:1465:ASN:HD21	3:N:1470:ARG:HD3	1.53	0.73
4:O:37:ASN:HD22	4:O:89:MET:HE2	1.53	0.73
1:A:8:ALA:HB1	1:B:224:TYR:CE1	2.24	0.73
3:D:6:ARG:HB3	3:D:6:ARG:HH11	1.51	0.73
3:D:544:TYR:O	3:D:548:ILE:HG12	1.88	0.73
3:D:728:LEU:HD13	3:D:745:MET:HE1	1.70	0.73
1:K:103:ALA:HB1	1:K:107:LYS:HD3	1.69	0.73
2:M:395:LYS:HE2	2:M:403:SER:HB2	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:603:VAL:HG21	2:M:643:VAL:HG11	1.70	0.73
3:N:807:ALA:HB2	3:N:833:GLU:OE1	1.89	0.73
1:A:42:ARG:NH2	1:B:34:VAL:HB	2.04	0.73
1:A:222:LEU:HD12	1:B:215:VAL:HB	1.69	0.73
1:B:185:ARG:HG3	1:B:190:THR:HG23	1.71	0.73
3:D:920:LEU:HB2	9:D:9488:HOH:O	1.88	0.73
2:C:1008:ARG:NH1	2:C:1020:PRO:HB3	2.04	0.73
3:D:1095:THR:O	3:D:1099:VAL:HG23	1.87	0.73
3:D:1412:LYS:O	3:D:1414:PRO:HD3	1.89	0.73
5:F:416:ARG:HB3	9:F:9582:HOH:O	1.89	0.73
1:L:57:TYR:HE1	1:L:163:ASN:HB2	1.53	0.73
2:M:362:GLY:HA3	2:M:367:LEU:HD23	1.71	0.73
2:M:710:ILE:HB	2:M:790:LEU:HD12	1.71	0.73
3:N:699:VAL:HG12	3:N:717:GLN:HA	1.69	0.73
5:P:234:LYS:HG3	9:P:3697:HOH:O	1.88	0.73
1:A:9:PRO:HD2	1:B:224:TYR:CZ	2.23	0.72
1:A:14:ARG:NH2	1:A:22:GLU:HB3	2.04	0.72
3:D:1310:ARG:NE	3:D:1327:ARG:HB3	2.04	0.72
2:M:264:PRO:HB3	2:M:289:THR:HG21	1.71	0.72
2:M:948:GLU:HA	9:M:9767:HOH:O	1.88	0.72
3:D:127:LEU:HD11	3:D:461:ILE:HD11	1.69	0.72
5:F:93:LEU:HD22	5:F:98:GLU:HB3	1.69	0.72
3:D:662:GLU:HB2	9:D:9514:HOH:O	1.89	0.72
2:M:626:ARG:NH1	2:M:637:LEU:HD12	2.04	0.72
2:M:651:LYS:HA	9:M:9639:HOH:O	1.89	0.72
3:N:44:LEU:HB3	3:N:525:ARG:HH21	1.54	0.72
3:N:87:ARG:HB3	3:N:523:ASP:HB2	1.71	0.72
3:N:1036:ARG:NH2	3:N:1042:ARG:HA	2.04	0.72
3:N:1112:CYS:HB2	3:N:1195:GLN:OE1	1.88	0.72
3:N:1381:VAL:HB	3:N:1389:LEU:O	1.87	0.72
1:A:175:ARG:NH2	1:A:202:ASP:HA	2.04	0.72
2:C:678:PRO:HG3	3:D:947:ILE:HD11	1.70	0.72
3:D:215:TYR:O	3:D:389:GLU:HB2	1.88	0.72
3:D:806:PHE:CE1	3:D:813:LEU:HB3	2.24	0.72
5:F:113:ILE:HA	5:F:116:LEU:HD12	1.70	0.72
1:K:222:LEU:HD11	1:L:218:LEU:HD23	1.72	0.72
2:M:71:TYR:H	2:M:71:TYR:HD2	1.36	0.72
2:M:1038:TRP:HE1	3:N:1463:LYS:HZ1	1.36	0.72
3:N:108:VAL:HG23	3:N:109:PRO:HD3	1.71	0.72
3:N:885:ILE:HG13	9:N:9868:HOH:O	1.89	0.72
3:N:1412:LYS:O	3:N:1414:PRO:HD3	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:165:LEU:HB2	9:M:9535:HOH:O	1.89	0.72
2:M:1082:PRO:HG2	3:N:1469:GLY:HA3	1.72	0.72
3:N:475:LYS:HA	3:N:478:LEU:HD12	1.70	0.72
3:N:1481:VAL:HG13	4:O:18:ARG:HE	1.54	0.72
1:A:145:ASP:HB3	9:A:9484:HOH:O	1.90	0.72
2:C:478:VAL:HA	2:C:506:ASN:O	1.90	0.72
3:N:65:ARG:HG3	3:N:66:GLN:H	1.53	0.72
2:C:993:PHE:HE1	2:C:995:MET:HG2	1.53	0.72
3:D:842:VAL:HG23	9:D:2618:HOH:O	1.89	0.72
2:M:605:LYS:HB2	2:M:610:ARG:NH1	2.00	0.72
2:M:897:LEU:HG	2:M:920:GLN:NE2	2.04	0.72
3:N:212:ARG:HA	9:N:2226:HOH:O	1.90	0.72
3:N:996:TRP:HA	3:N:999:THR:HG22	1.72	0.72
3:N:1090:ASP:HA	3:N:1093:TYR:HB2	1.72	0.72
4:O:51:LEU:HD12	4:O:52:GLU:H	1.55	0.72
1:B:36:LEU:O	1:B:39:PRO:HD2	1.89	0.72
2:C:8:ARG:HG2	9:C:9597:HOH:O	1.89	0.72
2:C:683:ASN:HA	2:C:687:ALA:HB3	1.71	0.72
2:M:679:PHE:HB3	9:M:9536:HOH:O	1.87	0.72
3:N:601:ARG:HG2	3:N:606:ILE:HD13	1.72	0.72
3:N:853:VAL:HG22	3:N:858:VAL:HG23	1.71	0.72
3:D:1292:VAL:HG23	3:D:1305:LEU:HD11	1.71	0.72
2:M:139:GLN:HB3	2:M:334:ARG:HD2	1.71	0.72
3:N:197:SER:HB2	3:N:205:TYR:CZ	2.25	0.72
1:A:8:ALA:HB1	1:B:224:TYR:HE1	1.54	0.72
1:A:42:ARG:HH11	2:C:978:ARG:HA	1.55	0.72
2:C:833:LEU:HD12	2:C:834:GLN:H	1.54	0.72
3:D:41:ARG:HD3	3:D:42:ASP:N	2.05	0.72
3:D:187:LYS:HE2	3:D:213:VAL:HG12	1.72	0.72
3:D:723:GLY:HA3	9:D:9551:HOH:O	1.90	0.72
3:D:978:TYR:HA	9:D:9513:HOH:O	1.89	0.72
3:D:1166:LEU:HD23	3:D:1166:LEU:H	1.54	0.72
3:D:1272:ALA:HA	3:D:1326:THR:HB	1.72	0.72
2:M:210:GLU:HA	9:M:2282:HOH:O	1.90	0.72
3:N:1382:THR:HG21	3:N:1418:LYS:NZ	2.05	0.72
2:C:728:HIS:HB3	2:C:729:LEU:HD12	1.72	0.71
2:M:367:LEU:HD23	2:M:371:LYS:HZ2	1.55	0.71
2:M:512:ARG:HB3	2:M:523:ILE:HD11	1.72	0.71
3:N:119:SER:H	3:N:123:LEU:HD22	1.54	0.71
2:C:108:ILE:HB	2:C:368:THR:OG1	1.88	0.71
2:C:504:GLU:HG2	9:C:9601:HOH:O	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:12:LEU:HD13	3:D:511:TRP:HB2	1.70	0.71
3:D:654:LYS:HB3	3:D:655:PRO:HD3	1.72	0.71
2:M:546:LEU:HD11	2:M:666:LEU:HD23	1.71	0.71
5:P:178:ARG:HD3	9:P:3512:HOH:O	1.87	0.71
1:A:49:PRO:HB3	1:A:148:VAL:HG22	1.71	0.71
2:C:987:ILE:HG23	3:D:948:THR:CG2	2.21	0.71
5:F:80:PRO:HA	5:F:83:GLN:HB2	1.70	0.71
2:M:572:ILE:HD11	2:M:698:ASP:HB3	1.71	0.71
3:N:771:SER:HB2	3:N:778:LEU:HD13	1.72	0.71
2:C:64:LEU:HD22	2:C:359:MET:HG3	1.72	0.71
3:D:534:ARG:HD3	9:F:9549:HOH:O	1.90	0.71
3:D:564:GLU:HA	3:D:567:ILE:HD12	1.73	0.71
1:A:46:SER:HB3	2:C:856:GLU:HG2	1.73	0.71
2:C:15:LEU:HD12	2:C:15:LEU:H	1.55	0.71
3:D:178:LEU:HD11	9:D:9843:HOH:O	1.89	0.71
1:K:226:SER:O	1:K:228:PRO:HD3	1.90	0.71
2:M:274:ARG:HD2	2:M:285:LEU:HB3	1.73	0.71
2:M:578:VAL:HG11	2:M:991:GLN:HB3	1.72	0.71
2:M:1000:MET:O	2:M:1003:ASP:HB3	1.91	0.71
2:C:30:LEU:HB3	2:C:44:ILE:HD12	1.72	0.71
3:D:982:PHE:HB3	9:D:2466:HOH:O	1.89	0.71
1:K:39:PRO:O	1:K:43:ILE:HG12	1.90	0.71
3:N:65:ARG:HA	9:N:2129:HOH:O	1.91	0.71
3:N:1145:TYR:HE2	3:N:1168:MET:HB2	1.56	0.71
3:D:100:ALA:HB2	9:D:9966:HOH:O	1.90	0.71
3:D:1136:LYS:HE3	3:D:1139:ASP:OD2	1.90	0.71
1:L:24:VAL:HG13	1:L:196:THR:HB	1.73	0.71
2:M:772:ARG:HB2	2:M:772:ARG:HH11	1.54	0.71
2:M:948:GLU:HB2	9:M:9817:HOH:O	1.90	0.71
5:P:102:LEU:HD13	5:P:187:LEU:HG	1.71	0.71
3:D:561:GLY:HA3	5:F:184:ARG:HH12	1.55	0.71
3:D:825:ALA:HB1	9:D:9486:HOH:O	1.91	0.71
2:M:36:PRO:HG2	2:M:70:GLU:HB3	1.70	0.71
2:M:769:PRO:HD2	9:N:2324:HOH:O	1.91	0.71
3:N:1404:ASN:HD22	3:N:1408:ILE:HD12	1.56	0.71
3:N:1434:TRP:CZ3	3:N:1457:ASP:HB2	2.26	0.71
2:C:557:ARG:CZ	2:C:879:ARG:HD3	2.20	0.71
2:C:670:GLN:O	2:C:672:VAL:HG12	1.91	0.71
3:D:165:LYS:HB3	3:D:395:VAL:HG11	1.71	0.71
3:D:955:VAL:HB	3:D:1011:PHE:HE1	1.56	0.71
3:D:1129:THR:HG23	3:D:1130:ARG:H	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:3474:HOH:O	1:L:42:ARG:HB3	1.91	0.71
2:M:199:VAL:HG13	2:M:235:LEU:HG	1.71	0.71
1:B:97:VAL:HG11	1:B:120:VAL:HG21	1.72	0.71
2:C:127:PHE:HA	9:C:9502:HOH:O	1.89	0.71
2:C:352:ALA:O	2:C:356:ARG:HG3	1.91	0.71
3:D:1266:ARG:O	3:D:1268:PRO:HD3	1.91	0.71
4:E:30:LEU:O	4:E:35:PHE:HA	1.90	0.71
3:N:962:GLN:HA	9:N:2437:HOH:O	1.90	0.71
5:P:163:LEU:HB3	5:P:174:LEU:HG	1.73	0.71
1:B:94:LEU:HD21	1:B:119:ASP:HB2	1.73	0.70
3:D:177:ALA:HB1	3:D:199:LEU:HD22	1.73	0.70
3:D:1307:LYS:H	3:D:1307:LYS:HD3	1.56	0.70
3:D:1464:GLU:HG2	9:D:2152:HOH:O	1.89	0.70
4:E:43:GLU:CD	4:E:43:GLU:H	1.99	0.70
5:F:88:ILE:HB	9:F:9492:HOH:O	1.90	0.70
2:M:409:ARG:HH22	7:M:8002:RPT:H18	1.55	0.70
1:A:10:VAL:HG12	1:A:12:THR:HG22	1.72	0.70
3:D:493:ARG:NE	3:D:1388:ARG:HB3	2.06	0.70
3:D:542:ASP:O	3:D:546:ARG:HG2	1.92	0.70
3:D:756:GLN:O	3:D:760:ARG:HG2	1.91	0.70
4:E:33:HIS:HB2	4:E:37:ASN:HD21	1.55	0.70
5:F:77:THR:O	5:F:81:VAL:HG23	1.90	0.70
5:F:371:LEU:HD22	5:F:375:LEU:HD22	1.73	0.70
2:M:150:PRO:HA	2:M:158:TYR:HB3	1.71	0.70
2:M:218:VAL:HA	2:M:221:LEU:HD23	1.71	0.70
2:M:704:HIS:HB2	2:M:831:ARG:HE	1.56	0.70
3:N:804:LEU:HB2	3:N:830:ALA:O	1.91	0.70
5:P:291:ILE:HG21	5:P:304:VAL:HG11	1.71	0.70
3:D:1220:ALA:HB1	3:D:1223:ILE:HD13	1.73	0.70
2:M:169:GLY:HA2	2:M:263:ASP:CB	2.20	0.70
1:B:99:LEU:HD21	1:B:122:ILE:HD11	1.72	0.70
2:C:611:ILE:HD11	2:C:641:PRO:HB3	1.73	0.70
3:D:233:LYS:HA	9:D:2088:HOH:O	1.90	0.70
5:F:398:ARG:HG2	5:F:402:ASN:HD22	1.56	0.70
1:K:19:GLU:HG3	9:K:4352:HOH:O	1.91	0.70
2:M:34:VAL:HB	2:M:38:LYS:HG3	1.73	0.70
2:M:151:ASP:HB2	2:M:157:ARG:O	1.91	0.70
2:M:1014:SER:HB3	2:M:1017:THR:O	1.90	0.70
3:N:884:ARG:HD2	9:N:9868:HOH:O	1.91	0.70
2:C:264:PRO:HB3	2:C:289:THR:HG21	1.74	0.70
3:D:161:LEU:HD23	3:D:449:SER:HB3	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:111:ASP:HA	9:M:2096:HOH:O	1.92	0.70
2:M:198:ARG:HH21	2:M:203:ASP:HB3	1.56	0.70
5:P:406:ARG:HA	5:P:409:LYS:HG2	1.72	0.70
2:C:554:ASP:OD2	2:C:556:ASN:HB3	1.91	0.70
3:D:1192:LEU:HD22	3:D:1345:GLU:HG2	1.73	0.70
3:N:153:LEU:HD11	3:N:158:TYR:N	2.06	0.70
2:C:1054:THR:HG22	2:C:1059:ASP:HB2	1.72	0.70
3:D:30:GLU:HB3	3:D:40:GLU:HB3	1.72	0.70
3:D:127:LEU:HD21	3:D:461:ILE:HD11	1.73	0.70
2:M:269:LEU:HD21	9:M:9709:HOH:O	1.90	0.70
2:M:767:PRO:HG2	9:M:2323:HOH:O	1.91	0.70
3:N:87:ARG:CB	3:N:523:ASP:HB2	2.21	0.70
2:C:376:ARG:HH12	5:F:285:GLU:HG2	1.57	0.70
2:C:773:LEU:HD13	9:F:9672:HOH:O	1.91	0.70
3:D:661:MET:HE3	3:D:673:ALA:HB1	1.72	0.70
2:M:328:LEU:HD23	2:M:437:ARG:HD3	1.74	0.70
2:M:1095:LEU:HB2	2:M:1097:LEU:CD2	2.22	0.70
3:N:966:GLU:HA	3:N:969:ARG:NH1	2.07	0.70
5:P:156:VAL:HA	5:P:159:ILE:HD12	1.72	0.70
5:P:291:ILE:HG23	5:P:304:VAL:HG21	1.74	0.70
1:B:27:PRO:HB3	1:B:192:LEU:HD22	1.74	0.70
2:C:110:GLU:HG2	2:C:369:PRO:CB	2.20	0.70
2:C:269:LEU:HD12	2:C:288:ARG:H	1.57	0.70
2:C:791:ARG:HB3	2:C:791:ARG:HH11	1.57	0.70
2:M:136:ILE:HG21	2:M:336:VAL:HG13	1.73	0.70
2:M:139:GLN:OE1	2:M:415:PRO:HD2	1.92	0.70
3:D:131:LYS:HE2	5:F:83:GLN:HE22	1.55	0.70
3:D:1493:LYS:O	3:D:1497:GLU:HG2	1.91	0.70
3:N:1033:GLN:HE21	3:N:1036:ARG:HD3	1.57	0.70
1:B:156:HIS:ND1	1:B:158:ILE:HG12	2.06	0.69
2:C:42:VAL:HG12	2:C:43:GLY:H	1.57	0.69
2:C:84:ARG:HH21	2:C:128:ILE:HD11	1.57	0.69
2:C:1109:VAL:HG23	3:D:3:LYS:HG2	1.73	0.69
4:E:9:LEU:HD13	4:E:19:LEU:HD11	1.73	0.69
3:N:1376:MET:HE3	3:N:1421:LEU:HD13	1.73	0.69
5:P:112:ALA:HA	5:P:173:TYR:HD2	1.56	0.69
2:C:1000:MET:HB3	2:C:1002:GLU:HG3	1.74	0.69
3:D:566:ILE:HG23	5:F:214:GLN:OE1	1.92	0.69
3:D:1269:LYS:HB3	9:D:2348:HOH:O	1.92	0.69
3:D:1285:GLU:CD	3:D:1285:GLU:H	2.00	0.69
2:M:182:VAL:HG12	2:M:193:LEU:HD13	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:704:ARG:HD2	3:N:705:ALA:H	1.57	0.69
3:N:1166:LEU:H	3:N:1166:LEU:HD23	1.56	0.69
1:A:117:VAL:HB	1:A:120:VAL:HG12	1.73	0.69
2:C:94:LEU:HD11	9:C:9738:HOH:O	1.91	0.69
2:M:68:PHE:HE1	2:M:96:ALA:HB1	1.56	0.69
2:M:157:ARG:HD2	2:M:314:THR:CG2	2.21	0.69
3:N:1393:GLN:HB2	3:N:1398:TRP:NE1	2.06	0.69
2:C:395:LYS:HE2	2:C:403:SER:HB2	1.74	0.69
2:C:420:ARG:HD3	2:C:422:ARG:HG3	1.73	0.69
5:F:358:LEU:HD21	5:F:370:LYS:HE3	1.74	0.69
2:M:385:PHE:HA	9:M:9823:HOH:O	1.92	0.69
3:N:643:GLY:HA3	3:N:727:GLN:HB2	1.72	0.69
3:D:100:ALA:HA	9:D:9738:HOH:O	1.91	0.69
1:K:101:LEU:HG	1:K:114:PHE:HA	1.72	0.69
1:L:97:VAL:HG11	1:L:120:VAL:HG21	1.72	0.69
2:M:197:LEU:HB3	2:M:202:TYR:HB2	1.75	0.69
2:M:1042:ALA:HB1	3:N:710:ARG:HE	1.58	0.69
1:B:89:PHE:HB3	1:B:94:LEU:HD13	1.75	0.69
2:C:706:GLU:HB3	2:C:708:TYR:CE1	2.26	0.69
3:D:153:LEU:CD1	3:D:157:GLU:HB2	2.23	0.69
3:D:1420:LEU:HD12	3:D:1421:LEU:N	2.07	0.69
5:F:131:VAL:HG12	5:F:181:GLU:HG3	1.74	0.69
1:K:206:THR:HG23	1:K:209:GLU:HB2	1.75	0.69
2:M:983:ILE:HG21	2:M:987:ILE:HD11	1.73	0.69
3:N:152:LEU:HD23	3:N:152:LEU:H	1.58	0.69
3:N:397:LYS:HG2	9:N:2231:HOH:O	1.91	0.69
3:N:1238:MET:HG2	3:N:1256:LEU:HD23	1.74	0.69
5:P:274:THR:O	5:P:278:LEU:HG	1.92	0.69
2:C:41:ASN:H	2:C:41:ASN:ND2	1.90	0.69
3:D:1324:PRO:HA	9:D:9544:HOH:O	1.92	0.69
5:F:144:ILE:HB	5:F:145:PRO:HD3	1.75	0.69
1:L:63:HIS:HB2	9:L:3319:HOH:O	1.91	0.69
2:M:881:ASN:HD22	2:M:881:ASN:H	1.39	0.69
3:N:1033:GLN:HE21	3:N:1036:ARG:HH11	1.40	0.69
3:N:1057:VAL:HG23	9:N:2261:HOH:O	1.92	0.69
3:N:1357:ARG:HG3	9:N:9798:HOH:O	1.93	0.69
2:C:889:HIS:HE1	3:D:951:ILE:H	1.40	0.69
2:C:1008:ARG:NH2	2:C:1028:GLY:HA2	2.08	0.69
2:C:1008:ARG:HH21	2:C:1028:GLY:HA2	1.58	0.69
3:D:427:VAL:CG2	3:D:435:VAL:HB	2.22	0.69
3:D:477:LEU:HD22	3:D:492:ALA:HB1	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:908:LYS:CB	3:D:1027:GLY:HA3	2.23	0.69
4:E:48:MET:HB2	4:E:54:LEU:HD12	1.75	0.69
2:M:678:PRO:HD2	9:N:9516:HOH:O	1.93	0.69
2:M:768:THR:HB	2:M:771:GLU:HB3	1.75	0.69
2:M:857:ASP:HB2	2:M:978:ARG:HG2	1.73	0.69
3:N:63:TYR:HB3	3:N:68:PHE:CE1	2.28	0.69
3:N:95:LEU:HD12	3:N:515:GLU:C	2.18	0.69
3:N:905:PRO:HD3	9:N:2419:HOH:O	1.91	0.69
4:O:10:PHE:HE2	4:O:16:LYS:HG3	1.58	0.69
2:C:1111:ILE:HG13	2:C:1112:PHE:H	1.57	0.69
3:D:1139:ASP:HB3	3:D:1357:ARG:NH2	2.08	0.69
1:K:49:PRO:HB3	1:K:148:VAL:HG22	1.75	0.69
1:L:112:ARG:HB3	1:L:112:ARG:NH1	2.07	0.69
2:C:367:LEU:HB3	2:C:371:LYS:HG2	1.75	0.69
3:D:625:TYR:O	3:D:749:VAL:HG23	1.92	0.69
3:D:709:HIS:NE2	3:D:711:LEU:HB2	2.07	0.69
3:D:1361:VAL:HG23	9:D:9531:HOH:O	1.93	0.69
5:P:361:LEU:HG	5:P:408:LEU:HD21	1.75	0.69
2:C:199:VAL:HG21	9:C:2083:HOH:O	1.92	0.68
3:D:561:GLY:HA3	5:F:184:ARG:HH22	1.58	0.68
3:D:1476:THR:HG23	4:E:21:VAL:HG22	1.76	0.68
2:M:670:GLN:O	2:M:672:VAL:HG12	1.93	0.68
3:N:793:THR:HB	3:N:879:ARG:HD3	1.74	0.68
2:C:96:ALA:HB2	9:C:9738:HOH:O	1.93	0.68
2:C:775:ARG:NH2	2:C:782:ALA:HB1	2.02	0.68
3:D:119:SER:HB2	3:D:123:LEU:N	2.06	0.68
3:D:699:VAL:HG12	3:D:717:GLN:HA	1.76	0.68
3:D:1118:ILE:HG21	3:D:1346:ARG:NH2	2.09	0.68
2:M:518:LYS:HA	9:M:9720:HOH:O	1.93	0.68
2:M:833:LEU:HD12	2:M:834:GLN:N	2.08	0.68
3:N:507:ASN:HB2	9:N:9590:HOH:O	1.92	0.68
2:C:305:PRO:HA	2:C:308:ARG:HB3	1.74	0.68
2:C:455:LEU:HD23	2:C:455:LEU:H	1.57	0.68
3:D:820:GLU:HB2	3:D:836:VAL:HG11	1.76	0.68
3:D:1404:ASN:ND2	3:D:1408:ILE:HD12	2.08	0.68
5:F:372:ARG:HB2	9:F:9526:HOH:O	1.93	0.68
5:P:144:ILE:HB	5:P:145:PRO:HD3	1.74	0.68
5:P:315:VAL:HA	9:P:4529:HOH:O	1.93	0.68
1:A:14:ARG:HH22	1:A:24:VAL:HG23	1.58	0.68
2:C:597:ALA:HB2	2:C:655:LEU:HD21	1.74	0.68
3:D:1452:ILE:HG12	9:D:9759:HOH:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:61:VAL:HA	9:K:3552:HOH:O	1.94	0.68
3:N:551:ASN:HA	9:N:9830:HOH:O	1.91	0.68
5:P:185:GLN:HA	5:P:188:ILE:HD12	1.75	0.68
2:C:1096:ALA:O	3:D:13:ALA:HB2	1.93	0.68
2:M:598:GLU:HB3	9:M:9583:HOH:O	1.93	0.68
3:N:1115:THR:HG22	9:N:2569:HOH:O	1.93	0.68
1:B:58:ILE:HB	1:B:61:VAL:HB	1.74	0.68
1:B:80:LEU:HD23	3:D:867:ARG:HH12	1.59	0.68
1:B:115:LEU:HB2	9:B:9609:HOH:O	1.93	0.68
3:D:153:LEU:HD12	3:D:154:THR:H	1.57	0.68
3:D:520:LEU:HD23	3:D:540:LEU:HD22	1.75	0.68
3:D:528:VAL:O	3:D:535:PHE:HA	1.92	0.68
3:D:877:PRO:HA	9:D:9580:HOH:O	1.91	0.68
3:D:996:TRP:CE3	3:D:999:THR:HG21	2.29	0.68
1:K:18:ARG:O	1:K:207:PRO:HD3	1.93	0.68
1:L:27:PRO:HB3	1:L:192:LEU:HD22	1.75	0.68
5:P:248:ASN:HA	5:P:251:ILE:HD12	1.76	0.68
2:C:292:ARG:HB2	2:C:299:LYS:HE2	1.74	0.68
3:D:209:ARG:NH2	3:D:397:LYS:HG3	2.09	0.68
3:D:628:ARG:HD3	3:D:744:GLN:NE2	2.08	0.68
5:F:166:LEU:HB3	5:F:170:HIS:HB2	1.76	0.68
2:M:915:LYS:HE2	9:M:9698:HOH:O	1.93	0.68
3:N:30:GLU:HG3	3:N:41:ARG:HG2	1.76	0.68
5:P:358:LEU:HD11	5:P:370:LYS:HZ2	1.59	0.68
3:D:538:SER:HB3	9:F:9546:HOH:O	1.92	0.68
3:D:584:ASN:HD21	3:D:589:ALA:HA	1.59	0.68
3:D:1236:LEU:HD11	3:D:1356:TYR:CE1	2.29	0.68
5:F:93:LEU:HG	5:F:190:ALA:HB1	1.76	0.68
5:F:152:ASP:HA	9:F:9491:HOH:O	1.94	0.68
2:M:326:ASP:HB2	2:M:431:HIS:ND1	2.09	0.68
2:M:683:ASN:HA	2:M:687:ALA:HB3	1.76	0.68
3:N:808:THR:HB	3:N:809:PRO:HD3	1.76	0.68
3:D:475:LYS:HG3	9:D:9989:HOH:O	1.92	0.68
3:D:988:ARG:HD2	3:D:989:TYR:N	2.09	0.68
2:C:432:ARG:HA	9:C:9669:HOH:O	1.94	0.68
2:C:755:LEU:HD22	2:C:825:VAL:HG11	1.76	0.68
3:D:86:ARG:HH11	3:D:86:ARG:HG2	1.58	0.68
1:K:95:GLN:HG2	1:K:146:ARG:NH1	2.08	0.68
2:M:773:LEU:HG	9:M:2483:HOH:O	1.93	0.68
4:O:30:LEU:O	4:O:35:PHE:HA	1.93	0.68
1:A:14:ARG:NH2	1:A:24:VAL:HG23	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:HIS:CE1	1:B:166:PRO:HB3	2.29	0.67
2:C:1042:ALA:HB3	3:D:710:ARG:HB3	1.76	0.67
3:D:490:ALA:HA	9:D:9583:HOH:O	1.93	0.67
3:D:611:GLN:HB3	3:D:616:GLN:NE2	2.09	0.67
5:F:212:LEU:HD11	9:F:9654:HOH:O	1.94	0.67
5:F:395:GLU:O	5:F:399:GLN:HB2	1.94	0.67
1:L:101:LEU:HD11	1:L:113:ASP:HB2	1.76	0.67
2:M:630:ARG:HA	2:M:705:ILE:HD11	1.75	0.67
3:N:119:SER:HB2	3:N:123:LEU:N	2.09	0.67
3:N:1422:MET:HE3	3:N:1426:LYS:HG2	1.76	0.67
5:P:228:GLU:HB3	9:P:4672:HOH:O	1.94	0.67
2:C:732:ALA:HA	2:C:735:ARG:NH1	2.09	0.67
2:C:833:LEU:HD12	2:C:834:GLN:N	2.08	0.67
3:D:483:HIS:HB2	3:D:484:PRO:HD3	1.76	0.67
3:D:708:LEU:O	3:D:1227:GLN:HG2	1.94	0.67
3:D:715:ALA:HB3	3:D:764:LEU:HA	1.73	0.67
2:M:422:ARG:HA	9:M:9874:HOH:O	1.91	0.67
2:M:575:GLN:HE21	2:M:671:ASN:HB2	1.59	0.67
2:M:672:VAL:HG23	2:M:868:ASP:HB2	1.76	0.67
3:N:187:LYS:HE2	3:N:213:VAL:HG12	1.76	0.67
3:N:1040:GLY:O	3:N:1060:SER:HB3	1.94	0.67
5:P:384:GLU:HA	9:P:4435:HOH:O	1.94	0.67
2:C:312:ALA:HB1	2:C:318:PRO:HG2	1.75	0.67
2:C:554:ASP:HB2	2:C:880:MET:HE3	1.77	0.67
2:C:724:ARG:HH22	2:C:734:LEU:HB3	1.60	0.67
1:L:116:PRO:HD2	9:L:4090:HOH:O	1.94	0.67
2:M:22:GLN:NE2	2:M:336:VAL:HG21	2.09	0.67
2:M:141:HIS:HB3	2:M:418:LEU:HD23	1.75	0.67
2:M:1093:GLN:HB3	3:N:90:MET:HE1	1.75	0.67
3:N:1271:LYS:HG2	3:N:1272:ALA:N	2.09	0.67
5:P:260:ILE:HD11	5:P:310:ILE:HG22	1.76	0.67
1:A:95:GLN:HG2	1:A:146:ARG:HH22	1.58	0.67
1:B:46:SER:O	1:B:148:VAL:HB	1.94	0.67
2:C:534:VAL:HB	2:C:538:GLN:OE1	1.93	0.67
3:D:1045:MET:CG	3:D:1073:SER:HA	2.24	0.67
3:D:1330:ILE:HA	9:D:2043:HOH:O	1.94	0.67
9:D:9593:HOH:O	5:F:222:ARG:HA	1.93	0.67
2:M:958:THR:OG1	2:M:961:GLU:HG2	1.94	0.67
3:N:754:PHE:HZ	4:O:21:VAL:HG13	1.59	0.67
3:N:1277:ILE:HD12	3:N:1301:LYS:HB2	1.76	0.67
5:P:76:SER:O	5:P:80:PRO:HD2	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:95:TYR:HA	9:C:2013:HOH:O	1.94	0.67
3:D:422:ALA:HB3	3:D:427:VAL:CG2	2.21	0.67
5:F:361:LEU:HD23	5:F:362:SER:H	1.59	0.67
2:M:45:GLN:HB2	2:M:71:TYR:CE1	2.30	0.67
2:M:358:ARG:HG3	2:M:361:MET:HE2	1.76	0.67
2:M:1021:LEU:HD21	5:P:332:PHE:HA	1.75	0.67
3:N:810:GLU:O	3:N:813:LEU:HG	1.94	0.67
3:N:898:GLU:HB2	3:N:921:ARG:HH22	1.59	0.67
3:D:754:PHE:HZ	4:E:21:VAL:HG13	1.60	0.67
2:M:23:VAL:HG12	9:M:9741:HOH:O	1.93	0.67
2:M:92:ALA:HB1	9:M:2197:HOH:O	1.94	0.67
2:M:140:ILE:HA	2:M:332:ARG:O	1.95	0.67
2:M:478:VAL:HA	2:M:506:ASN:O	1.95	0.67
2:M:815:LEU:HD23	9:M:9901:HOH:O	1.95	0.67
3:N:119:SER:OG	3:N:123:LEU:HD13	1.95	0.67
3:N:216:VAL:HG13	9:N:9526:HOH:O	1.94	0.67
3:N:529:GLN:HB2	9:N:9903:HOH:O	1.94	0.67
3:N:830:ALA:HA	9:N:9638:HOH:O	1.95	0.67
2:C:72:ARG:HE	2:C:97:ARG:HH12	1.42	0.67
2:C:882:LEU:HD23	2:C:885:ILE:HB	1.76	0.67
3:D:1280:VAL:HB	9:D:9793:HOH:O	1.95	0.67
1:K:43:ILE:HD11	1:L:35:THR:HG21	1.76	0.67
2:M:724:ARG:HG3	2:M:740:GLU:HA	1.75	0.67
3:N:1311:LEU:HD23	3:N:1311:LEU:H	1.60	0.67
3:N:1422:MET:HE2	3:N:1427:SER:HA	1.76	0.67
9:N:9768:HOH:O	5:P:254:GLN:HG2	1.95	0.67
4:O:51:LEU:HG	4:O:53:GLY:H	1.60	0.67
4:O:54:LEU:HD11	9:O:3983:HOH:O	1.93	0.67
2:C:1109:VAL:HG11	3:D:5:VAL:HG13	1.77	0.67
3:D:186:VAL:HG21	3:D:213:VAL:HB	1.76	0.67
3:D:834:THR:HG22	3:D:838:ARG:HD2	1.77	0.67
2:M:689:VAL:HG23	2:M:870:ILE:HB	1.77	0.67
2:M:758:ARG:HB3	2:M:788:THR:O	1.95	0.67
3:N:796:ARG:NH1	3:N:861:GLN:HB2	2.10	0.67
3:N:1194:CYS:HB2	9:N:9589:HOH:O	1.93	0.67
1:B:226:SER:HB3	9:B:9483:HOH:O	1.95	0.67
3:D:207:PHE:HB3	3:D:208:PRO:HD2	1.77	0.67
3:D:393:ILE:HG22	9:D:9798:HOH:O	1.95	0.67
5:F:275:ALA:HA	5:F:278:LEU:HD12	1.75	0.67
1:L:189:ARG:HG2	9:L:4538:HOH:O	1.94	0.67
2:M:346:VAL:HG12	2:M:350:ARG:HE	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1149:LEU:HD12	3:N:1161:GLU:O	1.93	0.67
3:N:1271:LYS:HG2	3:N:1272:ALA:H	1.59	0.67
1:B:78:ILE:HA	9:B:9525:HOH:O	1.94	0.67
2:C:1115:LEU:HD12	2:C:1115:LEU:H	1.60	0.67
3:D:1076:GLY:O	3:D:1079:LYS:HG3	1.95	0.67
3:D:1314:LYS:HD3	9:D:9730:HOH:O	1.94	0.67
3:N:207:PHE:HB3	3:N:208:PRO:HD2	1.76	0.67
3:N:464:LEU:HD11	9:N:9679:HOH:O	1.95	0.67
3:N:661:MET:HA	3:N:666:ILE:HD12	1.77	0.67
3:N:1484:THR:HG21	9:O:5601:HOH:O	1.95	0.67
2:C:881:ASN:H	2:C:881:ASN:HD22	1.44	0.66
3:D:1147:ARG:HB3	3:D:1188:VAL:HG21	1.77	0.66
5:F:321:ILE:HB	5:F:327:SER:OG	1.94	0.66
1:K:197:LEU:HD23	1:K:197:LEU:H	1.60	0.66
3:N:1337:GLU:HB3	9:N:9525:HOH:O	1.94	0.66
2:C:660:ALA:HB1	2:C:667:ALA:O	1.94	0.66
3:D:1209:LEU:HD22	3:D:1211:MET:HE2	1.75	0.66
4:E:33:HIS:HB2	4:E:37:ASN:ND2	2.11	0.66
2:M:186:VAL:HG23	2:M:187:ASN:H	1.60	0.66
2:M:686:ASP:HB2	9:N:2186:HOH:O	1.94	0.66
2:M:1000:MET:HB3	2:M:1002:GLU:HG3	1.75	0.66
3:N:135:LEU:HD13	3:N:147:VAL:HG23	1.75	0.66
3:N:426:LYS:HG3	3:N:434:ARG:NH1	2.10	0.66
3:N:559:ALA:HA	9:P:4212:HOH:O	1.94	0.66
1:B:51:THR:HB	9:B:9600:HOH:O	1.95	0.66
1:B:132:LEU:HD21	1:B:136:GLY:O	1.96	0.66
3:D:795:VAL:HG23	3:D:879:ARG:NH1	2.09	0.66
1:K:54:THR:HG21	9:K:3856:HOH:O	1.95	0.66
2:M:961:GLU:HG3	9:M:9678:HOH:O	1.94	0.66
3:N:41:ARG:HD3	3:N:42:ASP:H	1.60	0.66
4:O:78:ASN:HB3	9:O:3563:HOH:O	1.94	0.66
2:C:373:VAL:HG12	9:C:9971:HOH:O	1.95	0.66
2:C:708:TYR:HE2	2:C:793:PRO:HD2	1.60	0.66
3:D:531:ASP:C	3:D:533:GLY:H	2.00	0.66
3:D:1112:CYS:HA	9:D:2465:HOH:O	1.93	0.66
3:D:1399:ASP:O	3:D:1403:LEU:HB2	1.95	0.66
1:K:89:PHE:HB2	1:K:94:LEU:HD13	1.77	0.66
1:L:88:ARG:HB3	1:L:88:ARG:NH1	2.09	0.66
2:M:905:ILE:H	2:M:905:ILE:CD1	2.06	0.66
3:N:35:ARG:HD2	3:N:36:THR:N	2.09	0.66
3:N:185:VAL:HG13	9:N:9966:HOH:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:459:GLU:HA	9:N:9521:HOH:O	1.95	0.66
3:N:656:PHE:HB3	3:N:694:VAL:HG11	1.77	0.66
3:N:1091:SER:HA	9:N:9756:HOH:O	1.96	0.66
2:C:52:PHE:CG	2:C:68:PHE:HB2	2.31	0.66
2:C:101:ILE:HG23	2:C:107:LEU:HD22	1.76	0.66
2:C:197:LEU:HB3	2:C:202:TYR:HB2	1.77	0.66
2:C:503:LEU:HD12	2:C:505:GLY:H	1.60	0.66
3:D:770:LEU:HG	3:D:919:PHE:CE1	2.30	0.66
3:D:846:PRO:HB3	9:D:2128:HOH:O	1.94	0.66
3:D:850:LEU:HD12	3:D:850:LEU:H	1.59	0.66
1:A:86:VAL:HG21	1:A:202:ASP:O	1.96	0.66
3:D:924:MET:HG2	9:D:9500:HOH:O	1.94	0.66
4:E:36:LYS:HB3	9:E:9557:HOH:O	1.95	0.66
2:M:660:ALA:HB1	2:M:667:ALA:O	1.94	0.66
3:N:907:GLU:O	3:N:911:LEU:HD13	1.96	0.66
2:C:420:ARG:H	2:C:420:ARG:HD2	1.59	0.66
3:D:875:THR:HB	9:D:9975:HOH:O	1.96	0.66
3:D:1066:THR:HG22	3:D:1069:GLU:HG3	1.75	0.66
3:D:1097:LYS:HA	9:D:9591:HOH:O	1.94	0.66
3:D:1124:GLN:NE2	3:D:1135:ARG:HA	2.11	0.66
3:D:1432:LYS:NZ	3:D:1460:ILE:HG13	2.10	0.66
4:E:37:ASN:ND2	4:E:89:MET:HE2	2.09	0.66
5:F:108:GLU:HG3	5:F:176:ILE:HG21	1.78	0.66
2:M:292:ARG:HB2	2:M:299:LYS:HE2	1.78	0.66
3:N:953:ASP:OD1	3:N:1019:PRO:HG2	1.96	0.66
3:N:1129:THR:HA	9:N:2005:HOH:O	1.95	0.66
3:N:1301:LYS:HA	3:N:1301:LYS:HE3	1.75	0.66
5:P:88:ILE:HG23	9:P:4361:HOH:O	1.96	0.66
3:D:611:GLN:HG3	5:F:326:ASP:HB2	1.78	0.66
3:D:796:ARG:HH11	3:D:861:GLN:HB2	1.59	0.66
3:D:906:GLN:HB3	3:D:911:LEU:CD1	2.25	0.66
3:D:1031:ASN:HB3	3:D:1034:GLN:HG3	1.77	0.66
5:F:406:ARG:HA	5:F:409:LYS:HG2	1.78	0.66
2:M:347:GLY:HA2	2:M:350:ARG:HD2	1.76	0.66
3:N:1145:TYR:CE2	3:N:1168:MET:HB2	2.30	0.66
3:N:1209:LEU:HD23	3:N:1210:SER:N	2.11	0.66
1:B:38:ASN:O	1:B:41:ARG:HG2	1.96	0.66
2:C:182:VAL:HG12	2:C:193:LEU:HD13	1.78	0.66
2:C:405:ARG:HD2	2:C:442:GLU:OE1	1.96	0.66
2:C:703:ILE:HD11	2:C:830:LYS:HG2	1.78	0.66
2:C:724:ARG:HB3	2:C:724:ARG:HH11	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:176:ASP:HA	9:D:2419:HOH:O	1.96	0.66
3:D:462:GLN:HA	3:D:513:ILE:HD13	1.78	0.66
3:D:1262:LEU:HD23	3:D:1352:ILE:HG13	1.78	0.66
5:F:335:ASP:OD1	5:F:338:LEU:HB2	1.94	0.66
1:K:91:ASN:HB2	9:K:5800:HOH:O	1.94	0.66
2:M:939:ARG:HD3	2:M:982:PRO:HD3	1.77	0.66
3:N:535:PHE:HB3	5:P:314:PRO:HB3	1.78	0.66
3:N:1399:ASP:O	3:N:1403:LEU:HB2	1.95	0.66
1:B:180:GLN:HA	9:B:9698:HOH:O	1.94	0.66
2:C:256:TYR:CE1	2:C:293:PHE:HB2	2.30	0.66
2:C:1014:SER:HB3	2:C:1017:THR:O	1.95	0.66
3:D:924:MET:HB3	4:E:7:ASP:OD1	1.96	0.66
3:D:1096:ARG:HH11	3:D:1096:ARG:CB	2.08	0.66
3:D:1462:LEU:HD22	3:D:1472:ILE:HG23	1.78	0.66
3:N:984:THR:HG22	3:N:987:GLU:H	1.61	0.66
3:N:1166:LEU:HD12	3:N:1171:VAL:HG22	1.78	0.66
2:C:328:LEU:HB2	2:C:488:ALA:HB2	1.77	0.65
2:C:610:ARG:HB2	9:C:9703:HOH:O	1.96	0.65
3:D:131:LYS:HB3	3:D:456:MET:HE3	1.78	0.65
3:D:699:VAL:CG1	3:D:717:GLN:HG3	2.26	0.65
3:D:928:ALA:HA	3:D:931:LEU:HD12	1.78	0.65
3:D:1197:ARG:HG3	3:D:1198:TYR:H	1.61	0.65
3:D:1211:MET:HE3	3:D:1213:ARG:HG2	1.78	0.65
3:D:1462:LEU:HD22	3:D:1473:PRO:HD2	1.76	0.65
2:M:820:ARG:HB2	9:M:2167:HOH:O	1.95	0.65
2:M:1018:GLN:NE2	2:M:1060:ILE:HD11	2.07	0.65
2:C:146:VAL:HG22	2:C:162:ILE:HA	1.78	0.65
5:F:235:PHE:HA	9:F:9701:HOH:O	1.95	0.65
1:L:78:ILE:HG12	9:L:4728:HOH:O	1.97	0.65
2:M:89:THR:O	2:M:91:GLN:HG3	1.96	0.65
2:M:966:LEU:HD21	2:M:986:PRO:HG2	1.78	0.65
2:M:1084:SER:O	2:M:1087:VAL:HG12	1.95	0.65
3:N:28:LYS:HG3	3:N:29:PRO:HD2	1.78	0.65
3:N:1036:ARG:HH21	3:N:1042:ARG:CA	2.05	0.65
3:N:1471:LEU:HD12	3:N:1472:ILE:H	1.61	0.65
5:P:320:PRO:HB2	5:P:324:GLU:HG2	1.78	0.65
2:C:137:VAL:HG23	2:C:391:LEU:HG	1.77	0.65
2:C:478:VAL:HG13	2:C:506:ASN:HB3	1.78	0.65
1:K:41:ARG:O	1:K:45:LEU:HD12	1.96	0.65
3:N:1258:ARG:HH21	3:N:1351:GLU:HG2	1.62	0.65
5:P:404:ALA:HB2	9:P:3792:HOH:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:419:ARG:HD3	9:P:6175:HOH:O	1.95	0.65
1:B:73:GLU:HB3	1:B:77:GLU:CG	2.27	0.65
2:C:252:LYS:HE3	9:C:9859:HOH:O	1.95	0.65
2:C:328:LEU:HD22	2:C:433:THR:HG22	1.78	0.65
3:D:572:ARG:HD2	9:F:9689:HOH:O	1.95	0.65
3:D:1031:ASN:HA	9:D:2225:HOH:O	1.97	0.65
2:M:300:ASP:HB2	9:M:9603:HOH:O	1.95	0.65
2:M:305:PRO:HG3	2:M:308:ARG:HH21	1.61	0.65
2:M:451:LEU:HD12	2:M:451:LEU:H	1.58	0.65
2:M:454:SER:HB3	9:M:2089:HOH:O	1.95	0.65
2:M:479:VAL:HG21	2:M:503:LEU:HD11	1.78	0.65
3:N:875:THR:HG23	9:N:2072:HOH:O	1.95	0.65
3:N:1272:ALA:HA	3:N:1326:THR:HB	1.78	0.65
2:C:1060:ILE:HA	2:C:1063:ARG:NH1	2.12	0.65
3:D:1491:THR:O	3:D:1495:ILE:HD13	1.96	0.65
2:M:573:ARG:HG3	2:M:698:ASP:O	1.94	0.65
2:M:576:ALA:HB3	9:M:2073:HOH:O	1.96	0.65
3:N:480:GLU:OE2	3:N:484:PRO:HG2	1.97	0.65
3:N:1191:PRO:HA	9:N:9589:HOH:O	1.96	0.65
3:N:1462:LEU:HD22	3:N:1472:ILE:HG23	1.78	0.65
5:P:393:THR:HG22	5:P:394:ARG:H	1.61	0.65
1:A:11:PHE:CD1	1:B:225:PHE:HA	2.31	0.65
1:A:150:TYR:CE1	2:C:696:LYS:HA	2.32	0.65
3:D:190:GLU:HG3	3:D:210:ARG:NE	2.12	0.65
2:M:231:PRO:HG2	9:M:2420:HOH:O	1.95	0.65
2:M:310:LEU:HD13	9:M:9990:HOH:O	1.97	0.65
2:M:597:ALA:HB2	2:M:655:LEU:HD21	1.77	0.65
2:M:794:PRO:HB2	2:M:1027:PHE:CZ	2.31	0.65
3:N:105:VAL:HG12	3:N:106:LYS:NZ	2.11	0.65
3:N:117:ASP:HB2	3:N:495:ARG:NH2	2.12	0.65
3:N:137:PRO:HD2	3:N:453:ASP:CB	2.27	0.65
3:N:566:ILE:HG12	5:P:217:ASN:HD22	1.61	0.65
3:N:728:LEU:HD12	3:N:729:HIS:H	1.62	0.65
3:N:906:GLN:HB3	3:N:911:LEU:CD1	2.25	0.65
3:N:1147:ARG:HB3	3:N:1188:VAL:CG2	2.27	0.65
4:O:74:VAL:HG12	4:O:79:LEU:HD21	1.78	0.65
5:P:266:GLU:HA	5:P:269:ASN:HD22	1.60	0.65
1:B:77:GLU:HB2	3:D:872:ARG:HH21	1.62	0.65
2:C:798:GLY:H	2:C:827:VAL:HG11	1.62	0.65
2:C:1067:TYR:O	2:C:1071:ILE:HG12	1.97	0.65
3:D:630:VAL:HA	3:D:744:GLN:HG2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:980:MET:HG3	9:D:2017:HOH:O	1.96	0.65
3:D:1187:PRO:HG3	9:D:9606:HOH:O	1.96	0.65
5:F:314:PRO:HB2	9:F:9527:HOH:O	1.96	0.65
2:M:162:ILE:HB	2:M:172:ILE:HB	1.78	0.65
2:M:498:GLN:O	2:M:501:THR:HG23	1.96	0.65
2:M:833:LEU:HD12	2:M:834:GLN:H	1.62	0.65
3:N:536:ALA:HA	5:P:315:VAL:H	1.61	0.65
3:N:654:LYS:HB3	3:N:655:PRO:HD3	1.78	0.65
5:P:220:LEU:O	5:P:224:VAL:HG23	1.96	0.65
5:P:262:VAL:HG12	5:P:266:GLU:OE1	1.95	0.65
1:B:150:TYR:CD2	3:D:857:ILE:HG13	2.32	0.65
2:C:350:ARG:HB3	2:C:350:ARG:HH11	1.59	0.65
2:C:524:VAL:CG1	2:C:528:GLU:HB2	2.26	0.65
2:C:860:HIS:CD2	2:C:975:TYR:HB2	2.32	0.65
3:D:478:LEU:HD13	3:D:1388:ARG:NH2	2.12	0.65
5:F:351:SER:O	5:F:355:GLU:HB2	1.96	0.65
1:K:223:THR:HA	9:K:5661:HOH:O	1.95	0.65
3:N:127:LEU:HD12	3:N:128:TYR:N	2.11	0.65
3:N:171:LEU:HD22	3:N:390:PRO:HG3	1.79	0.65
3:N:427:VAL:CG2	3:N:435:VAL:HB	2.27	0.65
3:N:1213:ARG:HE	3:N:1213:ARG:N	1.95	0.65
3:N:1243:THR:OG1	3:N:1253:THR:HB	1.97	0.65
5:P:208:SER:HB2	5:P:211:ASP:OD1	1.96	0.65
5:P:222:ARG:HA	9:P:3420:HOH:O	1.96	0.65
1:B:68:ILE:HD12	1:B:71:VAL:HG21	1.78	0.65
2:C:115:LEU:HB3	9:C:9971:HOH:O	1.97	0.65
1:L:58:ILE:HB	1:L:61:VAL:HB	1.78	0.65
2:M:1072:LYS:HA	9:M:9641:HOH:O	1.97	0.65
3:N:136:ASP:CB	3:N:137:PRO:HD3	2.27	0.65
3:N:971:LEU:HA	3:N:974:ILE:HD12	1.79	0.65
3:N:1466:VAL:HG23	3:N:1472:ILE:HD11	1.79	0.65
1:B:101:LEU:HD21	1:B:113:ASP:HB3	1.78	0.65
2:C:181:VAL:HG11	9:C:2145:HOH:O	1.97	0.65
2:C:394:PHE:HB3	7:C:8001:RPT:H321	1.79	0.65
2:C:701:THR:HG23	2:C:832:LYS:HG3	1.79	0.65
2:C:910:LYS:HB2	2:C:913:GLU:OE1	1.97	0.65
3:D:546:ARG:O	3:D:550:ARG:HG2	1.97	0.65
2:M:583:LEU:O	2:M:587:VAL:HG23	1.96	0.65
2:M:739:GLU:HG3	9:M:9543:HOH:O	1.96	0.65
3:N:101:HIS:HD2	3:N:582:LEU:HD13	1.62	0.65
3:N:992:ILE:HB	9:N:9914:HOH:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:MET:C	1:B:125:PRO:HD3	2.22	0.64
2:C:433:THR:HA	9:C:9591:HOH:O	1.97	0.64
3:D:172:PRO:HD2	3:D:389:GLU:O	1.97	0.64
3:D:190:GLU:HG3	3:D:210:ARG:HE	1.62	0.64
3:D:1437:ALA:HA	3:D:1440:PHE:CE1	2.32	0.64
4:E:49:GLN:HB2	9:E:9593:HOH:O	1.96	0.64
2:M:95:TYR:CD2	2:M:114:PHE:HB3	2.32	0.64
3:N:756:GLN:O	3:N:760:ARG:HG2	1.95	0.64
5:P:361:LEU:HD22	5:P:366:ALA:HB2	1.79	0.64
2:C:971:LYS:HA	2:C:988:VAL:HA	1.79	0.64
3:D:396:VAL:HG21	3:D:447:VAL:HB	1.77	0.64
3:D:800:LYS:HE3	3:D:830:ALA:HB3	1.78	0.64
1:L:87:VAL:HG21	1:L:144:VAL:HG11	1.78	0.64
2:M:10:ARG:HH11	2:M:10:ARG:HA	1.62	0.64
2:M:409:ARG:HA	2:M:454:SER:HA	1.78	0.64
2:M:1034:GLU:HA	2:M:1037:VAL:HG23	1.78	0.64
3:N:434:ARG:HB2	3:N:447:VAL:HG22	1.79	0.64
3:N:715:ALA:O	3:N:764:LEU:HD12	1.97	0.64
2:C:676:ILE:HG23	3:D:948:THR:HB	1.80	0.64
3:D:122:GLU:O	3:D:126:VAL:HG23	1.98	0.64
3:D:1254:GLN:HG3	9:D:2555:HOH:O	1.96	0.64
1:L:80:LEU:HB3	3:N:867:ARG:NH2	2.13	0.64
2:M:198:ARG:HH12	2:M:231:PRO:HG3	1.62	0.64
3:N:543:LEU:HD22	3:N:580:ALA:HB1	1.78	0.64
1:A:20:TYR:HD2	1:A:21:GLY:N	1.95	0.64
2:C:71:TYR:HB2	9:C:9517:HOH:O	1.97	0.64
2:C:162:ILE:O	2:C:164:PRO:HD3	1.96	0.64
2:C:432:ARG:HD3	3:D:1048:PRO:HG2	1.79	0.64
2:C:650:ARG:HG3	2:C:653:ASP:HB2	1.78	0.64
3:D:208:PRO:HB2	3:D:395:VAL:HG13	1.78	0.64
3:D:996:TRP:HE3	3:D:999:THR:HG21	1.60	0.64
3:D:1046:GLN:HA	3:D:1052:THR:HA	1.80	0.64
5:F:163:LEU:HB3	5:F:174:LEU:HG	1.80	0.64
2:M:726:ILE:HG22	9:M:2191:HOH:O	1.98	0.64
3:N:428:LYS:HE3	3:N:434:ARG:HH12	1.63	0.64
1:B:85:LEU:HD12	1:B:124:ASN:HB3	1.78	0.64
2:C:197:LEU:HA	2:C:200:LEU:HD12	1.80	0.64
2:C:580:MET:HA	9:C:9544:HOH:O	1.97	0.64
2:C:678:PRO:O	3:D:943:THR:HA	1.97	0.64
3:D:804:LEU:HB2	3:D:830:ALA:O	1.98	0.64
1:L:33:GLY:O	1:L:195:LEU:HD22	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:13:ALA:HA	9:N:9515:HOH:O	1.98	0.64
3:N:672:ALA:HB2	5:P:420:ASP:OD1	1.98	0.64
3:N:975:GLU:O	3:N:979:GLU:HG3	1.97	0.64
5:P:80:PRO:HA	5:P:83:GLN:HB2	1.80	0.64
1:B:186:LEU:HD23	9:B:9707:HOH:O	1.96	0.64
2:C:677:MET:HE1	2:C:983:ILE:HD13	1.78	0.64
3:D:795:VAL:HG23	3:D:879:ARG:HH12	1.63	0.64
3:D:1377:LYS:O	3:D:1394:VAL:HA	1.97	0.64
5:F:291:ILE:HG23	5:F:304:VAL:HG21	1.79	0.64
1:L:123:MET:C	1:L:125:PRO:HD3	2.22	0.64
2:M:52:PHE:CD2	2:M:68:PHE:HB2	2.33	0.64
3:N:191:LEU:HD22	3:N:195:VAL:HG21	1.78	0.64
5:P:226:LYS:HB2	9:P:6226:HOH:O	1.96	0.64
5:P:279:GLN:HA	9:P:4921:HOH:O	1.97	0.64
2:C:76:PRO:HG3	9:C:2288:HOH:O	1.98	0.64
2:C:720:GLU:HG2	2:C:760:SER:HB3	1.80	0.64
3:D:178:LEU:HG	3:D:200:ASP:H	1.62	0.64
1:K:20:TYR:HD2	1:K:21:GLY:H	1.46	0.64
1:L:81:ASN:HB3	9:L:4066:HOH:O	1.97	0.64
1:L:89:PHE:HB2	1:L:94:LEU:HD13	1.78	0.64
3:N:817:GLU:O	3:N:821:VAL:HG23	1.98	0.64
3:N:1282:ARG:HD3	3:N:1295:GLU:OE2	1.98	0.64
1:A:177:VAL:O	2:C:864:GLY:HA3	1.97	0.64
1:B:180:GLN:HG3	9:B:9530:HOH:O	1.97	0.64
2:C:889:HIS:CE1	3:D:951:ILE:H	2.15	0.64
3:D:214:GLU:HG3	3:D:390:PRO:HB2	1.80	0.64
4:E:47:LYS:HA	4:E:54:LEU:HB3	1.80	0.64
1:L:32:PHE:HB2	9:L:5175:HOH:O	1.98	0.64
1:A:193:ASP:HA	9:A:9491:HOH:O	1.96	0.64
1:B:214:ALA:HA	1:B:217:ILE:HD12	1.79	0.64
2:C:595:LEU:HB3	9:C:9812:HOH:O	1.98	0.64
2:C:673:LEU:HD22	2:C:867:VAL:HA	1.79	0.64
2:C:1008:ARG:HE	2:C:1028:GLY:N	1.96	0.64
2:C:1098:ASP:HB2	3:D:21:TRP:CZ2	2.33	0.64
3:D:590:PRO:HA	9:D:9578:HOH:O	1.96	0.64
2:M:455:LEU:HD12	2:M:456:ALA:O	1.98	0.64
2:M:987:ILE:HG12	3:N:948:THR:HG21	1.80	0.64
2:M:1046:ALA:HB1	3:N:1471:LEU:HD11	1.80	0.64
3:N:795:VAL:HG11	3:N:863:VAL:HG13	1.79	0.64
5:P:305:GLU:HG2	9:P:3554:HOH:O	1.98	0.64
2:C:413:LEU:H	2:C:413:LEU:HD12	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:716:LYS:HD3	9:C:2019:HOH:O	1.96	0.64
2:C:926:PHE:O	2:C:930:LYS:HG3	1.97	0.64
2:C:1021:LEU:HD22	9:F:9484:HOH:O	1.98	0.64
3:D:395:VAL:HG12	9:D:2245:HOH:O	1.99	0.64
3:D:817:GLU:HG3	3:D:839:LEU:HD13	1.78	0.64
1:L:62:LEU:HD12	9:L:4737:HOH:O	1.97	0.64
2:M:511:GLU:O	2:M:526:PRO:HD3	1.98	0.64
2:M:838:LYS:HD2	2:M:846:LYS:HZ3	1.62	0.64
4:O:41:GLU:O	4:O:45:ARG:HG2	1.98	0.64
5:P:163:LEU:HB3	5:P:174:LEU:CG	2.28	0.64
2:C:250:ARG:HG2	2:C:253:ALA:HB3	1.79	0.63
2:C:379:GLU:O	2:C:383:ARG:HB3	1.97	0.63
2:C:605:LYS:HD3	2:C:610:ARG:NH1	2.13	0.63
2:C:730:SER:O	2:C:734:LEU:HD13	1.98	0.63
3:D:860:LEU:HD23	3:D:877:PRO:HB2	1.79	0.63
3:D:1124:GLN:NE2	3:D:1135:ARG:HG2	2.13	0.63
3:D:1152:GLU:CD	3:D:1159:ARG:HH12	2.06	0.63
2:M:612:VAL:HG22	2:M:622:GLU:HG3	1.80	0.63
2:M:694:LEU:HD11	2:M:868:ASP:HB3	1.80	0.63
3:N:185:VAL:CG1	3:N:191:LEU:HD21	2.28	0.63
3:N:1093:TYR:HA	9:N:2053:HOH:O	1.98	0.63
5:P:123:ASP:HB3	5:P:125:ASP:OD1	1.98	0.63
1:B:103:ALA:O	1:B:138:LEU:HD23	1.97	0.63
2:C:156:GLY:HA3	9:C:2245:HOH:O	1.97	0.63
2:C:399:ASN:HD22	2:C:399:ASN:N	1.96	0.63
2:C:404:LEU:HD22	2:C:591:SER:HB3	1.80	0.63
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.80	0.63
3:D:808:THR:HB	3:D:809:PRO:HD3	1.80	0.63
3:D:907:GLU:O	3:D:911:LEU:HD13	1.97	0.63
3:D:1465:ASN:HD21	3:D:1470:ARG:NH1	1.95	0.63
2:M:68:PHE:HZ	2:M:71:TYR:HB3	1.63	0.63
2:M:575:GLN:HA	2:M:662:GLU:OE2	1.98	0.63
3:N:984:THR:H	3:N:987:GLU:CD	2.06	0.63
2:C:816:LYS:HE2	2:C:819:VAL:HG21	1.78	0.63
3:D:396:VAL:HG11	9:D:9781:HOH:O	1.98	0.63
3:N:119:SER:H	3:N:123:LEU:HB2	1.63	0.63
3:N:1192:LEU:HD12	3:N:1346:ARG:HH21	1.63	0.63
1:A:42:ARG:NH1	2:C:978:ARG:HA	2.12	0.63
2:C:724:ARG:HB2	2:C:740:GLU:HG3	1.79	0.63
2:C:1067:TYR:CG	5:F:341:PRO:HB3	2.34	0.63
9:C:9697:HOH:O	4:E:31:LEU:HD11	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:109:VAL:HG23	9:K:3900:HOH:O	1.98	0.63
1:L:172:SER:HB3	9:L:4444:HOH:O	1.97	0.63
2:M:1056:LYS:O	3:N:624:ASP:HB2	1.98	0.63
2:M:1095:LEU:HD11	3:N:607:LEU:HD11	1.80	0.63
3:N:52:PRO:CG	3:N:78:VAL:HG13	2.27	0.63
3:N:125:GLN:HE22	3:N:587:ARG:HH21	1.46	0.63
3:N:535:PHE:O	5:P:315:VAL:N	2.30	0.63
3:N:1046:GLN:HA	3:N:1052:THR:HA	1.80	0.63
1:A:181:VAL:HG12	9:A:9491:HOH:O	1.97	0.63
2:C:355:VAL:CG2	2:C:372:LEU:HG	2.28	0.63
2:C:771:GLU:O	2:C:775:ARG:HG2	1.98	0.63
3:D:829:VAL:HA	9:D:2030:HOH:O	1.97	0.63
3:D:1272:ALA:HB2	9:D:2257:HOH:O	1.97	0.63
1:K:99:LEU:HB3	1:K:114:PHE:CD2	2.34	0.63
3:N:584:ASN:ND2	3:N:590:PRO:HD2	2.14	0.63
3:N:628:ARG:HD3	3:N:744:GLN:HE22	1.63	0.63
4:O:31:LEU:HD23	4:O:35:PHE:CE1	2.33	0.63
4:O:84:ARG:HB2	4:O:84:ARG:HH11	1.64	0.63
5:P:130:VAL:HG21	5:P:159:ILE:HG21	1.80	0.63
1:A:198:ARG:HD3	1:A:200:TRP:HH2	1.62	0.63
2:C:95:TYR:CD2	2:C:114:PHE:HB3	2.34	0.63
2:C:1066:ALA:O	2:C:1070:ILE:HG13	1.99	0.63
5:F:112:ALA:HA	5:F:173:TYR:HD2	1.63	0.63
2:M:19:THR:HG22	2:M:22:GLN:HB2	1.79	0.63
2:M:191:PHE:HZ	2:M:196:LEU:HB2	1.64	0.63
2:M:516:ARG:NE	3:N:1068:LEU:HD13	2.13	0.63
2:M:943:VAL:HA	9:M:2224:HOH:O	1.99	0.63
3:N:1465:ASN:ND2	3:N:1470:ARG:HD3	2.12	0.63
2:C:145:GLY:H	2:C:163:ILE:HG23	1.63	0.63
2:C:516:ARG:HD3	2:C:521:PRO:HA	1.81	0.63
2:C:595:LEU:HD23	2:C:655:LEU:HD12	1.81	0.63
2:C:724:ARG:HG3	2:C:741:GLY:N	2.07	0.63
2:C:949:LYS:CD	3:D:796:ARG:HH21	2.12	0.63
2:C:1034:GLU:HA	2:C:1037:VAL:HG23	1.81	0.63
2:C:1084:SER:O	2:C:1087:VAL:HG12	1.98	0.63
3:D:111:LYS:HD3	9:D:9759:HOH:O	1.97	0.63
3:D:135:LEU:HD13	3:D:147:VAL:HG23	1.80	0.63
3:D:551:ASN:O	3:D:555:LYS:HG3	1.98	0.63
3:D:705:ALA:HB3	3:D:706:PRO:HD3	1.79	0.63
3:D:1147:ARG:HB2	3:D:1166:LEU:HD21	1.80	0.63
2:M:443:THR:O	2:M:559:LEU:HD11	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:816:LYS:HB2	2:M:819:VAL:HG21	1.81	0.63
3:N:393:ILE:HD12	3:N:393:ILE:H	1.64	0.63
3:N:1095:THR:O	3:N:1099:VAL:HG23	1.99	0.63
3:N:1147:ARG:O	3:N:1165:TYR:HA	1.99	0.63
4:O:72:ARG:HD2	9:O:5366:HOH:O	1.98	0.63
2:C:25:SER:HB2	2:C:335:THR:HB	1.81	0.63
3:D:699:VAL:HG21	3:D:760:ARG:HB3	1.81	0.63
3:D:787:LEU:HD21	3:D:947:ILE:HD13	1.80	0.63
3:D:1290:LEU:HD13	3:D:1305:LEU:HD12	1.80	0.63
2:M:428:ARG:HG2	2:M:451:LEU:HG	1.81	0.63
2:M:863:ASP:OD2	2:M:865:THR:HG22	1.99	0.63
2:M:1115:LEU:HD12	2:M:1115:LEU:H	1.64	0.63
3:N:1159:ARG:HD3	9:N:9583:HOH:O	1.98	0.63
1:A:97:VAL:HG23	9:A:9486:HOH:O	1.98	0.63
3:D:393:ILE:H	3:D:393:ILE:HD12	1.64	0.63
3:D:584:ASN:HD22	3:D:584:ASN:C	2.07	0.63
3:D:1109:GLU:CD	3:D:1202:GLN:H	2.07	0.63
5:F:347:GLN:HG2	9:F:9631:HOH:O	1.98	0.63
1:K:78:ILE:HA	1:K:81:ASN:ND2	2.14	0.63
2:M:367:LEU:HB3	2:M:371:LYS:HG2	1.81	0.63
2:M:431:HIS:H	2:M:434:HIS:CE1	2.17	0.63
3:N:589:ALA:HB3	9:N:9549:HOH:O	1.98	0.63
3:N:800:LYS:HE3	3:N:830:ALA:HB3	1.80	0.63
3:N:1329:ALA:HA	9:N:9884:HOH:O	1.98	0.63
3:N:1500:LYS:HA	9:N:2479:HOH:O	1.99	0.63
2:C:151:ASP:HB2	2:C:157:ARG:O	1.98	0.62
2:C:305:PRO:HG3	2:C:308:ARG:NH2	2.14	0.62
2:C:721:ARG:HH21	2:C:783:ARG:HH21	1.47	0.62
2:C:1034:GLU:HG3	9:C:9762:HOH:O	1.98	0.62
3:D:126:VAL:HG22	9:D:2697:HOH:O	1.98	0.62
3:D:584:ASN:ND2	3:D:590:PRO:HD2	2.14	0.62
3:D:810:GLU:O	3:D:813:LEU:HG	1.98	0.62
5:F:273:ARG:HB3	9:F:9511:HOH:O	1.97	0.62
3:N:423:ASP:OD2	5:P:174:LEU:HD22	1.98	0.62
2:C:244:PRO:HB3	9:C:9757:HOH:O	1.99	0.62
2:C:557:ARG:HB2	9:C:9570:HOH:O	1.98	0.62
3:D:101:HIS:HD1	3:D:103:TRP:HB2	1.63	0.62
3:D:434:ARG:HB2	3:D:447:VAL:HG13	1.80	0.62
3:D:1495:ILE:HD11	9:E:9594:HOH:O	1.97	0.62
5:F:347:GLN:HG3	9:F:9808:HOH:O	1.99	0.62
2:M:603:VAL:HG21	2:M:643:VAL:CG1	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:802:ARG:HB3	9:M:9780:HOH:O	1.98	0.62
3:N:177:ALA:HB3	9:N:2388:HOH:O	1.99	0.62
3:N:760:ARG:HH21	4:O:3:GLU:CD	2.07	0.62
5:P:87:GLU:O	5:P:91:VAL:HG23	1.99	0.62
1:B:151:VAL:HG23	9:B:9528:HOH:O	1.99	0.62
2:C:503:LEU:HD13	2:C:507:ARG:O	1.99	0.62
2:C:606:VAL:HG22	2:C:645:VAL:HG22	1.81	0.62
2:C:672:VAL:CG2	2:C:868:ASP:HB2	2.30	0.62
2:C:675:ALA:HB2	2:C:867:VAL:HG11	1.81	0.62
1:K:67:THR:HG23	2:M:627:ARG:NH2	2.14	0.62
2:M:222:MET:HB3	9:M:9807:HOH:O	1.98	0.62
3:N:674:ARG:HG2	3:N:674:ARG:HH11	1.64	0.62
5:P:154:LYS:O	5:P:158:GLU:HG3	1.98	0.62
1:A:42:ARG:NH1	2:C:857:ASP:HB3	2.15	0.62
1:B:132:LEU:HG	1:B:136:GLY:HA3	1.80	0.62
2:C:313:LEU:HA	9:C:2113:HOH:O	1.98	0.62
2:C:554:ASP:HB2	2:C:880:MET:HB2	1.80	0.62
2:C:579:VAL:HB	2:C:890:LEU:CD2	2.28	0.62
3:D:26:VAL:HG11	3:D:44:LEU:HD23	1.82	0.62
3:D:36:THR:C	3:D:38:LYS:H	2.08	0.62
3:D:471:GLU:O	3:D:475:LYS:HD2	1.99	0.62
3:D:1436:SER:HB3	9:D:9596:HOH:O	1.98	0.62
2:M:15:LEU:H	2:M:15:LEU:HD12	1.64	0.62
2:M:308:ARG:HB3	9:M:9658:HOH:O	1.99	0.62
2:M:310:LEU:O	2:M:314:THR:HG23	1.99	0.62
3:N:1031:ASN:HB3	3:N:1034:GLN:CD	2.24	0.62
5:P:395:GLU:O	5:P:399:GLN:HB2	1.98	0.62
1:A:189:ARG:HB3	9:A:9613:HOH:O	1.99	0.62
9:A:9505:HOH:O	1:B:43:ILE:HD11	1.98	0.62
1:B:184:THR:HB	1:B:194:LYS:HZ3	1.64	0.62
3:D:146:PRO:HG2	9:D:9964:HOH:O	1.99	0.62
3:D:478:LEU:HD22	3:D:1388:ARG:CZ	2.28	0.62
3:D:679:ARG:HB2	3:D:682:ASP:OD2	2.00	0.62
3:D:860:LEU:HA	3:D:877:PRO:HB2	1.81	0.62
3:D:972:LEU:HD23	3:D:973:GLN:N	2.14	0.62
3:D:1399:ASP:HA	9:D:2529:HOH:O	1.99	0.62
1:K:62:LEU:HD12	9:K:3552:HOH:O	1.98	0.62
1:K:88:ARG:HD2	1:K:88:ARG:O	1.99	0.62
2:M:42:VAL:HG12	2:M:43:GLY:H	1.65	0.62
2:M:276:LYS:HB3	9:M:9769:HOH:O	1.99	0.62
2:M:1105:LYS:HG2	9:M:2030:HOH:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:373:LYS:HD3	5:P:378:GLY:C	2.25	0.62
1:A:74:ASP:HA	9:A:9598:HOH:O	1.99	0.62
1:A:120:VAL:HG13	9:A:9516:HOH:O	1.99	0.62
1:B:184:THR:HB	1:B:194:LYS:NZ	2.15	0.62
2:C:580:MET:HB3	2:C:584:GLU:OE2	2.00	0.62
2:C:724:ARG:NE	2:C:737:LEU:O	2.32	0.62
3:D:117:ASP:HB2	3:D:495:ARG:NH2	2.13	0.62
3:D:128:TYR:CE1	3:D:461:ILE:HG13	2.34	0.62
3:D:1342:GLU:HB3	9:D:9499:HOH:O	2.00	0.62
5:F:316:SER:HB3	5:F:318:GLU:O	2.00	0.62
1:L:26:GLU:HB3	9:L:3467:HOH:O	1.99	0.62
2:M:139:GLN:O	2:M:333:ILE:HA	2.00	0.62
2:M:433:THR:HG21	2:M:488:ALA:HB1	1.81	0.62
2:M:640:ARG:HB3	9:M:2138:HOH:O	1.99	0.62
2:M:770:GLU:HG2	3:N:65:ARG:NH2	2.15	0.62
2:M:971:LYS:HA	2:M:988:VAL:HA	1.81	0.62
3:N:1127:GLU:HB2	9:N:9636:HOH:O	1.99	0.62
5:P:321:ILE:HD11	5:P:329:TYR:HB2	1.81	0.62
2:C:376:ARG:NH1	5:F:285:GLU:HG2	2.15	0.62
3:D:179:VAL:HB	9:D:2419:HOH:O	1.99	0.62
1:L:5:LYS:HA	1:L:5:LYS:NZ	2.15	0.62
3:N:450:TYR:HB3	9:N:9938:HOH:O	1.99	0.62
3:N:633:VAL:HG22	3:N:635:PRO:HD3	1.82	0.62
2:C:398:THR:OG1	2:C:633:GLN:HG3	2.00	0.62
3:D:562:ALA:HB1	3:D:567:ILE:CD1	2.29	0.62
3:D:572:ARG:HH22	5:F:83:GLN:HG3	1.65	0.62
3:D:1238:MET:HE2	3:D:1257:PRO:HG3	1.81	0.62
4:E:12:MET:HE2	4:E:12:MET:HA	1.80	0.62
1:L:64:GLU:HG3	9:L:4182:HOH:O	1.99	0.62
2:M:97:ARG:HD2	9:M:9731:HOH:O	2.00	0.62
3:N:1493:LYS:O	3:N:1497:GLU:HG2	1.99	0.62
2:C:333:ILE:CD1	2:C:467:ILE:HG13	2.29	0.62
2:C:543:ASN:HD22	2:C:562:SER:HB3	1.64	0.62
2:C:569:VAL:HG23	2:C:635:THR:HG22	1.81	0.62
2:C:702:SER:HB2	9:C:9792:HOH:O	1.99	0.62
3:D:473:LEU:HD21	3:D:495:ARG:CZ	2.30	0.62
3:D:502:PHE:CE2	3:D:1452:ILE:HG13	2.35	0.62
3:D:675:ARG:O	3:D:678:GLU:HG2	1.99	0.62
3:D:1318:TYR:HB3	9:D:2293:HOH:O	1.99	0.62
4:E:41:GLU:HG2	9:E:9566:HOH:O	1.99	0.62
2:M:207:LEU:HD23	2:M:211:LEU:HD23	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:276:LYS:H	2:M:276:LYS:HD2	1.64	0.62
3:N:972:LEU:HD13	9:N:2036:HOH:O	2.00	0.62
3:N:1057:VAL:HG13	3:N:1069:GLU:HB3	1.81	0.62
4:O:62:THR:HA	4:O:65:MET:HE3	1.80	0.62
3:D:197:SER:CB	3:D:203:ALA:HB3	2.25	0.62
3:D:500:ARG:HH22	3:D:1388:ARG:NH1	1.97	0.62
3:D:1432:LYS:HG3	3:D:1433:SER:H	1.65	0.62
5:F:398:ARG:HG2	5:F:402:ASN:ND2	2.14	0.62
2:M:37:GLU:HA	9:M:2385:HOH:O	1.98	0.62
2:M:468:ARG:HD3	2:M:485:TYR:HB3	1.81	0.62
2:M:1095:LEU:HB2	2:M:1097:LEU:HD21	1.81	0.62
3:N:139:GLY:O	3:N:147:VAL:HB	2.00	0.62
3:N:692:GLU:HG2	3:N:720:LEU:HD12	1.81	0.62
2:C:178:PRO:HA	9:C:2061:HOH:O	1.99	0.61
2:C:298:PHE:HB3	9:C:2271:HOH:O	2.01	0.61
3:D:9:ARG:HA	3:D:1434:TRP:HH2	1.64	0.61
3:D:41:ARG:NH1	3:D:42:ASP:HB2	2.13	0.61
3:D:109:PRO:HD3	9:D:9821:HOH:O	2.00	0.61
3:D:402:PRO:HG2	3:D:444:VAL:HG11	1.80	0.61
3:D:877:PRO:O	3:D:880:ILE:HG22	1.99	0.61
3:D:1251:ASP:O	3:D:1270:ALA:HB3	1.99	0.61
2:M:157:ARG:HD3	2:M:158:TYR:N	2.15	0.61
2:M:630:ARG:HA	9:M:9812:HOH:O	2.00	0.61
2:M:939:ARG:HG3	9:M:9643:HOH:O	2.00	0.61
3:N:662:GLU:HB2	9:N:2066:HOH:O	2.00	0.61
3:N:728:LEU:HD22	3:N:745:MET:SD	2.40	0.61
4:O:47:LYS:HA	4:O:54:LEU:HB3	1.81	0.61
5:P:342:VAL:HB	9:P:5304:HOH:O	2.00	0.61
1:B:33:GLY:O	1:B:195:LEU:HD22	2.00	0.61
2:C:640:ARG:NH1	2:C:642:ARG:HH22	1.98	0.61
3:D:611:GLN:HB2	9:F:9660:HOH:O	2.00	0.61
3:D:817:GLU:HG2	3:D:840:LYS:HZ2	1.65	0.61
2:M:162:ILE:O	2:M:164:PRO:HD3	2.00	0.61
9:M:2401:HOH:O	5:P:409:LYS:HD2	1.98	0.61
2:C:84:ARG:NH2	2:C:128:ILE:HD11	2.15	0.61
2:C:389:SER:C	2:C:391:LEU:H	2.08	0.61
3:D:141:ILE:HG21	3:D:161:LEU:HD21	1.82	0.61
3:D:1304:LYS:HA	9:D:2093:HOH:O	2.00	0.61
3:N:421:LEU:HD12	3:N:435:VAL:HG11	1.81	0.61
3:N:705:ALA:HB3	3:N:706:PRO:HD3	1.82	0.61
2:C:480:THR:HG22	2:C:482:GLU:H	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:584:ASN:CG	3:D:590:PRO:HD2	2.25	0.61
3:D:1063:GLU:HG2	3:D:1064:GLY:N	2.14	0.61
3:D:1137:ARG:O	3:D:1141:GLU:HG3	2.00	0.61
3:D:1183:ILE:HG22	9:D:9811:HOH:O	2.00	0.61
2:M:149:THR:HG22	9:M:2395:HOH:O	2.00	0.61
2:M:178:PRO:HB3	9:M:9661:HOH:O	2.01	0.61
2:M:198:ARG:NH1	2:M:231:PRO:HG3	2.16	0.61
2:M:468:ARG:HD2	9:M:2017:HOH:O	1.98	0.61
2:M:720:GLU:HG2	2:M:760:SER:HB3	1.83	0.61
2:M:745:ILE:HG13	9:M:9989:HOH:O	2.00	0.61
3:N:957:PRO:HB3	3:N:959:GLU:OE1	2.00	0.61
3:N:1236:LEU:HA	9:N:2360:HOH:O	1.98	0.61
1:B:110:LYS:HG3	9:B:9511:HOH:O	1.99	0.61
3:D:1154:GLU:HG2	9:D:9504:HOH:O	2.00	0.61
3:D:1299:PHE:HB2	9:D:9955:HOH:O	1.98	0.61
5:F:100:VAL:HG21	9:F:9680:HOH:O	2.00	0.61
1:L:54:THR:HG22	1:L:158:ILE:HG13	1.82	0.61
2:M:437:ARG:CZ	2:M:488:ALA:HA	2.31	0.61
3:N:428:LYS:HE3	3:N:434:ARG:NH1	2.15	0.61
5:P:120:THR:HB	9:P:4895:HOH:O	2.00	0.61
5:P:166:LEU:O	5:P:171:LYS:HB2	2.00	0.61
2:C:62:GLY:O	2:C:103:LYS:HG3	2.00	0.61
2:C:197:LEU:HD12	2:C:207:LEU:HD11	1.81	0.61
2:C:218:VAL:HA	2:C:221:LEU:HD23	1.82	0.61
2:C:511:GLU:O	2:C:526:PRO:HD3	1.99	0.61
2:C:769:PRO:HG3	9:F:9763:HOH:O	1.99	0.61
3:D:501:ALA:HB2	9:D:9860:HOH:O	1.99	0.61
3:D:1135:ARG:HD3	9:D:2109:HOH:O	2.01	0.61
5:F:278:LEU:O	5:F:282:LEU:HG	2.00	0.61
2:M:431:HIS:CD2	2:M:433:THR:H	2.19	0.61
2:M:569:VAL:HG12	2:M:996:LYS:O	2.01	0.61
3:N:422:ALA:HB3	3:N:427:VAL:CG2	2.25	0.61
3:N:863:VAL:HG23	9:N:9553:HOH:O	2.01	0.61
3:N:1425:THR:HG23	3:N:1426:LYS:N	2.16	0.61
1:A:184:THR:HG23	1:A:192:LEU:HB2	1.83	0.61
1:B:26:GLU:HG2	1:B:27:PRO:HA	1.82	0.61
2:C:108:ILE:H	2:C:108:ILE:HD12	1.65	0.61
2:C:543:ASN:ND2	2:C:562:SER:HB3	2.16	0.61
3:D:668:PRO:HB2	9:F:9602:HOH:O	2.00	0.61
3:D:1403:LEU:O	3:D:1407:LEU:HB2	2.00	0.61
2:M:139:GLN:HE21	2:M:334:ARG:HD2	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:707:ARG:NH1	2:M:709:GLU:HB2	2.15	0.61
2:M:1115:LEU:HD23	3:N:85:VAL:HG13	1.82	0.61
3:N:208:PRO:HB2	3:N:395:VAL:HG22	1.81	0.61
3:N:618:LEU:HD22	9:N:2165:HOH:O	2.00	0.61
3:N:860:LEU:HA	3:N:877:PRO:HB2	1.82	0.61
3:N:983:LEU:HA	3:N:987:GLU:OE2	2.01	0.61
5:P:291:ILE:HB	9:P:3811:HOH:O	1.99	0.61
2:C:318:PRO:HD2	9:C:2113:HOH:O	2.00	0.61
2:C:625:LEU:HD11	2:C:641:PRO:HG3	1.82	0.61
3:D:760:ARG:HB2	9:E:9559:HOH:O	2.00	0.61
3:D:807:ALA:HB2	3:D:833:GLU:OE1	2.01	0.61
3:D:1412:LYS:HE3	9:D:2567:HOH:O	2.00	0.61
5:F:131:VAL:HG13	5:F:178:ARG:HD3	1.81	0.61
5:F:361:LEU:HD23	5:F:362:SER:N	2.14	0.61
2:M:140:ILE:HG22	2:M:333:ILE:HG13	1.83	0.61
2:M:148:PHE:HB3	9:M:9990:HOH:O	2.00	0.61
2:M:1017:THR:HG23	9:P:5990:HOH:O	2.01	0.61
3:N:15:PRO:HA	3:N:18:ILE:HG12	1.83	0.61
3:N:535:PHE:HB2	9:P:5489:HOH:O	1.99	0.61
3:N:950:GLY:H	3:N:953:ASP:HB2	1.66	0.61
3:N:984:THR:HB	3:N:987:GLU:OE1	2.01	0.61
3:N:1137:ARG:HA	3:N:1140:ILE:HD12	1.81	0.61
4:O:82:GLU:HG2	9:O:5722:HOH:O	2.01	0.61
5:P:372:ARG:HD2	9:P:5354:HOH:O	2.01	0.61
1:B:57:TYR:HB3	1:B:141:GLU:CG	2.29	0.61
2:C:498:GLN:O	2:C:501:THR:HG23	2.00	0.61
3:D:28:LYS:HD3	3:D:41:ARG:CZ	2.30	0.61
3:D:163:TYR:HB3	9:D:2435:HOH:O	2.01	0.61
3:D:774:SER:C	3:D:776:GLU:H	2.08	0.61
3:D:964:LEU:HD22	9:D:9566:HOH:O	2.01	0.61
3:D:1394:VAL:HB	3:D:1397:LYS:HD2	1.83	0.61
2:M:439:CYS:HB2	2:M:541:SER:HB3	1.82	0.61
2:M:510:ALA:HB3	2:M:513:VAL:HG23	1.81	0.61
2:M:773:LEU:O	2:M:777:ILE:HG13	2.01	0.61
3:N:45:PHE:HD1	3:N:86:ARG:HH22	1.48	0.61
3:N:82:LYS:HD3	9:N:2443:HOH:O	2.01	0.61
3:N:584:ASN:HB2	3:N:602:SER:OG	2.00	0.61
3:N:715:ALA:HB3	3:N:764:LEU:HA	1.82	0.61
1:A:58:ILE:HB	1:A:61:VAL:HB	1.83	0.61
2:C:342:ASP:O	2:C:346:VAL:HG23	2.00	0.61
2:C:377:PRO:HA	9:C:2397:HOH:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:601:ARG:HD2	5:F:328:PHE:CE1	2.33	0.61
2:M:611:ILE:HD11	2:M:641:PRO:HG3	1.82	0.61
2:M:806:LEU:HB2	9:M:9775:HOH:O	2.01	0.61
3:N:171:LEU:HB2	3:N:390:PRO:HA	1.82	0.61
3:N:543:LEU:HD23	9:N:9696:HOH:O	2.01	0.61
3:N:770:LEU:HB2	9:N:9545:HOH:O	2.01	0.61
5:P:208:SER:HB2	5:P:211:ASP:CG	2.25	0.61
1:A:20:TYR:HD2	1:A:21:GLY:H	1.48	0.60
2:C:260:LEU:HB2	2:C:291:ALA:HB1	1.83	0.60
2:C:789:SER:O	2:C:791:ARG:HG2	2.01	0.60
3:D:438:ASP:HB2	9:D:9897:HOH:O	2.01	0.60
1:L:101:LEU:HG	1:L:114:PHE:HA	1.81	0.60
2:M:321:GLU:HB3	9:M:9537:HOH:O	2.00	0.60
3:N:185:VAL:HG12	3:N:191:LEU:HD21	1.83	0.60
3:N:659:LYS:HE3	3:N:663:GLU:OE1	2.00	0.60
3:N:838:ARG:HB2	9:N:9806:HOH:O	2.01	0.60
3:N:1342:GLU:H	3:N:1342:GLU:CD	2.09	0.60
4:O:21:VAL:O	4:O:25:LYS:HG3	1.99	0.60
2:C:470:PRO:HB3	2:C:485:TYR:CZ	2.36	0.60
3:D:61:GLY:CA	3:D:64:LYS:HE3	2.31	0.60
3:D:119:SER:HB2	3:D:123:LEU:HB2	1.82	0.60
3:D:183:GLU:HA	3:D:186:VAL:HG12	1.82	0.60
3:D:1147:ARG:O	3:D:1165:TYR:HA	2.01	0.60
3:D:1422:MET:HE2	3:D:1427:SER:HA	1.83	0.60
1:L:36:LEU:O	1:L:39:PRO:HD2	2.01	0.60
1:L:103:ALA:HB1	1:L:107:LYS:HD2	1.83	0.60
2:M:772:ARG:HG3	2:M:773:LEU:N	2.15	0.60
2:M:841:ASN:ND2	2:M:844:GLY:H	1.99	0.60
3:N:481:MET:SD	3:N:1388:ARG:HG2	2.40	0.60
3:N:584:ASN:HD21	3:N:590:PRO:HB2	1.66	0.60
3:N:924:MET:HE1	4:O:10:PHE:CE1	2.36	0.60
4:O:50:THR:HB	9:O:3763:HOH:O	2.00	0.60
5:P:117:SER:HA	9:P:4895:HOH:O	2.01	0.60
5:P:225:GLU:HB3	9:P:3420:HOH:O	2.00	0.60
2:C:424:GLY:HA3	9:C:2382:HOH:O	2.02	0.60
3:D:1084:THR:HG21	9:D:2388:HOH:O	2.02	0.60
5:F:403:LYS:HA	5:F:403:LYS:NZ	2.16	0.60
1:L:101:LEU:HD21	1:L:113:ASP:HB3	1.83	0.60
1:L:110:LYS:HG3	9:L:5936:HOH:O	2.00	0.60
3:N:139:GLY:H	3:N:147:VAL:HG21	1.65	0.60
4:O:60:ALA:O	4:O:63:TRP:HB2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:209:PHE:O	5:P:213:ILE:HG13	2.00	0.60
1:A:5:LYS:O	1:A:8:ALA:HB2	2.01	0.60
2:C:29:ALA:HB2	2:C:337:GLY:CA	2.30	0.60
2:C:575:GLN:H	2:C:667:ALA:HB1	1.65	0.60
2:C:603:VAL:HG21	2:C:643:VAL:CG1	2.30	0.60
3:D:28:LYS:HB2	3:D:41:ARG:HD2	1.83	0.60
3:D:455:ARG:HG2	3:D:455:ARG:HH11	1.65	0.60
3:D:524:LEU:C	3:D:526:PRO:HD3	2.26	0.60
5:F:417:LYS:HA	9:F:9602:HOH:O	2.01	0.60
1:L:45:LEU:HD21	1:L:177:VAL:HG22	1.81	0.60
2:M:137:VAL:HG11	2:M:393:GLN:NE2	2.15	0.60
2:M:358:ARG:HH22	2:M:374:ASN:HB3	1.66	0.60
2:M:584:GLU:CD	2:M:584:GLU:H	2.08	0.60
3:N:829:VAL:HG23	9:N:2131:HOH:O	2.01	0.60
1:A:221:HIS:HA	1:A:224:TYR:CD2	2.36	0.60
1:B:212:ASN:O	1:B:215:VAL:HG22	2.01	0.60
2:C:122:THR:HA	9:C:9789:HOH:O	2.00	0.60
2:C:244:PRO:HG2	2:C:246:ASP:OD2	2.01	0.60
2:C:332:ARG:HA	2:C:465:GLY:O	2.02	0.60
2:C:431:HIS:H	2:C:434:HIS:CE1	2.19	0.60
3:D:105:VAL:HG21	3:D:128:TYR:HE2	1.66	0.60
1:L:184:THR:HG23	1:L:192:LEU:HB3	1.83	0.60
2:M:643:VAL:HG22	2:M:647:GLN:HE22	1.65	0.60
2:M:679:PHE:HD2	2:M:680:ASP:H	1.49	0.60
2:M:887:GLU:HB3	9:M:9573:HOH:O	2.01	0.60
2:M:944:LEU:HD21	2:M:963:LEU:HD22	1.84	0.60
2:M:1016:ILE:HG23	3:N:526:PRO:HG2	1.83	0.60
2:M:1109:VAL:HG11	3:N:5:VAL:HG22	1.84	0.60
3:N:36:THR:C	3:N:38:LYS:H	2.09	0.60
3:N:130:SER:HB3	3:N:132:TYR:CE1	2.36	0.60
3:N:141:ILE:HG12	3:N:449:SER:HA	1.84	0.60
3:N:1220:ALA:O	3:N:1224:VAL:HG23	2.00	0.60
1:B:80:LEU:HD23	3:D:867:ARG:NH1	2.17	0.60
2:C:513:VAL:HG13	9:C:9526:HOH:O	2.02	0.60
9:C:9676:HOH:O	3:D:621:LYS:HE2	2.02	0.60
3:D:87:ARG:HB3	3:D:523:ASP:CB	2.28	0.60
3:D:1336:LEU:HA	3:D:1344:VAL:HG22	1.83	0.60
5:F:317:LEU:O	5:F:329:TYR:HB3	2.01	0.60
2:M:212:GLY:HA3	2:M:218:VAL:HG23	1.82	0.60
2:M:571:LEU:HG	2:M:700:TYR:HA	1.83	0.60
2:M:674:VAL:HG23	2:M:869:VAL:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:752:GLY:H	2:M:792:VAL:HB	1.65	0.60
3:N:65:ARG:HB3	9:N:9605:HOH:O	2.01	0.60
3:N:73:CYS:HB3	3:N:76:CYS:O	2.02	0.60
3:N:210:ARG:NH1	3:N:398:ALA:HB3	2.07	0.60
3:N:402:PRO:HG2	3:N:444:VAL:HG11	1.83	0.60
3:N:704:ARG:CG	3:N:736:PHE:HB3	2.30	0.60
3:N:782:SER:O	3:N:786:ILE:HG13	2.02	0.60
3:N:1212:ALA:HB3	3:N:1213:ARG:HH21	1.66	0.60
3:N:1428:ALA:O	3:N:1431:THR:HG22	2.02	0.60
3:N:1459:LEU:HD22	3:N:1465:ASN:HD22	1.66	0.60
2:C:571:LEU:HD21	2:C:700:TYR:HD2	1.67	0.60
2:C:798:GLY:H	2:C:827:VAL:CG1	2.14	0.60
2:C:882:LEU:HD22	3:D:951:ILE:CD1	2.32	0.60
2:C:1052:MET:HE3	3:D:623:VAL:HG21	1.84	0.60
3:D:136:ASP:CB	3:D:137:PRO:HD3	2.31	0.60
1:L:41:ARG:HG2	1:L:177:VAL:HG21	1.84	0.60
1:L:212:ASN:O	1:L:215:VAL:HG22	2.01	0.60
2:M:256:TYR:CE1	2:M:293:PHE:HB2	2.37	0.60
2:M:609:ASN:HB2	9:M:9673:HOH:O	2.02	0.60
2:M:900:ARG:HD2	9:M:9963:HOH:O	2.02	0.60
2:M:1115:LEU:HD12	2:M:1115:LEU:N	2.17	0.60
3:N:964:LEU:HD22	3:N:1058:ARG:NH1	2.16	0.60
4:O:36:LYS:HB2	9:O:6252:HOH:O	2.01	0.60
4:O:76:GLY:N	4:O:79:LEU:HD22	2.16	0.60
2:C:269:LEU:HD12	2:C:288:ARG:N	2.16	0.60
2:C:740:GLU:HB2	9:C:2377:HOH:O	2.01	0.60
2:C:1086:ARG:HB3	2:C:1112:PHE:HE2	1.66	0.60
3:D:136:ASP:HB3	3:D:137:PRO:HD3	1.84	0.60
3:D:486:ARG:HH21	3:D:489:ARG:NH2	1.99	0.60
3:D:903:ASP:HA	9:D:9918:HOH:O	2.01	0.60
3:D:972:LEU:O	3:D:976:GLN:HG3	2.01	0.60
3:D:1082:ALA:O	3:D:1086:LEU:HD13	2.00	0.60
2:M:1115:LEU:HB3	3:N:85:VAL:HG12	1.83	0.60
3:N:831:GLY:HA3	9:N:9512:HOH:O	2.02	0.60
3:N:1491:THR:O	3:N:1495:ILE:HD13	2.00	0.60
1:A:213:GLN:O	1:A:217:ILE:HG13	2.02	0.60
1:B:38:ASN:OD1	2:C:979:THR:HA	2.02	0.60
2:C:395:LYS:HE3	2:C:407:LYS:HD2	1.83	0.60
2:C:470:PRO:HG2	2:C:538:GLN:OE1	2.02	0.60
9:C:9634:HOH:O	3:D:630:VAL:HG23	2.01	0.60
3:D:810:GLU:HA	3:D:813:LEU:HD23	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:149:GLY:O	1:K:171:PHE:HB2	2.02	0.60
2:M:776:SER:HB2	9:M:9826:HOH:O	2.01	0.60
3:N:183:GLU:HA	3:N:186:VAL:HG12	1.83	0.60
3:N:191:LEU:HD13	3:N:195:VAL:HG11	1.83	0.60
3:N:215:TYR:HB2	3:N:389:GLU:HA	1.84	0.60
3:N:631:ILE:O	3:N:632:VAL:HG23	2.02	0.60
5:P:415:THR:HB	9:P:3726:HOH:O	2.01	0.60
2:C:124:ASP:HB3	2:C:592:LEU:HD12	1.82	0.60
2:C:858:MET:SD	2:C:867:VAL:HG23	2.42	0.60
2:C:874:LEU:HD23	3:D:1023:MET:SD	2.42	0.60
2:C:1090:LYS:HE2	2:C:1112:PHE:CE1	2.37	0.60
3:D:569:ASN:OD1	5:F:80:PRO:HB3	2.02	0.60
3:D:965:GLU:HA	3:D:968:ASP:HB2	1.84	0.60
3:D:1468:LEU:HD13	3:D:1470:ARG:HD3	1.83	0.60
3:N:440:VAL:HG13	9:N:2153:HOH:O	2.01	0.60
3:N:502:PHE:CE1	3:N:509:PRO:HB3	2.37	0.60
3:N:1128:VAL:HG22	9:N:9749:HOH:O	2.00	0.60
1:A:36:LEU:O	1:A:39:PRO:HD2	2.02	0.59
1:A:150:TYR:HE1	2:C:696:LYS:HA	1.67	0.59
2:C:329:GLY:N	2:C:488:ALA:HB3	2.17	0.59
2:C:1000:MET:SD	2:C:1001:VAL:HG22	2.42	0.59
2:C:1043:TYR:HE2	3:D:768:ASN:OD1	1.85	0.59
2:C:1060:ILE:HD12	2:C:1063:ARG:NH1	2.15	0.59
3:D:61:GLY:HA3	3:D:64:LYS:HE3	1.84	0.59
3:D:702:LEU:HG	3:D:745:MET:HE3	1.83	0.59
3:D:844:ALA:O	3:D:867:ARG:HB3	2.01	0.59
3:D:1077:ALA:HB2	9:D:9550:HOH:O	2.02	0.59
3:D:1087:ARG:O	3:D:1091:SER:HB3	2.02	0.59
5:F:352:GLU:O	5:F:356:LYS:HG3	2.02	0.59
1:K:213:GLN:O	1:K:217:ILE:HG13	2.02	0.59
1:L:14:ARG:HB2	9:L:5263:HOH:O	2.02	0.59
2:M:66:LEU:HD22	2:M:372:LEU:HD23	1.83	0.59
2:M:500:ASN:HD21	3:N:1067:VAL:CG2	2.15	0.59
2:M:880:MET:HG2	3:N:1038:LEU:HD21	1.84	0.59
2:M:1024:LYS:HE2	9:M:9718:HOH:O	2.02	0.59
3:N:536:ALA:HA	5:P:315:VAL:O	2.02	0.59
3:N:543:LEU:O	3:N:546:ARG:HB2	2.02	0.59
3:N:898:GLU:HB2	3:N:921:ARG:NH2	2.16	0.59
3:N:1389:LEU:HD12	3:N:1390:LEU:H	1.67	0.59
4:O:25:LYS:HA	4:O:28:GLN:NE2	2.17	0.59
1:B:38:ASN:HB3	1:B:39:PRO:HD3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:LEU:HD12	1:B:114:PHE:CE1	2.37	0.59
1:B:151:VAL:HG22	1:B:155:LYS:HZ1	1.67	0.59
2:C:312:ALA:HB1	9:C:2264:HOH:O	2.03	0.59
3:D:703:ASN:ND2	3:D:704:ARG:H	2.00	0.59
3:D:1428:ALA:O	3:D:1431:THR:HG23	2.02	0.59
4:E:33:HIS:CD2	4:E:89:MET:HG2	2.37	0.59
1:K:218:LEU:O	1:K:222:LEU:HD23	2.02	0.59
3:N:774:SER:C	3:N:776:GLU:H	2.09	0.59
3:N:1000:THR:O	3:N:1003:VAL:HG22	2.02	0.59
1:B:58:ILE:HD13	1:B:140:MET:HB3	1.83	0.59
2:C:200:LEU:HB2	9:C:9888:HOH:O	2.02	0.59
2:C:1015:LEU:HD12	9:C:9604:HOH:O	2.01	0.59
3:D:9:ARG:HA	3:D:1434:TRP:CH2	2.38	0.59
3:D:75:ARG:HA	9:D:9977:HOH:O	2.02	0.59
3:D:98:PRO:HD3	9:D:9723:HOH:O	2.03	0.59
3:D:108:VAL:HB	3:D:109:PRO:HD3	1.83	0.59
3:D:537:THR:C	5:F:317:LEU:HB2	2.28	0.59
3:D:863:VAL:HA	9:D:9541:HOH:O	2.02	0.59
3:D:998:GLU:HA	9:D:9510:HOH:O	2.00	0.59
3:D:1243:THR:HB	3:D:1253:THR:HG22	1.83	0.59
9:K:3920:HOH:O	2:M:608:GLY:HA3	2.02	0.59
1:L:74:ASP:O	1:L:78:ILE:HG13	2.03	0.59
2:M:621:VAL:HG13	9:M:9824:HOH:O	2.02	0.59
3:N:133:ILE:HG21	3:N:454:ALA:CB	2.30	0.59
3:N:1146:GLY:HA3	3:N:1207:TYR:HB2	1.84	0.59
1:A:161:ARG:NH1	1:A:161:ARG:HB2	2.17	0.59
1:B:84:GLU:HG2	1:B:127:LEU:HD11	1.84	0.59
1:B:140:MET:HG2	9:B:9655:HOH:O	2.02	0.59
2:C:549:PHE:CD2	2:C:886:LEU:HB3	2.38	0.59
2:C:583:LEU:O	2:C:587:VAL:HG23	2.01	0.59
2:C:744:ARG:HG3	2:C:747:ALA:HB2	1.83	0.59
3:D:156:GLU:H	3:D:156:GLU:CD	2.10	0.59
3:D:813:LEU:O	3:D:817:GLU:HB2	2.02	0.59
5:F:402:ASN:O	5:F:406:ARG:HG3	2.01	0.59
1:K:11:PHE:CD1	1:L:225:PHE:HA	2.37	0.59
2:M:840:ALA:HB1	9:M:9563:HOH:O	2.01	0.59
3:N:1211:MET:SD	3:N:1213:ARG:HD2	2.41	0.59
3:N:1221:VAL:HB	9:N:9633:HOH:O	2.01	0.59
2:C:18:LEU:HD21	2:C:542:VAL:HG11	1.82	0.59
2:C:102:HIS:HB2	2:C:106:GLY:O	2.02	0.59
2:C:274:ARG:HB2	2:C:285:LEU:HD13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:595:LEU:HD11	9:C:9740:HOH:O	2.02	0.59
3:D:51:GLY:HA3	9:D:9784:HOH:O	2.02	0.59
3:D:530:VAL:HG11	9:F:9549:HOH:O	2.01	0.59
3:D:1119:SER:HA	3:D:1186:VAL:O	2.02	0.59
3:D:1145:TYR:HB2	3:D:1168:MET:HE1	1.83	0.59
1:L:90:LEU:HB3	9:L:4208:HOH:O	2.02	0.59
2:M:89:THR:HA	2:M:129:ILE:O	2.03	0.59
2:M:499:ALA:HA	9:M:2087:HOH:O	2.01	0.59
2:M:605:LYS:CB	2:M:610:ARG:HH12	2.03	0.59
3:N:8:VAL:HG11	9:N:9848:HOH:O	2.01	0.59
3:N:729:HIS:HE1	3:N:731:LEU:HG	1.66	0.59
3:N:950:GLY:O	3:N:953:ASP:N	2.31	0.59
3:N:975:GLU:HA	9:N:9710:HOH:O	2.03	0.59
3:N:1176:LYS:O	3:N:1176:LYS:HD3	2.02	0.59
3:N:1403:LEU:HD23	3:N:1407:LEU:HD22	1.83	0.59
1:A:226:SER:O	1:A:228:PRO:HD3	2.01	0.59
2:C:284:ARG:HG2	2:C:285:LEU:H	1.68	0.59
3:D:528:VAL:HG23	3:D:536:ALA:O	2.03	0.59
3:D:1420:LEU:HD12	3:D:1421:LEU:H	1.67	0.59
2:M:141:HIS:CE1	2:M:334:ARG:HE	2.20	0.59
2:M:333:ILE:HD13	2:M:467:ILE:HG13	1.85	0.59
2:M:617:ASP:HB2	9:M:2181:HOH:O	2.03	0.59
2:M:1042:ALA:HB3	3:N:710:ARG:HB3	1.84	0.59
2:C:383:ARG:HB2	2:C:383:ARG:CZ	2.31	0.59
3:D:793:THR:HG22	3:D:879:ARG:HA	1.84	0.59
4:E:48:MET:N	4:E:54:LEU:HB2	2.17	0.59
1:L:5:LYS:O	1:L:8:ALA:HB2	2.02	0.59
1:L:148:VAL:HG22	9:L:4917:HOH:O	2.02	0.59
2:M:689:VAL:CG2	2:M:870:ILE:HB	2.32	0.59
2:M:757:GLY:HA2	2:M:789:SER:HB3	1.85	0.59
3:N:546:ARG:HA	9:N:9543:HOH:O	2.01	0.59
3:N:573:MET:HG2	9:N:9529:HOH:O	2.01	0.59
3:N:1145:TYR:CD2	3:N:1168:MET:HE2	2.37	0.59
2:C:8:ARG:NH1	2:C:8:ARG:HB2	2.18	0.59
2:C:200:LEU:HD13	2:C:300:ASP:CG	2.28	0.59
2:C:276:LYS:O	2:C:280:LYS:HB2	2.02	0.59
3:D:139:GLY:O	3:D:147:VAL:HB	2.02	0.59
3:D:1124:GLN:HE21	3:D:1135:ARG:HA	1.67	0.59
3:D:1147:ARG:HB3	3:D:1188:VAL:CG2	2.32	0.59
3:D:1147:ARG:O	3:D:1166:LEU:HD23	2.02	0.59
1:K:9:PRO:HD2	1:L:224:TYR:CE1	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:94:LEU:HD21	1:L:119:ASP:HB2	1.84	0.59
2:M:260:LEU:HB2	2:M:291:ALA:HB1	1.85	0.59
2:M:541:SER:HB2	9:M:9944:HOH:O	2.03	0.59
3:N:884:ARG:HB2	9:N:2140:HOH:O	2.02	0.59
1:A:91:ASN:CG	1:A:92:PRO:HD2	2.27	0.59
2:C:6:PHE:HB2	9:C:2024:HOH:O	2.01	0.59
3:D:857:ILE:HA	9:D:2193:HOH:O	2.02	0.59
4:E:87:LYS:HB2	9:E:9519:HOH:O	2.01	0.59
5:F:256:ARG:CZ	5:F:260:ILE:HD12	2.32	0.59
1:K:36:LEU:O	1:K:39:PRO:HD2	2.03	0.59
1:L:18:ARG:NH2	1:L:123:MET:HE1	2.17	0.59
2:M:56:GLU:CG	2:M:64:LEU:HD23	2.33	0.59
3:N:59:ALA:HA	9:N:9941:HOH:O	2.02	0.59
3:N:172:PRO:HD2	3:N:389:GLU:O	2.03	0.59
3:N:441:ARG:O	3:N:443:VAL:HG23	2.02	0.59
3:N:820:GLU:HG2	3:N:825:ALA:O	2.03	0.59
3:N:1110:ALA:HB3	9:N:9637:HOH:O	2.01	0.59
4:O:48:MET:N	4:O:54:LEU:HB2	2.17	0.59
5:P:350:LEU:HA	9:P:3715:HOH:O	2.02	0.59
1:A:123:MET:C	1:A:125:PRO:HD3	2.28	0.59
1:B:194:LYS:HZ2	1:B:194:LYS:HB2	1.67	0.59
1:B:216:GLU:HB2	9:B:9598:HOH:O	2.03	0.59
2:C:376:ARG:HH22	5:F:285:GLU:HB3	1.67	0.59
2:C:708:TYR:HD1	2:C:708:TYR:H	1.49	0.59
2:C:874:LEU:HD21	3:D:787:LEU:CD2	2.32	0.59
3:D:817:GLU:HG2	3:D:840:LYS:NZ	2.17	0.59
3:D:1376:MET:HE3	3:D:1421:LEU:HA	1.85	0.59
5:F:85:LEU:HA	5:F:88:ILE:HD12	1.84	0.59
1:K:2:LEU:HD22	9:K:5005:HOH:O	2.03	0.59
1:K:94:LEU:HD11	1:K:119:ASP:HB3	1.84	0.59
1:L:137:ARG:NH1	1:L:137:ARG:HB3	2.18	0.59
2:M:129:ILE:HA	9:M:9795:HOH:O	2.02	0.59
2:M:139:GLN:HE22	2:M:415:PRO:HG2	1.68	0.59
2:M:437:ARG:NH1	2:M:488:ALA:HA	2.17	0.59
2:M:549:PHE:CD2	2:M:886:LEU:HB3	2.38	0.59
4:O:45:ARG:O	4:O:47:LYS:HE3	2.03	0.59
2:C:29:ALA:HB2	2:C:337:GLY:HA3	1.83	0.58
2:C:536:PRO:HD2	2:C:537:LYS:HD2	1.85	0.58
2:C:750:LYS:HD2	9:C:9787:HOH:O	2.02	0.58
2:C:1063:ARG:O	2:C:1066:ALA:HB3	2.02	0.58
3:D:116:LEU:HD23	3:D:468:LEU:HD11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:208:PRO:HB2	3:D:395:VAL:HG22	1.84	0.58
3:D:493:ARG:NH1	3:D:1390:LEU:HB2	2.17	0.58
3:N:1364:HIS:ND1	3:N:1366:LYS:HB2	2.18	0.58
5:P:385:GLU:O	5:P:397:ILE:HD13	2.03	0.58
2:C:655:LEU:HB2	9:C:9812:HOH:O	2.02	0.58
2:C:975:TYR:HA	2:C:982:PRO:HA	1.84	0.58
2:C:993:PHE:CE1	2:C:995:MET:HG2	2.37	0.58
2:C:1054:THR:HG22	2:C:1059:ASP:OD2	2.03	0.58
3:D:187:LYS:HD3	9:D:9662:HOH:O	2.01	0.58
3:D:908:LYS:CG	3:D:1027:GLY:HA3	2.33	0.58
3:D:1288:GLU:OE2	3:D:1289:LYS:HE3	2.03	0.58
5:F:404:ALA:HB3	9:F:9613:HOH:O	2.01	0.58
1:L:16:GLN:HB2	9:L:4742:HOH:O	2.01	0.58
3:N:422:ALA:H	3:N:427:VAL:CG1	2.16	0.58
3:N:1122:LEU:HD11	3:N:1186:VAL:HG23	1.84	0.58
3:N:1492:LEU:HD12	3:N:1493:LYS:NZ	2.18	0.58
5:P:88:ILE:CD1	5:P:193:ARG:HB2	2.31	0.58
5:P:96:LEU:HB2	9:P:5295:HOH:O	2.03	0.58
5:P:419:ARG:HG3	5:P:420:ASP:H	1.68	0.58
1:B:22:GLU:HG2	1:B:198:ARG:HG2	1.85	0.58
1:B:65:PHE:CD1	3:D:813:LEU:HD22	2.38	0.58
2:C:142:ARG:NH1	2:C:325:ILE:HG12	2.18	0.58
2:C:203:ASP:HB2	9:C:2302:HOH:O	2.03	0.58
2:C:431:HIS:CD2	2:C:433:THR:H	2.21	0.58
2:C:698:ASP:HA	9:C:9547:HOH:O	2.04	0.58
2:C:732:ALA:HB3	9:C:9678:HOH:O	2.04	0.58
3:D:101:HIS:CE1	3:D:582:LEU:HD22	2.38	0.58
3:D:601:ARG:NH2	3:D:612:GLY:HA2	2.19	0.58
3:D:671:LYS:HG2	9:F:9580:HOH:O	2.03	0.58
3:D:834:THR:HB	3:D:838:ARG:HB3	1.85	0.58
5:F:247:ILE:HG22	5:F:251:ILE:HD11	1.85	0.58
1:K:101:LEU:HD21	1:K:113:ASP:HB3	1.85	0.58
2:M:86:LYS:HE3	2:M:813:VAL:HG12	1.85	0.58
2:M:242:LEU:HD23	2:M:244:PRO:HD3	1.85	0.58
2:M:500:ASN:HB3	9:M:9721:HOH:O	2.03	0.58
9:M:9760:HOH:O	3:N:1047:LYS:HD3	2.03	0.58
3:N:177:ALA:HB1	3:N:199:LEU:HD22	1.84	0.58
3:N:440:VAL:HG23	9:N:9588:HOH:O	2.04	0.58
2:C:630:ARG:HA	2:C:705:ILE:HD11	1.85	0.58
3:D:148:GLU:HA	9:D:2669:HOH:O	2.03	0.58
3:D:704:ARG:NH1	3:D:738:ALA:HA	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1129:THR:HA	9:D:9663:HOH:O	2.03	0.58
3:D:1129:THR:HG22	9:D:2414:HOH:O	2.02	0.58
3:D:1136:LYS:HA	9:D:2534:HOH:O	2.03	0.58
3:D:1379:VAL:HG11	3:D:1395:LEU:HD23	1.85	0.58
9:D:2680:HOH:O	5:F:375:LEU:HD21	2.02	0.58
2:M:182:VAL:CG1	2:M:193:LEU:HD13	2.32	0.58
2:M:204:GLN:HB3	9:M:9981:HOH:O	2.03	0.58
2:M:263:ASP:HB2	2:M:264:PRO:HD3	1.85	0.58
3:N:211:VAL:HG13	3:N:393:ILE:HA	1.85	0.58
3:N:1262:LEU:CD2	3:N:1351:GLU:HG3	2.31	0.58
4:O:43:GLU:HG2	4:O:44:GLU:H	1.67	0.58
5:P:269:ASN:HB3	5:P:273:ARG:HH21	1.68	0.58
1:B:5:LYS:O	1:B:8:ALA:HB2	2.04	0.58
2:C:9:ILE:HG12	2:C:907:ASP:CG	2.29	0.58
2:C:104:ASP:HB2	9:C:9663:HOH:O	2.03	0.58
2:C:145:GLY:HA3	9:C:2408:HOH:O	2.04	0.58
2:C:816:LYS:HB2	2:C:819:VAL:HG21	1.84	0.58
5:F:205:ARG:HD2	5:F:251:ILE:HD13	1.85	0.58
5:F:393:THR:HG22	5:F:394:ARG:H	1.69	0.58
5:F:410:TYR:HD2	5:F:414:ARG:HH22	1.50	0.58
2:M:200:LEU:HD13	2:M:300:ASP:CG	2.28	0.58
2:M:890:LEU:HA	2:M:914:ILE:CD1	2.33	0.58
2:M:973:VAL:O	2:M:974:LEU:HD12	2.03	0.58
3:N:422:ALA:HB1	5:P:178:ARG:NH1	2.17	0.58
1:B:86:VAL:HA	9:B:9563:HOH:O	2.03	0.58
2:C:244:PRO:CD	2:C:245:GLY:H	2.15	0.58
2:C:838:LYS:HG3	2:C:997:LEU:HB2	1.85	0.58
3:D:380:GLU:O	3:D:382:GLU:N	2.36	0.58
3:D:574:LEU:O	3:D:578:VAL:HG23	2.03	0.58
3:D:759:ALA:HA	3:D:763:MET:HE2	1.84	0.58
3:D:788:GLY:O	3:D:792:ILE:HG22	2.02	0.58
3:D:804:LEU:HD23	3:D:804:LEU:H	1.68	0.58
3:D:1087:ARG:HA	3:D:1090:ASP:HB2	1.86	0.58
3:D:1146:GLY:HA3	3:D:1207:TYR:HB2	1.84	0.58
3:D:1279:GLY:O	3:D:1318:TYR:HA	2.03	0.58
2:M:525:SER:OG	2:M:528:GLU:HG3	2.04	0.58
2:M:672:VAL:CG2	2:M:868:ASP:HB2	2.33	0.58
3:N:104:PHE:CD2	3:N:1448:THR:HG23	2.38	0.58
3:N:470:LEU:HD23	9:N:9663:HOH:O	2.02	0.58
3:N:1441:GLN:NE2	3:N:1442:ASN:H	2.00	0.58
5:P:155:THR:HA	5:P:158:GLU:OE2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:291:ILE:O	5:P:295:MET:HB2	2.04	0.58
1:A:2:LEU:HB2	9:A:9681:HOH:O	2.03	0.58
2:C:15:LEU:HD13	2:C:583:LEU:HD11	1.85	0.58
2:C:176:VAL:C	2:C:178:PRO:HD3	2.28	0.58
2:C:469:THR:HG23	2:C:470:PRO:HD2	1.84	0.58
2:C:826:TYR:HD1	9:C:9672:HOH:O	1.85	0.58
3:D:996:TRP:CD2	3:D:1056:PRO:HG2	2.39	0.58
2:M:49:ARG:HH11	2:M:49:ARG:HB2	1.68	0.58
2:M:244:PRO:HG2	2:M:246:ASP:OD2	2.04	0.58
2:M:705:ILE:HD11	9:M:9812:HOH:O	2.03	0.58
2:M:1055:LEU:HD22	2:M:1066:ALA:HB2	1.84	0.58
3:N:616:GLN:OE1	3:N:619:LEU:HB3	2.03	0.58
3:N:805:GLU:HB3	9:N:9995:HOH:O	2.02	0.58
3:N:1102:THR:HG22	3:N:1222:GLY:HA2	1.84	0.58
5:P:260:ILE:HD11	5:P:310:ILE:CG2	2.32	0.58
5:P:294:ALA:HB2	9:P:3431:HOH:O	2.02	0.58
1:B:92:PRO:HA	1:B:146:ARG:NH1	2.18	0.58
2:C:497:ALA:HA	2:C:515:ALA:HA	1.86	0.58
2:C:526:PRO:HB2	9:C:9595:HOH:O	2.02	0.58
2:C:945:ARG:HB3	2:C:945:ARG:NH1	2.16	0.58
2:C:981:GLU:HG3	9:C:9552:HOH:O	2.04	0.58
2:C:1110:ASP:HA	9:C:9781:HOH:O	2.04	0.58
3:D:178:LEU:CD2	3:D:199:LEU:H	2.17	0.58
3:D:1372:VAL:HA	3:D:1375:MET:SD	2.44	0.58
5:F:370:LYS:HZ2	5:F:370:LYS:HB3	1.68	0.58
1:L:81:ASN:O	1:L:84:GLU:HB3	2.04	0.58
2:M:27:ARG:HD3	9:M:9741:HOH:O	2.03	0.58
2:M:49:ARG:HD3	9:M:9640:HOH:O	2.01	0.58
2:M:145:GLY:HA3	9:M:9769:HOH:O	2.02	0.58
2:M:772:ARG:HB2	2:M:772:ARG:NH1	2.19	0.58
2:M:1050:GLN:HG2	2:M:1079:PRO:HG2	1.85	0.58
3:N:119:SER:CB	3:N:123:LEU:HB2	2.34	0.58
3:N:462:GLN:HA	3:N:513:ILE:HD13	1.84	0.58
3:N:524:LEU:C	3:N:526:PRO:HD3	2.28	0.58
3:N:969:ARG:O	3:N:972:LEU:HB3	2.04	0.58
3:N:1119:SER:HA	3:N:1186:VAL:O	2.03	0.58
3:N:1124:GLN:N	3:N:1133:ARG:O	2.36	0.58
9:N:9535:HOH:O	5:P:326:ASP:HB2	2.03	0.58
1:B:14:ARG:HD2	9:B:9709:HOH:O	2.04	0.58
2:C:158:TYR:CE1	2:C:313:LEU:HG	2.38	0.58
2:C:302:VAL:C	2:C:305:PRO:HD2	2.29	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:679:PHE:C	3:D:943:THR:HG22	2.28	0.58
2:C:1003:ASP:HA	9:C:9634:HOH:O	2.04	0.58
3:D:139:GLY:H	3:D:147:VAL:HG21	1.69	0.58
3:D:211:VAL:HG22	3:D:393:ILE:HG23	1.85	0.58
3:D:1135:ARG:NH1	3:D:1357:ARG:HH22	2.02	0.58
3:D:1267:ARG:HH21	3:D:1331:ASP:CG	2.12	0.58
5:F:102:LEU:O	5:F:106:VAL:HG23	2.04	0.58
5:F:138:SER:O	5:F:141:VAL:HG12	2.04	0.58
2:M:841:ASN:OD1	2:M:845:ASN:HB3	2.04	0.58
9:M:2376:HOH:O	3:N:1079:LYS:HB2	2.04	0.58
3:N:535:PHE:CB	5:P:314:PRO:HB3	2.34	0.58
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.86	0.58
1:A:54:THR:HG22	1:A:158:ILE:HG13	1.85	0.58
1:B:47:SER:O	1:B:49:PRO:N	2.36	0.58
2:C:122:THR:HB	2:C:124:ASP:OD1	2.03	0.58
2:C:1115:LEU:HB3	3:D:85:VAL:HG13	1.85	0.58
3:D:131:LYS:HA	3:D:456:MET:HG3	1.85	0.58
3:D:476:GLU:HG2	9:D:9483:HOH:O	2.02	0.58
3:D:1198:TYR:OH	3:D:1432:LYS:HG2	2.04	0.58
1:K:117:VAL:HB	1:K:120:VAL:CG1	2.34	0.58
2:M:700:TYR:HB3	9:M:9662:HOH:O	2.04	0.58
2:M:755:LEU:HB2	2:M:790:LEU:HD22	1.85	0.58
2:M:846:LYS:HE3	9:M:9651:HOH:O	2.03	0.58
2:M:862:PRO:HA	2:M:975:TYR:CE1	2.38	0.58
2:M:913:GLU:HG3	9:M:9616:HOH:O	2.04	0.58
2:M:1037:VAL:HG13	2:M:1049:LEU:HD11	1.85	0.58
3:N:129:PHE:CE2	3:N:587:ARG:HD3	2.38	0.58
3:N:421:LEU:HD11	3:N:437:VAL:HG22	1.85	0.58
3:N:701:LEU:HD23	3:N:748:HIS:HB2	1.85	0.58
3:N:1213:ARG:HB2	3:N:1214:PRO:CD	2.33	0.58
2:C:601:GLY:HA2	2:C:616:GLU:HG2	1.85	0.57
2:C:694:LEU:HD11	2:C:868:ASP:HB3	1.85	0.57
2:C:802:ARG:HB2	9:C:9893:HOH:O	2.04	0.57
3:D:483:HIS:ND1	3:D:483:HIS:N	2.52	0.57
3:D:493:ARG:HH12	3:D:1390:LEU:H	1.51	0.57
4:E:26:ARG:HG2	4:E:67:GLU:OE1	2.03	0.57
5:F:136:LEU:HD12	5:F:137:GLY:N	2.19	0.57
1:L:226:SER:O	1:L:228:PRO:HD3	2.03	0.57
2:M:191:PHE:CZ	2:M:196:LEU:HB2	2.39	0.57
2:M:629:TYR:HB2	2:M:637:LEU:HG	1.86	0.57
3:N:105:VAL:HG13	3:N:124:GLU:OE1	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1280:VAL:HG22	9:N:9926:HOH:O	2.04	0.57
3:N:1475:GLY:O	3:N:1478:SER:HB3	2.04	0.57
4:O:70:THR:HG21	4:O:72:ARG:HH21	1.69	0.57
1:A:79:ILE:HD11	9:A:9511:HOH:O	2.04	0.57
1:A:80:LEU:HD22	9:A:9571:HOH:O	2.02	0.57
1:A:133:GLU:HB2	9:C:2067:HOH:O	2.04	0.57
1:A:158:ILE:HD13	9:A:9582:HOH:O	2.04	0.57
1:B:86:VAL:CG1	1:B:124:ASN:HD22	2.10	0.57
2:C:108:ILE:HD11	2:C:365:ASP:OD2	2.04	0.57
2:C:662:GLU:HG3	9:C:2147:HOH:O	2.04	0.57
2:C:720:GLU:HA	2:C:759:THR:O	2.04	0.57
3:D:1293:PHE:CD2	3:D:1302:GLU:HA	2.38	0.57
3:D:1376:MET:SD	3:D:1421:LEU:HD12	2.44	0.57
1:K:67:THR:HG21	2:M:609:ASN:HD21	1.69	0.57
3:N:181:ASP:OD2	3:N:199:LEU:HB2	2.05	0.57
3:N:408:GLU:HG3	9:N:9853:HOH:O	2.04	0.57
3:N:480:GLU:O	3:N:484:PRO:HD2	2.04	0.57
3:N:625:TYR:O	3:N:749:VAL:HG23	2.05	0.57
3:N:972:LEU:HD23	3:N:973:GLN:N	2.18	0.57
3:N:1109:GLU:OE1	3:N:1201:CYS:HB2	2.03	0.57
1:A:222:LEU:HD11	1:B:218:LEU:HD23	1.85	0.57
1:B:132:LEU:HD13	1:B:138:LEU:HD22	1.87	0.57
2:C:92:ALA:HB1	9:C:9550:HOH:O	2.03	0.57
2:C:99:GLN:HB2	9:C:2236:HOH:O	2.04	0.57
2:C:252:LYS:NZ	2:C:296:GLY:HA3	2.19	0.57
2:C:799:ILE:HB	9:C:9767:HOH:O	2.03	0.57
2:C:1005:MET:HB2	3:D:629:SER:HB2	1.85	0.57
3:D:137:PRO:HD2	3:D:453:ASP:CB	2.34	0.57
3:D:477:LEU:HD23	9:D:9483:HOH:O	2.03	0.57
3:D:704:ARG:HG2	3:D:736:PHE:HB3	1.84	0.57
3:D:1371:VAL:HG12	3:D:1375:MET:HE3	1.84	0.57
4:E:17:TYR:N	4:E:17:TYR:CD2	2.71	0.57
5:F:207:LEU:HB3	5:F:212:LEU:HG	1.86	0.57
5:F:369:LEU:HD23	9:F:9483:HOH:O	2.02	0.57
1:K:156:HIS:HD2	1:K:157:GLY:H	1.50	0.57
2:M:56:GLU:HG2	2:M:64:LEU:HD23	1.85	0.57
2:M:130:ASN:HB3	9:M:9727:HOH:O	2.04	0.57
2:M:798:GLY:H	2:M:827:VAL:HG11	1.68	0.57
3:N:572:ARG:NH2	5:P:83:GLN:HG3	2.13	0.57
3:N:584:ASN:CG	3:N:590:PRO:HD2	2.28	0.57
3:N:787:LEU:HD11	3:N:947:ILE:HG12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:804:LEU:HG	9:N:9546:HOH:O	2.04	0.57
5:P:264:MET:HE3	9:P:3779:HOH:O	2.03	0.57
5:P:408:LEU:O	5:P:412:GLU:HG2	2.03	0.57
1:A:72:LYS:HD2	1:A:73:GLU:OE2	2.05	0.57
2:C:101:ILE:HD12	2:C:107:LEU:HD13	1.86	0.57
2:C:897:LEU:HD23	2:C:899:GLN:NE2	2.19	0.57
3:D:369:ALA:HB3	9:D:2237:HOH:O	2.03	0.57
3:D:603:LEU:O	3:D:607:LEU:HD12	2.04	0.57
3:D:929:ARG:HD3	9:D:2352:HOH:O	2.04	0.57
1:K:20:TYR:CD2	1:K:21:GLY:N	2.73	0.57
1:L:36:LEU:HB3	9:L:4428:HOH:O	2.04	0.57
2:M:52:PHE:CG	2:M:68:PHE:HB2	2.39	0.57
2:M:269:LEU:HG	2:M:285:LEU:HD21	1.87	0.57
2:M:679:PHE:CD1	2:M:870:ILE:HD13	2.40	0.57
2:M:710:ILE:HD12	2:M:790:LEU:HB2	1.86	0.57
2:M:976:ASP:CB	2:M:979:THR:HG22	2.35	0.57
3:N:212:ARG:HD2	9:N:9862:HOH:O	2.03	0.57
3:N:950:GLY:C	3:N:952:ASP:N	2.58	0.57
3:N:1437:ALA:O	3:N:1446:VAL:HG21	2.04	0.57
5:P:419:ARG:HG3	5:P:420:ASP:N	2.20	0.57
1:A:114:PHE:HB3	9:A:9585:HOH:O	2.04	0.57
1:A:123:MET:O	1:A:125:PRO:HD3	2.04	0.57
1:A:222:LEU:HD12	1:B:215:VAL:CB	2.34	0.57
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.86	0.57
2:C:214:TYR:HD2	9:C:9769:HOH:O	1.87	0.57
2:C:598:GLU:O	2:C:651:LYS:HG3	2.04	0.57
2:C:841:ASN:HD21	2:C:845:ASN:N	2.03	0.57
3:D:817:GLU:O	3:D:821:VAL:HG23	2.04	0.57
3:D:1102:THR:HG22	3:D:1222:GLY:HA2	1.85	0.57
3:D:1431:THR:HG21	9:D:9888:HOH:O	2.04	0.57
3:D:1432:LYS:HZ1	3:D:1460:ILE:HG13	1.69	0.57
4:E:60:ALA:O	4:E:63:TRP:HB2	2.05	0.57
2:M:575:GLN:H	2:M:667:ALA:HB1	1.69	0.57
2:M:1114:GLY:N	2:M:1115:LEU:HD12	2.09	0.57
3:N:127:LEU:HD11	3:N:461:ILE:HD11	1.86	0.57
3:N:520:LEU:HD12	3:N:521:PRO:HD2	1.85	0.57
3:N:1281:VAL:HG23	3:N:1317:ASP:O	2.05	0.57
5:P:160:ASP:HB2	9:P:4343:HOH:O	2.03	0.57
1:A:107:LYS:HA	9:A:9530:HOH:O	2.03	0.57
2:C:580:MET:O	2:C:902:ILE:HA	2.04	0.57
2:C:643:VAL:HG13	2:C:647:GLN:OE1	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:57:GLU:CD	3:D:64:LYS:HE2	2.29	0.57
3:D:422:ALA:H	3:D:427:VAL:CG1	2.16	0.57
3:D:540:LEU:HD21	3:D:603:LEU:HD21	1.87	0.57
3:D:1289:LYS:HD2	9:D:9996:HOH:O	2.04	0.57
5:F:350:LEU:HD12	5:F:422:LEU:HD12	1.85	0.57
1:L:2:LEU:HD13	1:L:3:ASP:OD1	2.04	0.57
2:M:45:GLN:HG2	9:M:2429:HOH:O	2.03	0.57
2:M:274:ARG:HB2	2:M:285:LEU:HD13	1.87	0.57
2:M:838:LYS:HG3	2:M:997:LEU:HB2	1.87	0.57
2:M:841:ASN:C	2:M:841:ASN:HD22	2.12	0.57
2:M:1082:PRO:HA	9:M:9532:HOH:O	2.04	0.57
4:O:85:LEU:HD23	4:O:86:GLN:H	1.70	0.57
1:A:182:GLU:HG2	9:A:9502:HOH:O	2.03	0.57
2:C:208:ALA:O	2:C:218:VAL:HG21	2.05	0.57
3:D:1094:LEU:HB3	9:D:9776:HOH:O	2.04	0.57
5:F:205:ARG:HG2	9:F:9829:HOH:O	2.05	0.57
1:L:41:ARG:CZ	1:L:177:VAL:HG23	2.35	0.57
2:M:112:GLU:HG3	9:M:9726:HOH:O	2.03	0.57
2:M:143:SER:HB3	2:M:330:ASN:O	2.03	0.57
2:M:292:ARG:HD2	2:M:299:LYS:HG2	1.85	0.57
2:M:510:ALA:HB3	2:M:513:VAL:CG2	2.34	0.57
2:M:1104:GLU:HA	3:N:6:ARG:CD	2.35	0.57
3:N:119:SER:H	3:N:123:LEU:CD2	2.18	0.57
3:N:178:LEU:HD11	3:N:203:ALA:HB2	1.86	0.57
3:N:380:GLU:O	3:N:382:GLU:N	2.37	0.57
3:N:1103:HIS:HD2	3:N:1462:LEU:H	1.53	0.57
4:O:4:PRO:HG2	9:O:6061:HOH:O	2.05	0.57
5:P:223:ALA:HA	9:P:6226:HOH:O	2.05	0.57
2:C:599:GLU:HG2	2:C:600:ASP:N	2.20	0.57
2:C:837:ASP:OD1	2:C:996:LYS:HE3	2.04	0.57
2:C:882:LEU:HD22	3:D:951:ILE:HD13	1.86	0.57
3:D:658:LEU:HD11	3:D:674:ARG:HH11	1.69	0.57
5:F:361:LEU:HD12	5:F:408:LEU:HD11	1.87	0.57
1:K:227:ASN:HD22	1:K:227:ASN:N	2.01	0.57
2:M:49:ARG:HB2	2:M:49:ARG:NH1	2.20	0.57
3:N:820:GLU:HB2	3:N:836:VAL:HG11	1.87	0.57
4:O:48:MET:HB2	4:O:54:LEU:CD1	2.34	0.57
5:P:131:VAL:CG1	5:P:181:GLU:HG3	2.33	0.57
1:A:89:PHE:HE2	1:A:146:ARG:HD3	1.69	0.57
1:A:224:TYR:CD2	1:B:9:PRO:HG2	2.40	0.57
1:B:226:SER:O	1:B:228:PRO:HD3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:148:PHE:HZ	2:C:281:LEU:HD13	1.70	0.57
2:C:383:ARG:HB2	2:C:383:ARG:NH1	2.20	0.57
3:D:486:ARG:HA	3:D:489:ARG:HG2	1.87	0.57
3:D:572:ARG:NH2	5:F:83:GLN:HG3	2.20	0.57
3:D:650:LEU:HD13	3:D:688:TRP:HZ3	1.70	0.57
3:D:730:PRO:HA	3:D:733:CYS:SG	2.44	0.57
3:D:1236:LEU:HA	3:D:1359:GLN:OE1	2.04	0.57
3:D:1243:THR:OG1	3:D:1253:THR:HB	2.05	0.57
3:D:1304:LYS:HD2	9:D:2299:HOH:O	2.04	0.57
3:D:1350:GLU:O	3:D:1354:LYS:HG2	2.05	0.57
3:D:1353:GLN:HG3	9:D:2099:HOH:O	2.05	0.57
3:D:1393:GLN:HB2	3:D:1398:TRP:CZ2	2.39	0.57
3:D:1455:LYS:HD3	3:D:1456:LYS:N	2.19	0.57
1:L:209:GLU:HB3	9:L:3774:HOH:O	2.05	0.57
9:L:5963:HOH:O	3:N:721:VAL:HG12	2.05	0.57
2:M:147:TYR:HB3	2:M:323:ASP:OD2	2.05	0.57
3:N:875:THR:HG21	3:N:902:LEU:HD13	1.86	0.57
3:N:1090:ASP:O	3:N:1093:TYR:HB3	2.05	0.57
5:P:336:GLU:H	5:P:336:GLU:CD	2.12	0.57
2:C:64:LEU:HD13	2:C:359:MET:HG3	1.86	0.57
2:C:1071:ILE:HD13	3:D:655:PRO:HB3	1.87	0.57
2:M:736:ASP:HA	2:M:744:ARG:HD3	1.87	0.57
3:N:22:SER:HB3	9:N:9776:HOH:O	2.04	0.57
3:N:1049:SER:HB3	3:N:1051:GLU:OE2	2.04	0.57
5:P:256:ARG:HH12	5:P:313:GLU:HG2	1.70	0.57
1:A:198:ARG:C	1:A:199:ILE:HD12	2.31	0.56
2:C:513:VAL:HG23	9:C:2376:HOH:O	2.04	0.56
2:C:614:ARG:HG2	9:C:2116:HOH:O	2.04	0.56
3:D:191:LEU:HD22	3:D:195:VAL:HG21	1.87	0.56
3:D:399:ARG:HB2	3:D:444:VAL:HG13	1.86	0.56
5:F:166:LEU:O	5:F:171:LYS:HB2	2.04	0.56
2:M:439:CYS:SG	2:M:540:PHE:HB3	2.45	0.56
2:M:721:ARG:HG2	9:M:9686:HOH:O	2.05	0.56
4:O:66:LYS:HE3	9:O:4471:HOH:O	2.05	0.56
5:P:309:LYS:HA	5:P:312:GLN:HE21	1.70	0.56
5:P:403:LYS:HA	5:P:403:LYS:NZ	2.20	0.56
2:C:1076:VAL:HG23	3:D:752:SER:HA	1.87	0.56
3:D:81:THR:O	3:D:82:LYS:O	2.22	0.56
3:D:89:ARG:HA	9:D:9567:HOH:O	2.05	0.56
3:D:133:ILE:HG22	3:D:455:ARG:N	2.20	0.56
3:D:148:GLU:HG2	3:D:151:GLN:NE2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:470:LEU:HB2	3:D:503:LEU:HD11	1.87	0.56
3:D:510:GLU:O	3:D:513:ILE:HD12	2.05	0.56
3:D:695:ILE:HG21	3:D:720:LEU:HD11	1.87	0.56
3:D:967:ALA:O	3:D:995:LEU:HD21	2.04	0.56
3:D:1342:GLU:CD	3:D:1342:GLU:H	2.13	0.56
5:F:142:ARG:HB2	9:F:9491:HOH:O	2.05	0.56
5:F:208:SER:HA	9:F:9790:HOH:O	2.05	0.56
5:F:260:ILE:HG23	5:F:264:MET:HB2	1.85	0.56
1:K:20:TYR:HD2	1:K:21:GLY:N	2.03	0.56
2:M:231:PRO:HB2	9:M:9876:HOH:O	2.05	0.56
2:M:750:LYS:HG3	3:N:680:GLN:OE1	2.05	0.56
2:M:1079:PRO:HA	9:M:9805:HOH:O	2.05	0.56
3:N:395:VAL:HG23	9:N:2392:HOH:O	2.06	0.56
3:N:488:ARG:HB3	3:N:488:ARG:HH11	1.70	0.56
3:N:699:VAL:N	3:N:756:GLN:HE22	2.02	0.56
3:N:734:GLU:HB3	9:N:2085:HOH:O	2.04	0.56
3:N:1147:ARG:HB2	3:N:1166:LEU:HD21	1.86	0.56
3:N:1336:LEU:HD23	9:N:2315:HOH:O	2.04	0.56
3:N:1350:GLU:O	3:N:1354:LYS:HG2	2.04	0.56
5:P:299:TRP:HE3	9:P:3308:HOH:O	1.87	0.56
5:P:404:ALA:O	5:P:408:LEU:HD23	2.05	0.56
1:A:101:LEU:HD21	1:A:113:ASP:HB3	1.87	0.56
1:B:206:THR:CG2	1:B:209:GLU:H	2.19	0.56
2:C:172:ILE:H	2:C:172:ILE:HD12	1.70	0.56
2:C:332:ARG:NE	2:C:464:LEU:HD11	2.19	0.56
2:C:585:GLU:O	2:C:588:VAL:HG22	2.04	0.56
2:C:640:ARG:HH11	2:C:642:ARG:HH22	1.52	0.56
2:C:666:LEU:HD21	2:C:668:LEU:HD11	1.87	0.56
2:C:1101:THR:C	2:C:1102:LEU:HD12	2.30	0.56
9:C:9961:HOH:O	5:F:354:LEU:HD11	2.05	0.56
3:D:58:CYS:SG	3:D:59:ALA:N	2.78	0.56
3:D:486:ARG:HH21	3:D:489:ARG:CZ	2.18	0.56
3:D:512:MET:HE2	3:D:1452:ILE:HD11	1.88	0.56
3:D:607:LEU:HB3	3:D:614:PHE:HE2	1.70	0.56
3:D:1031:ASN:HB3	3:D:1034:GLN:CG	2.35	0.56
3:D:1087:ARG:HD3	3:D:1090:ASP:CB	2.34	0.56
3:D:1191:PRO:HB3	3:D:1370:ILE:HD13	1.87	0.56
3:D:1272:ALA:CA	3:D:1326:THR:HB	2.34	0.56
5:F:120:THR:HG22	5:F:122:LEU:HD13	1.87	0.56
5:F:401:GLU:O	5:F:405:LEU:HB2	2.05	0.56
1:K:5:LYS:O	1:K:8:ALA:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:145:GLY:O	2:M:163:ILE:HG23	2.04	0.56
2:M:516:ARG:NH1	3:N:1068:LEU:HD22	2.20	0.56
2:M:578:VAL:HG23	2:M:579:VAL:HG12	1.88	0.56
2:M:605:LYS:HD3	2:M:610:ARG:CZ	2.35	0.56
2:M:1008:ARG:NH1	2:M:1011:GLY:HA3	2.21	0.56
2:M:1063:ARG:O	2:M:1066:ALA:HB3	2.05	0.56
2:M:1085:PHE:CD2	3:N:1468:LEU:HA	2.40	0.56
3:N:80:VAL:HG12	3:N:81:THR:N	2.20	0.56
3:N:138:LYS:HA	9:N:9563:HOH:O	2.04	0.56
3:N:411:THR:HG23	3:N:429:SER:HB3	1.87	0.56
3:N:683:ILE:HG21	3:N:688:TRP:CZ3	2.41	0.56
3:N:865:THR:HG23	3:N:874:GLU:HG2	1.86	0.56
3:N:882:PHE:CE1	3:N:906:GLN:HG3	2.40	0.56
3:N:969:ARG:HB2	9:N:9844:HOH:O	2.05	0.56
3:N:1018:ASN:HB3	3:N:1021:TYR:HB3	1.87	0.56
3:N:1209:LEU:HD23	3:N:1210:SER:H	1.69	0.56
3:N:1279:GLY:O	3:N:1318:TYR:HA	2.05	0.56
3:N:1394:VAL:HG11	9:N:9728:HOH:O	2.04	0.56
5:P:289:GLU:O	5:P:293:GLU:HG3	2.05	0.56
5:P:355:GLU:HA	9:P:3471:HOH:O	2.05	0.56
5:P:401:GLU:O	5:P:405:LEU:HB2	2.05	0.56
1:B:57:TYR:HE1	1:B:163:ASN:HB2	1.69	0.56
1:B:150:TYR:CE2	3:D:857:ILE:HG13	2.40	0.56
2:C:275:TYR:CD2	2:C:276:LYS:HG3	2.41	0.56
3:D:424:GLY:HA2	3:D:435:VAL:O	2.05	0.56
3:D:1087:ARG:NH2	3:D:1238:MET:HB2	2.21	0.56
1:K:150:TYR:CE2	1:K:152:PRO:HG3	2.39	0.56
2:M:173:ASP:O	2:M:184:MET:HA	2.04	0.56
3:N:53:ILE:HG23	3:N:54:LYS:N	2.18	0.56
3:N:530:VAL:HG23	3:N:534:ARG:O	2.05	0.56
3:N:844:ALA:O	3:N:867:ARG:HB3	2.05	0.56
4:O:81:PRO:HB2	9:O:4797:HOH:O	2.05	0.56
5:P:230:LYS:HB2	9:P:4672:HOH:O	2.04	0.56
5:P:264:MET:O	5:P:267:THR:HB	2.05	0.56
2:C:227:PHE:HD2	2:C:230:ARG:HH21	1.54	0.56
2:C:338:GLU:HA	2:C:341:THR:HG22	1.88	0.56
2:C:498:GLN:NE2	3:D:1068:LEU:HD12	2.21	0.56
3:D:179:VAL:HG13	3:D:389:GLU:HG3	1.86	0.56
5:F:196:VAL:HG13	5:F:213:ILE:HD11	1.87	0.56
5:F:220:LEU:HD12	5:F:243:ILE:HD11	1.87	0.56
1:L:156:HIS:CE1	1:L:166:PRO:HB3	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:116:GLY:HA3	2:M:378:LEU:HD23	1.88	0.56
2:M:685:GLU:HG2	3:N:739:ASP:HB2	1.87	0.56
2:M:742:VAL:HG12	2:M:743:VAL:N	2.21	0.56
2:M:1071:ILE:HG13	9:M:9978:HOH:O	2.03	0.56
3:N:788:GLY:O	3:N:792:ILE:HG22	2.05	0.56
3:N:804:LEU:HD23	3:N:804:LEU:H	1.71	0.56
3:N:1122:LEU:O	3:N:1134:LEU:HD12	2.05	0.56
4:O:94:PRO:HA	9:O:5690:HOH:O	2.05	0.56
5:P:407:LYS:HA	9:P:3848:HOH:O	2.05	0.56
1:A:81:ASN:HA	1:A:84:GLU:OE2	2.06	0.56
2:C:89:THR:HA	2:C:129:ILE:O	2.06	0.56
2:C:114:PHE:H	2:C:114:PHE:HD1	1.53	0.56
2:C:565:GLN:HA	2:C:995:MET:HE1	1.87	0.56
2:C:648:ARG:HB3	9:C:2219:HOH:O	2.06	0.56
2:C:837:ASP:HA	2:C:999:HIS:HE1	1.71	0.56
2:C:1050:GLN:HG2	2:C:1079:PRO:HG2	1.88	0.56
3:D:10:ILE:HG13	3:D:1434:TRP:CE2	2.40	0.56
3:D:171:LEU:HB2	3:D:390:PRO:HA	1.86	0.56
3:D:901:GLN:HB2	9:D:2047:HOH:O	2.06	0.56
3:D:1091:SER:HA	9:D:2229:HOH:O	2.06	0.56
5:F:291:ILE:O	5:F:295:MET:HB2	2.06	0.56
2:M:41:ASN:HB2	9:M:2429:HOH:O	2.04	0.56
2:M:139:GLN:HG2	2:M:140:ILE:H	1.70	0.56
2:M:176:VAL:C	2:M:178:PRO:HD3	2.31	0.56
2:M:257:VAL:HG13	9:M:9572:HOH:O	2.06	0.56
3:N:570:GLU:OE2	5:P:214:GLN:HG3	2.05	0.56
3:N:661:MET:HG2	3:N:666:ILE:HD12	1.87	0.56
3:N:699:VAL:H	3:N:756:GLN:HE22	1.52	0.56
3:N:864:VAL:HG12	3:N:865:THR:H	1.68	0.56
3:N:1147:ARG:O	3:N:1166:LEU:HD23	2.05	0.56
5:P:226:LYS:HE3	9:P:4530:HOH:O	2.05	0.56
1:B:2:LEU:HD12	1:B:3:ASP:N	2.20	0.56
2:C:251:ASP:HB3	2:C:252:LYS:HD2	1.87	0.56
2:C:257:VAL:HG21	9:C:2339:HOH:O	2.05	0.56
3:D:68:PHE:HE2	9:D:2680:HOH:O	1.88	0.56
3:D:699:VAL:HG12	3:D:717:GLN:HG3	1.86	0.56
3:D:842:VAL:HG22	9:D:2270:HOH:O	2.05	0.56
3:D:963:TYR:CE2	3:D:1002:LYS:HB3	2.41	0.56
3:D:1366:LYS:O	3:D:1369:GLU:HB2	2.06	0.56
4:E:95:GLY:HA3	9:E:9521:HOH:O	2.05	0.56
1:K:58:ILE:HG21	1:K:68:ILE:HD11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:276:LYS:O	2:M:280:LYS:HB2	2.05	0.56
2:M:484:VAL:HA	9:M:9777:HOH:O	2.06	0.56
2:M:589:ARG:HH11	2:M:589:ARG:CB	2.17	0.56
2:M:789:SER:O	2:M:791:ARG:HG2	2.06	0.56
3:N:148:GLU:CB	3:N:151:GLN:HB2	2.34	0.56
3:N:714:GLN:HB2	3:N:736:PHE:HZ	1.71	0.56
3:N:814:ALA:HB2	9:N:9921:HOH:O	2.06	0.56
3:N:1429:LEU:HG	3:N:1441:GLN:HG3	1.88	0.56
3:N:1495:ILE:HG23	9:N:9711:HOH:O	2.06	0.56
5:P:323:ASP:C	5:P:325:LYS:H	2.14	0.56
1:A:128:HIS:HB2	9:A:9508:HOH:O	2.06	0.56
2:C:100:LEU:HD12	2:C:101:ILE:O	2.06	0.56
2:C:606:VAL:CG2	2:C:645:VAL:HG22	2.35	0.56
2:C:630:ARG:HH22	2:C:707:ARG:N	2.04	0.56
2:C:965:GLU:HG2	9:C:2373:HOH:O	2.06	0.56
2:C:1003:ASP:O	2:C:1005:MET:N	2.38	0.56
3:D:132:TYR:HA	9:D:9863:HOH:O	2.06	0.56
3:D:135:LEU:HD11	3:D:139:GLY:HA3	1.86	0.56
3:D:488:ARG:HG2	9:D:9629:HOH:O	2.06	0.56
3:D:799:LYS:H	3:D:826:PRO:HG2	1.71	0.56
3:D:971:LEU:O	3:D:975:GLU:HG3	2.06	0.56
5:F:234:LYS:CD	5:F:236:SER:HB3	2.35	0.56
5:F:385:GLU:O	5:F:397:ILE:HD13	2.05	0.56
5:F:418:LEU:HB2	9:F:9856:HOH:O	2.06	0.56
1:K:106:PRO:HD3	9:K:4154:HOH:O	2.06	0.56
3:N:1301:LYS:HD2	9:N:2174:HOH:O	2.05	0.56
1:A:7:LYS:HG3	9:A:9524:HOH:O	2.05	0.56
1:B:25:LEU:HD23	1:B:28:LEU:HD21	1.87	0.56
2:C:36:PRO:HB2	2:C:70:GLU:HG2	1.88	0.56
2:C:54:ILE:HB	9:C:9495:HOH:O	2.05	0.56
2:C:57:GLU:HB3	9:C:9973:HOH:O	2.05	0.56
2:C:265:ARG:HA	9:C:9902:HOH:O	2.04	0.56
3:D:33:ASN:HA	9:F:9729:HOH:O	2.05	0.56
3:D:142:LEU:HA	9:D:9874:HOH:O	2.05	0.56
3:D:790:TYR:HD2	3:D:906:GLN:O	1.89	0.56
3:D:1289:LYS:HB3	9:D:2542:HOH:O	2.06	0.56
3:D:1334:GLN:HA	9:D:9693:HOH:O	2.05	0.56
3:D:1335:LEU:HD21	9:D:9614:HOH:O	2.05	0.56
5:F:191:ASN:CA	5:F:194:LEU:HD23	2.34	0.56
1:L:137:ARG:HB3	1:L:137:ARG:HH11	1.71	0.56
2:M:442:GLU:HG3	9:M:9719:HOH:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:551:GLU:HA	2:M:906:PHE:CE2	2.41	0.56
3:N:68:PHE:O	3:N:71:LYS:HG2	2.05	0.56
3:N:161:LEU:HD22	3:N:452:ILE:HG21	1.88	0.56
3:N:574:LEU:O	3:N:578:VAL:HG23	2.05	0.56
3:N:1003:VAL:O	3:N:1007:VAL:HG13	2.06	0.56
3:N:1112:CYS:HB2	3:N:1195:GLN:CD	2.30	0.56
3:N:1204:CYS:HB3	9:N:9589:HOH:O	2.05	0.56
2:C:358:ARG:NH2	2:C:374:ASN:HB3	2.15	0.56
2:C:838:LYS:HD2	2:C:997:LEU:HD12	1.86	0.56
2:C:879:ARG:HB2	9:C:9557:HOH:O	2.06	0.56
3:D:126:VAL:HG12	3:D:132:TYR:HB2	1.88	0.56
3:D:192:ALA:O	3:D:195:VAL:HG23	2.05	0.56
3:D:724:GLN:C	3:D:724:GLN:HE21	2.13	0.56
3:D:806:PHE:CZ	3:D:813:LEU:HB3	2.40	0.56
3:D:1311:LEU:HD23	3:D:1311:LEU:H	1.71	0.56
4:E:26:ARG:O	4:E:29:GLN:HG3	2.06	0.56
4:E:64:ALA:HA	4:E:67:GLU:CD	2.31	0.56
5:F:234:LYS:HD3	5:F:236:SER:HB3	1.88	0.56
9:K:6004:HOH:O	1:L:43:ILE:HD13	2.05	0.56
2:M:145:GLY:C	2:M:163:ILE:HG23	2.31	0.56
2:M:1008:ARG:HD2	3:N:624:ASP:O	2.06	0.56
3:N:783:ARG:HE	3:N:1029:ARG:CD	2.18	0.56
3:N:949:ILE:HD11	3:N:1023:MET:CE	2.36	0.56
3:N:1280:VAL:O	3:N:1294:VAL:HA	2.06	0.56
2:C:236:ILE:HG13	9:C:9904:HOH:O	2.05	0.55
2:C:426:ASP:OD1	2:C:427:VAL:HG23	2.05	0.55
3:D:98:PRO:HG3	3:D:515:GLU:HB3	1.88	0.55
3:D:502:PHE:CE1	3:D:509:PRO:HB3	2.40	0.55
3:D:704:ARG:HD3	3:D:738:ALA:HB2	1.88	0.55
3:D:999:THR:O	3:D:1002:LYS:HB2	2.06	0.55
3:D:1209:LEU:HD22	3:D:1211:MET:CE	2.36	0.55
3:D:1369:GLU:O	3:D:1372:VAL:HG12	2.05	0.55
5:F:81:VAL:O	5:F:85:LEU:HG	2.06	0.55
1:L:103:ALA:HA	9:L:4911:HOH:O	2.06	0.55
1:L:206:THR:HG22	1:L:209:GLU:HG3	1.88	0.55
2:M:61:LYS:HD2	9:M:9929:HOH:O	2.06	0.55
2:M:206:THR:O	2:M:210:GLU:HG3	2.05	0.55
2:M:911:GLU:O	2:M:915:LYS:HG2	2.06	0.55
3:N:399:ARG:HB3	3:N:402:PRO:HG3	1.88	0.55
3:N:434:ARG:HB2	3:N:447:VAL:HG13	1.88	0.55
3:N:787:LEU:HD21	3:N:947:ILE:HD11	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1103:HIS:CD2	3:N:1463:LYS:H	2.24	0.55
3:N:1273:VAL:O	3:N:1325:LEU:HB2	2.06	0.55
3:N:1278:ASP:HB2	3:N:1318:TYR:HE1	1.70	0.55
5:P:195:VAL:HG11	5:P:217:ASN:OD1	2.06	0.55
1:B:73:GLU:HB3	1:B:77:GLU:HG2	1.86	0.55
2:C:269:LEU:O	2:C:269:LEU:HD23	2.06	0.55
2:C:292:ARG:HD2	2:C:299:LYS:CE	2.35	0.55
2:C:724:ARG:NH2	2:C:734:LEU:HB3	2.20	0.55
3:D:709:HIS:HE2	3:D:711:LEU:HB2	1.71	0.55
3:D:737:ASN:HA	9:D:9487:HOH:O	2.05	0.55
1:K:181:VAL:HG11	9:K:3503:HOH:O	2.05	0.55
1:K:227:ASN:HB2	9:K:5811:HOH:O	2.05	0.55
2:M:208:ALA:O	2:M:218:VAL:HG21	2.06	0.55
2:M:471:TYR:CE2	2:M:496:ILE:HG21	2.41	0.55
2:M:577:PRO:HA	2:M:993:PHE:HD2	1.72	0.55
2:M:748:GLU:HG3	9:M:2069:HOH:O	2.05	0.55
2:M:772:ARG:HE	5:P:373:LYS:HD2	1.70	0.55
2:M:772:ARG:NE	5:P:373:LYS:HD2	2.21	0.55
2:M:957:LYS:HG2	9:M:9678:HOH:O	2.05	0.55
2:M:1090:LYS:HE2	2:M:1112:PHE:HE1	1.71	0.55
3:N:390:PRO:HG2	9:N:2717:HOH:O	2.06	0.55
3:N:1401:GLU:OE1	3:N:1415:VAL:HG11	2.06	0.55
3:N:1459:LEU:HD22	3:N:1465:ASN:ND2	2.20	0.55
5:P:82:ARG:HG3	5:P:86:HIS:CE1	2.41	0.55
5:P:167:PRO:HB2	5:P:169:GLU:OE2	2.05	0.55
5:P:304:VAL:HG22	9:P:3308:HOH:O	2.06	0.55
2:C:115:LEU:HD22	2:C:373:VAL:HG11	1.88	0.55
2:C:758:ARG:HB3	2:C:788:THR:O	2.07	0.55
2:C:811:PRO:HD3	9:C:9578:HOH:O	2.05	0.55
2:C:976:ASP:CB	2:C:979:THR:HG22	2.37	0.55
2:C:1086:ARG:HH11	3:D:88:TYR:HE1	1.54	0.55
3:D:121:THR:HG23	9:D:2262:HOH:O	2.06	0.55
3:D:966:GLU:O	3:D:969:ARG:HG2	2.06	0.55
3:D:1004:THR:O	3:D:1007:VAL:HG22	2.06	0.55
3:D:1066:THR:CG2	3:D:1069:GLU:H	2.19	0.55
3:D:1097:LYS:HD3	9:D:9906:HOH:O	2.07	0.55
3:D:1364:HIS:NE2	3:D:1366:LYS:HE3	2.22	0.55
5:F:278:LEU:HD22	5:F:290:GLU:HB3	1.88	0.55
1:K:122:ILE:HD12	9:K:4736:HOH:O	2.05	0.55
2:M:18:LEU:HB2	2:M:590:ASP:HB3	1.87	0.55
2:M:1027:PHE:HA	9:M:9907:HOH:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:397:LYS:HB2	9:N:2381:HOH:O	2.05	0.55
3:N:1341:PRO:O	3:N:1344:VAL:HG23	2.06	0.55
1:A:75:VAL:N	9:A:9598:HOH:O	2.39	0.55
1:A:212:ASN:O	1:A:215:VAL:HG22	2.06	0.55
2:C:479:VAL:HG23	2:C:506:ASN:HA	1.88	0.55
2:C:555:ALA:HA	3:D:1070:TYR:OH	2.07	0.55
2:C:1015:LEU:HD22	5:F:333:ILE:HG21	1.88	0.55
3:D:698:LYS:HA	9:E:9480:HOH:O	2.06	0.55
3:D:959:GLU:H	3:D:959:GLU:CD	2.12	0.55
3:D:1094:LEU:HD23	3:D:1230:GLY:HA2	1.87	0.55
5:F:247:ILE:O	5:F:251:ILE:HG13	2.06	0.55
1:K:42:ARG:NH1	2:M:857:ASP:HB3	2.17	0.55
2:M:12:VAL:HG13	2:M:13:ILE:HG23	1.89	0.55
2:M:41:ASN:O	2:M:46:ALA:HB2	2.06	0.55
2:M:52:PHE:CE1	2:M:66:LEU:HG	2.42	0.55
2:M:239:PHE:CZ	2:M:254:VAL:HB	2.40	0.55
2:M:252:LYS:NZ	2:M:296:GLY:HA3	2.22	0.55
3:N:208:PRO:HB2	3:N:395:VAL:HG13	1.87	0.55
4:O:76:GLY:HA3	4:O:79:LEU:HD13	1.89	0.55
1:B:10:VAL:HG12	1:B:12:THR:HG23	1.87	0.55
2:C:198:ARG:NH2	2:C:203:ASP:HB3	2.22	0.55
2:C:460:ARG:HD2	2:C:485:TYR:CE2	2.41	0.55
2:C:544:THR:O	2:C:547:ILE:HG13	2.06	0.55
2:C:808:ARG:HG2	9:C:9965:HOH:O	2.05	0.55
3:D:119:SER:CB	3:D:123:LEU:HB2	2.37	0.55
3:D:536:ALA:HA	9:F:9527:HOH:O	2.07	0.55
3:D:764:LEU:HB3	9:D:9549:HOH:O	2.07	0.55
5:F:195:VAL:HG11	5:F:217:ASN:OD1	2.07	0.55
5:F:357:ALA:HA	9:F:9770:HOH:O	2.07	0.55
1:K:42:ARG:HG2	1:K:42:ARG:HH11	1.70	0.55
1:L:59:GLU:HG3	1:L:139:ASN:HB3	1.88	0.55
2:M:197:LEU:HD12	2:M:207:LEU:HD11	1.89	0.55
2:M:567:GLN:HB2	2:M:997:LEU:HD22	1.88	0.55
2:M:953:VAL:HG13	2:M:966:LEU:HD22	1.89	0.55
2:M:975:TYR:HA	2:M:982:PRO:HA	1.88	0.55
9:N:9664:HOH:O	4:O:5:GLY:HA2	2.06	0.55
5:P:278:LEU:HB2	5:P:286:PRO:HG2	1.88	0.55
1:B:95:GLN:HA	1:B:146:ARG:HD2	1.87	0.55
2:C:41:ASN:O	2:C:46:ALA:HB2	2.07	0.55
2:C:704:HIS:CD2	2:C:831:ARG:HH21	2.24	0.55
2:C:885:ILE:HD12	3:D:949:ILE:HB	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:18:ILE:HG21	3:D:516:ALA:O	2.07	0.55
3:D:135:LEU:CD1	3:D:147:VAL:HG23	2.37	0.55
3:D:462:GLN:HB3	9:D:9482:HOH:O	2.06	0.55
3:D:572:ARG:NH2	5:F:83:GLN:HE21	1.97	0.55
3:D:1412:LYS:HG2	3:D:1414:PRO:HG3	1.89	0.55
2:M:769:PRO:HB2	3:N:65:ARG:NH2	2.21	0.55
2:M:1104:GLU:HG3	3:N:6:ARG:HD2	1.88	0.55
3:N:104:PHE:CE2	3:N:1448:THR:HG23	2.41	0.55
3:N:434:ARG:HB2	3:N:447:VAL:CG2	2.35	0.55
3:N:679:ARG:HD3	3:N:682:ASP:OD2	2.06	0.55
5:P:135:ILE:O	5:P:135:ILE:HD13	2.06	0.55
1:A:191:ASP:O	1:A:192:LEU:HD23	2.07	0.55
1:B:65:PHE:HD1	3:D:813:LEU:HD22	1.72	0.55
1:B:132:LEU:HD22	9:B:9571:HOH:O	2.05	0.55
2:C:264:PRO:HB2	9:C:9939:HOH:O	2.07	0.55
3:D:785:ILE:H	3:D:785:ILE:HD12	1.72	0.55
3:D:823:LEU:HG	9:D:9683:HOH:O	2.07	0.55
2:M:26:TYR:O	2:M:30:LEU:HD12	2.06	0.55
2:M:462:ASP:HB3	2:M:468:ARG:CD	2.33	0.55
3:N:46:ASP:HB3	3:N:49:ILE:HG13	1.88	0.55
3:N:75:ARG:HH11	3:N:75:ARG:HG3	1.72	0.55
3:N:911:LEU:O	3:N:915:VAL:HG23	2.07	0.55
5:P:172:ARG:O	5:P:176:ILE:HD13	2.07	0.55
1:A:156:HIS:CD2	1:A:158:ILE:HG12	2.42	0.55
1:B:73:GLU:HB3	1:B:77:GLU:HG3	1.88	0.55
1:B:81:ASN:O	1:B:84:GLU:HB3	2.06	0.55
1:B:94:LEU:HD11	1:B:119:ASP:HB3	1.88	0.55
2:C:396:ASP:HA	2:C:633:GLN:HE22	1.72	0.55
2:C:529:VAL:HG21	9:C:9927:HOH:O	2.05	0.55
2:C:674:VAL:HG23	2:C:869:VAL:O	2.06	0.55
2:C:724:ARG:CD	2:C:740:GLU:HA	2.37	0.55
3:D:9:ARG:NH1	3:D:506:GLY:HA2	2.20	0.55
3:D:28:LYS:CB	3:D:41:ARG:HD2	2.37	0.55
3:D:145:VAL:HB	9:D:9524:HOH:O	2.05	0.55
3:D:1206:GLY:HA3	3:D:1366:LYS:NZ	2.22	0.55
3:D:1271:LYS:HG2	9:D:2043:HOH:O	2.06	0.55
2:M:549:PHE:CE2	2:M:886:LEU:HB3	2.42	0.55
2:M:1097:LEU:HD13	2:M:1097:LEU:N	2.22	0.55
3:N:28:LYS:HB2	3:N:41:ARG:HD2	1.89	0.55
3:N:630:VAL:HA	3:N:744:GLN:HG2	1.88	0.55
3:N:1220:ALA:HB1	3:N:1223:ILE:CD1	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:164:LYS:HA	5:P:171:LYS:HE3	1.88	0.55
5:P:234:LYS:HD3	5:P:236:SER:H	1.72	0.55
5:P:247:ILE:HG22	5:P:251:ILE:HD11	1.89	0.55
5:P:412:GLU:HG3	5:P:418:LEU:HD22	1.88	0.55
2:C:575:GLN:HB2	2:C:670:GLN:HG2	1.87	0.55
2:C:575:GLN:N	2:C:667:ALA:HB1	2.20	0.55
2:C:860:HIS:NE2	2:C:975:TYR:HB2	2.22	0.55
2:C:874:LEU:HD12	3:D:784:ASP:OD2	2.06	0.55
2:C:976:ASP:OD1	2:C:978:ARG:HD3	2.07	0.55
3:D:421:LEU:HD12	3:D:435:VAL:HG11	1.88	0.55
3:D:1101:VAL:HG22	3:D:1428:ALA:HB2	1.88	0.55
3:D:1115:THR:HG23	9:D:2006:HOH:O	2.06	0.55
3:D:1382:THR:HG21	3:D:1418:LYS:HE3	1.88	0.55
5:F:136:LEU:HB3	5:F:185:GLN:HE22	1.71	0.55
5:F:416:ARG:HB2	9:F:9697:HOH:O	2.06	0.55
1:L:41:ARG:HG3	9:L:4703:HOH:O	2.06	0.55
2:M:9:ILE:O	2:M:9:ILE:HG13	2.07	0.55
2:M:251:ASP:HB3	2:M:252:LYS:HD2	1.89	0.55
2:M:411:SER:OG	2:M:452:ILE:HG23	2.06	0.55
2:M:1048:THR:O	2:M:1052:MET:HE2	2.06	0.55
2:M:1117:SER:HB2	9:M:2359:HOH:O	2.07	0.55
3:N:424:GLY:HA3	9:N:2149:HOH:O	2.07	0.55
3:N:709:HIS:N	3:N:709:HIS:ND1	2.55	0.55
5:P:184:ARG:O	5:P:188:ILE:HG13	2.07	0.55
5:P:217:ASN:O	5:P:221:ILE:HG13	2.07	0.55
5:P:416:ARG:NH1	5:P:419:ARG:HB3	2.22	0.55
2:C:64:LEU:HA	9:C:9791:HOH:O	2.07	0.55
2:C:626:ARG:HH11	2:C:626:ARG:HB2	1.71	0.55
2:C:817:PRO:HB3	5:F:305:GLU:OE2	2.07	0.55
2:C:831:ARG:HA	9:C:9771:HOH:O	2.06	0.55
3:D:668:PRO:HD2	3:D:672:ALA:CB	2.37	0.55
5:F:323:ASP:C	5:F:325:LYS:H	2.15	0.55
1:K:123:MET:C	1:K:125:PRO:HD3	2.32	0.55
2:M:64:LEU:HD12	2:M:65:VAL:N	2.22	0.55
2:M:78:PHE:HB2	2:M:88:LEU:HD21	1.87	0.55
2:M:157:ARG:HD3	2:M:158:TYR:H	1.72	0.55
2:M:232:GLU:HG2	9:M:2023:HOH:O	2.07	0.55
2:M:244:PRO:HD2	2:M:245:GLY:H	1.72	0.55
2:M:363:SER:HB3	9:M:9637:HOH:O	2.06	0.55
3:N:119:SER:N	3:N:123:LEU:HB2	2.21	0.55
3:N:865:THR:CG2	3:N:874:GLU:HG2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:879:ARG:HH21	3:N:903:ASP:C	2.14	0.55
3:N:1281:VAL:HG21	3:N:1313:VAL:HG21	1.88	0.55
5:P:136:LEU:HB3	5:P:185:GLN:HE22	1.71	0.55
5:P:222:ARG:HH12	5:P:246:ALA:HB2	1.71	0.55
1:B:27:PRO:O	1:B:28:LEU:HD23	2.07	0.54
2:C:209:ARG:N	2:C:209:ARG:HD2	2.22	0.54
2:C:432:ARG:HG2	9:C:9920:HOH:O	2.06	0.54
2:C:1115:LEU:HD12	2:C:1115:LEU:N	2.22	0.54
3:D:148:GLU:CB	3:D:151:GLN:HB2	2.33	0.54
3:D:675:ARG:HD3	9:D:2158:HOH:O	2.06	0.54
4:E:92:ILE:HG21	9:E:9509:HOH:O	2.07	0.54
1:K:133:GLU:CD	2:M:605:LYS:HB3	2.33	0.54
1:L:39:PRO:O	1:L:43:ILE:HG12	2.08	0.54
2:M:144:PRO:HG3	9:M:9535:HOH:O	2.07	0.54
2:M:165:LEU:HD11	9:M:2143:HOH:O	2.07	0.54
2:M:580:MET:HB3	2:M:584:GLU:CD	2.30	0.54
3:N:12:LEU:HD22	3:N:511:TRP:HB2	1.89	0.54
3:N:71:LYS:HE3	9:N:9778:HOH:O	2.06	0.54
3:N:483:HIS:HB2	3:N:484:PRO:HD3	1.88	0.54
3:N:1011:PHE:HB3	3:N:1021:TYR:CD1	2.42	0.54
5:P:152:ASP:HB2	5:P:153:PRO:HD3	1.88	0.54
5:P:185:GLN:O	5:P:189:GLU:HG3	2.07	0.54
2:C:72:ARG:HH11	2:C:72:ARG:HG3	1.71	0.54
2:C:290:LEU:HB3	2:C:302:VAL:HG11	1.89	0.54
2:C:522:VAL:HG12	2:C:524:VAL:HG23	1.88	0.54
2:C:612:VAL:HG22	2:C:622:GLU:HA	1.89	0.54
3:D:119:SER:H	3:D:123:LEU:HD13	1.72	0.54
3:D:207:PHE:CB	3:D:208:PRO:HD2	2.34	0.54
3:D:519:VAL:HG13	3:D:544:TYR:CZ	2.42	0.54
3:D:775:GLY:HA2	9:D:2120:HOH:O	2.07	0.54
3:D:809:PRO:HB2	3:D:812:ALA:HB2	1.88	0.54
3:D:929:ARG:HH11	3:D:929:ARG:HG3	1.72	0.54
3:D:996:TRP:HB2	3:D:1044:LEU:HD11	1.89	0.54
3:D:1258:ARG:O	3:D:1262:LEU:HD13	2.08	0.54
3:D:1321:ALA:O	3:D:1339:LYS:HD3	2.07	0.54
2:M:313:LEU:HD12	2:M:313:LEU:O	2.07	0.54
2:M:405:ARG:HG2	9:M:2089:HOH:O	2.06	0.54
2:M:428:ARG:CZ	2:M:451:LEU:HD11	2.37	0.54
3:N:546:ARG:HG3	9:N:9696:HOH:O	2.08	0.54
3:N:550:ARG:NH1	3:N:573:MET:HB3	2.21	0.54
3:N:586:ARG:HD2	9:N:2319:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:996:TRP:O	3:N:999:THR:HG22	2.07	0.54
3:N:1242:HIS:CE1	3:N:1266:ARG:HD3	2.42	0.54
4:O:48:MET:HB2	4:O:54:LEU:HD12	1.89	0.54
2:C:206:THR:HG21	9:C:2105:HOH:O	2.07	0.54
2:C:212:GLY:HA3	2:C:218:VAL:HG23	1.89	0.54
2:C:715:THR:HG22	2:C:717:LEU:HG	1.90	0.54
2:C:1043:TYR:HE1	3:D:710:ARG:O	1.90	0.54
2:C:1062:GLY:HA2	9:C:9628:HOH:O	2.06	0.54
3:D:957:PRO:HG2	3:D:1007:VAL:HA	1.88	0.54
3:D:965:GLU:O	3:D:968:ASP:HB2	2.08	0.54
3:D:1307:LYS:HG2	3:D:1308:GLU:OE1	2.08	0.54
5:F:102:LEU:HD12	5:F:187:LEU:HG	1.89	0.54
5:F:125:ASP:HA	5:F:128:ARG:CZ	2.37	0.54
2:M:148:PHE:HZ	2:M:281:LEU:HD13	1.72	0.54
2:M:157:ARG:CD	2:M:314:THR:HG22	2.35	0.54
2:M:368:THR:HB	2:M:369:PRO:HD3	1.89	0.54
2:M:500:ASN:HD21	3:N:1067:VAL:HG23	1.73	0.54
2:M:584:GLU:O	2:M:588:VAL:HG13	2.07	0.54
2:M:675:ALA:HB2	2:M:867:VAL:HG11	1.88	0.54
2:M:721:ARG:NH2	2:M:785:VAL:HG21	2.22	0.54
2:M:862:PRO:HA	2:M:975:TYR:HE1	1.72	0.54
3:N:131:LYS:HG2	3:N:568:ARG:HG2	1.89	0.54
5:P:308:LEU:O	5:P:312:GLN:HG3	2.07	0.54
1:A:94:LEU:HB2	9:A:9536:HOH:O	2.06	0.54
1:B:105:GLY:O	1:B:132:LEU:HD23	2.06	0.54
1:B:184:THR:O	1:B:192:LEU:HB2	2.08	0.54
2:C:73:LEU:HB3	2:C:94:LEU:HD13	1.89	0.54
2:C:580:MET:HB3	2:C:584:GLU:CD	2.31	0.54
3:D:493:ARG:HH11	3:D:493:ARG:HG2	1.71	0.54
3:D:628:ARG:HD3	3:D:744:GLN:HE22	1.71	0.54
3:D:1104:GLU:HA	3:D:1461:GLY:HA2	1.88	0.54
3:D:1318:TYR:HD1	3:D:1319:VAL:H	1.55	0.54
3:D:1413:THR:HA	9:D:2122:HOH:O	2.07	0.54
1:K:58:ILE:HB	1:K:61:VAL:HB	1.89	0.54
1:K:67:THR:CG2	2:M:609:ASN:HD21	2.20	0.54
1:K:224:TYR:CD2	1:L:9:PRO:HG2	2.42	0.54
2:M:17:PRO:O	2:M:20:GLU:HB3	2.07	0.54
2:M:152:PRO:HG2	9:M:9934:HOH:O	2.06	0.54
2:M:455:LEU:CD1	2:M:459:ALA:HB3	2.37	0.54
2:M:988:VAL:HG13	9:M:9722:HOH:O	2.07	0.54
2:M:1034:GLU:HA	2:M:1037:VAL:CG2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:1076:VAL:CG2	3:N:752:SER:HB3	2.37	0.54
3:N:42:ASP:O	3:N:43:GLY:O	2.26	0.54
3:N:502:PHE:HZ	3:N:512:MET:HE3	1.71	0.54
3:N:514:LEU:HD23	9:N:9923:HOH:O	2.08	0.54
3:N:639:LEU:HD11	3:N:731:LEU:HD12	1.89	0.54
3:N:644:LEU:HD12	3:N:645:PRO:CD	2.35	0.54
3:N:829:VAL:HA	9:N:2355:HOH:O	2.06	0.54
3:N:1035:ILE:HG22	3:N:1039:CYS:SG	2.47	0.54
3:N:1404:ASN:ND2	3:N:1408:ILE:HD12	2.20	0.54
3:N:1478:SER:O	3:N:1482:ARG:HG3	2.07	0.54
4:O:61:GLU:HB2	4:O:65:MET:HE2	1.89	0.54
5:P:154:LYS:HD2	9:P:3317:HOH:O	2.07	0.54
5:P:332:PHE:HB2	9:P:5627:HOH:O	2.07	0.54
1:B:97:VAL:HG13	9:B:9502:HOH:O	2.07	0.54
2:C:437:ARG:O	2:C:467:ILE:HD13	2.08	0.54
2:C:736:ASP:O	2:C:744:ARG:HG2	2.07	0.54
2:C:859:PRO:O	2:C:867:VAL:HG22	2.08	0.54
3:D:116:LEU:O	3:D:118:LEU:HG	2.07	0.54
3:D:152:LEU:HD23	3:D:152:LEU:N	2.20	0.54
3:D:186:VAL:HG11	3:D:213:VAL:HB	1.89	0.54
3:D:730:PRO:HA	3:D:733:CYS:HG	1.71	0.54
3:D:1080:GLY:O	3:D:1084:THR:HG23	2.07	0.54
3:D:1412:LYS:HE2	3:D:1414:PRO:HG3	1.88	0.54
3:D:1478:SER:OG	3:D:1481:VAL:HG23	2.08	0.54
5:F:264:MET:O	5:F:267:THR:HB	2.07	0.54
1:K:54:THR:HG22	1:K:158:ILE:HG13	1.88	0.54
1:L:110:LYS:HZ3	1:L:110:LYS:HB2	1.71	0.54
2:M:83:CYS:HA	2:M:88:LEU:HD23	1.90	0.54
2:M:159:ILE:HG22	9:M:9660:HOH:O	2.06	0.54
2:M:198:ARG:NH2	2:M:203:ASP:HB3	2.21	0.54
2:M:335:THR:HG21	2:M:461:VAL:HG11	1.89	0.54
2:M:642:ARG:HG3	2:M:657:ASP:OD2	2.06	0.54
2:M:690:ILE:HG23	2:M:852:ILE:HA	1.90	0.54
2:M:704:HIS:CB	2:M:831:ARG:HE	2.19	0.54
2:M:1043:TYR:HE1	3:N:710:ARG:O	1.91	0.54
3:N:423:ASP:OD1	5:P:174:LEU:HD13	2.08	0.54
3:N:565:ILE:HD13	5:P:189:GLU:HG2	1.88	0.54
3:N:704:ARG:HG3	3:N:736:PHE:CB	2.33	0.54
3:N:1148:VAL:O	3:N:1189:ARG:HG2	2.06	0.54
3:N:1232:PRO:HB3	3:N:1361:VAL:HG21	1.88	0.54
3:N:1236:LEU:HD11	3:N:1356:TYR:CE1	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:201:LYS:HB2	9:P:4870:HOH:O	2.06	0.54
5:P:269:ASN:O	5:P:273:ARG:HG3	2.07	0.54
5:P:419:ARG:NH1	5:P:419:ARG:HB2	2.22	0.54
2:C:304:LEU:HD23	2:C:305:PRO:HD3	1.90	0.54
2:C:593:ALA:HA	9:C:9558:HOH:O	2.07	0.54
2:C:841:ASN:HD21	2:C:845:ASN:H	1.55	0.54
2:C:862:PRO:HG3	2:C:975:TYR:HE1	1.72	0.54
3:D:664:LYS:HD3	9:D:2194:HOH:O	2.07	0.54
3:D:709:HIS:HA	3:D:1227:GLN:HG2	1.90	0.54
3:D:1008:PHE:HZ	3:D:1032:PRO:HA	1.73	0.54
5:F:108:GLU:HG3	5:F:176:ILE:CG2	2.37	0.54
5:F:279:GLN:HB2	9:F:9647:HOH:O	2.07	0.54
2:M:260:LEU:HG	2:M:261:ILE:HG13	1.89	0.54
2:M:273:GLY:HA2	2:M:276:LYS:HD3	1.89	0.54
2:M:637:LEU:N	2:M:637:LEU:HD23	2.23	0.54
3:N:178:LEU:HG	3:N:200:ASP:H	1.71	0.54
3:N:427:VAL:HG21	3:N:435:VAL:HB	1.87	0.54
3:N:486:ARG:HA	3:N:489:ARG:HD3	1.89	0.54
3:N:799:LYS:O	3:N:799:LYS:HD3	2.07	0.54
3:N:1117:TYR:HB3	9:N:2569:HOH:O	2.07	0.54
3:N:1350:GLU:HG3	3:N:1354:LYS:HE3	1.88	0.54
5:P:264:MET:HB3	9:P:3779:HOH:O	2.07	0.54
1:B:86:VAL:HG12	1:B:124:ASN:ND2	2.08	0.54
1:B:101:LEU:HG	1:B:114:PHE:HA	1.89	0.54
2:C:123:GLU:HB2	9:C:2092:HOH:O	2.07	0.54
2:C:139:GLN:HG3	2:C:411:SER:O	2.07	0.54
2:C:405:ARG:NH2	2:C:566:THR:HG21	2.23	0.54
2:C:577:PRO:HG3	2:C:993:PHE:CD2	2.42	0.54
2:C:1090:LYS:HE3	3:D:88:TYR:O	2.06	0.54
3:D:178:LEU:HD21	3:D:199:LEU:H	1.73	0.54
3:D:427:VAL:HG21	3:D:435:VAL:HB	1.89	0.54
3:D:470:LEU:HD12	9:D:2635:HOH:O	2.07	0.54
3:D:852:ALA:O	3:D:857:ILE:HG12	2.07	0.54
3:D:899:LEU:HD12	3:D:900:ILE:HG23	1.89	0.54
3:D:1118:ILE:HG23	9:D:9597:HOH:O	2.08	0.54
3:D:1246:VAL:HG21	9:D:2550:HOH:O	2.06	0.54
3:D:1487:VAL:HA	9:D:9715:HOH:O	2.06	0.54
2:M:497:ALA:HA	2:M:515:ALA:HA	1.88	0.54
2:M:545:ASN:O	2:M:581:THR:HG21	2.07	0.54
2:M:730:SER:HB3	9:M:2237:HOH:O	2.07	0.54
2:M:798:GLY:H	2:M:827:VAL:CG1	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:1085:PHE:HE1	2:M:1111:ILE:HG21	1.73	0.54
3:N:690:ALA:O	3:N:694:VAL:HG23	2.08	0.54
3:N:1252:ILE:HD13	9:N:9977:HOH:O	2.08	0.54
3:N:1266:ARG:O	3:N:1268:PRO:HD3	2.08	0.54
5:P:159:ILE:O	5:P:163:LEU:HG	2.07	0.54
5:P:192:LEU:O	5:P:196:VAL:HG23	2.08	0.54
5:P:287:THR:N	5:P:290:GLU:OE1	2.41	0.54
2:C:124:ASP:CB	2:C:592:LEU:HD12	2.37	0.54
2:C:567:GLN:HB2	2:C:997:LEU:HD22	1.90	0.54
2:C:666:LEU:CD2	2:C:668:LEU:HD11	2.38	0.54
2:C:724:ARG:HD2	2:C:740:GLU:HA	1.89	0.54
3:D:465:LEU:HD13	9:D:2007:HOH:O	2.08	0.54
3:D:1065:LEU:HD11	3:D:1070:TYR:N	2.23	0.54
3:D:1211:MET:HE1	3:D:1216:SER:OG	2.08	0.54
3:D:1396:GLU:O	3:D:1400:VAL:HG23	2.08	0.54
4:E:25:LYS:O	4:E:29:GLN:HG2	2.08	0.54
5:F:132:ARG:O	5:F:136:LEU:HG	2.07	0.54
1:L:84:GLU:HG3	1:L:127:LEU:HD22	1.88	0.54
1:L:115:LEU:HD12	1:L:115:LEU:O	2.08	0.54
2:M:63:GLY:HA3	2:M:103:LYS:HE2	1.89	0.54
2:M:253:ALA:HB3	9:M:2207:HOH:O	2.08	0.54
2:M:432:ARG:CZ	2:M:519:GLY:HA3	2.38	0.54
2:M:759:THR:HB	2:M:785:VAL:HG21	1.88	0.54
2:M:897:LEU:HB3	2:M:899:GLN:NE2	2.19	0.54
3:N:81:THR:O	3:N:82:LYS:C	2.51	0.54
3:N:962:GLN:O	3:N:966:GLU:HG3	2.08	0.54
3:N:1103:HIS:HD2	3:N:1462:LEU:N	2.06	0.54
3:N:1372:VAL:HA	3:N:1375:MET:HG3	1.90	0.54
5:P:93:LEU:HA	5:P:98:GLU:OE1	2.08	0.54
2:C:176:VAL:HG12	2:C:182:VAL:HG13	1.89	0.54
2:C:877:PRO:HG3	3:D:1020:LEU:HD12	1.89	0.54
3:D:84:ILE:O	3:D:87:ARG:HG3	2.07	0.54
3:D:510:GLU:HB3	9:D:9600:HOH:O	2.08	0.54
3:D:561:GLY:HA3	5:F:184:ARG:NH1	2.23	0.54
3:D:850:LEU:O	3:D:853:VAL:HB	2.08	0.54
4:E:13:VAL:HG23	9:E:9552:HOH:O	2.06	0.54
4:E:48:MET:CB	4:E:54:LEU:HB2	2.38	0.54
5:F:356:LYS:O	5:F:360:LYS:HG2	2.07	0.54
2:M:537:LYS:HA	2:M:545:ASN:HD21	1.73	0.54
2:M:577:PRO:HG3	2:M:993:PHE:CE2	2.43	0.54
2:M:650:ARG:HD2	2:M:653:ASP:OD2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:687:ALA:C	2:M:688:ILE:HD12	2.33	0.54
2:M:1016:ILE:H	2:M:1016:ILE:HD13	1.71	0.54
2:M:1115:LEU:HD11	9:M:9579:HOH:O	2.07	0.54
3:N:871:LYS:HE2	9:N:9777:HOH:O	2.07	0.54
3:N:1058:ARG:HG3	3:N:1058:ARG:HH11	1.73	0.54
4:O:94:PRO:HG3	9:O:5923:HOH:O	2.06	0.54
1:A:93:SER:HB2	9:A:9533:HOH:O	2.06	0.54
2:C:794:PRO:HB3	9:C:9647:HOH:O	2.07	0.54
2:C:983:ILE:HG23	3:D:944:THR:O	2.08	0.54
3:D:42:ASP:O	3:D:43:GLY:O	2.25	0.54
3:D:399:ARG:NH2	3:D:432:TYR:HE2	2.06	0.54
3:D:400:VAL:CG1	3:D:441:ARG:HD3	2.38	0.54
3:D:404:GLU:HB3	3:D:414:ARG:CD	2.38	0.54
3:D:471:GLU:HG2	9:D:9659:HOH:O	2.07	0.54
3:D:502:PHE:CZ	3:D:509:PRO:HB3	2.42	0.54
1:K:27:PRO:HG2	1:K:186:LEU:HD22	1.90	0.54
1:K:198:ARG:HB2	1:K:200:TRP:CZ3	2.43	0.54
1:K:216:GLU:O	1:K:220:GLU:HG3	2.07	0.54
1:L:40:LEU:HD11	9:L:4428:HOH:O	2.08	0.54
2:M:580:MET:HB3	2:M:584:GLU:OE1	2.08	0.54
2:M:724:ARG:CG	2:M:740:GLU:HA	2.38	0.54
3:N:32:ILE:HG12	3:N:38:LYS:O	2.08	0.54
3:N:699:VAL:HG21	3:N:760:ARG:HB3	1.90	0.54
3:N:799:LYS:H	3:N:826:PRO:HG2	1.72	0.54
3:N:981:GLY:HA3	9:N:2378:HOH:O	2.07	0.54
3:N:999:THR:O	3:N:1002:LYS:HB2	2.08	0.54
3:N:1252:ILE:H	3:N:1252:ILE:HD12	1.72	0.54
3:N:1503:VAL:HG12	9:N:9617:HOH:O	2.08	0.54
4:O:85:LEU:HD23	4:O:86:GLN:N	2.23	0.54
5:P:102:LEU:O	5:P:106:VAL:HG23	2.08	0.54
5:P:184:ARG:HD3	5:P:188:ILE:HD11	1.90	0.54
1:A:50:GLY:O	1:A:146:ARG:HA	2.07	0.53
1:A:160:ASP:HB2	9:A:9521:HOH:O	2.08	0.53
1:B:137:ARG:HB2	9:B:9548:HOH:O	2.07	0.53
2:C:244:PRO:HG2	2:C:246:ASP:CG	2.33	0.53
2:C:436:GLY:HA2	2:C:538:GLN:O	2.08	0.53
2:C:536:PRO:HB2	2:C:905:ILE:HD13	1.89	0.53
2:C:1008:ARG:HE	2:C:1028:GLY:H	1.56	0.53
2:C:1070:ILE:HA	9:C:9807:HOH:O	2.07	0.53
3:D:149:LYS:HE3	9:D:2297:HOH:O	2.08	0.53
3:D:560:GLN:HG3	5:F:221:ILE:HG21	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1087:ARG:HD2	3:D:1256:LEU:HD22	1.90	0.53
3:D:1472:ILE:HG22	3:D:1474:ALA:H	1.73	0.53
4:E:88:GLU:HB2	9:E:9594:HOH:O	2.07	0.53
1:K:198:ARG:HD3	1:K:200:TRP:CH2	2.37	0.53
1:L:180:GLN:HG2	9:N:9580:HOH:O	2.07	0.53
2:M:208:ALA:HB1	2:M:218:VAL:HG13	1.90	0.53
2:M:460:ARG:O	2:M:468:ARG:HG3	2.08	0.53
2:M:604:ALA:HB3	2:M:612:VAL:O	2.08	0.53
2:M:714:ASP:HB2	9:M:2167:HOH:O	2.07	0.53
3:N:455:ARG:HH21	5:P:140:ARG:HD3	1.73	0.53
3:N:1379:VAL:HA	3:N:1420:LEU:HB2	1.91	0.53
2:C:242:LEU:HD23	9:C:9503:HOH:O	2.08	0.53
2:C:358:ARG:HB3	2:C:371:LYS:O	2.09	0.53
2:C:437:ARG:HG3	2:C:469:THR:OG1	2.07	0.53
2:C:464:LEU:O	2:C:466:PHE:N	2.40	0.53
2:C:553:ASP:HA	2:C:881:ASN:HA	1.89	0.53
2:C:926:PHE:CD2	2:C:930:LYS:HE2	2.43	0.53
2:C:937:ASP:HB2	2:C:940:GLU:HG3	1.89	0.53
3:D:424:GLY:HA2	3:D:436:GLU:HA	1.90	0.53
3:D:516:ALA:O	3:D:518:PRO:HD3	2.09	0.53
3:D:844:ALA:HA	3:D:867:ARG:NH1	2.22	0.53
3:D:1278:ASP:HB2	3:D:1318:TYR:HE1	1.72	0.53
3:D:1379:VAL:HG12	3:D:1419:PRO:HA	1.89	0.53
1:K:170:VAL:HG12	9:K:5166:HOH:O	2.07	0.53
2:M:163:ILE:HB	9:M:2375:HOH:O	2.08	0.53
2:M:254:VAL:HG13	2:M:258:TYR:HE1	1.73	0.53
2:M:460:ARG:HD3	9:M:2017:HOH:O	2.07	0.53
2:M:961:GLU:HA	9:M:9902:HOH:O	2.07	0.53
3:N:756:GLN:HE21	3:N:760:ARG:HD2	1.72	0.53
3:N:792:ILE:O	3:N:878:GLY:HA3	2.08	0.53
3:N:984:THR:HG23	3:N:986:ARG:H	1.73	0.53
3:N:1264:GLU:OE2	3:N:1424:VAL:HG12	2.08	0.53
4:O:90:GLU:HA	9:O:4524:HOH:O	2.08	0.53
5:P:291:ILE:CG2	5:P:304:VAL:HG21	2.38	0.53
1:A:34:VAL:HG21	2:C:939:ARG:HD2	1.90	0.53
2:C:72:ARG:HE	2:C:97:ARG:NH1	2.06	0.53
2:C:173:ASP:O	2:C:184:MET:HA	2.08	0.53
2:C:350:ARG:HG2	2:C:353:ARG:NH2	2.24	0.53
2:C:516:ARG:NH2	3:D:1068:LEU:HB3	2.23	0.53
2:C:625:LEU:CD1	2:C:641:PRO:HG3	2.38	0.53
2:C:927:GLY:HA2	2:C:930:LYS:HE3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:9784:HOH:O	3:D:943:THR:HG21	2.08	0.53
3:D:15:PRO:HA	3:D:18:ILE:HG12	1.90	0.53
3:D:89:ARG:O	3:D:521:PRO:HG3	2.08	0.53
3:D:647:ARG:NH1	3:D:650:LEU:HD23	2.24	0.53
3:D:769:LEU:H	3:D:769:LEU:HD12	1.74	0.53
3:D:789:LEU:O	3:D:792:ILE:HG23	2.08	0.53
3:D:1264:GLU:OE2	3:D:1424:VAL:N	2.41	0.53
3:D:1434:TRP:CZ3	3:D:1457:ASP:HB2	2.44	0.53
5:F:335:ASP:CG	5:F:338:LEU:HD12	2.33	0.53
1:K:14:ARG:HH12	1:K:24:VAL:HG23	1.73	0.53
1:K:19:GLU:H	1:K:19:GLU:CD	2.16	0.53
1:K:150:TYR:HE2	1:K:152:PRO:HG3	1.72	0.53
2:M:358:ARG:HB3	2:M:371:LYS:O	2.08	0.53
2:M:514:VAL:HG11	2:M:516:ARG:NH1	2.23	0.53
2:M:810:ASP:HB3	2:M:813:VAL:HG22	1.90	0.53
3:N:30:GLU:HB3	3:N:40:GLU:HB3	1.90	0.53
3:N:957:PRO:HG2	3:N:1007:VAL:HG12	1.91	0.53
3:N:1406:ARG:HH11	3:N:1406:ARG:HG3	1.73	0.53
1:A:30:ARG:NH2	1:A:191:ASP:HB2	2.24	0.53
1:A:81:ASN:HA	1:A:84:GLU:CD	2.33	0.53
1:B:83:LYS:HE2	1:B:168:ASP:HB2	1.89	0.53
2:C:41:ASN:ND2	2:C:41:ASN:N	2.55	0.53
2:C:741:GLY:HA3	9:C:9522:HOH:O	2.07	0.53
3:D:130:SER:HB3	3:D:132:TYR:CE1	2.43	0.53
3:D:526:PRO:O	3:D:537:THR:HA	2.08	0.53
3:D:633:VAL:C	3:D:635:PRO:HD3	2.33	0.53
5:F:307:THR:O	5:F:310:ILE:HG13	2.08	0.53
2:M:343:GLN:HG2	2:M:385:PHE:HB2	1.91	0.53
2:M:379:GLU:HG2	9:M:2388:HOH:O	2.07	0.53
2:M:642:ARG:HG3	2:M:654:LEU:HD21	1.91	0.53
2:M:662:GLU:HB3	9:M:9635:HOH:O	2.07	0.53
9:M:9722:HOH:O	3:N:948:THR:HB	2.08	0.53
3:N:436:GLU:HB2	3:N:445:ARG:HB2	1.89	0.53
3:N:583:ASP:OD2	3:N:604:THR:HG21	2.09	0.53
3:N:699:VAL:HG22	3:N:756:GLN:NE2	2.23	0.53
3:N:772:PRO:HA	9:N:9537:HOH:O	2.08	0.53
3:N:829:VAL:H	3:N:835:SER:HB2	1.73	0.53
3:N:1294:VAL:HB	9:N:2223:HOH:O	2.09	0.53
5:P:278:LEU:CB	5:P:286:PRO:HG2	2.38	0.53
1:A:156:HIS:CD2	1:A:157:GLY:N	2.76	0.53
3:D:126:VAL:O	3:D:132:TYR:HD1	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:171:LEU:HD22	3:D:390:PRO:HG3	1.90	0.53
3:D:800:LYS:HD3	3:D:804:LEU:HD13	1.90	0.53
3:D:955:VAL:HG11	3:D:1015:TYR:HE2	1.73	0.53
3:D:992:ILE:HD13	9:D:2530:HOH:O	2.08	0.53
1:K:44:LEU:O	1:K:174:VAL:HG21	2.08	0.53
1:K:83:LYS:HE2	1:K:168:ASP:H	1.73	0.53
1:L:218:LEU:O	1:L:222:LEU:HG	2.08	0.53
2:M:247:PRO:HB3	9:M:2135:HOH:O	2.08	0.53
2:M:549:PHE:CZ	2:M:886:LEU:HD12	2.44	0.53
2:M:1012:PRO:HD2	2:M:1021:LEU:O	2.09	0.53
2:M:1050:GLN:HG3	9:N:2259:HOH:O	2.07	0.53
3:N:9:ARG:HA	3:N:1455:LYS:O	2.07	0.53
3:N:102:ILE:HD13	3:N:586:ARG:HB2	1.88	0.53
3:N:103:TRP:HH2	3:N:1447:LEU:HD23	1.73	0.53
3:N:631:ILE:HG21	3:N:745:MET:SD	2.48	0.53
3:N:1263:PHE:HA	3:N:1375:MET:HE1	1.89	0.53
3:N:1289:LYS:HE2	9:N:9835:HOH:O	2.09	0.53
5:P:89:GLY:HA2	9:P:4587:HOH:O	2.08	0.53
1:A:7:LYS:HD3	9:A:9619:HOH:O	2.08	0.53
1:A:26:GLU:HB3	1:A:194:LYS:HG3	1.91	0.53
2:C:64:LEU:CD1	2:C:100:LEU:HD13	2.39	0.53
2:C:202:TYR:OH	2:C:304:LEU:HD22	2.09	0.53
2:C:517:ARG:NH1	2:C:522:VAL:HG11	2.24	0.53
2:C:722:ILE:HG12	2:C:757:GLY:O	2.09	0.53
2:C:853:LEU:HD23	2:C:858:MET:HB2	1.91	0.53
2:C:876:VAL:HB	3:D:949:ILE:HG13	1.91	0.53
2:C:1092:LEU:HD13	2:C:1099:VAL:HG21	1.91	0.53
9:C:9697:HOH:O	4:E:28:GLN:HG3	2.08	0.53
3:D:85:VAL:HB	9:D:9784:HOH:O	2.07	0.53
3:D:153:LEU:HD11	3:D:158:TYR:N	2.23	0.53
3:D:445:ARG:HG2	3:D:445:ARG:HH11	1.74	0.53
3:D:554:LEU:O	3:D:558:LEU:HG	2.09	0.53
3:D:963:TYR:CD2	3:D:1002:LYS:HB3	2.43	0.53
3:D:1066:THR:CG2	3:D:1069:GLU:HG3	2.38	0.53
3:D:1382:THR:HA	3:D:1389:LEU:HD13	1.91	0.53
4:E:31:LEU:HD12	4:E:32:ARG:HD3	1.89	0.53
4:E:41:GLU:HG3	9:E:9492:HOH:O	2.07	0.53
2:M:129:ILE:HG12	2:M:386:PHE:HB3	1.90	0.53
2:M:909:ALA:C	2:M:910:LYS:HD2	2.34	0.53
2:M:1093:GLN:HB3	3:N:90:MET:CE	2.38	0.53
3:N:52:PRO:HG3	3:N:78:VAL:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:169:TYR:HA	3:N:392:SER:HA	1.91	0.53
3:N:906:GLN:HE22	3:N:910:SER:HB2	1.72	0.53
3:N:1135:ARG:HG2	3:N:1136:LYS:HE3	1.90	0.53
5:P:234:LYS:HD2	5:P:236:SER:HB2	1.89	0.53
1:A:18:ARG:O	1:A:207:PRO:HD3	2.07	0.53
1:B:219:ARG:O	1:B:223:THR:HG23	2.09	0.53
3:D:633:VAL:HG22	3:D:635:PRO:CD	2.37	0.53
1:K:38:ASN:HB3	1:K:39:PRO:HD3	1.90	0.53
1:L:92:PRO:HD3	9:L:6230:HOH:O	2.08	0.53
2:M:79:PRO:HG2	2:M:82:GLU:HB2	1.90	0.53
2:M:195:LEU:HD12	2:M:234:ALA:HB1	1.90	0.53
2:M:710:ILE:HD11	2:M:758:ARG:CZ	2.39	0.53
2:M:772:ARG:HD2	5:P:373:LYS:HD2	1.91	0.53
2:M:838:LYS:HE2	2:M:997:LEU:HD12	1.90	0.53
2:M:876:VAL:HA	9:M:9508:HOH:O	2.08	0.53
2:M:1018:GLN:NE2	2:M:1063:ARG:HH22	2.07	0.53
3:N:809:PRO:HB2	3:N:812:ALA:HB2	1.90	0.53
2:C:739:GLU:HB3	9:C:9747:HOH:O	2.08	0.53
3:D:95:LEU:HD21	3:D:574:LEU:HD11	1.90	0.53
5:F:408:LEU:HA	5:F:411:HIS:CE1	2.43	0.53
1:L:149:GLY:O	1:L:171:PHE:HB2	2.08	0.53
1:L:170:VAL:C	1:L:172:SER:H	2.16	0.53
2:M:42:VAL:HA	9:M:2303:HOH:O	2.09	0.53
2:M:73:LEU:HD22	2:M:118:ILE:HD11	1.90	0.53
2:M:338:GLU:O	2:M:341:THR:HG22	2.08	0.53
2:M:987:ILE:HG23	9:M:9722:HOH:O	2.08	0.53
3:N:115:LEU:HD12	3:N:498:VAL:HG23	1.91	0.53
3:N:493:ARG:HG3	3:N:494:LYS:N	2.23	0.53
3:N:863:VAL:HG21	9:N:9770:HOH:O	2.07	0.53
3:N:1173:LEU:HD23	3:N:1174:LEU:HD23	1.90	0.53
3:N:1494:ALA:HB1	4:O:88:GLU:OE2	2.09	0.53
1:B:14:ARG:HG2	9:B:9567:HOH:O	2.08	0.53
2:C:6:PHE:CE2	2:C:913:GLU:HB3	2.44	0.53
2:C:405:ARG:HH12	2:C:563:ASN:HD22	1.53	0.53
2:C:409:ARG:HH12	7:C:8001:RPT:H18	1.74	0.53
2:C:496:ILE:H	2:C:496:ILE:HD12	1.74	0.53
2:C:625:LEU:HD13	2:C:639:GLN:O	2.08	0.53
3:D:178:LEU:HD22	9:D:9887:HOH:O	2.08	0.53
3:D:1395:LEU:HB3	9:D:9895:HOH:O	2.08	0.53
5:F:215:GLU:HG2	9:F:9503:HOH:O	2.08	0.53
5:F:282:LEU:HD12	5:F:284:ARG:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:54:ILE:HG22	2:M:66:LEU:HB3	1.90	0.53
2:M:166:PRO:HD3	2:M:265:ARG:HB2	1.90	0.53
2:M:610:ARG:HG2	9:M:9673:HOH:O	2.09	0.53
2:M:625:LEU:HD13	2:M:639:GLN:O	2.09	0.53
3:N:636:GLN:HB2	9:N:2002:HOH:O	2.09	0.53
3:N:681:ARG:HB3	3:N:681:ARG:HH11	1.74	0.53
5:P:138:SER:O	5:P:141:VAL:HG12	2.09	0.53
5:P:277:GLN:O	5:P:280:GLN:HB3	2.09	0.53
1:A:63:HIS:CD2	2:C:801:VAL:HG12	2.44	0.53
1:B:149:GLY:O	1:B:171:PHE:HB2	2.09	0.53
2:C:162:ILE:HD12	2:C:172:ILE:HB	1.91	0.53
2:C:405:ARG:HH21	2:C:566:THR:HG21	1.73	0.53
2:C:721:ARG:HA	9:C:9648:HOH:O	2.09	0.53
2:C:902:ILE:O	2:C:904:PRO:HD3	2.09	0.53
2:C:1002:GLU:HA	2:C:1006:HIS:HE1	1.73	0.53
3:D:143:ASN:HD21	3:D:145:VAL:HG12	1.74	0.53
3:D:576:GLU:HA	3:D:579:ASP:OD2	2.09	0.53
3:D:613:ARG:O	3:D:617:ASN:HB2	2.08	0.53
5:F:373:LYS:HB2	9:F:9672:HOH:O	2.08	0.53
1:K:123:MET:O	1:K:125:PRO:HD3	2.08	0.53
1:L:72:LYS:HE2	9:L:5229:HOH:O	2.09	0.53
2:M:254:VAL:HG21	9:M:9516:HOH:O	2.08	0.53
2:M:907:ASP:HA	9:M:2423:HOH:O	2.09	0.53
3:N:14:SER:HB2	3:N:16:GLU:HG2	1.91	0.53
3:N:204:LEU:HD21	9:N:9631:HOH:O	2.08	0.53
3:N:404:GLU:HB3	3:N:414:ARG:CZ	2.39	0.53
3:N:566:ILE:HG12	5:P:217:ASN:ND2	2.23	0.53
3:N:969:ARG:HA	9:N:2036:HOH:O	2.09	0.53
3:N:1189:ARG:HB3	3:N:1189:ARG:HH11	1.73	0.53
3:N:1459:LEU:HD13	3:N:1465:ASN:HD21	1.73	0.53
5:P:287:THR:C	5:P:289:GLU:H	2.16	0.53
1:A:44:LEU:O	1:A:174:VAL:HG21	2.09	0.52
2:C:601:GLY:O	2:C:648:ARG:HA	2.10	0.52
2:C:918:LEU:HB3	2:C:968:LEU:HD23	1.90	0.52
3:D:133:ILE:HG21	3:D:454:ALA:HB1	1.91	0.52
3:D:863:VAL:HG21	9:D:2215:HOH:O	2.09	0.52
3:D:1105:ILE:HG13	9:D:9769:HOH:O	2.08	0.52
4:E:17:TYR:O	4:E:21:VAL:HG23	2.10	0.52
5:F:107:GLU:HG2	9:F:9515:HOH:O	2.08	0.52
1:K:52:ALA:HA	9:K:3524:HOH:O	2.09	0.52
2:M:333:ILE:CD1	2:M:467:ILE:HG13	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:380:ALA:O	2:M:384:GLU:HB2	2.09	0.52
2:M:910:LYS:HG2	9:M:2099:HOH:O	2.08	0.52
2:M:1060:ILE:HG22	2:M:1061:GLU:N	2.25	0.52
3:N:699:VAL:HG12	3:N:717:GLN:CA	2.37	0.52
3:N:1047:LYS:HB3	3:N:1048:PRO:CD	2.40	0.52
3:N:1097:LYS:O	3:N:1101:VAL:HG23	2.08	0.52
3:N:1312:LEU:HB2	9:N:9707:HOH:O	2.10	0.52
3:N:1314:LYS:H	3:N:1314:LYS:NZ	2.02	0.52
3:N:1402:ALA:HB2	3:N:1415:VAL:CG2	2.39	0.52
3:N:1503:VAL:HG11	9:N:9596:HOH:O	2.09	0.52
4:O:79:LEU:HD11	9:O:4245:HOH:O	2.08	0.52
5:P:347:GLN:HG3	9:P:3973:HOH:O	2.09	0.52
1:A:91:ASN:HB3	9:A:9551:HOH:O	2.10	0.52
2:C:11:GLU:HG2	2:C:537:LYS:HZ1	1.75	0.52
2:C:708:TYR:CD1	2:C:708:TYR:N	2.77	0.52
2:C:732:ALA:HB1	2:C:735:ARG:NH2	2.24	0.52
2:C:811:PRO:HD2	2:C:813:VAL:HG22	1.91	0.52
3:D:95:LEU:HD12	3:D:517:VAL:HG23	1.90	0.52
3:D:131:LYS:O	3:D:133:ILE:HD13	2.09	0.52
3:D:957:PRO:CG	3:D:1007:VAL:HA	2.40	0.52
3:D:1068:LEU:HD23	3:D:1072:ILE:HG12	1.89	0.52
3:D:1274:ILE:HD11	3:D:1334:GLN:HB3	1.91	0.52
5:F:184:ARG:HE	5:F:188:ILE:HD11	1.74	0.52
5:F:368:VAL:HG12	9:F:9483:HOH:O	2.08	0.52
2:M:170:PRO:HG2	2:M:258:TYR:HD2	1.74	0.52
2:M:460:ARG:HB3	2:M:460:ARG:HH11	1.74	0.52
2:M:626:ARG:HA	9:M:9546:HOH:O	2.08	0.52
2:M:1101:THR:HB	3:N:5:VAL:HG13	1.92	0.52
3:N:215:TYR:HA	9:N:9773:HOH:O	2.09	0.52
3:N:633:VAL:C	3:N:635:PRO:HD3	2.34	0.52
3:N:781:PRO:HB2	3:N:911:LEU:HD23	1.91	0.52
3:N:800:LYS:HD2	9:N:2127:HOH:O	2.08	0.52
3:N:916:TYR:O	3:N:919:PHE:HB3	2.09	0.52
4:O:33:HIS:CG	4:O:89:MET:HG2	2.43	0.52
9:A:9609:HOH:O	2:C:856:GLU:HB3	2.09	0.52
2:C:346:VAL:HG12	9:C:9903:HOH:O	2.08	0.52
2:C:516:ARG:CZ	3:D:1068:LEU:HB3	2.39	0.52
2:C:778:PHE:HB3	9:C:2430:HOH:O	2.10	0.52
2:C:1055:LEU:HD21	2:C:1079:PRO:HG3	1.91	0.52
3:D:86:ARG:HG2	3:D:86:ARG:NH1	2.21	0.52
3:D:1192:LEU:HD21	3:D:1372:VAL:HG13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1231:GLU:HG2	3:D:1232:PRO:N	2.25	0.52
3:D:1496:GLU:HA	3:D:1499:ARG:HD2	1.90	0.52
5:F:127:ILE:HD11	9:F:9599:HOH:O	2.08	0.52
5:F:278:LEU:CB	5:F:286:PRO:HG2	2.39	0.52
1:K:30:ARG:HH11	1:K:30:ARG:HG3	1.74	0.52
1:K:224:TYR:HB3	1:L:9:PRO:HB2	1.91	0.52
1:L:7:LYS:HG3	9:L:5022:HOH:O	2.09	0.52
2:M:73:LEU:HD11	9:M:2198:HOH:O	2.08	0.52
2:M:376:ARG:HG2	9:M:2218:HOH:O	2.08	0.52
2:M:464:LEU:O	2:M:466:PHE:N	2.43	0.52
2:M:643:VAL:HG13	2:M:647:GLN:OE1	2.09	0.52
2:M:783:ARG:HB3	9:M:2452:HOH:O	2.08	0.52
2:M:801:VAL:O	2:M:802:ARG:HG3	2.10	0.52
2:M:937:ASP:HB3	2:M:940:GLU:H	1.73	0.52
2:M:1104:GLU:HA	3:N:6:ARG:HD2	1.92	0.52
3:N:462:GLN:HA	3:N:513:ILE:CD1	2.40	0.52
3:N:693:GLU:HA	4:O:48:MET:HE1	1.91	0.52
3:N:732:VAL:HG13	9:N:9614:HOH:O	2.09	0.52
3:N:1004:THR:O	3:N:1007:VAL:HG22	2.10	0.52
3:N:1104:GLU:O	3:N:1106:VAL:HG23	2.09	0.52
3:N:1382:THR:HG21	3:N:1418:LYS:HZ1	1.74	0.52
3:N:1493:LYS:HA	3:N:1496:GLU:CG	2.39	0.52
5:P:113:ILE:HG23	5:P:127:ILE:CG2	2.39	0.52
5:P:266:GLU:HA	5:P:269:ASN:ND2	2.24	0.52
5:P:403:LYS:HD2	9:P:3729:HOH:O	2.09	0.52
1:A:57:TYR:CE2	1:A:59:GLU:HA	2.45	0.52
1:A:149:GLY:O	1:A:171:PHE:HB2	2.09	0.52
1:A:161:ARG:HB2	1:A:161:ARG:HH11	1.72	0.52
2:C:165:LEU:HD13	9:C:9966:HOH:O	2.10	0.52
2:C:199:VAL:HG13	2:C:235:LEU:HG	1.91	0.52
2:C:693:GLU:HG3	9:C:9813:HOH:O	2.10	0.52
2:C:732:ALA:O	2:C:735:ARG:HG3	2.09	0.52
2:C:1033:GLY:HA2	3:D:619:LEU:O	2.09	0.52
3:D:104:PHE:CD2	3:D:1448:THR:HG23	2.44	0.52
3:D:420:VAL:HG13	5:F:164:LYS:HE2	1.91	0.52
3:D:584:ASN:ND2	3:D:589:ALA:HA	2.23	0.52
3:D:893:GLU:HA	9:D:9543:HOH:O	2.08	0.52
1:L:14:ARG:HG2	9:L:5424:HOH:O	2.08	0.52
2:M:902:ILE:O	2:M:904:PRO:HD3	2.10	0.52
2:M:998:TYR:CZ	2:M:1000:MET:HA	2.45	0.52
3:N:52:PRO:HB2	9:N:9523:HOH:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:207:PHE:CB	3:N:208:PRO:HD2	2.37	0.52
3:N:424:GLY:HA2	3:N:436:GLU:HA	1.91	0.52
5:P:264:MET:O	5:P:268:ILE:HG13	2.08	0.52
2:C:52:PHE:HB3	2:C:53:PRO:HD3	1.89	0.52
2:C:129:ILE:CG1	2:C:386:PHE:HB3	2.40	0.52
2:C:182:VAL:CG1	2:C:193:LEU:HD13	2.39	0.52
2:C:195:LEU:HD23	2:C:238:LEU:HG	1.91	0.52
2:C:328:LEU:HB2	2:C:488:ALA:CB	2.39	0.52
2:C:918:LEU:HD23	2:C:967:PHE:O	2.09	0.52
2:C:1042:ALA:CB	3:D:710:ARG:HB3	2.39	0.52
3:D:572:ARG:HB3	9:F:9505:HOH:O	2.09	0.52
3:D:1026:SER:C	3:D:1028:ALA:H	2.16	0.52
3:D:1144:LEU:HA	3:D:1147:ARG:HG3	1.90	0.52
2:M:366:SER:HB2	9:M:9558:HOH:O	2.09	0.52
2:M:643:VAL:HG13	2:M:647:GLN:CD	2.35	0.52
2:M:669:GLY:HA3	2:M:995:MET:HA	1.91	0.52
2:M:807:ARG:NH1	2:M:807:ARG:HB2	2.24	0.52
2:M:881:ASN:H	2:M:881:ASN:ND2	2.08	0.52
2:M:1005:MET:HB2	3:N:648:MET:HE3	1.91	0.52
3:N:35:ARG:HG2	3:N:35:ARG:HH11	1.74	0.52
3:N:629:SER:HB3	3:N:648:MET:HE1	1.90	0.52
3:N:1009:LYS:HG3	9:N:9751:HOH:O	2.08	0.52
3:N:1243:THR:HG22	3:N:1244:GLY:H	1.74	0.52
5:P:269:ASN:CB	5:P:273:ARG:HH21	2.23	0.52
1:A:46:SER:HB3	2:C:856:GLU:CG	2.38	0.52
1:B:123:MET:O	1:B:125:PRO:HD3	2.10	0.52
2:C:708:TYR:CE2	2:C:793:PRO:HD2	2.41	0.52
3:D:36:THR:HB	3:D:38:LYS:HG3	1.91	0.52
3:D:641:GLN:HB3	3:D:717:GLN:O	2.10	0.52
3:D:721:VAL:HA	9:D:9665:HOH:O	2.08	0.52
3:D:838:ARG:HH11	3:D:874:GLU:HB3	1.73	0.52
3:D:890:VAL:HG23	9:D:2176:HOH:O	2.08	0.52
3:D:926:LYS:HE2	9:D:9484:HOH:O	2.08	0.52
3:D:1341:PRO:HA	3:D:1344:VAL:HG23	1.91	0.52
5:F:166:LEU:HD13	5:F:170:HIS:HB2	1.92	0.52
1:L:50:GLY:O	1:L:146:ARG:HA	2.10	0.52
1:L:176:ARG:HB2	9:N:9671:HOH:O	2.08	0.52
2:M:176:VAL:HG12	2:M:182:VAL:HG13	1.91	0.52
2:M:1092:LEU:HD23	2:M:1097:LEU:HD23	1.92	0.52
3:N:972:LEU:HD11	9:N:9509:HOH:O	2.10	0.52
1:A:150:TYR:HE2	1:A:152:PRO:HG3	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:ARG:HB3	9:A:9641:HOH:O	2.10	0.52
2:C:682:TYR:HB3	2:C:689:VAL:HG22	1.92	0.52
2:C:813:VAL:HG13	9:C:9732:HOH:O	2.08	0.52
2:C:839:LEU:HD21	2:C:849:VAL:CG2	2.40	0.52
2:C:852:ILE:H	2:C:852:ILE:HD12	1.75	0.52
2:C:1081:VAL:HG21	2:C:1111:ILE:HG22	1.91	0.52
3:D:62:LYS:HE2	3:D:75:ARG:NH1	2.25	0.52
3:D:126:VAL:O	3:D:132:TYR:CD1	2.62	0.52
3:D:897:TRP:CH2	3:D:902:LEU:HD21	2.45	0.52
3:D:1047:LYS:HA	3:D:1053:PHE:CE1	2.45	0.52
3:D:1432:LYS:CG	3:D:1433:SER:H	2.22	0.52
4:E:29:GLN:HB3	9:E:9534:HOH:O	2.09	0.52
1:L:101:LEU:HB2	1:L:114:PHE:CD2	2.44	0.52
2:M:146:VAL:HG13	2:M:161:SER:O	2.09	0.52
2:M:177:GLU:HB2	9:M:9838:HOH:O	2.09	0.52
2:M:290:LEU:HB3	2:M:302:VAL:CG1	2.40	0.52
2:M:601:GLY:O	2:M:648:ARG:HA	2.10	0.52
2:M:694:LEU:CD1	2:M:868:ASP:HB3	2.39	0.52
2:M:1038:TRP:HH2	3:N:1096:ARG:HD2	1.74	0.52
3:N:122:GLU:HG2	9:N:2158:HOH:O	2.09	0.52
3:N:516:ALA:O	3:N:518:PRO:HD3	2.10	0.52
3:N:1018:ASN:O	3:N:1022:VAL:HG23	2.10	0.52
3:N:1109:GLU:HG2	3:N:1201:CYS:CA	2.38	0.52
2:C:4:LYS:HG2	9:C:9667:HOH:O	2.10	0.52
2:C:281:LEU:CD1	2:C:306:THR:HA	2.39	0.52
2:C:470:PRO:HB2	2:C:534:VAL:HG21	1.91	0.52
2:C:586:ARG:HD2	2:C:590:ASP:OD2	2.10	0.52
2:C:961:GLU:HA	9:C:2350:HOH:O	2.10	0.52
3:D:10:ILE:HG13	3:D:1434:TRP:CZ2	2.44	0.52
3:D:45:PHE:HD1	3:D:86:ARG:HH21	1.56	0.52
3:D:455:ARG:HG2	3:D:455:ARG:NH1	2.25	0.52
3:D:787:LEU:HD21	3:D:947:ILE:CD1	2.40	0.52
3:D:1011:PHE:HZ	3:D:1039:CYS:HG	1.56	0.52
3:D:1482:ARG:HB2	3:D:1483:PHE:CE1	2.44	0.52
9:D:2311:HOH:O	5:F:147:LEU:HD21	2.10	0.52
4:E:48:MET:HB3	4:E:54:LEU:HB2	1.92	0.52
2:M:69:LEU:HD21	2:M:99:GLN:NE2	2.25	0.52
2:M:578:VAL:CG2	2:M:579:VAL:HG12	2.40	0.52
2:M:636:ALA:HB3	9:M:9891:HOH:O	2.09	0.52
2:M:1038:TRP:HA	2:M:1041:GLU:HB2	1.91	0.52
2:M:1091:GLU:HA	3:N:520:LEU:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1177:ALA:HB3	3:N:1183:ILE:HD11	1.91	0.52
1:A:127:LEU:C	1:A:127:LEU:HD12	2.34	0.52
1:B:50:GLY:O	1:B:146:ARG:HA	2.10	0.52
2:C:34:VAL:CG1	2:C:38:LYS:HG3	2.40	0.52
2:C:198:ARG:HD3	9:C:9933:HOH:O	2.09	0.52
2:C:551:GLU:HB3	2:C:906:PHE:HD2	1.75	0.52
2:C:685:GLU:OE1	3:D:739:ASP:HA	2.10	0.52
2:C:721:ARG:HH21	2:C:783:ARG:NH2	2.07	0.52
2:C:752:GLY:C	2:C:791:ARG:HH12	2.18	0.52
3:D:213:VAL:HG11	9:D:9853:HOH:O	2.09	0.52
3:D:653:PHE:CE2	3:D:695:ILE:HG13	2.44	0.52
3:D:984:THR:HG22	3:D:987:GLU:CD	2.35	0.52
3:D:1003:VAL:O	3:D:1006:ALA:HB3	2.10	0.52
3:D:1379:VAL:O	3:D:1420:LEU:HD23	2.10	0.52
1:K:2:LEU:HD11	9:K:4002:HOH:O	2.09	0.52
2:M:137:VAL:HG22	2:M:391:LEU:O	2.10	0.52
2:M:142:ARG:NH1	2:M:325:ILE:HG12	2.25	0.52
2:M:413:LEU:HD12	2:M:413:LEU:N	2.25	0.52
2:M:752:GLY:O	3:N:679:ARG:HG2	2.10	0.52
2:M:840:ALA:HB2	2:M:846:LYS:HA	1.92	0.52
2:M:1016:ILE:HD13	2:M:1016:ILE:N	2.24	0.52
3:N:75:ARG:HB2	9:N:9539:HOH:O	2.10	0.52
3:N:183:GLU:HA	3:N:186:VAL:CG1	2.40	0.52
3:N:550:ARG:HH21	5:P:211:ASP:CG	2.18	0.52
5:P:128:ARG:HD3	9:P:3878:HOH:O	2.08	0.52
1:A:9:PRO:HB3	1:A:25:LEU:HD21	1.92	0.52
1:B:19:GLU:HG3	1:B:201:THR:O	2.09	0.52
2:C:212:GLY:C	2:C:215:GLY:H	2.18	0.52
2:C:461:VAL:HG23	9:C:9546:HOH:O	2.10	0.52
2:C:694:LEU:CD1	2:C:868:ASP:HB3	2.40	0.52
2:C:773:LEU:HB2	5:F:373:LYS:CB	2.39	0.52
3:D:30:GLU:HB3	3:D:40:GLU:CB	2.40	0.52
3:D:149:LYS:HA	9:D:9512:HOH:O	2.09	0.52
3:D:434:ARG:HB2	3:D:447:VAL:CG1	2.39	0.52
3:D:566:ILE:HD13	5:F:217:ASN:HB3	1.91	0.52
3:D:925:GLU:HG2	3:D:926:LYS:N	2.24	0.52
3:D:1166:LEU:HD12	3:D:1171:VAL:HG22	1.92	0.52
3:D:1280:VAL:O	3:D:1294:VAL:HA	2.10	0.52
5:F:358:LEU:CD2	5:F:370:LYS:HE3	2.40	0.52
5:F:408:LEU:O	5:F:412:GLU:HG2	2.10	0.52
1:L:125:PRO:HD2	9:L:4231:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:18:LEU:HD23	2:M:404:LEU:HD21	1.92	0.52
2:M:332:ARG:NH2	2:M:464:LEU:HD11	2.25	0.52
2:M:334:ARG:CZ	2:M:418:LEU:HD21	2.40	0.52
2:M:724:ARG:HG3	2:M:741:GLY:N	2.24	0.52
2:M:1035:MET:HG2	3:N:707:THR:O	2.09	0.52
3:N:135:LEU:HD11	3:N:452:ILE:HG13	1.91	0.52
3:N:658:LEU:O	3:N:661:MET:HB2	2.09	0.52
3:N:731:LEU:HB2	9:N:9614:HOH:O	2.10	0.52
3:N:1443:THR:HG23	9:N:2462:HOH:O	2.10	0.52
5:P:337:HIS:CD2	5:P:337:HIS:H	2.28	0.52
2:C:389:SER:C	2:C:391:LEU:N	2.68	0.51
2:C:742:VAL:HG12	2:C:743:VAL:N	2.25	0.51
3:D:97:THR:CG2	3:D:571:LYS:HD3	2.40	0.51
3:D:134:VAL:HG12	3:D:152:LEU:HB3	1.93	0.51
3:D:572:ARG:HH12	5:F:79:ASP:CG	2.18	0.51
3:D:592:THR:N	3:D:600:LEU:HD21	2.24	0.51
5:F:128:ARG:O	5:F:132:ARG:HG3	2.10	0.51
5:F:171:LYS:HE3	5:F:175:HIS:NE2	2.25	0.51
5:F:323:ASP:O	5:F:325:LYS:N	2.43	0.51
1:L:19:GLU:O	1:L:201:THR:HG23	2.09	0.51
1:L:170:VAL:HG23	9:L:5477:HOH:O	2.10	0.51
2:M:998:TYR:OH	2:M:1000:MET:HA	2.10	0.51
3:N:206:ARG:O	3:N:206:ARG:HD3	2.10	0.51
3:N:789:LEU:O	3:N:792:ILE:HG23	2.09	0.51
3:N:1366:LYS:O	3:N:1369:GLU:HB2	2.10	0.51
5:P:129:GLU:HB3	5:P:142:ARG:HH21	1.75	0.51
2:C:101:ILE:HG22	2:C:102:HIS:N	2.25	0.51
2:C:333:ILE:N	2:C:333:ILE:HD12	2.25	0.51
2:C:333:ILE:HD13	2:C:467:ILE:HG13	1.92	0.51
2:C:595:LEU:O	2:C:655:LEU:HG	2.10	0.51
2:C:710:ILE:HD11	2:C:758:ARG:NH2	2.26	0.51
2:C:1057:SER:HB2	3:D:622:ARG:O	2.09	0.51
3:D:105:VAL:HG12	3:D:106:LYS:HZ2	1.74	0.51
3:D:171:LEU:HD13	3:D:389:GLU:C	2.35	0.51
3:D:416:ALA:H	3:D:417:PRO:CD	2.23	0.51
3:D:478:LEU:HD21	3:D:500:ARG:HH21	1.75	0.51
3:D:480:GLU:O	3:D:484:PRO:HD2	2.10	0.51
3:D:491:LYS:HD3	3:D:492:ALA:N	2.26	0.51
3:D:505:SER:HB3	9:D:9680:HOH:O	2.09	0.51
3:D:553:ARG:HH12	5:F:211:ASP:HA	1.75	0.51
3:D:1240:THR:HA	9:D:2338:HOH:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1290:LEU:HD22	3:D:1291:SER:H	1.75	0.51
3:D:1417:TRP:HE1	3:D:1419:PRO:HG3	1.75	0.51
5:F:132:ARG:NH2	5:F:184:ARG:NH1	2.59	0.51
5:F:209:PHE:CE2	5:F:213:ILE:HD11	2.45	0.51
5:F:420:ASP:O	5:F:422:LEU:HD23	2.11	0.51
2:M:101:ILE:HG22	2:M:102:HIS:N	2.26	0.51
2:M:148:PHE:CZ	2:M:281:LEU:HD13	2.45	0.51
2:M:461:VAL:HG22	9:M:9987:HOH:O	2.10	0.51
9:M:2035:HOH:O	3:N:1456:LYS:HE2	2.10	0.51
3:N:123:LEU:HG	3:N:152:LEU:HD13	1.92	0.51
1:A:26:GLU:CB	1:A:194:LYS:HG3	2.41	0.51
2:C:65:VAL:HB	2:C:101:ILE:HB	1.92	0.51
2:C:89:THR:O	2:C:91:GLN:HG3	2.09	0.51
2:C:208:ALA:HB1	2:C:218:VAL:HG13	1.92	0.51
2:C:209:ARG:O	2:C:213:ALA:HB2	2.11	0.51
2:C:254:VAL:HG22	9:C:2339:HOH:O	2.10	0.51
2:C:436:GLY:HA3	2:C:469:THR:HG21	1.92	0.51
2:C:791:ARG:HB3	2:C:791:ARG:NH1	2.25	0.51
2:C:1030:GLN:HE22	3:D:628:ARG:NH2	2.08	0.51
3:D:974:ILE:HG22	9:D:9555:HOH:O	2.11	0.51
2:M:182:VAL:HB	2:M:192:PRO:HA	1.92	0.51
2:M:197:LEU:HD22	2:M:202:TYR:CD2	2.45	0.51
2:M:498:GLN:HG3	2:M:516:ARG:HH21	1.75	0.51
2:M:679:PHE:HD1	2:M:870:ILE:HD13	1.74	0.51
2:M:739:GLU:HA	9:M:2220:HOH:O	2.09	0.51
2:M:890:LEU:HA	2:M:914:ILE:HD11	1.91	0.51
2:M:1090:LYS:HG2	2:M:1112:PHE:CZ	2.44	0.51
3:N:196:VAL:HG13	3:N:202:VAL:CG1	2.40	0.51
3:N:404:GLU:OE1	3:N:414:ARG:HD3	2.10	0.51
3:N:423:ASP:HB2	5:P:178:ARG:CD	2.30	0.51
3:N:1066:THR:HG22	3:N:1069:GLU:HB2	1.90	0.51
3:N:1380:GLU:HG3	3:N:1381:VAL:H	1.75	0.51
1:A:227:ASN:ND2	1:A:227:ASN:H	2.09	0.51
1:B:106:PRO:HB3	9:B:9545:HOH:O	2.10	0.51
1:B:182:GLU:O	1:B:194:LYS:HB3	2.11	0.51
2:C:101:ILE:HG23	2:C:107:LEU:CD2	2.38	0.51
2:C:515:ALA:C	2:C:516:ARG:HG2	2.35	0.51
3:D:603:LEU:O	3:D:606:ILE:HB	2.10	0.51
3:D:794:GLN:HG2	3:D:905:PRO:HB3	1.91	0.51
3:D:1149:LEU:HD12	3:D:1161:GLU:O	2.11	0.51
3:D:1235:GLN:HB3	3:D:1359:GLN:HE22	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:150:TYR:CE1	2:M:696:LYS:HA	2.44	0.51
1:L:91:ASN:O	1:L:94:LEU:HD12	2.09	0.51
2:M:26:TYR:CE2	2:M:30:LEU:HD11	2.46	0.51
2:M:137:VAL:HG23	2:M:391:LEU:HG	1.91	0.51
2:M:257:VAL:HG22	9:M:9998:HOH:O	2.10	0.51
2:M:722:ILE:CD1	2:M:823:VAL:HG21	2.39	0.51
5:P:142:ARG:HH11	5:P:142:ARG:CB	2.22	0.51
5:P:306:GLU:O	5:P:310:ILE:HG13	2.10	0.51
5:P:323:ASP:O	5:P:325:LYS:N	2.43	0.51
1:A:24:VAL:HG22	1:A:196:THR:HB	1.92	0.51
2:C:83:CYS:HA	2:C:88:LEU:HD23	1.92	0.51
2:C:129:ILE:HD13	2:C:134:ARG:HB2	1.93	0.51
2:C:993:PHE:CD1	2:C:993:PHE:C	2.88	0.51
3:D:44:LEU:O	3:D:525:ARG:NH2	2.43	0.51
3:D:540:LEU:HA	3:D:543:LEU:HD12	1.92	0.51
3:D:807:ALA:HA	9:D:9904:HOH:O	2.10	0.51
3:D:887:ALA:HA	9:D:9543:HOH:O	2.09	0.51
3:D:1057:VAL:HA	3:D:1069:GLU:OE2	2.10	0.51
3:D:1066:THR:HG23	3:D:1068:LEU:H	1.75	0.51
3:D:1235:GLN:C	3:D:1359:GLN:HE22	2.18	0.51
3:D:1318:TYR:HD1	3:D:1319:VAL:N	2.09	0.51
5:F:132:ARG:HG2	5:F:181:GLU:OE1	2.10	0.51
1:K:94:LEU:HD21	1:K:119:ASP:HB2	1.93	0.51
1:L:121:GLU:HG3	9:L:3921:HOH:O	2.10	0.51
1:L:184:THR:O	1:L:192:LEU:HB2	2.10	0.51
2:M:52:PHE:HE1	2:M:66:LEU:HG	1.75	0.51
2:M:205:GLU:CD	2:M:206:THR:N	2.68	0.51
2:M:269:LEU:HD12	2:M:288:ARG:H	1.76	0.51
3:N:493:ARG:HH22	3:N:1388:ARG:HB3	1.76	0.51
3:N:637:LEU:HD11	3:N:642:CYS:N	2.26	0.51
3:N:1380:GLU:HG3	3:N:1381:VAL:N	2.25	0.51
4:O:37:ASN:ND2	4:O:89:MET:HE2	2.24	0.51
4:O:70:THR:HB	4:O:72:ARG:HE	1.75	0.51
5:P:93:LEU:HG	5:P:190:ALA:CB	2.40	0.51
5:P:416:ARG:HD2	5:P:419:ARG:HB3	1.91	0.51
1:A:219:ARG:CZ	1:B:219:ARG:HG2	2.41	0.51
1:B:18:ARG:O	1:B:207:PRO:HD3	2.11	0.51
1:B:23:PHE:HE2	1:B:199:ILE:HD12	1.76	0.51
2:C:132:ALA:HB1	2:C:632:ASN:ND2	2.23	0.51
2:C:208:ALA:HA	2:C:218:VAL:HG22	1.93	0.51
2:C:565:GLN:OE1	2:C:842:ARG:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:886:LEU:HD23	3:D:951:ILE:HG13	1.91	0.51
2:C:958:THR:HG23	2:C:961:GLU:H	1.74	0.51
2:C:1014:SER:HA	9:F:9484:HOH:O	2.11	0.51
2:C:1014:SER:OG	5:F:331:ASP:HA	2.11	0.51
3:D:704:ARG:HB2	3:D:736:PHE:CD2	2.46	0.51
3:D:890:VAL:HG11	3:D:922:LEU:HD13	1.93	0.51
3:D:1109:GLU:HG2	3:D:1201:CYS:CA	2.37	0.51
2:M:166:PRO:HG3	2:M:265:ARG:HE	1.74	0.51
2:M:879:ARG:HH12	3:N:1029:ARG:HH22	1.58	0.51
2:M:1086:ARG:HB3	2:M:1112:PHE:CE2	2.45	0.51
3:N:52:PRO:HG3	3:N:78:VAL:HG13	1.92	0.51
3:N:119:SER:HB2	3:N:123:LEU:CB	2.40	0.51
3:N:937:TYR:O	3:N:941:PHE:HD1	1.93	0.51
1:A:146:ARG:HD2	9:A:9500:HOH:O	2.10	0.51
2:C:332:ARG:HE	2:C:464:LEU:HD11	1.75	0.51
2:C:437:ARG:HA	2:C:467:ILE:HG21	1.91	0.51
2:C:495:THR:HB	2:C:530:GLU:HG3	1.93	0.51
2:C:663:ASN:HB2	9:C:2433:HOH:O	2.11	0.51
3:D:36:THR:O	3:D:38:LYS:N	2.44	0.51
3:D:154:THR:HA	9:D:9863:HOH:O	2.10	0.51
3:D:519:VAL:HG13	3:D:544:TYR:CE1	2.46	0.51
3:D:864:VAL:HG12	3:D:865:THR:H	1.75	0.51
3:D:970:LYS:HB2	3:D:970:LYS:NZ	2.25	0.51
3:D:1104:GLU:O	3:D:1106:VAL:HG23	2.10	0.51
3:D:1264:GLU:CD	3:D:1425:THR:H	2.19	0.51
3:D:1333:HIS:O	3:D:1336:LEU:HB3	2.10	0.51
5:F:287:THR:C	5:F:289:GLU:H	2.18	0.51
1:K:9:PRO:HB2	1:L:224:TYR:HB3	1.93	0.51
1:K:95:GLN:HG2	1:K:146:ARG:HH12	1.74	0.51
1:K:133:GLU:OE1	2:M:605:LYS:HB3	2.11	0.51
2:M:122:THR:HG21	9:M:2321:HOH:O	2.11	0.51
2:M:182:VAL:HG13	9:M:9636:HOH:O	2.08	0.51
2:M:232:GLU:O	2:M:235:LEU:HB2	2.10	0.51
2:M:759:THR:HB	2:M:785:VAL:CG2	2.41	0.51
2:M:877:PRO:HB3	3:N:1020:LEU:HD13	1.93	0.51
9:M:9978:HOH:O	5:P:345:ALA:HB1	2.09	0.51
3:N:191:LEU:HB3	3:N:195:VAL:HG21	1.93	0.51
3:N:421:LEU:HD12	3:N:435:VAL:CG1	2.41	0.51
3:N:539:ASP:HB3	9:N:9742:HOH:O	2.11	0.51
3:N:565:ILE:CD1	5:P:189:GLU:HG2	2.41	0.51
3:N:1492:LEU:O	3:N:1496:GLU:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:PHE:HD1	1:A:25:LEU:HD12	1.76	0.51
2:C:238:LEU:HB2	9:C:2083:HOH:O	2.11	0.51
2:C:549:PHE:CE2	2:C:886:LEU:HB3	2.46	0.51
2:C:876:VAL:HB	2:C:877:PRO:HD3	1.92	0.51
2:C:901:TYR:CE2	2:C:917:LEU:HD13	2.46	0.51
3:D:530:VAL:HB	3:D:534:ARG:CB	2.38	0.51
3:D:797:LYS:NZ	3:D:1016:PRO:HB3	2.26	0.51
3:D:829:VAL:HG21	9:D:9486:HOH:O	2.10	0.51
3:D:908:LYS:HG2	3:D:1027:GLY:HA3	1.91	0.51
3:D:1045:MET:HA	3:D:1045:MET:HE3	1.92	0.51
3:D:1292:VAL:H	3:D:1305:LEU:HD21	1.76	0.51
2:M:392:SER:O	7:M:8002:RPT:H371	2.11	0.51
2:M:437:ARG:C	2:M:438:ILE:HD12	2.35	0.51
2:M:676:ILE:HG23	9:M:9722:HOH:O	2.10	0.51
2:M:783:ARG:HG2	2:M:785:VAL:HG12	1.92	0.51
2:M:838:LYS:CD	2:M:846:LYS:HZ3	2.24	0.51
2:M:958:THR:HG23	9:M:9678:HOH:O	2.10	0.51
2:M:976:ASP:OD1	2:M:978:ARG:HG3	2.11	0.51
2:M:1104:GLU:H	2:M:1104:GLU:CD	2.19	0.51
3:N:527:MET:HE3	5:P:258:ILE:HD11	1.91	0.51
3:N:546:ARG:CZ	3:N:550:ARG:HH22	2.22	0.51
3:N:823:LEU:HD23	3:N:823:LEU:H	1.76	0.51
3:N:1020:LEU:HA	3:N:1023:MET:CE	2.41	0.51
1:A:70:GLY:HA2	1:A:133:GLU:OE2	2.09	0.51
2:C:292:ARG:HG2	9:C:2101:HOH:O	2.11	0.51
2:C:328:LEU:HD23	2:C:437:ARG:HD3	1.93	0.51
2:C:1027:PHE:HA	9:C:9777:HOH:O	2.10	0.51
3:D:704:ARG:HH11	3:D:738:ALA:HA	1.75	0.51
3:D:770:LEU:HG	3:D:919:PHE:HE1	1.75	0.51
3:D:1333:HIS:CE1	3:D:1421:LEU:HD23	2.45	0.51
4:E:91:ARG:HD2	9:E:9516:HOH:O	2.11	0.51
5:F:152:ASP:HB2	5:F:153:PRO:HD3	1.92	0.51
5:F:260:ILE:HG23	5:F:264:MET:CG	2.40	0.51
5:F:365:GLU:OE1	5:F:400:ILE:HD12	2.11	0.51
1:K:117:VAL:HG22	9:K:3709:HOH:O	2.10	0.51
2:M:744:ARG:HG3	2:M:747:ALA:HB2	1.93	0.51
2:M:777:ILE:HG22	2:M:778:PHE:CD1	2.45	0.51
3:N:180:LYS:O	3:N:184:GLU:HG3	2.11	0.51
3:N:183:GLU:O	3:N:186:VAL:HG12	2.11	0.51
3:N:423:ASP:HB3	5:P:175:HIS:HA	1.93	0.51
1:B:184:THR:HG23	1:B:192:LEU:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:28:ARG:HG3	2:C:40:GLU:OE1	2.10	0.51
2:C:520:GLU:HB2	9:C:2128:HOH:O	2.11	0.51
2:C:760:SER:O	2:C:785:VAL:HG22	2.10	0.51
2:C:1083:GLU:HG2	9:C:9596:HOH:O	2.11	0.51
2:C:1097:LEU:HD22	2:C:1097:LEU:H	1.76	0.51
3:D:49:ILE:HB	3:D:50:PHE:CD1	2.45	0.51
3:D:750:PRO:HB2	3:D:756:GLN:OE1	2.11	0.51
3:D:805:GLU:OE1	3:D:809:PRO:HD2	2.11	0.51
3:D:1410:GLU:HG2	9:D:2012:HOH:O	2.10	0.51
5:F:352:GLU:HG3	9:F:9610:HOH:O	2.11	0.51
1:L:109:VAL:HG21	1:L:138:LEU:HD21	1.92	0.51
1:L:215:VAL:HG21	9:L:5732:HOH:O	2.10	0.51
2:M:132:ALA:HB1	2:M:632:ASN:ND2	2.26	0.51
2:M:257:VAL:HA	9:M:2289:HOH:O	2.11	0.51
2:M:405:ARG:NH2	2:M:566:THR:HG21	2.26	0.51
2:M:774:LEU:HA	2:M:777:ILE:HD12	1.93	0.51
3:N:105:VAL:HG21	3:N:128:TYR:CE2	2.35	0.51
1:B:75:VAL:O	1:B:79:ILE:HG23	2.11	0.50
2:C:54:ILE:HG22	2:C:66:LEU:HB3	1.93	0.50
2:C:1052:MET:HG3	3:D:623:VAL:CG2	2.41	0.50
2:C:1081:VAL:HG12	2:C:1086:ARG:HE	1.76	0.50
3:D:566:ILE:HG23	5:F:217:ASN:HD22	1.77	0.50
3:D:1150:ALA:HA	9:D:2006:HOH:O	2.10	0.50
3:D:1478:SER:O	3:D:1482:ARG:HG3	2.10	0.50
2:M:420:ARG:H	2:M:420:ARG:CD	2.22	0.50
2:M:872:ASN:ND2	2:M:874:LEU:HB2	2.26	0.50
3:N:209:ARG:HG3	9:N:2381:HOH:O	2.09	0.50
5:P:101:GLU:HA	5:P:104:ARG:NH1	2.26	0.50
5:P:416:ARG:HB3	5:P:419:ARG:HG2	1.93	0.50
5:P:419:ARG:O	5:P:421:PHE:N	2.44	0.50
1:A:211:LEU:O	1:A:215:VAL:HG13	2.11	0.50
2:C:21:ILE:H	2:C:21:ILE:HD12	1.76	0.50
2:C:162:ILE:HB	2:C:172:ILE:HD13	1.93	0.50
2:C:263:ASP:HB2	2:C:264:PRO:HD3	1.92	0.50
2:C:338:GLU:O	2:C:341:THR:HG22	2.11	0.50
2:C:523:ILE:HG21	9:D:2662:HOH:O	2.12	0.50
2:C:572:ILE:HG21	2:C:703:ILE:HD13	1.93	0.50
2:C:971:LYS:HD2	2:C:986:PRO:HB2	1.92	0.50
3:D:161:LEU:HD13	3:D:452:ILE:HD12	1.94	0.50
3:D:965:GLU:HG3	3:D:969:ARG:NH2	2.23	0.50
3:D:1063:GLU:HG2	3:D:1064:GLY:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1136:LYS:HB2	3:D:1139:ASP:OD2	2.11	0.50
5:F:362:SER:HB2	9:F:9725:HOH:O	2.10	0.50
1:K:68:ILE:HA	9:K:4093:HOH:O	2.11	0.50
2:M:265:ARG:HB3	2:M:267:TYR:CE2	2.46	0.50
2:M:682:TYR:N	9:M:9536:HOH:O	2.44	0.50
2:M:841:ASN:HB2	9:M:9839:HOH:O	2.11	0.50
3:N:12:LEU:HB2	9:N:9590:HOH:O	2.11	0.50
3:N:603:LEU:O	3:N:606:ILE:HB	2.11	0.50
3:N:737:ASN:HA	9:N:9612:HOH:O	2.10	0.50
3:N:1026:SER:C	3:N:1028:ALA:H	2.17	0.50
3:N:1281:VAL:HG21	3:N:1313:VAL:CG2	2.40	0.50
1:A:18:ARG:HH11	1:A:123:MET:HE1	1.76	0.50
1:A:156:HIS:NE2	1:A:166:PRO:HB3	2.26	0.50
1:B:72:LYS:HE2	1:B:131:THR:OG1	2.11	0.50
2:C:80:GLN:HG2	2:C:90:TYR:CE2	2.47	0.50
2:C:625:LEU:O	2:C:627:ARG:N	2.45	0.50
3:D:132:TYR:HD2	9:D:9863:HOH:O	1.93	0.50
3:D:656:PHE:HB3	3:D:694:VAL:HG11	1.93	0.50
3:D:1324:PRO:HG3	3:D:1330:ILE:HD11	1.92	0.50
5:F:126:LEU:O	5:F:130:VAL:HG23	2.11	0.50
5:F:258:ILE:HB	9:F:9558:HOH:O	2.12	0.50
1:K:97:VAL:HG23	9:K:3291:HOH:O	2.11	0.50
2:M:91:GLN:CD	2:M:117:HIS:HB3	2.37	0.50
2:M:132:ALA:HB1	2:M:632:ASN:HD21	1.77	0.50
2:M:333:ILE:HD12	2:M:465:GLY:O	2.11	0.50
2:M:666:LEU:HD12	2:M:667:ALA:H	1.76	0.50
2:M:676:ILE:HG23	2:M:676:ILE:O	2.10	0.50
2:M:721:ARG:HH22	2:M:785:VAL:HG21	1.76	0.50
2:M:790:LEU:C	2:M:790:LEU:HD23	2.35	0.50
2:M:996:LYS:HD2	9:M:9662:HOH:O	2.11	0.50
2:M:1051:GLU:HG3	2:M:1055:LEU:HB2	1.92	0.50
3:N:14:SER:OG	3:N:17:LYS:HB2	2.11	0.50
3:N:39:PRO:HD2	9:N:2247:HOH:O	2.11	0.50
3:N:101:HIS:CD2	3:N:582:LEU:HD13	2.45	0.50
3:N:434:ARG:HB2	3:N:447:VAL:CG1	2.41	0.50
3:N:574:LEU:O	3:N:577:ALA:HB3	2.11	0.50
3:N:814:ALA:HB3	9:N:2003:HOH:O	2.11	0.50
3:N:1156:LEU:CD1	3:N:1176:LYS:HD2	2.41	0.50
3:N:1493:LYS:HD3	3:N:1496:GLU:OE2	2.12	0.50
4:O:51:LEU:HG	4:O:53:GLY:N	2.26	0.50
1:A:14:ARG:NH1	1:A:24:VAL:HG23	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:ASP:HB3	9:A:9649:HOH:O	2.10	0.50
1:B:13:VAL:HG13	1:B:23:PHE:CD1	2.46	0.50
1:B:189:ARG:HH11	1:B:189:ARG:HG3	1.75	0.50
2:C:425:PHE:HB2	9:C:9673:HOH:O	2.11	0.50
3:D:519:VAL:HA	3:D:544:TYR:OH	2.12	0.50
3:D:762:GLN:NE2	4:E:20:THR:HG21	2.26	0.50
3:D:1262:LEU:HD23	3:D:1352:ILE:CG1	2.40	0.50
4:E:64:ALA:O	4:E:67:GLU:HG3	2.12	0.50
5:F:112:ALA:HA	5:F:173:TYR:CD2	2.46	0.50
1:K:19:GLU:HB3	9:K:4176:HOH:O	2.11	0.50
2:M:462:ASP:HA	9:M:2351:HOH:O	2.12	0.50
3:N:108:VAL:CG2	3:N:109:PRO:HD3	2.40	0.50
3:N:119:SER:N	3:N:123:LEU:HD22	2.22	0.50
2:C:230:ARG:HG3	9:C:9560:HOH:O	2.11	0.50
2:C:436:GLY:O	2:C:459:ALA:HB2	2.12	0.50
2:C:1091:GLU:HG2	3:D:606:ILE:HG21	1.94	0.50
3:D:493:ARG:NH1	3:D:1390:LEU:H	2.08	0.50
3:D:826:PRO:HB3	3:D:828:LYS:NZ	2.27	0.50
5:F:111:GLU:O	5:F:115:LYS:HG2	2.11	0.50
1:L:180:GLN:HG3	9:L:3887:HOH:O	2.10	0.50
2:M:304:LEU:HD23	2:M:305:PRO:HD3	1.92	0.50
2:M:964:LYS:HB3	9:M:9902:HOH:O	2.11	0.50
3:N:131:LYS:HB3	9:N:2083:HOH:O	2.11	0.50
3:N:963:TYR:CD2	3:N:1002:LYS:HB3	2.46	0.50
3:N:1136:LYS:HE3	3:N:1136:LYS:H	1.76	0.50
1:B:38:ASN:HB2	9:B:9725:HOH:O	2.10	0.50
2:C:302:VAL:O	2:C:305:PRO:HD2	2.12	0.50
2:C:462:ASP:HA	9:C:9665:HOH:O	2.11	0.50
2:C:886:LEU:HG	3:D:951:ILE:HG13	1.93	0.50
3:D:500:ARG:HH22	3:D:1388:ARG:HH11	1.60	0.50
3:D:699:VAL:HG12	3:D:717:GLN:CA	2.40	0.50
3:D:1192:LEU:CD2	3:D:1345:GLU:HG2	2.39	0.50
5:F:109:GLY:O	5:F:113:ILE:HG13	2.12	0.50
2:M:160:ALA:O	2:M:173:ASP:HA	2.12	0.50
2:M:197:LEU:HD22	2:M:202:TYR:HD2	1.75	0.50
2:M:252:LYS:HZ3	2:M:296:GLY:HA3	1.75	0.50
2:M:260:LEU:HA	2:M:291:ALA:CB	2.42	0.50
2:M:768:THR:CB	2:M:771:GLU:HB3	2.41	0.50
2:M:841:ASN:HD21	2:M:845:ASN:H	1.59	0.50
2:M:984:GLU:HA	9:M:2224:HOH:O	2.10	0.50
2:M:1000:MET:HE2	9:M:9742:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:420:VAL:O	5:P:164:LYS:HD3	2.12	0.50
3:N:960:LYS:HB3	9:N:9922:HOH:O	2.12	0.50
4:O:32:ARG:HB3	9:O:5813:HOH:O	2.11	0.50
5:P:261:PRO:O	5:P:265:VAL:HG23	2.11	0.50
1:A:16:GLN:NE2	1:A:17:GLY:N	2.60	0.50
1:A:197:LEU:N	1:A:197:LEU:HD23	2.26	0.50
2:C:161:SER:HB3	9:C:2166:HOH:O	2.11	0.50
2:C:408:ARG:NH1	2:C:542:VAL:HG23	2.27	0.50
2:C:413:LEU:HD12	2:C:413:LEU:N	2.27	0.50
2:C:432:ARG:HD3	3:D:1048:PRO:CG	2.42	0.50
2:C:508:ILE:HG21	9:C:9927:HOH:O	2.12	0.50
2:C:561:GLY:HA3	2:C:842:ARG:O	2.11	0.50
2:C:724:ARG:CG	2:C:740:GLU:HA	2.42	0.50
2:C:1008:ARG:HE	2:C:1028:GLY:CA	2.24	0.50
3:D:18:ILE:HD12	3:D:518:PRO:CG	2.42	0.50
3:D:521:PRO:C	3:D:525:ARG:HH11	2.20	0.50
3:D:677:LEU:HD21	3:D:687:VAL:HG21	1.94	0.50
3:D:872:ARG:HB3	9:D:9540:HOH:O	2.11	0.50
3:D:1103:HIS:CD2	3:D:1463:LYS:H	2.30	0.50
3:D:1336:LEU:HD21	3:D:1419:PRO:O	2.12	0.50
5:F:220:LEU:HD21	9:F:9537:HOH:O	2.12	0.50
5:F:237:THR:HB	9:F:9628:HOH:O	2.11	0.50
1:K:184:THR:O	1:K:192:LEU:HD12	2.12	0.50
2:M:143:SER:HB2	2:M:332:ARG:HB2	1.93	0.50
2:M:435:TYR:C	2:M:437:ARG:H	2.18	0.50
2:M:637:LEU:HA	2:M:659:PRO:HG3	1.94	0.50
2:M:721:ARG:O	2:M:758:ARG:HA	2.11	0.50
2:M:821:GLU:HA	9:M:9975:HOH:O	2.12	0.50
2:M:872:ASN:HD21	2:M:874:LEU:HB2	1.76	0.50
2:M:939:ARG:HB3	2:M:982:PRO:HG3	1.94	0.50
3:N:546:ARG:NH1	3:N:550:ARG:HH22	2.09	0.50
3:N:559:ALA:O	5:P:132:ARG:NH2	2.44	0.50
3:N:957:PRO:CG	3:N:1007:VAL:HA	2.42	0.50
5:P:358:LEU:HD21	5:P:370:LYS:HE3	1.94	0.50
1:A:101:LEU:HD11	1:A:113:ASP:HB2	1.94	0.50
1:B:42:ARG:HG2	1:B:42:ARG:HH11	1.76	0.50
2:C:137:VAL:HG21	2:C:393:GLN:HE21	1.76	0.50
2:C:404:LEU:HD13	9:C:9579:HOH:O	2.12	0.50
2:C:630:ARG:HH22	2:C:707:ARG:HB2	1.76	0.50
7:C:8001:RPT:H422	9:C:9511:HOH:O	2.11	0.50
3:D:32:ILE:HD12	3:D:527:MET:HG2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:183:GLU:HA	3:D:186:VAL:CG1	2.42	0.50
3:D:211:VAL:HG13	3:D:393:ILE:HA	1.93	0.50
3:D:465:LEU:HD22	3:D:509:PRO:O	2.12	0.50
3:D:553:ARG:HH22	5:F:211:ASP:CG	2.19	0.50
3:D:1047:LYS:HB3	3:D:1048:PRO:CD	2.42	0.50
3:D:1047:LYS:HG2	3:D:1053:PHE:CE2	2.46	0.50
3:D:1283:ILE:N	3:D:1315:ASP:OD1	2.43	0.50
3:D:1440:PHE:HD1	3:D:1441:GLN:H	1.59	0.50
2:M:413:LEU:HD12	2:M:413:LEU:H	1.77	0.50
2:M:693:GLU:HA	2:M:696:LYS:HG3	1.94	0.50
2:M:808:ARG:HG2	2:M:808:ARG:HH11	1.75	0.50
2:M:1019:GLN:HE22	3:N:621:LYS:HA	1.76	0.50
3:N:12:LEU:HD11	3:N:512:MET:HG2	1.93	0.50
3:N:28:LYS:CB	3:N:41:ARG:HD2	2.42	0.50
3:N:950:GLY:O	3:N:951:ILE:C	2.54	0.50
3:N:959:GLU:HG3	3:N:1006:ALA:HB1	1.94	0.50
3:N:1045:MET:HA	9:N:2418:HOH:O	2.12	0.50
3:N:1169:ASP:HB2	9:N:2387:HOH:O	2.12	0.50
3:N:1462:LEU:HD22	3:N:1472:ILE:CG2	2.42	0.50
5:P:225:GLU:HG3	5:P:226:LYS:HG2	1.94	0.50
5:P:419:ARG:HB2	5:P:419:ARG:HH11	1.77	0.50
2:C:25:SER:CB	2:C:335:THR:HB	2.42	0.50
2:C:165:LEU:HD12	2:C:166:PRO:C	2.37	0.50
2:C:952:LEU:HB3	2:C:966:LEU:CD1	2.42	0.50
2:C:1005:MET:CE	3:D:648:MET:HB2	2.40	0.50
3:D:58:CYS:HA	3:D:78:VAL:HG11	1.93	0.50
3:D:521:PRO:O	3:D:525:ARG:HG2	2.12	0.50
3:D:561:GLY:HA3	5:F:184:ARG:NH2	2.25	0.50
3:D:607:LEU:HB3	3:D:614:PHE:CE2	2.47	0.50
3:D:637:LEU:HD12	3:D:641:GLN:OE1	2.12	0.50
3:D:796:ARG:NH1	3:D:861:GLN:HB2	2.25	0.50
3:D:1108:ARG:HH12	3:D:1460:ILE:HG22	1.77	0.50
3:D:1120:VAL:HB	3:D:1144:LEU:HD21	1.94	0.50
4:E:9:LEU:HD22	4:E:19:LEU:HD13	1.94	0.50
2:M:57:GLU:HG3	2:M:58:ASP:OD2	2.12	0.50
2:M:159:ILE:C	9:M:9990:HOH:O	2.55	0.50
2:M:289:THR:HG22	2:M:290:LEU:H	1.76	0.50
2:M:352:ALA:HA	2:M:355:VAL:HG12	1.92	0.50
2:M:367:LEU:O	2:M:372:LEU:HD13	2.12	0.50
2:M:479:VAL:CG2	2:M:503:LEU:HD11	2.41	0.50
2:M:594:ALA:HB1	2:M:654:LEU:HD12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:605:LYS:HD3	2:M:610:ARG:NH2	2.26	0.50
2:M:1016:ILE:CD1	5:P:317:LEU:HD21	2.42	0.50
3:N:10:ILE:HD11	3:N:1434:TRP:NE1	2.26	0.50
3:N:126:VAL:O	3:N:132:TYR:HD1	1.94	0.50
3:N:493:ARG:O	3:N:497:GLU:HG3	2.11	0.50
3:N:573:MET:SD	5:P:210:LEU:HD22	2.51	0.50
3:N:818:ARG:HG3	9:N:2703:HOH:O	2.11	0.50
3:N:966:GLU:HG2	9:N:9886:HOH:O	2.11	0.50
3:N:1047:LYS:HA	3:N:1053:PHE:CE1	2.47	0.50
3:N:1077:ALA:HA	9:N:9982:HOH:O	2.11	0.50
4:O:84:ARG:NH1	9:O:4797:HOH:O	2.44	0.50
1:A:59:GLU:HG3	1:A:139:ASN:CG	2.37	0.49
1:A:209:GLU:O	1:A:213:GLN:HG3	2.11	0.49
1:B:204:SER:HB2	9:B:9508:HOH:O	2.11	0.49
1:B:211:LEU:O	1:B:215:VAL:HG13	2.12	0.49
2:C:52:PHE:CD2	2:C:68:PHE:HB2	2.47	0.49
2:C:339:LEU:HD22	2:C:391:LEU:HD13	1.94	0.49
2:C:505:GLY:HA3	9:C:9890:HOH:O	2.11	0.49
2:C:557:ARG:NH1	2:C:879:ARG:HD3	2.26	0.49
2:C:817:PRO:C	2:C:819:VAL:H	2.20	0.49
2:C:976:ASP:HB2	2:C:979:THR:HG22	1.93	0.49
2:C:1012:PRO:HD2	2:C:1021:LEU:O	2.12	0.49
2:C:1015:LEU:HA	9:C:9604:HOH:O	2.12	0.49
3:D:818:ARG:HB3	9:D:9509:HOH:O	2.12	0.49
3:D:1009:LYS:HA	3:D:1012:GLU:OE2	2.12	0.49
5:F:142:ARG:HB3	5:F:142:ARG:HH11	1.76	0.49
1:K:184:THR:HG23	1:K:192:LEU:HB3	1.94	0.49
1:L:29:GLU:N	9:L:5175:HOH:O	2.45	0.49
2:M:68:PHE:HB3	9:M:9640:HOH:O	2.11	0.49
2:M:170:PRO:HG2	2:M:258:TYR:CD2	2.47	0.49
2:M:176:VAL:HG12	2:M:182:VAL:CG1	2.42	0.49
2:M:345:ARG:HB3	2:M:345:ARG:HH11	1.77	0.49
2:M:781:LYS:HG2	9:M:2296:HOH:O	2.11	0.49
2:M:807:ARG:HB2	2:M:807:ARG:CZ	2.40	0.49
3:N:191:LEU:HD12	3:N:211:VAL:HG21	1.92	0.49
3:N:550:ARG:NH1	3:N:550:ARG:HG3	2.26	0.49
3:N:619:LEU:HD13	9:N:9535:HOH:O	2.10	0.49
3:N:1172:HIS:HE1	9:N:2297:HOH:O	1.95	0.49
3:N:1278:ASP:HA	3:N:1319:VAL:O	2.12	0.49
2:C:54:ILE:CD1	2:C:356:ARG:HG2	2.35	0.49
2:C:367:LEU:O	2:C:371:LYS:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:441:VAL:HG12	2:C:559:LEU:HA	1.93	0.49
2:C:498:GLN:HG3	9:C:9731:HOH:O	2.12	0.49
2:C:569:VAL:HG12	2:C:996:LYS:O	2.12	0.49
2:C:690:ILE:CG2	2:C:852:ILE:HG23	2.39	0.49
2:C:745:ILE:HD11	9:C:9745:HOH:O	2.12	0.49
2:C:978:ARG:HD3	9:C:9846:HOH:O	2.11	0.49
2:C:1090:LYS:HG2	2:C:1112:PHE:CZ	2.47	0.49
3:D:608:SER:HB3	3:D:1443:THR:OG1	2.12	0.49
3:D:841:TYR:HB3	3:D:843:PHE:CE2	2.47	0.49
3:D:880:ILE:O	3:D:883:ALA:HB3	2.12	0.49
3:D:1072:ILE:O	3:D:1075:HIS:HD2	1.96	0.49
5:F:79:ASP:HB3	5:F:80:PRO:CD	2.41	0.49
5:F:323:ASP:HB3	5:F:325:LYS:HE3	1.93	0.49
5:F:411:HIS:HB2	9:F:9615:HOH:O	2.11	0.49
1:K:69:PRO:O	1:K:71:VAL:HG23	2.11	0.49
2:M:114:PHE:HD1	2:M:114:PHE:H	1.60	0.49
2:M:166:PRO:HD3	2:M:265:ARG:CB	2.42	0.49
2:M:376:ARG:HB3	2:M:377:PRO:HD3	1.95	0.49
2:M:671:ASN:HD21	2:M:993:PHE:HD2	1.60	0.49
2:M:820:ARG:HH11	2:M:820:ARG:HG2	1.76	0.49
2:M:1040:LEU:HG	2:M:1045:ALA:CB	2.42	0.49
3:N:602:SER:O	3:N:606:ILE:HG12	2.12	0.49
3:N:644:LEU:HB3	9:N:9610:HOH:O	2.11	0.49
3:N:924:MET:O	3:N:927:THR:HB	2.12	0.49
1:A:64:GLU:OE2	1:A:76:VAL:HG13	2.11	0.49
1:B:206:THR:HG22	1:B:209:GLU:H	1.77	0.49
2:C:197:LEU:HD22	2:C:202:TYR:HD2	1.77	0.49
2:C:669:GLY:HA3	2:C:995:MET:HA	1.93	0.49
2:C:768:THR:CB	2:C:771:GLU:HB3	2.42	0.49
2:C:983:ILE:HG22	2:C:987:ILE:HD11	1.94	0.49
2:C:1054:THR:HG22	2:C:1059:ASP:CB	2.41	0.49
3:D:154:THR:HG23	3:D:157:GLU:H	1.77	0.49
3:D:175:VAL:HG12	3:D:176:ASP:OD1	2.11	0.49
3:D:474:GLU:HG3	3:D:500:ARG:HE	1.77	0.49
3:D:1225:ALA:HA	3:D:1367:HIS:ND1	2.28	0.49
3:D:1455:LYS:HD3	3:D:1455:LYS:C	2.37	0.49
5:F:82:ARG:HA	9:F:9663:HOH:O	2.12	0.49
5:F:394:ARG:HG2	9:F:9632:HOH:O	2.12	0.49
1:K:9:PRO:HB3	1:K:25:LEU:HG	1.94	0.49
2:M:95:TYR:N	2:M:95:TYR:CD1	2.81	0.49
2:M:1006:HIS:O	3:N:648:MET:HE2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:93:ILE:CD1	3:N:548:ILE:HD11	2.42	0.49
3:N:399:ARG:HB2	3:N:444:VAL:HG13	1.94	0.49
3:N:795:VAL:CG1	3:N:863:VAL:HG13	2.42	0.49
3:N:1011:PHE:CD2	3:N:1021:TYR:HB2	2.47	0.49
3:N:1106:VAL:HG21	3:N:1474:ALA:HB2	1.93	0.49
4:O:47:LYS:N	4:O:54:LEU:HD22	2.27	0.49
5:P:132:ARG:O	5:P:136:LEU:HG	2.12	0.49
1:A:99:LEU:C	1:A:100:LEU:HD12	2.37	0.49
1:B:26:GLU:HG2	1:B:27:PRO:CA	2.42	0.49
2:C:51:THR:HB	2:C:348:LEU:HD23	1.94	0.49
2:C:207:LEU:HD22	2:C:221:LEU:HD22	1.94	0.49
2:C:328:LEU:CD2	2:C:437:ARG:HD3	2.43	0.49
2:C:516:ARG:NE	3:D:1068:LEU:HD13	2.27	0.49
2:C:584:GLU:HG2	9:C:9657:HOH:O	2.12	0.49
2:C:1013:TYR:HE1	2:C:1020:PRO:HG3	1.76	0.49
3:D:116:LEU:CD2	3:D:468:LEU:HD11	2.42	0.49
3:D:462:GLN:HG2	9:D:9936:HOH:O	2.12	0.49
3:D:678:GLU:HG3	3:D:679:ARG:HG3	1.94	0.49
3:D:696:HIS:HB2	4:E:48:MET:HE1	1.94	0.49
3:D:901:GLN:HG2	9:D:9763:HOH:O	2.12	0.49
3:D:1061:PHE:HE1	3:D:1065:LEU:HD23	1.78	0.49
3:D:1192:LEU:HD21	3:D:1372:VAL:CG1	2.42	0.49
3:D:1192:LEU:HD13	3:D:1345:GLU:HG2	1.94	0.49
3:D:1403:LEU:HD11	9:D:9892:HOH:O	2.11	0.49
5:F:272:SER:HB2	9:F:9540:HOH:O	2.11	0.49
2:M:54:ILE:O	2:M:54:ILE:HG23	2.13	0.49
2:M:56:GLU:HB2	2:M:64:LEU:HB3	1.94	0.49
2:M:121:MET:HB3	9:M:9714:HOH:O	2.12	0.49
2:M:209:ARG:O	2:M:213:ALA:HB2	2.12	0.49
2:M:571:LEU:HA	2:M:701:THR:O	2.13	0.49
2:M:627:ARG:O	2:M:638:ASP:HB3	2.13	0.49
2:M:640:ARG:HD3	2:M:642:ARG:HH22	1.76	0.49
2:M:752:GLY:HA3	3:N:679:ARG:HA	1.93	0.49
3:N:421:LEU:HD11	3:N:437:VAL:CG2	2.42	0.49
3:N:561:GLY:HA2	5:P:132:ARG:CZ	2.43	0.49
3:N:576:GLU:HA	3:N:579:ASP:OD2	2.12	0.49
3:N:1124:GLN:CG	3:N:1133:ARG:HD2	2.42	0.49
3:N:1333:HIS:O	3:N:1336:LEU:HB3	2.12	0.49
5:P:297:PRO:HB2	9:P:4687:HOH:O	2.13	0.49
5:P:328:PHE:O	5:P:331:ASP:N	2.35	0.49
2:C:146:VAL:HG13	2:C:161:SER:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:184:MET:HB2	2:C:193:LEU:HD12	1.95	0.49
2:C:260:LEU:HA	2:C:291:ALA:CB	2.42	0.49
2:C:301:GLU:O	2:C:305:PRO:HG2	2.13	0.49
3:D:212:ARG:HA	9:D:9662:HOH:O	2.11	0.49
3:D:434:ARG:HB2	3:D:447:VAL:HG22	1.94	0.49
3:D:860:LEU:HD23	3:D:877:PRO:CB	2.43	0.49
3:D:947:ILE:HD12	3:D:947:ILE:O	2.12	0.49
5:F:132:ARG:HG2	5:F:181:GLU:CD	2.36	0.49
5:F:217:ASN:O	5:F:221:ILE:HG13	2.12	0.49
5:F:252:ALA:HB1	5:F:265:VAL:HG21	1.93	0.49
5:F:419:ARG:O	5:F:421:PHE:N	2.46	0.49
2:M:34:VAL:CB	2:M:38:LYS:HG3	2.41	0.49
2:M:64:LEU:HD22	2:M:359:MET:HG3	1.95	0.49
2:M:98:LEU:HG	9:M:9996:HOH:O	2.12	0.49
2:M:388:ARG:HG3	9:M:9960:HOH:O	2.12	0.49
2:M:643:VAL:HG22	2:M:647:GLN:NE2	2.26	0.49
2:M:762:LYS:HD3	2:M:771:GLU:OE1	2.12	0.49
2:M:817:PRO:C	2:M:819:VAL:H	2.20	0.49
2:M:1079:PRO:HD3	9:M:2202:HOH:O	2.11	0.49
3:N:6:ARG:C	3:N:7:LYS:HG3	2.38	0.49
3:N:131:LYS:CG	3:N:568:ARG:HG2	2.42	0.49
3:N:976:GLN:HA	3:N:979:GLU:OE1	2.12	0.49
3:N:1216:SER:OG	4:O:15:SER:HA	2.12	0.49
1:A:42:ARG:HB3	9:B:9613:HOH:O	2.11	0.49
1:A:190:THR:HG22	9:A:9695:HOH:O	2.12	0.49
1:B:94:LEU:HD11	1:B:119:ASP:CB	2.42	0.49
1:B:192:LEU:HB3	9:B:9480:HOH:O	2.12	0.49
2:C:286:SER:HB3	2:C:299:LYS:CE	2.43	0.49
2:C:332:ARG:HB2	2:C:466:PHE:CE1	2.47	0.49
2:C:352:ALA:HA	2:C:355:VAL:HG12	1.94	0.49
2:C:620:LEU:O	2:C:620:LEU:HD22	2.13	0.49
2:C:703:ILE:CD1	2:C:830:LYS:HG2	2.43	0.49
2:C:783:ARG:HD3	9:C:9806:HOH:O	2.11	0.49
2:C:1034:GLU:HA	2:C:1037:VAL:CG2	2.41	0.49
3:D:131:LYS:HG3	9:D:9749:HOH:O	2.12	0.49
3:D:400:VAL:HG13	3:D:441:ARG:HD3	1.94	0.49
3:D:530:VAL:N	3:D:534:ARG:O	2.37	0.49
3:D:704:ARG:HB2	3:D:736:PHE:HD2	1.77	0.49
3:D:765:SER:O	3:D:767:HIS:N	2.46	0.49
3:D:770:LEU:HD22	3:D:777:PRO:HA	1.93	0.49
3:D:1156:LEU:HG	3:D:1177:ALA:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1295:GLU:HB3	3:D:1300:SER:CB	2.43	0.49
4:E:36:LYS:HD2	9:E:9566:HOH:O	2.11	0.49
5:F:115:LYS:HG3	5:F:173:TYR:CE2	2.48	0.49
1:L:65:PHE:HB2	9:L:5784:HOH:O	2.12	0.49
2:M:470:PRO:HB2	2:M:483:VAL:HG11	1.94	0.49
2:M:577:PRO:HA	2:M:993:PHE:CD2	2.48	0.49
2:M:876:VAL:O	2:M:879:ARG:O	2.31	0.49
2:M:1000:MET:SD	2:M:1001:VAL:HG22	2.52	0.49
3:N:131:LYS:HD2	5:P:83:GLN:NE2	2.27	0.49
3:N:396:VAL:HA	9:N:9955:HOH:O	2.11	0.49
3:N:550:ARG:HG3	3:N:550:ARG:HH11	1.76	0.49
3:N:699:VAL:HG22	3:N:756:GLN:HE22	1.77	0.49
3:N:1139:ASP:O	3:N:1142:ALA:HB3	2.12	0.49
3:N:1243:THR:HB	3:N:1253:THR:HG22	1.94	0.49
3:N:1353:GLN:O	3:N:1357:ARG:HD2	2.12	0.49
5:P:163:LEU:HB3	5:P:174:LEU:CD1	2.43	0.49
5:P:292:ALA:HB1	5:P:299:TRP:O	2.13	0.49
5:P:356:LYS:NZ	5:P:417:LYS:HE2	2.26	0.49
1:B:159:LYS:HD3	1:B:159:LYS:N	2.27	0.49
2:C:127:PHE:CE1	2:C:386:PHE:HE2	2.31	0.49
2:C:218:VAL:HG22	2:C:221:LEU:CD2	2.43	0.49
2:C:543:ASN:HD21	2:C:562:SER:C	2.19	0.49
2:C:712:ALA:O	2:C:820:ARG:HB2	2.12	0.49
3:D:447:VAL:HG12	9:D:9781:HOH:O	2.12	0.49
3:D:1495:ILE:HG12	4:E:80:VAL:HG11	1.93	0.49
1:L:13:VAL:HG13	1:L:23:PHE:CD1	2.48	0.49
2:M:353:ARG:HG2	9:M:9825:HOH:O	2.12	0.49
2:M:720:GLU:CD	2:M:758:ARG:HD2	2.38	0.49
2:M:976:ASP:HB3	2:M:979:THR:HG22	1.94	0.49
2:M:1070:ILE:HD13	9:N:2071:HOH:O	2.12	0.49
2:M:1118:LYS:HD2	9:N:9587:HOH:O	2.13	0.49
3:N:169:TYR:N	3:N:170:PRO:CD	2.76	0.49
5:P:82:ARG:HB2	9:P:5834:HOH:O	2.13	0.49
5:P:85:LEU:HD22	5:P:193:ARG:HD3	1.94	0.49
5:P:247:ILE:O	5:P:251:ILE:HG13	2.12	0.49
1:A:102:LYS:HG3	1:A:139:ASN:HB2	1.93	0.49
1:A:218:LEU:O	1:A:222:LEU:HD23	2.12	0.49
2:C:175:GLU:HB3	2:C:183:SER:OG	2.13	0.49
2:C:537:LYS:CD	2:C:537:LYS:H	2.26	0.49
2:C:676:ILE:HG23	2:C:676:ILE:O	2.12	0.49
2:C:722:ILE:HD12	2:C:805:ARG:CZ	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:769:PRO:HD2	9:D:2497:HOH:O	2.13	0.49
2:C:969:GLN:HB3	9:D:2069:HOH:O	2.13	0.49
2:C:1065:ALA:HB1	9:C:9619:HOH:O	2.12	0.49
3:D:156:GLU:CD	3:D:156:GLU:N	2.70	0.49
4:E:13:VAL:HG12	4:E:75:PHE:CE1	2.48	0.49
5:F:358:LEU:O	5:F:367:MET:HE1	2.13	0.49
1:L:129:ILE:HD13	9:L:4066:HOH:O	2.11	0.49
2:M:56:GLU:HB3	9:M:9605:HOH:O	2.12	0.49
2:M:212:GLY:C	2:M:215:GLY:H	2.21	0.49
2:M:671:ASN:HD22	2:M:993:PHE:HA	1.76	0.49
2:M:881:ASN:HD22	2:M:881:ASN:N	2.04	0.49
2:M:1068:GLU:OE1	5:P:345:ALA:HA	2.13	0.49
3:N:129:PHE:C	3:N:568:ARG:HH21	2.20	0.49
3:N:459:GLU:HG3	3:N:460:ALA:N	2.24	0.49
3:N:1066:THR:HG23	3:N:1069:GLU:H	1.78	0.49
5:P:350:LEU:O	5:P:354:LEU:HG	2.13	0.49
5:P:358:LEU:CD2	5:P:370:LYS:HE3	2.42	0.49
1:A:109:VAL:HG23	1:A:132:LEU:HD13	1.94	0.49
2:C:8:ARG:HB2	9:C:9660:HOH:O	2.13	0.49
2:C:57:GLU:HG3	2:C:58:ASP:OD2	2.13	0.49
2:C:444:PRO:HB3	7:C:8001:RPT:H302	1.95	0.49
2:C:684:PHE:HE2	3:D:733:CYS:HG	1.61	0.49
2:C:726:ILE:HG22	9:C:2076:HOH:O	2.12	0.49
2:C:777:ILE:HD12	9:C:9524:HOH:O	2.12	0.49
2:C:862:PRO:HA	2:C:975:TYR:CE1	2.48	0.49
3:D:149:LYS:HA	9:D:9954:HOH:O	2.12	0.49
3:D:230:TRP:HA	9:D:2088:HOH:O	2.13	0.49
3:D:462:GLN:HG3	3:D:513:ILE:HD13	1.94	0.49
3:D:478:LEU:HD21	3:D:500:ARG:NH2	2.28	0.49
3:D:928:ALA:O	3:D:931:LEU:HB2	2.13	0.49
3:D:1114:THR:HG23	3:D:1116:ASN:ND2	2.28	0.49
5:F:363:GLU:HA	5:F:367:MET:CE	2.37	0.49
2:M:21:ILE:H	2:M:21:ILE:HD12	1.77	0.49
2:M:474:VAL:HG11	2:M:529:VAL:HG12	1.95	0.49
2:M:546:LEU:O	2:M:546:LEU:HD23	2.13	0.49
3:N:18:ILE:HG23	3:N:518:PRO:CG	2.36	0.49
3:N:424:GLY:HA2	3:N:435:VAL:O	2.12	0.49
3:N:428:LYS:HB3	3:N:450:TYR:HE1	1.78	0.49
3:N:488:ARG:HB3	3:N:488:ARG:CZ	2.42	0.49
3:N:578:VAL:O	3:N:582:LEU:HD12	2.13	0.49
3:N:634:GLY:O	3:N:637:LEU:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:850:LEU:O	3:N:853:VAL:HB	2.13	0.49
3:N:880:ILE:O	3:N:883:ALA:HB3	2.13	0.49
3:N:1182:GLU:HG2	9:N:9579:HOH:O	2.11	0.49
3:N:1258:ARG:HH21	3:N:1351:GLU:CG	2.25	0.49
3:N:1492:LEU:HD12	3:N:1493:LYS:HZ2	1.78	0.49
1:A:14:ARG:CZ	1:A:24:VAL:HG23	2.43	0.49
1:A:191:ASP:O	1:A:191:ASP:CG	2.56	0.49
1:B:103:ALA:HB1	1:B:107:LYS:HD2	1.95	0.49
2:C:37:GLU:HA	9:C:9707:HOH:O	2.12	0.49
2:C:365:ASP:O	2:C:367:LEU:HD12	2.13	0.49
2:C:862:PRO:HG3	2:C:975:TYR:CE1	2.48	0.49
2:C:893:ALA:O	2:C:897:LEU:HB2	2.13	0.49
3:D:462:GLN:HA	3:D:513:ILE:CD1	2.41	0.49
3:D:809:PRO:O	3:D:812:ALA:HB3	2.13	0.49
3:D:1087:ARG:HH21	3:D:1238:MET:HB2	1.77	0.49
3:D:1267:ARG:HH22	3:D:1333:HIS:CD2	2.31	0.49
4:E:45:ARG:HB2	4:E:46:PRO:CD	2.43	0.49
5:F:117:SER:HB3	9:F:9892:HOH:O	2.13	0.49
1:K:68:ILE:HD13	1:K:138:LEU:HD13	1.94	0.49
1:K:91:ASN:CG	1:K:92:PRO:HD2	2.38	0.49
2:M:281:LEU:CD1	2:M:306:THR:HA	2.43	0.49
2:M:338:GLU:HA	2:M:341:THR:HG22	1.94	0.49
2:M:409:ARG:NH2	7:M:8002:RPT:H18	2.24	0.49
2:M:543:ASN:HD22	2:M:562:SER:HB3	1.77	0.49
2:M:928:LYS:HA	9:M:2129:HOH:O	2.12	0.49
3:N:463:GLN:O	3:N:467:GLU:HG3	2.13	0.49
3:N:843:PHE:CE1	3:N:864:VAL:HG11	2.48	0.49
3:N:949:ILE:HD11	3:N:1023:MET:HE2	1.94	0.49
3:N:996:TRP:HA	3:N:999:THR:CG2	2.40	0.49
3:N:1007:VAL:O	3:N:1010:ASN:HB3	2.12	0.49
3:N:1112:CYS:HA	3:N:1195:GLN:HE22	1.78	0.49
3:N:1489:GLN:O	3:N:1493:LYS:HG2	2.12	0.49
4:O:33:HIS:HB3	9:O:4524:HOH:O	2.10	0.49
5:P:356:LYS:O	5:P:360:LYS:HG2	2.12	0.49
5:P:361:LEU:HD13	5:P:366:ALA:CB	2.43	0.49
1:A:89:PHE:CZ	1:A:146:ARG:HB2	2.48	0.48
1:B:89:PHE:HB2	9:B:9688:HOH:O	2.13	0.48
1:B:101:LEU:HD12	1:B:114:PHE:CD1	2.48	0.48
2:C:396:ASP:HA	2:C:633:GLN:NE2	2.27	0.48
2:C:890:LEU:HD23	2:C:890:LEU:C	2.37	0.48
3:D:116:LEU:HB3	3:D:118:LEU:HD21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:186:VAL:HG23	3:D:211:VAL:CG1	2.43	0.48
3:D:423:ASP:OD2	5:F:174:LEU:HD22	2.13	0.48
3:D:669:ASN:O	3:D:672:ALA:HB3	2.12	0.48
3:D:896:ALA:HB2	9:D:9543:HOH:O	2.13	0.48
1:K:32:PHE:N	9:K:4346:HOH:O	2.40	0.48
2:M:720:GLU:HA	2:M:759:THR:O	2.13	0.48
3:N:237:LYS:HA	9:N:2400:HOH:O	2.13	0.48
3:N:958:GLU:O	3:N:961:LYS:HG2	2.13	0.48
3:N:998:GLU:HG2	9:N:9574:HOH:O	2.12	0.48
3:N:1068:LEU:C	3:N:1070:TYR:N	2.65	0.48
3:N:1318:TYR:HD1	3:N:1319:VAL:N	2.11	0.48
3:N:1382:THR:HG22	9:N:9550:HOH:O	2.13	0.48
2:C:231:PRO:HB3	9:C:9728:HOH:O	2.13	0.48
2:C:461:VAL:HG13	2:C:465:GLY:HA2	1.95	0.48
2:C:470:PRO:HB2	2:C:483:VAL:HG11	1.94	0.48
2:C:502:PRO:HB2	2:C:509:ALA:HB3	1.95	0.48
2:C:535:SER:O	2:C:538:GLN:HG2	2.13	0.48
2:C:570:PRO:CD	2:C:635:THR:HB	2.43	0.48
2:C:840:ALA:HB2	2:C:846:LYS:HA	1.94	0.48
3:D:86:ARG:O	3:D:86:ARG:HG3	2.12	0.48
3:D:105:VAL:HG12	3:D:106:LYS:NZ	2.28	0.48
3:D:1144:LEU:HB3	3:D:1166:LEU:HD11	1.95	0.48
4:E:26:ARG:HH11	4:E:29:GLN:NE2	2.10	0.48
5:F:123:ASP:H	5:F:126:LEU:HD22	1.79	0.48
5:F:192:LEU:O	5:F:192:LEU:HD23	2.13	0.48
5:F:282:LEU:HD11	5:F:286:PRO:HG3	1.96	0.48
5:F:369:LEU:HD11	5:F:401:GLU:HB2	1.96	0.48
1:L:74:ASP:OD2	1:L:76:VAL:HG23	2.13	0.48
2:M:242:LEU:HD13	9:M:2044:HOH:O	2.13	0.48
2:M:302:VAL:HB	9:M:9592:HOH:O	2.13	0.48
2:M:502:PRO:HB2	2:M:509:ALA:HB3	1.94	0.48
2:M:728:HIS:NE2	2:M:775:ARG:NH2	2.60	0.48
2:M:889:HIS:CD2	2:M:970:GLY:HA3	2.48	0.48
2:M:1015:LEU:HB2	5:P:334:PRO:O	2.13	0.48
2:M:1111:ILE:HG13	2:M:1112:PHE:N	2.25	0.48
3:N:506:GLY:C	3:N:507:ASN:HD22	2.21	0.48
3:N:671:LYS:HE2	9:N:2679:HOH:O	2.12	0.48
3:N:1275:SER:HB3	3:N:1325:LEU:CD1	2.43	0.48
2:C:56:GLU:HB3	9:C:9504:HOH:O	2.13	0.48
2:C:580:MET:O	2:C:903:SER:N	2.45	0.48
2:C:604:ALA:HB3	2:C:612:VAL:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:169:TYR:N	3:D:170:PRO:CD	2.77	0.48
3:D:170:PRO:HG2	9:D:2240:HOH:O	2.13	0.48
3:D:181:ASP:O	3:D:185:VAL:HG23	2.13	0.48
3:D:428:LYS:HD3	9:D:2416:HOH:O	2.12	0.48
3:D:631:ILE:O	3:D:632:VAL:HG23	2.13	0.48
3:D:847:ASP:HA	3:D:850:LEU:CD1	2.44	0.48
3:D:1097:LYS:O	3:D:1101:VAL:HG23	2.13	0.48
3:D:1159:ARG:HB3	3:D:1159:ARG:CZ	2.42	0.48
3:D:1188:VAL:HG22	3:D:1189:ARG:O	2.14	0.48
3:D:1281:VAL:HG21	3:D:1313:VAL:CG2	2.43	0.48
3:D:1281:VAL:HG21	3:D:1313:VAL:HG21	1.95	0.48
5:F:361:LEU:HD22	5:F:366:ALA:HB2	1.95	0.48
1:K:54:THR:HG23	1:K:156:HIS:CE1	2.47	0.48
1:K:91:ASN:O	1:K:94:LEU:HD12	2.12	0.48
1:L:100:LEU:O	1:L:115:LEU:HG	2.13	0.48
2:M:910:LYS:HD3	9:M:9697:HOH:O	2.13	0.48
3:N:12:LEU:HD22	3:N:511:TRP:CB	2.43	0.48
3:N:52:PRO:HD2	3:N:79:GLU:O	2.12	0.48
3:N:438:ASP:HB2	9:N:9821:HOH:O	2.13	0.48
3:N:563:PRO:HG3	5:P:188:ILE:HG21	1.96	0.48
3:N:777:PRO:HG2	3:N:915:VAL:HB	1.96	0.48
3:N:1198:TYR:HE2	3:N:1432:LYS:HE2	1.79	0.48
3:N:1356:TYR:CD2	3:N:1363:LEU:HD23	2.49	0.48
3:N:1406:ARG:HA	9:N:2372:HOH:O	2.13	0.48
3:N:1425:THR:HG23	3:N:1426:LYS:H	1.78	0.48
5:P:119:ILE:HD13	5:P:170:HIS:ND1	2.27	0.48
1:A:195:LEU:HD12	1:A:196:THR:N	2.27	0.48
1:B:36:LEU:C	1:B:39:PRO:HD2	2.37	0.48
2:C:56:GLU:HG2	2:C:64:LEU:HD23	1.94	0.48
2:C:704:HIS:HB2	2:C:831:ARG:NE	2.27	0.48
2:C:724:ARG:HG3	2:C:740:GLU:HA	1.95	0.48
2:C:775:ARG:HE	2:C:782:ALA:CB	2.25	0.48
2:C:954:THR:OG1	2:C:957:LYS:HG3	2.12	0.48
3:D:122:GLU:OE1	3:D:122:GLU:HA	2.13	0.48
3:D:525:ARG:HA	3:D:538:SER:HB2	1.94	0.48
3:D:754:PHE:HE2	3:D:1476:THR:HG21	1.79	0.48
3:D:1020:LEU:HA	3:D:1023:MET:HE3	1.95	0.48
3:D:1278:ASP:HA	3:D:1319:VAL:O	2.13	0.48
5:F:273:ARG:HA	5:F:276:ARG:HD2	1.94	0.48
1:L:23:PHE:O	1:L:196:THR:HA	2.14	0.48
2:M:45:GLN:CG	2:M:49:ARG:HH22	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:71:TYR:N	2:M:71:TYR:CD2	2.81	0.48
2:M:514:VAL:HG22	9:M:9787:HOH:O	2.13	0.48
2:M:683:ASN:HB2	9:M:9667:HOH:O	2.13	0.48
2:M:1097:LEU:N	2:M:1097:LEU:HD22	2.29	0.48
3:N:95:LEU:HD11	3:N:517:VAL:HG23	1.96	0.48
3:N:456:MET:C	9:N:2390:HOH:O	2.56	0.48
3:N:581:LEU:HD23	3:N:581:LEU:H	1.78	0.48
3:N:884:ARG:HD3	9:N:9544:HOH:O	2.13	0.48
3:N:1109:GLU:CD	3:N:1202:GLN:H	2.21	0.48
3:N:1304:LYS:HG2	9:N:2548:HOH:O	2.13	0.48
4:O:18:ARG:O	4:O:22:VAL:HG23	2.13	0.48
5:P:122:LEU:HD11	5:P:126:LEU:HD23	1.95	0.48
5:P:353:GLU:OE1	5:P:356:LYS:HE2	2.13	0.48
2:C:160:ALA:O	2:C:173:ASP:HA	2.13	0.48
2:C:470:PRO:HD3	2:C:485:TYR:CE2	2.49	0.48
2:C:820:ARG:HD3	9:C:2168:HOH:O	2.12	0.48
2:C:1005:MET:HE3	3:D:648:MET:HE3	1.96	0.48
2:C:1073:GLY:HA3	9:C:9551:HOH:O	2.13	0.48
3:D:911:LEU:O	3:D:915:VAL:HG23	2.14	0.48
3:D:1107:VAL:HG12	3:D:1217:ILE:HA	1.95	0.48
4:E:16:LYS:HA	9:E:9481:HOH:O	2.12	0.48
4:E:50:THR:HG22	9:E:9491:HOH:O	2.12	0.48
5:F:359:SER:C	5:F:361:LEU:H	2.21	0.48
2:M:165:LEU:HA	2:M:166:PRO:O	2.14	0.48
2:M:625:LEU:O	2:M:627:ARG:N	2.45	0.48
3:N:415:VAL:HG23	9:N:2389:HOH:O	2.13	0.48
3:N:546:ARG:NH2	3:N:550:ARG:HH12	2.12	0.48
3:N:714:GLN:OE1	3:N:765:SER:HA	2.13	0.48
3:N:1136:LYS:HB2	3:N:1139:ASP:OD2	2.13	0.48
1:B:170:VAL:O	1:B:170:VAL:HG23	2.13	0.48
2:C:426:ASP:HB2	9:C:2334:HOH:O	2.13	0.48
2:C:588:VAL:HG21	2:C:664:GLY:O	2.13	0.48
2:C:722:ILE:O	2:C:722:ILE:HG23	2.14	0.48
3:D:142:LEU:HB3	9:D:9718:HOH:O	2.13	0.48
3:D:790:TYR:CD1	3:D:1022:VAL:HG13	2.48	0.48
3:D:829:VAL:H	3:D:835:SER:HB2	1.78	0.48
3:D:1112:CYS:HB2	3:D:1195:GLN:OE1	2.14	0.48
3:D:1302:GLU:HG3	9:D:9628:HOH:O	2.14	0.48
3:D:1307:LYS:H	3:D:1307:LYS:CD	2.23	0.48
4:E:17:TYR:H	4:E:17:TYR:HD2	1.62	0.48
5:F:151:LEU:HB2	5:F:155:THR:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:278:LEU:HB2	5:F:286:PRO:HG2	1.95	0.48
1:L:206:THR:HG23	1:L:208:LEU:H	1.78	0.48
1:L:219:ARG:O	1:L:223:THR:HG23	2.13	0.48
2:M:102:HIS:HB2	2:M:106:GLY:O	2.14	0.48
2:M:205:GLU:OE2	2:M:206:THR:HB	2.14	0.48
2:M:260:LEU:HA	2:M:291:ALA:HB2	1.95	0.48
2:M:274:ARG:HB2	2:M:285:LEU:CD1	2.43	0.48
2:M:609:ASN:ND2	2:M:627:ARG:HE	2.12	0.48
2:M:1081:VAL:HB	2:M:1086:ARG:NE	2.29	0.48
3:N:27:GLU:O	3:N:28:LYS:HD2	2.13	0.48
3:N:152:LEU:HD21	9:N:9735:HOH:O	2.13	0.48
3:N:820:GLU:HA	3:N:825:ALA:O	2.14	0.48
3:N:1007:VAL:HG23	3:N:1008:PHE:N	2.28	0.48
3:N:1045:MET:HE1	9:N:9654:HOH:O	2.14	0.48
3:N:1303:TYR:HD2	9:N:2651:HOH:O	1.96	0.48
3:N:1459:LEU:HD13	3:N:1465:ASN:ND2	2.28	0.48
5:P:214:GLN:O	5:P:217:ASN:HB2	2.13	0.48
1:A:20:TYR:CD2	1:A:21:GLY:N	2.80	0.48
1:A:99:LEU:HB3	1:A:114:PHE:HD2	1.78	0.48
1:B:81:ASN:HD21	1:B:127:LEU:HG	1.78	0.48
1:B:124:ASN:HA	9:B:9533:HOH:O	2.14	0.48
2:C:108:ILE:HD12	2:C:108:ILE:N	2.28	0.48
2:C:196:LEU:HD11	2:C:303:PHE:CE1	2.49	0.48
2:C:299:LYS:HB3	9:C:9713:HOH:O	2.12	0.48
2:C:458:TYR:HB3	2:C:470:PRO:HG3	1.95	0.48
2:C:459:ALA:HB1	2:C:467:ILE:CG2	2.43	0.48
2:C:480:THR:HG22	2:C:481:ASP:N	2.28	0.48
2:C:952:LEU:HB3	2:C:966:LEU:HD11	1.95	0.48
2:C:1029:GLY:O	3:D:622:ARG:HD3	2.14	0.48
3:D:10:ILE:HD13	3:D:1447:LEU:HG	1.95	0.48
3:D:183:GLU:O	3:D:186:VAL:HG12	2.14	0.48
3:D:213:VAL:HG22	3:D:214:GLU:H	1.79	0.48
3:D:639:LEU:HD12	3:D:640:HIS:H	1.78	0.48
3:D:699:VAL:H	3:D:756:GLN:HE21	1.57	0.48
3:D:785:ILE:HG22	3:D:789:LEU:HD12	1.94	0.48
3:D:1209:LEU:HD21	4:E:16:LYS:HZ3	1.76	0.48
3:D:1232:PRO:HB3	3:D:1361:VAL:CG2	2.38	0.48
3:D:1406:ARG:C	3:D:1406:ARG:HD3	2.39	0.48
3:D:1432:LYS:HA	9:D:9581:HOH:O	2.13	0.48
5:F:261:PRO:O	5:F:265:VAL:HG23	2.14	0.48
1:K:83:LYS:HE2	1:K:168:ASP:N	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:185:ARG:HG3	1:L:190:THR:CG2	2.39	0.48
1:L:191:ASP:O	1:L:192:LEU:HG	2.13	0.48
2:M:195:LEU:HG	2:M:238:LEU:HG	1.96	0.48
2:M:431:HIS:HD2	2:M:433:THR:H	1.58	0.48
2:M:722:ILE:HG21	2:M:821:GLU:OE1	2.14	0.48
2:M:1043:TYR:HA	9:O:4679:HOH:O	2.13	0.48
2:M:1081:VAL:HB	2:M:1086:ARG:HE	1.78	0.48
3:N:103:TRP:CH2	3:N:1447:LEU:HD23	2.48	0.48
3:N:152:LEU:H	3:N:152:LEU:CD2	2.25	0.48
3:N:515:GLU:HB2	9:N:9820:HOH:O	2.13	0.48
3:N:629:SER:OG	3:N:726:ILE:HG13	2.14	0.48
3:N:633:VAL:HG22	3:N:635:PRO:CD	2.43	0.48
3:N:657:LEU:HG	3:N:661:MET:HE2	1.95	0.48
3:N:1305:LEU:HD21	3:N:1326:THR:OG1	2.14	0.48
3:N:1320:GLU:HG2	3:N:1339:LYS:HZ3	1.78	0.48
5:P:346:THR:HA	9:P:4114:HOH:O	2.12	0.48
2:C:42:VAL:HG12	2:C:43:GLY:N	2.26	0.48
2:C:64:LEU:HD12	2:C:100:LEU:HD13	1.95	0.48
2:C:627:ARG:HG3	2:C:628:PHE:H	1.77	0.48
2:C:931:GLY:HA3	9:C:2360:HOH:O	2.14	0.48
2:C:1051:GLU:HG3	2:C:1055:LEU:HD12	1.96	0.48
2:C:1089:VAL:O	2:C:1093:GLN:HG3	2.13	0.48
2:C:1115:LEU:HB3	3:D:85:VAL:CG1	2.44	0.48
3:D:1223:ILE:HD12	3:D:1223:ILE:N	2.20	0.48
4:E:54:LEU:HD23	4:E:54:LEU:O	2.14	0.48
5:F:128:ARG:HG2	9:F:9497:HOH:O	2.12	0.48
1:K:50:GLY:O	1:K:146:ARG:HA	2.13	0.48
1:L:20:TYR:HE2	1:L:198:ARG:HB3	1.78	0.48
2:M:54:ILE:HA	9:M:9582:HOH:O	2.13	0.48
2:M:578:VAL:HG13	2:M:671:ASN:CG	2.39	0.48
2:M:666:LEU:HD12	2:M:667:ALA:N	2.29	0.48
2:M:873:PRO:O	2:M:876:VAL:HG23	2.13	0.48
2:M:1021:LEU:HD22	5:P:331:ASP:O	2.14	0.48
2:M:1040:LEU:HG	2:M:1045:ALA:HB3	1.95	0.48
9:M:9830:HOH:O	5:P:351:SER:HA	2.14	0.48
3:N:186:VAL:HG13	3:N:187:LYS:N	2.29	0.48
3:N:462:GLN:HB2	3:N:513:ILE:HG21	1.95	0.48
3:N:694:VAL:HG13	9:N:2371:HOH:O	2.13	0.48
3:N:796:ARG:HA	9:N:9559:HOH:O	2.14	0.48
3:N:897:TRP:CZ2	3:N:902:LEU:HD21	2.48	0.48
3:N:967:ALA:O	3:N:995:LEU:HD21	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1087:ARG:HA	3:N:1090:ASP:HB2	1.95	0.48
3:N:1264:GLU:CD	3:N:1425:THR:HB	2.38	0.48
3:N:1353:GLN:HE21	3:N:1357:ARG:HE	1.61	0.48
1:A:14:ARG:HH12	1:A:24:VAL:HG23	1.79	0.48
1:B:27:PRO:C	1:B:28:LEU:HD23	2.39	0.48
2:C:444:PRO:HB3	7:C:8001:RPT:C30	2.44	0.48
2:C:649:VAL:HG23	9:C:9833:HOH:O	2.13	0.48
2:C:769:PRO:HB3	9:F:9559:HOH:O	2.12	0.48
2:C:1067:TYR:CE1	3:D:655:PRO:HG3	2.49	0.48
3:D:792:ILE:O	3:D:878:GLY:HA3	2.13	0.48
5:F:131:VAL:HG22	5:F:178:ARG:HD3	1.95	0.48
2:M:54:ILE:HB	9:M:2245:HOH:O	2.14	0.48
2:M:278:GLU:HB3	9:M:2020:HOH:O	2.14	0.48
2:M:455:LEU:HD13	2:M:459:ALA:HB3	1.94	0.48
2:M:564:MET:HG2	2:M:840:ALA:HB3	1.94	0.48
2:M:614:ARG:HG3	2:M:620:LEU:HD12	1.96	0.48
2:M:726:ILE:HG22	2:M:726:ILE:O	2.12	0.48
2:M:1015:LEU:HB3	2:M:1016:ILE:HD13	1.95	0.48
2:M:1033:GLY:O	2:M:1037:VAL:HG23	2.14	0.48
3:N:525:ARG:HD2	3:N:541:ASN:OD1	2.14	0.48
3:N:557:LEU:HD11	5:P:214:GLN:NE2	2.28	0.48
3:N:674:ARG:HG2	3:N:674:ARG:NH1	2.29	0.48
3:N:989:TYR:CZ	3:N:993:LEU:HD11	2.49	0.48
3:N:1023:MET:O	3:N:1028:ALA:HB3	2.14	0.48
3:N:1036:ARG:NH2	9:N:9654:HOH:O	2.47	0.48
5:P:93:LEU:HG	5:P:190:ALA:HB1	1.95	0.48
1:A:36:LEU:HD11	1:B:221:HIS:HB3	1.95	0.48
1:A:86:VAL:CG1	1:A:124:ASN:HB2	2.43	0.48
1:A:184:THR:HG23	1:A:192:LEU:HD12	1.96	0.48
2:C:91:GLN:OE1	2:C:117:HIS:HB3	2.13	0.48
2:C:144:PRO:HG2	2:C:265:ARG:NH1	2.25	0.48
2:C:184:MET:HB2	2:C:193:LEU:CD1	2.44	0.48
2:C:260:LEU:HA	2:C:291:ALA:HB2	1.95	0.48
2:C:380:ALA:O	2:C:384:GLU:HB2	2.13	0.48
2:C:445:GLU:HB2	2:C:559:LEU:HD21	1.95	0.48
2:C:630:ARG:HA	2:C:705:ILE:CD1	2.44	0.48
2:C:1036:GLU:HA	3:D:707:THR:HG21	1.96	0.48
3:D:27:GLU:HG3	3:D:28:LYS:HD2	1.96	0.48
3:D:42:ASP:O	3:D:46:ASP:HB2	2.13	0.48
3:D:1169:ASP:HB3	9:D:2071:HOH:O	2.13	0.48
3:D:1258:ARG:NH2	3:D:1262:LEU:HD11	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1280:VAL:HG12	3:D:1281:VAL:N	2.29	0.48
3:D:1379:VAL:HA	3:D:1420:LEU:HB3	1.95	0.48
3:D:1404:ASN:HB2	9:D:9939:HOH:O	2.14	0.48
3:D:1418:LYS:HG3	9:D:9914:HOH:O	2.13	0.48
5:F:277:GLN:O	5:F:280:GLN:HB3	2.14	0.48
5:F:388:ALA:HB1	9:F:9483:HOH:O	2.12	0.48
1:K:41:ARG:HH11	1:K:41:ARG:HG3	1.79	0.48
1:K:48:ILE:HD13	1:K:210:ALA:HB1	1.95	0.48
1:L:73:GLU:HB3	1:L:77:GLU:CG	2.43	0.48
1:L:132:LEU:HD21	1:L:136:GLY:O	2.14	0.48
2:M:189:ARG:HH22	2:M:243:ARG:HG2	1.78	0.48
2:M:432:ARG:NE	2:M:519:GLY:HA3	2.29	0.48
2:M:863:ASP:O	2:M:865:THR:N	2.47	0.48
2:M:953:VAL:HA	2:M:965:GLU:OE1	2.13	0.48
2:M:1043:TYR:OH	3:N:711:LEU:HD23	2.13	0.48
3:N:493:ARG:NH2	3:N:1388:ARG:HB3	2.28	0.48
3:N:794:GLN:NE2	3:N:795:VAL:O	2.47	0.48
3:N:970:LYS:NZ	3:N:970:LYS:HB2	2.29	0.48
3:N:1003:VAL:O	3:N:1006:ALA:HB3	2.13	0.48
3:N:1096:ARG:HG2	3:N:1096:ARG:NH1	2.29	0.48
3:N:1102:THR:HG22	3:N:1222:GLY:CA	2.44	0.48
3:N:1104:GLU:HA	3:N:1461:GLY:HA2	1.94	0.48
3:N:1263:PHE:CE2	3:N:1371:VAL:HG11	2.49	0.48
5:P:350:LEU:HD23	5:P:351:SER:N	2.29	0.48
1:A:63:HIS:HB3	2:C:746:GLY:CA	2.34	0.47
1:A:72:LYS:HB3	1:A:73:GLU:OE2	2.13	0.47
1:A:143:ARG:HD2	1:A:145:ASP:OD1	2.14	0.47
1:B:86:VAL:HG22	9:B:9508:HOH:O	2.14	0.47
2:C:182:VAL:HG11	9:C:9507:HOH:O	2.13	0.47
2:C:189:ARG:HH22	2:C:243:ARG:NH2	2.12	0.47
2:C:290:LEU:HB3	2:C:302:VAL:CG1	2.44	0.47
2:C:854:PRO:C	2:C:856:GLU:N	2.71	0.47
9:C:9669:HOH:O	3:D:1075:HIS:HE1	1.96	0.47
3:D:421:LEU:HD11	3:D:437:VAL:HG22	1.95	0.47
3:D:523:ASP:O	3:D:526:PRO:HG3	2.14	0.47
3:D:957:PRO:CD	3:D:1007:VAL:HG12	2.44	0.47
3:D:1259:VAL:O	3:D:1263:PHE:HD1	1.97	0.47
5:F:299:TRP:CE3	5:F:303:ARG:HD3	2.49	0.47
1:L:19:GLU:HG3	1:L:201:THR:O	2.14	0.47
2:M:287:GLY:O	2:M:288:ARG:C	2.56	0.47
2:M:345:ARG:HA	2:M:348:LEU:HB2	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:607:ASP:HB3	2:M:609:ASN:H	1.78	0.47
2:M:781:LYS:HG3	9:M:2053:HOH:O	2.14	0.47
2:M:1067:TYR:CE2	5:P:342:VAL:HA	2.49	0.47
2:M:1082:PRO:HG3	9:M:9510:HOH:O	2.13	0.47
2:M:1118:LYS:HB3	3:N:23:TYR:CE1	2.49	0.47
3:N:80:VAL:HG12	3:N:81:THR:H	1.77	0.47
3:N:122:GLU:O	3:N:126:VAL:HG23	2.13	0.47
3:N:730:PRO:HA	3:N:733:CYS:SG	2.54	0.47
3:N:965:GLU:HA	3:N:968:ASP:HB2	1.96	0.47
3:N:1209:LEU:HD22	3:N:1211:MET:HB3	1.96	0.47
3:N:1290:LEU:CD2	3:N:1291:SER:H	2.23	0.47
3:N:1292:VAL:O	3:N:1303:TYR:HB2	2.14	0.47
3:N:1493:LYS:HB2	9:N:9693:HOH:O	2.13	0.47
5:P:169:GLU:H	5:P:169:GLU:CD	2.22	0.47
5:P:234:LYS:CD	5:P:236:SER:H	2.27	0.47
5:P:417:LYS:HD2	9:P:4364:HOH:O	2.13	0.47
1:A:117:VAL:HB	1:A:120:VAL:CG1	2.41	0.47
1:B:133:GLU:HG3	9:B:9692:HOH:O	2.13	0.47
2:C:876:VAL:O	2:C:879:ARG:O	2.32	0.47
2:C:1086:ARG:HD3	2:C:1112:PHE:HD2	1.80	0.47
3:D:39:PRO:HB2	9:D:9934:HOH:O	2.14	0.47
3:D:110:SER:HB2	9:D:9697:HOH:O	2.13	0.47
3:D:445:ARG:HB3	9:D:9781:HOH:O	2.13	0.47
3:D:527:MET:HE2	5:F:258:ILE:HD11	1.96	0.47
3:D:671:LYS:O	3:D:671:LYS:HD3	2.14	0.47
3:D:756:GLN:HG2	9:E:9480:HOH:O	2.13	0.47
3:D:1044:LEU:HD21	3:D:1056:PRO:HG3	1.95	0.47
3:D:1087:ARG:CZ	3:D:1087:ARG:HB2	2.44	0.47
3:D:1173:LEU:HD23	3:D:1174:LEU:HD23	1.97	0.47
3:D:1240:THR:O	3:D:1257:PRO:HB3	2.13	0.47
3:D:1402:ALA:HB2	3:D:1415:VAL:CG2	2.44	0.47
3:D:1491:THR:HG22	9:E:9496:HOH:O	2.13	0.47
4:E:49:GLN:HA	4:E:51:LEU:O	2.14	0.47
5:F:352:GLU:HG2	9:F:9594:HOH:O	2.13	0.47
1:K:23:PHE:O	1:K:196:THR:HA	2.14	0.47
2:M:66:LEU:HD13	2:M:100:LEU:HB2	1.95	0.47
2:M:139:GLN:HE22	2:M:418:LEU:HD13	1.79	0.47
2:M:208:ALA:HA	2:M:218:VAL:HG22	1.96	0.47
2:M:331:ARG:NH1	2:M:427:VAL:HG13	2.29	0.47
2:M:381:ALA:HA	9:M:9949:HOH:O	2.13	0.47
2:M:474:VAL:HG23	2:M:478:VAL:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:678:PRO:HA	2:M:683:ASN:HD21	1.79	0.47
2:M:881:ASN:ND2	2:M:881:ASN:N	2.61	0.47
3:N:572:ARG:NH1	5:P:80:PRO:HD3	2.29	0.47
3:N:591:VAL:HG12	3:N:592:THR:O	2.14	0.47
3:N:668:PRO:HA	9:N:9706:HOH:O	2.14	0.47
3:N:1111:ASP:HA	9:N:9807:HOH:O	2.13	0.47
4:O:48:MET:CB	4:O:54:LEU:HB2	2.44	0.47
4:O:70:THR:CG2	4:O:72:ARG:HH21	2.27	0.47
5:P:193:ARG:HD2	9:P:3462:HOH:O	2.14	0.47
1:A:133:GLU:HA	9:A:9594:HOH:O	2.13	0.47
1:B:151:VAL:HB	1:B:169:ALA:HB3	1.96	0.47
2:C:52:PHE:HA	9:C:9979:HOH:O	2.13	0.47
2:C:197:LEU:HA	9:C:9888:HOH:O	2.14	0.47
2:C:285:LEU:HD23	2:C:285:LEU:O	2.14	0.47
2:C:367:LEU:HD22	9:C:2175:HOH:O	2.14	0.47
2:C:892:LEU:HD21	2:C:967:PHE:CE1	2.49	0.47
2:C:1090:LYS:HG2	2:C:1112:PHE:HZ	1.78	0.47
3:D:473:LEU:HD11	3:D:495:ARG:NH1	2.29	0.47
3:D:477:LEU:HD22	3:D:492:ALA:CB	2.42	0.47
3:D:843:PHE:CZ	3:D:864:VAL:HG11	2.49	0.47
3:D:1243:THR:HG22	3:D:1244:GLY:H	1.79	0.47
3:D:1394:VAL:HG21	3:D:1397:LYS:NZ	2.28	0.47
9:D:2394:HOH:O	4:E:54:LEU:HD11	2.14	0.47
4:E:59:ASN:HB3	4:E:62:THR:OG1	2.13	0.47
2:M:551:GLU:OE1	2:M:906:PHE:HA	2.14	0.47
3:N:474:GLU:O	3:N:478:LEU:HG	2.15	0.47
3:N:491:LYS:HG3	9:N:9963:HOH:O	2.13	0.47
3:N:664:LYS:HA	9:N:2138:HOH:O	2.14	0.47
3:N:776:GLU:OE1	3:N:912:LYS:HD3	2.14	0.47
4:O:54:LEU:HG	4:O:58:PRO:HD2	1.94	0.47
1:A:30:ARG:HH22	1:A:191:ASP:HB2	1.79	0.47
1:B:173:PRO:HB2	1:B:205:VAL:HG22	1.96	0.47
2:C:110:GLU:H	2:C:368:THR:HG21	1.79	0.47
2:C:134:ARG:HH21	2:C:394:PHE:N	2.12	0.47
2:C:925:TYR:CD1	2:C:925:TYR:C	2.92	0.47
9:C:9961:HOH:O	5:F:350:LEU:HD21	2.14	0.47
3:D:114:THR:O	3:D:495:ARG:HG3	2.15	0.47
3:D:501:ALA:HA	3:D:504:ASP:HB2	1.97	0.47
3:D:658:LEU:HD11	3:D:674:ARG:NH1	2.29	0.47
3:D:672:ALA:HA	5:F:420:ASP:OD2	2.15	0.47
3:D:836:VAL:HG12	9:D:9486:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1310:ARG:HG3	3:D:1327:ARG:CB	2.44	0.47
2:M:63:GLY:CA	2:M:103:LYS:HE2	2.45	0.47
2:M:478:VAL:HG13	2:M:506:ASN:HB3	1.95	0.47
2:M:841:ASN:HD22	2:M:843:HIS:H	1.60	0.47
3:N:834:THR:HB	3:N:838:ARG:HB3	1.95	0.47
3:N:1280:VAL:HG12	3:N:1281:VAL:N	2.29	0.47
3:N:1472:ILE:HG22	3:N:1474:ALA:H	1.78	0.47
2:C:16:PRO:HG2	2:C:460:ARG:HH12	1.79	0.47
2:C:19:THR:HG22	2:C:19:THR:O	2.15	0.47
2:C:256:TYR:HE1	2:C:293:PHE:HB2	1.76	0.47
2:C:352:ALA:O	2:C:355:VAL:HG12	2.15	0.47
2:C:413:LEU:H	2:C:413:LEU:CD1	2.25	0.47
2:C:420:ARG:HG2	2:C:421:GLU:H	1.79	0.47
2:C:945:ARG:HD3	2:C:949:LYS:HE3	1.96	0.47
3:D:171:LEU:HA	3:D:390:PRO:HA	1.96	0.47
3:D:584:ASN:HA	9:D:9901:HOH:O	2.15	0.47
3:D:659:LYS:O	3:D:659:LYS:HD3	2.14	0.47
3:D:891:GLU:N	9:D:9484:HOH:O	2.47	0.47
3:D:1326:THR:HG22	3:D:1327:ARG:N	2.30	0.47
3:D:1468:LEU:CD1	3:D:1470:ARG:HD3	2.43	0.47
1:K:34:VAL:HG21	9:M:2370:HOH:O	2.15	0.47
1:K:102:LYS:HG2	9:K:3922:HOH:O	2.13	0.47
1:L:84:GLU:HG3	1:L:127:LEU:CD2	2.44	0.47
2:M:393:GLN:HB3	7:M:8002:RPT:H343	1.97	0.47
2:M:602:GLU:HA	2:M:647:GLN:O	2.14	0.47
2:M:773:LEU:HD21	5:P:354:LEU:HD22	1.95	0.47
2:M:1030:GLN:HB2	3:N:626:SER:HB2	1.96	0.47
2:M:1102:LEU:HD11	3:N:9:ARG:HB2	1.97	0.47
3:N:656:PHE:CE2	3:N:698:LYS:HE3	2.49	0.47
3:N:728:LEU:HD12	3:N:729:HIS:N	2.30	0.47
3:N:826:PRO:HD2	3:N:829:VAL:HG22	1.95	0.47
3:N:848:GLU:HB3	9:N:9763:HOH:O	2.14	0.47
3:N:996:TRP:CE3	3:N:999:THR:HG21	2.50	0.47
3:N:1382:THR:HG21	3:N:1418:LYS:HZ2	1.77	0.47
5:P:236:SER:HB3	9:P:3697:HOH:O	2.14	0.47
5:P:361:LEU:HD21	5:P:404:ALA:HB1	1.95	0.47
1:A:38:ASN:HB3	1:A:39:PRO:HD3	1.95	0.47
1:A:57:TYR:CD1	1:A:161:ARG:HB3	2.50	0.47
1:A:219:ARG:NH1	1:B:219:ARG:HG2	2.29	0.47
1:B:191:ASP:O	1:B:192:LEU:HG	2.13	0.47
2:C:114:PHE:HB2	9:C:9593:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:537:LYS:HD2	2:C:537:LYS:H	1.80	0.47
2:C:1047:HIS:CD2	3:D:1471:LEU:HD11	2.50	0.47
2:C:1081:VAL:CG1	2:C:1086:ARG:HE	2.27	0.47
3:D:399:ARG:HH21	3:D:432:TYR:HE2	1.61	0.47
3:D:543:LEU:HA	3:D:546:ARG:HG3	1.96	0.47
3:D:601:ARG:CD	3:D:606:ILE:HD13	2.45	0.47
3:D:709:HIS:CD2	3:D:711:LEU:HB2	2.49	0.47
3:D:952:ASP:HA	3:D:1062:ARG:NH2	2.29	0.47
3:D:970:LYS:HD2	3:D:995:LEU:HD13	1.95	0.47
3:D:1302:GLU:OE2	3:D:1304:LYS:HG2	2.15	0.47
5:F:270:LYS:HB3	5:F:295:MET:HE3	1.96	0.47
1:K:18:ARG:O	1:K:201:THR:OG1	2.32	0.47
2:M:196:LEU:O	2:M:199:VAL:HB	2.15	0.47
2:M:197:LEU:CD1	2:M:207:LEU:HD11	2.45	0.47
2:M:227:PHE:HA	2:M:230:ARG:NE	2.22	0.47
2:M:269:LEU:HD11	2:M:287:GLY:HA2	1.97	0.47
2:M:802:ARG:CB	2:M:802:ARG:HH11	2.28	0.47
2:M:1019:GLN:NE2	3:N:621:LYS:HA	2.28	0.47
3:N:96:ALA:HB2	9:N:9830:HOH:O	2.13	0.47
3:N:563:PRO:O	3:N:567:ILE:HG13	2.13	0.47
3:N:719:VAL:N	9:N:9610:HOH:O	2.47	0.47
3:N:1352:ILE:CG2	3:N:1368:ILE:HD13	2.45	0.47
3:N:1476:THR:C	3:N:1478:SER:H	2.23	0.47
4:O:43:GLU:CD	4:O:43:GLU:H	2.23	0.47
5:P:142:ARG:NH1	5:P:150:THR:HG21	2.30	0.47
1:A:36:LEU:O	1:A:40:LEU:HG	2.15	0.47
1:B:32:PHE:HA	1:B:35:THR:OG1	2.15	0.47
1:B:72:LYS:HG2	9:B:9498:HOH:O	2.14	0.47
1:B:171:PHE:HD2	9:B:9528:HOH:O	1.96	0.47
1:B:190:THR:HG22	9:B:9536:HOH:O	2.14	0.47
2:C:48:PHE:O	2:C:52:PHE:HB2	2.15	0.47
2:C:55:GLU:HG2	9:C:2379:HOH:O	2.14	0.47
2:C:200:LEU:HD13	2:C:300:ASP:OD2	2.13	0.47
2:C:269:LEU:HD23	9:C:2225:HOH:O	2.15	0.47
2:C:285:LEU:HD12	2:C:288:ARG:O	2.14	0.47
2:C:328:LEU:HD11	2:C:434:HIS:HD2	1.79	0.47
2:C:352:ALA:C	2:C:355:VAL:HG12	2.39	0.47
2:C:451:LEU:H	2:C:451:LEU:HD12	1.79	0.47
2:C:612:VAL:HG22	2:C:622:GLU:HB2	1.97	0.47
2:C:636:ALA:C	2:C:637:LEU:HD23	2.40	0.47
2:C:654:LEU:HD13	2:C:664:GLY:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:673:LEU:CD2	2:C:867:VAL:HG12	2.45	0.47
2:C:676:ILE:CG2	2:C:988:VAL:HG22	2.45	0.47
2:C:816:LYS:HB3	9:C:9840:HOH:O	2.15	0.47
2:C:1006:HIS:N	2:C:1006:HIS:ND1	2.63	0.47
2:C:1008:ARG:NH2	2:C:1021:LEU:C	2.73	0.47
2:C:1016:ILE:HD12	3:D:526:PRO:HG2	1.96	0.47
2:C:1020:PRO:O	3:D:622:ARG:HD2	2.15	0.47
3:D:229:ALA:HB1	9:D:9916:HOH:O	2.14	0.47
3:D:421:LEU:HD12	3:D:435:VAL:CG1	2.44	0.47
3:D:501:ALA:HB1	3:D:1453:ALA:HA	1.97	0.47
3:D:601:ARG:HE	3:D:606:ILE:HA	1.78	0.47
3:D:894:LYS:HB2	9:D:9872:HOH:O	2.13	0.47
3:D:955:VAL:HB	3:D:1011:PHE:CE1	2.43	0.47
3:D:969:ARG:O	3:D:972:LEU:HB3	2.14	0.47
3:D:995:LEU:HA	9:D:2036:HOH:O	2.14	0.47
3:D:1041:LEU:HD12	3:D:1058:ARG:C	2.40	0.47
3:D:1151:ARG:HB2	9:D:9606:HOH:O	2.15	0.47
3:D:1220:ALA:HB1	3:D:1223:ILE:CD1	2.41	0.47
9:D:2189:HOH:O	5:F:145:PRO:HB3	2.14	0.47
1:L:111:ALA:HB3	1:L:124:ASN:O	2.15	0.47
2:M:194:VAL:HG21	2:M:221:LEU:HA	1.97	0.47
2:M:279:GLU:HA	9:M:9687:HOH:O	2.13	0.47
2:M:431:HIS:HB3	2:M:434:HIS:CD2	2.49	0.47
2:M:544:THR:O	2:M:547:ILE:HG13	2.15	0.47
2:M:619:ARG:HG3	9:M:9814:HOH:O	2.15	0.47
2:M:741:GLY:HA3	9:M:9845:HOH:O	2.13	0.47
2:M:768:THR:O	2:M:772:ARG:HB3	2.15	0.47
2:M:772:ARG:CD	5:P:373:LYS:HD2	2.44	0.47
2:M:833:LEU:HB2	9:M:9662:HOH:O	2.14	0.47
2:M:897:LEU:CD1	2:M:921:ALA:HA	2.44	0.47
2:M:910:LYS:HD2	2:M:910:LYS:N	2.30	0.47
2:M:925:TYR:CD1	2:M:925:TYR:C	2.91	0.47
2:M:984:GLU:HG3	3:N:944:THR:O	2.15	0.47
3:N:58:CYS:SG	3:N:59:ALA:N	2.88	0.47
3:N:75:ARG:HG3	3:N:75:ARG:NH1	2.27	0.47
3:N:440:VAL:HG12	3:N:441:ARG:N	2.30	0.47
3:N:610:LYS:HG2	3:N:611:GLN:HG2	1.96	0.47
3:N:684:LYS:HB3	3:N:686:GLU:HG3	1.96	0.47
3:N:704:ARG:CD	3:N:705:ALA:H	2.26	0.47
3:N:765:SER:C	3:N:767:HIS:H	2.22	0.47
3:N:982:PHE:HZ	9:N:2480:HOH:O	1.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1326:THR:HG22	3:N:1327:ARG:N	2.30	0.47
3:N:1376:MET:HE3	3:N:1421:LEU:CD1	2.43	0.47
5:P:82:ARG:HG2	9:P:4186:HOH:O	2.13	0.47
5:P:151:LEU:HB2	5:P:155:THR:OG1	2.15	0.47
5:P:412:GLU:OE1	5:P:418:LEU:HD13	2.15	0.47
1:A:18:ARG:HD3	1:A:123:MET:HE1	1.97	0.47
1:A:33:GLY:O	1:A:195:LEU:HD22	2.14	0.47
1:A:83:LYS:HE2	1:A:167:VAL:HG12	1.97	0.47
1:A:224:TYR:HB3	1:B:9:PRO:HB2	1.97	0.47
2:C:83:CYS:CA	2:C:88:LEU:HB3	2.39	0.47
2:C:129:ILE:HG12	2:C:386:PHE:HB3	1.97	0.47
2:C:137:VAL:O	2:C:391:LEU:HD11	2.15	0.47
2:C:232:GLU:O	2:C:235:LEU:HB2	2.14	0.47
2:C:886:LEU:CD2	3:D:951:ILE:HG13	2.44	0.47
3:D:28:LYS:O	3:D:43:GLY:HA2	2.15	0.47
3:D:436:GLU:HB2	3:D:445:ARG:HB3	1.95	0.47
3:D:539:ASP:OD2	5:F:318:GLU:HB2	2.14	0.47
3:D:1495:ILE:N	3:D:1495:ILE:HD12	2.29	0.47
5:F:74:LYS:HG3	9:F:9539:HOH:O	2.14	0.47
5:F:141:VAL:O	5:F:145:PRO:HD2	2.15	0.47
5:F:358:LEU:HD13	5:F:370:LYS:HG3	1.97	0.47
5:F:367:MET:HA	5:F:370:LYS:NZ	2.30	0.47
1:L:65:PHE:CD1	3:N:813:LEU:HD22	2.50	0.47
2:M:220:GLY:HA3	9:M:9540:HOH:O	2.15	0.47
2:M:277:ALA:HB1	9:M:2036:HOH:O	2.14	0.47
2:M:474:VAL:HG13	2:M:530:GLU:C	2.40	0.47
2:M:1076:VAL:HG21	3:N:752:SER:HB3	1.97	0.47
3:N:98:PRO:HG3	3:N:515:GLU:HB3	1.96	0.47
3:N:139:GLY:N	3:N:147:VAL:HG21	2.30	0.47
3:N:661:MET:CE	3:N:677:LEU:HD11	2.38	0.47
3:N:933:ALA:O	3:N:937:TYR:HD1	1.96	0.47
3:N:1223:ILE:HD12	3:N:1223:ILE:N	2.25	0.47
5:P:361:LEU:HD13	5:P:366:ALA:HB1	1.97	0.47
1:A:101:LEU:HD12	1:A:114:PHE:CD1	2.50	0.47
1:B:41:ARG:HB2	1:B:177:VAL:HG21	1.95	0.47
2:C:52:PHE:O	2:C:54:ILE:N	2.48	0.47
2:C:346:VAL:HB	9:C:2037:HOH:O	2.15	0.47
2:C:776:SER:HA	2:C:780:GLU:HB3	1.97	0.47
2:C:841:ASN:C	2:C:841:ASN:HD22	2.23	0.47
2:C:877:PRO:HG3	3:D:1020:LEU:CD1	2.44	0.47
2:C:1013:TYR:CE1	2:C:1020:PRO:HG3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1018:GLN:HG3	2:C:1060:ILE:HD13	1.97	0.47
3:D:843:PHE:CD1	3:D:849:ALA:HA	2.50	0.47
3:D:1129:THR:C	3:D:1130:ARG:HD2	2.40	0.47
3:D:1425:THR:HG23	3:D:1426:LYS:N	2.30	0.47
1:K:97:VAL:HG12	1:K:99:LEU:HD12	1.97	0.47
1:K:225:PHE:CE1	1:L:25:LEU:HD22	2.50	0.47
1:L:94:LEU:HD11	1:L:119:ASP:HB3	1.96	0.47
2:M:164:PRO:HD2	2:M:170:PRO:O	2.15	0.47
2:M:167:LYS:HD3	2:M:168:ARG:N	2.30	0.47
2:M:202:TYR:OH	2:M:304:LEU:HD22	2.14	0.47
2:M:371:LYS:HB2	9:M:9512:HOH:O	2.14	0.47
2:M:391:LEU:HD23	2:M:391:LEU:C	2.40	0.47
2:M:423:ALA:HB1	9:M:9593:HOH:O	2.15	0.47
2:M:543:ASN:ND2	2:M:562:SER:HB3	2.30	0.47
3:N:36:THR:O	3:N:38:LYS:N	2.46	0.47
3:N:137:PRO:HD2	3:N:453:ASP:HB2	1.97	0.47
5:P:184:ARG:NH2	9:P:3604:HOH:O	2.46	0.47
5:P:409:LYS:HE3	5:P:410:TYR:CD1	2.49	0.47
2:C:47:ALA:HA	2:C:50:GLU:OE2	2.15	0.47
2:C:56:GLU:CG	2:C:64:LEU:HD23	2.45	0.47
2:C:71:TYR:HD1	9:C:9517:HOH:O	1.97	0.47
2:C:144:PRO:HB2	9:C:9808:HOH:O	2.15	0.47
2:C:444:PRO:HG3	2:C:452:ILE:HD12	1.96	0.47
2:C:603:VAL:H	2:C:647:GLN:H	1.63	0.47
2:C:715:THR:HG22	9:C:2002:HOH:O	2.14	0.47
3:D:584:ASN:HB3	9:D:9515:HOH:O	2.15	0.47
5:F:85:LEU:HB2	9:F:9663:HOH:O	2.14	0.47
5:F:188:ILE:HA	9:F:9537:HOH:O	2.15	0.47
5:F:287:THR:HG23	5:F:289:GLU:H	1.80	0.47
5:F:340:SER:OG	5:F:342:VAL:HG23	2.15	0.47
1:L:189:ARG:NH1	1:L:189:ARG:HG3	2.30	0.47
2:M:96:ALA:HB3	9:M:9996:HOH:O	2.14	0.47
2:M:470:PRO:HB2	2:M:534:VAL:HG21	1.96	0.47
2:M:1098:ASP:HB2	3:N:21:TRP:HZ2	1.78	0.47
3:N:64:LYS:HE3	9:N:9919:HOH:O	2.14	0.47
3:N:135:LEU:CD1	3:N:147:VAL:HG23	2.42	0.47
3:N:186:VAL:HG11	3:N:213:VAL:HB	1.97	0.47
3:N:510:GLU:O	3:N:513:ILE:HD12	2.14	0.47
3:N:639:LEU:H	3:N:639:LEU:HD12	1.80	0.47
3:N:698:LYS:HA	3:N:756:GLN:NE2	2.30	0.47
3:N:703:ASN:ND2	3:N:704:ARG:H	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:844:ALA:HB3	3:N:848:GLU:OE2	2.15	0.47
3:N:1020:LEU:HA	3:N:1023:MET:HE3	1.97	0.47
3:N:1101:VAL:HG22	3:N:1428:ALA:HB2	1.97	0.47
4:O:5:GLY:HA3	4:O:8:LYS:HD2	1.96	0.47
1:A:206:THR:HG22	1:A:209:GLU:H	1.80	0.46
2:C:7:GLY:HA3	2:C:907:ASP:O	2.15	0.46
2:C:30:LEU:HD23	2:C:340:MET:HE2	1.95	0.46
2:C:287:GLY:O	2:C:288:ARG:C	2.58	0.46
2:C:305:PRO:HG3	2:C:308:ARG:HH22	1.80	0.46
2:C:471:TYR:CD2	2:C:533:ASP:HA	2.50	0.46
2:C:721:ARG:O	2:C:758:ARG:HA	2.14	0.46
3:D:95:LEU:CD2	3:D:574:LEU:HD11	2.45	0.46
3:D:104:PHE:CE2	3:D:1448:THR:HG23	2.49	0.46
3:D:210:ARG:NH1	3:D:398:ALA:HB3	2.30	0.46
3:D:650:LEU:HD22	3:D:688:TRP:CH2	2.50	0.46
3:D:1102:THR:HG22	3:D:1222:GLY:CA	2.44	0.46
4:E:70:THR:HB	9:E:9533:HOH:O	2.14	0.46
5:F:209:PHE:HE2	5:F:213:ILE:HD11	1.80	0.46
1:K:12:THR:HG23	1:K:24:VAL:HB	1.97	0.46
1:L:57:TYR:CE1	1:L:163:ASN:HB2	2.41	0.46
1:L:99:LEU:HA	9:L:4955:HOH:O	2.15	0.46
2:M:50:GLU:HA	2:M:266:ARG:NH1	2.31	0.46
2:M:170:PRO:HA	9:M:9800:HOH:O	2.14	0.46
2:M:269:LEU:HD12	2:M:288:ARG:HG3	1.97	0.46
2:M:671:ASN:ND2	2:M:993:PHE:HB2	2.30	0.46
2:M:929:ARG:HG3	2:M:929:ARG:HH11	1.80	0.46
2:M:966:LEU:HD11	2:M:986:PRO:HG2	1.96	0.46
2:M:1097:LEU:HD11	3:N:103:TRP:CZ3	2.50	0.46
3:N:31:THR:HG21	3:N:527:MET:HE2	1.96	0.46
3:N:87:ARG:HG3	3:N:88:TYR:CD2	2.50	0.46
3:N:551:ASN:O	3:N:555:LYS:HG3	2.14	0.46
3:N:968:ASP:O	3:N:971:LEU:HB3	2.15	0.46
3:N:972:LEU:O	3:N:976:GLN:HG3	2.14	0.46
3:N:1209:LEU:HD22	3:N:1211:MET:HE2	1.97	0.46
5:P:122:LEU:HA	9:P:4063:HOH:O	2.14	0.46
1:A:23:PHE:CD1	1:A:211:LEU:HD23	2.50	0.46
1:A:178:ALA:CB	2:C:864:GLY:H	2.28	0.46
1:B:56:VAL:HG13	1:B:142:VAL:HG12	1.96	0.46
1:B:85:LEU:HD13	1:B:127:LEU:HD23	1.97	0.46
2:C:8:ARG:HB2	2:C:8:ARG:HH11	1.80	0.46
2:C:49:ARG:HH11	2:C:49:ARG:CB	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:110:GLU:HB2	2:C:368:THR:CG2	2.45	0.46
2:C:208:ALA:HB1	2:C:218:VAL:CG1	2.45	0.46
2:C:911:GLU:HB3	2:C:912:PRO:HD3	1.97	0.46
3:D:105:VAL:HG23	9:D:9538:HOH:O	2.15	0.46
3:D:168:THR:HA	9:D:9616:HOH:O	2.15	0.46
3:D:442:ASN:HA	9:D:9677:HOH:O	2.14	0.46
3:D:503:LEU:HD23	3:D:508:ARG:HH12	1.80	0.46
3:D:574:LEU:O	3:D:577:ALA:HB3	2.15	0.46
3:D:720:LEU:H	3:D:720:LEU:CD1	2.23	0.46
3:D:1128:VAL:O	3:D:1129:THR:C	2.58	0.46
3:D:1402:ALA:HB2	3:D:1415:VAL:HG23	1.96	0.46
3:D:1437:ALA:O	3:D:1446:VAL:HG21	2.15	0.46
5:F:292:ALA:HB1	5:F:299:TRP:O	2.15	0.46
5:F:321:ILE:O	5:F:327:SER:HB3	2.15	0.46
1:K:25:LEU:HD23	1:K:25:LEU:C	2.40	0.46
2:M:101:ILE:HG22	2:M:102:HIS:H	1.80	0.46
2:M:185:LYS:HB3	2:M:188:LYS:O	2.15	0.46
2:M:352:ALA:O	2:M:356:ARG:HG3	2.16	0.46
2:M:498:GLN:CG	2:M:516:ARG:HH21	2.27	0.46
2:M:517:ARG:HG3	2:M:522:VAL:HG21	1.96	0.46
2:M:592:LEU:HD13	9:M:2275:HOH:O	2.14	0.46
2:M:770:GLU:HG2	3:N:65:ARG:HH22	1.79	0.46
2:M:810:ASP:HA	2:M:811:PRO:HD3	1.81	0.46
2:M:820:ARG:HG2	2:M:820:ARG:NH1	2.30	0.46
2:M:841:ASN:ND2	2:M:841:ASN:C	2.73	0.46
2:M:897:LEU:HD11	2:M:921:ALA:HA	1.96	0.46
3:N:50:PHE:HB3	3:N:522:PRO:HG2	1.97	0.46
3:N:196:VAL:HG12	9:N:9691:HOH:O	2.14	0.46
3:N:426:LYS:HD2	3:N:428:LYS:HZ1	1.80	0.46
5:P:77:THR:O	5:P:81:VAL:HG23	2.15	0.46
1:A:91:ASN:OD1	1:A:92:PRO:HD2	2.15	0.46
1:A:205:VAL:HG23	1:A:206:THR:N	2.31	0.46
9:B:9616:HOH:O	3:D:813:LEU:HD21	2.15	0.46
2:C:16:PRO:CG	2:C:460:ARG:HH12	2.28	0.46
2:C:642:ARG:HA	9:C:9967:HOH:O	2.15	0.46
2:C:757:GLY:HA2	2:C:789:SER:HB3	1.96	0.46
2:C:911:GLU:O	2:C:915:LYS:HG2	2.15	0.46
2:C:1030:GLN:HA	2:C:1030:GLN:NE2	2.29	0.46
2:C:1109:VAL:CG2	3:D:3:LYS:HG2	2.43	0.46
3:D:104:PHE:HB2	9:D:9538:HOH:O	2.15	0.46
3:D:196:VAL:HG13	3:D:202:VAL:CG1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:654:LYS:HD3	3:D:674:ARG:HH22	1.80	0.46
3:D:765:SER:C	3:D:767:HIS:H	2.24	0.46
3:D:844:ALA:O	3:D:867:ARG:HD2	2.15	0.46
3:D:859:ASP:O	3:D:877:PRO:HG2	2.16	0.46
5:F:123:ASP:HB2	5:F:126:LEU:HD13	1.98	0.46
1:L:133:GLU:HG3	1:L:134:GLU:HG2	1.97	0.46
2:M:342:ASP:O	2:M:346:VAL:HG23	2.16	0.46
2:M:403:SER:O	2:M:407:LYS:HG3	2.15	0.46
2:M:1067:TYR:HE2	5:P:342:VAL:HA	1.81	0.46
3:N:54:LYS:HG3	3:N:55:ASP:OD1	2.16	0.46
3:N:1124:GLN:HA	3:N:1125:PRO:HD3	1.70	0.46
3:N:1366:LYS:O	3:N:1370:ILE:HG12	2.16	0.46
3:N:1382:THR:OG1	3:N:1418:LYS:HE3	2.15	0.46
3:N:1403:LEU:O	3:N:1407:LEU:HB2	2.16	0.46
3:N:1422:MET:HE1	9:N:2491:HOH:O	2.16	0.46
3:N:1465:ASN:HD22	3:N:1465:ASN:HA	1.49	0.46
4:O:86:GLN:HE21	4:O:86:GLN:HB3	1.59	0.46
5:P:139:ALA:HA	9:P:3321:HOH:O	2.15	0.46
5:P:320:PRO:CB	5:P:324:GLU:HG2	2.45	0.46
5:P:363:GLU:HA	5:P:367:MET:CE	2.37	0.46
1:A:7:LYS:HD2	9:A:9499:HOH:O	2.15	0.46
1:B:150:TYR:HD2	3:D:857:ILE:HG13	1.77	0.46
2:C:498:GLN:CD	3:D:1068:LEU:HD12	2.41	0.46
2:C:961:GLU:HA	2:C:961:GLU:OE2	2.16	0.46
3:D:56:TYR:CE2	3:D:66:GLN:HA	2.50	0.46
3:D:68:PHE:O	3:D:71:LYS:HG2	2.15	0.46
3:D:422:ALA:O	3:D:427:VAL:HG21	2.16	0.46
3:D:552:ASN:HA	3:D:555:LYS:HE3	1.96	0.46
3:D:960:LYS:HG2	3:D:964:LEU:HD12	1.98	0.46
9:D:9547:HOH:O	5:F:349:LEU:HD12	2.15	0.46
4:E:58:PRO:HB2	9:E:9487:HOH:O	2.16	0.46
1:L:34:VAL:HG12	9:M:9557:HOH:O	2.15	0.46
2:M:22:GLN:HE22	2:M:336:VAL:HG21	1.79	0.46
2:M:861:LEU:HD22	2:M:863:ASP:OD1	2.16	0.46
2:M:897:LEU:HG	2:M:920:GLN:HE21	1.77	0.46
3:N:580:ALA:HA	3:N:584:ASN:OD1	2.15	0.46
3:N:647:ARG:CZ	9:N:2258:HOH:O	2.63	0.46
3:N:957:PRO:HG3	3:N:1007:VAL:HA	1.98	0.46
3:N:1129:THR:HG23	3:N:1130:ARG:H	1.81	0.46
3:N:1256:LEU:HA	3:N:1259:VAL:HG23	1.98	0.46
3:N:1431:THR:OG1	3:N:1432:LYS:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:317:LEU:O	5:P:329:TYR:HB3	2.15	0.46
5:P:416:ARG:CZ	5:P:419:ARG:HB3	2.46	0.46
1:A:9:PRO:HB3	1:A:25:LEU:CG	2.45	0.46
1:A:30:ARG:NH1	1:A:191:ASP:HB2	2.31	0.46
1:A:101:LEU:HG	1:A:114:PHE:CA	2.43	0.46
1:B:71:VAL:HG22	1:B:132:LEU:HD12	1.97	0.46
1:B:111:ALA:HB3	1:B:124:ASN:O	2.15	0.46
2:C:39:ARG:HG3	9:C:9773:HOH:O	2.15	0.46
2:C:127:PHE:O	2:C:133:ASP:HA	2.16	0.46
2:C:625:LEU:HB3	2:C:639:GLN:HB2	1.97	0.46
2:C:676:ILE:HG21	2:C:988:VAL:HG22	1.97	0.46
2:C:777:ILE:HG22	2:C:778:PHE:HD1	1.81	0.46
2:C:915:LYS:O	2:C:968:LEU:HD22	2.14	0.46
3:D:708:LEU:HA	3:D:708:LEU:HD23	1.73	0.46
3:D:820:GLU:HA	3:D:825:ALA:O	2.16	0.46
3:D:829:VAL:HG11	9:D:2252:HOH:O	2.15	0.46
3:D:1046:GLN:HB2	9:D:9695:HOH:O	2.15	0.46
3:D:1295:GLU:HG2	9:D:9793:HOH:O	2.15	0.46
3:D:1299:PHE:CD2	3:D:1299:PHE:N	2.84	0.46
3:D:1306:PRO:HG3	9:D:9577:HOH:O	2.16	0.46
3:D:1486:VAL:HG12	3:D:1487:VAL:N	2.30	0.46
2:M:17:PRO:O	2:M:20:GLU:N	2.46	0.46
2:M:429:ASP:HB3	9:M:9514:HOH:O	2.15	0.46
2:M:565:GLN:OE1	2:M:842:ARG:HG2	2.14	0.46
2:M:680:ASP:HB2	2:M:682:TYR:CE2	2.50	0.46
2:M:861:LEU:HD23	2:M:862:PRO:N	2.31	0.46
2:M:904:PRO:HG3	9:M:9623:HOH:O	2.16	0.46
2:M:1016:ILE:HD12	5:P:317:LEU:HD21	1.97	0.46
3:N:34:TYR:CE1	5:P:264:MET:HE2	2.51	0.46
3:N:107:ASP:O	3:N:108:VAL:C	2.59	0.46
3:N:416:ALA:HB3	3:N:417:PRO:HD3	1.97	0.46
3:N:562:ALA:HB1	3:N:567:ILE:CD1	2.45	0.46
3:N:1008:PHE:HB3	3:N:1012:GLU:OE2	2.15	0.46
3:N:1342:GLU:HB3	9:N:9577:HOH:O	2.15	0.46
5:P:127:ILE:HD11	9:P:4895:HOH:O	2.16	0.46
5:P:314:PRO:HD2	9:P:4162:HOH:O	2.15	0.46
1:A:43:ILE:HA	1:A:47:SER:OG	2.16	0.46
2:C:3:ILE:CD1	2:C:900:ARG:HB2	2.46	0.46
2:C:93:PRO:HB2	9:C:9537:HOH:O	2.14	0.46
2:C:115:LEU:HD12	2:C:378:LEU:HD22	1.97	0.46
2:C:129:ILE:HG12	2:C:386:PHE:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:145:GLY:C	2:C:163:ILE:HG23	2.40	0.46
2:C:777:ILE:HG22	2:C:778:PHE:CD1	2.51	0.46
2:C:1013:TYR:HB2	5:F:335:ASP:OD2	2.15	0.46
2:C:1101:THR:O	2:C:1102:LEU:HD12	2.15	0.46
3:D:22:SER:HB3	9:D:9666:HOH:O	2.16	0.46
3:D:93:ILE:HG12	3:D:548:ILE:HD12	1.98	0.46
3:D:208:PRO:CB	3:D:395:VAL:HG13	2.45	0.46
3:D:396:VAL:CG2	3:D:447:VAL:HB	2.42	0.46
3:D:397:LYS:NZ	3:D:399:ARG:HH21	2.13	0.46
3:D:512:MET:HE1	9:D:9759:HOH:O	2.16	0.46
3:D:581:LEU:HD12	3:D:603:LEU:HD12	1.96	0.46
3:D:860:LEU:O	3:D:877:PRO:HD2	2.16	0.46
3:D:983:LEU:HB2	9:D:9513:HOH:O	2.16	0.46
3:D:1139:ASP:O	3:D:1142:ALA:HB3	2.15	0.46
3:D:1258:ARG:HG3	3:D:1262:LEU:HD13	1.96	0.46
3:D:1331:ASP:OD1	3:D:1333:HIS:HB2	2.15	0.46
3:D:1346:ARG:HB2	3:D:1346:ARG:NH1	2.30	0.46
5:F:353:GLU:OE1	5:F:356:LYS:HD2	2.16	0.46
1:K:9:PRO:HG2	1:L:224:TYR:CD2	2.51	0.46
1:L:159:LYS:HD3	1:L:159:LYS:N	2.31	0.46
2:M:4:LYS:HE3	9:M:9956:HOH:O	2.15	0.46
2:M:409:ARG:HG2	9:M:2089:HOH:O	2.16	0.46
2:M:428:ARG:O	3:N:1078:ARG:NH1	2.49	0.46
3:N:388:HIS:H	5:P:97:GLU:HG3	1.79	0.46
3:N:434:ARG:HG3	9:N:9784:HOH:O	2.14	0.46
3:N:608:SER:OG	3:N:609:GLY:N	2.46	0.46
3:N:899:LEU:CD1	3:N:900:ILE:HG23	2.46	0.46
3:N:924:MET:HE3	4:O:7:ASP:OD1	2.16	0.46
3:N:928:ALA:O	3:N:931:LEU:HB2	2.16	0.46
3:N:1383:ASP:HB3	3:N:1416:ALA:H	1.81	0.46
4:O:4:PRO:HG3	9:O:5463:HOH:O	2.15	0.46
4:O:5:GLY:O	4:O:9:LEU:HG	2.15	0.46
1:A:86:VAL:HG23	1:A:202:ASP:OD1	2.16	0.46
1:B:123:MET:CG	9:B:9635:HOH:O	2.64	0.46
2:C:289:THR:HG22	2:C:290:LEU:H	1.80	0.46
2:C:289:THR:HG22	2:C:290:LEU:HD22	1.97	0.46
2:C:1049:LEU:HG	2:C:1053:LEU:HD11	1.96	0.46
2:C:1092:LEU:HD22	2:C:1099:VAL:CG2	2.46	0.46
3:D:468:LEU:HB3	9:D:9997:HOH:O	2.16	0.46
3:D:847:ASP:OD1	3:D:848:GLU:N	2.49	0.46
3:D:867:ARG:CB	3:D:867:ARG:HH11	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:919:PHE:HD2	3:D:919:PHE:O	1.98	0.46
3:D:1496:GLU:HA	3:D:1499:ARG:CD	2.45	0.46
4:E:54:LEU:HG	4:E:58:PRO:HG2	1.97	0.46
1:L:69:PRO:HB3	9:L:5138:HOH:O	2.16	0.46
1:L:123:MET:O	1:L:125:PRO:HD3	2.16	0.46
2:M:73:LEU:HB2	9:M:2197:HOH:O	2.15	0.46
2:M:575:GLN:HB3	2:M:670:GLN:HA	1.97	0.46
2:M:654:LEU:HD11	2:M:657:ASP:CG	2.40	0.46
2:M:952:LEU:HD22	2:M:952:LEU:N	2.29	0.46
9:M:2201:HOH:O	4:O:32:ARG:HD3	2.16	0.46
3:N:42:ASP:O	3:N:46:ASP:HB2	2.16	0.46
3:N:82:LYS:HB2	3:N:82:LYS:NZ	2.31	0.46
3:N:558:LEU:HD13	5:P:145:PRO:CB	2.41	0.46
3:N:1000:THR:HG23	3:N:1001:GLU:N	2.30	0.46
3:N:1300:SER:HB2	9:N:2406:HOH:O	2.15	0.46
3:N:1304:LYS:HB3	9:N:9487:HOH:O	2.15	0.46
4:O:61:GLU:H	4:O:61:GLU:HG3	1.49	0.46
5:P:215:GLU:O	5:P:218:GLN:HB3	2.16	0.46
5:P:343:ASP:HA	9:P:5842:HOH:O	2.15	0.46
1:B:89:PHE:CD1	1:B:120:VAL:HG22	2.50	0.46
2:C:524:VAL:HG22	9:C:2060:HOH:O	2.15	0.46
2:C:630:ARG:HE	2:C:705:ILE:CG1	2.29	0.46
2:C:705:ILE:HG22	2:C:827:VAL:O	2.16	0.46
2:C:1005:MET:CB	3:D:629:SER:HB2	2.45	0.46
3:D:44:LEU:HB3	3:D:525:ARG:NH2	2.22	0.46
3:D:1003:VAL:O	3:D:1007:VAL:HG13	2.16	0.46
3:D:1101:VAL:HG12	3:D:1374:GLN:HB3	1.97	0.46
3:D:1209:LEU:HD23	3:D:1211:MET:H	1.80	0.46
3:D:1359:GLN:HB3	3:D:1359:GLN:HE21	1.51	0.46
1:K:58:ILE:HD13	1:K:140:MET:HB3	1.96	0.46
1:L:23:PHE:CE1	1:L:208:LEU:HD13	2.50	0.46
2:M:137:VAL:O	2:M:391:LEU:HD21	2.15	0.46
2:M:343:GLN:HB2	9:M:9681:HOH:O	2.15	0.46
2:M:636:ALA:HB2	2:M:703:ILE:HG22	1.97	0.46
2:M:669:GLY:O	2:M:670:GLN:HG2	2.15	0.46
2:M:841:ASN:HD22	2:M:843:HIS:N	2.14	0.46
2:M:1054:THR:HG21	2:M:1079:PRO:HB3	1.96	0.46
3:N:181:ASP:O	3:N:185:VAL:HG23	2.16	0.46
3:N:191:LEU:HD22	3:N:195:VAL:CG2	2.45	0.46
3:N:441:ARG:O	3:N:443:VAL:N	2.49	0.46
3:N:669:ASN:O	3:N:672:ALA:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1252:ILE:HG22	3:N:1253:THR:H	1.81	0.46
4:O:45:ARG:HB2	4:O:46:PRO:CD	2.45	0.46
5:P:226:LYS:HB2	5:P:238:TYR:OH	2.16	0.46
5:P:319:THR:HG21	9:P:5402:HOH:O	2.16	0.46
1:A:13:VAL:HG12	1:A:15:THR:HG22	1.96	0.46
2:C:72:ARG:HB3	9:C:2179:HOH:O	2.15	0.46
2:C:252:LYS:HZ2	2:C:296:GLY:HA3	1.81	0.46
2:C:319:GLY:HA3	9:C:2214:HOH:O	2.16	0.46
2:C:435:TYR:C	2:C:437:ARG:H	2.24	0.46
2:C:595:LEU:HB2	9:C:2223:HOH:O	2.15	0.46
2:C:682:TYR:N	9:C:9490:HOH:O	2.49	0.46
2:C:705:ILE:HA	2:C:827:VAL:O	2.16	0.46
3:D:413:ASP:OD1	3:D:421:LEU:HD22	2.15	0.46
3:D:827:ILE:O	3:D:837:GLY:HA3	2.16	0.46
3:D:1277:ILE:CD1	3:D:1301:LYS:HB2	2.44	0.46
5:F:289:GLU:O	5:F:293:GLU:HG3	2.16	0.46
2:M:305:PRO:CG	2:M:308:ARG:HH21	2.25	0.46
2:M:329:GLY:N	2:M:488:ALA:HB3	2.31	0.46
2:M:599:GLU:HB2	9:M:9583:HOH:O	2.15	0.46
2:M:918:LEU:HD23	2:M:968:LEU:HA	1.96	0.46
3:N:704:ARG:CZ	3:N:737:ASN:O	2.64	0.46
5:P:290:GLU:H	5:P:290:GLU:CD	2.23	0.46
5:P:422:LEU:HD11	9:P:3715:HOH:O	2.16	0.46
1:A:86:VAL:HG12	1:A:124:ASN:HB2	1.98	0.46
1:A:195:LEU:CD1	1:A:197:LEU:HD22	2.40	0.46
1:B:106:PRO:HG3	1:B:134:GLU:CD	2.40	0.46
2:C:118:ILE:HG22	2:C:382:ILE:HD13	1.98	0.46
2:C:136:ILE:CG2	2:C:336:VAL:HG13	2.43	0.46
2:C:242:LEU:HA	9:C:9503:HOH:O	2.16	0.46
2:C:761:PHE:N	2:C:761:PHE:CD1	2.84	0.46
3:D:68:PHE:HA	3:D:71:LYS:NZ	2.31	0.46
3:D:107:ASP:O	3:D:108:VAL:C	2.59	0.46
3:D:591:VAL:HG12	3:D:592:THR:O	2.16	0.46
3:D:694:VAL:HG13	9:D:2053:HOH:O	2.16	0.46
3:D:1258:ARG:HH21	3:D:1351:GLU:HG2	1.81	0.46
2:M:146:VAL:HG11	2:M:306:THR:HG22	1.98	0.46
2:M:205:GLU:O	2:M:209:ARG:HD2	2.15	0.46
2:M:311:PHE:HB2	9:M:2157:HOH:O	2.16	0.46
2:M:438:ILE:HG22	2:M:439:CYS:O	2.16	0.46
2:M:675:ALA:CA	2:M:989:VAL:HG12	2.37	0.46
2:M:708:TYR:CD1	2:M:708:TYR:N	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:1090:LYS:HE2	2:M:1112:PHE:CE1	2.51	0.46
9:M:2448:HOH:O	5:P:283:GLY:HA2	2.15	0.46
3:N:31:THR:HB	3:N:32:ILE:H	1.62	0.46
3:N:213:VAL:HG22	3:N:214:GLU:H	1.81	0.46
3:N:411:THR:HG22	9:N:2263:HOH:O	2.16	0.46
3:N:667:ALA:HB2	9:N:2385:HOH:O	2.15	0.46
3:N:774:SER:C	3:N:776:GLU:N	2.74	0.46
3:N:1114:THR:HA	9:N:2201:HOH:O	2.16	0.46
3:N:1481:VAL:HG13	4:O:18:ARG:NE	2.27	0.46
5:P:102:LEU:HD22	5:P:183:ALA:O	2.15	0.46
1:A:9:PRO:HB3	1:A:25:LEU:HG	1.98	0.45
1:B:89:PHE:CD1	1:B:120:VAL:HG13	2.51	0.45
2:C:207:LEU:HD22	2:C:221:LEU:CD2	2.46	0.45
2:C:354:GLY:HA2	9:C:9624:HOH:O	2.15	0.45
2:C:860:HIS:HE2	2:C:975:TYR:HB2	1.81	0.45
3:D:235:ALA:HB3	9:D:2112:HOH:O	2.16	0.45
3:D:531:ASP:HB2	9:D:2123:HOH:O	2.16	0.45
3:D:564:GLU:HB2	9:F:9561:HOH:O	2.16	0.45
3:D:806:PHE:O	3:D:807:ALA:C	2.59	0.45
3:D:868:TYR:CG	3:D:869:MET:N	2.75	0.45
3:D:1043:GLY:O	3:D:1056:PRO:HB3	2.15	0.45
3:D:1106:VAL:HG21	3:D:1474:ALA:HB2	1.99	0.45
3:D:1221:VAL:O	3:D:1222:GLY:C	2.58	0.45
3:D:1346:ARG:HB2	3:D:1346:ARG:HH11	1.81	0.45
3:D:1403:LEU:HD12	9:D:2493:HOH:O	2.15	0.45
5:F:226:LYS:HE3	9:F:9804:HOH:O	2.17	0.45
5:F:362:SER:C	5:F:364:ARG:H	2.23	0.45
1:L:153:ALA:HA	1:L:156:HIS:NE2	2.30	0.45
2:M:60:GLY:HA2	9:M:9972:HOH:O	2.16	0.45
2:M:352:ALA:C	2:M:355:VAL:HG12	2.41	0.45
2:M:669:GLY:C	2:M:670:GLN:HG2	2.41	0.45
2:M:822:VAL:HG13	9:M:9775:HOH:O	2.15	0.45
2:M:1005:MET:HE1	3:N:645:PRO:HB2	1.98	0.45
3:N:586:ARG:HG2	9:N:2658:HOH:O	2.16	0.45
3:N:1122:LEU:HD23	3:N:1178:ALA:HB2	1.98	0.45
3:N:1495:ILE:O	3:N:1498:ALA:HB3	2.16	0.45
1:A:211:LEU:O	1:A:211:LEU:HD12	2.16	0.45
1:A:216:GLU:HG3	1:A:220:GLU:OE1	2.16	0.45
1:B:87:VAL:HA	9:B:9635:HOH:O	2.16	0.45
2:C:43:GLY:HA2	2:C:341:THR:OG1	2.16	0.45
2:C:339:LEU:HB3	2:C:385:PHE:HZ	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:471:TYR:HE1	2:C:491:GLU:OE2	1.99	0.45
2:C:578:VAL:HG21	2:C:991:GLN:O	2.16	0.45
2:C:742:VAL:HG23	9:C:2181:HOH:O	2.15	0.45
2:C:773:LEU:O	2:C:777:ILE:HG13	2.16	0.45
3:D:29:PRO:HG3	3:D:549:ASN:ND2	2.31	0.45
3:D:1007:VAL:HG23	3:D:1008:PHE:N	2.32	0.45
3:D:1290:LEU:CD2	3:D:1291:SER:H	2.28	0.45
5:F:316:SER:C	5:F:318:GLU:N	2.68	0.45
2:M:83:CYS:CA	2:M:88:LEU:HB3	2.42	0.45
2:M:603:VAL:HG23	2:M:647:GLN:O	2.16	0.45
2:M:811:PRO:HD3	9:M:9734:HOH:O	2.16	0.45
2:M:890:LEU:HA	2:M:914:ILE:HD13	1.96	0.45
2:M:893:ALA:O	2:M:897:LEU:HD22	2.16	0.45
2:M:1051:GLU:HG2	2:M:1056:LYS:CD	2.44	0.45
2:M:1086:ARG:HH11	2:M:1112:PHE:HA	1.82	0.45
3:N:156:GLU:O	3:N:159:ARG:HB3	2.17	0.45
3:N:523:ASP:O	3:N:526:PRO:HG3	2.17	0.45
3:N:765:SER:O	3:N:767:HIS:N	2.49	0.45
3:N:827:ILE:O	3:N:837:GLY:HA3	2.16	0.45
3:N:1087:ARG:HG2	3:N:1087:ARG:HH11	1.81	0.45
3:N:1246:VAL:HG21	9:N:2444:HOH:O	2.16	0.45
3:N:1272:ALA:CA	3:N:1326:THR:HB	2.44	0.45
3:N:1365:ASP:O	3:N:1369:GLU:HG3	2.16	0.45
4:O:69:LEU:O	4:O:69:LEU:HD23	2.16	0.45
5:P:132:ARG:NH1	5:P:136:LEU:HD21	2.27	0.45
1:A:9:PRO:HD2	1:B:224:TYR:CE1	2.52	0.45
1:A:206:THR:CG2	1:A:209:GLU:H	2.30	0.45
2:C:10:ARG:HH11	2:C:11:GLU:H	1.63	0.45
2:C:16:PRO:O	2:C:18:LEU:HD12	2.16	0.45
2:C:30:LEU:HD12	2:C:30:LEU:O	2.16	0.45
2:C:68:PHE:HZ	2:C:71:TYR:HB3	1.80	0.45
2:C:238:LEU:HD23	2:C:241:LEU:HB3	1.99	0.45
2:C:675:ALA:CA	2:C:989:VAL:HG12	2.40	0.45
2:C:873:PRO:O	2:C:876:VAL:HG23	2.16	0.45
3:D:115:LEU:HD22	3:D:502:PHE:HE1	1.80	0.45
3:D:135:LEU:HA	3:D:453:ASP:O	2.16	0.45
3:D:411:THR:HG23	9:D:9915:HOH:O	2.16	0.45
3:D:493:ARG:NH1	3:D:493:ARG:HG2	2.30	0.45
3:D:618:LEU:HD11	3:D:1463:LYS:HD2	1.97	0.45
3:D:750:PRO:O	3:D:756:GLN:OE1	2.35	0.45
3:D:799:LYS:N	3:D:826:PRO:HG2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1256:LEU:HA	3:D:1259:VAL:HG23	1.98	0.45
5:F:104:ARG:CZ	9:F:9749:HOH:O	2.64	0.45
5:F:220:LEU:O	5:F:224:VAL:HG23	2.15	0.45
1:K:184:THR:O	1:K:192:LEU:HB2	2.16	0.45
1:L:206:THR:HG23	1:L:208:LEU:N	2.31	0.45
2:M:52:PHE:O	2:M:54:ILE:N	2.50	0.45
2:M:68:PHE:CE1	2:M:96:ALA:HB1	2.44	0.45
2:M:77:PRO:HD3	2:M:93:PRO:HD3	1.98	0.45
2:M:713:ARG:NH2	2:M:819:VAL:HG22	2.32	0.45
2:M:768:THR:CG2	2:M:771:GLU:HB3	2.46	0.45
2:M:950:LEU:HB3	2:M:952:LEU:HD23	1.98	0.45
3:N:65:ARG:H	3:N:68:PHE:HZ	1.64	0.45
3:N:128:TYR:HB3	3:N:129:PHE:CD1	2.51	0.45
3:N:696:HIS:HB2	4:O:48:MET:CE	2.47	0.45
3:N:1012:GLU:HG3	3:N:1021:TYR:OH	2.15	0.45
3:N:1380:GLU:HB2	3:N:1420:LEU:HD23	1.98	0.45
3:N:1425:THR:CG2	3:N:1426:LYS:N	2.79	0.45
3:N:1500:LYS:O	3:N:1503:VAL:HG23	2.16	0.45
5:P:338:LEU:HB2	9:P:5459:HOH:O	2.16	0.45
1:A:111:ALA:HB3	1:A:124:ASN:O	2.16	0.45
1:B:189:ARG:HG3	9:B:9505:HOH:O	2.16	0.45
2:C:64:LEU:HB2	2:C:359:MET:SD	2.56	0.45
2:C:80:GLN:O	2:C:83:CYS:HB2	2.17	0.45
2:C:165:LEU:HA	2:C:166:PRO:O	2.16	0.45
2:C:261:ILE:HA	9:C:2458:HOH:O	2.17	0.45
2:C:455:LEU:O	2:C:541:SER:HB3	2.16	0.45
2:C:462:ASP:CG	2:C:463:GLU:H	2.24	0.45
2:C:598:GLU:HB2	2:C:615:TYR:OH	2.17	0.45
2:C:939:ARG:HG3	9:C:9564:HOH:O	2.16	0.45
3:D:153:LEU:HD11	3:D:157:GLU:HB2	1.97	0.45
3:D:191:LEU:HD22	3:D:195:VAL:HG11	1.98	0.45
3:D:427:VAL:HB	3:D:435:VAL:HB	1.99	0.45
3:D:462:GLN:HB2	3:D:513:ILE:HG21	1.98	0.45
3:D:661:MET:SD	3:D:687:VAL:HG22	2.57	0.45
3:D:862:ASP:O	3:D:877:PRO:HD3	2.16	0.45
3:D:926:LYS:HE3	9:D:9911:HOH:O	2.16	0.45
3:D:957:PRO:HG3	3:D:1010:ASN:HD22	1.81	0.45
3:D:965:GLU:HB2	9:D:9490:HOH:O	2.16	0.45
3:D:1278:ASP:HB2	3:D:1318:TYR:CE1	2.51	0.45
5:F:270:LYS:HB3	5:F:295:MET:CE	2.46	0.45
1:K:30:ARG:HG3	1:K:30:ARG:NH1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:127:PHE:O	2:M:133:ASP:HA	2.16	0.45
2:M:626:ARG:HG2	9:M:2116:HOH:O	2.15	0.45
2:M:905:ILE:HG22	2:M:906:PHE:CD1	2.52	0.45
3:N:95:LEU:HA	3:N:551:ASN:OD1	2.15	0.45
3:N:171:LEU:HB2	3:N:390:PRO:CA	2.47	0.45
3:N:171:LEU:HA	3:N:390:PRO:HA	1.97	0.45
3:N:400:VAL:C	3:N:402:PRO:HD3	2.42	0.45
3:N:427:VAL:HB	3:N:435:VAL:CG2	2.47	0.45
3:N:1128:VAL:O	3:N:1129:THR:C	2.58	0.45
3:N:1326:THR:HG22	3:N:1327:ARG:H	1.81	0.45
1:A:182:GLU:HB3	9:A:9489:HOH:O	2.17	0.45
2:C:9:ILE:HG13	2:C:9:ILE:O	2.16	0.45
2:C:115:LEU:HD22	2:C:373:VAL:CG1	2.46	0.45
2:C:140:ILE:CD1	2:C:412:ALA:HA	2.47	0.45
2:C:410:ILE:N	2:C:410:ILE:HD12	2.32	0.45
2:C:716:LYS:HE3	9:C:9571:HOH:O	2.16	0.45
2:C:839:LEU:N	2:C:839:LEU:HD23	2.31	0.45
2:C:1039:ALA:O	2:C:1043:TYR:HD1	1.98	0.45
3:D:153:LEU:HD13	3:D:157:GLU:HB2	1.98	0.45
3:D:1047:LYS:HD2	3:D:1051:GLU:CD	2.42	0.45
3:D:1341:PRO:O	3:D:1344:VAL:HG23	2.17	0.45
5:F:113:ILE:HG23	5:F:127:ILE:CG2	2.47	0.45
5:F:215:GLU:N	9:F:9503:HOH:O	2.48	0.45
5:F:393:THR:O	5:F:397:ILE:HG13	2.16	0.45
1:L:110:LYS:HD3	9:L:4382:HOH:O	2.16	0.45
2:M:64:LEU:HB2	2:M:359:MET:SD	2.56	0.45
2:M:110:GLU:CG	2:M:369:PRO:HG3	2.29	0.45
2:M:164:PRO:HG2	9:M:9517:HOH:O	2.17	0.45
2:M:267:TYR:HB2	2:M:272:ALA:CB	2.47	0.45
2:M:854:PRO:C	2:M:856:GLU:N	2.73	0.45
2:M:1036:GLU:O	2:M:1039:ALA:HB3	2.16	0.45
2:M:1085:PHE:O	2:M:1089:VAL:HG23	2.17	0.45
3:N:28:LYS:O	3:N:43:GLY:HA2	2.16	0.45
3:N:806:PHE:O	3:N:806:PHE:CG	2.69	0.45
3:N:984:THR:HG22	3:N:987:GLU:CG	2.40	0.45
3:N:1033:GLN:HB3	9:N:9622:HOH:O	2.17	0.45
3:N:1240:THR:O	3:N:1257:PRO:HB3	2.17	0.45
1:A:128:HIS:CE1	1:A:131:THR:HG23	2.51	0.45
1:A:218:LEU:HD23	1:B:222:LEU:HD21	1.99	0.45
1:B:27:PRO:HG2	1:B:186:LEU:CD1	2.46	0.45
1:B:86:VAL:HG13	1:B:123:MET:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:41:ASN:HD22	2:C:41:ASN:N	1.97	0.45
2:C:286:SER:HB3	2:C:299:LYS:HE3	1.98	0.45
2:C:631:SER:HB3	2:C:637:LEU:HD21	1.99	0.45
2:C:713:ARG:NH1	3:D:532:GLY:HA2	2.31	0.45
2:C:863:ASP:O	2:C:865:THR:N	2.50	0.45
2:C:1101:THR:HB	3:D:5:VAL:CG1	2.46	0.45
3:D:169:TYR:HA	3:D:392:SER:HA	1.99	0.45
3:D:171:LEU:HD11	3:D:388:HIS:CB	2.46	0.45
3:D:399:ARG:HB3	3:D:402:PRO:HG3	1.98	0.45
3:D:566:ILE:CG1	5:F:192:LEU:HD11	2.46	0.45
3:D:619:LEU:HB2	9:D:9516:HOH:O	2.15	0.45
3:D:659:LYS:HD3	3:D:659:LYS:C	2.41	0.45
3:D:729:HIS:ND1	3:D:730:PRO:N	2.64	0.45
3:D:1026:SER:C	3:D:1028:ALA:N	2.75	0.45
3:D:1467:ILE:HG13	9:D:9868:HOH:O	2.16	0.45
5:F:241:TRP:HA	5:F:244:ARG:NH1	2.31	0.45
5:F:263:HIS:HB2	9:F:9611:HOH:O	2.17	0.45
5:F:282:LEU:HB2	5:F:284:ARG:H	1.81	0.45
5:F:421:PHE:C	5:F:423:ASP:N	2.73	0.45
1:L:9:PRO:HB3	1:L:25:LEU:HG	1.98	0.45
1:L:94:LEU:HD11	9:L:4208:HOH:O	2.16	0.45
1:L:189:ARG:HG3	1:L:189:ARG:HH11	1.81	0.45
2:M:68:PHE:CZ	2:M:71:TYR:HB3	2.49	0.45
2:M:380:ALA:HA	2:M:383:ARG:HG2	1.99	0.45
2:M:516:ARG:NH2	3:N:1068:LEU:HB2	2.32	0.45
2:M:626:ARG:HB2	2:M:639:GLN:NE2	2.31	0.45
2:M:704:HIS:CG	2:M:831:ARG:HH21	2.34	0.45
2:M:897:LEU:HD22	2:M:921:ALA:HB2	1.98	0.45
2:M:1104:GLU:HA	3:N:6:ARG:HD3	1.97	0.45
3:N:179:VAL:HG22	3:N:389:GLU:HG3	1.99	0.45
3:N:651:GLU:OE1	3:N:651:GLU:HA	2.17	0.45
3:N:728:LEU:HD11	3:N:732:VAL:CG2	2.46	0.45
3:N:729:HIS:CE1	3:N:731:LEU:HG	2.47	0.45
3:N:1114:THR:HG23	3:N:1114:THR:O	2.16	0.45
3:N:1213:ARG:HD3	9:N:2343:HOH:O	2.15	0.45
3:N:1353:GLN:HE21	3:N:1353:GLN:HB3	1.54	0.45
3:N:1353:GLN:HE21	3:N:1357:ARG:NE	2.15	0.45
4:O:17:TYR:O	4:O:21:VAL:HG23	2.16	0.45
5:P:128:ARG:O	5:P:132:ARG:HG3	2.16	0.45
5:P:141:VAL:O	5:P:145:PRO:HD2	2.15	0.45
1:B:44:LEU:HD23	1:B:48:ILE:CD1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:LEU:HG	1:B:163:ASN:CG	2.41	0.45
1:B:101:LEU:HB2	1:B:114:PHE:CD2	2.51	0.45
2:C:326:ASP:HB2	2:C:431:HIS:ND1	2.32	0.45
2:C:693:GLU:OE2	2:C:855:VAL:HG21	2.17	0.45
2:C:704:HIS:CG	2:C:831:ARG:HE	2.34	0.45
2:C:1021:LEU:HG	2:C:1022:GLY:N	2.31	0.45
2:C:1060:ILE:HG23	2:C:1061:GLU:N	2.31	0.45
3:D:507:ASN:HB3	9:D:9971:HOH:O	2.17	0.45
3:D:639:LEU:CD1	3:D:640:HIS:H	2.29	0.45
3:D:666:ILE:H	3:D:666:ILE:HG13	1.61	0.45
3:D:700:VAL:HB	3:D:748:HIS:O	2.17	0.45
3:D:767:HIS:CD2	4:E:6:ILE:HG12	2.52	0.45
3:D:1084:THR:HG22	9:D:9646:HOH:O	2.17	0.45
3:D:1094:LEU:HD23	9:D:9776:HOH:O	2.16	0.45
3:D:1258:ARG:NE	3:D:1262:LEU:HD11	2.32	0.45
3:D:1312:LEU:HB2	9:D:2444:HOH:O	2.16	0.45
3:D:1383:ASP:HB3	3:D:1416:ALA:H	1.82	0.45
4:E:13:VAL:HG21	4:E:19:LEU:HB2	1.98	0.45
5:F:374:GLY:N	9:F:9672:HOH:O	2.49	0.45
1:K:20:TYR:CE2	1:K:22:GLU:HG2	2.52	0.45
2:M:3:ILE:HG21	9:M:2314:HOH:O	2.16	0.45
2:M:688:ILE:HD12	2:M:688:ILE:N	2.31	0.45
2:M:861:LEU:HD21	2:M:925:TYR:CE2	2.51	0.45
3:N:130:SER:O	3:N:568:ARG:NH2	2.50	0.45
3:N:197:SER:HB2	3:N:205:TYR:OH	2.17	0.45
3:N:379:ALA:HB2	9:N:9717:HOH:O	2.15	0.45
3:N:647:ARG:CZ	3:N:680:GLN:HE21	2.29	0.45
3:N:683:ILE:HG22	9:N:2260:HOH:O	2.16	0.45
3:N:701:LEU:H	3:N:701:LEU:HD22	1.82	0.45
3:N:989:TYR:HB2	9:N:9817:HOH:O	2.17	0.45
3:N:1312:LEU:CB	9:N:9707:HOH:O	2.64	0.45
3:N:1432:LYS:H	3:N:1432:LYS:HG3	1.48	0.45
3:N:1435:LEU:HD23	3:N:1464:GLU:HB2	1.98	0.45
4:O:70:THR:CB	4:O:72:ARG:HE	2.29	0.45
4:O:75:PHE:HD1	9:O:5601:HOH:O	1.99	0.45
5:P:392:VAL:CG1	5:P:396:ARG:HG3	2.47	0.45
1:A:100:LEU:N	9:A:9585:HOH:O	2.48	0.45
1:B:102:LYS:HE2	1:B:104:GLU:OE1	2.17	0.45
2:C:4:LYS:HB2	9:C:9680:HOH:O	2.17	0.45
2:C:114:PHE:CD1	2:C:114:PHE:N	2.84	0.45
2:C:886:LEU:CG	3:D:951:ILE:HG13	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1008:ARG:HH22	2:C:1021:LEU:C	2.25	0.45
3:D:127:LEU:HD21	3:D:461:ILE:CD1	2.44	0.45
3:D:637:LEU:HD11	3:D:641:GLN:HB2	1.99	0.45
3:D:728:LEU:HD13	3:D:745:MET:CE	2.45	0.45
3:D:764:LEU:HD12	3:D:765:SER:N	2.32	0.45
3:D:1264:GLU:OE2	3:D:1264:GLU:HA	2.16	0.45
4:E:25:LYS:HA	4:E:28:GLN:NE2	2.32	0.45
5:F:84:TYR:CD2	5:F:192:LEU:HD13	2.52	0.45
5:F:193:ARG:NH2	9:F:9492:HOH:O	2.50	0.45
1:L:5:LYS:HA	1:L:5:LYS:HZ2	1.80	0.45
2:M:1034:GLU:CA	2:M:1037:VAL:HG23	2.47	0.45
3:N:598:ARG:NH2	5:P:318:GLU:O	2.48	0.45
3:N:963:TYR:CE2	3:N:1002:LYS:HB3	2.52	0.45
3:N:996:TRP:O	3:N:1000:THR:HG22	2.17	0.45
3:N:1145:TYR:HD2	3:N:1168:MET:HE2	1.81	0.45
3:N:1348:LEU:HD13	3:N:1348:LEU:HA	1.81	0.45
4:O:33:HIS:CD2	4:O:89:MET:HG2	2.52	0.45
4:O:43:GLU:HG2	4:O:44:GLU:N	2.32	0.45
4:O:87:LYS:HE2	4:O:91:ARG:CZ	2.47	0.45
5:P:154:LYS:HE3	5:P:158:GLU:HG2	1.98	0.45
5:P:270:LYS:HE2	9:P:5582:HOH:O	2.17	0.45
5:P:372:ARG:HG2	9:P:6083:HOH:O	2.17	0.45
2:C:20:GLU:HG2	2:C:21:ILE:N	2.31	0.45
2:C:22:GLN:NE2	2:C:121:MET:HE2	2.32	0.45
2:C:70:GLU:HB2	2:C:97:ARG:HD2	1.98	0.45
2:C:89:THR:HG21	2:C:383:ARG:HH22	1.82	0.45
2:C:532:MET:HG3	2:C:533:ASP:N	2.32	0.45
2:C:1060:ILE:CG2	2:C:1061:GLU:N	2.80	0.45
2:C:1088:LEU:HA	2:C:1091:GLU:OE1	2.17	0.45
3:D:90:MET:N	9:D:9497:HOH:O	2.50	0.45
3:D:127:LEU:CD1	3:D:457:GLY:H	2.30	0.45
3:D:180:LYS:HG3	9:D:2419:HOH:O	2.17	0.45
3:D:853:VAL:HG22	3:D:858:VAL:HG23	1.99	0.45
5:F:196:VAL:HG13	5:F:213:ILE:CD1	2.46	0.45
1:K:41:ARG:NH1	1:K:177:VAL:HB	2.32	0.45
1:K:89:PHE:CB	1:K:94:LEU:HD13	2.45	0.45
1:K:91:ASN:H	1:K:94:LEU:HD12	1.82	0.45
2:M:52:PHE:HB3	2:M:53:PRO:HD3	1.99	0.45
2:M:290:LEU:HB3	2:M:302:VAL:HG12	1.98	0.45
2:M:842:ARG:HB2	9:M:9551:HOH:O	2.16	0.45
2:M:987:ILE:HG12	3:N:948:THR:CG2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:1039:ALA:O	2:M:1043:TYR:HD1	2.00	0.45
9:M:2262:HOH:O	3:N:3:LYS:HB3	2.17	0.45
3:N:55:ASP:HA	3:N:82:LYS:HE3	1.98	0.45
3:N:82:LYS:HD3	5:P:337:HIS:HB3	1.99	0.45
3:N:111:LYS:NZ	3:N:498:VAL:HG12	2.32	0.45
3:N:411:THR:HG21	9:N:9532:HOH:O	2.17	0.45
3:N:637:LEU:HD11	3:N:641:GLN:HB2	1.99	0.45
3:N:972:LEU:HD21	3:N:976:GLN:HE21	1.82	0.45
3:N:1026:SER:C	3:N:1028:ALA:N	2.75	0.45
3:N:1038:LEU:O	3:N:1060:SER:HB2	2.17	0.45
3:N:1137:ARG:O	3:N:1138:ALA:C	2.59	0.45
3:N:1175:ILE:O	3:N:1179:GLU:HG3	2.16	0.45
3:N:1211:MET:HG2	3:N:1213:ARG:NE	2.32	0.45
3:N:1390:LEU:HD22	9:N:2508:HOH:O	2.16	0.45
5:P:134:LYS:HA	9:P:4179:HOH:O	2.16	0.45
1:A:133:GLU:CG	1:A:134:GLU:N	2.76	0.45
1:A:197:LEU:HD23	1:A:197:LEU:H	1.82	0.45
1:B:77:GLU:HB2	3:D:872:ARG:NH2	2.30	0.45
2:C:196:LEU:HD21	2:C:303:PHE:CG	2.52	0.45
2:C:211:LEU:HD11	2:C:308:ARG:CB	2.37	0.45
2:C:810:ASP:HA	2:C:811:PRO:HD3	1.78	0.45
2:C:896:PHE:O	2:C:924:VAL:HG11	2.17	0.45
2:C:1051:GLU:HG2	2:C:1056:LYS:HG3	1.98	0.45
2:C:1102:LEU:HD23	2:C:1106:ASP:C	2.42	0.45
3:D:87:ARG:CB	3:D:523:ASP:HB2	2.35	0.45
3:D:141:ILE:CG2	3:D:161:LEU:HD21	2.45	0.45
3:D:165:LYS:CB	3:D:395:VAL:HG11	2.44	0.45
3:D:188:GLY:HA2	9:D:2289:HOH:O	2.17	0.45
3:D:645:PRO:HG3	3:D:725:SER:O	2.16	0.45
3:D:795:VAL:HG11	3:D:863:VAL:HG13	1.99	0.45
3:D:895:VAL:O	3:D:899:LEU:HG	2.17	0.45
3:D:1065:LEU:C	3:D:1065:LEU:HD12	2.42	0.45
3:D:1115:THR:HG21	3:D:1151:ARG:NH2	2.32	0.45
3:D:1283:ILE:HB	3:D:1315:ASP:OD2	2.17	0.45
3:D:1325:LEU:C	9:D:2444:HOH:O	2.58	0.45
3:D:1462:LEU:N	3:D:1462:LEU:HD23	2.31	0.45
3:D:1466:VAL:CG2	3:D:1472:ILE:HD11	2.39	0.45
5:F:291:ILE:CG2	5:F:304:VAL:HG21	2.46	0.45
5:F:416:ARG:NH1	9:F:9866:HOH:O	2.46	0.45
1:K:111:ALA:HB3	1:K:124:ASN:O	2.17	0.45
1:L:122:ILE:HD12	1:L:122:ILE:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:227:PHE:HB3	9:M:9899:HOH:O	2.17	0.45
2:M:283:ILE:HG23	9:M:2206:HOH:O	2.17	0.45
2:M:571:LEU:HD12	2:M:701:THR:O	2.17	0.45
2:M:770:GLU:HB2	9:N:2049:HOH:O	2.17	0.45
2:M:1029:GLY:HA3	3:N:623:VAL:O	2.17	0.45
3:N:18:ILE:HG21	3:N:516:ALA:O	2.17	0.45
3:N:52:PRO:CB	3:N:80:VAL:HG13	2.30	0.45
3:N:55:ASP:HB3	3:N:82:LYS:HE3	1.98	0.45
3:N:161:LEU:HD13	3:N:452:ILE:HD13	1.99	0.45
3:N:882:PHE:O	3:N:886:VAL:HG23	2.17	0.45
2:C:98:LEU:HD12	2:C:98:LEU:N	2.32	0.44
2:C:186:VAL:HG23	2:C:187:ASN:N	2.25	0.44
2:C:359:MET:HA	9:C:2175:HOH:O	2.17	0.44
2:C:578:VAL:HG11	2:C:991:GLN:HB3	2.00	0.44
2:C:648:ARG:HG2	9:C:9825:HOH:O	2.17	0.44
3:D:39:PRO:HG2	3:D:47:GLU:OE2	2.17	0.44
3:D:83:SER:O	3:D:86:ARG:HB3	2.17	0.44
3:D:99:ALA:HB1	3:D:575:GLN:CD	2.43	0.44
3:D:396:VAL:HG13	3:D:447:VAL:HA	1.98	0.44
3:D:685:ASP:HB3	9:D:9826:HOH:O	2.16	0.44
3:D:804:LEU:HD23	3:D:804:LEU:N	2.30	0.44
3:D:1090:ASP:HA	3:D:1093:TYR:HB2	1.97	0.44
3:D:1392:GLY:N	9:D:9923:HOH:O	2.49	0.44
3:D:1418:LYS:HB3	9:D:9806:HOH:O	2.16	0.44
3:D:1492:LEU:HD12	3:D:1493:LYS:NZ	2.31	0.44
5:F:365:GLU:CD	5:F:397:ILE:HA	2.42	0.44
1:K:199:ILE:N	1:K:199:ILE:HD12	2.32	0.44
2:M:239:PHE:HD1	9:M:9955:HOH:O	1.99	0.44
2:M:473:ARG:HG2	2:M:473:ARG:HH11	1.81	0.44
2:M:542:VAL:HG23	9:M:9944:HOH:O	2.16	0.44
2:M:686:ASP:N	9:N:2186:HOH:O	2.49	0.44
2:M:772:ARG:HH21	5:P:378:GLY:HA2	1.81	0.44
2:M:983:ILE:CG2	2:M:987:ILE:HD11	2.45	0.44
2:M:1085:PHE:CZ	3:N:1468:LEU:HG	2.52	0.44
2:M:1088:LEU:HD23	2:M:1089:VAL:N	2.31	0.44
3:N:36:THR:C	3:N:38:LYS:N	2.75	0.44
3:N:462:GLN:HB3	9:N:9521:HOH:O	2.17	0.44
3:N:601:ARG:HG2	3:N:606:ILE:CD1	2.46	0.44
3:N:895:VAL:HG11	3:N:922:LEU:HD21	1.99	0.44
3:N:1149:LEU:HD11	3:N:1160:LEU:HB3	1.99	0.44
3:N:1237:THR:N	9:N:2360:HOH:O	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:TYR:HE1	1:B:168:ASP:HB3	1.82	0.44
2:C:176:VAL:HG11	9:C:9635:HOH:O	2.17	0.44
2:C:405:ARG:HB3	9:C:9528:HOH:O	2.16	0.44
2:C:681:GLY:C	3:D:635:PRO:HG2	2.43	0.44
3:D:506:GLY:HA3	3:D:1454:GLY:HA3	2.00	0.44
3:D:520:LEU:CD2	3:D:540:LEU:HD22	2.47	0.44
3:D:553:ARG:NH1	5:F:211:ASP:HA	2.32	0.44
3:D:587:ARG:HD3	9:D:9502:HOH:O	2.18	0.44
3:D:1244:GLY:HA2	9:D:2331:HOH:O	2.17	0.44
3:D:1263:PHE:CZ	3:D:1352:ILE:HD13	2.52	0.44
3:D:1271:LYS:HB2	9:D:2687:HOH:O	2.17	0.44
3:D:1348:LEU:O	3:D:1349:VAL:C	2.58	0.44
5:F:172:ARG:O	5:F:176:ILE:HD13	2.16	0.44
5:F:192:LEU:O	5:F:196:VAL:HG23	2.17	0.44
5:F:222:ARG:HD2	5:F:242:TRP:CE3	2.52	0.44
5:F:229:TYR:HE1	9:F:9586:HOH:O	2.00	0.44
5:F:234:LYS:HD3	5:F:236:SER:H	1.82	0.44
5:F:303:ARG:NH2	9:F:9668:HOH:O	2.50	0.44
1:L:150:TYR:H	3:N:855:HIS:CE1	2.35	0.44
2:M:428:ARG:HD3	2:M:449:ILE:O	2.17	0.44
2:M:753:ASP:O	2:M:792:VAL:HG23	2.17	0.44
2:M:1008:ARG:NH2	2:M:1020:PRO:HB3	2.32	0.44
3:N:22:SER:HA	3:N:90:MET:O	2.18	0.44
3:N:416:ALA:H	3:N:417:PRO:CD	2.31	0.44
3:N:610:LYS:HB3	9:N:2113:HOH:O	2.16	0.44
3:N:630:VAL:HG12	3:N:631:ILE:N	2.30	0.44
3:N:1045:MET:HG2	3:N:1073:SER:CA	2.41	0.44
5:P:358:LEU:O	5:P:367:MET:HE1	2.17	0.44
1:A:85:LEU:HD12	1:A:86:VAL:N	2.32	0.44
1:A:97:VAL:HG12	1:A:99:LEU:HD12	1.99	0.44
1:A:165:ILE:HD12	1:A:165:ILE:O	2.16	0.44
1:B:95:GLN:HG3	1:B:146:ARG:HD2	2.00	0.44
2:C:136:ILE:HG23	2:C:391:LEU:CD2	2.47	0.44
2:C:433:THR:CG2	2:C:488:ALA:HB1	2.40	0.44
2:C:474:VAL:HG13	2:C:530:GLU:C	2.42	0.44
9:C:9809:HOH:O	5:F:349:LEU:HB2	2.16	0.44
3:D:61:GLY:HA2	3:D:64:LYS:HE3	1.98	0.44
3:D:131:LYS:HE2	5:F:83:GLN:NE2	2.29	0.44
3:D:168:THR:OG1	3:D:393:ILE:HB	2.17	0.44
3:D:477:LEU:HD11	3:D:495:ARG:HD3	1.98	0.44
3:D:619:LEU:O	3:D:619:LEU:HD23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:619:LEU:HD12	9:D:9516:HOH:O	2.16	0.44
3:D:785:ILE:HD12	3:D:785:ILE:N	2.32	0.44
3:D:1256:LEU:O	3:D:1257:PRO:C	2.59	0.44
3:D:1379:VAL:CG1	3:D:1395:LEU:HD23	2.47	0.44
3:D:1472:ILE:HA	3:D:1473:PRO:HD3	1.84	0.44
3:D:1491:THR:HG22	9:E:9527:HOH:O	2.17	0.44
5:F:307:THR:HA	5:F:310:ILE:HD11	1.98	0.44
1:K:63:HIS:HB3	9:K:5125:HOH:O	2.16	0.44
1:K:198:ARG:HG2	9:K:3473:HOH:O	2.18	0.44
2:M:58:ASP:O	2:M:59:LYS:HG3	2.17	0.44
2:M:422:ARG:NH1	9:M:2004:HOH:O	2.51	0.44
2:M:557:ARG:NE	2:M:560:MET:SD	2.90	0.44
2:M:609:ASN:CG	2:M:627:ARG:HH21	2.26	0.44
2:M:677:MET:HE3	2:M:678:PRO:O	2.17	0.44
2:M:793:PRO:O	2:M:794:PRO:C	2.61	0.44
2:M:794:PRO:HB2	2:M:1027:PHE:HZ	1.82	0.44
3:N:44:LEU:HB3	3:N:525:ARG:NH2	2.26	0.44
3:N:978:TYR:HD1	9:N:9888:HOH:O	2.00	0.44
3:N:1238:MET:HE1	3:N:1241:PHE:N	2.32	0.44
3:N:1377:LYS:HE2	9:N:9728:HOH:O	2.16	0.44
4:O:33:HIS:HB2	4:O:37:ASN:ND2	2.32	0.44
5:P:376:ILE:HG22	5:P:377:ASP:OD1	2.17	0.44
1:A:63:HIS:HA	9:A:9482:HOH:O	2.17	0.44
1:A:104:GLU:HB3	9:A:9622:HOH:O	2.15	0.44
1:A:198:ARG:HB2	1:A:200:TRP:CH2	2.52	0.44
2:C:140:ILE:HD11	2:C:412:ALA:HA	1.99	0.44
2:C:492:ASP:HB3	2:C:518:LYS:HD2	1.99	0.44
2:C:755:LEU:HD12	2:C:791:ARG:C	2.42	0.44
2:C:913:GLU:O	2:C:916:GLU:HB3	2.17	0.44
3:D:432:TYR:HB3	3:D:448:GLU:HA	1.99	0.44
3:D:699:VAL:CG2	3:D:760:ARG:HB3	2.47	0.44
3:D:701:LEU:HD11	3:D:763:MET:HE3	1.99	0.44
3:D:805:GLU:HA	9:D:9963:HOH:O	2.16	0.44
3:D:838:ARG:HE	3:D:838:ARG:HB2	1.54	0.44
3:D:843:PHE:CE1	3:D:864:VAL:HG11	2.53	0.44
3:D:995:LEU:HD12	9:D:2036:HOH:O	2.16	0.44
3:D:996:TRP:HE3	3:D:999:THR:CG2	2.26	0.44
3:D:1239:ARG:HH22	3:D:1254:GLN:HB2	1.82	0.44
4:E:40:LEU:O	4:E:40:LEU:HD22	2.17	0.44
4:E:70:THR:HG22	4:E:71:GLY:N	2.32	0.44
1:L:73:GLU:HB3	1:L:77:GLU:HG3	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:208:ALA:HB1	2:M:218:VAL:CG1	2.47	0.44
2:M:611:ILE:HD12	2:M:611:ILE:N	2.32	0.44
2:M:723:THR:HG23	2:M:725:ASP:HB2	1.98	0.44
2:M:728:HIS:C	2:M:729:LEU:HD12	2.43	0.44
2:M:1060:ILE:CG2	2:M:1061:GLU:N	2.80	0.44
2:M:1115:LEU:HD21	3:N:84:ILE:HD12	2.00	0.44
3:N:29:PRO:HG3	3:N:549:ASN:ND2	2.33	0.44
3:N:546:ARG:CZ	3:N:550:ARG:NH2	2.81	0.44
3:N:800:LYS:HG2	9:N:9629:HOH:O	2.17	0.44
3:N:864:VAL:HG12	3:N:865:THR:N	2.30	0.44
3:N:1114:THR:CG2	3:N:1195:GLN:HB3	2.48	0.44
3:N:1153:VAL:HG12	3:N:1155:VAL:HG22	2.00	0.44
3:N:1173:LEU:CD2	3:N:1174:LEU:HD23	2.47	0.44
4:O:49:GLN:HA	4:O:51:LEU:O	2.18	0.44
5:P:141:VAL:HB	9:P:4054:HOH:O	2.18	0.44
5:P:173:TYR:HE2	9:P:5021:HOH:O	2.00	0.44
5:P:273:ARG:NH2	9:P:3957:HOH:O	2.50	0.44
1:A:72:LYS:HA	2:C:608:GLY:N	2.32	0.44
1:A:88:ARG:O	1:A:88:ARG:HG2	2.17	0.44
2:C:73:LEU:HD12	2:C:73:LEU:O	2.16	0.44
2:C:79:PRO:HB3	9:C:2096:HOH:O	2.16	0.44
2:C:93:PRO:HB3	9:C:9910:HOH:O	2.18	0.44
2:C:309:TYR:CE2	2:C:321:GLU:HB3	2.53	0.44
2:C:793:PRO:O	2:C:794:PRO:C	2.60	0.44
3:D:10:ILE:HD11	3:D:1434:TRP:NE1	2.33	0.44
3:D:630:VAL:O	3:D:726:ILE:HG13	2.17	0.44
3:D:630:VAL:CA	3:D:744:GLN:HG2	2.47	0.44
3:D:1045:MET:HG2	3:D:1072:ILE:O	2.17	0.44
3:D:1209:LEU:HD22	3:D:1211:MET:SD	2.57	0.44
3:D:1288:GLU:OE1	3:D:1289:LYS:HG3	2.17	0.44
5:F:366:ALA:HB3	5:F:367:MET:CE	2.42	0.44
1:L:41:ARG:NH1	1:L:177:VAL:HG23	2.32	0.44
2:M:253:ALA:O	2:M:256:TYR:HB2	2.17	0.44
2:M:769:PRO:HB2	3:N:65:ARG:CZ	2.48	0.44
2:M:1086:ARG:HB3	2:M:1112:PHE:HE2	1.82	0.44
3:N:29:PRO:HG3	3:N:549:ASN:HD21	1.82	0.44
3:N:396:VAL:HG13	3:N:446:VAL:O	2.18	0.44
3:N:519:VAL:N	9:N:9660:HOH:O	2.50	0.44
4:O:33:HIS:HA	9:O:5072:HOH:O	2.18	0.44
5:P:84:TYR:HD1	9:P:3565:HOH:O	2.00	0.44
5:P:100:VAL:HG12	5:P:104:ARG:HH12	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:203:THR:HG22	5:P:204:GLY:N	2.32	0.44
5:P:286:PRO:HD3	9:P:4921:HOH:O	2.17	0.44
1:A:7:LYS:NZ	1:A:188:GLN:HE22	2.15	0.44
1:B:83:LYS:HE3	1:B:167:VAL:HG12	1.99	0.44
1:B:142:VAL:HG23	1:B:142:VAL:O	2.17	0.44
1:B:143:ARG:CD	1:B:158:ILE:HG21	2.48	0.44
1:B:143:ARG:HD3	1:B:158:ILE:HG21	1.98	0.44
2:C:195:LEU:HB3	9:C:9594:HOH:O	2.16	0.44
2:C:313:LEU:HD12	2:C:313:LEU:O	2.17	0.44
2:C:525:SER:OG	2:C:527:GLU:HG3	2.17	0.44
2:C:726:ILE:HG22	2:C:726:ILE:O	2.17	0.44
2:C:816:LYS:O	2:C:819:VAL:HB	2.18	0.44
3:D:211:VAL:HG13	3:D:393:ILE:HG23	1.99	0.44
3:D:441:ARG:O	3:D:443:VAL:N	2.50	0.44
3:D:531:ASP:C	3:D:533:GLY:N	2.70	0.44
3:D:780:LYS:HE2	9:D:2356:HOH:O	2.18	0.44
3:D:917:GLN:HA	9:D:9488:HOH:O	2.16	0.44
3:D:1173:LEU:HD23	3:D:1174:LEU:N	2.32	0.44
4:E:12:MET:HA	4:E:12:MET:CE	2.45	0.44
4:E:89:MET:HE3	4:E:93:TYR:CD1	2.53	0.44
5:F:398:ARG:HB3	9:F:9487:HOH:O	2.18	0.44
5:F:412:GLU:HG3	5:F:418:LEU:HD22	1.99	0.44
5:F:421:PHE:C	5:F:423:ASP:H	2.26	0.44
1:K:216:GLU:OE1	1:K:219:ARG:HD2	2.17	0.44
2:M:189:ARG:HH22	2:M:243:ARG:CD	2.31	0.44
2:M:211:LEU:CD1	2:M:308:ARG:HG3	2.48	0.44
2:M:428:ARG:HH21	2:M:451:LEU:HD21	1.82	0.44
2:M:498:GLN:HB3	2:M:500:ASN:OD1	2.18	0.44
2:M:561:GLY:HA3	2:M:842:ARG:O	2.17	0.44
2:M:816:LYS:HB2	2:M:819:VAL:CG2	2.46	0.44
3:N:102:ILE:HG13	9:N:2374:HOH:O	2.15	0.44
3:N:526:PRO:HB2	5:P:317:LEU:HD11	2.00	0.44
3:N:806:PHE:O	3:N:807:ALA:C	2.59	0.44
3:N:972:LEU:HD23	3:N:972:LEU:C	2.43	0.44
5:P:101:GLU:O	5:P:105:LYS:HG3	2.17	0.44
1:B:1:MET:HE1	9:B:9547:HOH:O	2.16	0.44
2:C:41:ASN:HA	2:C:45:GLN:OE1	2.17	0.44
2:C:597:ALA:HB2	2:C:655:LEU:CD2	2.45	0.44
2:C:1087:VAL:HG13	2:C:1091:GLU:OE2	2.17	0.44
3:D:643:GLY:CA	3:D:727:GLN:HB2	2.46	0.44
3:D:719:VAL:HG23	3:D:719:VAL:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1155:VAL:CG1	3:D:1177:ALA:HB1	2.46	0.44
3:D:1374:GLN:HG2	9:D:9769:HOH:O	2.17	0.44
4:E:9:LEU:HD22	4:E:19:LEU:CD1	2.47	0.44
5:F:94:LEU:HD23	5:F:95:THR:N	2.33	0.44
5:F:226:LYS:HD2	5:F:242:TRP:CZ2	2.52	0.44
5:F:256:ARG:NE	5:F:260:ILE:HD12	2.33	0.44
5:F:320:PRO:C	5:F:321:ILE:HD13	2.42	0.44
5:F:372:ARG:HD3	9:F:9526:HOH:O	2.17	0.44
1:L:124:ASN:ND2	1:L:127:LEU:HD22	2.32	0.44
2:M:113:VAL:HG12	2:M:115:LEU:HD23	1.98	0.44
2:M:309:TYR:HA	2:M:312:ALA:HB3	1.99	0.44
2:M:438:ILE:HD11	2:M:467:ILE:HD12	1.99	0.44
2:M:964:LYS:HE2	9:M:9902:HOH:O	2.17	0.44
2:M:1013:TYR:CE1	2:M:1020:PRO:HG3	2.52	0.44
2:M:1038:TRP:HD1	2:M:1041:GLU:OE1	2.00	0.44
2:M:1083:GLU:N	9:M:9532:HOH:O	2.47	0.44
3:N:175:VAL:HA	3:N:389:GLU:OE1	2.17	0.44
3:N:484:PRO:O	3:N:489:ARG:HD2	2.18	0.44
3:N:568:ARG:O	3:N:569:ASN:C	2.61	0.44
3:N:666:ILE:HG23	3:N:686:GLU:OE2	2.17	0.44
3:N:681:ARG:HH11	3:N:681:ARG:CB	2.30	0.44
3:N:824:ASN:HB3	9:N:9554:HOH:O	2.18	0.44
3:N:1063:GLU:HB3	9:N:2380:HOH:O	2.17	0.44
3:N:1156:LEU:HD13	3:N:1176:LYS:HD2	2.00	0.44
3:N:1217:ILE:H	3:N:1217:ILE:HG13	1.44	0.44
3:N:1353:GLN:HB3	3:N:1357:ARG:NE	2.32	0.44
3:N:1503:VAL:HG22	9:N:2327:HOH:O	2.18	0.44
5:P:128:ARG:HB2	5:P:128:ARG:CZ	2.48	0.44
5:P:413:SER:HA	5:P:416:ARG:HD3	1.98	0.44
1:A:106:PRO:HG3	1:A:133:GLU:O	2.18	0.44
1:B:158:ILE:HD13	1:B:158:ILE:HA	1.84	0.44
2:C:444:PRO:HD2	2:C:452:ILE:O	2.18	0.44
2:C:474:VAL:HG13	2:C:530:GLU:O	2.18	0.44
2:C:493:ARG:HD2	9:C:9650:HOH:O	2.17	0.44
2:C:1103:ASP:N	2:C:1107:ASN:O	2.51	0.44
3:D:50:PHE:HB3	3:D:522:PRO:HG2	1.99	0.44
3:D:470:LEU:HD11	3:D:509:PRO:HG3	2.00	0.44
3:D:629:SER:OG	3:D:630:VAL:N	2.50	0.44
3:D:867:ARG:HB3	3:D:867:ARG:HH11	1.83	0.44
3:D:1087:ARG:HB3	3:D:1234:THR:HG23	1.99	0.44
3:D:1236:LEU:HD12	3:D:1256:LEU:CD1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1310:ARG:HG3	3:D:1327:ARG:HB3	1.99	0.44
1:K:30:ARG:HD2	9:K:4362:HOH:O	2.17	0.44
1:K:88:ARG:HB3	9:K:3485:HOH:O	2.16	0.44
2:M:264:PRO:HB3	2:M:289:THR:CG2	2.46	0.44
2:M:704:HIS:O	2:M:705:ILE:HG23	2.17	0.44
2:M:1032:PHE:HA	9:M:2368:HOH:O	2.17	0.44
3:N:29:PRO:HG3	9:N:9768:HOH:O	2.17	0.44
3:N:126:VAL:HG12	3:N:132:TYR:HB2	1.99	0.44
3:N:525:ARG:HB2	3:N:538:SER:OG	2.18	0.44
3:N:546:ARG:NH1	3:N:550:ARG:NH2	2.65	0.44
3:N:641:GLN:HB3	3:N:717:GLN:O	2.18	0.44
3:N:645:PRO:HB3	3:N:723:GLY:O	2.17	0.44
3:N:679:ARG:NH2	3:N:681:ARG:HD2	2.33	0.44
3:N:951:ILE:HG23	3:N:1062:ARG:HH21	1.82	0.44
3:N:1209:LEU:HD21	4:O:16:LYS:NZ	2.33	0.44
1:B:48:ILE:HD13	1:B:210:ALA:HB1	2.00	0.44
1:B:109:VAL:HG22	9:B:9571:HOH:O	2.17	0.44
1:B:112:ARG:HB3	1:B:112:ARG:CZ	2.47	0.44
2:C:7:GLY:HA3	2:C:907:ASP:CG	2.43	0.44
2:C:25:SER:OG	2:C:337:GLY:N	2.48	0.44
2:C:139:GLN:HE22	2:C:415:PRO:CD	2.31	0.44
2:C:139:GLN:HE22	2:C:415:PRO:HD3	1.82	0.44
2:C:333:ILE:O	2:C:465:GLY:HA3	2.17	0.44
2:C:630:ARG:HE	2:C:705:ILE:HG13	1.82	0.44
2:C:816:LYS:HB2	2:C:819:VAL:CG2	2.47	0.44
2:C:1052:MET:HE1	2:C:1056:LYS:NZ	2.33	0.44
3:D:175:VAL:HG11	3:D:218:LYS:H	1.83	0.44
3:D:396:VAL:HG13	3:D:446:VAL:O	2.18	0.44
3:D:400:VAL:HA	3:D:442:ASN:O	2.18	0.44
3:D:1068:LEU:HD23	3:D:1068:LEU:O	2.18	0.44
3:D:1281:VAL:HG23	3:D:1317:ASP:O	2.18	0.44
3:D:1332:PRO:HB2	3:D:1421:LEU:HD22	2.00	0.44
1:K:198:ARG:HB2	1:K:200:TRP:CH2	2.53	0.44
1:L:151:VAL:HB	1:L:169:ALA:HB3	1.99	0.44
2:M:62:GLY:O	2:M:103:LYS:HG3	2.18	0.44
2:M:165:LEU:HA	2:M:165:LEU:HD12	1.88	0.44
2:M:269:LEU:O	2:M:269:LEU:HD23	2.18	0.44
2:M:464:LEU:HD12	2:M:464:LEU:HA	1.80	0.44
2:M:704:HIS:CG	2:M:831:ARG:HE	2.36	0.44
2:M:910:LYS:HB3	2:M:912:PRO:HD2	2.00	0.44
2:M:930:LYS:HA	9:M:9525:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:979:THR:HG23	2:M:981:GLU:HB2	1.99	0.44
2:M:1042:ALA:CB	3:N:710:ARG:HE	2.29	0.44
3:N:33:ASN:O	3:N:36:THR:O	2.36	0.44
3:N:661:MET:SD	3:N:673:ALA:HB1	2.57	0.44
3:N:684:LYS:C	3:N:686:GLU:H	2.24	0.44
3:N:767:HIS:NE2	4:O:6:ILE:HD13	2.33	0.44
3:N:832:ARG:HG2	9:N:9674:HOH:O	2.18	0.44
3:N:1109:GLU:HG2	3:N:1202:GLN:H	1.83	0.44
3:N:1192:LEU:HD22	3:N:1345:GLU:OE2	2.18	0.44
3:N:1243:THR:HG1	3:N:1253:THR:HB	1.83	0.44
3:N:1438:ALA:N	3:N:1446:VAL:HG11	2.33	0.44
2:C:71:TYR:H	2:C:71:TYR:HD2	1.65	0.43
2:C:110:GLU:HB2	2:C:368:THR:HG22	1.99	0.43
2:C:195:LEU:HD12	2:C:234:ALA:HB1	1.99	0.43
2:C:235:LEU:HA	9:C:2083:HOH:O	2.18	0.43
2:C:360:LEU:HD12	9:C:9600:HOH:O	2.18	0.43
2:C:712:ALA:HB1	9:C:2168:HOH:O	2.18	0.43
2:C:863:ASP:OD1	2:C:865:THR:HG22	2.18	0.43
3:D:16:GLU:HA	3:D:19:ARG:NH1	2.33	0.43
3:D:101:HIS:ND1	3:D:103:TRP:HB2	2.31	0.43
3:D:191:LEU:HB3	3:D:195:VAL:HG21	2.00	0.43
3:D:216:VAL:HG12	9:D:9947:HOH:O	2.17	0.43
3:D:525:ARG:N	3:D:526:PRO:HD3	2.33	0.43
3:D:569:ASN:HD21	5:F:210:LEU:HD22	1.82	0.43
3:D:650:LEU:HD22	3:D:688:TRP:CZ3	2.53	0.43
3:D:669:ASN:HB3	9:D:9547:HOH:O	2.17	0.43
3:D:1057:VAL:HA	3:D:1069:GLU:CD	2.43	0.43
3:D:1314:LYS:HZ3	3:D:1317:ASP:H	1.66	0.43
3:D:1393:GLN:HB2	3:D:1398:TRP:HZ2	1.81	0.43
3:D:1496:GLU:O	3:D:1500:LYS:HG3	2.17	0.43
4:E:52:GLU:HB3	4:E:55:PHE:CZ	2.53	0.43
5:F:319:THR:HB	5:F:321:ILE:HD11	1.99	0.43
2:M:195:LEU:CD2	2:M:238:LEU:HG	2.48	0.43
2:M:241:LEU:HD23	9:M:9797:HOH:O	2.18	0.43
2:M:380:ALA:O	2:M:383:ARG:HG2	2.18	0.43
2:M:418:LEU:N	2:M:418:LEU:HD12	2.33	0.43
2:M:670:GLN:HG3	2:M:700:TYR:CE2	2.53	0.43
2:M:916:GLU:O	2:M:919:ALA:HB3	2.18	0.43
2:M:1090:LYS:HD2	3:N:90:MET:SD	2.58	0.43
3:N:111:LYS:HZ1	3:N:498:VAL:HG12	1.83	0.43
3:N:637:LEU:HD12	3:N:641:GLN:OE1	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:994:GLN:HE21	3:N:994:GLN:HA	1.83	0.43
3:N:1047:LYS:HB3	3:N:1048:PRO:HD2	2.00	0.43
3:N:1112:CYS:HB3	3:N:1201:CYS:SG	2.57	0.43
5:P:134:LYS:HG3	5:P:178:ARG:NH2	2.33	0.43
5:P:223:ALA:HB2	5:P:242:TRP:HB2	1.99	0.43
5:P:370:LYS:HD2	5:P:370:LYS:C	2.43	0.43
1:A:2:LEU:O	1:A:6:LEU:HB3	2.18	0.43
1:A:63:HIS:HE1	9:C:2299:HOH:O	2.00	0.43
1:A:101:LEU:HG	1:A:113:ASP:C	2.43	0.43
1:B:143:ARG:NH1	1:B:158:ILE:HG23	2.33	0.43
2:C:68:PHE:HE1	2:C:96:ALA:HB1	1.82	0.43
2:C:111:ASP:HB3	2:C:112:GLU:OE2	2.18	0.43
2:C:232:GLU:HG3	2:C:235:LEU:CD1	2.48	0.43
2:C:443:THR:HG23	2:C:449:ILE:HG13	1.99	0.43
2:C:460:ARG:HD2	2:C:485:TYR:CD2	2.52	0.43
2:C:535:SER:HB2	2:C:537:LYS:HD3	2.00	0.43
2:C:557:ARG:NH1	2:C:879:ARG:HG2	2.33	0.43
2:C:572:ILE:CG2	2:C:703:ILE:HD13	2.49	0.43
2:C:674:VAL:HG12	2:C:990:GLY:O	2.18	0.43
2:C:689:VAL:HB	2:C:870:ILE:CG1	2.36	0.43
2:C:838:LYS:HG3	2:C:838:LYS:O	2.18	0.43
3:D:6:ARG:HH11	3:D:6:ARG:CB	2.24	0.43
3:D:513:ILE:HA	9:D:9738:HOH:O	2.18	0.43
3:D:705:ALA:CB	3:D:706:PRO:HD3	2.45	0.43
3:D:1023:MET:O	3:D:1028:ALA:HB3	2.18	0.43
3:D:1031:ASN:O	3:D:1034:GLN:HB2	2.17	0.43
3:D:1042:ARG:O	3:D:1057:VAL:HB	2.18	0.43
3:D:1267:ARG:HH22	3:D:1333:HIS:HD2	1.65	0.43
9:D:9603:HOH:O	5:F:337:HIS:HB3	2.18	0.43
4:E:54:LEU:HA	4:E:58:PRO:HG2	2.01	0.43
1:K:209:GLU:O	1:K:213:GLN:HG3	2.19	0.43
2:M:728:HIS:CE1	2:M:775:ARG:HH12	2.36	0.43
3:N:115:LEU:HD12	3:N:499:VAL:HG22	1.99	0.43
3:N:454:ALA:C	3:N:455:ARG:HD2	2.43	0.43
3:N:1068:LEU:O	3:N:1069:GLU:C	2.59	0.43
3:N:1096:ARG:HG2	3:N:1096:ARG:HH11	1.82	0.43
4:O:82:GLU:O	4:O:85:LEU:HD22	2.18	0.43
5:P:85:LEU:HD22	5:P:193:ARG:CD	2.48	0.43
1:A:18:ARG:NH2	1:A:88:ARG:NH2	2.65	0.43
1:A:66:SER:O	1:A:75:VAL:HG23	2.19	0.43
2:C:190:LYS:HG3	9:C:9876:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:577:PRO:HG3	2:C:993:PHE:CE2	2.54	0.43
2:C:1044:GLY:HA3	4:E:17:TYR:CE1	2.53	0.43
3:D:553:ARG:CZ	9:F:9503:HOH:O	2.65	0.43
3:D:553:ARG:NE	9:D:9572:HOH:O	2.51	0.43
3:D:805:GLU:OE1	3:D:805:GLU:O	2.37	0.43
3:D:853:VAL:CG2	3:D:858:VAL:HG23	2.48	0.43
3:D:1154:GLU:HB2	9:D:9708:HOH:O	2.18	0.43
3:D:1413:THR:HG22	9:D:2035:HOH:O	2.18	0.43
4:E:61:GLU:OE2	4:E:62:THR:N	2.52	0.43
5:F:115:LYS:HG3	5:F:173:TYR:HE2	1.82	0.43
5:F:230:LYS:HD3	9:F:9882:HOH:O	2.17	0.43
5:F:241:TRP:HA	5:F:244:ARG:HH12	1.83	0.43
5:F:282:LEU:CD1	5:F:286:PRO:HG3	2.49	0.43
5:F:295:MET:HB3	5:F:299:TRP:CG	2.53	0.43
5:F:305:GLU:O	5:F:309:LYS:HG3	2.18	0.43
1:K:9:PRO:HD2	1:L:224:TYR:CZ	2.53	0.43
1:L:100:LEU:HB2	1:L:115:LEU:CD2	2.44	0.43
2:M:461:VAL:HG13	2:M:465:GLY:HA2	1.99	0.43
2:M:625:LEU:HD22	2:M:639:GLN:HB3	2.00	0.43
2:M:674:VAL:O	2:M:989:VAL:HA	2.17	0.43
2:M:707:ARG:HH12	2:M:709:GLU:CB	2.21	0.43
2:M:1097:LEU:H	2:M:1097:LEU:HD22	1.83	0.43
3:N:153:LEU:HD11	3:N:158:TYR:CA	2.48	0.43
3:N:852:ALA:O	3:N:857:ILE:HG12	2.18	0.43
3:N:899:LEU:HD12	3:N:900:ILE:HG23	1.99	0.43
3:N:915:VAL:HG13	3:N:931:LEU:HD21	2.00	0.43
3:N:996:TRP:HE3	3:N:999:THR:HG21	1.83	0.43
5:P:211:ASP:OD1	5:P:211:ASP:N	2.51	0.43
1:A:18:ARG:HD3	1:A:123:MET:CE	2.48	0.43
2:C:580:MET:HB2	2:C:902:ILE:HG12	1.99	0.43
2:C:607:ASP:HB3	2:C:610:ARG:H	1.84	0.43
2:C:861:LEU:HD23	2:C:862:PRO:N	2.34	0.43
2:C:938:LYS:N	9:C:9976:HOH:O	2.51	0.43
3:D:90:MET:HE3	3:D:90:MET:HB3	1.84	0.43
3:D:130:SER:O	3:D:568:ARG:NH2	2.50	0.43
3:D:703:ASN:ND2	3:D:704:ARG:N	2.66	0.43
3:D:762:GLN:HE21	4:E:20:THR:HG21	1.83	0.43
3:D:838:ARG:HD3	3:D:874:GLU:HB3	2.00	0.43
3:D:890:VAL:HG21	3:D:922:LEU:CD1	2.49	0.43
3:D:1107:VAL:O	3:D:1218:GLY:N	2.49	0.43
3:D:1495:ILE:O	3:D:1498:ALA:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:46:PRO:C	4:E:54:LEU:HD22	2.44	0.43
1:K:101:LEU:HG	1:K:114:PHE:CA	2.43	0.43
1:K:156:HIS:CD2	1:K:157:GLY:N	2.86	0.43
1:K:197:LEU:H	1:K:197:LEU:CD2	2.30	0.43
2:M:36:PRO:HG2	2:M:70:GLU:CB	2.46	0.43
2:M:132:ALA:HB2	9:M:2414:HOH:O	2.18	0.43
2:M:175:GLU:HB3	2:M:183:SER:OG	2.18	0.43
2:M:389:SER:HB2	9:M:9823:HOH:O	2.17	0.43
2:M:603:VAL:H	2:M:647:GLN:H	1.66	0.43
2:M:957:LYS:HA	9:M:2387:HOH:O	2.18	0.43
2:M:1067:TYR:CE1	3:N:655:PRO:HB3	2.54	0.43
2:M:1100:GLN:HE21	2:M:1100:GLN:HB2	1.69	0.43
3:N:693:GLU:O	4:O:48:MET:HE1	2.18	0.43
3:N:835:SER:N	9:N:9806:HOH:O	2.52	0.43
3:N:1135:ARG:HD3	3:N:1139:ASP:HB2	1.98	0.43
3:N:1403:LEU:HD23	3:N:1407:LEU:CD2	2.47	0.43
3:N:1449:GLU:HG2	9:N:9651:HOH:O	2.18	0.43
5:P:412:GLU:HA	9:P:3726:HOH:O	2.17	0.43
1:A:32:PHE:HD2	9:A:9505:HOH:O	2.01	0.43
1:A:42:ARG:CZ	9:A:9609:HOH:O	2.66	0.43
1:A:73:GLU:OE2	1:A:73:GLU:N	2.52	0.43
1:A:89:PHE:HB2	9:A:9536:HOH:O	2.17	0.43
1:A:109:VAL:O	1:A:129:ILE:HB	2.18	0.43
1:B:27:PRO:HG2	1:B:186:LEU:HD12	2.01	0.43
2:C:3:ILE:HA	2:C:900:ARG:O	2.19	0.43
2:C:174:LEU:CD2	2:C:184:MET:HG3	2.48	0.43
2:C:443:THR:OG1	2:C:444:PRO:HD2	2.18	0.43
2:C:598:GLU:HB2	2:C:615:TYR:CZ	2.53	0.43
2:C:722:ILE:HD13	2:C:722:ILE:C	2.43	0.43
2:C:752:GLY:H	2:C:792:VAL:HB	1.83	0.43
2:C:780:GLU:CD	2:C:781:LYS:HG3	2.43	0.43
2:C:880:MET:HE3	2:C:880:MET:HB2	1.88	0.43
2:C:1036:GLU:HG3	3:D:707:THR:OG1	2.18	0.43
3:D:129:PHE:CD2	3:D:587:ARG:CZ	3.01	0.43
3:D:131:LYS:HG3	3:D:568:ARG:HG2	2.00	0.43
3:D:210:ARG:HG3	3:D:398:ALA:HB3	2.00	0.43
3:D:459:GLU:O	3:D:463:GLN:HG2	2.18	0.43
3:D:520:LEU:HD12	3:D:521:PRO:CD	2.38	0.43
3:D:537:THR:HG22	9:F:9527:HOH:O	2.17	0.43
3:D:566:ILE:HG12	5:F:217:ASN:ND2	2.33	0.43
3:D:569:ASN:ND2	5:F:210:LEU:HD22	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:591:VAL:HG11	9:D:2452:HOH:O	2.17	0.43
3:D:615:ARG:HH11	3:D:615:ARG:HG3	1.82	0.43
3:D:625:TYR:N	3:D:625:TYR:CD1	2.86	0.43
3:D:638:LYS:C	3:D:729:HIS:HD2	2.26	0.43
3:D:639:LEU:HD22	3:D:766:ALA:CB	2.48	0.43
3:D:797:LYS:HZ3	3:D:1016:PRO:HB3	1.84	0.43
3:D:1206:GLY:HA3	3:D:1366:LYS:HZ3	1.82	0.43
2:M:189:ARG:HG2	2:M:189:ARG:HH11	1.83	0.43
2:M:385:PHE:O	2:M:389:SER:HB3	2.19	0.43
2:M:610:ARG:HH11	2:M:610:ARG:HG3	1.83	0.43
2:M:625:LEU:HD22	2:M:639:GLN:CB	2.48	0.43
2:M:802:ARG:HB3	2:M:802:ARG:HH11	1.84	0.43
2:M:913:GLU:O	2:M:916:GLU:HB3	2.19	0.43
2:M:1015:LEU:HD12	5:P:335:ASP:OD1	2.19	0.43
2:M:1075:ASP:HB2	4:O:31:LEU:HD12	2.00	0.43
3:N:1031:ASN:O	3:N:1035:ILE:HG12	2.18	0.43
3:N:1203:LYS:HB2	9:N:9807:HOH:O	2.18	0.43
5:P:245:GLN:HA	9:P:3671:HOH:O	2.17	0.43
5:P:421:PHE:C	5:P:423:ASP:H	2.26	0.43
1:B:23:PHE:O	1:B:196:THR:HA	2.19	0.43
1:B:84:GLU:HB3	1:B:127:LEU:HD21	2.00	0.43
2:C:10:ARG:NH1	2:C:11:GLU:H	2.16	0.43
2:C:27:ARG:HD2	9:C:9549:HOH:O	2.18	0.43
2:C:44:ILE:HA	2:C:344:PHE:CE1	2.54	0.43
2:C:476:GLY:C	2:C:478:VAL:H	2.27	0.43
2:C:525:SER:OG	2:C:528:GLU:HG3	2.18	0.43
2:C:679:PHE:O	3:D:943:THR:HG22	2.18	0.43
2:C:722:ILE:HD12	2:C:805:ARG:NH2	2.32	0.43
2:C:1036:GLU:O	2:C:1039:ALA:HB3	2.18	0.43
2:C:1115:LEU:CB	3:D:85:VAL:HG13	2.48	0.43
3:D:112:ILE:O	3:D:116:LEU:HB2	2.18	0.43
3:D:178:LEU:CG	3:D:200:ASP:H	2.28	0.43
3:D:187:LYS:HG2	9:D:9853:HOH:O	2.19	0.43
3:D:440:VAL:HG12	3:D:441:ARG:N	2.33	0.43
3:D:475:LYS:O	3:D:479:GLU:HG2	2.18	0.43
3:D:502:PHE:C	9:D:2635:HOH:O	2.61	0.43
3:D:598:ARG:NH2	5:F:318:GLU:O	2.51	0.43
3:D:746:ALA:HB2	9:D:9498:HOH:O	2.19	0.43
3:D:908:LYS:HA	3:D:911:LEU:HD22	2.01	0.43
3:D:1114:THR:HG23	3:D:1114:THR:O	2.17	0.43
3:D:1264:GLU:HG2	3:D:1266:ARG:NH2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1364:HIS:CE1	3:D:1366:LYS:HG3	2.53	0.43
3:D:1394:VAL:HB	3:D:1397:LYS:CD	2.47	0.43
4:E:26:ARG:HA	4:E:29:GLN:OE1	2.18	0.43
5:F:187:LEU:HD21	9:F:9584:HOH:O	2.17	0.43
5:F:205:ARG:HD2	5:F:251:ILE:HG21	2.01	0.43
1:K:32:PHE:O	1:K:36:LEU:HG	2.19	0.43
1:K:66:SER:O	1:K:75:VAL:HG23	2.18	0.43
1:L:124:ASN:HD22	1:L:127:LEU:HD22	1.83	0.43
2:M:21:ILE:HD12	2:M:21:ILE:N	2.33	0.43
2:M:26:TYR:CD2	2:M:30:LEU:HD11	2.54	0.43
2:M:148:PHE:HB2	9:M:9837:HOH:O	2.19	0.43
2:M:150:PRO:CA	2:M:158:TYR:HB3	2.43	0.43
2:M:230:ARG:HB2	9:M:9523:HOH:O	2.19	0.43
2:M:243:ARG:HG2	9:M:9816:HOH:O	2.18	0.43
2:M:301:GLU:O	2:M:305:PRO:HG2	2.19	0.43
2:M:335:THR:CG2	2:M:461:VAL:HG11	2.49	0.43
2:M:433:THR:CG2	2:M:488:ALA:HB1	2.47	0.43
2:M:697:ARG:HB2	9:M:9519:HOH:O	2.19	0.43
2:M:1008:ARG:HB2	2:M:1027:PHE:HB2	2.00	0.43
2:M:1086:ARG:NH1	2:M:1112:PHE:HA	2.33	0.43
3:N:96:ALA:CB	9:N:9830:HOH:O	2.66	0.43
3:N:469:ASP:OD1	3:N:471:GLU:HB2	2.19	0.43
3:N:949:ILE:HD11	3:N:1023:MET:HE1	2.01	0.43
3:N:992:ILE:O	3:N:995:LEU:HB3	2.19	0.43
3:N:1033:GLN:NE2	3:N:1036:ARG:HH11	2.10	0.43
3:N:1123:PHE:CD1	3:N:1134:LEU:HA	2.54	0.43
3:N:1294:VAL:O	3:N:1300:SER:HA	2.19	0.43
3:N:1312:LEU:HD21	9:N:2005:HOH:O	2.18	0.43
5:P:100:VAL:HG11	9:P:6003:HOH:O	2.17	0.43
5:P:356:LYS:HZ1	5:P:417:LYS:HE2	1.84	0.43
5:P:358:LEU:HD11	5:P:367:MET:SD	2.58	0.43
1:A:90:LEU:HD21	9:A:9569:HOH:O	2.18	0.43
1:A:227:ASN:N	1:A:227:ASN:HD22	2.16	0.43
2:C:162:ILE:HD12	2:C:172:ILE:CB	2.49	0.43
2:C:551:GLU:HG3	2:C:552:HIS:CD2	2.54	0.43
2:C:602:GLU:HA	2:C:647:GLN:O	2.19	0.43
2:C:874:LEU:CD2	3:D:1023:MET:SD	3.06	0.43
2:C:877:PRO:HG2	3:D:1023:MET:CE	2.48	0.43
2:C:890:LEU:HD21	2:C:901:TYR:CD1	2.53	0.43
3:D:130:SER:HB2	9:D:9649:HOH:O	2.18	0.43
3:D:570:GLU:HB2	5:F:214:GLN:NE2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:965:GLU:HA	3:D:965:GLU:OE1	2.18	0.43
3:D:1299:PHE:H	3:D:1299:PHE:HD2	1.66	0.43
3:D:1487:VAL:O	4:E:73:LEU:HA	2.18	0.43
4:E:43:GLU:CD	4:E:43:GLU:N	2.72	0.43
4:E:89:MET:HE3	4:E:93:TYR:CE1	2.53	0.43
5:F:194:LEU:HD22	5:F:194:LEU:N	2.33	0.43
5:F:209:PHE:HD1	9:F:9815:HOH:O	2.01	0.43
5:F:214:GLN:O	5:F:217:ASN:HB2	2.19	0.43
5:F:274:THR:O	5:F:278:LEU:HG	2.18	0.43
1:L:127:LEU:HD12	1:L:128:HIS:H	1.84	0.43
1:L:132:LEU:HG	1:L:136:GLY:HA3	1.99	0.43
2:M:91:GLN:HB3	2:M:118:ILE:C	2.44	0.43
2:M:185:LYS:HG2	2:M:190:LYS:HG2	2.01	0.43
2:M:189:ARG:HH22	2:M:243:ARG:CG	2.32	0.43
2:M:431:HIS:HB3	2:M:434:HIS:NE2	2.34	0.43
2:M:566:THR:HG22	2:M:566:THR:O	2.19	0.43
2:M:911:GLU:OE2	3:N:1062:ARG:NE	2.51	0.43
3:N:436:GLU:HB2	3:N:445:ARG:CB	2.48	0.43
3:N:481:MET:SD	3:N:493:ARG:HA	2.58	0.43
3:N:643:GLY:CA	3:N:727:GLN:HB2	2.42	0.43
3:N:693:GLU:HA	4:O:48:MET:CE	2.48	0.43
3:N:1144:LEU:HA	3:N:1147:ARG:HG3	2.01	0.43
5:P:258:ILE:HG13	9:P:3765:HOH:O	2.18	0.43
5:P:401:GLU:O	5:P:405:LEU:HD13	2.19	0.43
1:B:88:ARG:NH1	9:B:9562:HOH:O	2.51	0.43
2:C:100:LEU:HD22	2:C:372:LEU:HD22	2.01	0.43
2:C:199:VAL:HG13	2:C:235:LEU:CD2	2.48	0.43
2:C:552:HIS:CD2	2:C:886:LEU:HD12	2.52	0.43
2:C:660:ALA:O	2:C:667:ALA:O	2.37	0.43
2:C:1005:MET:O	2:C:1005:MET:HG3	2.18	0.43
3:D:2:LYS:HB3	3:D:3:LYS:NZ	2.33	0.43
3:D:33:ASN:O	3:D:36:THR:O	2.36	0.43
3:D:55:ASP:HB3	3:D:56:TYR:H	1.57	0.43
3:D:637:LEU:HD11	3:D:642:CYS:N	2.34	0.43
3:D:781:PRO:HB3	3:D:785:ILE:CG2	2.49	0.43
3:D:884:ARG:HA	9:D:9724:HOH:O	2.18	0.43
3:D:1369:GLU:O	3:D:1370:ILE:C	2.60	0.43
3:D:1377:LYS:HB3	3:D:1378:TYR:CE1	2.54	0.43
3:D:1472:ILE:HG22	3:D:1474:ALA:O	2.19	0.43
5:F:316:SER:HB2	5:F:319:THR:OG1	2.19	0.43
1:K:203:GLY:HA2	9:K:4352:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:220:GLU:HB2	9:K:5313:HOH:O	2.18	0.43
1:L:84:GLU:HB2	9:N:9942:HOH:O	2.18	0.43
1:L:145:ASP:O	1:L:171:PHE:HE1	2.02	0.43
2:M:218:VAL:HG22	2:M:221:LEU:CD2	2.48	0.43
2:M:663:ASN:HD22	2:M:663:ASN:HA	1.65	0.43
2:M:1018:GLN:HE21	2:M:1063:ARG:HH22	1.66	0.43
2:M:1103:ASP:N	2:M:1107:ASN:O	2.52	0.43
3:N:99:ALA:HA	3:N:575:GLN:HE22	1.83	0.43
3:N:422:ALA:O	3:N:427:VAL:HG21	2.18	0.43
3:N:644:LEU:N	9:N:9610:HOH:O	2.50	0.43
3:N:834:THR:HG22	3:N:838:ARG:HD2	2.01	0.43
3:N:890:VAL:HG11	3:N:922:LEU:HD13	1.99	0.43
4:O:70:THR:CG2	4:O:72:ARG:HE	2.31	0.43
5:P:393:THR:O	5:P:397:ILE:HG13	2.18	0.43
2:C:432:ARG:HG2	2:C:432:ARG:H	1.65	0.43
2:C:689:VAL:O	2:C:869:VAL:HG23	2.19	0.43
2:C:691:SER:HA	2:C:858:MET:HE3	2.00	0.43
2:C:854:PRO:O	2:C:856:GLU:N	2.52	0.43
3:D:535:PHE:O	5:F:315:VAL:HG22	2.18	0.43
3:D:639:LEU:N	3:D:729:HIS:CD2	2.86	0.43
3:D:641:GLN:HG2	9:D:9590:HOH:O	2.18	0.43
3:D:734:GLU:HA	9:D:9487:HOH:O	2.19	0.43
3:D:1047:LYS:HE3	3:D:1051:GLU:HB2	2.01	0.43
3:D:1066:THR:O	3:D:1070:TYR:HB2	2.19	0.43
3:D:1148:VAL:HG13	3:D:1163:GLY:O	2.19	0.43
3:D:1264:GLU:OE2	3:D:1424:VAL:HG12	2.19	0.43
3:D:1292:VAL:O	3:D:1303:TYR:HB2	2.19	0.43
4:E:29:GLN:CB	4:E:33:HIS:NE2	2.82	0.43
5:F:313:GLU:H	5:F:313:GLU:HG2	1.47	0.43
1:K:198:ARG:C	1:K:199:ILE:HD12	2.44	0.43
1:L:58:ILE:HD13	1:L:140:MET:HB3	2.01	0.43
2:M:65:VAL:HB	2:M:101:ILE:HB	2.00	0.43
2:M:85:GLU:HA	9:M:9565:HOH:O	2.18	0.43
2:M:926:PHE:O	2:M:930:LYS:HG3	2.18	0.43
2:M:1115:LEU:N	2:M:1115:LEU:CD1	2.82	0.43
3:N:45:PHE:N	9:N:9567:HOH:O	2.51	0.43
3:N:749:VAL:HA	3:N:750:PRO:HD3	1.86	0.43
3:N:1033:GLN:NE2	3:N:1036:ARG:HD3	2.27	0.43
3:N:1125:PRO:HB2	3:N:1126:ASP:H	1.64	0.43
3:N:1221:VAL:O	3:N:1222:GLY:C	2.62	0.43
3:N:1264:GLU:OE2	3:N:1425:THR:HB	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1334:GLN:HG3	9:N:2654:HOH:O	2.18	0.43
3:N:1441:GLN:CD	3:N:1442:ASN:HB2	2.43	0.43
5:P:143:HIS:HB2	5:P:152:ASP:OD1	2.19	0.43
5:P:197:SER:O	5:P:200:LYS:HB3	2.18	0.43
5:P:287:THR:O	5:P:289:GLU:N	2.51	0.43
1:A:99:LEU:HB3	1:A:114:PHE:CD2	2.54	0.43
1:A:176:ARG:O	1:A:200:TRP:HE3	2.02	0.43
1:B:72:LYS:HD3	9:B:9705:HOH:O	2.18	0.43
2:C:172:ILE:HD12	2:C:172:ILE:N	2.33	0.43
2:C:289:THR:HB	9:C:9939:HOH:O	2.19	0.43
2:C:327:HIS:O	2:C:330:ASN:HB2	2.19	0.43
2:C:357:GLU:HB2	9:C:9624:HOH:O	2.19	0.43
2:C:1008:ARG:NH2	2:C:1021:LEU:O	2.50	0.43
2:C:1034:GLU:CA	2:C:1037:VAL:HG23	2.48	0.43
9:C:2220:HOH:O	3:D:758:GLU:HB3	2.18	0.43
3:D:131:LYS:CB	3:D:456:MET:HE3	2.47	0.43
3:D:473:LEU:HD11	3:D:495:ARG:HH12	1.82	0.43
3:D:563:PRO:HB3	9:D:9517:HOH:O	2.18	0.43
3:D:679:ARG:HB2	3:D:682:ASP:CG	2.44	0.43
3:D:806:PHE:O	3:D:806:PHE:CD1	2.72	0.43
3:D:957:PRO:HG2	3:D:1007:VAL:HG12	2.01	0.43
3:D:1106:VAL:HG12	3:D:1107:VAL:N	2.34	0.43
3:D:1219:GLU:HG2	3:D:1220:ALA:N	2.33	0.43
3:D:1239:ARG:NH2	3:D:1254:GLN:HB2	2.34	0.43
3:D:1274:ILE:H	3:D:1274:ILE:HG13	1.54	0.43
1:L:92:PRO:HB3	9:L:5570:HOH:O	2.19	0.43
2:M:227:PHE:O	2:M:230:ARG:HD3	2.19	0.43
2:M:302:VAL:C	2:M:305:PRO:HD2	2.44	0.43
2:M:651:LYS:HD2	9:M:2254:HOH:O	2.19	0.43
2:M:859:PRO:O	2:M:867:VAL:HG22	2.19	0.43
2:M:1004:LYS:O	2:M:1006:HIS:ND1	2.52	0.43
2:M:1021:LEU:CD2	5:P:332:PHE:HA	2.45	0.43
2:M:1109:VAL:HG21	3:N:3:LYS:O	2.19	0.43
3:N:452:ILE:HG23	3:N:452:ILE:O	2.19	0.43
3:N:500:ARG:HH11	3:N:500:ARG:HG3	1.84	0.43
3:N:957:PRO:CG	3:N:1007:VAL:HG12	2.49	0.43
3:N:1256:LEU:O	3:N:1257:PRO:C	2.62	0.43
1:B:41:ARG:HG3	1:B:42:ARG:N	2.34	0.42
2:C:36:PRO:CB	2:C:70:GLU:HG2	2.48	0.42
2:C:308:ARG:HG2	2:C:308:ARG:HH11	1.84	0.42
2:C:441:VAL:O	2:C:559:LEU:HD12	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:674:VAL:O	2:C:989:VAL:HA	2.19	0.42
2:C:979:THR:HG23	2:C:981:GLU:HB2	2.00	0.42
2:C:1049:LEU:HG	2:C:1053:LEU:CD1	2.49	0.42
2:C:1067:TYR:CZ	2:C:1071:ILE:HD11	2.54	0.42
2:C:1105:LYS:O	2:C:1107:ASN:N	2.52	0.42
9:C:9491:HOH:O	3:D:613:ARG:HG3	2.18	0.42
3:D:474:GLU:CG	3:D:500:ARG:HE	2.32	0.42
3:D:647:ARG:O	3:D:647:ARG:HD3	2.19	0.42
3:D:684:LYS:C	3:D:686:GLU:H	2.27	0.42
3:D:952:ASP:HA	3:D:1062:ARG:HH21	1.83	0.42
3:D:984:THR:CG2	3:D:987:GLU:H	2.31	0.42
5:F:234:LYS:HD2	5:F:236:SER:HB3	2.00	0.42
5:F:373:LYS:HG2	9:F:9532:HOH:O	2.19	0.42
5:F:392:VAL:HA	9:F:9723:HOH:O	2.18	0.42
1:L:143:ARG:NH1	1:L:158:ILE:HG23	2.33	0.42
2:M:250:ARG:HG2	9:M:2207:HOH:O	2.19	0.42
2:M:331:ARG:CZ	2:M:427:VAL:HG13	2.49	0.42
2:M:1043:TYR:C	2:M:1045:ALA:H	2.27	0.42
3:N:754:PHE:CG	4:O:24:ALA:HB1	2.54	0.42
3:N:783:ARG:HE	3:N:1029:ARG:HD3	1.84	0.42
3:N:989:TYR:HA	9:N:9914:HOH:O	2.19	0.42
3:N:1282:ARG:NH1	9:N:2080:HOH:O	2.51	0.42
3:N:1379:VAL:HG12	3:N:1419:PRO:HA	2.01	0.42
3:N:1471:LEU:HD12	3:N:1472:ILE:N	2.31	0.42
3:N:1493:LYS:HA	3:N:1496:GLU:HG2	1.99	0.42
5:P:102:LEU:HD23	5:P:183:ALA:HA	2.01	0.42
1:A:143:ARG:HG3	1:A:144:VAL:N	2.32	0.42
2:C:69:LEU:HB2	2:C:97:ARG:HB2	2.01	0.42
2:C:91:GLN:HG2	2:C:119:PRO:HG3	2.01	0.42
2:C:378:LEU:HD11	2:C:382:ILE:HD11	2.01	0.42
2:C:676:ILE:HG22	2:C:988:VAL:O	2.19	0.42
2:C:708:TYR:HE2	2:C:793:PRO:CD	2.30	0.42
2:C:715:THR:CG2	2:C:717:LEU:HG	2.49	0.42
2:C:1010:THR:HG21	5:F:341:PRO:CG	2.49	0.42
3:D:10:ILE:CD1	3:D:1447:LEU:HG	2.49	0.42
3:D:397:LYS:HZ3	3:D:399:ARG:HH21	1.66	0.42
3:D:426:LYS:HB2	9:D:2623:HOH:O	2.20	0.42
3:D:462:GLN:NE2	3:D:513:ILE:HB	2.34	0.42
3:D:498:VAL:HG12	9:D:9841:HOH:O	2.18	0.42
3:D:591:VAL:CG1	3:D:597:ASP:HA	2.49	0.42
3:D:996:TRP:CG	3:D:1056:PRO:HG2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1031:ASN:O	3:D:1032:PRO:C	2.62	0.42
3:D:1147:ARG:HH22	3:D:1369:GLU:CD	2.27	0.42
3:D:1403:LEU:HD23	3:D:1407:LEU:HD22	2.00	0.42
5:F:340:SER:O	5:F:342:VAL:N	2.52	0.42
5:F:401:GLU:O	5:F:405:LEU:HD13	2.18	0.42
1:K:11:PHE:HD2	1:L:228:PRO:HA	1.84	0.42
1:K:58:ILE:HG21	1:K:68:ILE:CD1	2.48	0.42
2:M:166:PRO:HB2	9:M:9802:HOH:O	2.19	0.42
2:M:380:ALA:HB2	9:M:2136:HOH:O	2.19	0.42
2:M:751:PRO:HA	2:M:792:VAL:CG1	2.49	0.42
2:M:984:GLU:OE1	3:N:945:SER:HA	2.19	0.42
2:M:1015:LEU:HA	5:P:335:ASP:HB2	2.01	0.42
2:M:1043:TYR:HA	3:N:710:ARG:NH2	2.34	0.42
2:M:1090:LYS:HG2	2:M:1112:PHE:HZ	1.83	0.42
3:N:42:ASP:O	3:N:49:ILE:HD12	2.18	0.42
3:N:619:LEU:HD23	3:N:619:LEU:C	2.45	0.42
3:N:777:PRO:HD2	3:N:912:LYS:HG2	2.01	0.42
3:N:793:THR:O	3:N:879:ARG:NH1	2.52	0.42
3:N:799:LYS:HE2	3:N:824:ASN:O	2.19	0.42
3:N:1144:LEU:HD13	3:N:1174:LEU:HD12	2.01	0.42
3:N:1319:VAL:O	3:N:1319:VAL:HG23	2.19	0.42
3:N:1478:SER:OG	3:N:1480:PHE:HB3	2.19	0.42
5:P:161:GLN:NE2	9:P:3901:HOH:O	2.52	0.42
5:P:169:GLU:HA	5:P:172:ARG:NH2	2.34	0.42
5:P:240:THR:O	5:P:244:ARG:HG3	2.20	0.42
1:A:88:ARG:HD2	1:A:123:MET:HE2	2.02	0.42
1:B:107:LYS:HB2	9:B:9631:HOH:O	2.19	0.42
1:B:124:ASN:OD1	1:B:127:LEU:HB2	2.19	0.42
1:B:150:TYR:HD1	1:B:169:ALA:O	2.02	0.42
2:C:72:ARG:HG3	2:C:72:ARG:NH1	2.32	0.42
2:C:271:GLU:C	2:C:273:GLY:H	2.27	0.42
2:C:474:VAL:HG23	2:C:478:VAL:O	2.18	0.42
2:C:663:ASN:HD22	2:C:663:ASN:HA	1.60	0.42
2:C:697:ARG:O	2:C:699:PHE:N	2.53	0.42
2:C:1090:LYS:NZ	3:D:90:MET:HG3	2.34	0.42
3:D:119:SER:HB2	3:D:123:LEU:CB	2.48	0.42
3:D:167:GLU:HB2	9:D:9804:HOH:O	2.19	0.42
3:D:513:ILE:HG13	9:D:2007:HOH:O	2.18	0.42
3:D:613:ARG:HA	3:D:613:ARG:HD2	1.90	0.42
3:D:955:VAL:O	3:D:1039:CYS:HB3	2.20	0.42
4:E:46:PRO:CB	4:E:63:TRP:NE1	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:135:ILE:O	5:F:135:ILE:HD13	2.19	0.42
5:F:401:GLU:HG3	5:F:405:LEU:HD22	2.01	0.42
1:K:173:PRO:HB3	1:K:204:SER:HB3	2.01	0.42
1:L:101:LEU:HD12	1:L:114:PHE:CD1	2.55	0.42
1:L:206:THR:CG2	1:L:209:GLU:H	2.26	0.42
2:M:352:ALA:O	2:M:355:VAL:HG12	2.19	0.42
2:M:437:ARG:HG2	2:M:467:ILE:HG22	2.02	0.42
2:M:690:ILE:CG2	2:M:852:ILE:HG12	2.49	0.42
2:M:802:ARG:HB3	2:M:802:ARG:NH1	2.34	0.42
2:M:897:LEU:CD2	2:M:921:ALA:HB2	2.50	0.42
2:M:1095:LEU:O	2:M:1096:ALA:C	2.62	0.42
3:N:127:LEU:HB3	3:N:132:TYR:O	2.18	0.42
3:N:520:LEU:CD1	3:N:521:PRO:HD2	2.49	0.42
3:N:520:LEU:O	3:N:525:ARG:NH1	2.52	0.42
3:N:734:GLU:OE1	3:N:782:SER:HB2	2.18	0.42
3:N:951:ILE:HG23	3:N:1062:ARG:NH2	2.35	0.42
3:N:1106:VAL:HB	3:N:1108:ARG:HH21	1.84	0.42
4:O:44:GLU:HG3	9:O:5061:HOH:O	2.20	0.42
4:O:59:ASN:ND2	9:O:5180:HOH:O	2.52	0.42
4:O:79:LEU:HD12	4:O:79:LEU:HA	1.93	0.42
1:A:9:PRO:HB3	1:A:25:LEU:CD2	2.49	0.42
1:A:26:GLU:HG2	1:A:27:PRO:HG3	2.00	0.42
1:B:86:VAL:HG13	1:B:86:VAL:O	2.17	0.42
1:B:207:PRO:HB2	9:B:9532:HOH:O	2.18	0.42
1:B:213:GLN:HE21	1:B:213:GLN:HB2	1.58	0.42
2:C:11:GLU:HG2	2:C:537:LYS:NZ	2.34	0.42
2:C:31:GLN:HB3	2:C:71:TYR:OH	2.19	0.42
2:C:69:LEU:HD12	2:C:97:ARG:HB2	2.01	0.42
2:C:253:ALA:O	2:C:256:TYR:HB2	2.19	0.42
2:C:270:GLY:O	2:C:271:GLU:HG2	2.18	0.42
2:C:578:VAL:HG13	2:C:671:ASN:OD1	2.19	0.42
2:C:852:ILE:HD12	2:C:852:ILE:N	2.34	0.42
3:D:112:ILE:C	3:D:112:ILE:HD12	2.44	0.42
3:D:581:LEU:CD1	3:D:603:LEU:HD12	2.50	0.42
3:D:704:ARG:CD	3:D:705:ALA:H	2.32	0.42
3:D:757:ALA:CB	4:E:24:ALA:HB2	2.50	0.42
3:D:786:ILE:HD13	3:D:1027:GLY:C	2.44	0.42
3:D:817:GLU:CD	3:D:839:LEU:HD22	2.44	0.42
3:D:844:ALA:HB3	3:D:848:GLU:OE2	2.18	0.42
3:D:914:LEU:HD22	3:D:930:LEU:HD21	2.00	0.42
3:D:1205:TYR:HE1	3:D:1221:VAL:HG13	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1467:ILE:HG22	9:D:9522:HOH:O	2.19	0.42
4:E:14:ASP:HB2	9:E:9493:HOH:O	2.18	0.42
5:F:87:GLU:HB3	9:F:9506:HOH:O	2.20	0.42
2:M:35:PRO:HD2	2:M:38:LYS:CG	2.49	0.42
2:M:80:GLN:O	2:M:83:CYS:HB2	2.19	0.42
2:M:246:ASP:HB2	9:M:9955:HOH:O	2.19	0.42
2:M:352:ALA:HA	2:M:355:VAL:CG1	2.49	0.42
2:M:361:MET:HG2	9:M:2349:HOH:O	2.18	0.42
2:M:706:GLU:HB3	2:M:708:TYR:CE1	2.54	0.42
2:M:808:ARG:HA	9:M:9526:HOH:O	2.19	0.42
2:M:1000:MET:HG3	7:M:8002:RPT:H472	2.00	0.42
2:M:1044:GLY:C	3:N:762:GLN:HE22	2.27	0.42
2:M:1115:LEU:H	2:M:1115:LEU:CD1	2.31	0.42
3:N:7:LYS:HG2	3:N:1458:GLU:CD	2.45	0.42
3:N:9:ARG:HG3	3:N:1456:LYS:HG2	2.01	0.42
3:N:93:ILE:HD13	3:N:548:ILE:HD11	2.01	0.42
3:N:95:LEU:HD11	3:N:517:VAL:CG2	2.50	0.42
3:N:563:PRO:HG2	3:N:566:ILE:HB	2.01	0.42
3:N:892:ASP:HB3	3:N:895:VAL:CG2	2.49	0.42
3:N:1111:ASP:HB2	3:N:1203:LYS:HG3	2.02	0.42
3:N:1133:ARG:HB2	9:N:9762:HOH:O	2.18	0.42
3:N:1402:ALA:HB1	9:N:2424:HOH:O	2.18	0.42
9:N:9815:HOH:O	5:P:140:ARG:HB2	2.19	0.42
5:P:122:LEU:HD12	9:P:4063:HOH:O	2.18	0.42
5:P:361:LEU:HD23	5:P:362:SER:N	2.35	0.42
1:B:49:PRO:HB3	1:B:148:VAL:HG13	2.01	0.42
1:B:103:ALA:HB1	1:B:107:LYS:CE	2.49	0.42
2:C:77:PRO:HD2	2:C:91:GLN:O	2.20	0.42
2:C:276:LYS:HG2	9:C:2408:HOH:O	2.19	0.42
2:C:431:HIS:CD2	2:C:433:THR:HG1	2.38	0.42
2:C:577:PRO:HB2	2:C:580:MET:HG3	2.01	0.42
2:C:668:LEU:O	2:C:669:GLY:C	2.62	0.42
2:C:710:ILE:HD12	2:C:790:LEU:HB2	2.01	0.42
2:C:744:ARG:HA	9:C:9908:HOH:O	2.19	0.42
2:C:774:LEU:HD21	9:C:9684:HOH:O	2.18	0.42
2:C:876:VAL:HG11	2:C:885:ILE:HD11	2.02	0.42
2:C:956:GLY:HA2	9:C:9712:HOH:O	2.19	0.42
2:C:1067:TYR:CE1	2:C:1071:ILE:HD11	2.55	0.42
3:D:34:TYR:O	3:D:35:ARG:C	2.62	0.42
3:D:102:ILE:HG13	9:D:9521:HOH:O	2.19	0.42
3:D:500:ARG:HG3	9:D:9797:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:704:ARG:NH1	3:D:737:ASN:O	2.53	0.42
3:D:1087:ARG:CG	3:D:1234:THR:HA	2.19	0.42
3:D:1183:ILE:O	3:D:1183:ILE:HD12	2.20	0.42
3:D:1274:ILE:HA	9:D:9544:HOH:O	2.17	0.42
3:D:1412:LYS:HG3	9:D:9570:HOH:O	2.18	0.42
3:D:1434:TRP:CZ3	3:D:1455:LYS:HB3	2.54	0.42
3:D:1451:ALA:O	3:D:1452:ILE:C	2.63	0.42
5:F:348:SER:OG	5:F:349:LEU:N	2.53	0.42
1:K:229:GLN:HE21	1:K:229:GLN:HB2	1.68	0.42
1:L:68:ILE:HG23	9:L:6170:HOH:O	2.18	0.42
1:L:101:LEU:HG	1:L:113:ASP:C	2.44	0.42
1:L:119:ASP:HB3	9:L:4208:HOH:O	2.17	0.42
1:L:142:VAL:HG23	1:L:142:VAL:O	2.20	0.42
2:M:50:GLU:HA	2:M:266:ARG:CZ	2.50	0.42
2:M:444:PRO:HB3	7:M:8002:RPT:H302	2.01	0.42
2:M:571:LEU:HD12	2:M:701:THR:C	2.44	0.42
2:M:798:GLY:HA2	9:M:2295:HOH:O	2.18	0.42
2:M:801:VAL:C	2:M:802:ARG:HG3	2.44	0.42
3:N:106:LYS:HB3	3:N:586:ARG:NH1	2.34	0.42
3:N:209:ARG:NH2	3:N:397:LYS:HG3	2.34	0.42
3:N:508:ARG:HG3	9:N:2034:HOH:O	2.18	0.42
3:N:679:ARG:HB3	9:N:9725:HOH:O	2.19	0.42
3:N:838:ARG:HD3	3:N:874:GLU:HB3	2.00	0.42
3:N:1047:LYS:HG2	3:N:1053:PHE:CE1	2.55	0.42
3:N:1065:LEU:C	3:N:1065:LEU:HD12	2.43	0.42
3:N:1122:LEU:O	3:N:1135:ARG:N	2.45	0.42
3:N:1231:GLU:HB3	3:N:1232:PRO:HD3	2.00	0.42
4:O:31:LEU:HD23	4:O:35:PHE:CD1	2.54	0.42
5:P:88:ILE:HG21	5:P:193:ARG:CZ	2.50	0.42
5:P:131:VAL:HG13	5:P:178:ARG:HG2	2.02	0.42
5:P:132:ARG:HG2	5:P:181:GLU:CD	2.44	0.42
5:P:359:SER:C	5:P:361:LEU:H	2.27	0.42
5:P:411:HIS:HA	5:P:414:ARG:HG3	2.01	0.42
1:A:9:PRO:HG2	1:B:224:TYR:CD2	2.55	0.42
1:A:32:PHE:HB2	9:A:9526:HOH:O	2.19	0.42
1:B:123:MET:HG2	9:B:9635:HOH:O	2.20	0.42
1:B:140:MET:HG3	9:B:9666:HOH:O	2.19	0.42
2:C:172:ILE:HA	2:C:185:LYS:O	2.18	0.42
2:C:254:VAL:HG13	2:C:258:TYR:HE1	1.84	0.42
2:C:614:ARG:HG3	2:C:620:LEU:HB3	2.02	0.42
2:C:658:GLY:N	2:C:661:SER:OG	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:964:LYS:HB2	9:C:2350:HOH:O	2.19	0.42
2:C:1091:GLU:CD	3:D:613:ARG:HG2	2.43	0.42
3:D:474:GLU:CD	3:D:500:ARG:HE	2.28	0.42
3:D:501:ALA:HB1	3:D:1453:ALA:CB	2.49	0.42
3:D:715:ALA:HB3	3:D:764:LEU:CA	2.47	0.42
3:D:1040:GLY:O	3:D:1060:SER:HB3	2.20	0.42
3:D:1065:LEU:HD11	3:D:1069:GLU:C	2.45	0.42
3:D:1074:SER:O	3:D:1077:ALA:HB3	2.20	0.42
3:D:1109:GLU:HG2	3:D:1202:GLN:H	1.85	0.42
3:D:1344:VAL:HG11	3:D:1421:LEU:HD13	2.01	0.42
5:F:295:MET:HA	5:F:295:MET:HE2	2.02	0.42
1:K:18:ARG:HG2	9:K:4001:HOH:O	2.19	0.42
2:M:86:LYS:CE	2:M:813:VAL:HG12	2.49	0.42
2:M:90:TYR:CE2	2:M:120:LEU:HB2	2.55	0.42
2:M:393:GLN:HB2	7:M:8002:RPT:O9	2.20	0.42
2:M:405:ARG:HD2	2:M:442:GLU:OE1	2.19	0.42
2:M:546:LEU:HD23	2:M:842:ARG:HH11	1.85	0.42
2:M:689:VAL:O	2:M:869:VAL:HG23	2.20	0.42
2:M:729:LEU:HB3	9:M:2237:HOH:O	2.20	0.42
2:M:928:LYS:HD2	9:M:2219:HOH:O	2.18	0.42
2:M:1078:GLU:HA	2:M:1079:PRO:HD3	1.93	0.42
3:N:645:PRO:HA	3:N:721:VAL:O	2.19	0.42
3:N:676:MET:HE1	3:N:684:LYS:HG3	2.00	0.42
3:N:739:ASP:O	3:N:743:ASP:OD2	2.37	0.42
3:N:964:LEU:HD22	3:N:1058:ARG:HH12	1.81	0.42
3:N:1283:ILE:N	3:N:1315:ASP:OD1	2.52	0.42
3:N:1341:PRO:HA	3:N:1344:VAL:HG23	2.01	0.42
3:N:1394:VAL:HG21	3:N:1397:LYS:HE3	2.02	0.42
5:P:136:LEU:HD12	5:P:137:GLY:N	2.35	0.42
5:P:336:GLU:CD	5:P:336:GLU:N	2.77	0.42
5:P:352:GLU:O	5:P:356:LYS:HG3	2.19	0.42
2:C:94:LEU:HD21	9:C:9517:HOH:O	2.19	0.42
2:C:137:VAL:O	2:C:391:LEU:HD21	2.20	0.42
2:C:559:LEU:HD23	2:C:560:MET:N	2.35	0.42
2:C:798:GLY:HA3	2:C:828:ALA:O	2.20	0.42
2:C:833:LEU:HD11	2:C:849:VAL:HG21	2.02	0.42
2:C:886:LEU:HD23	2:C:886:LEU:HA	1.92	0.42
3:D:93:ILE:HD12	3:D:519:VAL:HG22	2.02	0.42
3:D:169:TYR:N	3:D:170:PRO:HD2	2.35	0.42
3:D:584:ASN:HD21	3:D:589:ALA:CA	2.30	0.42
3:D:619:LEU:HD23	3:D:619:LEU:C	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:959:GLU:CD	3:D:959:GLU:N	2.76	0.42
3:D:1034:GLN:O	3:D:1037:GLN:HG3	2.19	0.42
3:D:1041:LEU:O	3:D:1041:LEU:HD23	2.19	0.42
3:D:1065:LEU:HD12	3:D:1066:THR:N	2.34	0.42
3:D:1463:LYS:HD3	3:D:1463:LYS:HA	1.85	0.42
5:F:300:ASP:CG	5:F:301:ALA:N	2.78	0.42
1:L:95:GLN:NE2	1:L:95:GLN:H	2.18	0.42
1:L:116:PRO:HD3	9:L:6307:HOH:O	2.19	0.42
2:M:93:PRO:HG3	2:M:117:HIS:HE1	1.83	0.42
2:M:141:HIS:HB2	9:M:9692:HOH:O	2.19	0.42
2:M:455:LEU:HD12	2:M:459:ALA:HB3	2.00	0.42
2:M:654:LEU:HD11	2:M:657:ASP:HA	2.00	0.42
2:M:815:LEU:HD21	2:M:820:ARG:O	2.19	0.42
3:N:135:LEU:HD11	3:N:139:GLY:HA3	2.02	0.42
3:N:154:THR:HG23	3:N:157:GLU:H	1.83	0.42
3:N:187:LYS:HA	3:N:187:LYS:HD3	1.87	0.42
3:N:411:THR:HG23	3:N:429:SER:CB	2.49	0.42
3:N:957:PRO:CD	3:N:1007:VAL:HG12	2.49	0.42
3:N:1037:GLN:OE1	3:N:1042:ARG:HB3	2.20	0.42
3:N:1110:ALA:O	3:N:1111:ASP:C	2.61	0.42
3:N:1148:VAL:HG21	3:N:1203:LYS:HA	2.02	0.42
3:N:1283:ILE:HG23	3:N:1290:LEU:HD21	2.00	0.42
3:N:1315:ASP:HB2	9:N:9493:HOH:O	2.20	0.42
1:A:7:LYS:HB2	9:A:9499:HOH:O	2.18	0.42
1:B:84:GLU:HG2	1:B:127:LEU:CD1	2.49	0.42
2:C:101:ILE:HG22	2:C:102:HIS:H	1.85	0.42
2:C:135:VAL:O	2:C:392:SER:HA	2.19	0.42
2:C:343:GLN:HA	9:C:2037:HOH:O	2.19	0.42
2:C:420:ARG:HG2	2:C:421:GLU:N	2.34	0.42
2:C:755:LEU:CD2	2:C:825:VAL:HG11	2.47	0.42
2:C:881:ASN:H	2:C:881:ASN:ND2	2.15	0.42
2:C:1102:LEU:HD23	2:C:1106:ASP:CA	2.50	0.42
3:D:23:TYR:OH	3:D:89:ARG:NE	2.53	0.42
3:D:209:ARG:CZ	3:D:397:LYS:HG3	2.49	0.42
3:D:415:VAL:N	9:D:2009:HOH:O	2.51	0.42
3:D:430:ASP:CG	3:D:431:VAL:H	2.28	0.42
3:D:491:LYS:HB2	9:D:9973:HOH:O	2.19	0.42
3:D:661:MET:HE3	3:D:673:ALA:CB	2.45	0.42
3:D:1047:LYS:HA	3:D:1053:PHE:CZ	2.55	0.42
3:D:1109:GLU:CG	3:D:1202:GLN:H	2.33	0.42
3:D:1292:VAL:N	3:D:1305:LEU:HD21	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:87:LYS:HD2	9:E:9516:HOH:O	2.20	0.42
5:F:131:VAL:CG1	5:F:181:GLU:HG3	2.48	0.42
1:L:18:ARG:O	1:L:207:PRO:HD3	2.19	0.42
1:L:85:LEU:HD12	1:L:86:VAL:N	2.35	0.42
1:L:103:ALA:O	1:L:138:LEU:HD23	2.19	0.42
2:M:290:LEU:HD22	2:M:302:VAL:HG11	2.00	0.42
2:M:316:GLY:O	2:M:318:PRO:HD3	2.19	0.42
2:M:380:ALA:HA	2:M:383:ARG:CD	2.50	0.42
2:M:405:ARG:HH21	2:M:409:ARG:NH2	2.18	0.42
2:M:443:THR:HG23	2:M:449:ILE:HG13	2.02	0.42
2:M:496:ILE:H	2:M:496:ILE:HD12	1.85	0.42
2:M:537:LYS:HE3	2:M:905:ILE:HD11	2.02	0.42
2:M:660:ALA:O	2:M:667:ALA:O	2.38	0.42
2:M:721:ARG:HH11	2:M:721:ARG:HG3	1.85	0.42
2:M:727:PRO:HB3	9:M:2452:HOH:O	2.19	0.42
2:M:815:LEU:HD11	2:M:819:VAL:HG12	2.02	0.42
2:M:1008:ARG:NH1	2:M:1011:GLY:CA	2.82	0.42
2:M:1032:PHE:HD1	9:M:2368:HOH:O	2.03	0.42
3:N:115:LEU:CD1	3:N:498:VAL:HG23	2.50	0.42
3:N:799:LYS:N	3:N:826:PRO:HG2	2.34	0.42
3:N:950:GLY:C	3:N:953:ASP:H	2.23	0.42
3:N:1459:LEU:HD22	3:N:1465:ASN:HA	2.01	0.42
3:N:1481:VAL:C	3:N:1483:PHE:N	2.78	0.42
5:P:276:ARG:HB2	9:P:4488:HOH:O	2.19	0.42
1:B:28:LEU:HB2	1:B:193:ASP:HB2	2.01	0.42
2:C:14:PRO:HA	9:C:2347:HOH:O	2.20	0.42
2:C:75:GLU:O	2:C:93:PRO:HG2	2.19	0.42
2:C:150:PRO:CA	2:C:158:TYR:HB3	2.34	0.42
2:C:384:GLU:HA	2:C:388:ARG:HH21	1.85	0.42
2:C:406:HIS:ND1	2:C:406:HIS:O	2.52	0.42
2:C:599:GLU:HG2	2:C:600:ASP:H	1.84	0.42
3:D:203:ALA:HB2	9:D:9843:HOH:O	2.20	0.42
3:D:491:LYS:HG3	9:D:9655:HOH:O	2.19	0.42
3:D:1011:PHE:HZ	3:D:1039:CYS:SG	2.42	0.42
3:D:1031:ASN:OD1	3:D:1033:GLN:N	2.53	0.42
5:F:220:LEU:HB2	5:F:243:ILE:HD11	2.01	0.42
5:F:326:ASP:HB2	9:F:9660:HOH:O	2.20	0.42
1:K:32:PHE:HB2	9:K:4346:HOH:O	2.20	0.42
1:K:44:LEU:CD2	1:K:199:ILE:HG12	2.49	0.42
1:K:53:VAL:HG21	1:K:82:LEU:HB3	2.01	0.42
2:M:103:LYS:HG2	9:M:9553:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:199:VAL:HG13	2:M:235:LEU:CG	2.44	0.42
2:M:305:PRO:HA	2:M:308:ARG:HB2	2.01	0.42
2:M:495:THR:HG21	2:M:524:VAL:HG21	2.01	0.42
2:M:571:LEU:HD12	2:M:701:THR:N	2.34	0.42
2:M:983:ILE:O	2:M:984:GLU:C	2.63	0.42
2:M:1059:ASP:OD2	2:M:1079:PRO:HA	2.20	0.42
3:N:6:ARG:HG2	9:N:9676:HOH:O	2.19	0.42
3:N:120:ALA:HB1	9:N:2018:HOH:O	2.20	0.42
3:N:477:LEU:HD21	3:N:495:ARG:HD3	2.00	0.42
3:N:546:ARG:NH2	3:N:550:ARG:HH22	2.17	0.42
3:N:637:LEU:HD11	3:N:641:GLN:C	2.45	0.42
3:N:654:LYS:CB	3:N:655:PRO:HD3	2.48	0.42
3:N:782:SER:N	3:N:785:ILE:HD13	2.34	0.42
3:N:828:LYS:N	3:N:828:LYS:HD3	2.34	0.42
3:N:1074:SER:O	3:N:1077:ALA:HB3	2.19	0.42
3:N:1141:GLU:HB3	3:N:1168:MET:HE1	2.01	0.42
5:P:113:ILE:HG23	5:P:127:ILE:HG22	2.01	0.42
5:P:175:HIS:O	5:P:179:GLU:HG2	2.20	0.42
1:A:110:LYS:HB2	9:A:9528:HOH:O	2.19	0.42
1:A:199:ILE:N	9:A:9498:HOH:O	2.52	0.42
1:B:132:LEU:CD1	1:B:138:LEU:HD22	2.48	0.42
1:B:217:ILE:O	1:B:221:HIS:ND1	2.53	0.42
2:C:64:LEU:HD13	2:C:359:MET:CG	2.50	0.42
2:C:137:VAL:HG22	2:C:391:LEU:O	2.20	0.42
2:C:207:LEU:HD13	2:C:221:LEU:HD13	2.02	0.42
2:C:218:VAL:HG22	2:C:221:LEU:HD23	2.00	0.42
2:C:258:TYR:O	2:C:290:LEU:HG	2.20	0.42
2:C:289:THR:O	2:C:291:ALA:N	2.53	0.42
2:C:466:PHE:HD2	9:C:9744:HOH:O	2.03	0.42
2:C:742:VAL:HG12	2:C:743:VAL:H	1.84	0.42
2:C:1056:LYS:CD	3:D:623:VAL:HG13	2.45	0.42
3:D:15:PRO:HG3	9:D:9862:HOH:O	2.20	0.42
3:D:142:LEU:HD12	3:D:142:LEU:O	2.20	0.42
3:D:159:ARG:NH1	3:D:159:ARG:HB2	2.34	0.42
3:D:434:ARG:HB2	3:D:447:VAL:CG2	2.50	0.42
3:D:634:GLY:O	3:D:637:LEU:HB3	2.19	0.42
3:D:675:ARG:HH22	5:F:420:ASP:HA	1.84	0.42
3:D:681:ARG:NH1	9:D:2081:HOH:O	2.53	0.42
3:D:992:ILE:O	3:D:995:LEU:HB3	2.20	0.42
3:D:1118:ILE:HG21	3:D:1346:ARG:CZ	2.50	0.42
3:D:1176:LYS:HA	3:D:1179:GLU:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:138:SER:HB2	5:F:140:ARG:HG2	2.02	0.42
1:K:209:GLU:C	1:K:213:GLN:HE21	2.28	0.42
1:L:165:ILE:HA	1:L:166:PRO:HD3	1.94	0.42
1:L:195:LEU:HD12	1:L:196:THR:N	2.34	0.42
2:M:47:ALA:O	2:M:50:GLU:HB3	2.20	0.42
2:M:172:ILE:N	2:M:172:ILE:HD12	2.35	0.42
2:M:276:LYS:HE3	9:M:9970:HOH:O	2.20	0.42
2:M:405:ARG:HH21	2:M:409:ARG:HH21	1.68	0.42
2:M:430:VAL:HG13	3:N:1075:HIS:ND1	2.35	0.42
2:M:575:GLN:C	2:M:667:ALA:HB1	2.45	0.42
2:M:591:SER:HB2	9:M:2161:HOH:O	2.18	0.42
2:M:752:GLY:C	9:M:9759:HOH:O	2.62	0.42
2:M:790:LEU:HD23	2:M:791:ARG:N	2.34	0.42
2:M:1050:GLN:HA	2:M:1053:LEU:HD12	2.02	0.42
3:N:28:LYS:HD3	3:N:41:ARG:NH1	2.34	0.42
3:N:450:TYR:HA	9:N:9669:HOH:O	2.18	0.42
3:N:1007:VAL:CG2	3:N:1008:PHE:N	2.82	0.42
3:N:1317:ASP:OD2	3:N:1317:ASP:N	2.49	0.42
3:N:1423:GLY:O	3:N:1426:LYS:N	2.53	0.42
3:N:1441:GLN:NE2	3:N:1442:ASN:HB2	2.35	0.42
5:P:340:SER:O	5:P:342:VAL:N	2.52	0.42
1:A:64:GLU:O	1:A:64:GLU:HG2	2.20	0.41
1:B:19:GLU:O	1:B:200:TRP:HA	2.20	0.41
2:C:244:PRO:CD	2:C:245:GLY:N	2.82	0.41
2:C:418:LEU:O	2:C:419:THR:C	2.61	0.41
2:C:555:ALA:HB2	3:D:1070:TYR:CE2	2.55	0.41
2:C:666:LEU:HG	2:C:668:LEU:HD11	2.02	0.41
2:C:713:ARG:HH12	3:D:532:GLY:HA2	1.85	0.41
3:D:123:LEU:HD12	9:D:9569:HOH:O	2.19	0.41
3:D:568:ARG:O	3:D:569:ASN:C	2.63	0.41
3:D:672:ALA:HB2	9:F:9494:HOH:O	2.18	0.41
3:D:683:ILE:HA	9:D:9956:HOH:O	2.19	0.41
3:D:1351:GLU:HA	3:D:1354:LYS:HG2	2.01	0.41
4:E:84:ARG:NH1	4:E:84:ARG:HB2	2.35	0.41
5:F:281:GLU:HB3	9:F:9529:HOH:O	2.20	0.41
5:F:350:LEU:O	5:F:354:LEU:HB2	2.20	0.41
5:F:366:ALA:CB	5:F:367:MET:HE2	2.45	0.41
5:F:370:LYS:HB3	5:F:370:LYS:NZ	2.34	0.41
5:F:370:LYS:NZ	5:F:371:LEU:HG	2.35	0.41
1:K:156:HIS:HD2	1:K:157:GLY:N	2.18	0.41
1:L:156:HIS:HE1	1:L:166:PRO:HB3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:188:GLN:N	9:L:5782:HOH:O	2.53	0.41
2:M:203:ASP:OD1	2:M:205:GLU:HG3	2.19	0.41
2:M:460:ARG:HD2	2:M:485:TYR:CD2	2.55	0.41
2:M:525:SER:HA	9:M:2109:HOH:O	2.20	0.41
2:M:744:ARG:HE	2:M:747:ALA:HB2	1.86	0.41
2:M:877:PRO:HG3	3:N:1023:MET:CE	2.49	0.41
2:M:1044:GLY:HA3	4:O:17:TYR:CD1	2.55	0.41
9:M:9879:HOH:O	5:P:334:PRO:HG2	2.18	0.41
3:N:63:TYR:HE1	3:N:74:GLU:OE1	2.03	0.41
3:N:105:VAL:HG12	3:N:106:LYS:HZ1	1.85	0.41
3:N:153:LEU:HD12	3:N:154:THR:N	2.35	0.41
3:N:605:ASP:HB3	9:N:9598:HOH:O	2.19	0.41
3:N:653:PHE:CE2	3:N:695:ILE:HG13	2.53	0.41
3:N:734:GLU:HB2	9:N:9534:HOH:O	2.19	0.41
3:N:1066:THR:HG22	3:N:1069:GLU:OE1	2.20	0.41
3:N:1259:VAL:HG22	3:N:1355:VAL:HG21	2.02	0.41
4:O:54:LEU:HA	4:O:58:PRO:HG2	2.00	0.41
5:P:392:VAL:HG12	5:P:396:ARG:HG3	2.02	0.41
1:A:23:PHE:O	1:A:196:THR:HA	2.19	0.41
1:A:30:ARG:NH1	2:C:938:LYS:HE2	2.35	0.41
1:A:79:ILE:O	1:A:83:LYS:HG3	2.20	0.41
1:A:89:PHE:HZ	1:A:146:ARG:HB2	1.83	0.41
1:B:34:VAL:HA	9:B:9725:HOH:O	2.19	0.41
2:C:124:ASP:OD1	2:C:125:GLY:N	2.53	0.41
2:C:578:VAL:N	2:C:671:ASN:OD1	2.53	0.41
2:C:787:ASP:OD1	2:C:787:ASP:C	2.64	0.41
3:D:106:LYS:HD3	3:D:106:LYS:HA	1.81	0.41
3:D:196:VAL:HG13	3:D:202:VAL:HG13	2.01	0.41
3:D:983:LEU:CB	9:D:9513:HOH:O	2.68	0.41
3:D:1090:ASP:HA	3:D:1093:TYR:CB	2.49	0.41
3:D:1129:THR:O	3:D:1130:ARG:HD2	2.20	0.41
3:D:1294:VAL:O	3:D:1300:SER:HA	2.19	0.41
3:D:1465:ASN:ND2	3:D:1470:ARG:NH1	2.66	0.41
5:F:82:ARG:HD3	9:F:9734:HOH:O	2.20	0.41
5:F:149:GLU:OE1	5:F:149:GLU:HA	2.19	0.41
1:K:36:LEU:HB2	1:K:195:LEU:CD2	2.50	0.41
1:K:57:TYR:CZ	1:K:161:ARG:HD2	2.55	0.41
1:K:156:HIS:CD2	1:K:157:GLY:H	2.33	0.41
1:K:197:LEU:HD23	1:K:197:LEU:N	2.33	0.41
1:L:44:LEU:O	1:L:174:VAL:HG21	2.18	0.41
1:L:177:VAL:HB	9:L:4703:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:54:ILE:HG12	2:M:56:GLU:HG2	2.02	0.41
2:M:162:ILE:HG21	2:M:172:ILE:HD13	2.02	0.41
2:M:167:LYS:HE3	2:M:168:ARG:NH2	2.35	0.41
2:M:260:LEU:HG	2:M:261:ILE:CG1	2.49	0.41
2:M:398:THR:O	2:M:399:ASN:HB3	2.20	0.41
2:M:459:ALA:HB1	2:M:467:ILE:CG2	2.50	0.41
2:M:933:GLY:HA2	9:M:9889:HOH:O	2.19	0.41
2:M:1007:ALA:HB2	3:N:648:MET:CG	2.50	0.41
9:M:9622:HOH:O	3:N:791:TYR:HE2	2.03	0.41
3:N:235:ALA:HB1	9:N:9519:HOH:O	2.20	0.41
3:N:481:MET:HB2	3:N:1388:ARG:HH21	1.84	0.41
3:N:871:LYS:HB3	3:N:873:LEU:HD11	2.02	0.41
3:N:1084:THR:HG23	9:N:9666:HOH:O	2.20	0.41
3:N:1495:ILE:HG12	4:O:80:VAL:HG11	2.00	0.41
5:P:321:ILE:HG13	5:P:332:PHE:HE1	1.86	0.41
5:P:365:GLU:CD	5:P:397:ILE:HA	2.45	0.41
1:B:92:PRO:HA	1:B:146:ARG:CZ	2.50	0.41
2:C:145:GLY:O	2:C:163:ILE:HG23	2.20	0.41
2:C:185:LYS:HG2	2:C:190:LYS:HG2	2.03	0.41
2:C:193:LEU:HB2	9:C:9507:HOH:O	2.21	0.41
2:C:194:VAL:HG21	2:C:221:LEU:HA	2.01	0.41
2:C:461:VAL:N	9:C:9546:HOH:O	2.53	0.41
2:C:734:LEU:HA	2:C:737:LEU:HD12	2.02	0.41
2:C:768:THR:HG23	9:C:9533:HOH:O	2.20	0.41
2:C:769:PRO:O	2:C:772:ARG:HB3	2.20	0.41
2:C:943:VAL:HG11	2:C:973:VAL:HG22	2.03	0.41
3:D:49:ILE:HB	3:D:50:PHE:CE1	2.55	0.41
3:D:146:PRO:HA	9:D:9718:HOH:O	2.20	0.41
3:D:389:GLU:O	3:D:389:GLU:HG2	2.20	0.41
3:D:396:VAL:HG23	9:D:9579:HOH:O	2.20	0.41
3:D:521:PRO:HA	3:D:522:PRO:HD3	1.84	0.41
3:D:940:THR:O	3:D:943:THR:HG23	2.20	0.41
3:D:1227:GLN:C	3:D:1229:ILE:N	2.78	0.41
3:D:1378:TYR:CD1	3:D:1378:TYR:N	2.87	0.41
3:D:1429:LEU:HG	3:D:1441:GLN:OE1	2.19	0.41
2:M:18:LEU:C	2:M:20:GLU:H	2.29	0.41
2:M:208:ALA:HA	2:M:221:LEU:HD21	2.01	0.41
2:M:211:LEU:HD13	2:M:308:ARG:HG3	2.02	0.41
2:M:339:LEU:HD22	2:M:391:LEU:HD13	2.02	0.41
2:M:403:SER:OG	2:M:404:LEU:N	2.54	0.41
2:M:498:GLN:O	2:M:532:MET:SD	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:1008:ARG:HH21	2:M:1029:GLY:H	1.68	0.41
3:N:2:LYS:HB3	3:N:3:LYS:CE	2.50	0.41
3:N:56:TYR:HB3	9:N:2129:HOH:O	2.20	0.41
3:N:639:LEU:N	3:N:729:HIS:CD2	2.88	0.41
3:N:678:GLU:HG3	3:N:679:ARG:HG3	2.03	0.41
3:N:681:ARG:HB3	3:N:681:ARG:NH1	2.36	0.41
3:N:684:LYS:HG2	9:N:2365:HOH:O	2.20	0.41
3:N:813:LEU:HD12	3:N:814:ALA:N	2.35	0.41
3:N:1061:PHE:HE1	3:N:1065:LEU:HD23	1.85	0.41
3:N:1472:ILE:HA	3:N:1473:PRO:HD3	1.87	0.41
5:P:303:ARG:HG2	9:P:3308:HOH:O	2.20	0.41
5:P:340:SER:O	5:P:341:PRO:C	2.63	0.41
5:P:364:ARG:NH1	5:P:392:VAL:HG21	2.35	0.41
1:A:128:HIS:NE2	1:A:131:THR:HG23	2.34	0.41
2:C:3:ILE:HD13	2:C:900:ARG:HB2	2.02	0.41
2:C:22:GLN:O	2:C:121:MET:HE1	2.21	0.41
2:C:63:GLY:HA3	2:C:103:LYS:CG	2.50	0.41
2:C:239:PHE:CE1	2:C:250:ARG:HB3	2.55	0.41
2:C:308:ARG:HG3	9:C:9545:HOH:O	2.20	0.41
2:C:332:ARG:CZ	2:C:464:LEU:HD11	2.50	0.41
2:C:717:LEU:HD11	9:C:2279:HOH:O	2.20	0.41
2:C:843:HIS:CD2	2:C:884:GLN:HA	2.55	0.41
2:C:1019:GLN:H	2:C:1019:GLN:HG2	1.65	0.41
2:C:1020:PRO:HD2	2:C:1057:SER:OG	2.21	0.41
2:C:1059:ASP:CG	2:C:1062:GLY:HA3	2.45	0.41
3:D:145:VAL:CG2	3:D:146:PRO:HD2	2.37	0.41
3:D:441:ARG:HG2	3:D:442:ASN:N	2.35	0.41
3:D:468:LEU:HD22	9:D:2533:HOH:O	2.20	0.41
3:D:493:ARG:HE	3:D:1388:ARG:HB3	1.80	0.41
3:D:683:ILE:N	3:D:683:ILE:HD12	2.35	0.41
3:D:765:SER:OG	3:D:766:ALA:N	2.52	0.41
3:D:774:SER:C	3:D:776:GLU:N	2.74	0.41
3:D:786:ILE:HD13	3:D:908:LYS:HB3	2.02	0.41
3:D:984:THR:HG22	3:D:987:GLU:H	1.84	0.41
3:D:1031:ASN:O	3:D:1035:ILE:HG12	2.20	0.41
3:D:1097:LYS:NZ	9:D:9536:HOH:O	2.53	0.41
5:F:115:LYS:HG2	9:F:9676:HOH:O	2.20	0.41
1:K:184:THR:HG23	1:K:192:LEU:CB	2.50	0.41
1:L:7:LYS:HA	9:L:5355:HOH:O	2.20	0.41
2:M:192:PRO:C	2:M:194:VAL:H	2.28	0.41
2:M:207:LEU:HD22	2:M:221:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:367:LEU:HD23	2:M:371:LYS:NZ	2.31	0.41
2:M:865:THR:HA	2:M:866:PRO:HD3	1.90	0.41
3:N:30:GLU:HB3	3:N:40:GLU:CB	2.50	0.41
3:N:34:TYR:HE1	5:P:264:MET:HE2	1.84	0.41
3:N:196:VAL:HG13	3:N:202:VAL:HG11	2.02	0.41
3:N:426:LYS:CD	3:N:428:LYS:HZ1	2.33	0.41
3:N:501:ALA:HA	3:N:504:ASP:HB2	2.02	0.41
3:N:1275:SER:HB3	3:N:1325:LEU:HD11	2.01	0.41
3:N:1352:ILE:HG22	3:N:1368:ILE:HD13	2.03	0.41
3:N:1396:GLU:O	3:N:1400:VAL:HG23	2.20	0.41
5:P:163:LEU:HB3	5:P:174:LEU:HD11	2.01	0.41
1:A:36:LEU:C	1:A:39:PRO:HD2	2.45	0.41
2:C:124:ASP:CG	2:C:407:LYS:NZ	2.78	0.41
2:C:208:ALA:HA	2:C:221:LEU:HD21	2.02	0.41
2:C:413:LEU:CD2	2:C:448:ASN:HD21	2.17	0.41
2:C:634:GLY:HA3	9:C:2295:HOH:O	2.20	0.41
2:C:668:LEU:O	2:C:993:PHE:CZ	2.73	0.41
2:C:1115:LEU:H	2:C:1115:LEU:CD1	2.31	0.41
3:D:89:ARG:HB3	9:D:9497:HOH:O	2.20	0.41
3:D:459:GLU:HA	9:D:9482:HOH:O	2.20	0.41
3:D:525:ARG:HA	3:D:538:SER:CB	2.51	0.41
3:D:591:VAL:HG22	9:D:9851:HOH:O	2.18	0.41
3:D:1098:LEU:HD12	3:D:1098:LEU:N	2.35	0.41
3:D:1314:LYS:NZ	3:D:1317:ASP:HB2	2.35	0.41
3:D:1319:VAL:HG11	3:D:1325:LEU:HD11	2.02	0.41
3:D:1369:GLU:HA	3:D:1372:VAL:HG12	2.02	0.41
3:D:1379:VAL:HA	3:D:1420:LEU:CB	2.50	0.41
3:D:1481:VAL:HB	9:E:9482:HOH:O	2.20	0.41
5:F:119:ILE:HG12	9:F:9493:HOH:O	2.20	0.41
5:F:124:PRO:C	5:F:128:ARG:NH2	2.79	0.41
5:F:226:LYS:HB2	5:F:238:TYR:OH	2.20	0.41
5:F:256:ARG:HD3	5:F:260:ILE:HB	2.02	0.41
1:K:44:LEU:HD21	1:K:199:ILE:HG12	2.03	0.41
1:K:59:GLU:HG3	1:K:139:ASN:HB3	2.03	0.41
1:K:211:LEU:O	1:K:214:ALA:HB3	2.20	0.41
1:K:212:ASN:O	1:K:215:VAL:HG22	2.21	0.41
1:L:100:LEU:HD12	1:L:115:LEU:HD21	2.02	0.41
1:L:208:LEU:H	1:L:208:LEU:CD2	2.33	0.41
2:M:444:PRO:HD2	2:M:452:ILE:O	2.20	0.41
2:M:462:ASP:N	9:M:2120:HOH:O	2.54	0.41
2:M:545:ASN:HB3	2:M:583:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:742:VAL:HG12	2:M:743:VAL:H	1.85	0.41
2:M:899:GLN:HG3	2:M:901:TYR:OH	2.20	0.41
3:N:50:PHE:CB	3:N:522:PRO:HG2	2.51	0.41
3:N:90:MET:HE3	3:N:518:PRO:HB3	2.03	0.41
3:N:105:VAL:HG12	3:N:106:LYS:HZ2	1.86	0.41
3:N:177:ALA:HB1	3:N:199:LEU:HB3	2.03	0.41
3:N:444:VAL:O	3:N:446:VAL:HG23	2.20	0.41
3:N:1310:ARG:HB3	9:N:9491:HOH:O	2.20	0.41
1:A:121:GLU:HB3	9:A:9529:HOH:O	2.20	0.41
1:A:140:MET:HE3	1:A:142:VAL:HG11	2.01	0.41
2:C:92:ALA:HB2	9:C:2288:HOH:O	2.21	0.41
2:C:107:LEU:HB3	9:C:2236:HOH:O	2.19	0.41
2:C:279:GLU:HG3	2:C:280:LYS:N	2.34	0.41
2:C:630:ARG:NH2	2:C:707:ARG:HB2	2.36	0.41
2:C:684:PHE:HA	3:D:784:ASP:OD1	2.21	0.41
2:C:813:VAL:HG12	9:C:9512:HOH:O	2.21	0.41
2:C:937:ASP:HB2	2:C:940:GLU:H	1.86	0.41
2:C:1044:GLY:HA3	4:E:17:TYR:HE1	1.85	0.41
2:C:1095:LEU:O	2:C:1096:ALA:C	2.64	0.41
2:C:1105:LYS:HD2	2:C:1107:ASN:HD21	1.86	0.41
2:C:1111:ILE:HG13	2:C:1112:PHE:N	2.29	0.41
3:D:168:THR:O	3:D:393:ILE:N	2.52	0.41
3:D:400:VAL:HG21	3:D:441:ARG:NH1	2.28	0.41
3:D:578:VAL:O	3:D:582:LEU:HD12	2.21	0.41
3:D:614:PHE:HB3	9:D:9835:HOH:O	2.20	0.41
3:D:1303:TYR:CD1	3:D:1325:LEU:HD23	2.56	0.41
1:K:28:LEU:HD11	1:K:36:LEU:HD12	2.02	0.41
1:K:208:LEU:O	1:K:211:LEU:HB3	2.21	0.41
1:L:23:PHE:HZ	1:L:207:PRO:HB2	1.86	0.41
2:M:172:ILE:HD12	2:M:172:ILE:H	1.84	0.41
2:M:367:LEU:HA	2:M:371:LYS:HB2	2.03	0.41
2:M:374:ASN:ND2	2:M:377:PRO:HD3	2.36	0.41
2:M:512:ARG:HA	9:M:2109:HOH:O	2.20	0.41
2:M:872:ASN:OD1	2:M:873:PRO:HD2	2.20	0.41
2:M:1032:PHE:CD2	2:M:1052:MET:HG2	2.56	0.41
3:N:171:LEU:HD13	3:N:389:GLU:C	2.46	0.41
3:N:176:ASP:HB2	9:N:2270:HOH:O	2.19	0.41
3:N:603:LEU:O	3:N:607:LEU:HD12	2.20	0.41
3:N:637:LEU:CD1	3:N:641:GLN:HB2	2.50	0.41
3:N:943:THR:HA	9:N:9516:HOH:O	2.20	0.41
4:O:72:ARG:N	9:O:3347:HOH:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:151:LEU:HB2	5:P:155:THR:H	1.86	0.41
5:P:377:ASP:O	5:P:378:GLY:C	2.64	0.41
1:A:30:ARG:CZ	1:A:191:ASP:HB2	2.50	0.41
1:A:59:GLU:CD	1:A:139:ASN:ND2	2.79	0.41
1:A:72:LYS:HA	2:C:608:GLY:CA	2.50	0.41
1:B:81:ASN:ND2	1:B:128:HIS:O	2.54	0.41
1:B:156:HIS:CE1	1:B:158:ILE:H	2.39	0.41
2:C:48:PHE:HE2	9:C:9738:HOH:O	2.03	0.41
2:C:66:LEU:HD13	2:C:100:LEU:HB2	2.03	0.41
2:C:399:ASN:N	2:C:399:ASN:ND2	2.66	0.41
2:C:504:GLU:HB2	2:C:507:ARG:HB2	2.01	0.41
2:C:509:ALA:HB1	9:C:9815:HOH:O	2.21	0.41
2:C:710:ILE:HD11	2:C:758:ARG:HH21	1.84	0.41
2:C:945:ARG:O	2:C:948:GLU:HG3	2.20	0.41
2:C:957:LYS:NZ	9:C:2373:HOH:O	2.53	0.41
2:C:1083:GLU:O	2:C:1087:VAL:HB	2.21	0.41
3:D:95:LEU:CD1	3:D:517:VAL:HG23	2.51	0.41
3:D:1362:LYS:HD3	3:D:1362:LYS:HA	1.93	0.41
4:E:93:TYR:HA	4:E:94:PRO:HD3	1.80	0.41
5:F:273:ARG:HG2	5:F:276:ARG:NH1	2.35	0.41
5:F:278:LEU:HB3	5:F:286:PRO:HG2	2.03	0.41
5:F:409:LYS:HG3	5:F:410:TYR:N	2.35	0.41
1:K:127:LEU:HD12	1:K:128:HIS:N	2.35	0.41
1:K:185:ARG:HD3	9:K:4032:HOH:O	2.21	0.41
1:L:29:GLU:OE2	1:L:189:ARG:NH2	2.53	0.41
1:L:176:ARG:NH2	3:N:884:ARG:NE	2.69	0.41
2:M:31:GLN:O	2:M:34:VAL:HG23	2.21	0.41
2:M:290:LEU:HD23	2:M:290:LEU:H	1.86	0.41
2:M:627:ARG:HA	9:M:9521:HOH:O	2.19	0.41
2:M:707:ARG:HH11	2:M:824:ARG:CG	2.33	0.41
2:M:775:ARG:NH1	5:P:423:ASP:O	2.54	0.41
2:M:1025:ALA:HA	9:M:9518:HOH:O	2.20	0.41
3:N:92:HIS:HA	3:N:519:VAL:HG23	2.02	0.41
3:N:462:GLN:HE21	3:N:513:ILE:CD1	2.34	0.41
3:N:639:LEU:HD12	3:N:729:HIS:NE2	2.35	0.41
3:N:668:PRO:HD2	3:N:672:ALA:CB	2.50	0.41
3:N:838:ARG:HH11	3:N:874:GLU:HB3	1.84	0.41
3:N:956:ILE:HD13	3:N:960:LYS:NZ	2.36	0.41
5:P:370:LYS:NZ	5:P:370:LYS:HB3	2.36	0.41
1:A:150:TYR:CD1	2:C:696:LYS:HG2	2.55	0.41
1:B:22:GLU:HG2	1:B:198:ARG:CG	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:LEU:HD23	1:B:48:ILE:HD12	2.03	0.41
1:B:45:LEU:HD21	1:B:177:VAL:HG13	2.02	0.41
1:B:101:LEU:HG	1:B:113:ASP:C	2.45	0.41
1:B:165:ILE:HG12	9:B:9537:HOH:O	2.20	0.41
2:C:22:GLN:NE2	2:C:336:VAL:HG21	2.36	0.41
2:C:151:ASP:CG	2:C:152:PRO:HD2	2.45	0.41
2:C:347:GLY:HA2	9:C:9903:HOH:O	2.19	0.41
2:C:352:ALA:HA	2:C:355:VAL:CG1	2.50	0.41
2:C:355:VAL:HB	9:C:9756:HOH:O	2.20	0.41
2:C:376:ARG:HH22	5:F:285:GLU:CB	2.33	0.41
2:C:438:ILE:HG22	2:C:439:CYS:O	2.21	0.41
2:C:472:ARG:HD2	2:C:480:THR:O	2.21	0.41
2:C:759:THR:HA	9:C:9930:HOH:O	2.21	0.41
2:C:881:ASN:HD22	2:C:881:ASN:N	2.07	0.41
2:C:889:HIS:CD2	2:C:970:GLY:HA3	2.56	0.41
2:C:1008:ARG:HH21	2:C:1028:GLY:CA	2.32	0.41
3:D:101:HIS:CE1	3:D:582:LEU:HD13	2.56	0.41
3:D:482:LYS:HB3	3:D:483:HIS:ND1	2.36	0.41
3:D:553:ARG:HD3	9:F:9503:HOH:O	2.20	0.41
3:D:760:ARG:NH1	4:E:59:ASN:OD1	2.53	0.41
3:D:800:LYS:HG2	9:D:2552:HOH:O	2.20	0.41
3:D:847:ASP:HA	3:D:850:LEU:HD13	2.03	0.41
3:D:1046:GLN:HG2	3:D:1052:THR:HG22	2.03	0.41
5:F:215:GLU:HG3	5:F:250:ALA:CB	2.51	0.41
5:F:324:GLU:HA	9:F:9742:HOH:O	2.21	0.41
5:F:340:SER:O	5:F:341:PRO:C	2.64	0.41
1:K:86:VAL:HG12	1:K:124:ASN:HB2	2.02	0.41
1:K:227:ASN:H	1:K:227:ASN:ND2	2.07	0.41
2:M:18:LEU:HD22	2:M:590:ASP:HB2	2.02	0.41
2:M:195:LEU:O	2:M:199:VAL:HG23	2.20	0.41
2:M:374:ASN:HD21	2:M:377:PRO:HD3	1.85	0.41
2:M:418:LEU:O	2:M:419:THR:C	2.64	0.41
2:M:443:THR:OG1	2:M:444:PRO:HD2	2.19	0.41
2:M:1064:ASN:ND2	5:P:344:ALA:HB2	2.36	0.41
3:N:400:VAL:HA	3:N:442:ASN:O	2.20	0.41
3:N:534:ARG:HD2	5:P:315:VAL:CG2	2.51	0.41
3:N:694:VAL:HG22	9:N:2371:HOH:O	2.20	0.41
3:N:1053:PHE:HD2	9:N:9968:HOH:O	2.02	0.41
5:P:309:LYS:HA	5:P:312:GLN:NE2	2.35	0.41
5:P:328:PHE:HD2	5:P:328:PHE:HA	1.77	0.41
1:A:127:LEU:HD12	1:A:128:HIS:C	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:GLY:HA2	9:A:9515:HOH:O	2.20	0.41
1:A:156:HIS:HE1	1:A:167:VAL:O	2.03	0.41
1:A:184:THR:HG23	1:A:192:LEU:CB	2.49	0.41
1:B:12:THR:OG1	1:B:24:VAL:HB	2.21	0.41
1:B:88:ARG:C	1:B:88:ARG:HD3	2.46	0.41
1:B:103:ALA:HB1	1:B:107:LYS:CD	2.51	0.41
1:B:219:ARG:HD3	9:B:9524:HOH:O	2.20	0.41
2:C:29:ALA:HB2	2:C:337:GLY:HA2	2.01	0.41
2:C:127:PHE:HE1	2:C:386:PHE:HE2	1.68	0.41
2:C:129:ILE:HB	2:C:134:ARG:HG3	2.01	0.41
2:C:170:PRO:HG2	2:C:258:TYR:CD2	2.56	0.41
2:C:176:VAL:O	2:C:178:PRO:HD3	2.20	0.41
2:C:242:LEU:HD23	2:C:242:LEU:HA	1.92	0.41
2:C:267:TYR:HB2	2:C:272:ALA:CB	2.51	0.41
2:C:378:LEU:O	2:C:382:ILE:HG13	2.21	0.41
2:C:471:TYR:HD2	2:C:533:ASP:HA	1.85	0.41
2:C:575:GLN:C	2:C:667:ALA:HB1	2.46	0.41
2:C:593:ALA:HB1	2:C:658:GLY:HA3	2.02	0.41
2:C:597:ALA:O	2:C:652:GLY:N	2.54	0.41
2:C:670:GLN:HE22	2:C:699:PHE:C	2.29	0.41
2:C:745:ILE:HD12	9:C:2126:HOH:O	2.21	0.41
2:C:862:PRO:CG	2:C:975:TYR:HE1	2.34	0.41
2:C:881:ASN:ND2	2:C:881:ASN:N	2.69	0.41
2:C:1004:LYS:O	2:C:1005:MET:C	2.64	0.41
3:D:53:ILE:O	3:D:53:ILE:HG12	2.20	0.41
3:D:60:CYS:HA	9:D:2600:HOH:O	2.20	0.41
3:D:156:GLU:O	3:D:159:ARG:HB3	2.21	0.41
3:D:185:VAL:CG1	3:D:191:LEU:HD21	2.51	0.41
3:D:399:ARG:HG3	9:D:9991:HOH:O	2.21	0.41
3:D:441:ARG:O	3:D:443:VAL:HG23	2.21	0.41
3:D:653:PHE:CD1	3:D:653:PHE:N	2.86	0.41
3:D:704:ARG:CB	3:D:736:PHE:HB3	2.51	0.41
3:D:783:ARG:NE	3:D:1029:ARG:CZ	2.84	0.41
3:D:818:ARG:HD2	9:D:9809:HOH:O	2.20	0.41
3:D:890:VAL:HG13	3:D:926:LYS:HD3	2.03	0.41
3:D:967:ALA:HB2	9:D:2079:HOH:O	2.21	0.41
3:D:1047:LYS:HD2	3:D:1051:GLU:OE1	2.21	0.41
3:D:1060:SER:O	3:D:1063:GLU:O	2.39	0.41
3:D:1143:GLY:HA2	9:D:9689:HOH:O	2.20	0.41
3:D:1156:LEU:HD21	3:D:1177:ALA:HA	2.02	0.41
3:D:1299:PHE:N	3:D:1299:PHE:HD2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1383:ASP:HB2	3:D:1416:ALA:HB3	2.02	0.41
3:D:1438:ALA:N	3:D:1446:VAL:HG11	2.35	0.41
3:D:1480:PHE:HE2	9:E:9493:HOH:O	2.04	0.41
3:D:1481:VAL:C	3:D:1483:PHE:N	2.76	0.41
4:E:26:ARG:NH1	4:E:29:GLN:NE2	2.68	0.41
4:E:90:GLU:HB3	9:E:9562:HOH:O	2.20	0.41
5:F:74:LYS:HD3	5:F:74:LYS:HA	1.95	0.41
5:F:79:ASP:HB3	5:F:80:PRO:HD2	2.02	0.41
5:F:108:GLU:OE1	5:F:108:GLU:HA	2.20	0.41
5:F:227:PHE:CZ	5:F:229:TYR:HA	2.56	0.41
1:K:30:ARG:HG2	9:K:4745:HOH:O	2.21	0.41
1:K:69:PRO:C	1:K:71:VAL:H	2.29	0.41
1:K:102:LYS:HD2	9:K:3447:HOH:O	2.19	0.41
1:K:133:GLU:OE2	2:M:605:LYS:HB3	2.21	0.41
2:M:64:LEU:HD22	2:M:359:MET:SD	2.61	0.41
2:M:132:ALA:HA	9:M:2436:HOH:O	2.20	0.41
2:M:172:ILE:HA	2:M:185:LYS:O	2.20	0.41
2:M:492:ASP:HB3	2:M:518:LYS:HG2	2.02	0.41
2:M:798:GLY:HA3	2:M:828:ALA:O	2.20	0.41
2:M:808:ARG:HG2	2:M:808:ARG:NH1	2.35	0.41
2:M:854:PRO:O	2:M:856:GLU:N	2.54	0.41
2:M:911:GLU:O	2:M:914:ILE:HG22	2.21	0.41
2:M:917:LEU:HD12	9:M:2374:HOH:O	2.19	0.41
3:N:31:THR:HG21	3:N:527:MET:CE	2.51	0.41
3:N:44:LEU:HG	9:N:9808:HOH:O	2.19	0.41
3:N:115:LEU:CD1	3:N:499:VAL:HG22	2.51	0.41
3:N:178:LEU:HD11	9:N:9572:HOH:O	2.21	0.41
3:N:179:VAL:HG23	9:N:9797:HOH:O	2.21	0.41
3:N:223:LEU:N	3:N:365:ASP:O	2.50	0.41
3:N:413:ASP:OD1	3:N:419:ASP:HA	2.21	0.41
3:N:827:ILE:HB	3:N:828:LYS:HD3	2.02	0.41
3:N:891:GLU:CD	3:N:891:GLU:H	2.29	0.41
3:N:1031:ASN:O	3:N:1032:PRO:C	2.63	0.41
3:N:1106:VAL:HA	9:N:9633:HOH:O	2.21	0.41
3:N:1154:GLU:HG3	3:N:1159:ARG:HG2	2.02	0.41
3:N:1282:ARG:HA	3:N:1315:ASP:OD1	2.21	0.41
3:N:1348:LEU:O	3:N:1349:VAL:C	2.64	0.41
3:N:1462:LEU:CD2	3:N:1473:PRO:HD2	2.51	0.41
9:N:2443:HOH:O	5:P:337:HIS:HA	2.20	0.41
5:P:119:ILE:HD13	5:P:170:HIS:CG	2.56	0.41
5:P:337:HIS:H	5:P:337:HIS:HD2	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:409:LYS:HE3	5:P:410:TYR:HD1	1.85	0.41
2:C:51:THR:HG22	2:C:51:THR:O	2.21	0.41
2:C:91:GLN:HA	2:C:119:PRO:HA	2.03	0.41
2:C:264:PRO:HB3	2:C:289:THR:CG2	2.48	0.41
2:C:585:GLU:HB2	9:C:2332:HOH:O	2.21	0.41
2:C:601:GLY:HA3	2:C:615:TYR:HA	2.03	0.41
2:C:605:LYS:HG2	2:C:612:VAL:HB	2.03	0.41
2:C:660:ALA:O	2:C:667:ALA:HB3	2.21	0.41
2:C:722:ILE:HG23	2:C:805:ARG:NH2	2.36	0.41
2:C:878:SER:HB3	3:D:1029:ARG:NH1	2.35	0.41
2:C:958:THR:CG2	2:C:961:GLU:HG2	2.50	0.41
2:C:1039:ALA:HB2	3:D:707:THR:HG21	2.02	0.41
2:C:1067:TYR:CB	5:F:341:PRO:HB3	2.50	0.41
3:D:27:GLU:HG3	3:D:27:GLU:O	2.20	0.41
3:D:29:PRO:HG3	3:D:549:ASN:HD21	1.86	0.41
3:D:393:ILE:HD12	3:D:393:ILE:N	2.31	0.41
3:D:398:ALA:C	9:D:9991:HOH:O	2.62	0.41
3:D:606:ILE:O	3:D:613:ARG:HB2	2.21	0.41
3:D:629:SER:HB3	3:D:726:ILE:HD11	2.03	0.41
3:D:645:PRO:HB3	3:D:723:GLY:O	2.21	0.41
3:D:683:ILE:HD12	3:D:683:ILE:H	1.86	0.41
5:F:115:LYS:HD3	5:F:118:GLU:OE2	2.21	0.41
5:F:244:ARG:HB2	5:F:244:ARG:HH11	1.86	0.41
5:F:317:LEU:O	5:F:317:LEU:HD23	2.21	0.41
5:F:399:GLN:HB3	9:F:9591:HOH:O	2.19	0.41
5:F:408:LEU:HA	5:F:411:HIS:ND1	2.36	0.41
1:K:19:GLU:O	1:K:200:TRP:HA	2.20	0.41
1:K:185:ARG:HD2	1:K:185:ARG:O	2.21	0.41
2:M:78:PHE:CB	2:M:88:LEU:HD21	2.49	0.41
2:M:136:ILE:CG2	2:M:336:VAL:HG13	2.46	0.41
2:M:405:ARG:C	2:M:407:LYS:H	2.28	0.41
2:M:512:ARG:HD3	2:M:523:ILE:HD11	2.01	0.41
2:M:739:GLU:HG3	9:M:9499:HOH:O	2.21	0.41
9:M:9830:HOH:O	5:P:354:LEU:HD12	2.21	0.41
3:N:125:GLN:NE2	3:N:587:ARG:HH21	2.16	0.41
3:N:965:GLU:HB2	9:N:2437:HOH:O	2.19	0.41
3:N:1335:LEU:HD21	3:N:1343:ALA:CB	2.51	0.41
3:N:1425:THR:CG2	3:N:1426:LYS:H	2.33	0.41
3:N:1460:ILE:O	3:N:1464:GLU:CD	2.64	0.41
3:N:1503:VAL:HG13	9:N:2327:HOH:O	2.20	0.41
4:O:42:PRO:HD3	9:O:4549:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:73:LEU:N	9:O:3347:HOH:O	2.54	0.41
5:P:151:LEU:O	5:P:155:THR:HB	2.21	0.41
5:P:218:GLN:HA	5:P:221:ILE:CD1	2.52	0.41
1:A:150:TYR:CE2	1:A:152:PRO:HG3	2.55	0.40
1:B:89:PHE:HD1	1:B:120:VAL:HG13	1.85	0.40
1:B:191:ASP:OD1	1:B:191:ASP:N	2.55	0.40
2:C:252:LYS:HZ3	2:C:296:GLY:HA3	1.85	0.40
2:C:307:LEU:HG	2:C:311:PHE:CE2	2.56	0.40
2:C:333:ILE:HD11	2:C:467:ILE:HG13	2.02	0.40
2:C:396:ASP:O	2:C:403:SER:N	2.54	0.40
2:C:479:VAL:HG23	2:C:506:ASN:CA	2.51	0.40
2:C:571:LEU:C	2:C:573:ARG:N	2.78	0.40
2:C:1002:GLU:HA	2:C:1006:HIS:CE1	2.56	0.40
2:C:1033:GLY:O	2:C:1037:VAL:HG23	2.21	0.40
3:D:34:TYR:O	3:D:37:LEU:HD23	2.21	0.40
3:D:769:LEU:HD12	3:D:769:LEU:N	2.36	0.40
3:D:836:VAL:HA	3:D:839:LEU:HB2	2.04	0.40
3:D:912:LYS:HE3	9:D:2356:HOH:O	2.21	0.40
3:D:1120:VAL:HA	3:D:1121:PRO:HD3	1.84	0.40
3:D:1339:LYS:HB3	3:D:1343:ALA:CB	2.51	0.40
3:D:1393:GLN:CB	3:D:1398:TRP:HE1	2.33	0.40
4:E:36:LYS:HA	4:E:36:LYS:HD3	1.82	0.40
5:F:105:LYS:HE2	5:F:179:GLU:O	2.21	0.40
5:F:336:GLU:HB2	9:F:9817:HOH:O	2.21	0.40
1:K:46:SER:HA	9:K:5849:HOH:O	2.21	0.40
1:L:86:VAL:HG13	1:L:86:VAL:O	2.20	0.40
1:L:110:LYS:HB2	1:L:110:LYS:NZ	2.36	0.40
2:M:5:ARG:H	2:M:5:ARG:HG3	1.77	0.40
2:M:63:GLY:HA3	2:M:103:LYS:CG	2.51	0.40
2:M:276:LYS:H	2:M:276:LYS:CD	2.32	0.40
2:M:418:LEU:HD12	2:M:418:LEU:H	1.86	0.40
2:M:601:GLY:HA3	2:M:615:TYR:HA	2.02	0.40
2:M:654:LEU:HD21	2:M:657:ASP:OD2	2.20	0.40
2:M:900:ARG:NE	9:M:2073:HOH:O	2.54	0.40
2:M:922:PHE:CD2	2:M:964:LYS:HD3	2.57	0.40
2:M:1049:LEU:O	2:M:1053:LEU:HG	2.21	0.40
2:M:1105:LYS:O	2:M:1107:ASN:N	2.54	0.40
3:N:32:ILE:HG12	3:N:38:LYS:C	2.46	0.40
3:N:40:GLU:OE1	3:N:40:GLU:HA	2.21	0.40
3:N:53:ILE:HB	3:N:86:ARG:HD3	2.02	0.40
3:N:134:VAL:HG12	3:N:152:LEU:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:550:ARG:NE	9:N:9529:HOH:O	2.54	0.40
3:N:702:LEU:HD23	3:N:716:PHE:CD1	2.55	0.40
3:N:706:PRO:HA	9:N:9787:HOH:O	2.21	0.40
3:N:731:LEU:CD1	3:N:931:LEU:HB3	2.51	0.40
3:N:838:ARG:HG2	3:N:865:THR:OG1	2.22	0.40
3:N:881:LEU:HD12	9:N:9868:HOH:O	2.20	0.40
3:N:980:MET:HB3	3:N:982:PHE:CE1	2.56	0.40
3:N:1065:LEU:HD12	3:N:1066:THR:N	2.37	0.40
3:N:1171:VAL:O	3:N:1171:VAL:HG12	2.21	0.40
3:N:1346:ARG:HG2	9:N:9698:HOH:O	2.21	0.40
3:N:1362:LYS:HB3	9:N:9810:HOH:O	2.21	0.40
5:P:147:LEU:HG	9:P:3632:HOH:O	2.20	0.40
5:P:270:LYS:HB3	5:P:295:MET:HE3	2.04	0.40
5:P:409:LYS:HG3	5:P:410:TYR:N	2.35	0.40
1:A:150:TYR:HD1	2:C:696:LYS:HG2	1.87	0.40
1:A:179:PHE:HD2	9:A:9593:HOH:O	2.03	0.40
1:B:101:LEU:HB2	1:B:114:PHE:CE2	2.56	0.40
2:C:2:GLU:HG2	9:C:9602:HOH:O	2.21	0.40
2:C:70:GLU:N	9:C:9625:HOH:O	2.53	0.40
2:C:251:ASP:C	2:C:252:LYS:HD2	2.45	0.40
2:C:265:ARG:HD3	2:C:267:TYR:HB3	2.04	0.40
2:C:267:TYR:CD2	2:C:267:TYR:N	2.89	0.40
2:C:379:GLU:HG3	9:C:2275:HOH:O	2.20	0.40
2:C:605:LYS:CG	2:C:612:VAL:HB	2.52	0.40
2:C:1045:ALA:HB1	2:C:1048:THR:HB	2.03	0.40
2:C:1068:GLU:HG2	9:C:2111:HOH:O	2.21	0.40
2:C:1096:ALA:HB2	3:D:101:HIS:CD2	2.56	0.40
3:D:31:THR:HB	3:D:32:ILE:H	1.63	0.40
3:D:603:LEU:HA	3:D:606:ILE:HG13	2.03	0.40
3:D:1087:ARG:NH1	3:D:1234:THR:O	2.54	0.40
3:D:1254:GLN:HA	3:D:1254:GLN:OE1	2.21	0.40
5:F:370:LYS:HD2	5:F:370:LYS:C	2.47	0.40
1:K:34:VAL:HG23	9:K:3503:HOH:O	2.20	0.40
1:L:105:GLY:O	1:L:132:LEU:HB3	2.21	0.40
2:M:129:ILE:HD12	2:M:129:ILE:N	2.36	0.40
2:M:408:ARG:O	2:M:454:SER:HB2	2.21	0.40
2:M:449:ILE:C	2:M:451:LEU:HD12	2.46	0.40
2:M:547:ILE:HA	2:M:548:PRO:HD3	1.90	0.40
2:M:771:GLU:HB2	9:P:5420:HOH:O	2.21	0.40
2:M:942:GLU:O	2:M:945:ARG:HB3	2.21	0.40
3:N:463:GLN:HE21	3:N:463:GLN:HA	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:471:GLU:HG2	9:N:2578:HOH:O	2.21	0.40
3:N:502:PHE:CD1	3:N:509:PRO:HB3	2.56	0.40
3:N:809:PRO:O	3:N:812:ALA:HB3	2.21	0.40
3:N:849:ALA:O	3:N:853:VAL:HG23	2.21	0.40
3:N:927:THR:O	3:N:931:LEU:HG	2.21	0.40
3:N:1295:GLU:HB2	3:N:1300:SER:OG	2.22	0.40
3:N:1379:VAL:HA	3:N:1420:LEU:CB	2.50	0.40
5:P:421:PHE:C	5:P:423:ASP:N	2.78	0.40
2:C:140:ILE:H	2:C:140:ILE:HD12	1.86	0.40
2:C:192:PRO:C	2:C:194:VAL:H	2.29	0.40
2:C:258:TYR:HD2	9:C:2316:HOH:O	2.04	0.40
2:C:732:ALA:HB2	9:C:9752:HOH:O	2.21	0.40
2:C:746:GLY:C	2:C:799:ILE:HG22	2.46	0.40
2:C:1037:VAL:HG13	2:C:1049:LEU:HD11	2.02	0.40
2:C:1039:ALA:HB2	3:D:707:THR:CG2	2.51	0.40
2:C:1043:TYR:C	2:C:1045:ALA:H	2.29	0.40
2:C:1055:LEU:CD2	2:C:1079:PRO:HG3	2.51	0.40
2:C:1115:LEU:HD23	3:D:85:VAL:HG13	2.03	0.40
3:D:671:LYS:N	9:D:9547:HOH:O	2.46	0.40
3:D:770:LEU:HB2	3:D:1210:SER:O	2.21	0.40
3:D:919:PHE:C	3:D:919:PHE:CD2	2.98	0.40
3:D:929:ARG:HB3	9:D:2176:HOH:O	2.21	0.40
3:D:1148:VAL:HG21	3:D:1203:LYS:HA	2.03	0.40
3:D:1264:GLU:HG2	3:D:1266:ARG:HH21	1.86	0.40
3:D:1432:LYS:CG	3:D:1433:SER:N	2.83	0.40
5:F:403:LYS:HA	5:F:403:LYS:HZ2	1.84	0.40
1:K:106:PRO:HB3	9:K:3754:HOH:O	2.20	0.40
1:K:152:PRO:HB3	2:M:832:LYS:NZ	2.36	0.40
1:L:30:ARG:HH11	1:L:30:ARG:HG2	1.86	0.40
2:M:109:LYS:HE2	9:M:2096:HOH:O	2.21	0.40
2:M:163:ILE:HB	2:M:171:TRP:CZ2	2.56	0.40
2:M:200:LEU:HD22	2:M:300:ASP:OD1	2.21	0.40
2:M:212:GLY:HA3	2:M:218:VAL:CG2	2.49	0.40
2:M:642:ARG:HH11	2:M:642:ARG:HG2	1.86	0.40
2:M:693:GLU:HA	2:M:693:GLU:OE1	2.21	0.40
2:M:1002:GLU:HG3	2:M:1002:GLU:H	1.57	0.40
3:N:8:VAL:HG12	3:N:9:ARG:N	2.37	0.40
3:N:87:ARG:HD2	3:N:88:TYR:HE2	1.86	0.40
3:N:823:LEU:HD23	3:N:823:LEU:N	2.36	0.40
3:N:866:VAL:HG12	3:N:867:ARG:N	2.37	0.40
3:N:1043:GLY:N	9:N:9654:HOH:O	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1192:LEU:HD13	3:N:1345:GLU:HB3	2.03	0.40
3:N:1264:GLU:HG2	3:N:1266:ARG:CZ	2.51	0.40
3:N:1344:VAL:O	3:N:1345:GLU:C	2.64	0.40
5:P:155:THR:HG22	5:P:156:VAL:N	2.35	0.40
1:A:19:GLU:O	1:A:200:TRP:HA	2.21	0.40
2:C:34:VAL:HB	2:C:38:LYS:HG3	2.02	0.40
2:C:54:ILE:HG12	2:C:56:GLU:HG2	2.03	0.40
2:C:209:ARG:NH2	2:C:222:MET:HE1	2.37	0.40
2:C:864:GLY:C	9:C:9519:HOH:O	2.64	0.40
2:C:916:GLU:O	2:C:919:ALA:HB3	2.22	0.40
2:C:1051:GLU:HG2	2:C:1056:LYS:HD2	2.03	0.40
2:C:1069:ALA:HA	9:C:2111:HOH:O	2.21	0.40
3:D:598:ARG:HD3	5:F:320:PRO:HD3	2.03	0.40
3:D:742:GLY:HA3	9:D:9931:HOH:O	2.22	0.40
3:D:1000:THR:CG2	3:D:1001:GLU:N	2.84	0.40
3:D:1037:GLN:OE1	3:D:1042:ARG:NE	2.53	0.40
3:D:1066:THR:HG22	3:D:1069:GLU:H	1.86	0.40
3:D:1238:MET:CE	3:D:1257:PRO:HG3	2.50	0.40
3:D:1258:ARG:HE	3:D:1351:GLU:HG3	1.86	0.40
5:F:85:LEU:HA	9:F:9492:HOH:O	2.21	0.40
5:F:163:LEU:HB3	5:F:174:LEU:CG	2.50	0.40
5:F:343:ASP:O	5:F:346:THR:HB	2.21	0.40
1:K:23:PHE:HB2	1:K:197:LEU:HD23	2.03	0.40
2:M:126:SER:HB3	2:M:395:LYS:NZ	2.37	0.40
2:M:230:ARG:HA	2:M:231:PRO:HD3	1.80	0.40
2:M:323:ASP:HA	9:M:9868:HOH:O	2.21	0.40
2:M:410:ILE:HD12	2:M:410:ILE:N	2.37	0.40
2:M:520:GLU:HA	2:M:521:PRO:HD3	1.80	0.40
2:M:602:GLU:HB3	9:M:9999:HOH:O	2.21	0.40
2:M:1030:GLN:CB	3:N:626:SER:HB2	2.52	0.40
2:M:1046:ALA:HB3	3:N:1476:THR:HG22	2.02	0.40
3:N:210:ARG:O	3:N:394:LEU:O	2.40	0.40
3:N:562:ALA:HB1	3:N:567:ILE:HD11	2.02	0.40
3:N:602:SER:O	3:N:603:LEU:C	2.63	0.40
3:N:861:GLN:N	3:N:861:GLN:CD	2.80	0.40
3:N:867:ARG:NH1	9:N:9942:HOH:O	2.54	0.40
3:N:1161:GLU:HG2	3:N:1164:ARG:HB2	2.02	0.40
3:N:1166:LEU:HD12	3:N:1171:VAL:CG2	2.50	0.40
3:N:1209:LEU:C	3:N:1211:MET:N	2.79	0.40
3:N:1223:ILE:O	3:N:1224:VAL:C	2.65	0.40
5:P:210:LEU:HA	5:P:213:ILE:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:215:GLU:OE2	5:P:254:GLN:NE2	2.53	0.40
5:P:408:LEU:HA	5:P:411:HIS:CE1	2.55	0.40
2:C:271:GLU:C	2:C:273:GLY:N	2.79	0.40
2:C:527:GLU:HB3	9:C:9801:HOH:O	2.21	0.40
2:C:971:LYS:HB3	2:C:987:ILE:C	2.47	0.40
2:C:1013:TYR:CZ	2:C:1063:ARG:NE	2.89	0.40
2:C:1016:ILE:CD1	3:D:526:PRO:HG2	2.52	0.40
3:D:3:LYS:CD	3:D:3:LYS:H	2.34	0.40
3:D:52:PRO:HG3	3:D:78:VAL:HG13	2.03	0.40
3:D:169:TYR:HA	3:D:392:SER:CB	2.52	0.40
3:D:396:VAL:HG22	9:D:9613:HOH:O	2.20	0.40
3:D:566:ILE:HG13	5:F:192:LEU:HD11	2.04	0.40
3:D:704:ARG:HB2	3:D:736:PHE:HB3	2.02	0.40
3:D:773:ALA:HB2	3:D:1228:SER:HB3	2.04	0.40
3:D:1171:VAL:O	3:D:1171:VAL:HG12	2.21	0.40
3:D:1362:LYS:HB3	9:D:9652:HOH:O	2.22	0.40
3:D:1423:GLY:O	3:D:1426:LYS:N	2.54	0.40
3:D:1497:GLU:OE1	3:D:1500:LYS:HD2	2.22	0.40
4:E:17:TYR:N	4:E:17:TYR:HD2	2.17	0.40
5:F:194:LEU:CD2	5:F:194:LEU:H	2.34	0.40
5:F:373:LYS:HD3	5:F:378:GLY:C	2.46	0.40
1:K:38:ASN:ND2	1:K:38:ASN:C	2.79	0.40
1:K:217:ILE:HG13	1:K:217:ILE:H	1.70	0.40
1:L:152:PRO:HG2	3:N:857:ILE:HD12	2.03	0.40
2:M:44:ILE:HA	9:M:2405:HOH:O	2.22	0.40
2:M:285:LEU:HG	2:M:287:GLY:O	2.21	0.40
2:M:728:HIS:HE1	2:M:775:ARG:HH12	1.68	0.40
2:M:979:THR:HG23	2:M:981:GLU:N	2.19	0.40
3:N:172:PRO:HA	3:N:173:PRO:HD3	1.66	0.40
3:N:429:SER:C	9:N:2567:HOH:O	2.64	0.40
3:N:956:ILE:HD13	3:N:960:LYS:HZ3	1.86	0.40
3:N:1115:THR:C	9:N:2569:HOH:O	2.65	0.40
3:N:1280:VAL:HG12	3:N:1281:VAL:H	1.86	0.40
3:N:1320:GLU:HG2	3:N:1339:LYS:NZ	2.36	0.40
5:P:179:GLU:HG3	9:P:5874:HOH:O	2.21	0.40
5:P:361:LEU:HD12	5:P:408:LEU:HG	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	227/315 (72%)	201 (88%)	21 (9%)	5 (2%)	5	9
1	B	227/315 (72%)	198 (87%)	23 (10%)	6 (3%)	4	7
1	K	227/315 (72%)	200 (88%)	23 (10%)	4 (2%)	6	12
1	L	227/315 (72%)	203 (89%)	20 (9%)	4 (2%)	6	12
2	C	1117/1119 (100%)	907 (81%)	157 (14%)	53 (5%)	2	2
2	M	1117/1119 (100%)	906 (81%)	158 (14%)	53 (5%)	2	2
3	D	1388/1524 (91%)	1108 (80%)	207 (15%)	73 (5%)	1	1
3	N	1388/1524 (91%)	1105 (80%)	208 (15%)	75 (5%)	1	1
4	E	93/99 (94%)	75 (81%)	15 (16%)	3 (3%)	3	4
4	O	93/99 (94%)	75 (81%)	15 (16%)	3 (3%)	3	4
5	F	341/423 (81%)	285 (84%)	38 (11%)	18 (5%)	1	1
5	P	341/423 (81%)	287 (84%)	38 (11%)	16 (5%)	2	2
All	All	6786/7590 (89%)	5550 (82%)	923 (14%)	313 (5%)	2	2

All (313) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	B	29	GLU
1	B	48	ILE
2	C	152	PRO
2	C	178	PRO
2	C	231	PRO
2	C	244	PRO
2	C	262	ALA
2	C	288	ARG
2	C	290	LEU
2	C	422	ARG
2	C	462	ASP

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Mol	Chain	Res	Type
2	C	465	GLY
2	C	548	PRO
2	C	680	ASP
2	C	864	GLY
2	C	908	GLY
2	C	1004	LYS
3	D	40	GLU
3	D	43	GLY
3	D	55	ASP
3	D	82	LYS
3	D	137	PRO
3	D	208	PRO
3	D	209	ARG
3	D	238	PRO
3	D	246	PRO
3	D	370	ALA
3	D	373	PRO
3	D	381	ALA
3	D	385	VAL
3	D	440	VAL
3	D	504	ASP
3	D	705	ALA
3	D	766	ALA
3	D	832	ARG
3	D	844	ALA
3	D	1028	ALA
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	147	LEU
5	F	153	PRO
5	F	324	GLU
5	F	341	PRO
5	F	390	PHE
1	K	29	GLU
1	L	29	GLU
2	M	152	PRO
2	M	178	PRO
2	M	231	PRO

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Mol	Chain	Res	Type
2	M	244	PRO
2	M	261	ILE
2	M	262	ALA
2	M	288	ARG
2	M	290	LEU
2	M	422	ARG
2	M	462	ASP
2	M	465	GLY
2	M	680	ASP
2	M	864	GLY
2	M	908	GLY
3	N	40	GLU
3	N	43	GLY
3	N	55	ASP
3	N	82	LYS
3	N	137	PRO
3	N	208	PRO
3	N	209	ARG
3	N	217	LYS
3	N	238	PRO
3	N	246	PRO
3	N	370	ALA
3	N	373	PRO
3	N	381	ALA
3	N	385	VAL
3	N	440	VAL
3	N	504	ASP
3	N	705	ALA
3	N	766	ALA
3	N	832	ARG
3	N	844	ALA
3	N	1028	ALA
3	N	1125	PRO
3	N	1129	THR
3	N	1208	ASP
3	N	1243	THR
3	N	1441	GLN
4	O	42	PRO
4	O	58	PRO
5	P	147	LEU
5	P	153	PRO
5	P	324	GLU

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Mol	Chain	Res	Type
5	P	390	PHE
1	A	187	GLY
1	B	187	GLY
2	C	18	LEU
2	C	59	LYS
2	C	156	GLY
2	C	170	PRO
2	C	261	ILE
2	C	363	SER
2	C	369	PRO
2	C	626	ARG
2	C	627	ARG
2	C	1106	ASP
3	D	96	ALA
3	D	98	PRO
3	D	165	LYS
3	D	220	ARG
3	D	231	VAL
3	D	417	PRO
3	D	594	PRO
3	D	609	GLY
3	D	783	ARG
3	D	803	GLY
3	D	822	ALA
3	D	1020	LEU
4	E	53	GLY
5	F	326	ASP
1	K	187	GLY
1	L	187	GLY
2	M	59	LYS
2	M	156	GLY
2	M	363	SER
2	M	369	PRO
2	M	413	LEU
2	M	447	ALA
2	M	548	PRO
2	M	626	ARG
2	M	1106	ASP
3	N	31	THR
3	N	37	LEU
3	N	98	PRO
3	N	165	LYS

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Mol	Chain	Res	Type
3	N	220	ARG
3	N	417	PRO
3	N	594	PRO
3	N	609	GLY
3	N	783	ARG
3	N	803	GLY
3	N	822	ALA
4	O	53	GLY
5	P	326	ASP
5	P	341	PRO
1	A	106	PRO
1	A	188	GLN
1	B	106	PRO
2	C	74	GLY
2	C	164	PRO
2	C	251	ASP
2	C	273	GLY
2	C	447	ALA
2	C	517	ARG
2	C	727	PRO
2	C	783	ARG
2	C	1007	ALA
3	D	31	THR
3	D	37	LEU
3	D	120	ALA
3	D	170	PRO
3	D	424	GLY
3	D	451	ASP
3	D	1248	GLY
3	D	1286	THR
3	D	1349	VAL
5	F	288	TYR
5	F	420	ASP
1	L	106	PRO
2	M	74	GLY
2	M	164	PRO
2	M	170	PRO
2	M	251	ASP
2	M	423	ALA
2	M	517	ARG
2	M	529	VAL
2	M	627	ARG

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Mol	Chain	Res	Type
2	M	727	PRO
3	N	96	ALA
3	N	120	ALA
3	N	170	PRO
3	N	231	VAL
3	N	424	GLY
3	N	530	VAL
3	N	1338	ALA
3	N	1349	VAL
3	N	1389	LEU
5	P	232	ARG
5	P	288	TYR
5	P	420	ASP
2	C	180	GLY
2	C	400	PRO
2	C	413	LEU
2	C	781	LYS
2	C	1097	LEU
3	D	46	ASP
3	D	415	VAL
3	D	416	ALA
3	D	509	PRO
3	D	522	PRO
3	D	530	VAL
3	D	1338	ALA
3	D	1385	GLY
3	D	1389	LEU
5	F	232	ARG
5	F	286	PRO
5	F	297	PRO
5	F	329	TYR
5	F	393	THR
1	K	106	PRO
2	M	180	GLY
2	M	223	ASP
2	M	273	GLY
2	M	455	LEU
2	M	781	LYS
2	M	1007	ALA
2	M	1097	LEU
3	N	24	GLY
3	N	415	VAL

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Mol	Chain	Res	Type
3	N	416	ALA
3	N	451	ASP
3	N	509	PRO
3	N	522	PRO
3	N	782	SER
3	N	1019	PRO
3	N	1064	GLY
3	N	1248	GLY
3	N	1385	GLY
5	P	286	PRO
5	P	297	PRO
1	B	188	GLN
2	C	399	ASN
2	C	529	VAL
2	C	905	ILE
3	D	24	GLY
3	D	161	LEU
3	D	808	THR
3	D	1019	PRO
3	D	1064	GLY
3	D	1213	ARG
3	D	1241	PHE
3	D	1315	ASP
3	D	1379	VAL
5	F	97	GLU
5	F	416	ARG
2	M	18	LEU
3	N	161	LEU
3	N	533	GLY
3	N	808	THR
3	N	1241	PHE
3	N	1286	THR
3	N	1315	ASP
3	N	1341	PRO
5	P	184	ARG
5	P	393	THR
1	B	9	PRO
2	C	79	PRO
2	C	779	GLY
3	D	425	GLY
3	D	782	SER
3	D	1288	GLU

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Mol	Chain	Res	Type
5	F	167	PRO
5	F	293	GLU
2	M	79	PRO
2	M	705	ILE
2	M	779	GLY
2	M	1059	ASP
3	N	1213	ARG
3	N	1390	LEU
5	P	416	ARG
2	C	424	GLY
3	D	368	VAL
3	D	1306	PRO
1	K	9	PRO
2	M	399	ASN
3	N	368	VAL
3	N	425	GLY
5	P	167	PRO
1	A	9	PRO
2	C	1076	VAL
3	D	1446	VAL
1	L	9	PRO
2	M	646	GLY
3	N	173	PRO
3	N	1306	PRO
3	N	1379	VAL
3	N	1446	VAL
5	P	314	PRO
3	D	136	ASP
2	M	767	PRO
2	M	905	ILE
2	M	1076	VAL
2	C	53	PRO
2	C	835	VAL
3	D	173	PRO
3	D	781	PRO
2	M	17	PRO
2	M	415	PRO
3	N	136	ASP
3	N	169	TYR
3	N	1268	PRO
2	C	17	PRO
2	C	377	PRO

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Mol	Chain	Res	Type
2	C	646	GLY
2	C	767	PRO
3	D	526	PRO
5	F	314	PRO
2	M	377	PRO
2	C	166	PRO
2	M	166	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%)	156 (77%)	46 (23%)	1	1
1	B	202/273 (74%)	163 (81%)	39 (19%)	1	2
1	K	202/273 (74%)	161 (80%)	41 (20%)	1	2
1	L	202/273 (74%)	154 (76%)	48 (24%)	1	1
2	C	941/941 (100%)	708 (75%)	233 (25%)	1	1
2	M	941/941 (100%)	719 (76%)	222 (24%)	1	1
3	D	1123/1279 (88%)	851 (76%)	272 (24%)	1	1
3	N	1123/1279 (88%)	847 (75%)	276 (25%)	1	1
4	E	83/87 (95%)	62 (75%)	21 (25%)	0	1
4	O	83/87 (95%)	62 (75%)	21 (25%)	0	1
5	F	295/370 (80%)	228 (77%)	67 (23%)	1	1
5	P	295/370 (80%)	236 (80%)	59 (20%)	1	2
All	All	5692/6446 (88%)	4347 (76%)	1345 (24%)	1	1

All (1345) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	5	LYS
1	A	9	PRO

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Mol	Chain	Res	Type
1	A	12	THR
1	A	15	THR
1	A	26	GLU
1	A	34	VAL
1	A	44	LEU
1	A	45	LEU
1	A	47	SER
1	A	66	SER
1	A	73	GLU
1	A	74	ASP
1	A	86	VAL
1	A	96	THR
1	A	101	LEU
1	A	104	GLU
1	A	112	ARG
1	A	115	LEU
1	A	121	GLU
1	A	127	LEU
1	A	133	GLU
1	A	137	ARG
1	A	142	VAL
1	A	155	LYS
1	A	161	ARG
1	A	163	ASN
1	A	165	ILE
1	A	167	VAL
1	A	170	VAL
1	A	184	THR
1	A	186	LEU
1	A	188	GLN
1	A	190	THR
1	A	191	ASP
1	A	195	LEU
1	A	196	THR
1	A	197	LEU
1	A	198	ARG
1	A	205	VAL
1	A	206	THR
1	A	208	LEU
1	A	211	LEU
1	A	223	THR
1	A	227	ASN

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Mol	Chain	Res	Type
1	A	229	GLN
1	B	5	LYS
1	B	7	LYS
1	B	9	PRO
1	B	26	GLU
1	B	30	ARG
1	B	41	ARG
1	B	64	GLU
1	B	65	PHE
1	B	68	ILE
1	B	73	GLU
1	B	77	GLU
1	B	80	LEU
1	B	89	PHE
1	B	92	PRO
1	B	94	LEU
1	B	95	GLN
1	B	96	THR
1	B	101	LEU
1	B	110	LYS
1	B	121	GLU
1	B	124	ASN
1	B	128	HIS
1	B	133	GLU
1	B	140	MET
1	B	141	GLU
1	B	146	ARG
1	B	158	ILE
1	B	159	LYS
1	B	162	ILE
1	B	190	THR
1	B	194	LYS
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	229	GLN
2	C	1	MET
2	C	5	ARG

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Mol	Chain	Res	Type
2	C	8	ARG
2	C	9	ILE
2	C	10	ARG
2	C	20	GLU
2	C	22	GLN
2	C	26	TYR
2	C	30	LEU
2	C	31	GLN
2	C	34	VAL
2	C	37	GLU
2	C	41	ASN
2	C	48	PHE
2	C	49	ARG
2	C	81	ASP
2	C	82	GLU
2	C	87	ASP
2	C	95	TYR
2	C	98	LEU
2	C	99	GLN
2	C	100	LEU
2	C	103	LYS
2	C	104	ASP
2	C	105	THR
2	C	108	ILE
2	C	110	GLU
2	C	114	PHE
2	C	115	LEU
2	C	133	ASP
2	C	135	VAL
2	C	137	VAL
2	C	139	GLN
2	C	140	ILE
2	C	144	PRO
2	C	149	THR
2	C	150	PRO
2	C	152	PRO
2	C	157	ARG
2	C	158	TYR
2	C	161	SER
2	C	163	ILE
2	C	168	ARG
2	C	170	PRO

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Mol	Chain	Res	Type
2	C	172	ILE
2	C	178	PRO
2	C	179	ASN
2	C	194	VAL
2	C	196	LEU
2	C	205	GLU
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	250	ARG
2	C	252	LYS
2	C	254	VAL
2	C	257	VAL
2	C	260	LEU
2	C	267	TYR
2	C	268	ASP
2	C	279	GLU
2	C	285	LEU
2	C	286	SER
2	C	290	LEU
2	C	297	GLU
2	C	304	LEU
2	C	308	ARG
2	C	321	GLU
2	C	323	ASP
2	C	327	HIS
2	C	340	MET
2	C	343	GLN
2	C	350	ARG
2	C	357	GLU
2	C	359	MET
2	C	360	LEU
2	C	364	GLU
2	C	365	ASP
2	C	367	LEU
2	C	379	GLU
2	C	383	ARG
2	C	384	GLU

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Mol	Chain	Res	Type
2	C	392	SER
2	C	393	GLN
2	C	394	PHE
2	C	399	ASN
2	C	400	PRO
2	C	408	ARG
2	C	413	LEU
2	C	419	THR
2	C	420	ARG
2	C	422	ARG
2	C	426	ASP
2	C	432	ARG
2	C	443	THR
2	C	451	LEU
2	C	452	ILE
2	C	453	THR
2	C	474	VAL
2	C	479	VAL
2	C	482	GLU
2	C	486	MET
2	C	487	THR
2	C	496	ILE
2	C	502	PRO
2	C	503	LEU
2	C	508	ILE
2	C	517	ARG
2	C	524	VAL
2	C	527	GLU
2	C	533	ASP
2	C	537	LYS
2	C	542	VAL
2	C	548	PRO
2	C	554	ASP
2	C	559	LEU
2	C	564	MET
2	C	565	GLN
2	C	566	THR
2	C	584	GLU
2	C	589	ARG
2	C	620	LEU
2	C	621	VAL
2	C	622	GLU

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Mol	Chain	Res	Type
2	C	633	GLN
2	C	637	LEU
2	C	640	ARG
2	C	645	VAL
2	C	654	LEU
2	C	655	LEU
2	C	663	ASN
2	C	668	LEU
2	C	671	ASN
2	C	672	VAL
2	C	674	VAL
2	C	684	PHE
2	C	691	SER
2	C	693	GLU
2	C	698	ASP
2	C	699	PHE
2	C	705	ILE
2	C	708	TYR
2	C	714	ASP
2	C	722	ILE
2	C	724	ARG
2	C	725	ASP
2	C	727	PRO
2	C	730	SER
2	C	740	GLU
2	C	744	ARG
2	C	749	VAL
2	C	754	ILE
2	C	759	THR
2	C	768	THR
2	C	771	GLU
2	C	773	LEU
2	C	780	GLU
2	C	785	VAL
2	C	791	ARG
2	C	794	PRO
2	C	796	GLU
2	C	799	ILE
2	C	800	VAL
2	C	804	VAL
2	C	808	ARG
2	C	820	ARG

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Mol	Chain	Res	Type
2	C	821	GLU
2	C	829	GLN
2	C	832	LYS
2	C	834	GLN
2	C	835	VAL
2	C	839	LEU
2	C	841	ASN
2	C	852	ILE
2	C	853	LEU
2	C	858	MET
2	C	862	PRO
2	C	863	ASP
2	C	870	ILE
2	C	877	PRO
2	C	881	ASN
2	C	882	LEU
2	C	886	LEU
2	C	904	PRO
2	C	905	ILE
2	C	907	ASP
2	C	914	ILE
2	C	916	GLU
2	C	923	GLU
2	C	925	TYR
2	C	934	PHE
2	C	938	LYS
2	C	939	ARG
2	C	945	ARG
2	C	948	GLU
2	C	950	LEU
2	C	953	VAL
2	C	959	PRO
2	C	963	LEU
2	C	966	LEU
2	C	978	ARG
2	C	981	GLU
2	C	984	GLU
2	C	988	VAL
2	C	993	PHE
2	C	995	MET
2	C	1000	MET
2	C	1006	HIS

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Mol	Chain	Res	Type
2	C	1008	ARG
2	C	1016	ILE
2	C	1018	GLN
2	C	1019	GLN
2	C	1021	LEU
2	C	1026	GLN
2	C	1035	MET
2	C	1052	MET
2	C	1054	THR
2	C	1060	ILE
2	C	1074	GLU
2	C	1076	VAL
2	C	1081	VAL
2	C	1082	PRO
2	C	1083	GLU
2	C	1087	VAL
2	C	1092	LEU
2	C	1098	ASP
2	C	1103	ASP
2	C	1106	ASP
2	C	1109	VAL
3	D	3	LYS
3	D	5	VAL
3	D	6	ARG
3	D	9	ARG
3	D	12	LEU
3	D	14	SER
3	D	15	PRO
3	D	16	GLU
3	D	25	GLU
3	D	27	GLU
3	D	28	LYS
3	D	29	PRO
3	D	31	THR
3	D	41	ARG
3	D	42	ASP
3	D	47	GLU
3	D	53	ILE
3	D	55	ASP
3	D	56	TYR
3	D	58	CYS
3	D	62	LYS

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Mol	Chain	Res	Type
3	D	71	LYS
3	D	76	CYS
3	D	80	VAL
3	D	82	LYS
3	D	85	VAL
3	D	86	ARG
3	D	87	ARG
3	D	89	ARG
3	D	95	LEU
3	D	97	THR
3	D	101	HIS
3	D	102	ILE
3	D	112	ILE
3	D	115	LEU
3	D	117	ASP
3	D	118	LEU
3	D	122	GLU
3	D	127	LEU
3	D	133	ILE
3	D	143	ASN
3	D	145	VAL
3	D	150	ARG
3	D	153	LEU
3	D	155	ASP
3	D	156	GLU
3	D	162	ARG
3	D	166	GLN
3	D	170	PRO
3	D	171	LEU
3	D	185	VAL
3	D	199	LEU
3	D	205	TYR
3	D	208	PRO
3	D	209	ARG
3	D	211	VAL
3	D	389	GLU
3	D	393	ILE
3	D	394	LEU
3	D	395	VAL
3	D	404	GLU
3	D	405	ASP
3	D	411	THR

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Mol	Chain	Res	Type
3	D	413	ASP
3	D	421	LEU
3	D	427	VAL
3	D	432	TYR
3	D	444	VAL
3	D	445	ARG
3	D	447	VAL
3	D	452	ILE
3	D	456	MET
3	D	459	GLU
3	D	473	LEU
3	D	475	LYS
3	D	478	LEU
3	D	481	MET
3	D	483	HIS
3	D	486	ARG
3	D	488	ARG
3	D	491	LYS
3	D	504	ASP
3	D	513	ILE
3	D	521	PRO
3	D	528	VAL
3	D	529	GLN
3	D	535	PHE
3	D	537	THR
3	D	540	LEU
3	D	542	ASP
3	D	554	LEU
3	D	565	ILE
3	D	569	ASN
3	D	571	LYS
3	D	576	GLU
3	D	584	ASN
3	D	590	PRO
3	D	594	PRO
3	D	600	LEU
3	D	618	LEU
3	D	636	GLN
3	D	639	LEU
3	D	641	GLN
3	D	651	GLU
3	D	661	MET

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Mol	Chain	Res	Type
3	D	675	ARG
3	D	676	MET
3	D	682	ASP
3	D	687	VAL
3	D	695	ILE
3	D	702	LEU
3	D	704	ARG
3	D	713	ILE
3	D	716	PHE
3	D	719	VAL
3	D	724	GLN
3	D	739	ASP
3	D	749	VAL
3	D	764	LEU
3	D	770	LEU
3	D	780	LYS
3	D	781	PRO
3	D	792	ILE
3	D	793	THR
3	D	794	GLN
3	D	796	ARG
3	D	797	LYS
3	D	800	LYS
3	D	805	GLU
3	D	810	GLU
3	D	813	LEU
3	D	824	ASN
3	D	828	LYS
3	D	829	VAL
3	D	832	ARG
3	D	836	VAL
3	D	838	ARG
3	D	839	LEU
3	D	851	LEU
3	D	862	ASP
3	D	863	VAL
3	D	864	VAL
3	D	865	THR
3	D	867	ARG
3	D	879	ARG
3	D	880	ILE
3	D	888	GLU

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Mol	Chain	Res	Type
3	D	891	GLU
3	D	902	LEU
3	D	910	SER
3	D	914	LEU
3	D	915	VAL
3	D	917	GLN
3	D	922	LEU
3	D	927	THR
3	D	929	ARG
3	D	944	THR
3	D	951	ILE
3	D	952	ASP
3	D	953	ASP
3	D	957	PRO
3	D	959	GLU
3	D	961	LYS
3	D	968	ASP
3	D	970	LYS
3	D	972	LEU
3	D	985	ASP
3	D	987	GLU
3	D	999	THR
3	D	1001	GLU
3	D	1003	VAL
3	D	1026	SER
3	D	1029	ARG
3	D	1032	PRO
3	D	1041	LEU
3	D	1042	ARG
3	D	1051	GLU
3	D	1058	ARG
3	D	1060	SER
3	D	1065	LEU
3	D	1068	LEU
3	D	1079	LYS
3	D	1087	ARG
3	D	1095	THR
3	D	1096	ARG
3	D	1109	GLU
3	D	1112	CYS
3	D	1116	ASN
3	D	1127	GLU

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Mol	Chain	Res	Type
3	D	1132	LEU
3	D	1135	ARG
3	D	1139	ASP
3	D	1144	LEU
3	D	1151	ARG
3	D	1160	LEU
3	D	1161	GLU
3	D	1164	ARG
3	D	1166	LEU
3	D	1167	SER
3	D	1173	LEU
3	D	1176	LYS
3	D	1183	ILE
3	D	1188	VAL
3	D	1195	GLN
3	D	1207	TYR
3	D	1209	LEU
3	D	1211	MET
3	D	1215	VAL
3	D	1223	ILE
3	D	1227	GLN
3	D	1231	GLU
3	D	1238	MET
3	D	1242	HIS
3	D	1243	THR
3	D	1251	ASP
3	D	1258	ARG
3	D	1259	VAL
3	D	1260	ILE
3	D	1264	GLU
3	D	1267	ARG
3	D	1269	LYS
3	D	1274	ILE
3	D	1276	GLU
3	D	1288	GLU
3	D	1290	LEU
3	D	1299	PHE
3	D	1305	LEU
3	D	1306	PRO
3	D	1307	LYS
3	D	1314	LYS
3	D	1317	ASP

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Mol	Chain	Res	Type
3	D	1331	ASP
3	D	1337	GLU
3	D	1344	VAL
3	D	1345	GLU
3	D	1346	ARG
3	D	1348	LEU
3	D	1350	GLU
3	D	1353	GLN
3	D	1359	GLN
3	D	1363	LEU
3	D	1365	ASP
3	D	1368	ILE
3	D	1376	MET
3	D	1378	TYR
3	D	1382	THR
3	D	1387	SER
3	D	1389	LEU
3	D	1401	GLU
3	D	1403	LEU
3	D	1415	VAL
3	D	1419	PRO
3	D	1420	LEU
3	D	1421	LEU
3	D	1424	VAL
3	D	1435	LEU
3	D	1440	PHE
3	D	1447	LEU
3	D	1452	ILE
3	D	1455	LYS
3	D	1456	LYS
3	D	1460	ILE
3	D	1462	LEU
3	D	1463	LYS
3	D	1465	ASN
3	D	1466	VAL
3	D	1479	ASP
3	D	1481	VAL
3	D	1485	GLN
3	D	1488	ASP
3	D	1496	GLU
3	D	1501	GLU
4	E	12	MET

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Mol	Chain	Res	Type
4	E	14	ASP
4	E	20	THR
4	E	28	GLN
4	E	29	GLN
4	E	30	LEU
4	E	31	LEU
4	E	33	HIS
4	E	40	LEU
4	E	42	PRO
4	E	43	GLU
4	E	45	ARG
4	E	56	ASP
4	E	57	ASP
4	E	59	ASN
4	E	61	GLU
4	E	66	LYS
4	E	67	GLU
4	E	81	PRO
4	E	84	ARG
4	E	87	LYS
5	F	83	GLN
5	F	84	TYR
5	F	86	HIS
5	F	90	GLN
5	F	91	VAL
5	F	97	GLU
5	F	101	GLU
5	F	111	GLU
5	F	125	ASP
5	F	126	LEU
5	F	127	ILE
5	F	135	ILE
5	F	136	LEU
5	F	142	ARG
5	F	145	PRO
5	F	149	GLU
5	F	154	LYS
5	F	164	LYS
5	F	170	HIS
5	F	174	LEU
5	F	176	ILE
5	F	181	GLU

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Mol	Chain	Res	Type
5	F	184	ARG
5	F	186	HIS
5	F	187	LEU
5	F	192	LEU
5	F	203	THR
5	F	207	LEU
5	F	208	SER
5	F	234	LYS
5	F	240	THR
5	F	244	ARG
5	F	245	GLN
5	F	260	ILE
5	F	261	PRO
5	F	264	MET
5	F	280	GLN
5	F	282	LEU
5	F	290	GLU
5	F	295	MET
5	F	297	PRO
5	F	302	LYS
5	F	310	ILE
5	F	313	GLU
5	F	328	PHE
5	F	331	ASP
5	F	336	GLU
5	F	337	HIS
5	F	340	SER
5	F	341	PRO
5	F	342	VAL
5	F	347	GLN
5	F	349	LEU
5	F	355	GLU
5	F	363	GLU
5	F	365	GLU
5	F	370	LYS
5	F	392	VAL
5	F	393	THR
5	F	396	ARG
5	F	399	GLN
5	F	403	LYS
5	F	406	ARG
5	F	408	LEU

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Mol	Chain	Res	Type
5	F	410	TYR
5	F	414	ARG
5	F	422	LEU
1	K	5	LYS
1	K	9	PRO
1	K	12	THR
1	K	18	ARG
1	K	19	GLU
1	K	26	GLU
1	K	29	GLU
1	K	44	LEU
1	K	54	THR
1	K	60	ASP
1	K	62	LEU
1	K	67	THR
1	K	71	VAL
1	K	73	GLU
1	K	79	ILE
1	K	84	GLU
1	K	89	PHE
1	K	90	LEU
1	K	92	PRO
1	K	94	LEU
1	K	101	LEU
1	K	112	ARG
1	K	115	LEU
1	K	121	GLU
1	K	127	LEU
1	K	142	VAL
1	K	146	ARG
1	K	165	ILE
1	K	167	VAL
1	K	180	GLN
1	K	184	THR
1	K	186	LEU
1	K	196	THR
1	K	197	LEU
1	K	198	ARG
1	K	206	THR
1	K	211	LEU
1	K	216	GLU
1	K	219	ARG

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Mol	Chain	Res	Type
1	K	223	THR
1	K	227	ASN
1	L	1	MET
1	L	2	LEU
1	L	4	SER
1	L	5	LYS
1	L	7	LYS
1	L	9	PRO
1	L	24	VAL
1	L	26	GLU
1	L	29	GLU
1	L	38	ASN
1	L	41	ARG
1	L	47	SER
1	L	55	SER
1	L	62	LEU
1	L	69	PRO
1	L	73	GLU
1	L	77	GLU
1	L	80	LEU
1	L	88	ARG
1	L	89	PHE
1	L	92	PRO
1	L	94	LEU
1	L	95	GLN
1	L	100	LEU
1	L	101	LEU
1	L	108	GLU
1	L	112	ARG
1	L	121	GLU
1	L	123	MET
1	L	126	ASP
1	L	138	LEU
1	L	141	GLU
1	L	159	LYS
1	L	160	ASP
1	L	167	VAL
1	L	177	VAL
1	L	181	VAL
1	L	182	GLU
1	L	190	THR
1	L	191	ASP

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Mol	Chain	Res	Type
1	L	192	LEU
1	L	197	LEU
1	L	201	THR
1	L	204	SER
1	L	206	THR
1	L	208	LEU
1	L	213	GLN
1	L	220	GLU
2	M	4	LYS
2	M	5	ARG
2	M	10	ARG
2	M	22	GLN
2	M	30	LEU
2	M	31	GLN
2	M	33	ASP
2	M	34	VAL
2	M	48	PHE
2	M	49	ARG
2	M	51	THR
2	M	71	TYR
2	M	79	PRO
2	M	82	GLU
2	M	86	LYS
2	M	91	GLN
2	M	95	TYR
2	M	98	LEU
2	M	99	GLN
2	M	100	LEU
2	M	102	HIS
2	M	104	ASP
2	M	105	THR
2	M	107	LEU
2	M	108	ILE
2	M	110	GLU
2	M	114	PHE
2	M	115	LEU
2	M	133	ASP
2	M	134	ARG
2	M	140	ILE
2	M	143	SER
2	M	149	THR
2	M	152	PRO

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Mol	Chain	Res	Type
2	M	157	ARG
2	M	158	TYR
2	M	163	ILE
2	M	167	LYS
2	M	168	ARG
2	M	178	PRO
2	M	182	VAL
2	M	184	MET
2	M	189	ARG
2	M	193	LEU
2	M	194	VAL
2	M	198	ARG
2	M	209	ARG
2	M	211	LEU
2	M	218	VAL
2	M	221	LEU
2	M	222	MET
2	M	230	ARG
2	M	235	LEU
2	M	237	ARG
2	M	238	LEU
2	M	239	PHE
2	M	243	ARG
2	M	252	LYS
2	M	254	VAL
2	M	260	LEU
2	M	267	TYR
2	M	276	LYS
2	M	279	GLU
2	M	285	LEU
2	M	290	LEU
2	M	295	ASP
2	M	297	GLU
2	M	304	LEU
2	M	309	TYR
2	M	321	GLU
2	M	322	VAL
2	M	328	LEU
2	M	345	ARG
2	M	348	LEU
2	M	351	LEU
2	M	359	MET

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Mol	Chain	Res	Type
2	M	360	LEU
2	M	365	ASP
2	M	367	LEU
2	M	368	THR
2	M	371	LYS
2	M	374	ASN
2	M	384	GLU
2	M	393	GLN
2	M	397	GLU
2	M	413	LEU
2	M	415	PRO
2	M	420	ARG
2	M	422	ARG
2	M	426	ASP
2	M	427	VAL
2	M	430	VAL
2	M	443	THR
2	M	451	LEU
2	M	452	ILE
2	M	455	LEU
2	M	460	ARG
2	M	468	ARG
2	M	469	THR
2	M	474	VAL
2	M	479	VAL
2	M	480	THR
2	M	482	GLU
2	M	486	MET
2	M	496	ILE
2	M	500	ASN
2	M	503	LEU
2	M	507	ARG
2	M	514	VAL
2	M	523	ILE
2	M	524	VAL
2	M	538	GLN
2	M	540	PHE
2	M	542	VAL
2	M	545	ASN
2	M	546	LEU
2	M	563	ASN
2	M	564	MET

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Mol	Chain	Res	Type
2	M	571	LEU
2	M	579	VAL
2	M	583	LEU
2	M	584	GLU
2	M	586	ARG
2	M	588	VAL
2	M	589	ARG
2	M	590	ASP
2	M	595	LEU
2	M	599	GLU
2	M	603	VAL
2	M	605	LYS
2	M	607	ASP
2	M	620	LEU
2	M	626	ARG
2	M	627	ARG
2	M	633	GLN
2	M	635	THR
2	M	637	LEU
2	M	645	VAL
2	M	654	LEU
2	M	657	ASP
2	M	663	ASN
2	M	668	LEU
2	M	672	VAL
2	M	684	PHE
2	M	689	VAL
2	M	690	ILE
2	M	697	ARG
2	M	699	PHE
2	M	713	ARG
2	M	717	LEU
2	M	727	PRO
2	M	729	LEU
2	M	730	SER
2	M	735	ARG
2	M	737	LEU
2	M	739	GLU
2	M	749	VAL
2	M	750	LYS
2	M	754	ILE
2	M	755	LEU

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Mol	Chain	Res	Type
2	M	762	LYS
2	M	772	ARG
2	M	773	LEU
2	M	775	ARG
2	M	780	GLU
2	M	785	VAL
2	M	799	ILE
2	M	805	ARG
2	M	807	ARG
2	M	808	ARG
2	M	813	VAL
2	M	821	GLU
2	M	822	VAL
2	M	825	VAL
2	M	834	GLN
2	M	835	VAL
2	M	839	LEU
2	M	841	ASN
2	M	853	LEU
2	M	862	PRO
2	M	863	ASP
2	M	874	LEU
2	M	881	ASN
2	M	886	LEU
2	M	897	LEU
2	M	910	LYS
2	M	911	GLU
2	M	937	ASP
2	M	941	VAL
2	M	942	GLU
2	M	950	LEU
2	M	958	THR
2	M	966	LEU
2	M	975	TYR
2	M	981	GLU
2	M	984	GLU
2	M	988	VAL
2	M	997	LEU
2	M	999	HIS
2	M	1000	MET
2	M	1002	GLU
2	M	1003	ASP

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Mol	Chain	Res	Type
2	M	1009	SER
2	M	1016	ILE
2	M	1026	GLN
2	M	1035	MET
2	M	1040	LEU
2	M	1058	ASP
2	M	1060	ILE
2	M	1074	GLU
2	M	1076	VAL
2	M	1079	PRO
2	M	1081	VAL
2	M	1087	VAL
2	M	1092	LEU
2	M	1095	LEU
2	M	1097	LEU
2	M	1098	ASP
2	M	1100	GLN
2	M	1103	ASP
2	M	1117	SER
2	M	1118	LYS
3	N	3	LYS
3	N	6	ARG
3	N	12	LEU
3	N	15	PRO
3	N	27	GLU
3	N	32	ILE
3	N	34	TYR
3	N	35	ARG
3	N	41	ARG
3	N	52	PRO
3	N	53	ILE
3	N	55	ASP
3	N	56	TYR
3	N	66	GLN
3	N	71	LYS
3	N	76	CYS
3	N	78	VAL
3	N	80	VAL
3	N	82	LYS
3	N	85	VAL
3	N	87	ARG
3	N	97	THR

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Mol	Chain	Res	Type
3	N	102	ILE
3	N	103	TRP
3	N	106	LYS
3	N	108	VAL
3	N	112	ILE
3	N	117	ASP
3	N	123	LEU
3	N	128	TYR
3	N	133	ILE
3	N	141	ILE
3	N	142	LEU
3	N	145	VAL
3	N	148	GLU
3	N	153	LEU
3	N	161	LEU
3	N	162	ARG
3	N	166	GLN
3	N	169	TYR
3	N	170	PRO
3	N	171	LEU
3	N	172	PRO
3	N	185	VAL
3	N	190	GLU
3	N	199	LEU
3	N	205	TYR
3	N	208	PRO
3	N	210	ARG
3	N	389	GLU
3	N	393	ILE
3	N	394	LEU
3	N	395	VAL
3	N	413	ASP
3	N	414	ARG
3	N	419	ASP
3	N	427	VAL
3	N	430	ASP
3	N	432	TYR
3	N	442	ASN
3	N	444	VAL
3	N	447	VAL
3	N	450	TYR
3	N	456	MET

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Mol	Chain	Res	Type
3	N	459	GLU
3	N	463	GLN
3	N	465	LEU
3	N	473	LEU
3	N	475	LYS
3	N	481	MET
3	N	486	ARG
3	N	488	ARG
3	N	493	ARG
3	N	502	PHE
3	N	503	LEU
3	N	505	SER
3	N	509	PRO
3	N	513	ILE
3	N	521	PRO
3	N	528	VAL
3	N	530	VAL
3	N	534	ARG
3	N	554	LEU
3	N	565	ILE
3	N	567	ILE
3	N	569	ASN
3	N	576	GLU
3	N	590	PRO
3	N	592	THR
3	N	594	PRO
3	N	601	ARG
3	N	602	SER
3	N	616	GLN
3	N	617	ASN
3	N	629	SER
3	N	632	VAL
3	N	641	GLN
3	N	651	GLU
3	N	652	LEU
3	N	666	ILE
3	N	674	ARG
3	N	676	MET
3	N	677	LEU
3	N	681	ARG
3	N	688	TRP
3	N	692	GLU

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Mol	Chain	Res	Type
3	N	695	ILE
3	N	701	LEU
3	N	704	ARG
3	N	709	HIS
3	N	710	ARG
3	N	713	ILE
3	N	716	PHE
3	N	721	VAL
3	N	739	ASP
3	N	749	VAL
3	N	754	PHE
3	N	758	GLU
3	N	770	LEU
3	N	778	LEU
3	N	785	ILE
3	N	786	ILE
3	N	787	LEU
3	N	792	ILE
3	N	794	GLN
3	N	796	ARG
3	N	797	LYS
3	N	799	LYS
3	N	800	LYS
3	N	805	GLU
3	N	828	LYS
3	N	829	VAL
3	N	836	VAL
3	N	847	ASP
3	N	863	VAL
3	N	864	VAL
3	N	865	THR
3	N	868	TYR
3	N	869	MET
3	N	876	SER
3	N	879	ARG
3	N	880	ILE
3	N	886	VAL
3	N	888	GLU
3	N	890	VAL
3	N	891	GLU
3	N	897	TRP
3	N	899	LEU

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Mol	Chain	Res	Type
3	N	907	GLU
3	N	914	LEU
3	N	917	GLN
3	N	942	SER
3	N	947	ILE
3	N	949	ILE
3	N	951	ILE
3	N	959	GLU
3	N	970	LYS
3	N	971	LEU
3	N	972	LEU
3	N	975	GLU
3	N	984	THR
3	N	990	ASP
3	N	991	GLN
3	N	994	GLN
3	N	999	THR
3	N	1020	LEU
3	N	1032	PRO
3	N	1033	GLN
3	N	1034	GLN
3	N	1035	ILE
3	N	1039	CYS
3	N	1051	GLU
3	N	1052	THR
3	N	1058	ARG
3	N	1060	SER
3	N	1063	GLU
3	N	1065	LEU
3	N	1068	LEU
3	N	1083	ASP
3	N	1084	THR
3	N	1087	ARG
3	N	1090	ASP
3	N	1095	THR
3	N	1096	ARG
3	N	1101	VAL
3	N	1102	THR
3	N	1104	GLU
3	N	1109	GLU
3	N	1112	CYS
3	N	1115	THR

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Mol	Chain	Res	Type
3	N	1119	SER
3	N	1127	GLU
3	N	1129	THR
3	N	1130	ARG
3	N	1135	ARG
3	N	1136	LYS
3	N	1141	GLU
3	N	1144	LEU
3	N	1151	ARG
3	N	1164	ARG
3	N	1166	LEU
3	N	1183	ILE
3	N	1189	ARG
3	N	1195	GLN
3	N	1207	TYR
3	N	1208	ASP
3	N	1213	ARG
3	N	1216	SER
3	N	1217	ILE
3	N	1231	GLU
3	N	1235	GLN
3	N	1238	MET
3	N	1243	THR
3	N	1252	ILE
3	N	1254	GLN
3	N	1256	LEU
3	N	1259	VAL
3	N	1262	LEU
3	N	1264	GLU
3	N	1267	ARG
3	N	1269	LYS
3	N	1274	ILE
3	N	1286	THR
3	N	1295	GLU
3	N	1297	GLU
3	N	1299	PHE
3	N	1301	LYS
3	N	1306	PRO
3	N	1307	LYS
3	N	1308	GLU
3	N	1311	LEU
3	N	1312	LEU

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Mol	Chain	Res	Type
3	N	1314	LYS
3	N	1317	ASP
3	N	1331	ASP
3	N	1332	PRO
3	N	1337	GLU
3	N	1344	VAL
3	N	1348	LEU
3	N	1353	GLN
3	N	1355	VAL
3	N	1363	LEU
3	N	1372	VAL
3	N	1380	GLU
3	N	1382	THR
3	N	1387	SER
3	N	1389	LEU
3	N	1391	GLU
3	N	1395	LEU
3	N	1399	ASP
3	N	1401	GLU
3	N	1403	LEU
3	N	1412	LYS
3	N	1418	LYS
3	N	1419	PRO
3	N	1420	LEU
3	N	1424	VAL
3	N	1431	THR
3	N	1432	LYS
3	N	1433	SER
3	N	1435	LEU
3	N	1439	SER
3	N	1441	GLN
3	N	1447	LEU
3	N	1455	LYS
3	N	1456	LYS
3	N	1460	ILE
3	N	1465	ASN
3	N	1466	VAL
3	N	1476	THR
3	N	1478	SER
3	N	1481	VAL
3	N	1483	PHE
3	N	1485	GLN

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Mol	Chain	Res	Type
3	N	1488	ASP
3	N	1501	GLU
4	O	12	MET
4	O	14	ASP
4	O	15	SER
4	O	32	ARG
4	O	41	GLU
4	O	42	PRO
4	O	45	ARG
4	O	51	LEU
4	O	54	LEU
4	O	57	ASP
4	O	59	ASN
4	O	61	GLU
4	O	66	LYS
4	O	70	THR
4	O	72	ARG
4	O	79	LEU
4	O	82	GLU
4	O	84	ARG
4	O	85	LEU
4	O	86	GLN
4	O	89	MET
5	P	83	GLN
5	P	84	TYR
5	P	86	HIS
5	P	87	GLU
5	P	91	VAL
5	P	96	LEU
5	P	101	GLU
5	P	107	GLU
5	P	108	GLU
5	P	125	ASP
5	P	126	LEU
5	P	132	ARG
5	P	135	ILE
5	P	136	LEU
5	P	142	ARG
5	P	144	ILE
5	P	145	PRO
5	P	150	THR
5	P	164	LYS

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Mol	Chain	Res	Type
5	P	174	LEU
5	P	181	GLU
5	P	184	ARG
5	P	186	HIS
5	P	187	LEU
5	P	203	THR
5	P	207	LEU
5	P	212	LEU
5	P	214	GLN
5	P	220	LEU
5	P	225	GLU
5	P	231	ARG
5	P	234	LYS
5	P	240	THR
5	P	245	GLN
5	P	260	ILE
5	P	262	VAL
5	P	277	GLN
5	P	280	GLN
5	P	285	GLU
5	P	289	GLU
5	P	295	MET
5	P	319	THR
5	P	327	SER
5	P	328	PHE
5	P	337	HIS
5	P	341	PRO
5	P	347	GLN
5	P	350	LEU
5	P	353	GLU
5	P	363	GLU
5	P	365	GLU
5	P	370	LYS
5	P	392	VAL
5	P	393	THR
5	P	399	GLN
5	P	403	LYS
5	P	410	TYR
5	P	419	ARG
5	P	420	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (179) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	81	ASN
1	A	156	HIS
1	A	163	ASN
1	A	180	GLN
1	A	188	GLN
1	A	227	ASN
1	A	229	GLN
1	B	81	ASN
1	B	95	GLN
1	B	124	ASN
1	B	163	ASN
1	B	212	ASN
1	B	213	GLN
2	C	22	GLN
2	C	41	ASN
2	C	187	ASN
2	C	343	GLN
2	C	399	ASN
2	C	498	GLN
2	C	543	ASN
2	C	552	HIS
2	C	563	ASN
2	C	609	ASN
2	C	632	ASN
2	C	663	ASN
2	C	670	GLN
2	C	834	GLN
2	C	841	ASN
2	C	845	ASN
2	C	881	ASN
2	C	884	GLN
2	C	889	HIS
2	C	899	GLN
2	C	962	GLN
2	C	969	GLN
2	C	999	HIS
2	C	1018	GLN
2	C	1019	GLN
2	C	1030	GLN
2	C	1047	HIS
2	C	1050	GLN
2	C	1107	ASN

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Mol	Chain	Res	Type
3	D	143	ASN
3	D	151	GLN
3	D	507	ASN
3	D	549	ASN
3	D	560	GLN
3	D	584	ASN
3	D	616	GLN
3	D	636	GLN
3	D	703	ASN
3	D	724	GLN
3	D	756	GLN
3	D	768	ASN
3	D	794	GLN
3	D	824	ASN
3	D	976	GLN
3	D	994	GLN
3	D	1018	ASN
3	D	1025	GLN
3	D	1033	GLN
3	D	1075	HIS
3	D	1103	HIS
3	D	1116	ASN
3	D	1124	GLN
3	D	1202	GLN
3	D	1242	HIS
3	D	1323	GLN
3	D	1333	HIS
3	D	1353	GLN
3	D	1359	GLN
3	D	1374	GLN
3	D	1404	ASN
3	D	1442	ASN
3	D	1465	ASN
4	E	28	GLN
4	E	37	ASN
4	E	86	GLN
5	F	83	GLN
5	F	90	GLN
5	F	170	HIS
5	F	185	GLN
5	F	186	HIS
5	F	217	ASN

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Mol	Chain	Res	Type
5	F	218	GLN
5	F	245	GLN
5	F	312	GLN
5	F	399	GLN
5	F	402	ASN
1	K	38	ASN
1	K	156	HIS
1	K	180	GLN
1	K	213	GLN
1	K	227	ASN
1	K	229	GLN
1	L	38	ASN
1	L	63	HIS
1	L	95	GLN
1	L	212	ASN
1	L	227	ASN
1	L	229	GLN
2	M	22	GLN
2	M	99	GLN
2	M	117	HIS
2	M	139	GLN
2	M	343	GLN
2	M	374	ASN
2	M	434	HIS
2	M	448	ASN
2	M	506	ASN
2	M	575	GLN
2	M	609	ASN
2	M	632	ASN
2	M	639	GLN
2	M	663	ASN
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	920	GLN
2	M	969	GLN
2	M	1018	GLN
2	M	1019	GLN
3	N	101	HIS

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Mol	Chain	Res	Type
3	N	151	GLN
3	N	462	GLN
3	N	463	GLN
3	N	507	ASN
3	N	549	ASN
3	N	552	ASN
3	N	560	GLN
3	N	640	HIS
3	N	703	ASN
3	N	727	GLN
3	N	737	ASN
3	N	748	HIS
3	N	756	GLN
3	N	768	ASN
3	N	794	GLN
3	N	816	HIS
3	N	855	HIS
3	N	906	GLN
3	N	917	GLN
3	N	976	GLN
3	N	994	GLN
3	N	1033	GLN
3	N	1103	HIS
3	N	1116	ASN
3	N	1184	GLN
3	N	1202	GLN
3	N	1235	GLN
3	N	1242	HIS
3	N	1323	GLN
3	N	1334	GLN
3	N	1353	GLN
3	N	1359	GLN
3	N	1393	GLN
3	N	1404	ASN
3	N	1441	GLN
3	N	1465	ASN
4	O	28	GLN
4	O	29	GLN
4	O	37	ASN
4	O	86	GLN
5	P	83	GLN
5	P	86	HIS

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Mol	Chain	Res	Type
5	P	90	GLN
5	P	161	GLN
5	P	185	GLN
5	P	191	ASN
5	P	269	ASN
5	P	279	GLN
5	P	312	GLN
5	P	337	HIS
5	P	399	GLN
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 493 ligands modelled in this entry, 491 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	RPT	M	8002	-	68,68,68	2.61	22 (32%)	101,101,101	1.24	10 (9%)
7	RPT	C	8001	-	68,68,68	2.53	23 (33%)	101,101,101	1.24	12 (11%)

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	RPT	M	8002	-	-	22/64/96/96	0/6/6/6
7	RPT	C	8001	-	-	12/64/96/96	0/6/6/6

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	8002	RPT	C39-N4	6.87	1.59	1.47
7	M	8002	RPT	C42-N4	6.73	1.59	1.47
7	C	8001	RPT	O6-C27	6.22	1.58	1.43
7	C	8001	RPT	O5-C29	6.18	1.55	1.39
7	M	8002	RPT	O5-C29	6.04	1.54	1.39
7	M	8002	RPT	C2-C1	5.69	1.52	1.38
7	C	8001	RPT	C42-N4	5.44	1.57	1.47
7	C	8001	RPT	C39-N4	5.31	1.57	1.47
7	M	8002	RPT	C8-C9	5.16	1.58	1.43
7	C	8001	RPT	C8-C9	5.12	1.57	1.43
7	C	8001	RPT	C10-C9	5.00	1.54	1.42
7	M	8002	RPT	C5-C10	4.99	1.53	1.42
7	M	8002	RPT	O6-C27	4.94	1.55	1.43
7	C	8001	RPT	C2-C1	4.92	1.50	1.38
7	C	8001	RPT	C5-C10	4.92	1.53	1.42
7	M	8002	RPT	C10-C9	4.69	1.54	1.42
7	M	8002	RPT	C38-N4	4.58	1.60	1.48
7	C	8001	RPT	C3-C4	4.52	1.48	1.40
7	M	8002	RPT	C3-C2	4.09	1.48	1.41
7	M	8002	RPT	C40-N3	4.04	1.54	1.46
7	C	8001	RPT	O4-C11	3.85	1.27	1.21
7	C	8001	RPT	C24-C25	3.59	1.63	1.54
7	M	8002	RPT	O5-C12	3.58	1.58	1.42
7	M	8002	RPT	C3-C4	3.57	1.46	1.40
7	M	8002	RPT	C24-C25	3.45	1.62	1.54
7	C	8001	RPT	O5-C12	3.42	1.57	1.42
7	C	8001	RPT	C40-N3	3.41	1.52	1.46
7	M	8002	RPT	O4-C11	3.22	1.26	1.21
7	C	8001	RPT	C3-C2	3.10	1.46	1.41
7	M	8002	RPT	C1-C9	3.00	1.51	1.43
7	M	8002	RPT	C8-C7	2.97	1.53	1.40
7	C	8001	RPT	C1-C9	2.92	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	8001	RPT	C8-C7	2.87	1.52	1.40
7	M	8002	RPT	C27-C28	2.78	1.59	1.50
7	C	8001	RPT	C38-N4	2.75	1.55	1.48
7	C	8001	RPT	C27-C28	2.68	1.59	1.50
7	C	8001	RPT	O7-C25	2.65	1.48	1.44
7	C	8001	RPT	C41-N3	2.60	1.51	1.46
7	M	8002	RPT	C41-N3	2.57	1.51	1.46
7	C	8001	RPT	C45-C38	2.50	1.59	1.53
7	C	8001	RPT	C3-C43	2.31	1.51	1.46
7	M	8002	RPT	C32-C22	2.29	1.58	1.53
7	M	8002	RPT	O2-C8	-2.29	1.28	1.35
7	M	8002	RPT	C3-C43	2.19	1.51	1.46
7	C	8001	RPT	C32-C22	2.03	1.57	1.53

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	8002	RPT	C24-C23-C22	3.76	121.68	115.41
7	C	8001	RPT	C2-N1-C15	3.35	134.26	124.06
7	C	8001	RPT	C24-C23-C22	3.31	120.92	115.41
7	M	8002	RPT	C20-C21-C22	3.26	121.58	114.97
7	C	8001	RPT	C25-O7-C35	3.22	122.72	117.72
7	M	8002	RPT	C34-C26-C25	-3.08	105.97	111.40
7	C	8001	RPT	C20-C21-C22	3.05	121.16	114.97
7	M	8002	RPT	C31-C20-C19	-3.04	103.02	109.91
7	M	8002	RPT	C2-N1-C15	2.95	133.05	124.06
7	C	8001	RPT	C31-C20-C19	-2.86	103.44	109.91
7	M	8002	RPT	C25-O7-C35	2.63	121.81	117.72
7	C	8001	RPT	C3-C2-N1	-2.62	114.84	119.33
7	C	8001	RPT	C26-C27-C28	2.51	117.54	112.11
7	C	8001	RPT	C34-C26-C25	-2.40	107.18	111.40
7	M	8002	RPT	C32-C22-C23	-2.27	106.97	111.43
7	C	8001	RPT	C5-C10-C9	-2.22	116.04	119.77
7	C	8001	RPT	C12-O5-C29	2.19	123.22	117.84
7	M	8002	RPT	C5-C10-C9	-2.13	116.21	119.77
7	C	8001	RPT	C37-O6-C27	2.09	117.78	112.99
7	C	8001	RPT	C32-C22-C23	-2.07	107.37	111.43
7	M	8002	RPT	C31-C20-C21	2.06	115.85	111.45
7	M	8002	RPT	C3-C2-N1	-2.02	115.88	119.33

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	8001	RPT	C26-C27-C28-C29
7	C	8001	RPT	C26-C27-O6-C37
7	C	8001	RPT	C28-C27-O6-C37
7	M	8002	RPT	C28-C27-O6-C37
7	M	8002	RPT	C44-C38-N4-C39
7	M	8002	RPT	C45-C38-N4-C39
7	M	8002	RPT	C45-C38-N4-C42
7	M	8002	RPT	C16-C17-C18-C19
7	M	8002	RPT	C3-C2-N1-C15
7	C	8001	RPT	C16-C17-C18-C19
7	C	8001	RPT	C3-C2-N1-C15
7	C	8001	RPT	C18-C19-C20-C31
7	C	8001	RPT	C19-C20-C21-C22
7	M	8002	RPT	C19-C20-C21-C22
7	M	8002	RPT	C31-C20-C21-C22
7	C	8001	RPT	C43-N2-N3-C40
7	C	8001	RPT	C43-N2-N3-C41
7	M	8002	RPT	C43-N2-N3-C40
7	M	8002	RPT	C43-N2-N3-C41
7	C	8001	RPT	O6-C27-C28-C29
7	M	8002	RPT	C33-C24-C25-C26
7	M	8002	RPT	C18-C19-C20-C21
7	M	8002	RPT	C23-C24-C25-C26
7	M	8002	RPT	C26-C27-C28-C29
7	M	8002	RPT	O6-C27-C28-C29
7	M	8002	RPT	C18-C19-C20-C31
7	M	8002	RPT	C44-C38-N4-C42
7	M	8002	RPT	C31-C20-C21-O10
7	C	8001	RPT	C23-C24-C25-C26
7	C	8001	RPT	C28-C29-O5-C12
7	M	8002	RPT	C28-C29-O5-C12
7	M	8002	RPT	C1-C2-N1-C15
7	M	8002	RPT	C33-C24-C25-O7
7	M	8002	RPT	C23-C24-C25-O7

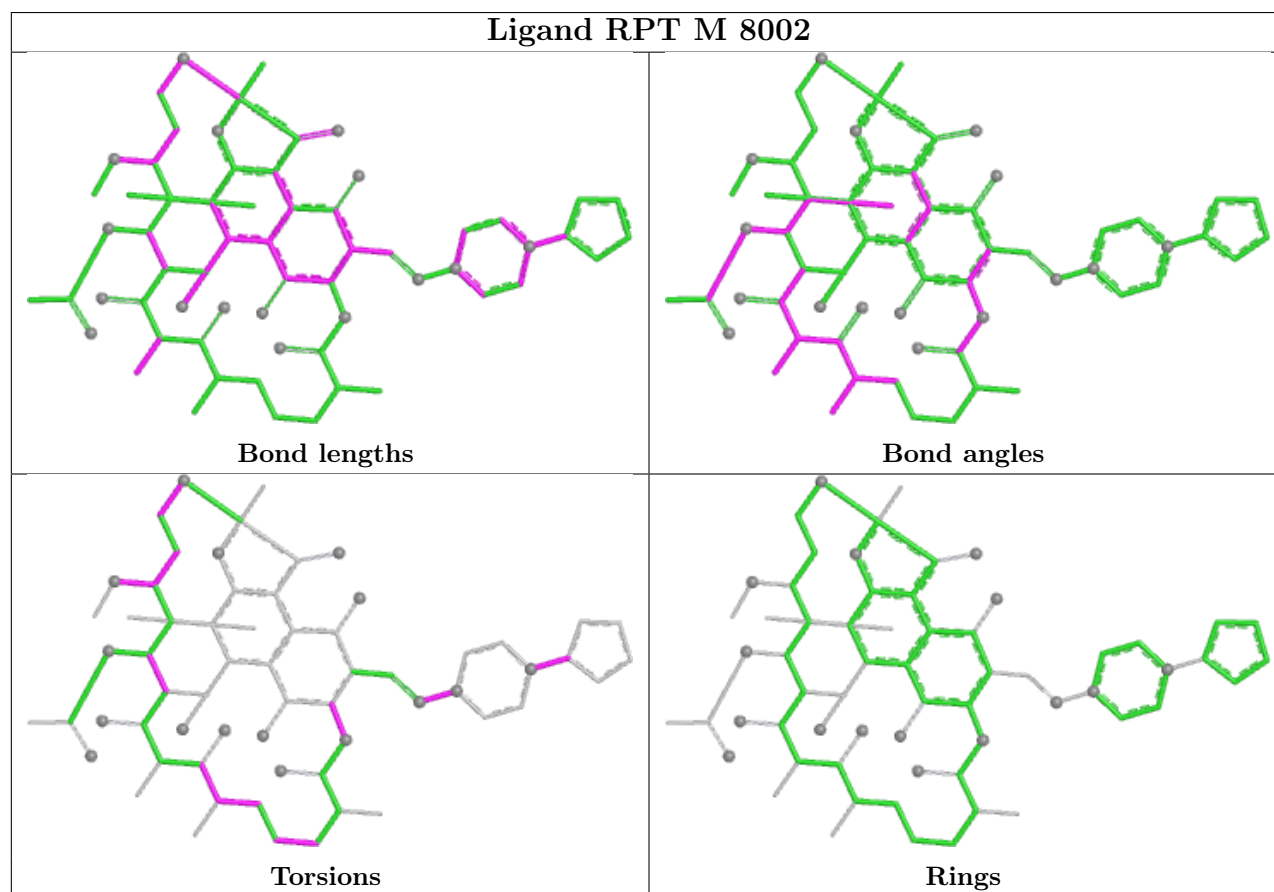
There are no ring outliers.

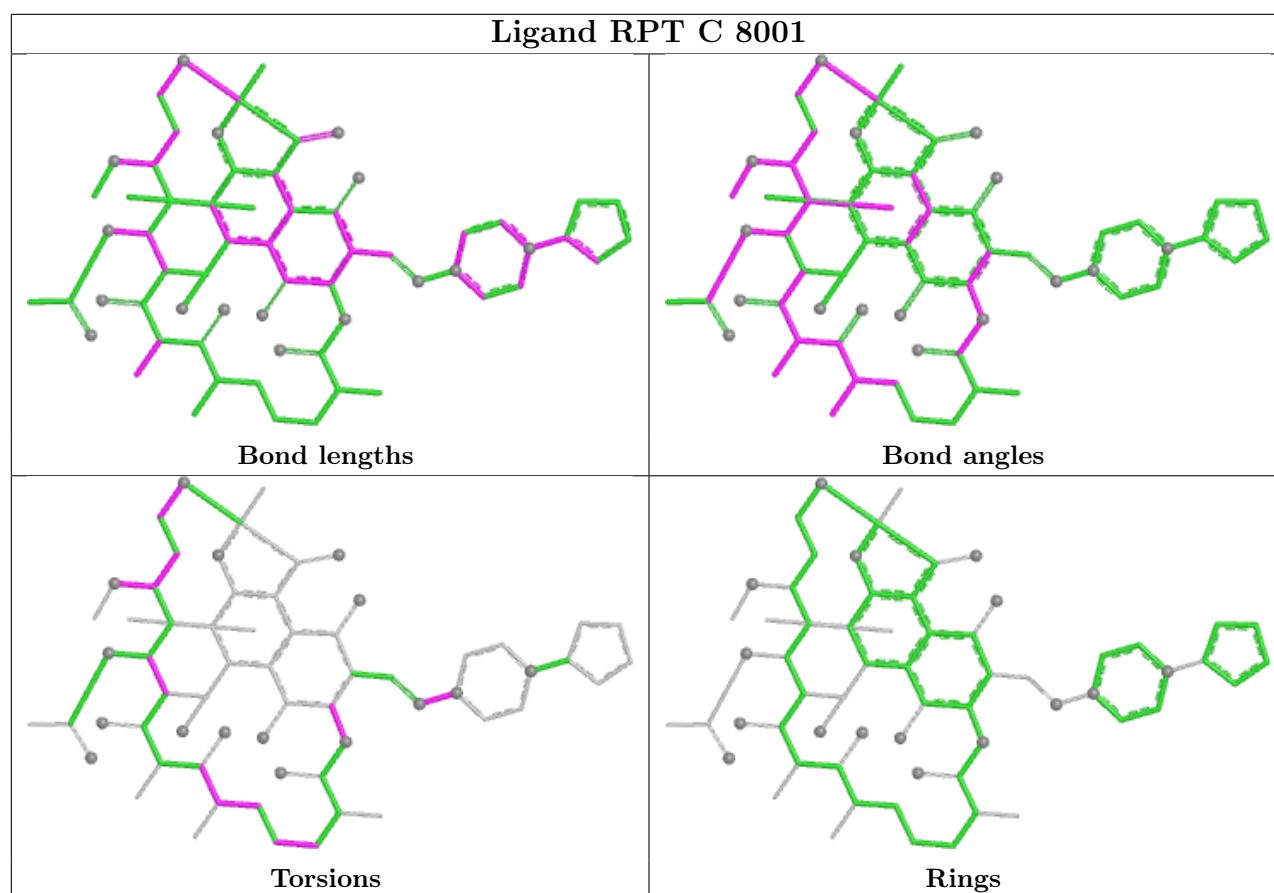
2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	M	8002	RPT	7	0
7	C	8001	RPT	5	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-1.62	0 100 100	27, 63, 91, 115	0
1	B	229/315 (72%)	-1.49	0 100 100	48, 93, 115, 119	0
1	K	229/315 (72%)	-1.62	0 100 100	34, 65, 94, 134	0
1	L	229/315 (72%)	-1.55	0 100 100	52, 92, 110, 131	0
2	C	1119/1119 (100%)	-1.59	0 100 100	21, 75, 106, 118	0
2	M	1119/1119 (100%)	-1.58	0 100 100	25, 79, 109, 122	0
3	D	1392/1524 (91%)	-1.60	0 100 100	24, 65, 112, 132	0
3	N	1392/1524 (91%)	-1.57	0 100 100	25, 69, 117, 138	0
4	E	95/99 (95%)	-1.50	0 100 100	42, 83, 108, 126	0
4	O	95/99 (95%)	-1.56	0 100 100	46, 80, 107, 114	0
5	F	345/423 (81%)	-1.57	0 100 100	49, 84, 110, 127	0
5	P	345/423 (81%)	-1.55	0 100 100	63, 89, 114, 124	0
All	All	6818/7590 (89%)	-1.58	0 100 100	21, 75, 112, 138	0

There are no RSRZ outliers to report.

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 ⓘ

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
6	MG	D	9177	1/1	0.98	0.03	64,64,64,64	0
6	MG	A	9043	1/1	0.99	0.01	37,37,37,37	0
6	MG	A	9153	1/1	0.99	0.04	66,66,66,66	0
6	MG	A	9171	1/1	0.99	0.03	58,58,58,58	0
6	MG	A	9380	1/1	0.99	0.03	44,44,44,44	0
6	MG	B	9080	1/1	0.99	0.02	56,56,56,56	0
6	MG	B	9093	1/1	0.99	0.02	40,40,40,40	0
6	MG	C	9021	1/1	0.99	0.04	37,37,37,37	0
6	MG	C	9047	1/1	0.99	0.03	53,53,53,53	0
6	MG	C	9067	1/1	0.99	0.02	57,57,57,57	0
6	MG	C	9112	1/1	0.99	0.03	39,39,39,39	0
6	MG	C	9122	1/1	0.99	0.03	56,56,56,56	0
6	MG	C	9160	1/1	0.99	0.05	44,44,44,44	0
6	MG	C	9175	1/1	0.99	0.02	68,68,68,68	0
6	MG	C	9340	1/1	0.99	0.04	60,60,60,60	0
6	MG	C	9360	1/1	0.99	0.03	53,53,53,53	0
6	MG	C	9362	1/1	0.99	0.02	55,55,55,55	0
6	MG	C	9454	1/1	0.99	0.04	55,55,55,55	0
6	MG	C	9462	1/1	0.99	0.04	43,43,43,43	0
6	MG	C	9463	1/1	0.99	0.02	55,55,55,55	0
6	MG	D	9024	1/1	0.99	0.02	36,36,36,36	0
6	MG	D	9030	1/1	0.99	0.04	48,48,48,48	0
6	MG	D	9082	1/1	0.99	0.02	60,60,60,60	0
6	MG	D	9137	1/1	0.99	0.04	47,47,47,47	0
6	MG	D	9140	1/1	0.99	0.03	40,40,40,40	0
6	MG	D	9152	1/1	0.99	0.03	67,67,67,67	0
6	MG	D	9163	1/1	0.99	0.03	52,52,52,52	0
6	MG	D	9167	1/1	0.99	0.02	49,49,49,49	0
6	MG	D	9173	1/1	0.99	0.04	48,48,48,48	0
6	MG	A	9016	1/1	0.99	0.02	36,36,36,36	0
6	MG	D	9330	1/1	0.99	0.02	39,39,39,39	0
6	MG	D	9348	1/1	0.99	0.02	57,57,57,57	0
6	MG	D	9349	1/1	0.99	0.01	33,33,33,33	0
6	MG	D	9367	1/1	0.99	0.04	31,31,31,31	0
6	MG	D	9459	1/1	0.99	0.04	54,54,54,54	0
6	MG	D	9480	1/1	0.99	0.03	55,55,55,55	0
6	MG	E	9045	1/1	0.99	0.02	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	F	9008	1/1	0.99	0.02	40,40,40,40	0
6	MG	F	9099	1/1	0.99	0.01	56,56,56,56	0
6	MG	F	9148	1/1	0.99	0.02	54,54,54,54	0
6	MG	F	9159	1/1	0.99	0.02	57,57,57,57	0
6	MG	F	9370	1/1	0.99	0.03	46,46,46,46	0
6	MG	F	9389	1/1	0.99	0.04	53,53,53,53	0
6	MG	K	9188	1/1	0.99	0.02	40,40,40,40	0
6	MG	K	9433	1/1	0.99	0.03	50,50,50,50	0
6	MG	L	9245	1/1	0.99	0.02	62,62,62,62	0
6	MG	L	9246	1/1	0.99	0.02	52,52,52,52	0
6	MG	L	9283	1/1	0.99	0.02	59,59,59,59	0
6	MG	L	9289	1/1	0.99	0.02	62,62,62,62	0
6	MG	L	9414	1/1	0.99	0.02	51,51,51,51	0
6	MG	M	9201	1/1	0.99	0.02	45,45,45,45	0
6	MG	M	9210	1/1	0.99	0.02	41,41,41,41	0
6	MG	M	9220	1/1	0.99	0.03	51,51,51,51	0
6	MG	M	9263	1/1	0.99	0.04	56,56,56,56	0
6	MG	M	9272	1/1	0.99	0.02	45,45,45,45	0
6	MG	M	9310	1/1	0.99	0.03	46,46,46,46	0
6	MG	M	9324	1/1	0.99	0.04	41,41,41,41	0
6	MG	M	9406	1/1	0.99	0.03	67,67,67,67	0
6	MG	M	9416	1/1	0.99	0.03	45,45,45,45	0
6	MG	M	9440	1/1	0.99	0.03	50,50,50,50	0
6	MG	M	9442	1/1	0.99	0.04	59,59,59,59	0
6	MG	M	9447	1/1	0.99	0.02	64,64,64,64	0
6	MG	M	9452	1/1	0.99	0.02	42,42,42,42	0
6	MG	M	9475	1/1	0.99	0.04	62,62,62,62	0
6	MG	N	9185	1/1	0.99	0.02	56,56,56,56	0
6	MG	N	9200	1/1	0.99	0.02	38,38,38,38	0
6	MG	N	9207	1/1	0.99	0.02	41,41,41,41	0
6	MG	N	9211	1/1	0.99	0.02	44,44,44,44	0
6	MG	N	9217	1/1	0.99	0.02	48,48,48,48	0
6	MG	N	9238	1/1	0.99	0.07	43,43,43,43	0
6	MG	N	9253	1/1	0.99	0.02	42,42,42,42	0
6	MG	N	9308	1/1	0.99	0.02	55,55,55,55	0
6	MG	N	9313	1/1	0.99	0.04	43,43,43,43	0
6	MG	N	9317	1/1	0.99	0.03	43,43,43,43	0
6	MG	N	9425	1/1	0.99	0.02	46,46,46,46	0
6	MG	N	9426	1/1	0.99	0.04	41,41,41,41	0
6	MG	N	9427	1/1	0.99	0.02	58,58,58,58	0
6	MG	N	9445	1/1	0.99	0.03	51,51,51,51	0
6	MG	N	9449	1/1	0.99	0.03	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	N	9465	1/1	0.99	0.03	49,49,49,49	0
6	MG	N	9476	1/1	0.99	0.03	54,54,54,54	0
6	MG	P	9226	1/1	0.99	0.05	43,43,43,43	0
6	MG	P	9228	1/1	0.99	0.03	43,43,43,43	0
6	MG	P	9280	1/1	0.99	0.02	51,51,51,51	0
6	MG	P	9282	1/1	0.99	0.03	56,56,56,56	0
6	MG	P	9325	1/1	0.99	0.02	49,49,49,49	0
6	MG	P	9436	1/1	0.99	0.02	49,49,49,49	0
6	MG	C	9119	1/1	1.00	0.02	43,43,43,43	0
6	MG	A	9081	1/1	1.00	0.03	40,40,40,40	0
6	MG	C	9126	1/1	1.00	0.03	46,46,46,46	0
6	MG	C	9128	1/1	1.00	0.02	52,52,52,52	0
6	MG	C	9138	1/1	1.00	0.03	43,43,43,43	0
6	MG	C	9142	1/1	1.00	0.02	48,48,48,48	0
6	MG	C	9143	1/1	1.00	0.01	35,35,35,35	0
6	MG	C	9145	1/1	1.00	0.01	66,66,66,66	0
6	MG	C	9149	1/1	1.00	0.02	48,48,48,48	0
6	MG	C	9154	1/1	1.00	0.04	43,43,43,43	0
6	MG	A	9088	1/1	1.00	0.02	36,36,36,36	0
6	MG	C	9162	1/1	1.00	0.03	50,50,50,50	0
6	MG	C	9164	1/1	1.00	0.01	49,49,49,49	0
6	MG	C	9168	1/1	1.00	0.03	45,45,45,45	0
6	MG	C	9169	1/1	1.00	0.02	42,42,42,42	0
6	MG	C	9170	1/1	1.00	0.03	41,41,41,41	0
6	MG	A	9097	1/1	1.00	0.01	34,34,34,34	0
6	MG	C	9176	1/1	1.00	0.03	28,28,28,28	0
6	MG	C	9178	1/1	1.00	0.03	39,39,39,39	0
6	MG	A	9106	1/1	1.00	0.01	38,38,38,38	0
6	MG	C	9350	1/1	1.00	0.01	60,60,60,60	0
6	MG	C	9353	1/1	1.00	0.01	48,48,48,48	0
6	MG	C	9355	1/1	1.00	0.02	58,58,58,58	0
6	MG	A	9111	1/1	1.00	0.03	35,35,35,35	0
6	MG	C	9361	1/1	1.00	0.03	41,41,41,41	0
6	MG	A	9124	1/1	1.00	0.02	39,39,39,39	0
6	MG	C	9366	1/1	1.00	0.01	41,41,41,41	0
6	MG	C	9371	1/1	1.00	0.01	54,54,54,54	0
6	MG	C	9372	1/1	1.00	0.06	61,61,61,61	0
6	MG	C	9377	1/1	1.00	0.02	44,44,44,44	0
6	MG	C	9381	1/1	1.00	0.01	53,53,53,53	0
6	MG	C	9391	1/1	1.00	0.04	60,60,60,60	0
6	MG	C	9394	1/1	1.00	0.03	33,33,33,33	0
6	MG	A	9125	1/1	1.00	0.01	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	C	9455	1/1	1.00	0.03	40,40,40,40	0
6	MG	C	9461	1/1	1.00	0.04	50,50,50,50	0
6	MG	A	9012	1/1	1.00	0.03	47,47,47,47	0
6	MG	A	9156	1/1	1.00	0.02	43,43,43,43	0
6	MG	C	9464	1/1	1.00	0.02	48,48,48,48	0
6	MG	C	9487	1/1	1.00	0.02	32,32,32,32	0
6	MG	D	9001	1/1	1.00	0.03	36,36,36,36	0
6	MG	D	9005	1/1	1.00	0.02	40,40,40,40	0
6	MG	D	9006	1/1	1.00	0.02	40,40,40,40	0
6	MG	D	9009	1/1	1.00	0.01	43,43,43,43	0
6	MG	D	9011	1/1	1.00	0.01	33,33,33,33	0
6	MG	D	9014	1/1	1.00	0.01	41,41,41,41	0
6	MG	D	9017	1/1	1.00	0.02	42,42,42,42	0
6	MG	D	9018	1/1	1.00	0.01	39,39,39,39	0
6	MG	D	9023	1/1	1.00	0.01	34,34,34,34	0
6	MG	A	9013	1/1	1.00	0.01	44,44,44,44	0
6	MG	D	9028	1/1	1.00	0.01	34,34,34,34	0
6	MG	D	9029	1/1	1.00	0.01	33,33,33,33	0
6	MG	A	9332	1/1	1.00	0.02	35,35,35,35	0
6	MG	D	9034	1/1	1.00	0.01	41,41,41,41	0
6	MG	D	9036	1/1	1.00	0.01	44,44,44,44	0
6	MG	D	9038	1/1	1.00	0.04	39,39,39,39	0
6	MG	D	9039	1/1	1.00	0.02	44,44,44,44	0
6	MG	D	9041	1/1	1.00	0.01	47,47,47,47	0
6	MG	D	9052	1/1	1.00	0.01	65,65,65,65	0
6	MG	D	9054	1/1	1.00	0.01	44,44,44,44	0
6	MG	D	9058	1/1	1.00	0.02	38,38,38,38	0
6	MG	D	9062	1/1	1.00	0.02	47,47,47,47	0
6	MG	D	9063	1/1	1.00	0.04	33,33,33,33	0
6	MG	D	9064	1/1	1.00	0.01	44,44,44,44	0
6	MG	D	9069	1/1	1.00	0.01	48,48,48,48	0
6	MG	D	9070	1/1	1.00	0.03	33,33,33,33	0
6	MG	D	9072	1/1	1.00	0.02	32,32,32,32	0
6	MG	D	9073	1/1	1.00	0.03	34,34,34,34	0
6	MG	D	9077	1/1	1.00	0.03	35,35,35,35	0
6	MG	A	9342	1/1	1.00	0.01	39,39,39,39	0
6	MG	D	9084	1/1	1.00	0.01	37,37,37,37	0
6	MG	D	9085	1/1	1.00	0.02	49,49,49,49	0
6	MG	D	9087	1/1	1.00	0.05	43,43,43,43	0
6	MG	D	9089	1/1	1.00	0.04	36,36,36,36	0
6	MG	D	9091	1/1	1.00	0.03	27,27,27,27	0
6	MG	D	9095	1/1	1.00	0.03	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	D	9096	1/1	1.00	0.02	60,60,60,60	0
6	MG	D	9100	1/1	1.00	0.05	43,43,43,43	0
6	MG	D	9102	1/1	1.00	0.03	44,44,44,44	0
6	MG	D	9108	1/1	1.00	0.01	51,51,51,51	0
6	MG	D	9113	1/1	1.00	0.02	34,34,34,34	0
6	MG	D	9117	1/1	1.00	0.02	48,48,48,48	0
6	MG	D	9118	1/1	1.00	0.02	44,44,44,44	0
6	MG	D	9120	1/1	1.00	0.03	31,31,31,31	0
6	MG	D	9121	1/1	1.00	0.01	35,35,35,35	0
6	MG	D	9127	1/1	1.00	0.01	48,48,48,48	0
6	MG	D	9129	1/1	1.00	0.01	42,42,42,42	0
6	MG	D	9130	1/1	1.00	0.01	51,51,51,51	0
6	MG	D	9132	1/1	1.00	0.02	43,43,43,43	0
6	MG	D	9133	1/1	1.00	0.02	42,42,42,42	0
6	MG	D	9134	1/1	1.00	0.02	47,47,47,47	0
6	MG	D	9135	1/1	1.00	0.02	50,50,50,50	0
6	MG	A	9345	1/1	1.00	0.02	41,41,41,41	0
6	MG	A	9352	1/1	1.00	0.01	46,46,46,46	0
6	MG	D	9141	1/1	1.00	0.03	50,50,50,50	0
6	MG	D	9144	1/1	1.00	0.03	39,39,39,39	0
6	MG	D	9146	1/1	1.00	0.02	31,31,31,31	0
6	MG	D	9147	1/1	1.00	0.02	41,41,41,41	0
6	MG	D	9150	1/1	1.00	0.01	31,31,31,31	0
6	MG	D	9151	1/1	1.00	0.01	57,57,57,57	0
6	MG	A	9354	1/1	1.00	0.02	37,37,37,37	0
6	MG	D	9158	1/1	1.00	0.04	60,60,60,60	0
6	MG	D	9161	1/1	1.00	0.02	57,57,57,57	0
6	MG	A	9357	1/1	1.00	0.02	54,54,54,54	0
6	MG	D	9165	1/1	1.00	0.04	32,32,32,32	0
6	MG	D	9166	1/1	1.00	0.02	40,40,40,40	0
6	MG	A	9368	1/1	1.00	0.02	43,43,43,43	0
6	MG	A	9002	1/1	1.00	0.01	31,31,31,31	0
6	MG	D	9174	1/1	1.00	0.02	47,47,47,47	0
6	MG	A	9384	1/1	1.00	0.02	39,39,39,39	0
6	MG	D	9328	1/1	1.00	0.03	30,30,30,30	0
6	MG	D	9329	1/1	1.00	0.02	33,33,33,33	0
6	MG	A	9395	1/1	1.00	0.03	50,50,50,50	0
6	MG	D	9331	1/1	1.00	0.01	43,43,43,43	0
6	MG	D	9333	1/1	1.00	0.05	33,33,33,33	0
6	MG	D	9334	1/1	1.00	0.01	54,54,54,54	0
6	MG	D	9335	1/1	1.00	0.02	52,52,52,52	0
6	MG	D	9336	1/1	1.00	0.02	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	D	9337	1/1	1.00	0.02	53,53,53,53	0
6	MG	D	9338	1/1	1.00	0.02	42,42,42,42	0
6	MG	D	9339	1/1	1.00	0.01	37,37,37,37	0
6	MG	D	9341	1/1	1.00	0.02	41,41,41,41	0
6	MG	D	9343	1/1	1.00	0.03	59,59,59,59	0
6	MG	D	9344	1/1	1.00	0.03	55,55,55,55	0
6	MG	D	9346	1/1	1.00	0.02	47,47,47,47	0
6	MG	D	9347	1/1	1.00	0.01	49,49,49,49	0
6	MG	A	9460	1/1	1.00	0.03	55,55,55,55	0
6	MG	A	9477	1/1	1.00	0.02	52,52,52,52	0
6	MG	D	9351	1/1	1.00	0.01	43,43,43,43	0
6	MG	D	9364	1/1	1.00	0.02	47,47,47,47	0
6	MG	D	9365	1/1	1.00	0.02	41,41,41,41	0
6	MG	B	9032	1/1	1.00	0.05	34,34,34,34	0
6	MG	D	9369	1/1	1.00	0.01	49,49,49,49	0
6	MG	D	9373	1/1	1.00	0.03	51,51,51,51	0
6	MG	D	9374	1/1	1.00	0.02	41,41,41,41	0
6	MG	D	9379	1/1	1.00	0.03	47,47,47,47	0
6	MG	D	9385	1/1	1.00	0.01	35,35,35,35	0
6	MG	D	9386	1/1	1.00	0.03	40,40,40,40	0
6	MG	D	9388	1/1	1.00	0.01	37,37,37,37	0
6	MG	D	9392	1/1	1.00	0.02	52,52,52,52	0
6	MG	D	9396	1/1	1.00	0.04	62,62,62,62	0
6	MG	D	9397	1/1	1.00	0.02	51,51,51,51	0
6	MG	D	9453	1/1	1.00	0.02	38,38,38,38	0
6	MG	D	9456	1/1	1.00	0.02	55,55,55,55	0
6	MG	B	9033	1/1	1.00	0.01	33,33,33,33	0
6	MG	B	9040	1/1	1.00	0.01	36,36,36,36	0
6	MG	E	9007	1/1	1.00	0.01	40,40,40,40	0
6	MG	B	9056	1/1	1.00	0.01	43,43,43,43	0
6	MG	E	9074	1/1	1.00	0.01	59,59,59,59	0
6	MG	E	9155	1/1	1.00	0.02	44,44,44,44	0
6	MG	E	9479	1/1	1.00	0.01	62,62,62,62	0
6	MG	B	9059	1/1	1.00	0.03	48,48,48,48	0
6	MG	F	9035	1/1	1.00	0.01	40,40,40,40	0
6	MG	F	9048	1/1	1.00	0.02	41,41,41,41	0
6	MG	F	9057	1/1	1.00	0.03	30,30,30,30	0
6	MG	F	9060	1/1	1.00	0.02	41,41,41,41	0
6	MG	F	9098	1/1	1.00	0.02	54,54,54,54	0
6	MG	A	9027	1/1	1.00	0.04	37,37,37,37	0
6	MG	F	9101	1/1	1.00	0.03	44,44,44,44	0
6	MG	F	9105	1/1	1.00	0.01	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	F	9109	1/1	1.00	0.02	60,60,60,60	0
6	MG	F	9123	1/1	1.00	0.03	37,37,37,37	0
6	MG	F	9139	1/1	1.00	0.02	38,38,38,38	0
6	MG	B	9083	1/1	1.00	0.01	40,40,40,40	0
6	MG	F	9157	1/1	1.00	0.02	42,42,42,42	0
6	MG	A	9010	1/1	1.00	0.01	30,30,30,30	0
6	MG	F	9172	1/1	1.00	0.01	51,51,51,51	0
6	MG	F	9356	1/1	1.00	0.01	37,37,37,37	0
6	MG	F	9363	1/1	1.00	0.02	53,53,53,53	0
6	MG	B	9094	1/1	1.00	0.02	38,38,38,38	0
6	MG	F	9375	1/1	1.00	0.01	36,36,36,36	0
6	MG	F	9376	1/1	1.00	0.02	62,62,62,62	0
6	MG	F	9382	1/1	1.00	0.03	40,40,40,40	0
6	MG	F	9383	1/1	1.00	0.04	48,48,48,48	0
6	MG	F	9387	1/1	1.00	0.03	53,53,53,53	0
6	MG	B	9103	1/1	1.00	0.01	43,43,43,43	0
6	MG	F	9390	1/1	1.00	0.02	46,46,46,46	0
6	MG	F	9393	1/1	1.00	0.01	38,38,38,38	0
6	MG	F	9481	1/1	1.00	0.03	57,57,57,57	0
6	MG	K	9180	1/1	1.00	0.04	42,42,42,42	0
6	MG	B	9104	1/1	1.00	0.02	45,45,45,45	0
6	MG	K	9191	1/1	1.00	0.01	32,32,32,32	0
6	MG	K	9213	1/1	1.00	0.01	43,43,43,43	0
6	MG	K	9223	1/1	1.00	0.03	32,32,32,32	0
6	MG	K	9244	1/1	1.00	0.03	44,44,44,44	0
6	MG	K	9251	1/1	1.00	0.02	43,43,43,43	0
6	MG	K	9257	1/1	1.00	0.03	58,58,58,58	0
6	MG	K	9264	1/1	1.00	0.02	42,42,42,42	0
6	MG	K	9290	1/1	1.00	0.01	51,51,51,51	0
6	MG	K	9301	1/1	1.00	0.02	43,43,43,43	0
6	MG	K	9405	1/1	1.00	0.01	56,56,56,56	0
6	MG	K	9410	1/1	1.00	0.11	36,36,36,36	0
6	MG	K	9413	1/1	1.00	0.02	54,54,54,54	0
6	MG	K	9432	1/1	1.00	0.02	49,49,49,49	0
6	MG	B	9110	1/1	1.00	0.02	49,49,49,49	0
6	MG	K	9438	1/1	1.00	0.01	52,52,52,52	0
6	MG	K	9469	1/1	1.00	0.01	50,50,50,50	0
6	MG	K	9470	1/1	1.00	0.04	55,55,55,55	0
6	MG	L	9182	1/1	1.00	0.02	47,47,47,47	0
6	MG	L	9183	1/1	1.00	0.01	37,37,37,37	0
6	MG	L	9218	1/1	1.00	0.03	33,33,33,33	0
6	MG	B	9116	1/1	1.00	0.03	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	B	9131	1/1	1.00	0.04	33,33,33,33	0
6	MG	L	9252	1/1	1.00	0.01	45,45,45,45	0
6	MG	L	9278	1/1	1.00	0.01	44,44,44,44	0
6	MG	B	9136	1/1	1.00	0.03	47,47,47,47	0
6	MG	B	9358	1/1	1.00	0.04	39,39,39,39	0
6	MG	L	9306	1/1	1.00	0.02	57,57,57,57	0
6	MG	L	9307	1/1	1.00	0.02	35,35,35,35	0
6	MG	L	9309	1/1	1.00	0.01	49,49,49,49	0
6	MG	L	9314	1/1	1.00	0.01	56,56,56,56	0
6	MG	B	9359	1/1	1.00	0.04	52,52,52,52	0
6	MG	L	9421	1/1	1.00	0.02	53,53,53,53	0
6	MG	L	9437	1/1	1.00	0.04	40,40,40,40	0
6	MG	L	9466	1/1	1.00	0.02	49,49,49,49	0
6	MG	M	9190	1/1	1.00	0.01	29,29,29,29	0
6	MG	M	9195	1/1	1.00	0.03	34,34,34,34	0
6	MG	M	9196	1/1	1.00	0.02	42,42,42,42	0
6	MG	B	9378	1/1	1.00	0.01	47,47,47,47	0
6	MG	M	9203	1/1	1.00	0.01	32,32,32,32	0
6	MG	M	9205	1/1	1.00	0.04	38,38,38,38	0
6	MG	M	9208	1/1	1.00	0.03	39,39,39,39	0
6	MG	B	9457	1/1	1.00	0.04	43,43,43,43	0
6	MG	M	9212	1/1	1.00	0.02	32,32,32,32	0
6	MG	M	9219	1/1	1.00	0.03	47,47,47,47	0
6	MG	B	9458	1/1	1.00	0.03	44,44,44,44	0
6	MG	M	9222	1/1	1.00	0.03	35,35,35,35	0
6	MG	M	9224	1/1	1.00	0.01	40,40,40,40	0
6	MG	M	9225	1/1	1.00	0.02	56,56,56,56	0
6	MG	M	9227	1/1	1.00	0.01	35,35,35,35	0
6	MG	M	9230	1/1	1.00	0.01	50,50,50,50	0
6	MG	M	9234	1/1	1.00	0.02	53,53,53,53	0
6	MG	M	9237	1/1	1.00	0.02	52,52,52,52	0
6	MG	M	9239	1/1	1.00	0.03	34,34,34,34	0
6	MG	M	9241	1/1	1.00	0.03	36,36,36,36	0
6	MG	M	9242	1/1	1.00	0.03	35,35,35,35	0
6	MG	M	9247	1/1	1.00	0.04	51,51,51,51	0
6	MG	M	9248	1/1	1.00	0.02	48,48,48,48	0
6	MG	M	9250	1/1	1.00	0.01	38,38,38,38	0
6	MG	M	9256	1/1	1.00	0.02	56,56,56,56	0
6	MG	M	9260	1/1	1.00	0.02	36,36,36,36	0
6	MG	M	9261	1/1	1.00	0.01	47,47,47,47	0
6	MG	B	9478	1/1	1.00	0.01	61,61,61,61	0
6	MG	M	9268	1/1	1.00	0.02	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	C	9003	1/1	1.00	0.02	38,38,38,38	0
6	MG	M	9273	1/1	1.00	0.03	44,44,44,44	0
6	MG	M	9275	1/1	1.00	0.01	55,55,55,55	0
6	MG	M	9281	1/1	1.00	0.01	49,49,49,49	0
6	MG	M	9284	1/1	1.00	0.01	54,54,54,54	0
6	MG	M	9294	1/1	1.00	0.05	52,52,52,52	0
6	MG	M	9295	1/1	1.00	0.01	42,42,42,42	0
6	MG	M	9299	1/1	1.00	0.04	43,43,43,43	0
6	MG	M	9300	1/1	1.00	0.01	39,39,39,39	0
6	MG	M	9305	1/1	1.00	0.02	46,46,46,46	0
6	MG	C	9004	1/1	1.00	0.02	39,39,39,39	0
6	MG	M	9312	1/1	1.00	0.01	37,37,37,37	0
6	MG	M	9319	1/1	1.00	0.01	41,41,41,41	0
6	MG	M	9320	1/1	1.00	0.04	34,34,34,34	0
6	MG	M	9321	1/1	1.00	0.02	41,41,41,41	0
6	MG	C	9015	1/1	1.00	0.03	38,38,38,38	0
6	MG	M	9400	1/1	1.00	0.01	40,40,40,40	0
6	MG	M	9401	1/1	1.00	0.02	37,37,37,37	0
6	MG	C	9019	1/1	1.00	0.01	57,57,57,57	0
6	MG	M	9407	1/1	1.00	0.02	35,35,35,35	0
6	MG	M	9409	1/1	1.00	0.02	36,36,36,36	0
6	MG	M	9411	1/1	1.00	0.02	47,47,47,47	0
6	MG	M	9412	1/1	1.00	0.02	43,43,43,43	0
6	MG	C	9020	1/1	1.00	0.01	34,34,34,34	0
6	MG	M	9424	1/1	1.00	0.02	34,34,34,34	0
6	MG	M	9434	1/1	1.00	0.03	34,34,34,34	0
6	MG	A	9066	1/1	1.00	0.01	47,47,47,47	0
6	MG	M	9441	1/1	1.00	0.03	45,45,45,45	0
6	MG	C	9022	1/1	1.00	0.01	37,37,37,37	0
6	MG	C	9025	1/1	1.00	0.02	39,39,39,39	0
6	MG	C	9026	1/1	1.00	0.01	42,42,42,42	0
6	MG	M	9471	1/1	1.00	0.03	47,47,47,47	0
6	MG	M	9474	1/1	1.00	0.04	49,49,49,49	0
6	MG	C	9031	1/1	1.00	0.03	40,40,40,40	0
6	MG	M	9485	1/1	1.00	0.04	54,54,54,54	0
6	MG	M	9486	1/1	1.00	0.05	48,48,48,48	0
6	MG	N	9179	1/1	1.00	0.02	33,33,33,33	0
6	MG	N	9181	1/1	1.00	0.01	47,47,47,47	0
6	MG	N	9184	1/1	1.00	0.01	29,29,29,29	0
6	MG	C	9037	1/1	1.00	0.01	51,51,51,51	0
6	MG	N	9186	1/1	1.00	0.01	49,49,49,49	0
6	MG	N	9187	1/1	1.00	0.01	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	N	9192	1/1	1.00	0.01	62,62,62,62	0
6	MG	N	9193	1/1	1.00	0.01	34,34,34,34	0
6	MG	N	9194	1/1	1.00	0.01	51,51,51,51	0
6	MG	N	9199	1/1	1.00	0.01	35,35,35,35	0
6	MG	C	9042	1/1	1.00	0.01	47,47,47,47	0
6	MG	N	9204	1/1	1.00	0.01	44,44,44,44	0
6	MG	N	9206	1/1	1.00	0.01	31,31,31,31	0
6	MG	C	9044	1/1	1.00	0.01	34,34,34,34	0
6	MG	C	9046	1/1	1.00	0.02	38,38,38,38	0
6	MG	N	9214	1/1	1.00	0.03	33,33,33,33	0
6	MG	N	9215	1/1	1.00	0.02	32,32,32,32	0
6	MG	A	9068	1/1	1.00	0.03	39,39,39,39	0
6	MG	N	9221	1/1	1.00	0.01	44,44,44,44	0
6	MG	N	9229	1/1	1.00	0.03	41,41,41,41	0
6	MG	N	9231	1/1	1.00	0.01	52,52,52,52	0
6	MG	N	9232	1/1	1.00	0.02	47,47,47,47	0
6	MG	N	9233	1/1	1.00	0.03	62,62,62,62	0
6	MG	N	9236	1/1	1.00	0.02	39,39,39,39	0
6	MG	C	9049	1/1	1.00	0.01	46,46,46,46	0
6	MG	N	9240	1/1	1.00	0.02	46,46,46,46	0
6	MG	N	9243	1/1	1.00	0.01	35,35,35,35	0
6	MG	N	9249	1/1	1.00	0.02	45,45,45,45	0
6	MG	C	9050	1/1	1.00	0.01	37,37,37,37	0
6	MG	N	9259	1/1	1.00	0.01	34,34,34,34	0
6	MG	N	9262	1/1	1.00	0.03	51,51,51,51	0
6	MG	N	9265	1/1	1.00	0.02	61,61,61,61	0
6	MG	N	9267	1/1	1.00	0.01	42,42,42,42	0
6	MG	N	9269	1/1	1.00	0.04	42,42,42,42	0
6	MG	N	9270	1/1	1.00	0.02	39,39,39,39	0
6	MG	N	9271	1/1	1.00	0.03	43,43,43,43	0
6	MG	N	9274	1/1	1.00	0.01	40,40,40,40	0
6	MG	N	9276	1/1	1.00	0.02	61,61,61,61	0
6	MG	N	9279	1/1	1.00	0.02	54,54,54,54	0
6	MG	N	9286	1/1	1.00	0.01	31,31,31,31	0
6	MG	N	9287	1/1	1.00	0.02	53,53,53,53	0
6	MG	N	9288	1/1	1.00	0.04	49,49,49,49	0
6	MG	N	9291	1/1	1.00	0.02	64,64,64,64	0
6	MG	N	9292	1/1	1.00	0.02	56,56,56,56	0
6	MG	N	9293	1/1	1.00	0.01	42,42,42,42	0
6	MG	N	9298	1/1	1.00	0.02	55,55,55,55	0
6	MG	N	9302	1/1	1.00	0.01	31,31,31,31	0
6	MG	N	9303	1/1	1.00	0.03	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	N	9304	1/1	1.00	0.01	47,47,47,47	0
6	MG	C	9051	1/1	1.00	0.03	37,37,37,37	0
6	MG	N	9311	1/1	1.00	0.02	39,39,39,39	0
6	MG	C	9053	1/1	1.00	0.02	30,30,30,30	0
6	MG	N	9316	1/1	1.00	0.04	37,37,37,37	0
6	MG	C	9055	1/1	1.00	0.03	38,38,38,38	0
6	MG	N	9318	1/1	1.00	0.04	34,34,34,34	0
6	MG	N	9322	1/1	1.00	0.02	54,54,54,54	0
6	MG	N	9323	1/1	1.00	0.04	38,38,38,38	0
6	MG	N	9326	1/1	1.00	0.02	62,62,62,62	0
6	MG	N	9327	1/1	1.00	0.02	40,40,40,40	0
6	MG	N	9398	1/1	1.00	0.02	48,48,48,48	0
6	MG	N	9402	1/1	1.00	0.02	45,45,45,45	0
6	MG	N	9403	1/1	1.00	0.01	34,34,34,34	0
6	MG	N	9404	1/1	1.00	0.01	55,55,55,55	0
6	MG	N	9408	1/1	1.00	0.02	45,45,45,45	0
6	MG	N	9415	1/1	1.00	0.02	42,42,42,42	0
6	MG	N	9417	1/1	1.00	0.02	39,39,39,39	0
6	MG	N	9418	1/1	1.00	0.01	49,49,49,49	0
6	MG	N	9419	1/1	1.00	0.02	51,51,51,51	0
6	MG	N	9422	1/1	1.00	0.02	56,56,56,56	0
6	MG	N	9423	1/1	1.00	0.02	58,58,58,58	0
6	MG	C	9061	1/1	1.00	0.02	34,34,34,34	0
6	MG	C	9065	1/1	1.00	0.01	37,37,37,37	0
6	MG	A	9075	1/1	1.00	0.03	36,36,36,36	0
6	MG	N	9428	1/1	1.00	0.01	42,42,42,42	0
6	MG	N	9429	1/1	1.00	0.03	45,45,45,45	0
6	MG	N	9430	1/1	1.00	0.05	57,57,57,57	0
6	MG	N	9431	1/1	1.00	0.03	39,39,39,39	0
6	MG	N	9435	1/1	1.00	0.01	53,53,53,53	0
6	MG	N	9443	1/1	1.00	0.01	54,54,54,54	0
6	MG	N	9444	1/1	1.00	0.02	49,49,49,49	0
6	MG	C	9071	1/1	1.00	0.02	42,42,42,42	0
6	MG	N	9448	1/1	1.00	0.02	51,51,51,51	0
6	MG	C	9076	1/1	1.00	0.03	33,33,33,33	0
6	MG	N	9450	1/1	1.00	0.02	48,48,48,48	0
6	MG	N	9451	1/1	1.00	0.05	41,41,41,41	0
6	MG	C	9079	1/1	1.00	0.03	38,38,38,38	0
6	MG	N	9467	1/1	1.00	0.09	35,35,35,35	0
6	MG	N	9468	1/1	1.00	0.03	55,55,55,55	0
6	MG	N	9472	1/1	1.00	0.01	56,56,56,56	0
6	MG	N	9473	1/1	1.00	0.02	51,51,51,51	0

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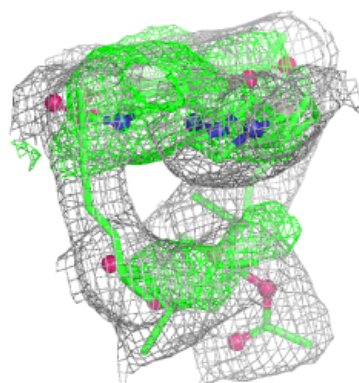
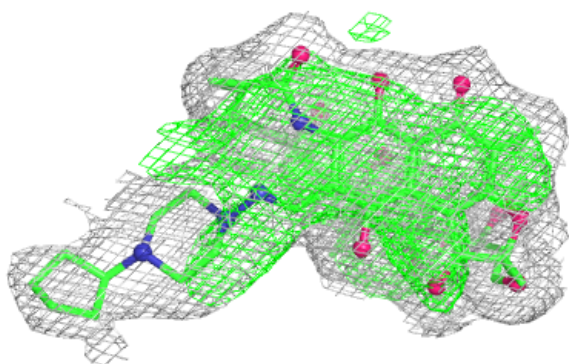
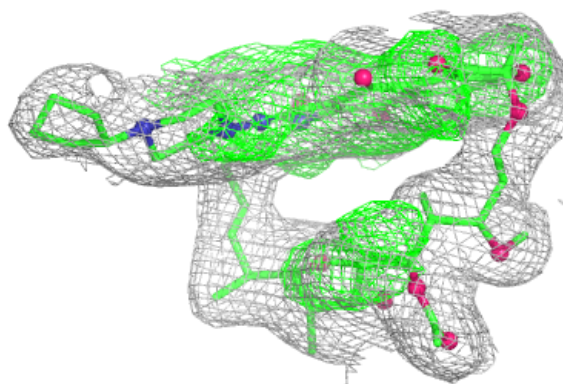
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	C	9086	1/1	1.00	0.02	39,39,39,39	0
6	MG	N	9484	1/1	1.00	0.02	37,37,37,37	0
6	MG	O	9197	1/1	1.00	0.04	57,57,57,57	0
6	MG	O	9198	1/1	1.00	0.01	36,36,36,36	0
6	MG	O	9254	1/1	1.00	0.02	39,39,39,39	0
6	MG	O	9266	1/1	1.00	0.01	47,47,47,47	0
6	MG	O	9296	1/1	1.00	0.03	42,42,42,42	0
6	MG	O	9420	1/1	1.00	0.05	51,51,51,51	0
6	MG	O	9439	1/1	1.00	0.01	56,56,56,56	0
6	MG	O	9483	1/1	1.00	0.03	63,63,63,63	0
6	MG	P	9189	1/1	1.00	0.05	49,49,49,49	0
6	MG	P	9202	1/1	1.00	0.02	49,49,49,49	0
6	MG	P	9209	1/1	1.00	0.02	46,46,46,46	0
6	MG	P	9216	1/1	1.00	0.01	48,48,48,48	0
6	MG	C	9090	1/1	1.00	0.03	47,47,47,47	0
6	MG	C	9092	1/1	1.00	0.03	44,44,44,44	0
6	MG	P	9235	1/1	1.00	0.01	40,40,40,40	0
6	MG	P	9255	1/1	1.00	0.04	34,34,34,34	0
6	MG	P	9258	1/1	1.00	0.01	51,51,51,51	0
6	MG	P	9277	1/1	1.00	0.03	41,41,41,41	0
6	MG	C	9107	1/1	1.00	0.01	42,42,42,42	0
6	MG	A	9078	1/1	1.00	0.04	66,66,66,66	0
6	MG	P	9285	1/1	1.00	0.02	56,56,56,56	0
6	MG	P	9297	1/1	1.00	0.01	45,45,45,45	0
6	MG	P	9315	1/1	1.00	0.03	35,35,35,35	0
6	MG	C	9114	1/1	1.00	0.04	30,30,30,30	0
6	MG	P	9399	1/1	1.00	0.01	34,34,34,34	0
6	MG	C	9115	1/1	1.00	0.01	36,36,36,36	0
6	MG	P	9446	1/1	1.00	0.01	34,34,34,34	0
6	MG	P	9482	1/1	1.00	0.02	48,48,48,48	0
7	RPT	C	8001	63/63	1.00	0.04	26,40,66,82	0
7	RPT	M	8002	63/63	1.00	0.03	33,45,55,57	0
8	ZN	D	7058	1/1	1.00	0.02	106,106,106,106	0
8	ZN	D	7112	1/1	1.00	0.03	80,80,80,80	0
8	ZN	N	7059	1/1	1.00	0.01	93,93,93,93	0
8	ZN	N	7113	1/1	1.00	0.01	84,84,84,84	0

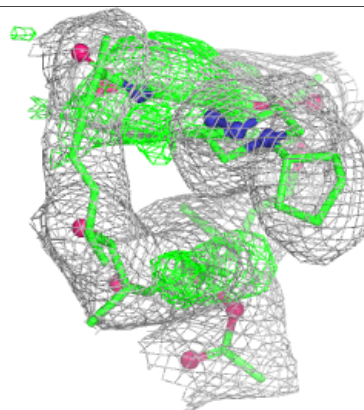
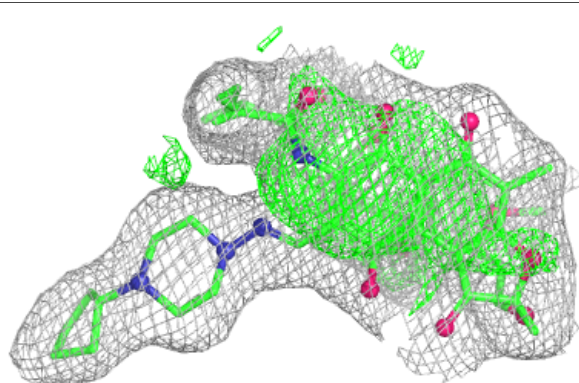
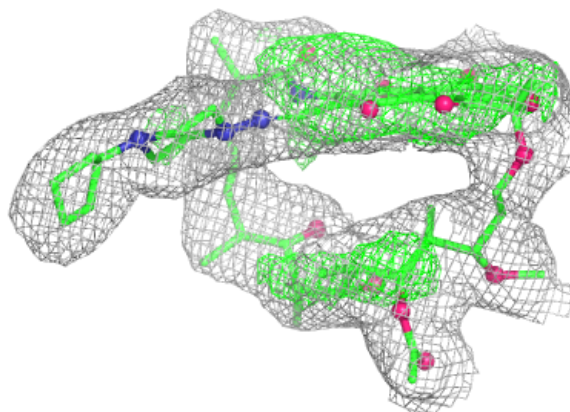
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around RPT C 8001:

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

**Electron density around RPT M 8002:**

$2mF_o-DF_c$ (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.